



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:28 PM GMT

PDB ID : 4V5I
Title : STRUCTURE OF THE PHAGE P2 BASEPLATE IN ITS ACTIVATED CONFORMATION WITH CA
Authors : Sciara, G.; Bebeacua, C.; Bron, P.; Tremblay, D.; Ortiz-Lombardia, M.; Lichiere, J.; vanHeel, M.; Campanacci, V.; Moineau, S.; Cambillau, C.
Deposited on : 2010-02-05
Resolution : 5.46 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : trunk26765
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

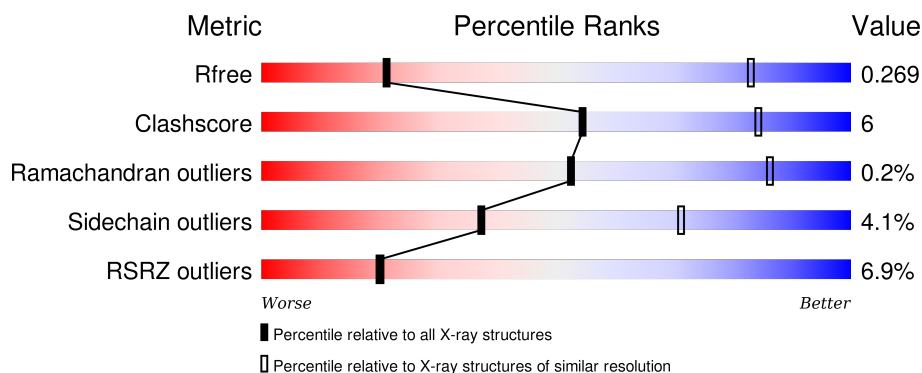
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.46 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1013 (7.10-3.62)
Clashscore	102246	1020 (7.10-3.70)
Ramachandran outliers	100387	1013 (7.10-3.64)
Sidechain outliers	100360	1011 (7.10-3.62)
RSRZ outliers	91569	1012 (7.10-3.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A0	372	<div> <div>13%</div> <div>84%</div> <div>14%</div> </div>
1	AY	372	<div> <div>11%</div> <div>86%</div> <div>12%</div> </div>
1	AZ	372	<div> <div>11%</div> <div>83%</div> <div>16%</div> </div>
1	B0	372	<div> <div>9%</div> <div>85%</div> <div>14%</div> </div>
1	BY	372	<div> <div>5%</div> <div>86%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	BZ	372	
2	AA	263	
2	AB	263	
2	AC	263	
2	AD	263	
2	AE	263	
2	AF	263	
2	AG	263	
2	AH	263	
2	AI	263	
2	AJ	263	
2	AK	263	
2	AL	263	
2	AM	263	
2	AN	263	
2	AO	263	
2	AP	263	
2	AQ	263	
2	AR	263	
2	BA	263	
2	BB	263	
2	BC	263	
2	BD	263	
2	BE	263	
2	BF	263	

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Mol	Chain	Length	Quality of chain
2	BG	263	
2	BH	263	
2	BI	263	
2	BJ	263	
2	BK	263	
2	BL	263	
2	BM	263	
2	BN	263	
2	BO	263	
2	BP	263	
2	BQ	263	
2	BR	263	
3	AS	298	
3	AT	298	
3	AU	298	
3	AV	298	
3	AW	298	
3	AX	298	
3	BS	298	
3	BT	298	
3	BU	298	
3	BV	298	
3	BW	298	
3	BX	298	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 119484 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ORF16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A0	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	AY	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	AZ	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	B0	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	BY	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	BZ	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			

- Molecule 2 is a protein called PUTATIVE RECEPTOR BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AA	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AB	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AC	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AD	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AE	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AF	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AG	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AH	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AI	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AJ	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AK	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AL	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AM	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AN	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AO	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AP	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AQ	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AR	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BA	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BB	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BC	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BD	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BE	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BF	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BG	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BH	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BI	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BJ	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BK	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BL	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BM	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BN	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BO	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BP	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BQ	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BR	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0

- Molecule 3 is a protein called ORF15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AS	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	AT	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	AU	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	AV	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	AW	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	AX	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	BS	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	BT	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	BU	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	BV	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	BW	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	BX	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0

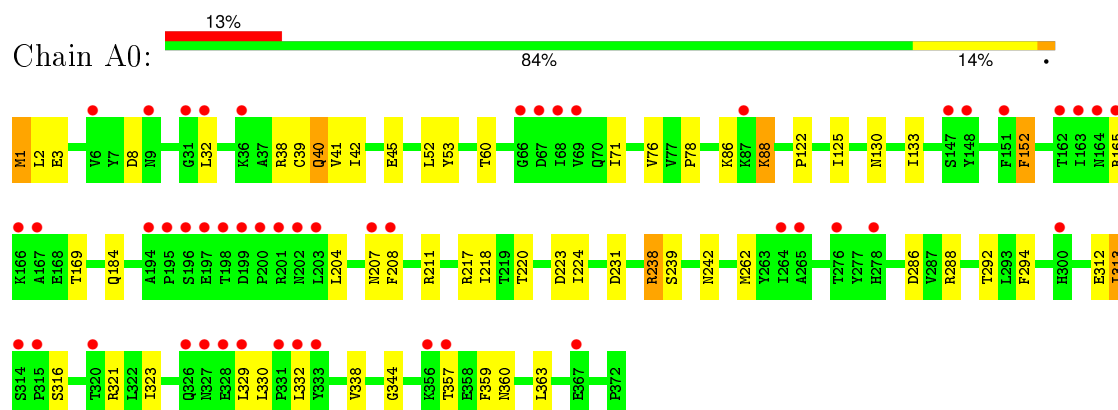
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	BU	1	Total	Ca	0	0
			1	1		
4	BT	1	Total	Ca	0	0
			1	1		
4	AV	1	Total	Ca	0	0
			1	1		
4	BV	1	Total	Ca	0	0
			1	1		
4	AW	1	Total	Ca	0	0
			1	1		
4	AT	1	Total	Ca	0	0
			1	1		
4	BS	1	Total	Ca	0	0
			1	1		
4	AU	1	Total	Ca	0	0
			1	1		
4	AX	1	Total	Ca	0	0
			1	1		
4	BW	1	Total	Ca	0	0
			1	1		
4	BX	1	Total	Ca	0	0
			1	1		
4	AS	1	Total	Ca	0	0
			1	1		

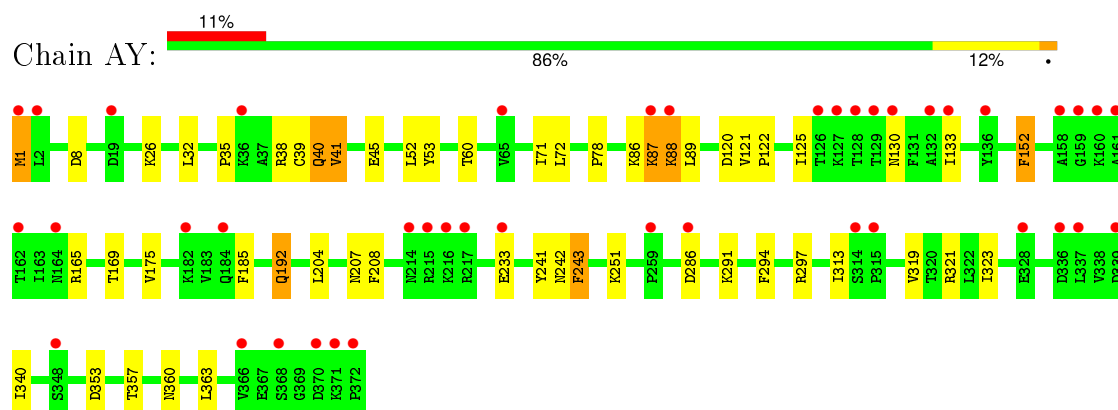
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

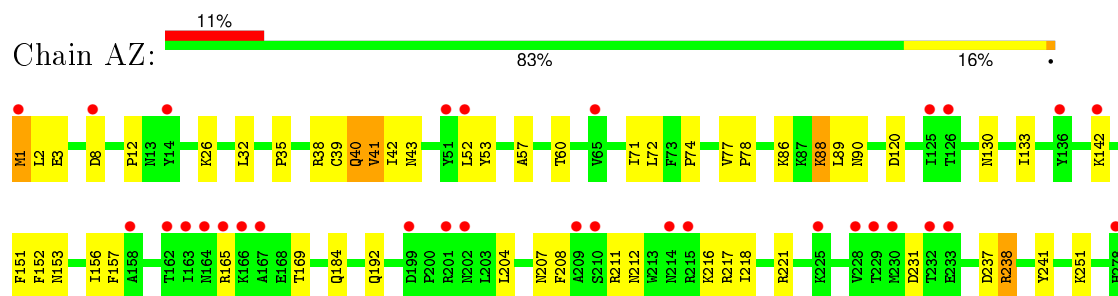
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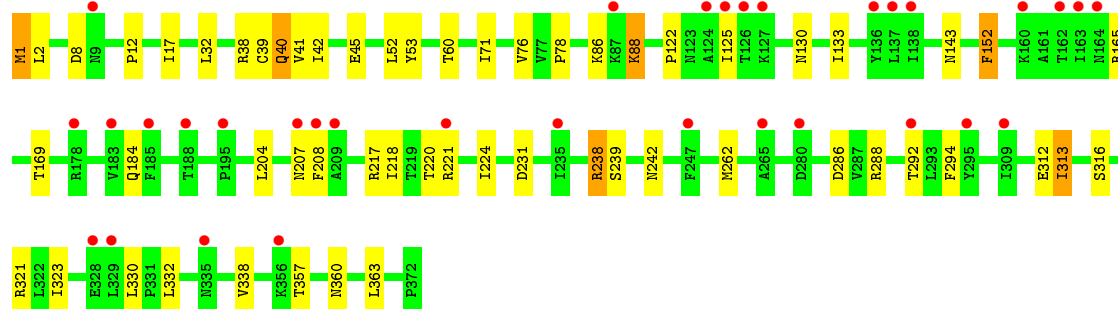
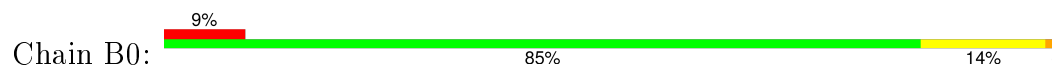


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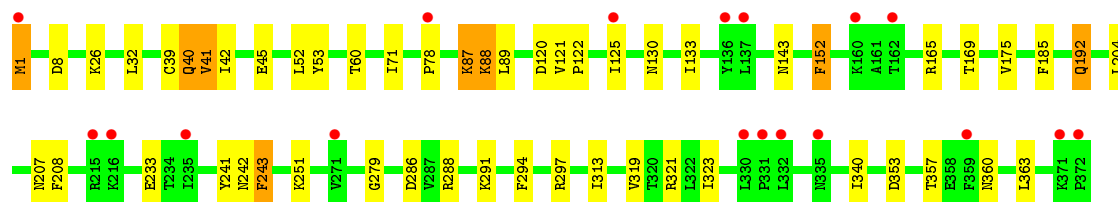
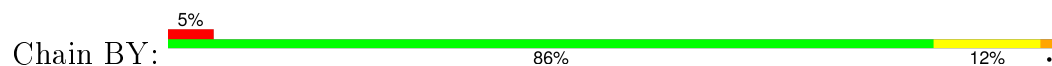




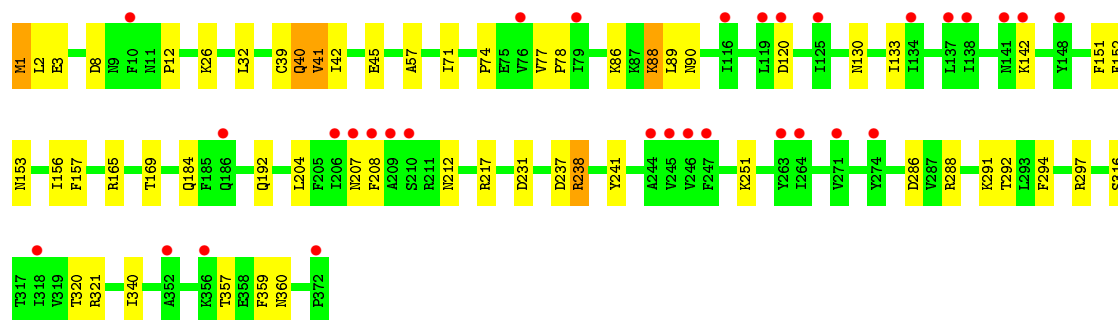
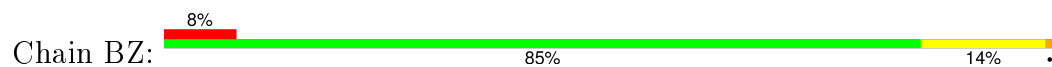
• Molecule 1: ORF16



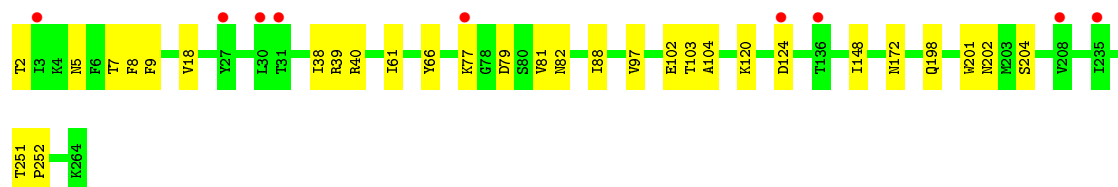
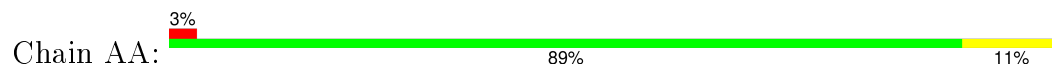
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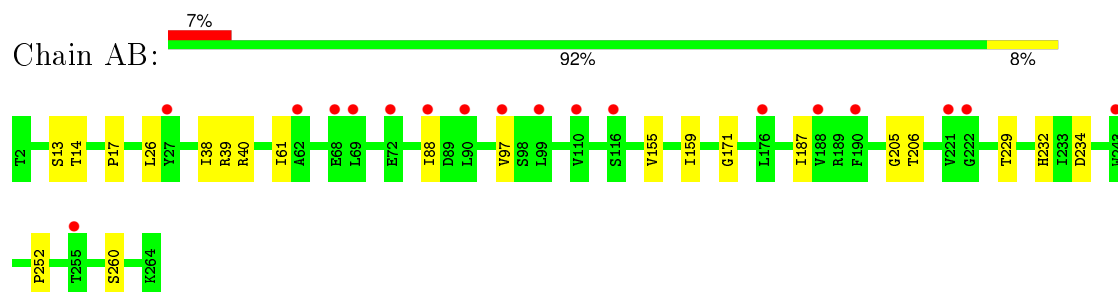
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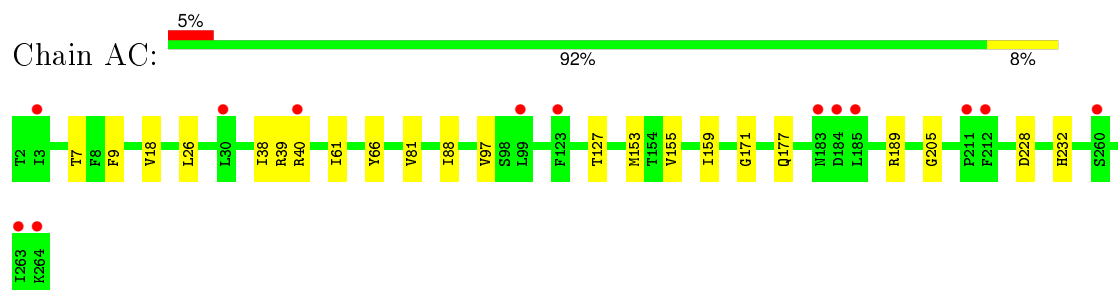
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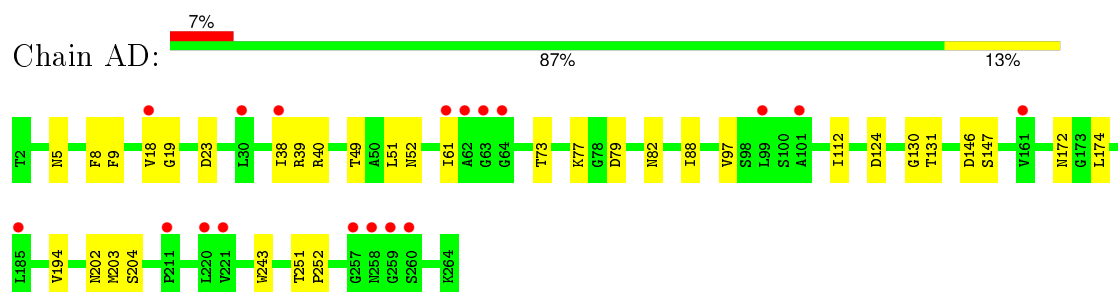
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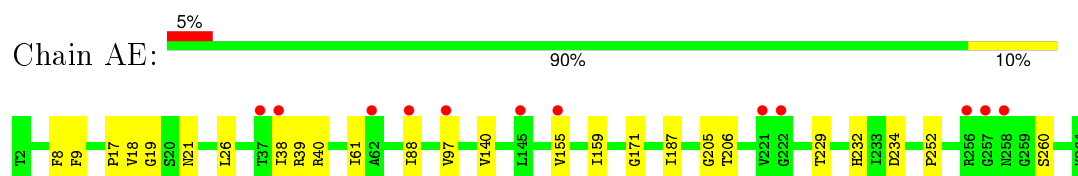
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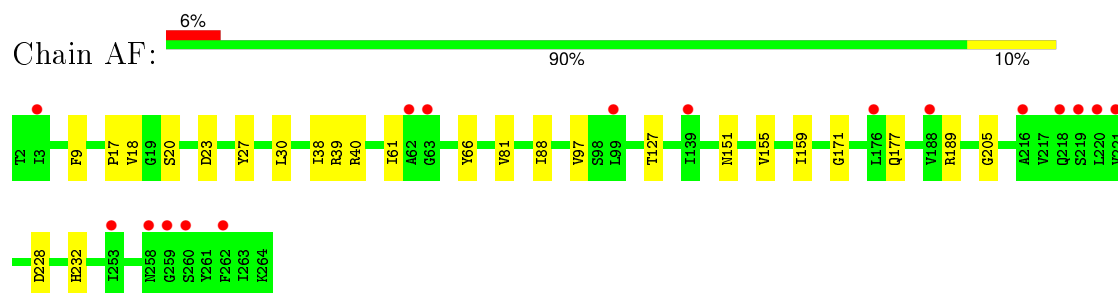
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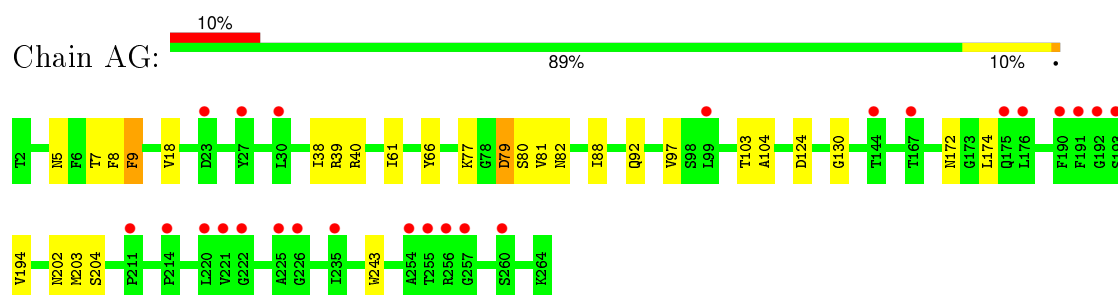
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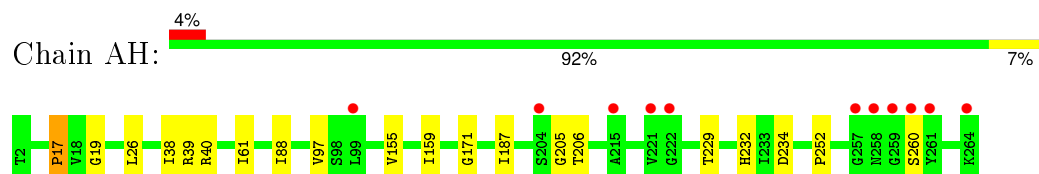
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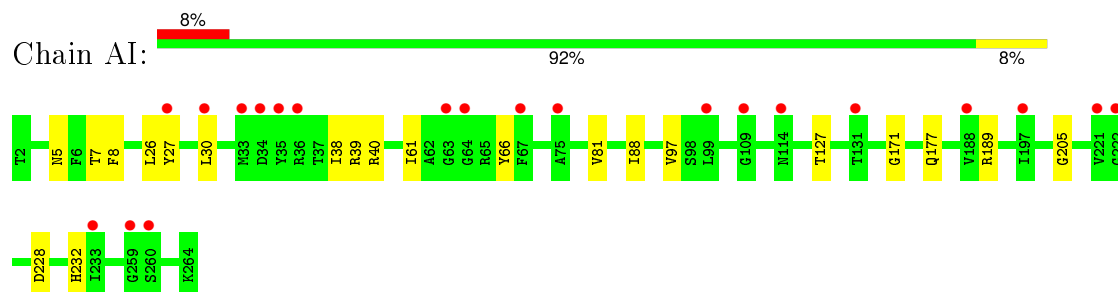
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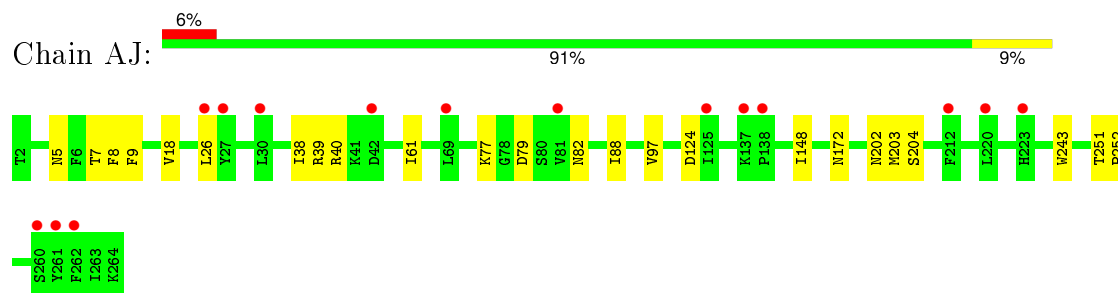
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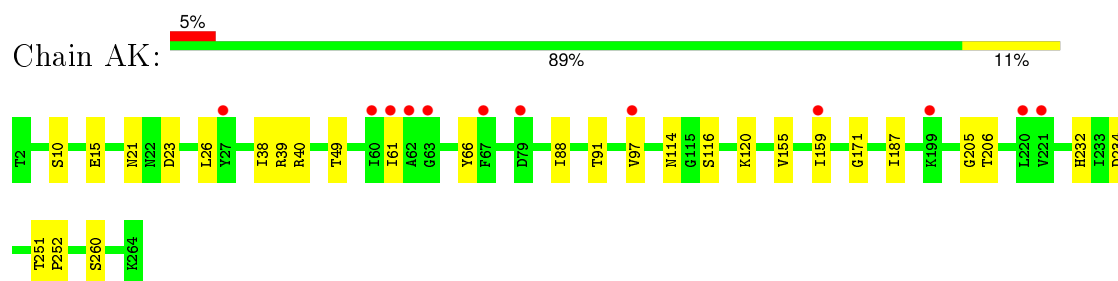
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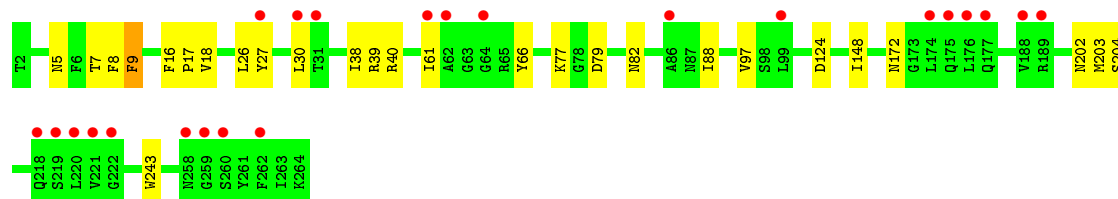
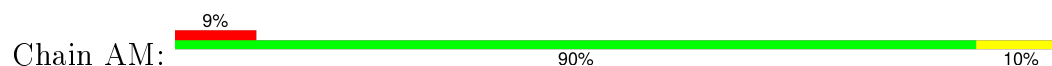


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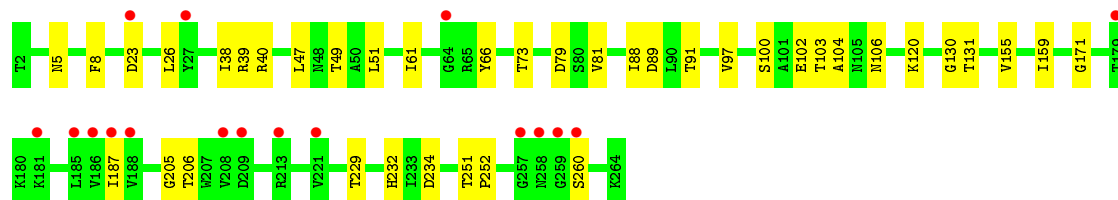
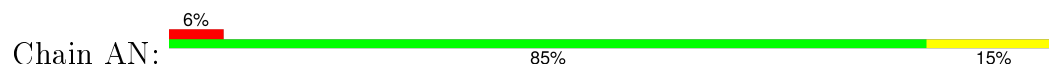




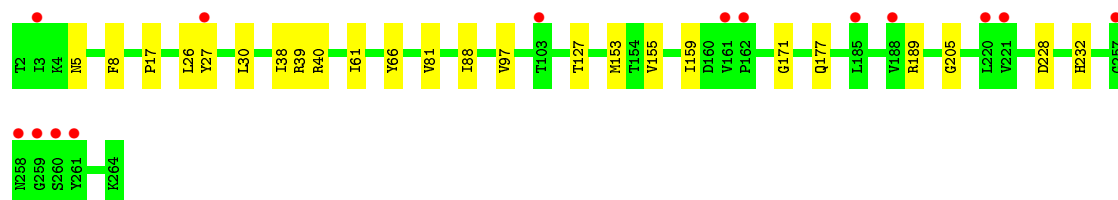
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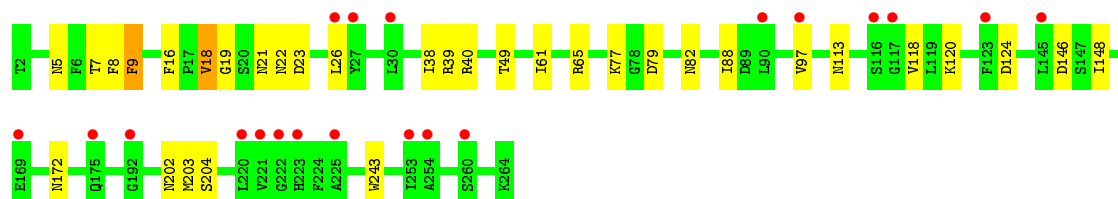
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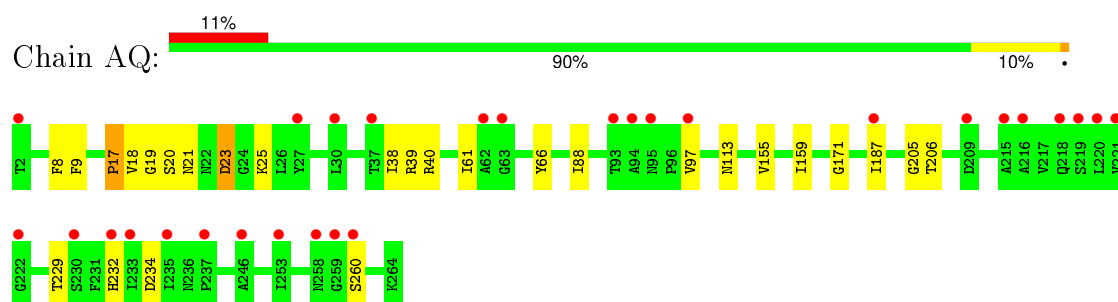
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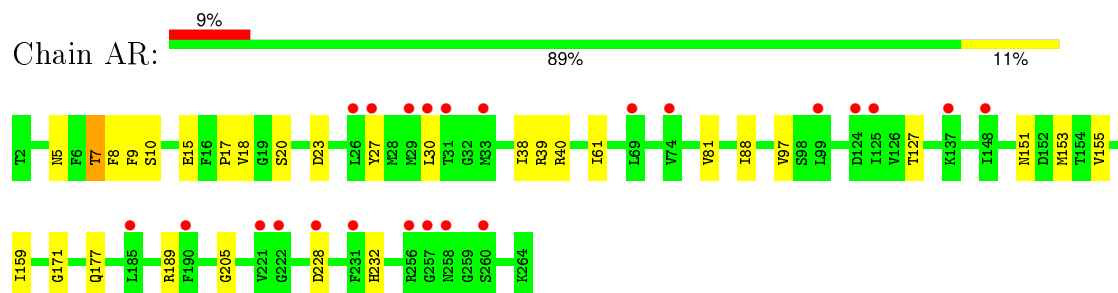
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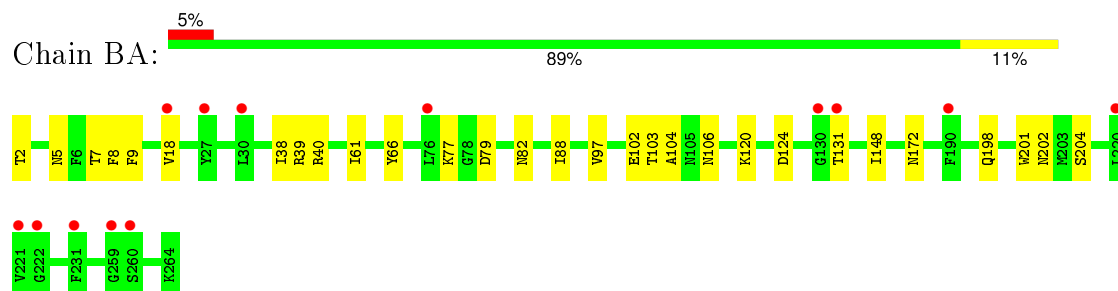
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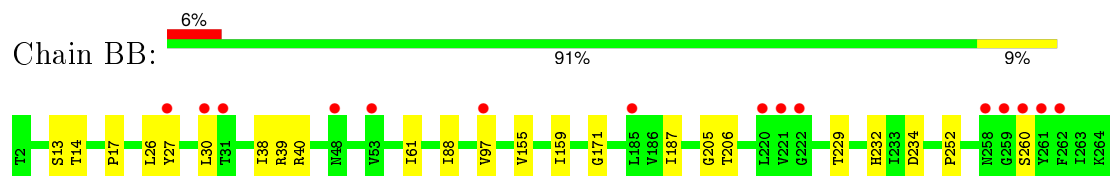
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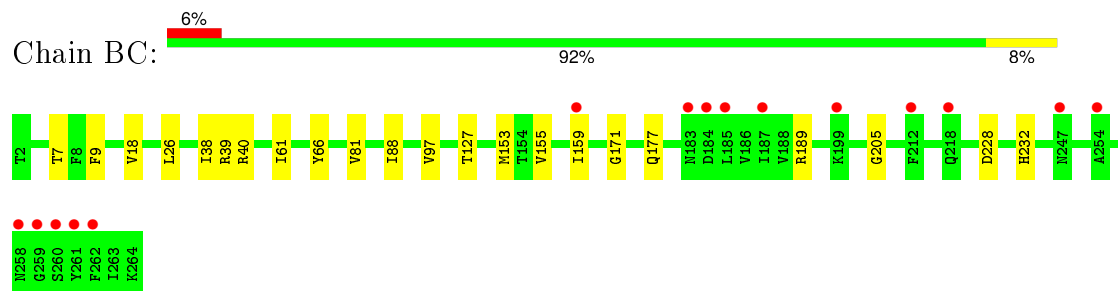
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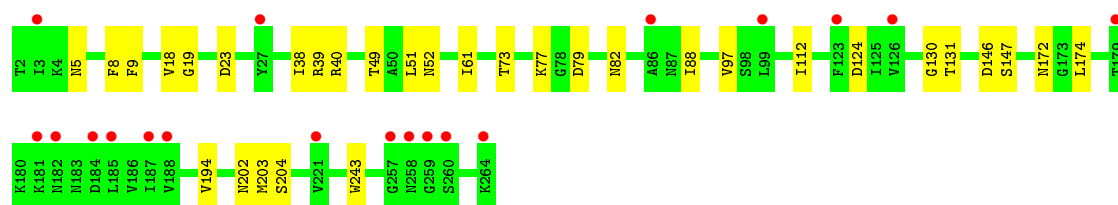


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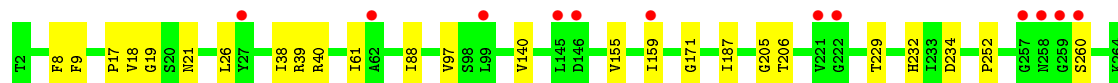
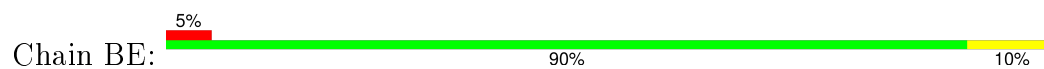


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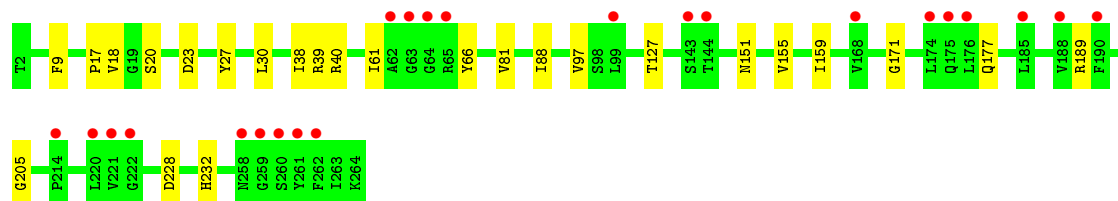
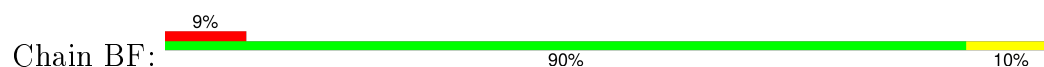




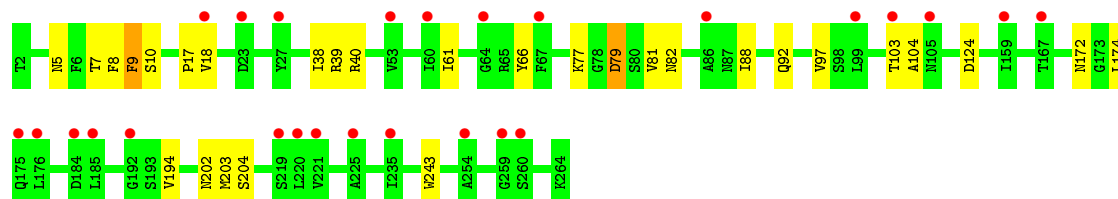
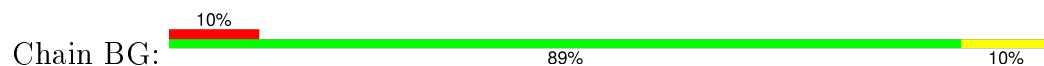
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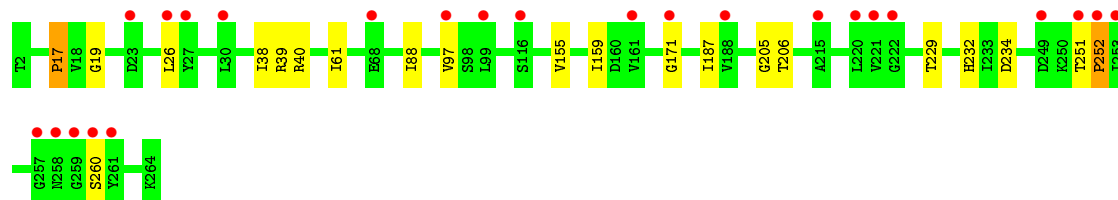
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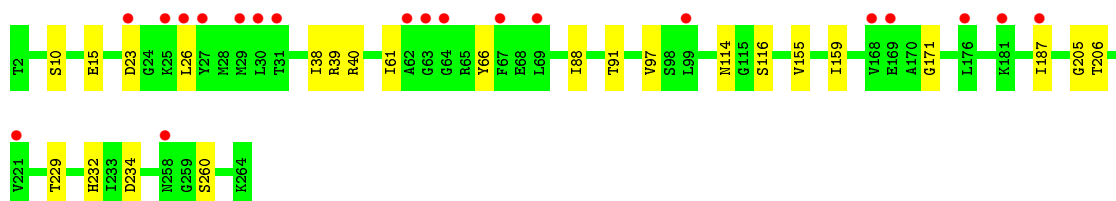




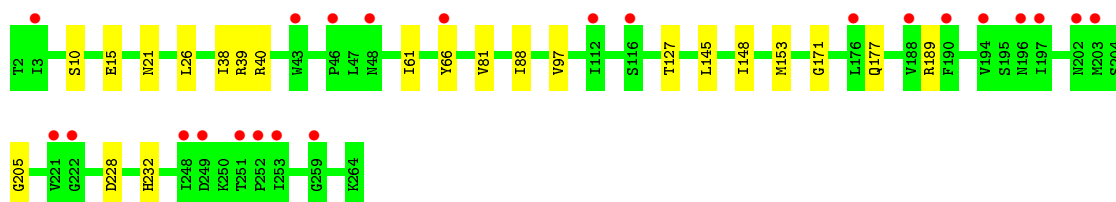
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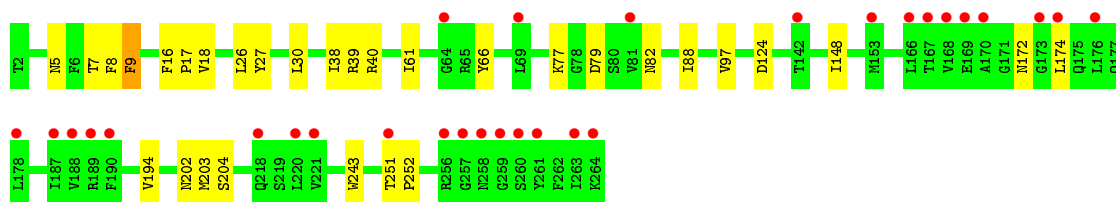
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• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

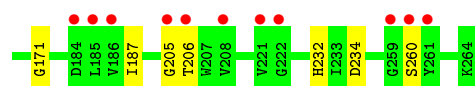


• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

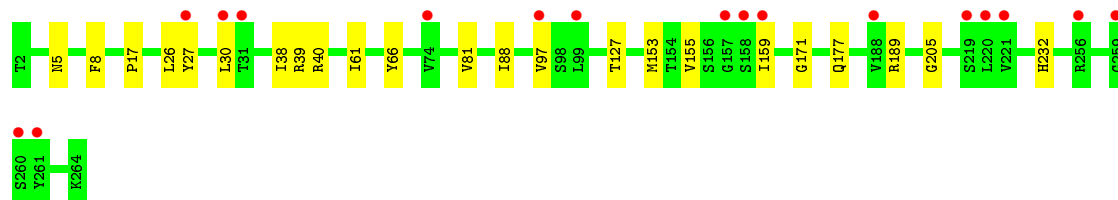


• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

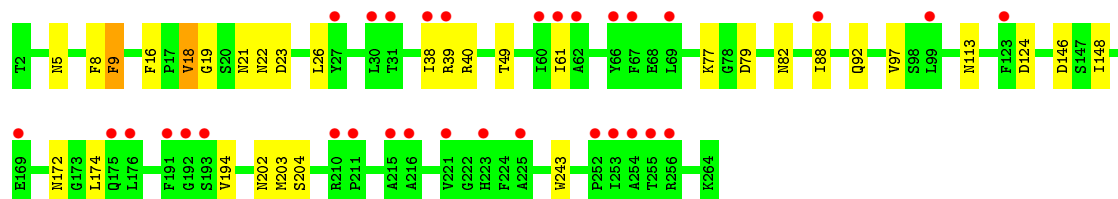
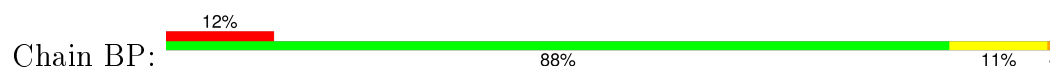




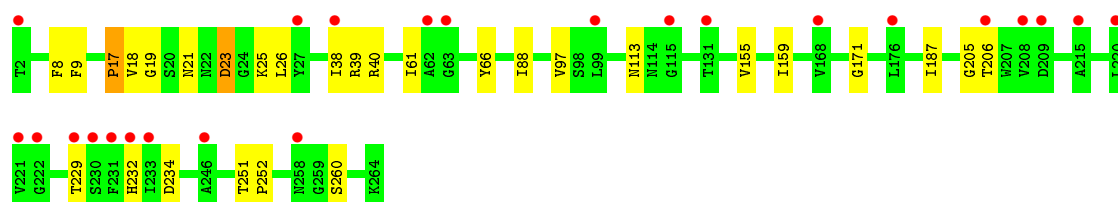
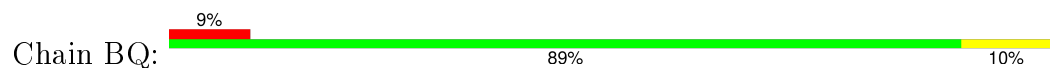
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



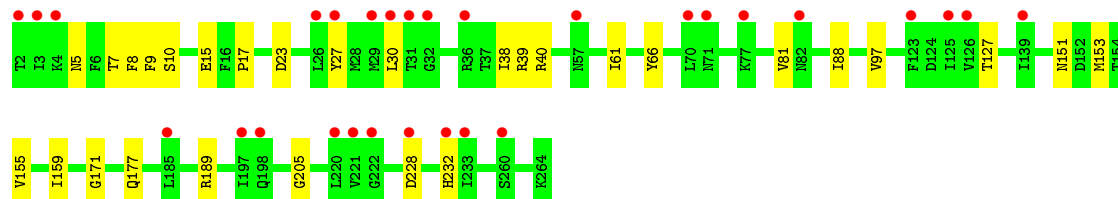
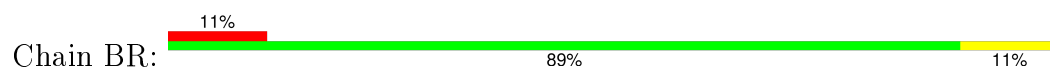
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



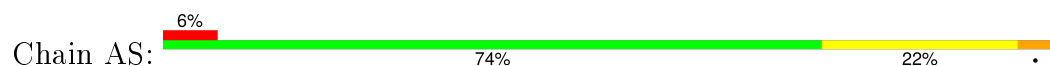
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

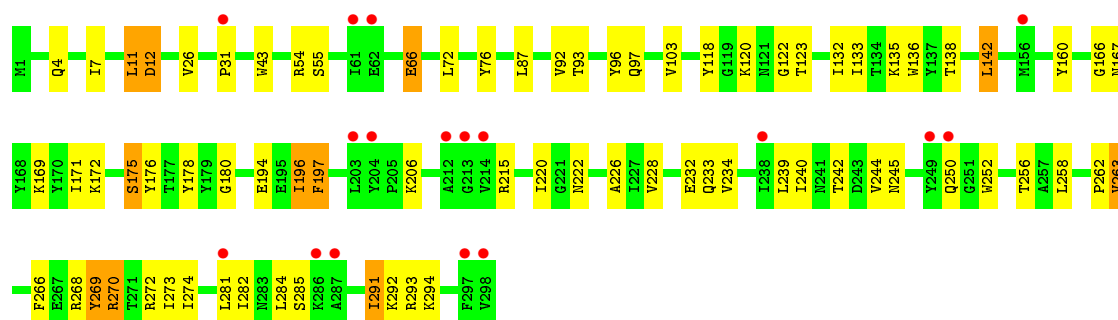


• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

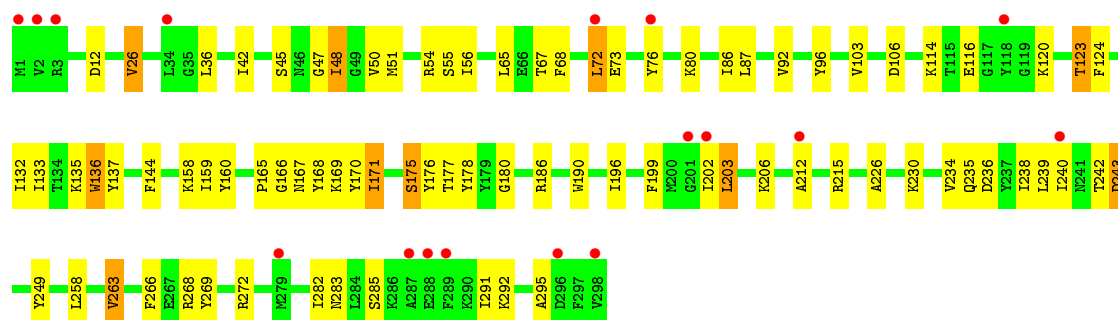
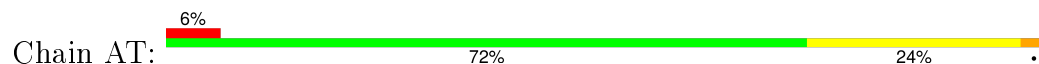


• Molecule 3: ORF15

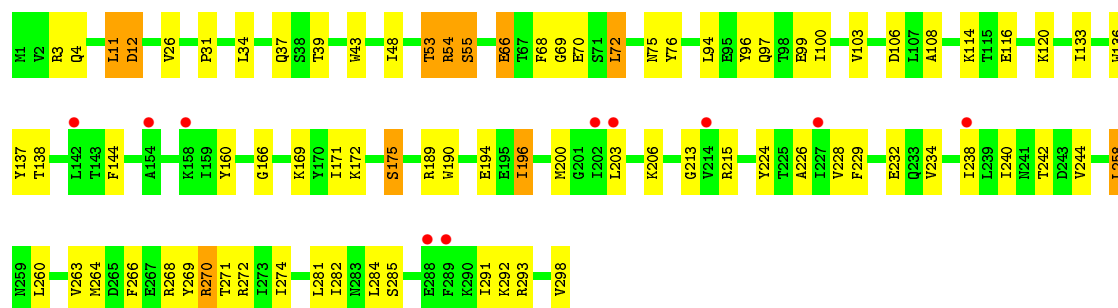
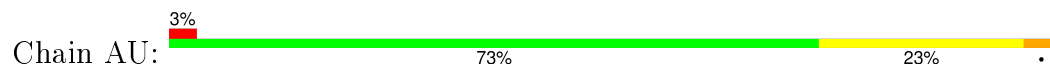




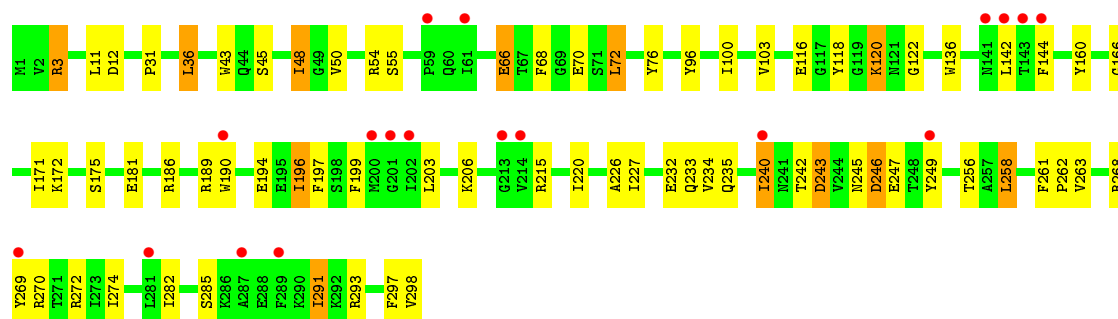
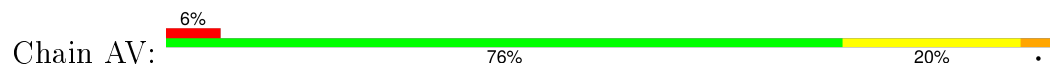
• Molecule 3: ORF15



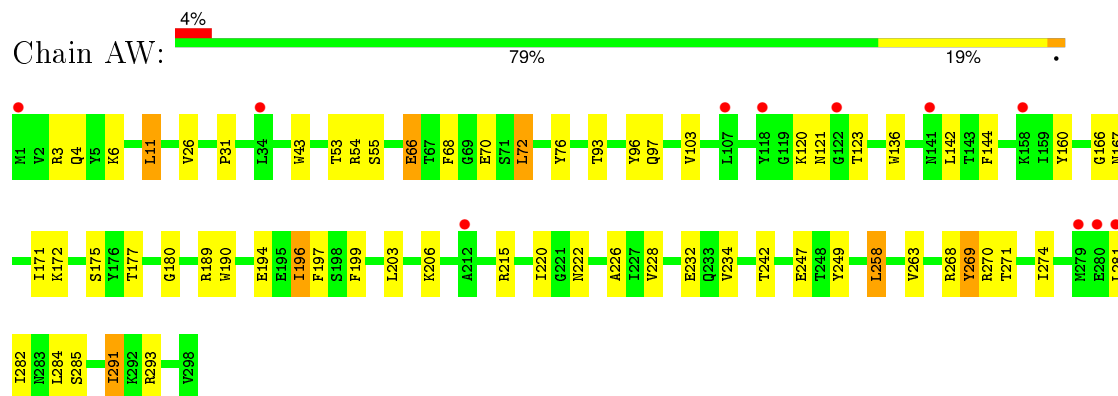
• Molecule 3: ORF15



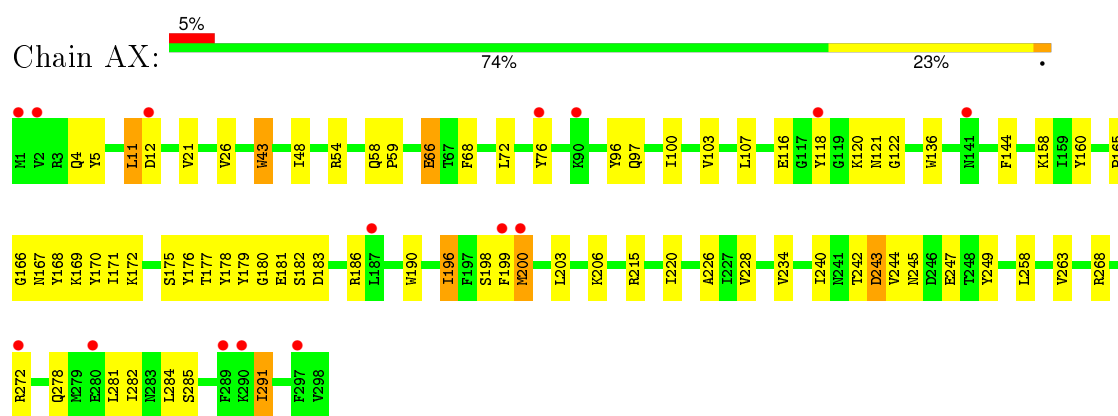
• Molecule 3: ORF15



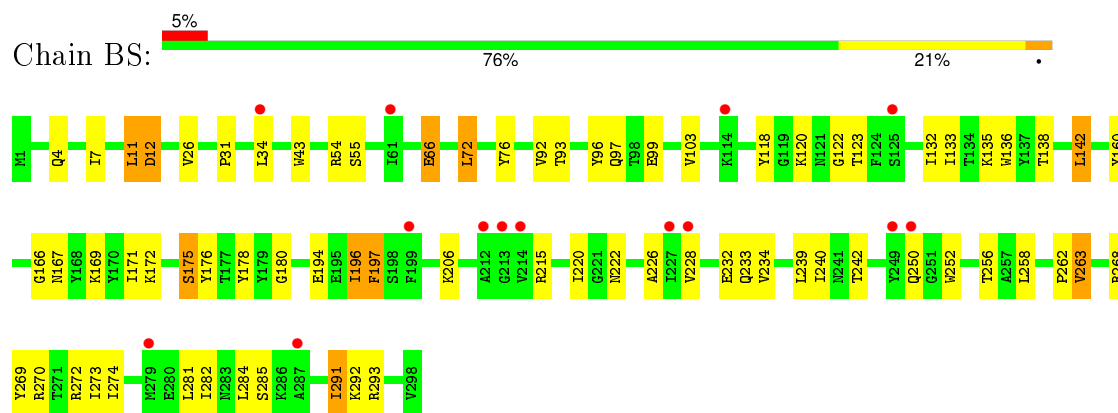
- Molecule 3: ORF15



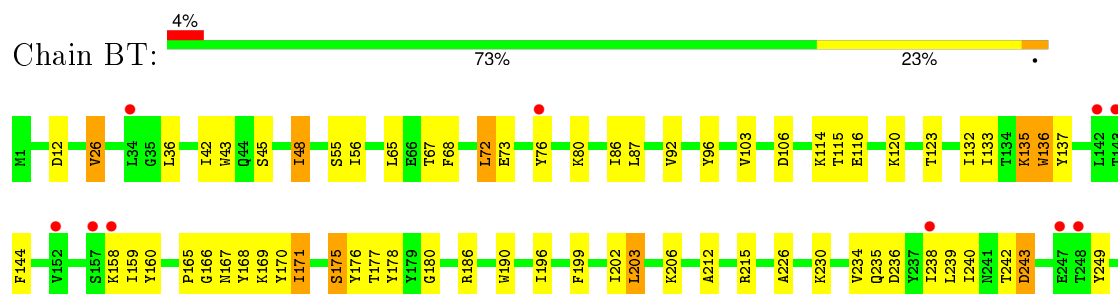
- Molecule 3: ORF15

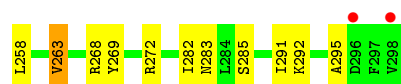


- Molecule 3: ORF15

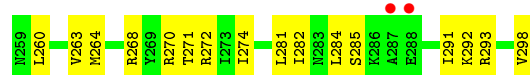
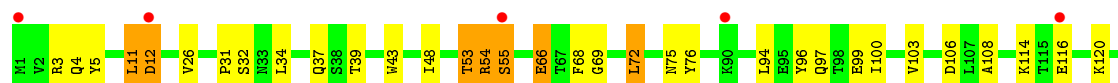
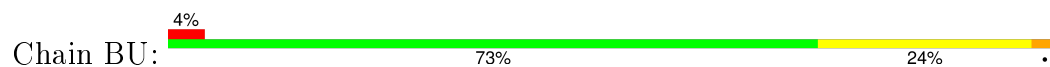


- Molecule 3: ORF15

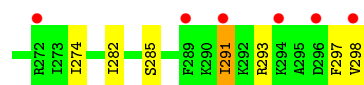
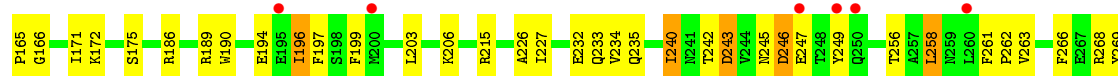
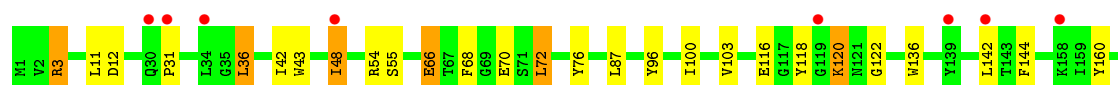
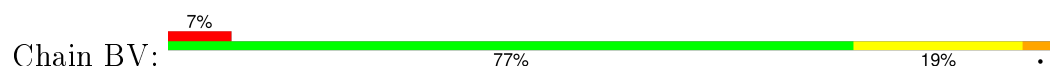




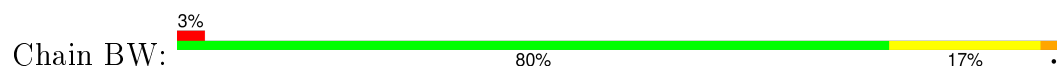
• Molecule 3: ORF15



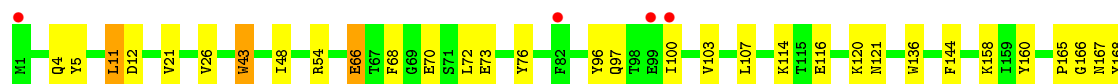
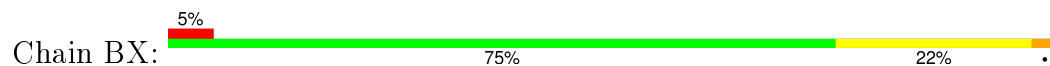
• Molecule 3: ORF15

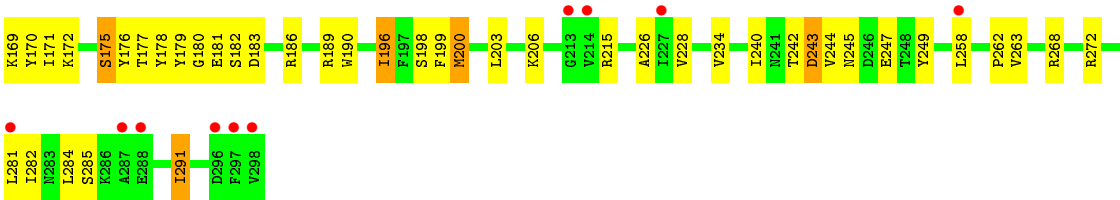


• Molecule 3: ORF15



• Molecule 3: ORF15





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	219.52Å 219.34Å 392.43Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	44.56 – 5.46 44.56 – 5.46	Depositor EDS
% Data completeness (in resolution range)	91.0 (44.56-5.46) 90.9 (44.56-5.46)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 5.38Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.291 , 0.297 0.269 , 0.269	Depositor DCC
R_{free} test set	5616 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	205.9	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 403.8	EDS
Estimated twinning fraction	0.409 for k,h,-l 0.399 for -k,-h,-l 0.408 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	3 of 112350 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	119484	wwPDB-VP
Average B, all atoms (Å ²)	343.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A0	0.38	0/3069	0.64	0/4175
1	AY	0.38	0/3069	0.65	0/4175
1	AZ	0.37	0/3069	0.63	0/4175
1	B0	0.38	0/3069	0.64	0/4175
1	BY	0.38	0/3069	0.65	0/4175
1	BZ	0.37	0/3069	0.63	0/4175
2	AA	0.32	0/2048	0.63	0/2791
2	AB	0.36	0/2048	0.58	0/2791
2	AC	0.35	0/2048	0.59	0/2791
2	AD	0.32	0/2048	0.61	0/2791
2	AE	0.36	0/2048	0.58	0/2791
2	AF	0.36	0/2048	0.58	0/2791
2	AG	0.32	0/2048	0.62	0/2791
2	AH	0.37	0/2048	0.58	0/2791
2	AI	0.37	0/2048	0.58	0/2791
2	AJ	0.34	0/2048	0.63	0/2791
2	AK	0.36	0/2048	0.59	0/2791
2	AL	0.36	0/2048	0.58	0/2791
2	AM	0.34	0/2048	0.63	0/2791
2	AN	0.36	0/2048	0.58	0/2791
2	AO	0.36	0/2048	0.58	0/2791
2	AP	0.34	0/2048	0.63	0/2791
2	AQ	0.37	0/2048	0.58	0/2791
2	AR	0.37	0/2048	0.59	0/2791
2	BA	0.32	0/2048	0.63	0/2791
2	BB	0.36	0/2048	0.58	0/2791
2	BC	0.35	0/2048	0.59	0/2791
2	BD	0.32	0/2048	0.61	0/2791
2	BE	0.36	0/2048	0.58	0/2791
2	BF	0.36	0/2048	0.58	0/2791
2	BG	0.32	0/2048	0.62	0/2791
2	BH	0.37	0/2048	0.58	0/2791

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	BI	0.37	0/2048	0.58	0/2791
2	BJ	0.34	0/2048	0.63	0/2791
2	BK	0.35	0/2048	0.59	0/2791
2	BL	0.36	0/2048	0.58	0/2791
2	BM	0.34	0/2048	0.63	0/2791
2	BN	0.36	0/2048	0.58	0/2791
2	BO	0.36	0/2048	0.58	0/2791
2	BP	0.34	0/2048	0.63	0/2791
2	BQ	0.37	0/2048	0.58	0/2791
2	BR	0.37	0/2048	0.59	0/2791
3	AS	0.36	0/2485	0.69	0/3356
3	AT	0.36	0/2485	0.69	0/3356
3	AU	0.35	0/2485	0.67	0/3356
3	AV	0.36	0/2485	0.67	0/3356
3	AW	0.35	0/2485	0.66	0/3356
3	AX	0.36	0/2485	0.67	0/3356
3	BS	0.36	0/2485	0.69	0/3356
3	BT	0.36	0/2485	0.69	0/3356
3	BU	0.35	0/2485	0.67	0/3356
3	BV	0.36	0/2485	0.67	0/3356
3	BW	0.35	0/2485	0.66	0/3356
3	BX	0.36	0/2485	0.67	0/3356
All	All	0.36	0/121962	0.62	0/165798

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	3000	0	2956	55	0
1	AY	3000	0	2956	37	0
1	AZ	3000	0	2956	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B0	3000	0	2956	45	0
1	BY	3000	0	2956	36	0
1	BZ	3000	0	2956	53	0
2	AA	2008	0	1971	22	0
2	AB	2008	0	1971	16	0
2	AC	2008	0	1971	15	0
2	AD	2008	0	1971	55	0
2	AE	2008	0	1971	34	0
2	AF	2008	0	1971	20	0
2	AG	2008	0	1971	34	0
2	AH	2008	0	1971	9	0
2	AI	2008	0	1971	10	0
2	AJ	2008	0	1971	11	0
2	AK	2008	0	1971	15	0
2	AL	2008	0	1971	10	0
2	AM	2008	0	1971	15	0
2	AN	2008	0	1971	38	0
2	AO	2008	0	1971	13	0
2	AP	2008	0	1971	35	0
2	AQ	2008	0	1971	42	0
2	AR	2008	0	1971	32	0
2	BA	2008	0	1971	18	0
2	BB	2008	0	1971	17	0
2	BC	2008	0	1971	15	0
2	BD	2008	0	1971	46	0
2	BE	2008	0	1971	35	0
2	BF	2008	0	1971	21	0
2	BG	2008	0	1971	25	0
2	BH	2008	0	1971	11	0
2	BI	2008	0	1971	10	0
2	BJ	2008	0	1971	10	0
2	BK	2008	0	1971	12	0
2	BL	2008	0	1971	11	0
2	BM	2008	0	1971	16	0
2	BN	2008	0	1971	37	0
2	BO	2008	0	1971	12	0
2	BP	2008	0	1971	23	0
2	BQ	2008	0	1971	31	0
2	BR	2008	0	1971	23	0
3	AS	2432	0	2392	115	0
3	AT	2432	0	2392	107	0
3	AU	2432	0	2392	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AV	2432	0	2392	98	0
3	AW	2432	0	2392	74	0
3	AX	2432	0	2392	141	0
3	BS	2432	0	2392	96	0
3	BT	2432	0	2392	102	0
3	BU	2432	0	2392	92	0
3	BV	2432	0	2392	95	0
3	BW	2432	0	2392	74	0
3	BX	2432	0	2392	112	0
4	AS	1	0	0	0	0
4	AT	1	0	0	0	0
4	AU	1	0	0	0	0
4	AV	1	0	0	0	0
4	AW	1	0	0	0	0
4	AX	1	0	0	0	0
4	BS	1	0	0	0	0
4	BT	1	0	0	0	0
4	BU	1	0	0	0	0
4	BV	1	0	0	0	0
4	BW	1	0	0	0	0
4	BX	1	0	0	0	0
All	All	119484	0	117396	1505	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1505) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AW:120:LYS:HD3	3:BV:68:PHE:CE1	1.26	1.65
3:AV:68:PHE:CD1	3:BW:120:LYS:HD3	1.30	1.61
3:AV:68:PHE:CE1	3:BW:120:LYS:HD3	1.28	1.58
3:AU:68:PHE:CE1	3:BX:120:LYS:HD3	1.37	1.54
3:AW:120:LYS:HD3	3:BV:68:PHE:CD1	1.42	1.54
3:AX:120:LYS:HD3	3:BU:68:PHE:CE1	1.40	1.51
2:AD:52:ASN:CG	3:AS:258:LEU:HD22	1.30	1.47
3:AV:68:PHE:CE1	3:BW:120:LYS:CD	2.01	1.43
2:AD:52:ASN:ND2	3:AS:258:LEU:HD22	1.28	1.43
1:A0:42:ILE:HB	3:AX:43:TRP:CZ2	1.51	1.41
3:AW:120:LYS:CD	3:BV:68:PHE:CE1	2.04	1.39
3:AV:68:PHE:CD1	3:BW:120:LYS:CD	2.08	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AG:103:THR:CB	1:AZ:78:PRO:HG3	1.53	1.36
3:AV:120:LYS:HZ2	3:BW:66:GLU:CG	1.42	1.32
1:B0:42:ILE:HB	3:BX:43:TRP:CZ2	1.66	1.30
2:AG:103:THR:HB	1:AZ:78:PRO:CG	1.62	1.30
2:BD:52:ASN:CG	3:BS:258:LEU:HD22	1.51	1.28
3:AV:120:LYS:NZ	3:BW:66:GLU:CG	1.99	1.24
2:AD:73:THR:CB	3:AS:256:THR:HG21	1.68	1.22
2:AD:131:THR:HG22	3:AS:262:PRO:O	1.38	1.21
2:BD:52:ASN:ND2	3:BS:258:LEU:HD22	1.54	1.21
1:A0:42:ILE:CB	3:AX:43:TRP:HZ2	1.55	1.20
2:BD:52:ASN:CG	3:BS:258:LEU:CD2	2.10	1.20
3:AW:66:GLU:CG	3:BV:120:LYS:HZ2	1.54	1.20
3:AW:120:LYS:CD	3:BV:68:PHE:CD1	2.21	1.19
2:BD:130:GLY:O	3:BS:262:PRO:HB3	1.39	1.19
3:AU:68:PHE:CE1	3:BX:120:LYS:CD	2.25	1.19
2:BD:131:THR:HG22	3:BS:262:PRO:O	1.42	1.18
2:AB:13:SER:O	3:AS:169:LYS:HD2	1.44	1.16
2:BD:130:GLY:O	3:BS:262:PRO:CB	1.93	1.15
2:BB:13:SER:O	3:BS:169:LYS:HD2	1.46	1.15
3:AW:66:GLU:CG	3:BV:120:LYS:NZ	2.10	1.15
2:AD:130:GLY:O	3:AS:262:PRO:HB3	1.34	1.15
1:A0:88:LYS:NZ	2:AN:104:ALA:HB3	1.62	1.14
3:AX:120:LYS:CD	3:BU:68:PHE:CE1	2.29	1.12
2:AD:130:GLY:O	3:AS:262:PRO:HB2	1.42	1.12
2:AD:52:ASN:ND2	3:AS:258:LEU:CD2	2.03	1.11
2:BD:73:THR:CB	3:BS:256:THR:HG21	1.81	1.10
2:AQ:18:VAL:HG12	3:AX:168:TYR:O	1.50	1.10
2:AQ:17:PRO:HB3	3:AX:167:ASN:HD22	1.11	1.09
3:AV:68:PHE:CE1	3:BW:120:LYS:CG	2.35	1.08
2:AQ:17:PRO:HB3	3:AX:169:LYS:HE3	1.35	1.08
2:BG:103:THR:CB	1:BZ:78:PRO:HG3	1.83	1.07
2:BN:131:THR:HG22	3:BV:262:PRO:O	1.52	1.07
2:BB:13:SER:C	3:BS:169:LYS:HD2	1.74	1.07
3:AV:120:LYS:NZ	3:BW:66:GLU:HG3	1.69	1.06
3:AW:66:GLU:HG2	3:BV:120:LYS:HZ2	1.09	1.06
2:BB:13:SER:O	3:BS:169:LYS:CD	2.04	1.06
2:BB:13:SER:O	3:BS:169:LYS:CE	2.03	1.06
2:AD:52:ASN:CB	3:AS:258:LEU:HD22	1.86	1.05
2:AB:13:SER:O	3:AS:169:LYS:CD	2.03	1.05
1:A0:86:LYS:NZ	2:AN:81:VAL:HB	1.70	1.05
2:AB:13:SER:O	3:AS:169:LYS:CE	2.05	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AQ:18:VAL:O	3:AX:167:ASN:HA	1.57	1.04
1:B0:42:ILE:CB	3:BX:43:TRP:HZ2	1.71	1.03
2:AB:13:SER:C	3:AS:169:LYS:HD2	1.78	1.03
3:AS:197:PHE:CD1	3:AT:48:ILE:HG22	1.93	1.03
2:AD:52:ASN:CG	3:AS:258:LEU:HD23	1.72	1.02
2:BG:103:THR:HB	1:BZ:78:PRO:HG3	1.03	1.02
2:BN:130:GLY:O	3:BV:262:PRO:HB3	1.60	1.02
3:BS:242:THR:CG2	3:BS:272:ARG:HG3	1.90	1.02
3:AV:120:LYS:HZ2	3:BW:66:GLU:HG2	0.85	1.01
3:AS:242:THR:CG2	3:AS:272:ARG:HG3	1.90	1.01
2:AD:52:ASN:CB	3:AS:258:LEU:CD2	2.38	1.00
3:AU:120:LYS:HZ1	3:BX:66:GLU:HG3	1.22	1.00
3:AW:120:LYS:CG	3:BV:68:PHE:CE1	2.44	0.99
3:AW:120:LYS:CD	3:BV:68:PHE:HE1	1.59	0.99
2:BG:103:THR:HB	1:BZ:78:PRO:CG	1.91	0.99
3:AW:120:LYS:CG	3:BV:68:PHE:HE1	1.75	0.98
2:AD:73:THR:HB	3:AS:256:THR:CG2	1.94	0.97
3:AS:66:GLU:HG3	3:BT:120:LYS:NZ	1.78	0.97
2:AQ:19:GLY:HA2	3:AX:166:GLY:O	1.65	0.97
3:AV:68:PHE:HE1	3:BW:120:LYS:CG	1.71	0.97
2:AD:73:THR:HB	3:AS:256:THR:HG21	1.47	0.97
1:B0:42:ILE:HB	3:BX:43:TRP:HZ2	0.80	0.96
3:AU:53:THR:CG2	1:AZ:359:PHE:HB3	1.95	0.96
2:BQ:17:PRO:HB3	3:BX:167:ASN:HD22	1.29	0.96
3:BT:116:GLU:HB2	3:BU:31:PRO:HD2	1.48	0.96
1:BY:169:THR:HG21	1:BZ:294:PHE:CE2	2.00	0.96
3:AX:66:GLU:HG3	3:BU:120:LYS:HZ1	1.31	0.95
2:BN:51:LEU:HD12	3:BV:262:PRO:HG2	1.46	0.95
2:BA:103:THR:HB	1:BY:78:PRO:HG3	1.46	0.95
3:AV:68:PHE:CD1	3:BW:120:LYS:HB3	2.03	0.94
3:AV:68:PHE:HE1	3:BW:120:LYS:HG2	1.30	0.94
2:AN:131:THR:HG22	3:AV:262:PRO:O	1.65	0.94
2:BE:17:PRO:CB	3:BT:167:ASN:HD22	1.79	0.94
3:AV:68:PHE:HE1	3:BW:120:LYS:CD	1.64	0.93
2:BB:13:SER:O	3:BS:169:LYS:NZ	2.02	0.93
2:AD:73:THR:CG2	3:AS:256:THR:HG21	1.99	0.92
2:AP:18:VAL:HG13	3:AX:158:LYS:O	1.70	0.92
2:BD:52:ASN:CB	3:BS:258:LEU:HD22	2.01	0.91
3:AW:66:GLU:HG3	3:BV:120:LYS:NZ	1.83	0.91
3:AV:68:PHE:CE1	3:BW:120:LYS:HG2	2.02	0.91
2:AD:52:ASN:OD1	3:AS:258:LEU:HD23	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AE:17:PRO:CB	3:AT:167:ASN:HD22	1.81	0.91
2:BE:17:PRO:HB3	3:BT:167:ASN:HD22	1.36	0.91
3:AV:68:PHE:HD1	3:BW:120:LYS:CD	1.77	0.90
3:AV:43:TRP:CD1	1:AZ:42:ILE:HD13	2.07	0.90
2:AE:17:PRO:HB3	3:AT:167:ASN:HD22	1.37	0.89
3:AT:116:GLU:HB2	3:AU:31:PRO:HD2	1.53	0.89
2:BD:73:THR:HB	3:BS:256:THR:HG21	1.52	0.89
2:AA:103:THR:HB	1:AY:78:PRO:HG3	1.53	0.89
2:AG:103:THR:CG2	1:AZ:78:PRO:HG3	2.01	0.89
3:AW:120:LYS:HB3	3:BV:68:PHE:CD1	2.08	0.88
3:AV:120:LYS:NZ	3:BW:66:GLU:HG2	1.72	0.88
2:AQ:17:PRO:HG3	3:AX:169:LYS:HE2	1.55	0.88
2:AQ:19:GLY:CA	3:AX:166:GLY:O	2.21	0.88
3:AU:68:PHE:CD1	3:BX:120:LYS:HD3	2.09	0.87
1:A0:88:LYS:HZ1	2:AN:104:ALA:HB3	1.36	0.87
2:BD:130:GLY:O	3:BS:262:PRO:HB2	1.75	0.86
2:BE:18:VAL:HG12	3:BT:168:TYR:O	1.75	0.85
2:AQ:17:PRO:HB3	3:AX:167:ASN:ND2	1.91	0.85
2:BD:73:THR:HB	3:BS:256:THR:CG2	2.05	0.85
2:BD:52:ASN:ND2	3:BS:258:LEU:CD2	2.33	0.85
3:AW:66:GLU:HG2	3:BV:120:LYS:NZ	1.80	0.85
3:AU:53:THR:HG21	1:AZ:359:PHE:HB3	1.58	0.85
1:A0:86:LYS:HZ2	2:AN:81:VAL:HB	1.40	0.85
2:AA:104:ALA:HB2	1:AY:88:LYS:NZ	1.91	0.85
2:BQ:17:PRO:HB3	3:BX:169:LYS:HE3	1.59	0.85
3:AS:133:ILE:HA	3:AT:42:ILE:HG21	1.59	0.85
2:AQ:17:PRO:CB	3:AX:167:ASN:HD22	1.89	0.84
2:BE:19:GLY:HA2	3:BT:166:GLY:O	1.76	0.84
3:AW:120:LYS:HG2	3:BV:68:PHE:HE1	1.41	0.84
2:AE:17:PRO:CB	3:AT:167:ASN:HB2	2.08	0.84
2:BN:73:THR:OG1	3:BV:256:THR:HG21	1.76	0.84
3:AU:68:PHE:CZ	3:BX:120:LYS:HD3	2.11	0.84
2:AB:13:SER:O	3:AS:169:LYS:NZ	2.10	0.84
3:AU:66:GLU:HG2	3:BX:120:LYS:HE2	1.60	0.83
3:AX:120:LYS:HD3	3:BU:68:PHE:CD1	2.13	0.83
2:AQ:18:VAL:CG1	3:AX:168:TYR:O	2.25	0.83
3:AU:120:LYS:NZ	3:BX:66:GLU:HG3	1.92	0.83
1:A0:86:LYS:HZ1	2:AN:81:VAL:HB	1.42	0.83
3:AS:197:PHE:CD1	3:AT:48:ILE:CG2	2.61	0.83
1:A0:294:PHE:CE2	1:AZ:169:THR:HG21	2.13	0.83
2:AQ:21:ASN:OD1	3:AX:165:PRO:HG2	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AN:51:LEU:HD12	3:AV:262:PRO:HG2	1.59	0.82
3:AU:120:LYS:NZ	3:BX:66:GLU:CG	2.42	0.82
2:BE:17:PRO:CB	3:BT:167:ASN:HB2	2.10	0.82
2:AE:18:VAL:HG12	3:AT:168:TYR:O	1.79	0.82
2:BE:9:PHE:HA	3:BT:170:TYR:O	1.79	0.82
2:AE:19:GLY:HA2	3:AT:166:GLY:O	1.80	0.81
3:AW:120:LYS:NZ	3:BV:66:GLU:HG3	1.94	0.81
3:AU:120:LYS:HZ1	3:BX:66:GLU:CG	1.93	0.81
3:AX:120:LYS:HE2	3:BU:66:GLU:HG2	1.63	0.81
2:AE:17:PRO:HB2	3:AT:167:ASN:HB2	1.62	0.81
2:AE:9:PHE:HA	3:AT:170:TYR:O	1.80	0.81
3:AW:120:LYS:HE2	3:BV:66:GLU:HG2	1.61	0.81
2:BQ:18:VAL:HG12	3:BX:168:TYR:O	1.79	0.81
2:AD:73:THR:CB	3:AS:256:THR:CG2	2.49	0.81
2:AD:52:ASN:HD22	3:AS:258:LEU:HD22	1.46	0.81
1:B0:239:SER:HB2	1:B0:312:GLU:O	1.81	0.81
2:BE:17:PRO:HB3	3:BT:167:ASN:ND2	1.96	0.80
2:AG:103:THR:HB	1:AZ:78:PRO:HG3	0.82	0.80
3:AT:73:GLU:HG3	3:AU:100:ILE:HG23	1.61	0.80
2:AG:79:ASP:O	1:AZ:212:ASN:ND2	2.14	0.80
2:BE:17:PRO:HB2	3:BT:167:ASN:HB2	1.64	0.80
3:BS:242:THR:HG22	3:BS:272:ARG:HG3	1.64	0.80
2:AC:9:PHE:HA	3:AS:178:TYR:HB2	1.62	0.80
2:BE:17:PRO:HB3	3:BT:169:LYS:HE3	1.64	0.79
3:AW:120:LYS:HG2	3:BV:68:PHE:CE1	2.15	0.79
1:A0:239:SER:HB2	1:A0:312:GLU:O	1.81	0.79
3:AV:68:PHE:CD1	3:BW:120:LYS:CG	2.62	0.79
2:BQ:18:VAL:O	3:BX:167:ASN:HA	1.81	0.79
1:A0:42:ILE:HD13	3:AX:43:TRP:NE1	1.97	0.79
2:BD:52:ASN:CG	3:BS:258:LEU:HD23	2.01	0.79
2:AE:17:PRO:HB3	3:AT:167:ASN:ND2	1.97	0.79
3:AV:66:GLU:HG2	3:BW:120:LYS:HE2	1.65	0.79
2:AN:130:GLY:O	3:AV:262:PRO:HB3	1.81	0.79
2:BB:14:THR:HA	3:BS:169:LYS:HE2	1.63	0.79
3:AW:120:LYS:CD	3:BV:68:PHE:HD1	1.91	0.79
3:AS:66:GLU:HG3	3:BT:120:LYS:HZ1	1.42	0.78
2:AF:17:PRO:HA	3:AT:177:THR:HG22	1.65	0.78
3:AS:142:LEU:HD12	3:AS:291:ILE:HD12	1.65	0.78
3:AS:273:ILE:HD11	3:AT:48:ILE:HD12	1.65	0.78
3:AS:66:GLU:CG	3:BT:120:LYS:NZ	2.45	0.78
2:BF:17:PRO:HA	3:BT:177:THR:HG22	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AY:169:THR:HG21	1:AZ:294:PHE:CE2	2.19	0.78
3:BS:142:LEU:HD12	3:BS:291:ILE:HD12	1.65	0.78
2:AN:49:THR:HB	3:AV:258:LEU:HD21	1.64	0.78
1:A0:330:LEU:HB2	3:AV:261:PHE:CE2	2.19	0.78
3:AW:120:LYS:HZ1	3:BV:66:GLU:HG3	1.46	0.77
3:AX:120:LYS:HD3	3:BU:68:PHE:CZ	2.16	0.77
3:AT:120:LYS:NZ	3:BS:66:GLU:HG3	1.98	0.77
2:AN:73:THR:OG1	3:AV:256:THR:HG21	1.85	0.77
2:BE:21:ASN:OD1	3:BT:165:PRO:HG2	1.84	0.77
3:AS:242:THR:HG22	3:AS:272:ARG:HG3	1.64	0.77
2:BN:49:THR:O	3:BV:258:LEU:HD21	1.85	0.77
2:AD:73:THR:HG21	3:AS:256:THR:HG21	1.65	0.77
2:BD:52:ASN:CB	3:BS:258:LEU:CD2	2.61	0.77
3:AX:66:GLU:HG3	3:BU:120:LYS:NZ	2.00	0.76
2:AG:79:ASP:C	1:AZ:212:ASN:HD21	1.89	0.76
3:AV:68:PHE:HD1	3:BW:120:LYS:HB3	1.45	0.76
2:AQ:19:GLY:HA2	3:AX:166:GLY:C	2.05	0.76
3:BU:242:THR:CG2	3:BU:272:ARG:HG3	2.16	0.76
3:AU:242:THR:CG2	3:AU:272:ARG:HG3	2.16	0.76
2:BQ:19:GLY:HA2	3:BX:166:GLY:O	1.85	0.76
3:AW:66:GLU:CB	3:BV:120:LYS:HZ2	1.98	0.76
3:AX:120:LYS:HD3	3:BU:68:PHE:HE1	1.37	0.75
3:AS:66:GLU:HG2	3:BT:120:LYS:HE2	1.69	0.75
3:AX:66:GLU:CG	3:BU:120:LYS:NZ	2.49	0.75
2:BR:9:PHE:CE2	3:BX:181:GLU:HG3	2.21	0.75
2:AD:73:THR:OG1	3:AS:256:THR:HG21	1.86	0.75
1:B0:88:LYS:NZ	2:BN:104:ALA:HB3	2.01	0.75
2:AE:17:PRO:HB3	3:AT:169:LYS:HE3	1.68	0.75
2:AE:21:ASN:OD1	3:AT:165:PRO:HG2	1.87	0.75
3:AU:53:THR:HG23	1:AZ:359:PHE:HB3	1.69	0.74
2:AP:65:ARG:NH2	3:AX:181:GLU:OE2	2.19	0.74
2:BC:9:PHE:HA	3:BS:178:TYR:HB2	1.68	0.74
3:AW:120:LYS:NZ	3:BV:66:GLU:CG	2.50	0.74
3:AV:68:PHE:CD1	3:BW:120:LYS:CB	2.70	0.74
3:BU:53:THR:CG2	1:BZ:359:PHE:HB3	2.17	0.74
3:BS:197:PHE:CD1	3:BT:48:ILE:HG22	2.22	0.74
2:AQ:18:VAL:C	3:AX:167:ASN:HA	2.06	0.74
2:BR:9:PHE:CZ	3:BX:181:GLU:HG3	2.23	0.74
2:BD:73:THR:OG1	3:BS:256:THR:HG21	1.88	0.74
2:AC:9:PHE:CD1	3:AS:180:GLY:HA2	2.23	0.73
3:AW:120:LYS:HB3	3:BV:68:PHE:HD1	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AR:23:ASP:OD2	3:AX:176:TYR:OH	2.06	0.73
1:A0:38:ARG:NH2	3:AW:269:TYR:O	2.21	0.73
2:AR:9:PHE:CE1	3:AX:180:GLY:CA	2.72	0.73
3:BS:31:PRO:HD2	3:BX:116:GLU:HB2	1.70	0.73
2:AD:131:THR:HB	3:AS:263:VAL:HG23	1.71	0.72
2:AD:131:THR:CG2	3:AS:262:PRO:O	2.31	0.72
3:AV:66:GLU:HG3	3:BW:120:LYS:NZ	2.04	0.72
1:A0:1:MET:SD	3:AX:48:ILE:HD13	2.30	0.72
3:AS:66:GLU:HG3	3:BT:120:LYS:HZ3	1.53	0.72
3:AV:48:ILE:HD13	1:AZ:1:MET:SD	2.30	0.72
2:AG:81:VAL:HB	1:AZ:86:LYS:NZ	2.05	0.72
3:AU:68:PHE:HE1	3:BX:120:LYS:HD3	1.40	0.71
3:AS:244:VAL:HG21	3:AT:50:VAL:HG22	1.72	0.71
1:B0:294:PHE:CE2	1:BZ:169:THR:HG21	2.25	0.71
2:AC:18:VAL:HG13	3:AS:176:TYR:CZ	2.26	0.71
2:AQ:17:PRO:CB	3:AX:169:LYS:HE3	2.17	0.71
2:AQ:9:PHE:HA	3:AX:170:TYR:O	1.91	0.71
2:AR:9:PHE:CE1	3:AX:180:GLY:HA2	2.26	0.71
1:B0:42:ILE:HD13	3:BX:43:TRP:NE1	2.06	0.70
2:AA:104:ALA:HB2	1:AY:88:LYS:HZ3	1.56	0.70
2:BC:9:PHE:CD1	3:BS:180:GLY:HA2	2.27	0.70
1:A0:211:ARG:NH2	2:AN:79:ASP:HB2	2.06	0.70
3:AU:68:PHE:HE1	3:BX:120:LYS:CG	2.05	0.70
2:AP:113:ASN:O	3:AX:186:ARG:NH2	2.24	0.70
3:AX:66:GLU:CG	3:BU:120:LYS:HZ1	2.00	0.70
2:AQ:18:VAL:O	3:AX:167:ASN:CA	2.38	0.70
2:AA:77:LYS:H	2:AA:82:ASN:HD21	1.39	0.70
2:AD:73:THR:HB	3:AS:256:THR:HG23	1.72	0.70
2:BE:17:PRO:HG3	3:BT:169:LYS:HE2	1.74	0.70
3:AW:121:ASN:HD21	3:BV:68:PHE:HB3	1.57	0.69
3:AS:242:THR:HG22	3:AS:272:ARG:CG	2.21	0.69
2:AP:22:ASN:HD21	3:AX:182:SER:CB	2.04	0.69
3:BT:80:LYS:HE3	3:BU:298:VAL:HG22	1.74	0.69
2:BP:18:VAL:HG13	3:BX:158:LYS:O	1.91	0.69
2:AB:14:THR:HA	3:AS:169:LYS:HE2	1.73	0.69
3:BS:242:THR:HG22	3:BS:272:ARG:CG	2.22	0.69
2:BE:18:VAL:O	3:BT:167:ASN:HA	1.93	0.69
3:AV:120:LYS:NZ	3:BW:66:GLU:CB	2.55	0.69
2:BE:19:GLY:CA	3:BT:166:GLY:O	2.40	0.69
3:AS:120:LYS:HG2	3:BT:68:PHE:CE1	2.28	0.69
3:AS:197:PHE:HD1	3:AT:48:ILE:CG2	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A0:294:PHE:HE2	1:AZ:169:THR:HG21	1.57	0.69
3:AV:70:GLU:HG2	3:BW:70:GLU:HG2	1.74	0.69
2:BA:77:LYS:H	2:BA:82:ASN:HD21	1.39	0.69
3:BT:45:SER:OG	1:BY:1:MET:HB3	1.94	0.68
2:AD:73:THR:HG21	3:AS:256:THR:CG2	2.23	0.68
1:B0:88:LYS:HZ1	2:BN:104:ALA:HB3	1.59	0.68
3:AS:250:GLN:HE21	3:AS:252:TRP:HE1	1.42	0.68
3:AW:120:LYS:CE	3:BV:66:GLU:HG2	2.23	0.68
2:AD:52:ASN:HB2	3:AS:258:LEU:HD22	1.71	0.68
3:BS:250:GLN:HE21	3:BS:252:TRP:HE1	1.42	0.68
2:AR:17:PRO:HA	3:AX:177:THR:HG22	1.74	0.68
3:AU:68:PHE:CD1	3:BX:120:LYS:CD	2.72	0.68
2:AD:77:LYS:H	2:AD:82:ASN:HD21	1.42	0.68
3:AU:66:GLU:HB3	3:BX:120:LYS:HZ3	1.58	0.68
3:BV:43:TRP:CD1	1:BZ:42:ILE:HD13	2.28	0.68
3:AT:80:LYS:HE3	3:AU:298:VAL:HG22	1.75	0.68
2:AP:77:LYS:H	2:AP:82:ASN:HD21	1.41	0.68
2:BP:77:LYS:H	2:BP:82:ASN:HD21	1.41	0.68
3:AV:120:LYS:HZ1	3:BW:66:GLU:CG	2.05	0.67
2:AQ:23:ASP:OD2	3:AX:168:TYR:HE2	1.78	0.67
2:AM:77:LYS:H	2:AM:82:ASN:HD21	1.42	0.67
2:AD:73:THR:CG2	3:AS:256:THR:CG2	2.72	0.67
3:AS:31:PRO:HD2	3:AX:116:GLU:HB2	1.75	0.67
2:AF:18:VAL:O	3:AT:175:SER:OG	2.10	0.67
2:AG:103:THR:HB	1:AZ:78:PRO:CB	2.25	0.67
3:BW:142:LEU:HG	3:BW:291:ILE:HD12	1.77	0.67
3:AT:120:LYS:HZ3	3:BS:66:GLU:HG3	1.59	0.67
2:AP:19:GLY:HA3	3:AX:180:GLY:O	1.95	0.67
3:AU:68:PHE:CE1	3:BX:120:LYS:CG	2.77	0.67
2:BN:130:GLY:O	3:BV:262:PRO:CB	2.41	0.66
3:AW:70:GLU:HG2	3:BV:70:GLU:HG2	1.75	0.66
2:BJ:77:LYS:H	2:BJ:82:ASN:HD21	1.41	0.66
3:AX:120:LYS:HZ3	3:BU:66:GLU:HB3	1.59	0.66
2:BN:49:THR:HG21	3:BV:235:GLN:NE2	2.10	0.66
2:BN:49:THR:HB	3:BV:258:LEU:HD21	1.75	0.66
2:BD:23:ASP:OD2	3:BT:178:TYR:HE1	1.77	0.66
2:BD:77:LYS:H	2:BD:82:ASN:HD21	1.42	0.66
2:AJ:77:LYS:H	2:AJ:82:ASN:HD21	1.41	0.66
3:AS:66:GLU:CG	3:BT:120:LYS:HZ3	2.07	0.66
2:BM:77:LYS:H	2:BM:82:ASN:HD21	1.42	0.66
3:AU:271:THR:HA	1:AZ:3:GLU:HG3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AV:120:LYS:HZ3	3:BW:66:GLU:HG3	1.61	0.66
2:BC:18:VAL:HG13	3:BS:176:TYR:CZ	2.31	0.66
2:AD:52:ASN:ND2	3:AS:258:LEU:HB3	2.10	0.66
1:BZ:238:ARG:HG3	1:BZ:316:SER:HA	1.78	0.66
3:BT:73:GLU:HG3	3:BU:100:ILE:HG23	1.77	0.66
3:AS:133:ILE:HG13	3:AT:42:ILE:HD13	1.78	0.66
3:AU:269:TYR:O	1:AZ:38:ARG:NH2	2.27	0.66
2:AG:77:LYS:H	2:AG:82:ASN:HD21	1.42	0.66
2:BG:77:LYS:H	2:BG:82:ASN:HD21	1.42	0.66
2:BQ:17:PRO:HG3	3:BX:169:LYS:HE2	1.78	0.66
2:AE:18:VAL:O	3:AT:167:ASN:HA	1.96	0.66
3:AW:142:LEU:HG	3:AW:291:ILE:HD12	1.77	0.66
3:AW:120:LYS:CB	3:BV:68:PHE:CD1	2.80	0.65
2:AE:17:PRO:HB2	3:AT:167:ASN:CB	2.25	0.65
2:AA:104:ALA:HB2	1:AY:88:LYS:HZ2	1.60	0.65
2:AD:51:LEU:CD1	3:AS:262:PRO:HG2	2.26	0.65
2:AP:22:ASN:ND2	3:AX:182:SER:OG	2.30	0.65
3:BU:76:TYR:HB3	3:BV:100:ILE:HD11	1.78	0.65
2:BD:52:ASN:OD1	3:BS:258:LEU:HD23	1.95	0.65
2:AN:49:THR:HB	3:AV:258:LEU:CD2	2.26	0.65
3:AS:244:VAL:CG2	3:AT:50:VAL:HG22	2.27	0.65
1:AZ:238:ARG:HG3	1:AZ:316:SER:HA	1.78	0.65
1:BZ:89:LEU:HD22	1:BZ:192:GLN:HG3	1.79	0.65
3:AV:120:LYS:HZ1	3:BW:66:GLU:CB	2.09	0.65
3:AW:66:GLU:CB	3:BV:120:LYS:NZ	2.58	0.65
2:AE:17:PRO:HG3	3:AT:169:LYS:HE2	1.77	0.65
2:BN:49:THR:HG21	3:BV:235:GLN:HE22	1.62	0.65
3:BU:53:THR:HG21	1:BZ:359:PHE:HB3	1.79	0.65
2:BD:131:THR:HA	3:BS:262:PRO:HB2	1.78	0.65
2:BA:120:LYS:HE2	3:BS:222:ASN:ND2	2.12	0.64
1:AY:152:PHE:HB2	1:AY:208:PHE:HB2	1.80	0.64
1:AY:243:PHE:HA	1:AY:313:ILE:HD11	1.79	0.64
3:AX:120:LYS:CG	3:BU:68:PHE:HE1	2.11	0.64
3:BS:250:GLN:NE2	3:BS:252:TRP:HE1	1.96	0.64
2:AQ:23:ASP:OD2	3:AX:168:TYR:CE2	2.50	0.64
2:AQ:17:PRO:HB3	3:AX:169:LYS:CE	2.20	0.64
3:AX:120:LYS:HZ3	3:BU:66:GLU:CB	2.10	0.64
1:AZ:89:LEU:HD22	1:AZ:192:GLN:HG3	1.79	0.64
3:AU:68:PHE:CD1	3:BX:120:LYS:HB3	2.33	0.64
3:AS:250:GLN:NE2	3:AS:252:TRP:HE1	1.96	0.64
2:AE:19:GLY:CA	3:AT:166:GLY:O	2.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AG:79:ASP:CA	1:AZ:212:ASN:HD21	2.11	0.63
1:BY:152:PHE:HB2	1:BY:208:PHE:HB2	1.80	0.63
3:AV:66:GLU:CG	3:BW:120:LYS:NZ	2.62	0.63
3:BV:116:GLU:HB2	3:BW:31:PRO:HD2	1.79	0.63
2:BD:73:THR:CG2	3:BS:256:THR:HG21	2.28	0.63
2:BE:17:PRO:HB2	3:BT:167:ASN:CB	2.26	0.63
2:AD:23:ASP:OD2	3:AT:178:TYR:HE1	1.82	0.63
3:BV:247:GLU:OE1	3:BV:249:TYR:HE2	1.82	0.63
3:AU:68:PHE:HD1	3:BX:120:LYS:HB3	1.63	0.63
3:AV:247:GLU:OE1	3:AV:249:TYR:HE2	1.82	0.63
2:AD:51:LEU:HD11	3:AS:262:PRO:HG2	1.81	0.63
3:AX:11:LEU:HD23	3:AX:12:ASP:H	1.64	0.63
3:AW:66:GLU:HG3	3:BV:120:LYS:HZ3	1.64	0.63
3:AT:120:LYS:HE2	3:BS:66:GLU:HG2	1.80	0.63
1:BY:243:PHE:HA	1:BY:313:ILE:HD11	1.79	0.63
3:BX:11:LEU:HD23	3:BX:12:ASP:H	1.63	0.63
2:AQ:17:PRO:HG3	3:AX:169:LYS:CE	2.27	0.62
1:A0:152:PHE:HB2	1:A0:208:PHE:HB2	1.81	0.62
3:AU:224:TYR:HB2	1:AZ:74:PRO:HB2	1.81	0.62
2:AD:52:ASN:CB	3:AS:258:LEU:HD21	2.27	0.62
3:AV:45:SER:CB	1:AZ:42:ILE:HG22	2.29	0.62
3:AV:66:GLU:HG3	3:BW:120:LYS:HZ1	1.63	0.62
2:BD:73:THR:CB	3:BS:256:THR:CG2	2.63	0.62
1:A0:330:LEU:HB2	3:AV:261:PHE:HE2	1.64	0.62
1:BY:241:TYR:HB2	1:BY:291:LYS:HD2	1.81	0.62
2:AP:9:PHE:HA	3:AX:160:TYR:O	1.99	0.62
2:BR:23:ASP:OD2	3:BX:176:TYR:OH	2.17	0.62
2:BB:17:PRO:HB3	3:BS:167:ASN:HB2	1.81	0.62
3:AX:120:LYS:CD	3:BU:68:PHE:CD1	2.77	0.62
1:A0:88:LYS:HE2	2:AN:106:ASN:OD1	1.99	0.62
3:AU:271:THR:HA	1:AZ:3:GLU:CG	2.30	0.62
3:AV:68:PHE:HD1	3:BW:120:LYS:CB	2.09	0.62
2:AF:23:ASP:OD2	3:AT:176:TYR:OH	2.17	0.62
3:AU:120:LYS:HE2	3:BX:66:GLU:HG2	1.82	0.62
1:B0:152:PHE:HB2	1:B0:208:PHE:HB2	1.81	0.61
3:AS:245:ASN:OD1	3:AT:51:MET:N	2.26	0.61
3:AV:66:GLU:HG2	3:BW:120:LYS:CE	2.30	0.61
1:A0:88:LYS:HZ2	2:AN:104:ALA:HB3	1.62	0.61
3:AU:66:GLU:CB	3:BX:120:LYS:HZ3	2.13	0.61
3:BX:199:PHE:N	3:BX:242:THR:OG1	2.33	0.61
3:AW:215:ARG:HB3	3:AW:282:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A0:88:LYS:NZ	2:AN:104:ALA:CB	2.52	0.61
3:BW:215:ARG:HB3	3:BW:282:ILE:HD11	1.83	0.61
3:AS:215:ARG:HB3	3:AS:282:ILE:HD11	1.82	0.61
3:AX:247:GLU:OE1	3:AX:249:TYR:HE2	1.83	0.61
1:A0:3:GLU:HG3	3:AW:271:THR:HA	1.83	0.61
2:AQ:19:GLY:HA3	3:AX:166:GLY:O	2.01	0.61
3:AT:120:LYS:HZ3	3:BS:66:GLU:CG	2.14	0.61
1:BZ:90:ASN:HD22	1:BZ:192:GLN:NE2	1.99	0.61
1:AY:241:TYR:HB2	1:AY:291:LYS:HD2	1.81	0.61
2:AD:131:THR:O	3:AS:263:VAL:HG23	2.01	0.60
2:BD:51:LEU:CD1	3:BS:262:PRO:HG2	2.31	0.60
3:AS:269:TYR:O	1:AY:38:ARG:NH2	2.29	0.60
2:AA:104:ALA:CB	1:AY:88:LYS:NZ	2.63	0.60
3:BU:53:THR:HG23	1:BZ:359:PHE:HB3	1.84	0.60
1:B0:294:PHE:HE2	1:BZ:169:THR:HG21	1.66	0.60
1:AZ:90:ASN:HD22	1:AZ:192:GLN:NE2	1.99	0.60
3:BT:235:GLN:HE22	3:BT:258:LEU:HD12	1.66	0.60
2:BG:81:VAL:HB	1:BZ:86:LYS:NZ	2.16	0.60
3:AT:235:GLN:HE22	3:AT:258:LEU:HD12	1.66	0.60
3:BX:247:GLU:OE1	3:BX:249:TYR:HE2	1.83	0.60
3:AV:68:PHE:CE1	3:BW:120:LYS:CE	2.83	0.60
3:AX:120:LYS:CG	3:BU:68:PHE:CE1	2.84	0.60
3:AU:53:THR:HG21	1:AZ:359:PHE:CB	2.29	0.60
2:AE:17:PRO:CB	3:AT:167:ASN:ND2	2.58	0.60
2:AA:104:ALA:HB3	1:AY:88:LYS:HD2	1.84	0.60
3:AV:50:VAL:HG11	1:AZ:60:THR:HG22	1.84	0.60
3:BU:137:TYR:HD1	3:BU:292:LYS:HB2	1.66	0.60
2:AP:23:ASP:OD2	3:AX:178:TYR:HE1	1.85	0.60
3:AW:121:ASN:ND2	3:BV:68:PHE:HB3	2.16	0.60
3:AU:66:GLU:CG	3:BX:120:LYS:NZ	2.64	0.60
2:BE:17:PRO:CB	3:BT:167:ASN:ND2	2.56	0.60
3:BX:12:ASP:HB2	3:BX:200:MET:HG3	1.84	0.60
3:BX:199:PHE:CE1	3:BX:242:THR:HG21	2.37	0.60
3:AS:206:LYS:HG3	3:AS:285:SER:HB3	1.84	0.60
3:BS:215:ARG:HB3	3:BS:282:ILE:HD11	1.82	0.60
1:A0:42:ILE:HD13	3:AX:43:TRP:HE1	1.65	0.60
2:AR:18:VAL:HG12	3:AX:176:TYR:O	2.02	0.60
2:BF:23:ASP:OD2	3:BT:176:TYR:OH	2.18	0.60
2:BD:52:ASN:HB2	3:BS:258:LEU:HD22	1.82	0.59
2:AR:9:PHE:CZ	3:AX:181:GLU:HG3	2.37	0.59
3:AX:12:ASP:HB2	3:AX:200:MET:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AG:92:GLN:NE2	3:AU:189:ARG:CZ	2.65	0.59
3:AU:66:GLU:HG3	3:BX:120:LYS:HZ1	1.66	0.59
3:AV:171:ILE:HG22	3:AV:172:LYS:H	1.68	0.59
2:AD:49:THR:CG2	3:AS:233:GLN:HB2	2.32	0.59
3:BS:206:LYS:HG3	3:BS:285:SER:HB3	1.84	0.59
2:AG:79:ASP:O	1:AZ:212:ASN:CG	2.40	0.59
2:BN:49:THR:HB	3:BV:258:LEU:CD2	2.32	0.59
3:BX:215:ARG:HB3	3:BX:282:ILE:HD11	1.84	0.59
3:AX:199:PHE:CE1	3:AX:242:THR:HG21	2.37	0.59
3:AU:137:TYR:HD1	3:AU:292:LYS:HB2	1.66	0.59
3:AV:68:PHE:HB3	3:BW:121:ASN:HD21	1.66	0.59
2:BA:104:ALA:HB2	1:BY:88:LYS:NZ	2.17	0.59
3:AX:199:PHE:N	3:AX:242:THR:OG1	2.33	0.59
3:BU:215:ARG:HB3	3:BU:282:ILE:HD11	1.83	0.59
3:AU:120:LYS:CE	3:BX:66:GLU:HG2	2.33	0.59
2:BQ:19:GLY:CA	3:BX:166:GLY:O	2.49	0.59
3:AU:215:ARG:HB3	3:AU:282:ILE:HD11	1.83	0.59
2:AD:131:THR:HA	3:AS:262:PRO:HB2	1.84	0.59
3:BV:247:GLU:OE1	3:BV:249:TYR:CE2	2.56	0.59
3:BS:273:ILE:HD11	3:BT:48:ILE:HD12	1.83	0.58
3:AX:215:ARG:HB3	3:AX:282:ILE:HD11	1.84	0.58
3:AT:73:GLU:CG	3:AU:100:ILE:HG23	2.31	0.58
1:BZ:41:VAL:HG23	1:BZ:57:ALA:HB1	1.85	0.58
2:BG:79:ASP:O	1:BZ:212:ASN:ND2	2.37	0.58
2:AP:21:ASN:HB3	3:AX:181:GLU:CD	2.23	0.58
1:AZ:41:VAL:HG23	1:AZ:57:ALA:HB1	1.85	0.58
3:AX:120:LYS:NZ	3:BU:66:GLU:CG	2.66	0.58
2:AN:51:LEU:HD12	3:AV:262:PRO:CG	2.33	0.58
3:AU:238:ILE:HG22	3:AU:240:ILE:HG23	1.85	0.58
3:AV:226:ALA:HB3	3:AV:268:ARG:HB3	1.85	0.58
2:AN:120:LYS:HE2	3:AW:222:ASN:ND2	2.18	0.58
2:AR:88:ILE:HG12	2:AR:97:VAL:HG22	1.85	0.58
3:AV:116:GLU:HB2	3:AW:31:PRO:HD2	1.84	0.58
2:AR:9:PHE:CE2	3:AX:181:GLU:HG3	2.38	0.58
3:AT:45:SER:OG	1:AY:1:MET:HB3	2.04	0.58
2:AF:88:ILE:HG12	2:AF:97:VAL:HG22	1.86	0.58
3:BU:238:ILE:HG22	3:BU:240:ILE:HG23	1.85	0.58
1:BZ:153:ASN:HB3	1:BZ:156:ILE:HG12	1.85	0.58
2:AC:88:ILE:HG12	2:AC:97:VAL:HG22	1.85	0.58
3:BS:196:ILE:HG13	3:BS:274:ILE:HB	1.85	0.58
2:BQ:21:ASN:OD1	3:BX:165:PRO:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BO:88:ILE:HG12	2:BO:97:VAL:HG22	1.85	0.58
3:BV:171:ILE:HG22	3:BV:172:LYS:H	1.68	0.58
3:AU:68:PHE:HB3	3:BX:121:ASN:HD21	1.68	0.57
2:AE:18:VAL:HG13	3:AT:168:TYR:CD2	2.38	0.57
3:AV:247:GLU:OE1	3:AV:249:TYR:CE2	2.56	0.57
2:AD:49:THR:HG22	3:AS:233:GLN:HB2	1.85	0.57
3:AW:120:LYS:CG	3:BV:68:PHE:CD1	2.78	0.57
1:A0:330:LEU:HB2	3:AV:261:PHE:CD2	2.39	0.57
2:AI:88:ILE:HG12	2:AI:97:VAL:HG22	1.85	0.57
1:AZ:153:ASN:HB3	1:AZ:156:ILE:HG12	1.85	0.57
3:AU:66:GLU:HG2	3:BX:120:LYS:CE	2.30	0.57
3:AS:66:GLU:HG2	3:BT:120:LYS:CE	2.34	0.57
2:AG:81:VAL:HB	1:AZ:86:LYS:HZ1	1.69	0.57
3:BV:226:ALA:HB3	3:BV:268:ARG:HB3	1.85	0.57
3:AX:206:LYS:HG3	3:AX:285:SER:HB3	1.86	0.57
2:AO:88:ILE:HG12	2:AO:97:VAL:HG22	1.85	0.57
3:BU:114:LYS:NZ	3:BV:298:VAL:O	2.37	0.57
2:BN:51:LEU:HD12	3:BV:262:PRO:CG	2.26	0.57
2:BE:18:VAL:HG13	3:BT:168:TYR:CD2	2.39	0.57
2:BF:18:VAL:O	3:BT:175:SER:OG	2.07	0.57
2:BF:88:ILE:HG12	2:BF:97:VAL:HG22	1.86	0.57
2:AQ:21:ASN:CG	3:AX:165:PRO:HG2	2.24	0.57
2:AR:20:SER:HA	3:AX:170:TYR:CD1	2.40	0.57
2:BR:9:PHE:CE1	3:BX:180:GLY:CA	2.87	0.57
3:AS:196:ILE:HG13	3:AS:274:ILE:HB	1.85	0.57
1:B0:86:LYS:NZ	2:BN:81:VAL:HB	2.19	0.57
2:BR:88:ILE:HG12	2:BR:97:VAL:HG22	1.85	0.57
2:AR:9:PHE:CZ	3:AX:180:GLY:C	2.78	0.57
2:AA:120:LYS:HE2	3:AS:222:ASN:ND2	2.19	0.57
2:AP:21:ASN:CB	3:AX:181:GLU:HG2	2.35	0.57
1:A0:78:PRO:HG3	2:AN:103:THR:HB	1.87	0.57
3:AU:196:ILE:HG22	3:AU:293:ARG:HD3	1.87	0.57
2:BI:88:ILE:HG12	2:BI:97:VAL:HG22	1.85	0.57
3:AV:68:PHE:HB3	3:BW:121:ASN:ND2	2.20	0.56
3:BT:73:GLU:HB2	3:BU:99:GLU:CD	2.25	0.56
2:BC:88:ILE:HG12	2:BC:97:VAL:HG22	1.85	0.56
2:BR:17:PRO:HA	3:BX:177:THR:HG22	1.87	0.56
2:AD:131:THR:HG22	3:AS:262:PRO:C	2.18	0.56
3:BU:240:ILE:HD12	3:BU:240:ILE:O	2.05	0.56
3:AW:206:LYS:HG3	3:AW:285:SER:HB3	1.87	0.56
3:AV:206:LYS:HG3	3:AV:285:SER:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AT:266:PHE:CD1	1:AZ:221:ARG:HB2	2.40	0.56
3:AT:240:ILE:HD12	3:AT:240:ILE:O	2.06	0.56
2:AR:23:ASP:OD2	3:AX:176:TYR:CE2	2.58	0.56
3:BX:206:LYS:HG3	3:BX:285:SER:HB3	1.86	0.56
2:AL:88:ILE:HG12	2:AL:97:VAL:HG22	1.86	0.56
3:BW:206:LYS:HG3	3:BW:285:SER:HB3	1.87	0.56
1:A0:41:VAL:HG11	1:A0:71:ILE:HG12	1.87	0.56
2:BD:19:GLY:HA2	3:BT:180:GLY:O	2.05	0.56
2:AM:26:LEU:HD13	2:AN:66:TYR:HB2	1.88	0.56
3:AU:76:TYR:HB3	3:AV:100:ILE:HD11	1.86	0.56
2:AC:18:VAL:HG13	3:AS:176:TYR:CE2	2.41	0.56
2:AE:187:ILE:HG12	2:AE:260:SER:HB3	1.88	0.56
2:AK:10:SER:HA	2:AK:15:GLU:HB2	1.88	0.56
3:BW:76:TYR:HB3	3:BX:100:ILE:HD11	1.87	0.56
3:AS:270:ARG:NH1	1:AY:72:LEU:HD22	2.21	0.56
2:AN:187:ILE:HG12	2:AN:260:SER:HB3	1.88	0.56
3:AX:120:LYS:CD	3:BU:68:PHE:HE1	2.01	0.56
2:BQ:18:VAL:CG1	3:BX:168:TYR:O	2.52	0.56
2:BN:51:LEU:CD1	3:BV:262:PRO:HG2	2.28	0.56
2:BL:88:ILE:HG12	2:BL:97:VAL:HG22	1.86	0.56
2:AB:17:PRO:HB3	3:AS:167:ASN:HB2	1.88	0.56
3:BU:196:ILE:HG22	3:BU:293:ARG:HD3	1.87	0.56
2:BE:187:ILE:HG12	2:BE:260:SER:HB3	1.88	0.56
3:AX:120:LYS:HB3	3:BU:68:PHE:HD1	1.71	0.55
3:AX:247:GLU:OE1	3:AX:249:TYR:CE2	2.59	0.55
2:BN:120:LYS:NZ	3:BW:220:ILE:O	2.34	0.55
2:BB:88:ILE:HG12	2:BB:97:VAL:HG22	1.88	0.55
2:BM:26:LEU:HD13	2:BN:66:TYR:HB2	1.88	0.55
3:BU:224:TYR:HB2	1:BZ:74:PRO:HB2	1.88	0.55
3:BV:206:LYS:HG3	3:BV:285:SER:HB3	1.87	0.55
3:BX:247:GLU:OE1	3:BX:249:TYR:CE2	2.59	0.55
3:BX:240:ILE:O	3:BX:240:ILE:HD12	2.07	0.55
3:AU:66:GLU:HG3	3:BX:120:LYS:NZ	2.22	0.55
3:AX:120:LYS:CE	3:BU:66:GLU:HG2	2.33	0.55
1:B0:42:ILE:HD13	3:BX:43:TRP:HE1	1.69	0.55
2:AQ:18:VAL:O	3:AX:168:TYR:N	2.39	0.55
3:AS:197:PHE:HB2	3:AT:48:ILE:HG21	1.88	0.55
1:A0:88:LYS:CE	2:AN:106:ASN:OD1	2.54	0.55
2:BG:103:THR:CG2	1:BZ:78:PRO:HG3	2.35	0.55
3:AT:120:LYS:NZ	3:BS:66:GLU:CG	2.66	0.55
2:AB:155:VAL:HG21	2:AB:159:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BT:240:ILE:HD12	3:BT:240:ILE:O	2.06	0.55
3:AX:120:LYS:HB3	3:BU:68:PHE:CD1	2.41	0.55
3:BT:160:TYR:HB3	3:BT:166:GLY:HA3	1.89	0.55
2:AN:47:LEU:HD22	3:AV:233:GLN:CD	2.26	0.55
3:AU:120:LYS:NZ	3:BX:66:GLU:HG2	2.22	0.55
1:AZ:41:VAL:HG11	1:AZ:71:ILE:HG12	1.88	0.55
3:AU:240:ILE:O	3:AU:240:ILE:HD12	2.05	0.55
3:AU:108:ALA:HB2	3:AU:133:ILE:HD11	1.89	0.55
2:AD:131:THR:HB	3:AS:263:VAL:CG2	2.37	0.55
2:BF:23:ASP:OD2	3:BT:176:TYR:CE2	2.60	0.55
2:BN:187:ILE:HG12	2:BN:260:SER:HB3	1.88	0.55
2:BH:187:ILE:HG12	2:BH:260:SER:HB3	1.88	0.55
3:AX:240:ILE:O	3:AX:240:ILE:HD12	2.07	0.55
2:AQ:187:ILE:HG12	2:AQ:260:SER:HB3	1.88	0.55
3:BU:160:TYR:HB3	3:BU:166:GLY:HA3	1.89	0.55
2:AK:88:ILE:HG12	2:AK:97:VAL:HG22	1.89	0.55
2:AD:52:ASN:ND2	3:AS:258:LEU:CB	2.70	0.55
3:AS:87:LEU:O	3:AT:54:ARG:NH1	2.40	0.55
1:B0:41:VAL:HG11	1:B0:71:ILE:HG12	1.88	0.55
2:AG:92:GLN:HE21	3:AU:189:ARG:NE	2.05	0.54
2:AB:88:ILE:HG12	2:AB:97:VAL:HG22	1.88	0.54
2:AN:89:ASP:OD2	3:AW:189:ARG:NH1	2.33	0.54
3:AT:123:THR:HG21	3:BS:120:LYS:HD2	1.89	0.54
3:AX:120:LYS:NZ	3:BU:66:GLU:HG3	2.23	0.54
1:BY:243:PHE:CD1	1:BY:243:PHE:C	2.80	0.54
2:BK:10:SER:HA	2:BK:15:GLU:HB2	1.87	0.54
2:BK:187:ILE:HG12	2:BK:260:SER:HB3	1.88	0.54
2:AG:80:SER:OG	1:AZ:211:ARG:HD2	2.07	0.54
2:BQ:187:ILE:HG12	2:BQ:260:SER:HB3	1.88	0.54
2:AB:187:ILE:HG12	2:AB:260:SER:HB3	1.88	0.54
3:AX:66:GLU:HG2	3:BU:120:LYS:HE2	1.89	0.54
2:AC:18:VAL:CG1	3:AS:176:TYR:CZ	2.90	0.54
1:AY:243:PHE:C	1:AY:243:PHE:CD1	2.80	0.54
3:BT:106:ASP:O	3:BT:133:ILE:HB	2.07	0.54
2:AP:5:ASN:HB3	2:AP:8:PHE:CD1	2.42	0.54
2:AE:88:ILE:HG12	2:AE:97:VAL:HG22	1.89	0.54
3:AU:160:TYR:HB3	3:AU:166:GLY:HA3	1.89	0.54
2:AK:187:ILE:HG12	2:AK:260:SER:HB3	1.88	0.54
2:AH:88:ILE:HG12	2:AH:97:VAL:HG22	1.89	0.54
2:AH:187:ILE:HG12	2:AH:260:SER:HB3	1.88	0.54
3:AS:160:TYR:HB3	3:AS:166:GLY:HA3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BT:215:ARG:HB3	3:BT:282:ILE:HD11	1.89	0.54
2:BQ:88:ILE:HG12	2:BQ:97:VAL:HG22	1.89	0.54
2:BD:73:THR:HB	3:BS:256:THR:HG23	1.87	0.54
1:BZ:41:VAL:HG11	1:BZ:71:ILE:HG12	1.88	0.54
2:BQ:17:PRO:HB3	3:BX:167:ASN:ND2	2.12	0.54
3:BX:167:ASN:ND2	3:BX:169:LYS:HE3	2.23	0.54
2:BA:104:ALA:HB2	1:BY:88:LYS:HZ2	1.72	0.54
2:AM:88:ILE:HG12	2:AM:97:VAL:HG22	1.90	0.54
3:AX:226:ALA:HB3	3:AX:268:ARG:HB3	1.89	0.54
3:AT:160:TYR:HB3	3:AT:166:GLY:HA3	1.89	0.54
2:AN:49:THR:O	3:AV:258:LEU:HD21	2.08	0.54
2:BP:5:ASN:HB3	2:BP:8:PHE:CD1	2.42	0.54
3:AT:215:ARG:HB3	3:AT:282:ILE:HD11	1.89	0.54
2:BK:88:ILE:HG12	2:BK:97:VAL:HG22	1.89	0.54
1:A0:294:PHE:CE2	1:AZ:169:THR:CG2	2.88	0.53
3:BU:242:THR:HG23	3:BU:272:ARG:HG3	1.87	0.53
3:AU:242:THR:HG23	3:AU:272:ARG:HG3	1.87	0.53
3:BU:55:SER:HB3	1:BZ:359:PHE:CE1	2.44	0.53
2:AQ:8:PHE:O	3:AX:170:TYR:HB2	2.07	0.53
2:AQ:88:ILE:HG12	2:AQ:97:VAL:HG22	1.89	0.53
1:A0:344:GLY:HA3	3:AV:270:ARG:HH11	1.73	0.53
2:BB:187:ILE:HG12	2:BB:260:SER:HB3	1.88	0.53
3:BS:160:TYR:HB3	3:BS:166:GLY:HA3	1.89	0.53
3:AT:106:ASP:O	3:AT:133:ILE:HB	2.08	0.53
2:BN:131:THR:CG2	3:BV:262:PRO:O	2.42	0.53
2:BF:17:PRO:HA	3:BT:177:THR:CG2	2.37	0.53
2:AP:21:ASN:H	3:AX:181:GLU:HG2	1.73	0.53
2:AN:47:LEU:HD22	3:AV:233:GLN:NE2	2.23	0.53
2:BB:155:VAL:HG21	2:BB:159:ILE:HD11	1.88	0.53
3:AW:120:LYS:HZ3	3:BV:66:GLU:CG	2.21	0.53
3:AX:121:ASN:HD21	3:BU:68:PHE:HB3	1.73	0.53
1:B0:238:ARG:HG3	1:B0:316:SER:HA	1.89	0.53
1:B0:169:THR:HG21	1:BY:294:PHE:CE2	2.42	0.53
3:BT:114:LYS:HB3	3:BU:34:LEU:HB2	1.90	0.53
3:AX:167:ASN:ND2	3:AX:169:LYS:HE3	2.23	0.53
2:BE:88:ILE:HG12	2:BE:97:VAL:HG22	1.89	0.53
2:AD:19:GLY:HA2	3:AT:180:GLY:O	2.08	0.53
2:AN:47:LEU:HB3	3:AV:233:GLN:OE1	2.09	0.53
1:A0:45:GLU:HA	1:A0:357:THR:HG22	1.91	0.53
2:AG:88:ILE:HG12	2:AG:97:VAL:HG22	1.90	0.53
2:AJ:88:ILE:HG12	2:AJ:97:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BH:88:ILE:HG12	2:BH:97:VAL:HG22	1.89	0.53
3:BU:108:ALA:HB2	3:BU:133:ILE:HD11	1.89	0.53
3:BS:133:ILE:HA	3:BT:42:ILE:HG21	1.91	0.53
2:AN:88:ILE:HG12	2:AN:97:VAL:HG22	1.89	0.53
2:AA:5:ASN:HB3	2:AA:8:PHE:CD1	2.44	0.53
2:BN:47:LEU:HB3	3:BV:233:GLN:OE1	2.09	0.53
2:AP:26:LEU:HD13	2:AQ:66:TYR:HB2	1.91	0.53
2:BA:120:LYS:HE2	3:BS:222:ASN:HD21	1.74	0.53
3:BX:226:ALA:HB3	3:BX:268:ARG:HB3	1.89	0.53
3:AT:206:LYS:HG3	3:AT:285:SER:HB3	1.91	0.53
2:BF:18:VAL:HG12	3:BT:176:TYR:O	2.10	0.53
3:AW:68:PHE:CE1	3:BV:120:LYS:HD2	2.44	0.52
3:AX:160:TYR:HB3	3:AX:166:GLY:HA3	1.91	0.52
2:BD:5:ASN:HB3	2:BD:8:PHE:CD1	2.44	0.52
2:BP:88:ILE:HG12	2:BP:97:VAL:HG22	1.91	0.52
1:A0:238:ARG:HG3	1:A0:316:SER:HA	1.90	0.52
3:AX:183:ASP:O	3:AX:186:ARG:HG3	2.09	0.52
3:AW:196:ILE:HG13	3:AW:274:ILE:HB	1.90	0.52
1:B0:45:GLU:HA	1:B0:357:THR:HG22	1.91	0.52
2:AD:5:ASN:HB3	2:AD:8:PHE:CD1	2.44	0.52
3:AW:66:GLU:HB3	3:BV:120:LYS:NZ	2.24	0.52
2:AF:17:PRO:CA	3:AT:177:THR:HG22	2.36	0.52
3:BU:55:SER:HB3	1:BZ:359:PHE:HE1	1.74	0.52
2:BQ:25:LYS:HE2	2:BQ:113:ASN:HB3	1.91	0.52
2:BN:88:ILE:HG12	2:BN:97:VAL:HG22	1.89	0.52
2:AP:88:ILE:HG12	2:AP:97:VAL:HG22	1.91	0.52
3:BT:206:LYS:HG3	3:BT:285:SER:HB3	1.91	0.52
2:BP:26:LEU:HD13	2:BQ:66:TYR:HB2	1.91	0.52
2:BA:5:ASN:HB3	2:BA:8:PHE:CD1	2.44	0.52
2:BJ:88:ILE:HG12	2:BJ:97:VAL:HG22	1.91	0.52
2:BR:9:PHE:CE1	3:BX:180:GLY:HA2	2.44	0.52
2:AP:21:ASN:HB3	3:AX:181:GLU:HG2	1.92	0.52
1:AZ:241:TYR:HB2	1:AZ:291:LYS:HD2	1.91	0.52
2:BG:88:ILE:HG12	2:BG:97:VAL:HG22	1.90	0.52
2:AF:23:ASP:OD2	3:AT:176:TYR:CE2	2.63	0.52
3:BW:196:ILE:HG13	3:BW:274:ILE:HB	1.90	0.52
3:AT:230:LYS:HG3	3:AT:263:VAL:HG22	1.91	0.52
3:BX:183:ASP:O	3:BX:186:ARG:HG3	2.09	0.52
3:AV:142:LEU:HG	3:AV:291:ILE:HD12	1.90	0.52
3:AW:66:GLU:HB3	3:BV:120:LYS:HZ2	1.70	0.52
3:AU:116:GLU:HB2	3:AV:31:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BE:17:PRO:HB2	3:BT:167:ASN:HD22	1.72	0.52
3:BV:142:LEU:HG	3:BV:291:ILE:HD12	1.90	0.52
1:BY:89:LEU:HD22	1:BY:192:GLN:HG3	1.92	0.52
2:AA:148:ILE:HB	2:AC:153:MET:HG3	1.92	0.52
3:AW:66:GLU:CG	3:BV:120:LYS:HZ3	2.15	0.52
2:AQ:18:VAL:HG13	3:AX:168:TYR:CD2	2.45	0.52
2:AQ:20:SER:OG	3:AX:165:PRO:O	2.18	0.52
3:AV:43:TRP:CZ2	1:AZ:43:ASN:HB2	2.45	0.52
1:B0:12:PRO:HB2	1:BY:288:ARG:NH2	2.25	0.52
3:BT:230:LYS:HG3	3:BT:263:VAL:HG22	1.91	0.52
2:BL:145:LEU:HD13	2:BL:148:ILE:HD11	1.91	0.52
3:AW:160:TYR:HB3	3:AW:166:GLY:HA3	1.92	0.52
3:AU:281:LEU:HB3	3:AU:284:LEU:HD12	1.92	0.52
1:BZ:241:TYR:HB2	1:BZ:291:LYS:HD2	1.91	0.52
2:BR:9:PHE:HE2	3:BX:181:GLU:HG3	1.72	0.51
3:BT:132:ILE:HD13	3:BT:135:LYS:HG3	1.92	0.51
3:BW:226:ALA:HB3	3:BW:268:ARG:HB3	1.92	0.51
2:BP:5:ASN:O	2:BP:16:PHE:HB3	2.10	0.51
2:AA:88:ILE:HG12	2:AA:97:VAL:HG22	1.92	0.51
1:A0:42:ILE:HD13	3:AX:43:TRP:CE2	2.44	0.51
3:BS:242:THR:HG23	3:BS:272:ARG:HG3	1.89	0.51
3:BX:160:TYR:HB3	3:BX:166:GLY:HA3	1.91	0.51
2:AP:5:ASN:O	2:AP:16:PHE:HB3	2.11	0.51
1:BY:32:LEU:HD11	1:BY:204:LEU:HB2	1.92	0.51
2:AQ:25:LYS:HE2	2:AQ:113:ASN:HB3	1.92	0.51
2:BM:88:ILE:HG12	2:BM:97:VAL:HG22	1.90	0.51
2:AD:52:ASN:HD21	3:AS:258:LEU:HB3	1.75	0.51
3:AS:266:PHE:CG	1:AY:35:PRO:HD2	2.46	0.51
3:AT:87:LEU:HA	3:AU:54:ARG:NH1	2.25	0.51
2:BA:88:ILE:HG12	2:BA:97:VAL:HG22	1.92	0.51
3:AT:132:ILE:HD13	3:AT:135:LYS:HG3	1.92	0.51
2:AN:100:SER:HB3	3:AW:220:ILE:HG21	1.92	0.51
2:AI:177:GLN:HB3	2:AI:189:ARG:HB2	1.93	0.51
2:BA:148:ILE:HB	2:BC:153:MET:HG3	1.92	0.51
3:AT:199:PHE:N	3:AT:242:THR:OG1	2.39	0.51
2:AQ:17:PRO:CB	3:AX:169:LYS:CE	2.84	0.51
2:BI:177:GLN:HB3	2:BI:189:ARG:HB2	1.93	0.51
3:BW:160:TYR:HB3	3:BW:166:GLY:HA3	1.92	0.51
3:AS:270:ARG:HG3	1:AY:72:LEU:HB3	1.93	0.51
3:BX:144:PHE:HB3	3:BX:190:TRP:CE2	2.45	0.51
2:AL:145:LEU:HD13	2:AL:148:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AC:177:GLN:HB3	2:AC:189:ARG:HB2	1.93	0.51
2:BF:177:GLN:HB3	2:BF:189:ARG:HB2	1.93	0.51
2:BO:177:GLN:HB3	2:BO:189:ARG:HB2	1.93	0.51
3:AX:167:ASN:HD22	3:AX:169:LYS:HE3	1.76	0.51
3:BX:167:ASN:HD22	3:BX:169:LYS:HE3	1.76	0.51
3:AX:66:GLU:HG2	3:BU:120:LYS:NZ	2.26	0.51
2:BG:10:SER:N	3:BU:160:TYR:O	2.30	0.51
1:AZ:157:PHE:HE2	1:AZ:208:PHE:HB3	1.76	0.51
1:AY:89:LEU:HD22	1:AY:192:GLN:HG3	1.92	0.51
2:BC:177:GLN:HB3	2:BC:189:ARG:HB2	1.93	0.51
2:BQ:9:PHE:HA	3:BX:170:TYR:O	2.11	0.51
3:AW:120:LYS:CB	3:BV:68:PHE:HD1	2.21	0.50
2:AB:13:SER:O	3:AS:169:LYS:HE2	2.05	0.50
3:AS:244:VAL:HG21	3:AT:50:VAL:CG2	2.40	0.50
1:AY:32:LEU:HD11	1:AY:204:LEU:HB2	1.92	0.50
3:BS:171:ILE:HG22	3:BS:172:LYS:H	1.76	0.50
2:BN:89:ASP:OD2	3:BW:189:ARG:NH1	2.37	0.50
1:BY:120:ASP:HB2	1:BZ:292:THR:HB	1.93	0.50
3:AX:66:GLU:HG2	3:BU:120:LYS:CE	2.40	0.50
3:AT:73:GLU:HB2	3:AU:99:GLU:CD	2.30	0.50
2:BN:102:GLU:OE1	3:BW:222:ASN:ND2	2.40	0.50
1:A0:32:LEU:HD11	1:A0:204:LEU:HB2	1.93	0.50
2:AO:177:GLN:HB3	2:AO:189:ARG:HB2	1.93	0.50
3:AX:144:PHE:HB3	3:AX:190:TRP:CE2	2.45	0.50
1:A0:42:ILE:HB	3:AX:43:TRP:HZ2	0.61	0.50
2:AQ:20:SER:HA	3:AX:160:TYR:CD1	2.46	0.50
2:AF:17:PRO:HA	3:AT:177:THR:CG2	2.38	0.50
3:BS:197:PHE:HD1	3:BT:48:ILE:HG22	1.76	0.50
3:AV:45:SER:HB2	1:AZ:42:ILE:HG22	1.92	0.50
3:BU:138:THR:O	3:BU:292:LYS:HA	2.11	0.50
3:BT:238:ILE:HG22	3:BT:240:ILE:HG23	1.94	0.50
3:AT:124:PHE:O	3:BS:120:LYS:NZ	2.43	0.50
2:BP:113:ASN:O	3:BX:186:ARG:NH2	2.44	0.50
2:AP:120:LYS:NZ	3:AX:220:ILE:O	2.37	0.50
1:BZ:157:PHE:HE2	1:BZ:208:PHE:HB3	1.76	0.50
3:AV:120:LYS:HZ1	3:BW:66:GLU:HB3	1.75	0.50
3:AU:116:GLU:OE2	3:AV:3:ARG:HG3	2.11	0.50
2:AD:88:ILE:HG12	2:AD:97:VAL:HG22	1.93	0.50
1:B0:122:PRO:HD2	1:B0:125:ILE:HD12	1.94	0.50
3:BU:281:LEU:HB3	3:BU:284:LEU:HD12	1.92	0.50
3:BT:87:LEU:HA	3:BU:54:ARG:NH1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BM:9:PHE:HB2	3:BW:180:GLY:HA2	1.92	0.50
3:BT:243:ASP:OD1	3:BT:243:ASP:C	2.50	0.50
3:BU:196:ILE:HG13	3:BU:274:ILE:HB	1.94	0.50
2:BA:102:GLU:OE2	3:BS:220:ILE:HD12	2.12	0.50
1:A0:288:ARG:NH2	1:AZ:12:PRO:HB2	2.27	0.50
2:BB:13:SER:C	3:BS:169:LYS:CD	2.59	0.50
3:AU:266:PHE:CG	1:AZ:35:PRO:HD2	2.47	0.50
3:AS:4:GLN:HB2	3:AS:97:GLN:HB3	1.93	0.50
1:B0:32:LEU:HD11	1:B0:204:LEU:HB2	1.93	0.50
3:AW:226:ALA:HB3	3:AW:268:ARG:HB3	1.92	0.50
2:AA:81:VAL:HB	1:AY:86:LYS:NZ	2.27	0.50
2:AP:21:ASN:HB3	3:AX:181:GLU:CG	2.42	0.50
3:AV:196:ILE:HG13	3:AV:274:ILE:HB	1.94	0.50
2:AO:171:GLY:HA3	2:AO:205:GLY:H	1.77	0.50
2:BD:88:ILE:HG12	2:BD:97:VAL:HG22	1.93	0.50
3:AT:36:LEU:HD22	3:AT:56:ILE:HD11	1.93	0.50
2:BL:177:GLN:HB3	2:BL:189:ARG:HB2	1.93	0.50
1:AY:39:CYS:HB2	1:AY:60:THR:OG1	2.12	0.50
2:AJ:5:ASN:HB3	2:AJ:8:PHE:CD1	2.47	0.50
3:BV:240:ILE:C	3:BV:240:ILE:HD12	2.32	0.50
3:BV:96:TYR:HB3	3:BV:103:VAL:HG23	1.94	0.50
2:BK:116:SER:OG	3:BV:186:ARG:O	2.29	0.50
3:AU:68:PHE:HE1	3:BX:120:LYS:HG2	1.76	0.49
1:B0:76:VAL:HG11	1:B0:88:LYS:HD2	1.94	0.49
2:AR:9:PHE:CE1	3:AX:180:GLY:N	2.80	0.49
2:AR:177:GLN:HB3	2:AR:189:ARG:HB2	1.93	0.49
2:BR:177:GLN:HB3	2:BR:189:ARG:HB2	1.93	0.49
3:BV:48:ILE:HG21	1:BZ:1:MET:HE1	1.92	0.49
2:BO:171:GLY:HA3	2:BO:205:GLY:H	1.77	0.49
3:AU:171:ILE:HG22	3:AU:172:LYS:H	1.77	0.49
2:AL:177:GLN:HB3	2:AL:189:ARG:HB2	1.93	0.49
2:AA:172:ASN:HD21	2:AA:204:SER:H	1.60	0.49
2:BA:172:ASN:HD21	2:BA:204:SER:H	1.60	0.49
2:BF:17:PRO:CA	3:BT:177:THR:HG22	2.37	0.49
2:AP:22:ASN:HD21	3:AX:182:SER:HB3	1.77	0.49
3:AX:199:PHE:CZ	3:AX:242:THR:HG21	2.47	0.49
1:B0:86:LYS:HZ2	2:BN:81:VAL:HB	1.75	0.49
2:BN:120:LYS:HE2	3:BW:222:ASN:ND2	2.27	0.49
3:AT:199:PHE:H	3:AT:242:THR:HG1	1.57	0.49
1:A0:218:ILE:HB	1:A0:338:VAL:HG12	1.95	0.49
3:AS:171:ILE:HG22	3:AS:172:LYS:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BS:4:GLN:HB2	3:BS:97:GLN:HB3	1.93	0.49
2:AF:177:GLN:HB3	2:AF:189:ARG:HB2	1.93	0.49
3:AV:43:TRP:HE1	1:AZ:42:ILE:HB	1.77	0.49
3:BX:199:PHE:CZ	3:BX:242:THR:HG21	2.47	0.49
3:AU:138:THR:O	3:AU:292:LYS:HA	2.11	0.49
1:AZ:152:PHE:CB	1:AZ:208:PHE:HB2	2.42	0.49
3:AW:120:LYS:CE	3:BV:68:PHE:CE1	2.90	0.49
3:AX:120:LYS:HZ1	3:BU:66:GLU:HG3	1.77	0.49
3:BS:197:PHE:CD1	3:BT:48:ILE:CG2	2.94	0.49
2:AQ:39:ARG:HB2	2:AQ:61:ILE:HB	1.94	0.49
3:AW:76:TYR:HB3	3:AX:100:ILE:HD11	1.94	0.49
3:BS:11:LEU:O	3:BS:12:ASP:CG	2.51	0.49
3:BW:4:GLN:HB2	3:BW:97:GLN:HB3	1.94	0.49
1:A0:122:PRO:HD2	1:A0:125:ILE:HD12	1.94	0.49
1:A0:242:ASN:O	1:A0:313:ILE:HD12	2.12	0.49
3:BS:196:ILE:HG22	3:BS:293:ARG:HD3	1.95	0.49
3:BX:171:ILE:HG22	3:BX:172:LYS:H	1.77	0.49
1:BY:45:GLU:HA	1:BY:357:THR:HG22	1.95	0.49
3:AU:270:ARG:NH1	1:AZ:72:LEU:HD22	2.28	0.49
2:AI:171:GLY:HA3	2:AI:205:GLY:H	1.77	0.49
3:AX:171:ILE:HG22	3:AX:172:LYS:H	1.77	0.49
3:BT:36:LEU:HD22	3:BT:56:ILE:HD11	1.93	0.49
3:AT:243:ASP:C	3:AT:243:ASP:OD1	2.50	0.49
2:AR:7:THR:HA	3:AX:178:TYR:CE2	2.47	0.49
3:BV:196:ILE:HG13	3:BV:274:ILE:HB	1.94	0.49
1:BZ:152:PHE:CB	1:BZ:208:PHE:HB2	2.42	0.49
2:AK:39:ARG:HB2	2:AK:61:ILE:HB	1.94	0.49
2:AN:39:ARG:HB2	2:AN:61:ILE:HB	1.94	0.49
3:AW:4:GLN:HB2	3:AW:97:GLN:HB3	1.94	0.49
1:A0:76:VAL:HG11	1:A0:88:LYS:HD2	1.94	0.49
2:AF:18:VAL:HG12	3:AT:176:TYR:O	2.12	0.49
2:BC:18:VAL:HG13	3:BS:176:TYR:CE2	2.47	0.49
3:AU:196:ILE:HG13	3:AU:274:ILE:HB	1.94	0.49
2:AF:171:GLY:HA3	2:AF:205:GLY:H	1.77	0.49
2:AP:118:VAL:HG23	3:AX:278:GLN:NE2	2.27	0.49
2:BQ:39:ARG:HB2	2:BQ:61:ILE:HB	1.94	0.49
3:BU:171:ILE:HG22	3:BU:172:LYS:H	1.77	0.49
2:AD:52:ASN:HB2	3:AS:258:LEU:CD2	2.30	0.49
3:AU:53:THR:HG21	1:AZ:359:PHE:CA	2.43	0.49
2:AG:79:ASP:CB	1:AZ:212:ASN:HD21	2.25	0.49
2:BC:18:VAL:CG1	3:BS:176:TYR:CZ	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BG:79:ASP:C	1:BZ:212:ASN:HD21	2.16	0.49
2:BN:100:SER:HB3	3:BW:220:ILE:HG21	1.95	0.49
3:AS:11:LEU:O	3:AS:12:ASP:CG	2.51	0.49
1:B0:218:ILE:HB	1:B0:338:VAL:HG12	1.95	0.49
2:BF:171:GLY:HA3	2:BF:205:GLY:H	1.77	0.49
2:BM:17:PRO:HA	3:BW:177:THR:HG22	1.95	0.49
2:AK:91:THR:HG21	3:AV:189:ARG:HB2	1.93	0.49
2:BP:22:ASN:HD21	3:BX:182:SER:CB	2.25	0.49
1:BY:169:THR:HG21	1:BZ:294:PHE:CZ	2.47	0.49
3:AS:133:ILE:HA	3:AT:42:ILE:CG2	2.39	0.49
1:BY:39:CYS:HB2	1:BY:60:THR:OG1	2.12	0.49
2:AJ:26:LEU:HD13	2:AK:66:TYR:HB2	1.94	0.49
3:AV:240:ILE:C	3:AV:240:ILE:HD12	2.32	0.49
2:BJ:26:LEU:HD13	2:BK:66:TYR:HB2	1.94	0.49
2:BC:171:GLY:HA3	2:BC:205:GLY:H	1.77	0.49
2:AR:171:GLY:HA3	2:AR:205:GLY:H	1.77	0.49
1:AY:233:GLU:HB2	1:AY:321:ARG:HH21	1.78	0.49
3:BU:229:PHE:CD1	3:BU:264:MET:HB3	2.48	0.49
2:BJ:5:ASN:HB3	2:BJ:8:PHE:CD1	2.47	0.49
3:BT:199:PHE:CE1	3:BT:242:THR:HG21	2.48	0.49
3:AU:229:PHE:CD1	3:AU:264:MET:HB3	2.48	0.49
3:AT:199:PHE:CE1	3:AT:242:THR:HG21	2.48	0.49
2:BG:92:GLN:HE21	3:BU:189:ARG:NE	2.11	0.49
2:BH:19:GLY:HA2	3:BU:166:GLY:O	2.13	0.48
2:BQ:8:PHE:O	3:BX:170:TYR:HB2	2.12	0.48
3:BT:199:PHE:N	3:BT:242:THR:OG1	2.39	0.48
2:BN:39:ARG:HB2	2:BN:61:ILE:HB	1.93	0.48
1:B0:242:ASN:O	1:B0:313:ILE:HD12	2.12	0.48
3:BV:87:LEU:HA	3:BW:54:ARG:NH1	2.28	0.48
2:BL:171:GLY:HA3	2:BL:205:GLY:H	1.77	0.48
2:BH:39:ARG:HB2	2:BH:61:ILE:HB	1.95	0.48
3:BX:242:THR:O	3:BX:272:ARG:HD3	2.13	0.48
3:AT:238:ILE:HG22	3:AT:240:ILE:HG23	1.94	0.48
2:BI:171:GLY:HA3	2:BI:205:GLY:H	1.77	0.48
1:BY:233:GLU:HB2	1:BY:321:ARG:HH21	1.77	0.48
1:A0:184:GLN:HE22	1:A0:217:ARG:HH22	1.61	0.48
3:BT:76:TYR:HE1	3:BU:96:TYR:OH	1.96	0.48
2:BQ:17:PRO:HB3	3:BX:169:LYS:CE	2.38	0.48
2:AR:17:PRO:HA	3:AX:177:THR:CG2	2.43	0.48
3:BV:215:ARG:HB3	3:BV:282:ILE:HD11	1.95	0.48
3:AT:212:ALA:HB2	3:AT:283:ASN:HD22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AE:39:ARG:HB2	2:AE:61:ILE:HB	1.94	0.48
3:AU:114:LYS:NZ	3:AV:298:VAL:O	2.45	0.48
2:BH:17:PRO:HB3	3:BU:169:LYS:HE3	1.94	0.48
2:AH:39:ARG:HB2	2:AH:61:ILE:HB	1.94	0.48
3:BV:36:LEU:HD21	3:BV:297:PHE:HB2	1.96	0.48
1:B0:288:ARG:NH2	1:BZ:12:PRO:HB2	2.28	0.48
2:BD:52:ASN:ND2	3:BS:258:LEU:HB3	2.29	0.48
3:AU:272:ARG:NH1	1:AZ:40:GLN:OE1	2.46	0.48
2:BR:9:PHE:CZ	3:BX:180:GLY:C	2.87	0.48
1:B0:294:PHE:CE2	1:BZ:169:THR:CG2	2.96	0.48
2:BG:104:ALA:HB3	1:BZ:88:LYS:HD2	1.94	0.48
2:BE:39:ARG:HB2	2:BE:61:ILE:HB	1.95	0.48
1:B0:184:GLN:HE22	1:B0:217:ARG:HH22	1.61	0.48
2:AN:49:THR:HG21	3:AV:235:GLN:NE2	2.29	0.48
3:AT:120:LYS:HZ1	3:BS:66:GLU:HG3	1.75	0.48
3:AS:196:ILE:HG22	3:AS:293:ARG:HD3	1.95	0.48
3:BX:281:LEU:HB3	3:BX:284:LEU:HD12	1.96	0.48
3:AV:243:ASP:OD1	3:AV:243:ASP:C	2.52	0.48
1:A0:231:ASP:OD2	1:A0:321:ARG:NH1	2.47	0.48
2:AC:171:GLY:HA3	2:AC:205:GLY:H	1.77	0.48
1:AY:45:GLU:HA	1:AY:357:THR:HG22	1.95	0.48
3:BS:96:TYR:HH	3:BX:76:TYR:HE1	1.62	0.48
2:BE:18:VAL:CG1	3:BT:168:TYR:O	2.54	0.48
2:BR:9:PHE:HZ	3:BX:181:GLU:HG3	1.76	0.48
2:BD:23:ASP:OD2	3:BT:178:TYR:CE1	2.62	0.48
1:AZ:237:ASP:C	1:AZ:238:ARG:HG2	2.33	0.48
2:BN:47:LEU:HD22	3:BV:233:GLN:CD	2.34	0.48
2:BG:92:GLN:NE2	3:BU:189:ARG:CZ	2.77	0.48
2:AR:10:SER:HA	2:AR:15:GLU:HB2	1.96	0.48
1:BY:122:PRO:HD2	1:BY:125:ILE:HD12	1.96	0.48
2:BK:39:ARG:HB2	2:BK:61:ILE:HB	1.94	0.48
3:AV:36:LEU:HD21	3:AV:297:PHE:HB2	1.96	0.48
3:BV:144:PHE:HB3	3:BV:190:TRP:CE2	2.49	0.48
3:AS:242:THR:O	3:AS:272:ARG:HD3	2.14	0.48
1:B0:231:ASP:OD2	1:B0:321:ARG:NH1	2.47	0.48
2:BR:10:SER:HA	2:BR:15:GLU:HB2	1.96	0.48
3:AT:26:VAL:HG23	3:AT:67:THR:HG22	1.96	0.48
3:BT:26:VAL:HG23	3:BT:67:THR:HG22	1.96	0.48
3:AS:239:LEU:C	3:AS:239:LEU:HD23	2.34	0.48
2:AR:9:PHE:CZ	3:AX:181:GLU:N	2.82	0.48
1:BZ:237:ASP:C	1:BZ:238:ARG:HG2	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BS:239:LEU:HD23	3:BS:239:LEU:C	2.35	0.48
2:BR:171:GLY:HA3	2:BR:205:GLY:H	1.77	0.48
1:AY:122:PRO:HD2	1:AY:125:ILE:HD12	1.96	0.48
2:BD:131:THR:O	3:BS:263:VAL:HG23	2.13	0.48
3:BS:242:THR:O	3:BS:272:ARG:HD3	2.14	0.48
3:AX:68:PHE:CE1	3:BU:120:LYS:HD3	2.48	0.48
3:AU:106:ASP:O	3:AU:133:ILE:HB	2.14	0.48
3:BU:116:GLU:HB2	3:BV:31:PRO:HD2	1.95	0.48
3:BW:11:LEU:HD12	3:BW:93:THR:HG21	1.96	0.48
2:AK:116:SER:OG	3:AV:186:ARG:O	2.32	0.48
2:BB:39:ARG:HB2	2:BB:61:ILE:HB	1.95	0.48
2:BP:9:PHE:HA	3:BX:160:TYR:O	2.13	0.47
3:AU:194:GLU:HB2	3:AU:293:ARG:HD2	1.96	0.47
3:BT:226:ALA:HB3	3:BT:268:ARG:HB3	1.95	0.47
2:BR:27:TYR:HA	2:BR:30:LEU:HD12	1.96	0.47
2:BI:27:TYR:HA	2:BI:30:LEU:HD12	1.96	0.47
3:AV:96:TYR:HB3	3:AV:103:VAL:HG23	1.94	0.47
3:AU:120:LYS:HD3	3:BX:68:PHE:CE1	2.49	0.47
2:AP:19:GLY:CA	3:AX:180:GLY:O	2.62	0.47
2:AR:23:ASP:OD2	3:AX:176:TYR:CZ	2.67	0.47
3:AX:242:THR:O	3:AX:272:ARG:HD3	2.13	0.47
1:A0:169:THR:HG21	1:AY:294:PHE:CE2	2.49	0.47
3:BT:212:ALA:HB2	3:BT:283:ASN:HD22	1.79	0.47
3:BV:243:ASP:C	3:BV:243:ASP:OD1	2.52	0.47
3:AW:11:LEU:HD12	3:AW:93:THR:HG21	1.96	0.47
2:AP:148:ILE:HB	2:AR:153:MET:HG3	1.96	0.47
3:AW:171:ILE:HG22	3:AW:172:LYS:H	1.79	0.47
3:AV:215:ARG:HB3	3:AV:282:ILE:HD11	1.95	0.47
3:AU:66:GLU:CG	3:BX:120:LYS:CE	2.92	0.47
2:AQ:17:PRO:CG	3:AX:169:LYS:CE	2.93	0.47
3:BT:199:PHE:H	3:BT:242:THR:HG1	1.57	0.47
2:AR:27:TYR:HA	2:AR:30:LEU:HD12	1.96	0.47
2:AB:39:ARG:HB2	2:AB:61:ILE:HB	1.95	0.47
1:BZ:231:ASP:OD2	1:BZ:321:ARG:NH1	2.47	0.47
3:AT:226:ALA:HB3	3:AT:268:ARG:HB3	1.95	0.47
2:BN:73:THR:CB	3:BV:256:THR:HG21	2.44	0.47
3:BW:171:ILE:HG22	3:BW:172:LYS:H	1.79	0.47
2:AB:13:SER:C	3:AS:169:LYS:CD	2.62	0.47
2:BD:73:THR:HG21	3:BS:256:THR:HG21	1.94	0.47
3:BU:194:GLU:HB2	3:BU:293:ARG:HD2	1.96	0.47
3:BU:106:ASP:O	3:BU:133:ILE:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AU:11:LEU:O	3:AU:12:ASP:CG	2.52	0.47
3:AS:281:LEU:HB3	3:AS:284:LEU:HD12	1.96	0.47
2:AL:171:GLY:HA3	2:AL:205:GLY:H	1.77	0.47
3:AX:281:LEU:HB3	3:AX:284:LEU:HD12	1.96	0.47
3:AV:66:GLU:CG	3:BW:120:LYS:HZ3	2.26	0.47
2:AD:77:LYS:H	2:AD:82:ASN:ND2	2.12	0.47
3:AV:144:PHE:HB3	3:AV:190:TRP:CE2	2.49	0.47
3:AV:160:TYR:HB3	3:AV:166:GLY:HA3	1.95	0.47
3:BU:11:LEU:O	3:BU:12:ASP:CG	2.52	0.47
3:BV:160:TYR:HB3	3:BV:166:GLY:HA3	1.95	0.47
1:AZ:231:ASP:OD2	1:AZ:321:ARG:NH1	2.47	0.47
2:BD:51:LEU:HD12	3:BS:262:PRO:HG2	1.95	0.47
2:BE:18:VAL:C	3:BT:167:ASN:HA	2.35	0.47
3:AU:244:VAL:HG11	1:AZ:1:MET:HE1	1.96	0.47
2:AD:23:ASP:OD2	3:AT:178:TYR:CE1	2.67	0.47
3:BS:281:LEU:HB3	3:BS:284:LEU:HD12	1.96	0.47
3:BX:4:GLN:HB2	3:BX:97:GLN:HB3	1.96	0.47
3:BS:72:LEU:HD22	3:BS:76:TYR:CE2	2.50	0.47
1:A0:359:PHE:O	3:AW:53:THR:HG21	2.14	0.47
2:BF:23:ASP:OD2	3:BT:176:TYR:HE2	1.97	0.47
3:AV:196:ILE:HD13	3:AV:291:ILE:HG12	1.97	0.47
2:AI:27:TYR:HA	2:AI:30:LEU:HD12	1.96	0.47
2:BD:19:GLY:CA	3:BT:180:GLY:O	2.63	0.47
3:BV:196:ILE:HD13	3:BV:291:ILE:HG12	1.97	0.47
2:AP:172:ASN:HD21	2:AP:204:SER:H	1.63	0.47
3:AX:196:ILE:HD13	3:AX:291:ILE:HG13	1.97	0.47
3:BX:72:LEU:HD22	3:BX:76:TYR:CE2	2.50	0.47
3:BV:243:ASP:OD1	3:BV:245:ASN:N	2.48	0.47
3:AV:43:TRP:NE1	1:AZ:42:ILE:HB	2.30	0.46
2:BE:9:PHE:HD2	3:BT:170:TYR:C	2.18	0.46
2:BG:172:ASN:HD21	2:BG:204:SER:H	1.63	0.46
2:BP:148:ILE:HB	2:BR:153:MET:HG3	1.96	0.46
2:AM:5:ASN:HB3	2:AM:8:PHE:CD1	2.50	0.46
2:AH:17:PRO:HB3	3:AU:169:LYS:HE3	1.97	0.46
3:BX:196:ILE:HD13	3:BX:291:ILE:HG13	1.97	0.46
3:BW:72:LEU:HD22	3:BW:76:TYR:CE2	2.50	0.46
2:BM:5:ASN:HB3	2:BM:8:PHE:CD1	2.51	0.46
2:BP:172:ASN:HD21	2:BP:204:SER:H	1.63	0.46
2:AA:102:GLU:OE2	3:AS:220:ILE:HD12	2.15	0.46
2:AG:79:ASP:O	1:AZ:212:ASN:OD1	2.32	0.46
2:AG:172:ASN:HD21	2:AG:204:SER:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BU:72:LEU:HD22	3:BU:76:TYR:CE2	2.51	0.46
3:AS:194:GLU:HB2	3:AS:293:ARG:HD2	1.97	0.46
3:BV:196:ILE:HG22	3:BV:293:ARG:HD3	1.98	0.46
3:BT:242:THR:O	3:BT:272:ARG:HD3	2.16	0.46
3:AX:96:TYR:HB3	3:AX:103:VAL:HG23	1.98	0.46
3:AS:72:LEU:HD22	3:AS:76:TYR:CE2	2.50	0.46
2:AQ:17:PRO:CA	3:AX:169:LYS:HD3	2.46	0.46
2:BA:77:LYS:H	2:BA:82:ASN:ND2	2.11	0.46
2:BG:81:VAL:HB	1:BZ:86:LYS:HZ1	1.79	0.46
3:AT:242:THR:O	3:AT:272:ARG:HD3	2.16	0.46
1:A0:292:THR:HB	1:AZ:120:ASP:HB2	1.97	0.46
3:AV:68:PHE:HD1	3:BW:120:LYS:HD2	1.72	0.46
2:BQ:17:PRO:CB	3:BX:167:ASN:HD22	2.13	0.46
2:BE:19:GLY:HA2	3:BT:166:GLY:C	2.35	0.46
2:AE:9:PHE:HD2	3:AT:170:TYR:C	2.18	0.46
2:BQ:19:GLY:HA2	3:BX:166:GLY:C	2.35	0.46
3:AW:72:LEU:HD22	3:AW:76:TYR:CE2	2.50	0.46
2:BA:131:THR:HG22	3:BX:262:PRO:O	2.16	0.46
1:A0:130:ASN:HA	1:A0:133:ILE:HD12	1.98	0.46
2:AM:172:ASN:HD21	2:AM:204:SER:H	1.62	0.46
2:BB:13:SER:O	3:BS:169:LYS:HE2	2.07	0.46
2:AR:9:PHE:CD1	3:AX:180:GLY:HA2	2.51	0.46
3:BV:72:LEU:HD22	3:BV:76:TYR:CE2	2.50	0.46
1:AZ:130:ASN:HA	1:AZ:133:ILE:HD12	1.98	0.46
2:BE:171:GLY:HA3	2:BE:205:GLY:H	1.81	0.46
2:AD:112:ILE:O	3:AT:186:ARG:NH1	2.46	0.46
2:BP:77:LYS:H	2:BP:82:ASN:ND2	2.12	0.46
2:AA:81:VAL:HB	1:AY:86:LYS:HZ1	1.81	0.46
3:AV:243:ASP:OD1	3:AV:245:ASN:N	2.48	0.46
2:BD:172:ASN:HD21	2:BD:204:SER:H	1.64	0.46
3:BU:69:GLY:H	3:BU:75:ASN:HD21	1.64	0.46
3:AT:96:TYR:HB3	3:AT:103:VAL:HG23	1.98	0.46
2:BM:148:ILE:HB	2:BO:153:MET:HG3	1.98	0.46
3:AU:206:LYS:HG3	3:AU:285:SER:HB3	1.98	0.46
3:AV:196:ILE:HG22	3:AV:293:ARG:HD3	1.98	0.46
3:BS:194:GLU:HB2	3:BS:293:ARG:HD2	1.97	0.46
3:BT:76:TYR:CE1	3:BU:96:TYR:OH	2.68	0.46
2:AE:26:LEU:HD13	2:AF:66:TYR:HB2	1.98	0.46
3:AX:72:LEU:HD22	3:AX:76:TYR:CE2	2.51	0.46
3:AV:72:LEU:HD22	3:AV:76:TYR:CE2	2.50	0.46
2:AR:5:ASN:HB3	2:AR:8:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BK:171:GLY:HA3	2:BK:205:GLY:H	1.81	0.46
2:BH:171:GLY:HA3	2:BH:205:GLY:H	1.81	0.46
3:BT:96:TYR:HB3	3:BT:103:VAL:HG23	1.98	0.46
2:AE:171:GLY:HA3	2:AE:205:GLY:H	1.81	0.46
3:AU:72:LEU:HD22	3:AU:76:TYR:CE2	2.51	0.45
3:BU:229:PHE:CD1	3:BU:260:LEU:HB3	2.52	0.45
2:BE:26:LEU:HD13	2:BF:66:TYR:HB2	1.98	0.45
3:BW:144:PHE:HB3	3:BW:190:TRP:CE2	2.52	0.45
1:B0:130:ASN:HA	1:B0:133:ILE:HD12	1.98	0.45
2:BQ:17:PRO:HG3	3:BX:169:LYS:CE	2.45	0.45
2:AE:18:VAL:HG13	3:AT:168:TYR:CE2	2.51	0.45
3:BU:242:THR:CG2	3:BU:272:ARG:CG	2.93	0.45
3:AU:229:PHE:CD1	3:AU:260:LEU:HB3	2.52	0.45
1:AY:251:LYS:HG2	1:AY:297:ARG:HD3	1.97	0.45
1:AY:130:ASN:HA	1:AY:133:ILE:HD12	1.99	0.45
2:BR:5:ASN:HB3	2:BR:8:PHE:CD1	2.51	0.45
1:BZ:130:ASN:HA	1:BZ:133:ILE:HD12	1.98	0.45
2:BG:17:PRO:HA	3:BU:159:ILE:HG22	1.98	0.45
3:AX:4:GLN:HB2	3:AX:97:GLN:HB3	1.96	0.45
1:A0:42:ILE:CB	3:AX:43:TRP:CZ2	2.47	0.45
2:AE:8:PHE:O	3:AT:170:TYR:HB2	2.15	0.45
2:BG:77:LYS:H	2:BG:82:ASN:ND2	2.12	0.45
2:BO:17:PRO:CB	3:BW:167:ASN:HB2	2.47	0.45
3:BU:206:LYS:HG3	3:BU:285:SER:HB3	1.97	0.45
2:AD:172:ASN:HD21	2:AD:204:SER:H	1.64	0.45
3:AW:120:LYS:CE	3:BV:66:GLU:CG	2.92	0.45
1:BY:169:THR:HG21	1:BZ:294:PHE:HE2	1.71	0.45
2:BE:8:PHE:O	3:BT:170:TYR:HB2	2.16	0.45
2:AP:113:ASN:C	3:AX:186:ARG:NH2	2.68	0.45
2:AJ:172:ASN:HD21	2:AJ:204:SER:H	1.63	0.45
2:AB:26:LEU:HD13	2:AC:66:TYR:HB2	1.98	0.45
3:BX:96:TYR:HB3	3:BX:103:VAL:HG23	1.98	0.45
3:AT:72:LEU:HD22	3:AT:76:TYR:CE2	2.51	0.45
3:AU:96:TYR:HB3	3:AU:103:VAL:HG23	1.99	0.45
3:BU:4:GLN:HB2	3:BU:97:GLN:HB3	1.97	0.45
3:AV:120:LYS:NZ	3:BW:66:GLU:HB3	2.28	0.45
1:A0:329:LEU:HB3	3:AV:261:PHE:CG	2.52	0.45
3:AU:229:PHE:CE1	3:AU:264:MET:HB3	2.52	0.45
2:BJ:148:ILE:HB	2:BL:153:MET:HG3	1.99	0.45
3:AU:4:GLN:HB2	3:AU:97:GLN:HB3	1.97	0.45
1:B0:1:MET:SD	3:BX:48:ILE:HD13	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B0:78:PRO:HG3	2:BN:103:THR:HB	1.98	0.45
3:BT:144:PHE:HB3	3:BT:190:TRP:CE2	2.52	0.45
2:BJ:172:ASN:HD21	2:BJ:204:SER:H	1.63	0.45
3:AU:69:GLY:H	3:AU:75:ASN:HD21	1.64	0.45
2:BN:52:ASN:ND2	3:BV:258:LEU:HG	2.32	0.45
3:AT:240:ILE:HG22	3:AT:249:TYR:HD1	1.82	0.45
3:BS:11:LEU:HD12	3:BS:93:THR:HG21	1.99	0.45
3:BT:72:LEU:HD22	3:BT:76:TYR:CE2	2.51	0.45
2:BQ:171:GLY:HA3	2:BQ:205:GLY:H	1.81	0.45
2:AP:39:ARG:HB2	2:AP:61:ILE:HB	1.99	0.45
2:AM:27:TYR:HA	2:AM:30:LEU:HD12	1.99	0.45
1:BY:130:ASN:HA	1:BY:133:ILE:HD12	1.99	0.45
2:AG:77:LYS:H	2:AG:82:ASN:ND2	2.12	0.45
2:BA:106:ASN:OD1	1:BY:88:LYS:HD2	2.17	0.45
2:BM:27:TYR:HA	2:BM:30:LEU:HD12	1.99	0.45
3:BU:144:PHE:HB3	3:BU:190:TRP:CE2	2.52	0.45
2:AJ:148:ILE:HB	2:AL:153:MET:HG3	1.99	0.45
2:BP:22:ASN:ND2	3:BX:182:SER:OG	2.43	0.45
3:AW:144:PHE:HB3	3:AW:190:TRP:CE2	2.52	0.45
2:AM:17:PRO:HA	3:AW:177:THR:HG22	1.98	0.45
2:BD:77:LYS:H	2:BD:82:ASN:ND2	2.12	0.45
2:AG:9:PHE:HA	3:AU:160:TYR:HB2	1.98	0.45
3:BU:116:GLU:OE2	3:BV:3:ARG:HG3	2.16	0.45
3:AT:76:TYR:HE1	3:AU:96:TYR:OH	2.00	0.45
3:AU:144:PHE:HB3	3:AU:190:TRP:CE2	2.52	0.45
2:AD:146:ASP:O	2:AF:151:ASN:HB2	2.17	0.45
1:BY:251:LYS:HG2	1:BY:297:ARG:HD3	1.97	0.45
2:AR:81:VAL:HG22	2:AR:127:THR:HG23	1.99	0.45
2:BM:172:ASN:HD21	2:BM:204:SER:H	1.62	0.45
2:BD:51:LEU:HD11	3:BS:262:PRO:HG2	1.97	0.45
3:AT:136:TRP:HB2	3:AT:295:ALA:O	2.17	0.45
2:AB:171:GLY:HA3	2:AB:205:GLY:H	1.81	0.45
2:BR:81:VAL:HG22	2:BR:127:THR:HG23	1.99	0.45
2:BB:171:GLY:HA3	2:BB:205:GLY:H	1.81	0.45
2:BP:19:GLY:HA3	3:BX:180:GLY:O	2.17	0.44
2:AR:23:ASP:OD2	3:AX:176:TYR:HE2	1.99	0.44
3:AU:266:PHE:CD2	1:AZ:35:PRO:HD2	2.52	0.44
3:BW:194:GLU:HB2	3:BW:293:ARG:HD2	1.99	0.44
2:BC:81:VAL:HG22	2:BC:127:THR:HG23	1.99	0.44
2:BN:171:GLY:HA3	2:BN:205:GLY:H	1.81	0.44
2:AJ:39:ARG:HB2	2:AJ:61:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AH:171:GLY:HA3	2:AH:205:GLY:H	1.81	0.44
2:AA:77:LYS:H	2:AA:82:ASN:ND2	2.11	0.44
2:AM:148:ILE:HB	2:AO:153:MET:HG3	1.98	0.44
2:AQ:171:GLY:HA3	2:AQ:205:GLY:H	1.81	0.44
2:BD:146:ASP:O	2:BF:151:ASN:HB2	2.17	0.44
2:BP:39:ARG:HB2	2:BP:61:ILE:HB	1.99	0.44
2:BQ:251:THR:HA	2:BQ:252:PRO:HD3	1.86	0.44
3:BS:197:PHE:HD1	3:BT:48:ILE:CG2	2.30	0.44
3:BT:240:ILE:HG22	3:BT:249:TYR:HD1	1.82	0.44
3:AS:239:LEU:HD23	3:AS:240:ILE:N	2.32	0.44
2:AG:104:ALA:HB3	1:AZ:88:LYS:HD2	1.98	0.44
1:A0:220:THR:HG21	1:A0:332:LEU:HD21	2.00	0.44
1:BY:1:MET:HG3	1:BY:40:GLN:HB2	2.00	0.44
3:BU:96:TYR:HB3	3:BU:103:VAL:HG23	1.99	0.44
2:AO:81:VAL:HG22	2:AO:127:THR:HG23	1.99	0.44
2:AA:39:ARG:HB2	2:AA:61:ILE:HB	2.00	0.44
2:AC:81:VAL:HG22	2:AC:127:THR:HG23	1.99	0.44
2:BH:26:LEU:HD13	2:BI:66:TYR:HB2	1.99	0.44
3:AT:144:PHE:HB3	3:AT:190:TRP:CE2	2.52	0.44
3:AX:120:LYS:CE	3:BU:66:GLU:CG	2.96	0.44
3:BU:271:THR:HA	1:BZ:3:GLU:HG3	1.99	0.44
2:AA:172:ASN:ND2	2:AA:204:SER:H	2.16	0.44
3:BU:229:PHE:CE1	3:BU:264:MET:HB3	2.52	0.44
3:BV:76:TYR:HE1	3:BW:96:TYR:HH	1.63	0.44
3:AW:247:GLU:OE1	3:AW:249:TYR:HE2	2.01	0.44
1:AZ:184:GLN:HE22	1:AZ:217:ARG:HH22	1.66	0.44
3:AU:70:GLU:HG2	3:BX:70:GLU:HG2	1.99	0.44
3:AU:55:SER:HB3	1:AZ:359:PHE:CE1	2.53	0.44
2:BF:20:SER:HA	3:BT:170:TYR:CD1	2.53	0.44
3:AU:242:THR:CG2	3:AU:272:ARG:CG	2.93	0.44
3:AV:194:GLU:HB2	3:AV:293:ARG:HD2	1.99	0.44
3:AS:11:LEU:HD12	3:AS:93:THR:HG21	1.99	0.44
3:BS:239:LEU:HD23	3:BS:240:ILE:N	2.33	0.44
1:B0:220:THR:HG21	1:B0:332:LEU:HD21	2.00	0.44
2:AF:81:VAL:HG22	2:AF:127:THR:HG23	1.99	0.44
2:BG:39:ARG:HB2	2:BG:61:ILE:HB	2.00	0.44
1:BZ:251:LYS:HG2	1:BZ:297:ARG:HD3	1.98	0.44
2:BK:26:LEU:HD13	2:BL:66:TYR:HB2	2.00	0.44
2:BB:26:LEU:HD13	2:BC:66:TYR:HB2	1.99	0.44
2:AN:171:GLY:HA3	2:AN:205:GLY:H	1.81	0.44
2:AK:171:GLY:HA3	2:AK:205:GLY:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BA:39:ARG:HB2	2:BA:61:ILE:HB	2.00	0.44
2:BI:81:VAL:HG22	2:BI:127:THR:HG23	1.99	0.44
3:AS:138:THR:O	3:AS:292:LYS:HA	2.17	0.44
1:B0:262:MET:SD	1:BZ:142:LYS:HG2	2.57	0.44
3:AX:5:TYR:HB3	3:AX:21:VAL:HG23	2.00	0.44
2:BG:9:PHE:HA	3:BU:160:TYR:HB2	1.98	0.44
3:BT:136:TRP:HB2	3:BT:295:ALA:O	2.17	0.44
2:BQ:18:VAL:C	3:BX:167:ASN:HA	2.36	0.44
3:AT:76:TYR:CE1	3:AU:96:TYR:OH	2.70	0.44
1:AZ:251:LYS:HG2	1:AZ:297:ARG:HD3	1.98	0.44
2:BL:39:ARG:HB2	2:BL:61:ILE:HB	2.00	0.44
2:AL:39:ARG:HB2	2:AL:61:ILE:HB	2.00	0.44
2:BM:66:TYR:HB2	2:BO:26:LEU:HD13	1.99	0.44
2:AG:39:ARG:HB2	2:AG:61:ILE:HB	2.00	0.44
2:AG:81:VAL:HB	1:AZ:86:LYS:HZ2	1.82	0.44
2:BH:17:PRO:HB3	3:BU:169:LYS:CE	2.48	0.44
2:BC:39:ARG:HB2	2:BC:61:ILE:HB	2.00	0.44
2:BD:112:ILE:O	3:BT:186:ARG:NH1	2.45	0.44
1:BZ:32:LEU:HD11	1:BZ:204:LEU:HB2	1.99	0.44
1:B0:39:CYS:HB2	1:B0:60:THR:OG1	2.18	0.44
3:BS:138:THR:O	3:BS:292:LYS:HA	2.17	0.44
3:AW:194:GLU:HB2	3:AW:293:ARG:HD2	1.99	0.44
1:AZ:1:MET:HG3	1:AZ:40:GLN:HB2	2.00	0.43
2:AR:9:PHE:CZ	3:AX:180:GLY:HA2	2.53	0.43
1:A0:1:MET:HG3	1:A0:40:GLN:HB2	2.00	0.43
1:B0:1:MET:HG3	1:B0:40:GLN:HB2	2.00	0.43
2:BL:81:VAL:HG22	2:BL:127:THR:HG23	2.00	0.43
2:AH:26:LEU:HD13	2:AI:66:TYR:HB2	1.99	0.43
2:BO:81:VAL:HG22	2:BO:127:THR:HG23	1.99	0.43
2:AM:39:ARG:HB2	2:AM:61:ILE:HB	2.00	0.43
3:BV:194:GLU:HB2	3:BV:293:ARG:HD2	1.99	0.43
2:AK:114:ASN:O	3:AV:186:ARG:CD	2.66	0.43
1:A0:262:MET:SD	1:AZ:142:LYS:HG2	2.57	0.43
2:BO:39:ARG:HB2	2:BO:61:ILE:HB	2.01	0.43
2:BF:81:VAL:HG22	2:BF:127:THR:HG23	1.99	0.43
2:AK:49:THR:HB	3:AU:258:LEU:HD21	2.00	0.43
1:BY:41:VAL:HG11	1:BY:71:ILE:HG12	2.00	0.43
2:BE:155:VAL:HG21	2:BE:159:ILE:HD11	2.00	0.43
2:AM:66:TYR:HB2	2:AO:26:LEU:HD13	1.99	0.43
2:BO:27:TYR:HA	2:BO:30:LEU:HD12	2.00	0.43
2:BD:39:ARG:HB2	2:BD:61:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BD:49:THR:CG2	3:BS:233:GLN:HB2	2.49	0.43
2:AD:51:LEU:HD12	3:AS:262:PRO:HG2	2.00	0.43
1:B0:12:PRO:HB2	1:BY:288:ARG:CZ	2.47	0.43
2:AD:39:ARG:HB2	2:AD:61:ILE:HB	2.00	0.43
3:BX:5:TYR:HB3	3:BX:21:VAL:HG23	2.00	0.43
3:AV:66:GLU:CG	3:BW:120:LYS:CE	2.95	0.43
2:AQ:20:SER:HA	3:AX:160:TYR:CE1	2.53	0.43
2:AE:18:VAL:C	3:AT:167:ASN:HA	2.39	0.43
2:AF:9:PHE:CB	3:AT:180:GLY:HA2	2.48	0.43
2:AO:39:ARG:HB2	2:AO:61:ILE:HB	2.00	0.43
2:AL:81:VAL:HG22	2:AL:127:THR:HG23	2.00	0.43
2:AA:66:TYR:HB2	2:AC:26:LEU:HD13	1.99	0.43
1:A0:39:CYS:HB2	1:A0:60:THR:OG1	2.18	0.43
2:AM:9:PHE:HB2	3:AW:180:GLY:HA2	2.01	0.43
2:AH:155:VAL:HG21	2:AH:159:ILE:HD11	2.00	0.43
2:AG:92:GLN:HE21	3:AU:189:ARG:CZ	2.31	0.43
1:AY:1:MET:HG3	1:AY:40:GLN:HB2	1.99	0.43
2:AH:19:GLY:HA2	3:AU:166:GLY:O	2.19	0.43
1:AY:41:VAL:HG11	1:AY:71:ILE:HG12	2.00	0.43
2:BF:155:VAL:HG21	2:BF:159:ILE:HD11	2.01	0.43
2:AQ:155:VAL:HG21	2:AQ:159:ILE:HD11	2.01	0.43
3:BS:96:TYR:HB3	3:BS:103:VAL:HG23	1.99	0.43
1:AZ:32:LEU:HD11	1:AZ:204:LEU:HB2	1.99	0.43
1:B0:17:ILE:HD13	1:BY:279:GLY:O	2.18	0.43
2:BF:39:ARG:HB2	2:BF:61:ILE:HB	2.00	0.43
2:AE:155:VAL:HG21	2:AE:159:ILE:HD11	2.00	0.43
2:AI:81:VAL:HG22	2:AI:127:THR:HG23	1.99	0.43
2:AK:21:ASN:H	3:AV:181:GLU:HG2	1.83	0.43
1:BZ:184:GLN:HE22	1:BZ:217:ARG:HH22	1.66	0.43
2:BJ:39:ARG:HB2	2:BJ:61:ILE:HB	1.99	0.43
2:AP:49:THR:HB	3:AW:258:LEU:HD21	2.00	0.43
2:AG:79:ASP:OD1	1:AZ:216:LYS:HB2	2.18	0.43
3:BU:271:THR:HA	1:BZ:3:GLU:CG	2.49	0.43
3:AT:171:ILE:H	3:AT:175:SER:HA	1.84	0.43
2:BM:77:LYS:H	2:BM:82:ASN:ND2	2.13	0.43
3:AW:196:ILE:HD11	3:AW:199:PHE:HD1	1.83	0.43
3:BV:48:ILE:HD13	1:BZ:1:MET:SD	2.59	0.43
3:BT:43:TRP:HD1	1:BY:42:ILE:HB	1.84	0.43
2:AK:26:LEU:HD13	2:AL:66:TYR:HB2	2.00	0.43
2:BI:39:ARG:HB2	2:BI:61:ILE:HB	2.00	0.43
2:BP:92:GLN:HE21	3:BX:189:ARG:NE	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BA:66:TYR:HB2	2:BC:26:LEU:HD13	1.99	0.43
3:BT:137:TYR:CE1	3:BT:292:LYS:HD2	2.54	0.43
1:BY:121:VAL:HG11	1:BY:175:VAL:HG21	2.01	0.43
3:AS:96:TYR:HB3	3:AS:103:VAL:HG23	1.99	0.43
2:BE:18:VAL:HG13	3:BT:168:TYR:CE2	2.54	0.43
2:AE:17:PRO:CB	3:AT:167:ASN:CB	2.86	0.43
2:AE:17:PRO:HG3	3:AT:169:LYS:CE	2.48	0.43
3:BW:196:ILE:HD11	3:BW:199:PHE:HD1	1.83	0.43
1:B0:143:ASN:O	1:BY:288:ARG:NH1	2.51	0.43
2:BG:172:ASN:ND2	2:BG:204:SER:H	2.17	0.43
2:AI:39:ARG:HB2	2:AI:61:ILE:HB	2.00	0.43
2:BL:21:ASN:OD1	3:BV:165:PRO:HG2	2.19	0.43
3:BW:247:GLU:OE1	3:BW:249:TYR:HE2	2.01	0.43
3:AS:118:TYR:HB3	3:AS:122:GLY:HA2	1.99	0.43
2:AC:39:ARG:HB2	2:AC:61:ILE:HB	2.00	0.43
1:B0:221:ARG:HB2	3:BV:266:PHE:HB3	2.00	0.43
2:AD:52:ASN:ND2	3:AS:258:LEU:CG	2.77	0.43
2:BA:172:ASN:ND2	2:BA:204:SER:H	2.16	0.43
2:AJ:251:THR:HA	2:AJ:252:PRO:HD3	1.87	0.43
2:AO:155:VAL:HG21	2:AO:159:ILE:HD11	2.01	0.43
2:BO:155:VAL:HG21	2:BO:159:ILE:HD11	2.01	0.43
3:AU:66:GLU:CB	3:BX:120:LYS:NZ	2.82	0.43
2:AP:7:THR:HG23	3:AX:160:TYR:CE2	2.54	0.43
3:BX:196:ILE:HD11	3:BX:199:PHE:HD1	1.84	0.43
3:BX:198:SER:HA	3:BX:242:THR:OG1	2.19	0.43
2:AA:120:LYS:HE2	3:AS:222:ASN:HD21	1.84	0.43
2:BN:91:THR:HG21	3:BW:189:ARG:HB2	2.01	0.43
2:AG:172:ASN:ND2	2:AG:204:SER:H	2.17	0.43
2:BR:39:ARG:HB2	2:BR:61:ILE:HB	2.00	0.43
2:AF:23:ASP:OD2	3:AT:176:TYR:HE2	2.01	0.42
2:AJ:77:LYS:H	2:AJ:82:ASN:ND2	2.12	0.42
3:BU:203:LEU:HB2	3:BU:238:ILE:HB	2.01	0.42
2:AN:26:LEU:HD13	2:AO:66:TYR:HB2	2.01	0.42
3:BS:118:TYR:HB3	3:BS:122:GLY:HA2	2.00	0.42
2:BK:91:THR:HG21	3:BV:189:ARG:HB2	2.01	0.42
3:BT:171:ILE:H	3:BT:175:SER:HA	1.84	0.42
3:BU:203:LEU:HD13	3:BU:213:GLY:HA2	2.01	0.42
3:BW:96:TYR:HB3	3:BW:103:VAL:HG23	2.01	0.42
3:BX:243:ASP:OD1	3:BX:245:ASN:N	2.52	0.42
2:AO:27:TYR:HA	2:AO:30:LEU:HD12	2.00	0.42
2:AF:27:TYR:HA	2:AF:30:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AG:174:LEU:HB2	2:AG:194:VAL:HG22	2.01	0.42
3:AW:96:TYR:HB3	3:AW:103:VAL:HG23	2.01	0.42
2:BO:5:ASN:HB3	2:BO:8:PHE:CD1	2.54	0.42
2:AN:155:VAL:HG21	2:AN:159:ILE:HD11	2.01	0.42
3:AX:243:ASP:OD1	3:AX:245:ASN:N	2.52	0.42
2:BN:155:VAL:HG21	2:BN:159:ILE:HD11	2.01	0.42
2:BH:155:VAL:HG21	2:BH:159:ILE:HD11	2.01	0.42
2:BQ:155:VAL:HG21	2:BQ:159:ILE:HD11	2.00	0.42
2:AO:5:ASN:HB3	2:AO:8:PHE:CD1	2.54	0.42
3:AU:120:LYS:HZ3	3:BX:66:GLU:CG	2.29	0.42
2:AR:9:PHE:CZ	3:AX:180:GLY:CA	3.03	0.42
2:AD:19:GLY:CA	3:AT:180:GLY:O	2.67	0.42
3:BT:43:TRP:CD1	1:BY:42:ILE:HB	2.54	0.42
3:BV:118:TYR:HB3	3:BV:122:GLY:HA2	2.02	0.42
3:BS:34:LEU:HB2	3:BX:114:LYS:HB3	2.00	0.42
2:AG:203:MET:SD	2:AG:243:TRP:HB2	2.59	0.42
3:AS:66:GLU:CG	3:BT:120:LYS:CE	2.96	0.42
2:AG:92:GLN:NE2	3:AU:189:ARG:NE	2.67	0.42
3:AU:203:LEU:HD13	3:AU:213:GLY:HA2	2.01	0.42
2:BQ:9:PHE:CE1	3:BX:172:LYS:HB2	2.54	0.42
3:BW:247:GLU:OE1	3:BW:249:TYR:CE2	2.73	0.42
2:AR:39:ARG:HB2	2:AR:61:ILE:HB	2.00	0.42
3:BU:226:ALA:HB3	3:BU:268:ARG:HB3	2.01	0.42
2:AD:147:SER:HB2	2:AE:140:VAL:HG22	2.02	0.42
2:BG:203:MET:SD	2:BG:243:TRP:HB2	2.59	0.42
2:BR:155:VAL:HG21	2:BR:159:ILE:HD11	2.02	0.42
2:BM:39:ARG:HB2	2:BM:61:ILE:HB	2.00	0.42
2:BQ:18:VAL:HG13	3:BX:168:TYR:CD2	2.54	0.42
2:AF:20:SER:HA	3:AT:170:TYR:CD1	2.54	0.42
2:AM:77:LYS:H	2:AM:82:ASN:ND2	2.13	0.42
3:BW:199:PHE:CE1	3:BW:242:THR:HG21	2.55	0.42
3:BW:196:ILE:HD13	3:BW:291:ILE:HG12	2.02	0.42
1:BZ:1:MET:HG3	1:BZ:40:GLN:HB2	2.00	0.42
3:AV:118:TYR:HB3	3:AV:122:GLY:HA2	2.02	0.42
2:BC:155:VAL:HG21	2:BC:159:ILE:HD11	2.02	0.42
3:AT:137:TYR:CE1	3:AT:292:LYS:HD2	2.54	0.42
2:AF:39:ARG:HB2	2:AF:61:ILE:HB	2.00	0.42
2:BF:27:TYR:HA	2:BF:30:LEU:HD12	2.01	0.42
1:A0:76:VAL:HG21	1:A0:88:LYS:HE3	2.02	0.42
2:BJ:77:LYS:H	2:BJ:82:ASN:ND2	2.12	0.42
3:AW:199:PHE:CE1	3:AW:242:THR:HG21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AX:196:ILE:HD11	3:AX:199:PHE:HD1	1.84	0.42
1:AZ:241:TYR:CD2	1:AZ:241:TYR:N	2.88	0.42
2:BK:114:ASN:O	3:BV:186:ARG:CD	2.68	0.42
2:AC:155:VAL:HG21	2:AC:159:ILE:HD11	2.02	0.42
2:BN:26:LEU:HD13	2:BO:66:TYR:HB2	2.01	0.42
1:B0:38:ARG:NH2	3:BW:269:TYR:O	2.48	0.42
2:AQ:20:SER:N	3:AX:160:TYR:CD1	2.88	0.42
2:AP:21:ASN:N	3:AX:181:GLU:HG2	2.34	0.42
2:AR:18:VAL:CG1	3:AX:176:TYR:O	2.65	0.42
3:AU:203:LEU:HB2	3:AU:238:ILE:HB	2.01	0.42
2:AN:91:THR:HG21	3:AW:189:ARG:HB2	2.01	0.42
2:AM:5:ASN:O	2:AM:16:PHE:HB3	2.20	0.42
2:AK:155:VAL:HG21	2:AK:159:ILE:HD11	2.02	0.42
3:AT:114:LYS:HB3	3:AU:34:LEU:HB2	2.02	0.42
3:AS:132:ILE:HG21	3:AS:135:LYS:HB2	2.00	0.42
2:BQ:23:ASP:OD2	3:BX:168:TYR:HE2	2.03	0.42
2:BE:17:PRO:CB	3:BT:167:ASN:CB	2.87	0.42
3:AW:196:ILE:HD13	3:AW:291:ILE:HG12	2.02	0.42
1:BZ:77:VAL:O	1:BZ:89:LEU:HB3	2.20	0.42
3:AX:198:SER:HA	3:AX:242:THR:OG1	2.19	0.42
3:AT:86:ILE:HA	3:AT:92:VAL:HG21	2.01	0.42
1:BY:52:LEU:HD23	1:BY:53:TYR:CE2	2.55	0.42
2:AR:155:VAL:HG21	2:AR:159:ILE:HD11	2.02	0.42
2:BP:23:ASP:OD2	3:BX:178:TYR:HE1	2.03	0.42
2:AI:5:ASN:HB3	2:AI:8:PHE:CD1	2.55	0.42
2:BP:49:THR:HB	3:BW:258:LEU:HD21	2.01	0.42
3:BT:86:ILE:HA	3:BT:92:VAL:HG21	2.01	0.42
2:AE:18:VAL:CG1	3:AT:168:TYR:O	2.59	0.41
1:AZ:77:VAL:O	1:AZ:89:LEU:HB3	2.20	0.41
3:AS:266:PHE:CD2	1:AY:35:PRO:HD2	2.55	0.41
3:AV:199:PHE:CZ	3:AV:242:THR:HG21	2.55	0.41
3:BU:131:ASP:HB3	3:BV:42:ILE:HD12	2.01	0.41
3:BS:132:ILE:HG21	3:BS:135:LYS:HB2	2.00	0.41
2:BD:147:SER:HB2	2:BE:140:VAL:HG22	2.02	0.41
3:BS:99:GLU:OE2	3:BX:73:GLU:HB2	2.19	0.41
3:AS:294:LYS:HD2	3:AT:47:GLY:O	2.19	0.41
3:AU:53:THR:HG21	1:AZ:359:PHE:C	2.41	0.41
2:BR:9:PHE:CZ	3:BX:181:GLU:N	2.88	0.41
2:AP:77:LYS:H	2:AP:82:ASN:ND2	2.12	0.41
3:BT:87:LEU:HA	3:BU:54:ARG:HH11	1.85	0.41
2:AK:251:THR:HA	2:AK:252:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BD:203:MET:SD	2:BD:243:TRP:HB2	2.60	0.41
2:AF:155:VAL:HG21	2:AF:159:ILE:HD11	2.01	0.41
3:BT:202:ILE:HG12	3:BT:239:LEU:HD12	2.01	0.41
2:BD:73:THR:CG2	3:BS:256:THR:CG2	2.98	0.41
3:BV:199:PHE:CZ	3:BV:242:THR:HG21	2.55	0.41
3:AW:247:GLU:OE1	3:AW:249:TYR:CE2	2.73	0.41
2:BG:66:TYR:HB2	2:BI:26:LEU:HD13	2.02	0.41
3:BW:281:LEU:HB3	3:BW:284:LEU:HD12	2.03	0.41
2:BI:5:ASN:HB3	2:BI:8:PHE:CD1	2.55	0.41
2:BE:21:ASN:CG	3:BT:165:PRO:HG2	2.40	0.41
3:BT:199:PHE:HB3	3:BT:291:ILE:HD13	2.02	0.41
2:BK:155:VAL:HG21	2:BK:159:ILE:HD11	2.02	0.41
1:A0:323:ILE:HA	1:A0:363:LEU:O	2.20	0.41
2:BG:5:ASN:HB3	2:BG:8:PHE:CD1	2.56	0.41
1:AY:323:ILE:HA	1:AY:363:LEU:O	2.20	0.41
1:A0:52:LEU:HD23	1:A0:53:TYR:CE2	2.55	0.41
2:AQ:229:THR:HB	2:AR:228:ASP:HB2	2.03	0.41
2:AJ:203:MET:SD	2:AJ:243:TRP:HB2	2.61	0.41
3:AT:202:ILE:HG12	3:AT:239:LEU:HD12	2.00	0.41
1:AY:121:VAL:HG11	1:AY:175:VAL:HG21	2.01	0.41
2:AD:203:MET:SD	2:AD:243:TRP:HB2	2.60	0.41
2:BQ:23:ASP:OD2	3:BX:168:TYR:CE2	2.74	0.41
2:BP:21:ASN:HB3	3:BX:181:GLU:CD	2.41	0.41
1:B0:76:VAL:HG21	1:B0:88:LYS:HE3	2.02	0.41
3:AT:203:LEU:HD21	3:AT:240:ILE:HG13	2.03	0.41
2:BN:100:SER:CB	3:BW:220:ILE:HG21	2.51	0.41
1:B0:288:ARG:CZ	1:BZ:12:PRO:HB2	2.50	0.41
3:BS:99:GLU:CD	3:BX:73:GLU:HB2	2.41	0.41
2:AD:251:THR:HA	2:AD:252:PRO:HD3	1.96	0.41
1:B0:323:ILE:HA	1:B0:363:LEU:O	2.20	0.41
2:BM:251:THR:HA	2:BM:252:PRO:HD3	1.90	0.41
2:BQ:229:THR:HB	2:BR:228:ASP:HB2	2.03	0.41
2:AE:19:GLY:HA2	3:AT:166:GLY:C	2.39	0.41
2:AP:5:ASN:HD21	2:AQ:97:VAL:HB	1.85	0.41
1:BZ:241:TYR:CD2	1:BZ:241:TYR:N	2.88	0.41
2:BD:172:ASN:ND2	2:BD:204:SER:H	2.19	0.41
2:AA:251:THR:HA	2:AA:252:PRO:HD3	1.95	0.41
2:AG:5:ASN:HB3	2:AG:8:PHE:CD1	2.56	0.41
2:BJ:203:MET:SD	2:BJ:243:TRP:HB2	2.60	0.41
1:B0:330:LEU:HB2	3:BV:261:PHE:CE2	2.55	0.41
1:A0:223:ASP:CG	3:AV:272:ARG:HH12	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BG:174:LEU:HB2	2:BG:194:VAL:HG22	2.02	0.41
2:BE:9:PHE:CA	3:BT:170:TYR:O	2.61	0.41
2:AP:21:ASN:CG	3:AX:181:GLU:HG2	2.41	0.41
1:BZ:89:LEU:CD2	1:BZ:192:GLN:HG3	2.49	0.41
3:AT:199:PHE:HB3	3:AT:291:ILE:HD13	2.02	0.41
3:AS:171:ILE:H	3:AS:175:SER:HA	1.86	0.41
3:BU:171:ILE:H	3:BU:175:SER:HA	1.86	0.41
2:BM:5:ASN:O	2:BM:16:PHE:HB3	2.20	0.41
3:AV:76:TYR:HE1	3:AW:96:TYR:HH	1.63	0.41
2:AG:66:TYR:HB2	2:AI:26:LEU:HD13	2.02	0.41
2:AK:120:LYS:NZ	3:AV:220:ILE:O	2.48	0.41
2:BQ:26:LEU:HD13	2:BR:66:TYR:HB2	2.03	0.41
1:AY:52:LEU:HD23	1:AY:53:TYR:CE2	2.55	0.41
3:BT:115:THR:HG22	3:BU:32:SER:O	2.21	0.41
1:BY:323:ILE:HA	1:BY:363:LEU:O	2.20	0.41
3:AS:7:ILE:HG23	3:AS:92:VAL:CG1	2.51	0.41
3:BV:246:ASP:O	3:BV:246:ASP:CG	2.59	0.41
2:BD:73:THR:HG21	3:BS:256:THR:CG2	2.51	0.41
3:BU:272:ARG:NH1	1:BZ:3:GLU:OE1	2.54	0.41
2:AN:102:GLU:OE1	3:AW:222:ASN:ND2	2.46	0.41
2:AP:172:ASN:ND2	2:AP:204:SER:H	2.19	0.41
2:BB:229:THR:HB	2:BC:228:ASP:HB2	2.03	0.41
1:BY:143:ASN:O	1:BZ:288:ARG:NH1	2.53	0.41
1:AY:120:ASP:HB2	1:AZ:292:THR:HB	2.03	0.41
2:BM:203:MET:SD	2:BM:243:TRP:HB2	2.61	0.41
2:BP:174:LEU:HB2	2:BP:194:VAL:HG22	2.03	0.41
3:AU:226:ALA:HB3	3:AU:268:ARG:HB3	2.01	0.41
3:AX:58:GLN:HA	3:AX:59:PRO:HD3	1.99	0.41
2:AE:17:PRO:HB2	3:AT:167:ASN:HD22	1.76	0.41
3:AT:158:LYS:HD2	3:AT:176:TYR:CE1	2.56	0.41
3:AU:271:THR:HA	1:AZ:3:GLU:HG2	2.02	0.41
1:AY:185:PHE:CE2	1:AY:208:PHE:HA	2.56	0.41
2:BF:23:ASP:OD2	3:BT:176:TYR:CZ	2.74	0.41
1:AY:87:LYS:HZ1	1:AY:89:LEU:HD23	1.86	0.41
3:BV:240:ILE:CD1	3:BV:242:THR:HG23	2.51	0.41
1:AZ:52:LEU:HD23	1:AZ:53:TYR:CE2	2.56	0.41
2:AM:203:MET:SD	2:AM:243:TRP:HB2	2.61	0.41
2:AH:229:THR:HB	2:AI:228:ASP:HB2	2.03	0.41
3:AV:246:ASP:O	3:AV:246:ASP:CG	2.59	0.41
2:BP:146:ASP:O	2:BR:151:ASN:HB2	2.21	0.41
2:BH:251:THR:HA	2:BH:252:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AW:281:LEU:HB3	3:AW:284:LEU:HD12	2.03	0.41
2:BM:174:LEU:HB2	2:BM:194:VAL:HG22	2.03	0.41
3:AS:242:THR:HG23	3:AS:272:ARG:HG3	1.89	0.41
2:AE:9:PHE:CA	3:AT:170:TYR:O	2.61	0.41
3:BT:158:LYS:HD2	3:BT:176:TYR:CE1	2.56	0.41
3:BT:203:LEU:HD21	3:BT:240:ILE:HG13	2.02	0.41
3:AT:87:LEU:HA	3:AU:54:ARG:HH11	1.84	0.41
3:BS:171:ILE:H	3:BS:175:SER:HA	1.86	0.41
2:BP:172:ASN:ND2	2:BP:204:SER:H	2.19	0.41
2:AJ:172:ASN:ND2	2:AJ:204:SER:H	2.19	0.41
2:AN:229:THR:HB	2:AO:228:ASP:HB2	2.03	0.41
2:AA:198:GLN:HB2	2:AA:201:TRP:CD1	2.56	0.41
2:BL:10:SER:HA	2:BL:15:GLU:HB2	2.03	0.41
2:AN:251:THR:HA	2:AN:252:PRO:HD3	1.90	0.41
2:AB:229:THR:HB	2:AC:228:ASP:HB2	2.03	0.41
3:AT:68:PHE:CE1	3:BS:120:LYS:HG2	2.56	0.40
1:BY:87:LYS:HZ1	1:BY:89:LEU:HD23	1.86	0.40
3:BX:171:ILE:H	3:BX:175:SER:HA	1.86	0.40
2:AM:172:ASN:ND2	2:AM:204:SER:H	2.19	0.40
3:AS:226:ALA:HB3	3:AS:268:ARG:HB3	2.03	0.40
2:AE:229:THR:HB	2:AF:228:ASP:HB2	2.03	0.40
2:AG:130:GLY:HA3	1:AZ:218:ILE:HG23	2.02	0.40
2:BD:174:LEU:HB2	2:BD:194:VAL:HG22	2.03	0.40
2:BA:198:GLN:HB2	2:BA:201:TRP:CD1	2.56	0.40
2:AG:79:ASP:CB	1:AZ:212:ASN:ND2	2.85	0.40
2:AL:10:SER:HA	2:AL:15:GLU:HB2	2.03	0.40
1:BZ:45:GLU:HA	1:BZ:357:THR:HG22	2.03	0.40
2:BJ:174:LEU:HB2	2:BJ:194:VAL:HG22	2.04	0.40
2:BB:27:TYR:HA	2:BB:30:LEU:HD12	2.03	0.40
2:AP:146:ASP:O	2:AR:151:ASN:HB2	2.21	0.40
3:BS:7:ILE:HG23	3:BS:92:VAL:CG1	2.51	0.40
2:AO:17:PRO:CB	3:AW:167:ASN:HB2	2.51	0.40
2:AL:5:ASN:HB3	2:AL:8:PHE:CD1	2.56	0.40
1:B0:52:LEU:HD23	1:B0:53:TYR:CE2	2.56	0.40
2:BE:17:PRO:HG3	3:BT:169:LYS:CE	2.46	0.40
1:A0:3:GLU:CG	3:AW:271:THR:HA	2.51	0.40
3:AV:240:ILE:CD1	3:AV:242:THR:HG23	2.51	0.40
3:AX:118:TYR:HB3	3:AX:122:GLY:HA2	2.04	0.40
3:BS:226:ALA:HB3	3:BS:268:ARG:HB3	2.03	0.40
2:AP:203:MET:SD	2:AP:243:TRP:HB2	2.61	0.40
3:AU:171:ILE:H	3:AU:175:SER:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BE:229:THR:HB	2:BF:228:ASP:HB2	2.03	0.40
2:AD:174:LEU:HB2	2:AD:194:VAL:HG22	2.02	0.40
2:BH:229:THR:HB	2:BI:228:ASP:HB2	2.03	0.40
2:AQ:17:PRO:N	3:AX:169:LYS:HD3	2.36	0.40
3:BT:116:GLU:OE2	3:BU:5:TYR:CE2	2.74	0.40
1:BY:185:PHE:CE2	1:BY:208:PHE:HA	2.56	0.40
2:BF:9:PHE:CB	3:BT:180:GLY:HA2	2.52	0.40
3:AS:270:ARG:CZ	1:AY:72:LEU:HD22	2.51	0.40
2:BG:9:PHE:HB2	3:BU:166:GLY:CA	2.51	0.40
3:AT:132:ILE:HG21	3:AT:135:LYS:HB2	2.04	0.40
3:BW:171:ILE:H	3:BW:175:SER:HA	1.86	0.40
2:BN:5:ASN:HB3	2:BN:8:PHE:CD1	2.57	0.40
2:BK:229:THR:HB	2:BL:228:ASP:HB2	2.03	0.40
2:BP:203:MET:SD	2:BP:243:TRP:HB2	2.61	0.40
1:B0:292:THR:HB	1:BZ:120:ASP:HB2	2.03	0.40
2:AN:5:ASN:HB3	2:AN:8:PHE:CD1	2.57	0.40
3:AW:3:ARG:HD2	3:AW:3:ARG:C	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	370/372 (100%)	358 (97%)	12 (3%)	0	100	100
1	AY	370/372 (100%)	355 (96%)	15 (4%)	0	100	100
1	AZ	370/372 (100%)	358 (97%)	12 (3%)	0	100	100
1	B0	370/372 (100%)	358 (97%)	12 (3%)	0	100	100
1	BY	370/372 (100%)	355 (96%)	15 (4%)	0	100	100
1	BZ	370/372 (100%)	357 (96%)	13 (4%)	0	100	100
2	AA	261/263 (99%)	254 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	AC	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	AD	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	AE	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AF	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AG	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	AH	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AI	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AJ	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	AK	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AL	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	AM	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	AN	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	AO	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AP	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	AQ	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	AR	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	BA	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	BB	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	BC	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	BD	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	BE	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BF	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BG	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	BH	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BI	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BJ	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	BK	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BL	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	BM	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	BN	261/263 (99%)	247 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BO	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BP	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	BQ	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	BR	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
3	AS	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	26	71
3	AT	296/298 (99%)	273 (92%)	21 (7%)	2 (1%)	26	71
3	AU	296/298 (99%)	274 (93%)	20 (7%)	2 (1%)	26	71
3	AV	296/298 (99%)	275 (93%)	19 (6%)	2 (1%)	26	71
3	AW	296/298 (99%)	280 (95%)	14 (5%)	2 (1%)	26	71
3	AX	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	26	71
3	BS	296/298 (99%)	278 (94%)	16 (5%)	2 (1%)	26	71
3	BT	296/298 (99%)	273 (92%)	21 (7%)	2 (1%)	26	71
3	BU	296/298 (99%)	274 (93%)	20 (7%)	2 (1%)	26	71
3	BV	296/298 (99%)	275 (93%)	19 (6%)	2 (1%)	26	71
3	BW	296/298 (99%)	280 (95%)	14 (5%)	2 (1%)	26	71
3	BX	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	26	71
All	All	15168/15276 (99%)	14418 (95%)	726 (5%)	24 (0%)	52	86

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AS	175	SER
3	AT	175	SER
3	AU	175	SER
3	AV	175	SER
3	AW	175	SER
3	AX	175	SER
3	BS	175	SER
3	BT	175	SER
3	BU	175	SER
3	BV	175	SER
3	BW	175	SER
3	BX	175	SER
3	AS	136	TRP
3	AU	136	TRP
3	AV	136	TRP

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Mol	Chain	Res	Type
3	AW	136	TRP
3	AX	136	TRP
3	BS	136	TRP
3	BU	136	TRP
3	BV	136	TRP
3	BW	136	TRP
3	BX	136	TRP
3	AT	136	TRP
3	BT	136	TRP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	337/337 (100%)	324 (96%)	13 (4%)	39	72
1	AY	337/337 (100%)	319 (95%)	18 (5%)	28	65
1	AZ	337/337 (100%)	321 (95%)	16 (5%)	32	68
1	B0	337/337 (100%)	324 (96%)	13 (4%)	39	72
1	BY	337/337 (100%)	319 (95%)	18 (5%)	28	65
1	BZ	337/337 (100%)	321 (95%)	16 (5%)	32	68
2	AA	227/227 (100%)	218 (96%)	9 (4%)	38	71
2	AB	227/227 (100%)	221 (97%)	6 (3%)	54	80
2	AC	227/227 (100%)	223 (98%)	4 (2%)	66	87
2	AD	227/227 (100%)	220 (97%)	7 (3%)	47	77
2	AE	227/227 (100%)	221 (97%)	6 (3%)	54	80
2	AF	227/227 (100%)	224 (99%)	3 (1%)	76	90
2	AG	227/227 (100%)	219 (96%)	8 (4%)	43	75
2	AH	227/227 (100%)	220 (97%)	7 (3%)	47	77
2	AI	227/227 (100%)	223 (98%)	4 (2%)	66	87
2	AJ	227/227 (100%)	219 (96%)	8 (4%)	43	75
2	AK	227/227 (100%)	221 (97%)	6 (3%)	54	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AL	227/227 (100%)	223 (98%)	4 (2%)	66	87
2	AM	227/227 (100%)	219 (96%)	8 (4%)	43	75
2	AN	227/227 (100%)	221 (97%)	6 (3%)	54	80
2	AO	227/227 (100%)	224 (99%)	3 (1%)	76	90
2	AP	227/227 (100%)	220 (97%)	7 (3%)	47	77
2	AQ	227/227 (100%)	220 (97%)	7 (3%)	47	77
2	AR	227/227 (100%)	223 (98%)	4 (2%)	66	87
2	BA	227/227 (100%)	218 (96%)	9 (4%)	38	71
2	BB	227/227 (100%)	221 (97%)	6 (3%)	54	80
2	BC	227/227 (100%)	223 (98%)	4 (2%)	66	87
2	BD	227/227 (100%)	220 (97%)	7 (3%)	47	77
2	BE	227/227 (100%)	221 (97%)	6 (3%)	54	80
2	BF	227/227 (100%)	224 (99%)	3 (1%)	76	90
2	BG	227/227 (100%)	219 (96%)	8 (4%)	43	75
2	BH	227/227 (100%)	220 (97%)	7 (3%)	47	77
2	BI	227/227 (100%)	223 (98%)	4 (2%)	66	87
2	BJ	227/227 (100%)	219 (96%)	8 (4%)	43	75
2	BK	227/227 (100%)	221 (97%)	6 (3%)	54	80
2	BL	227/227 (100%)	223 (98%)	4 (2%)	66	87
2	BM	227/227 (100%)	219 (96%)	8 (4%)	43	75
2	BN	227/227 (100%)	221 (97%)	6 (3%)	54	80
2	BO	227/227 (100%)	224 (99%)	3 (1%)	76	90
2	BP	227/227 (100%)	220 (97%)	7 (3%)	47	77
2	BQ	227/227 (100%)	220 (97%)	7 (3%)	47	77
2	BR	227/227 (100%)	223 (98%)	4 (2%)	66	87
3	AS	264/265 (100%)	246 (93%)	18 (7%)	20	57
3	AT	264/265 (100%)	248 (94%)	16 (6%)	23	61
3	AU	264/265 (100%)	241 (91%)	23 (9%)	13	46
3	AV	264/265 (100%)	241 (91%)	23 (9%)	13	46
3	AW	264/265 (100%)	244 (92%)	20 (8%)	16	53
3	AX	264/265 (100%)	247 (94%)	17 (6%)	22	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	BS	264/265 (100%)	245 (93%)	19 (7%)	18	55
3	BT	264/265 (100%)	247 (94%)	17 (6%)	22	59
3	BU	264/265 (100%)	241 (91%)	23 (9%)	13	46
3	BV	264/265 (100%)	241 (91%)	23 (9%)	13	46
3	BW	264/265 (100%)	244 (92%)	20 (8%)	16	53
3	BX	264/265 (100%)	247 (94%)	17 (6%)	22	59
All	All	13362/13374 (100%)	12818 (96%)	544 (4%)	37	71

All (544) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A0	1	MET
1	A0	2	LEU
1	A0	8	ASP
1	A0	40	GLN
1	A0	88	LYS
1	A0	152	PHE
1	A0	165	ARG
1	A0	207	ASN
1	A0	224	ILE
1	A0	238	ARG
1	A0	286	ASP
1	A0	313	ILE
1	A0	360	ASN
2	AA	2	THR
2	AA	7	THR
2	AA	9	PHE
2	AA	18	VAL
2	AA	38	ILE
2	AA	40	ARG
2	AA	79	ASP
2	AA	124	ASP
2	AA	202	ASN
2	AB	38	ILE
2	AB	40	ARG
2	AB	206	THR
2	AB	232	HIS
2	AB	234	ASP
2	AB	252	PRO
2	AC	7	THR

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Mol	Chain	Res	Type
2	AC	38	ILE
2	AC	40	ARG
2	AC	232	HIS
2	AD	9	PHE
2	AD	18	VAL
2	AD	38	ILE
2	AD	40	ARG
2	AD	79	ASP
2	AD	124	ASP
2	AD	202	ASN
2	AE	38	ILE
2	AE	40	ARG
2	AE	206	THR
2	AE	232	HIS
2	AE	234	ASP
2	AE	252	PRO
2	AF	38	ILE
2	AF	40	ARG
2	AF	232	HIS
2	AG	7	THR
2	AG	9	PHE
2	AG	18	VAL
2	AG	38	ILE
2	AG	40	ARG
2	AG	79	ASP
2	AG	124	ASP
2	AG	202	ASN
2	AH	17	PRO
2	AH	38	ILE
2	AH	40	ARG
2	AH	206	THR
2	AH	232	HIS
2	AH	234	ASP
2	AH	252	PRO
2	AI	7	THR
2	AI	38	ILE
2	AI	40	ARG
2	AI	232	HIS
2	AJ	7	THR
2	AJ	9	PHE
2	AJ	18	VAL
2	AJ	38	ILE

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Mol	Chain	Res	Type
2	AJ	40	ARG
2	AJ	79	ASP
2	AJ	124	ASP
2	AJ	202	ASN
2	AK	23	ASP
2	AK	38	ILE
2	AK	40	ARG
2	AK	206	THR
2	AK	232	HIS
2	AK	234	ASP
2	AL	26	LEU
2	AL	38	ILE
2	AL	40	ARG
2	AL	232	HIS
2	AM	7	THR
2	AM	9	PHE
2	AM	18	VAL
2	AM	38	ILE
2	AM	40	ARG
2	AM	79	ASP
2	AM	124	ASP
2	AM	202	ASN
2	AN	23	ASP
2	AN	38	ILE
2	AN	40	ARG
2	AN	206	THR
2	AN	232	HIS
2	AN	234	ASP
2	AO	38	ILE
2	AO	40	ARG
2	AO	232	HIS
2	AP	9	PHE
2	AP	18	VAL
2	AP	38	ILE
2	AP	40	ARG
2	AP	79	ASP
2	AP	124	ASP
2	AP	202	ASN
2	AQ	17	PRO
2	AQ	23	ASP
2	AQ	38	ILE
2	AQ	40	ARG

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Mol	Chain	Res	Type
2	AQ	206	THR
2	AQ	232	HIS
2	AQ	234	ASP
2	AR	7	THR
2	AR	38	ILE
2	AR	40	ARG
2	AR	232	HIS
3	AS	11	LEU
3	AS	12	ASP
3	AS	26	VAL
3	AS	43	TRP
3	AS	54	ARG
3	AS	55	SER
3	AS	66	GLU
3	AS	123	THR
3	AS	142	LEU
3	AS	196	ILE
3	AS	197	PHE
3	AS	228	VAL
3	AS	232	GLU
3	AS	234	VAL
3	AS	263	VAL
3	AS	269	TYR
3	AS	270	ARG
3	AS	291	ILE
3	AT	12	ASP
3	AT	26	VAL
3	AT	48	ILE
3	AT	55	SER
3	AT	65	LEU
3	AT	72	LEU
3	AT	123	THR
3	AT	159	ILE
3	AT	171	ILE
3	AT	196	ILE
3	AT	203	LEU
3	AT	234	VAL
3	AT	236	ASP
3	AT	243	ASP
3	AT	263	VAL
3	AT	269	TYR
3	AU	3	ARG

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Mol	Chain	Res	Type
3	AU	11	LEU
3	AU	12	ASP
3	AU	26	VAL
3	AU	37	GLN
3	AU	39	THR
3	AU	43	TRP
3	AU	48	ILE
3	AU	53	THR
3	AU	54	ARG
3	AU	55	SER
3	AU	66	GLU
3	AU	72	LEU
3	AU	94	LEU
3	AU	196	ILE
3	AU	200	MET
3	AU	228	VAL
3	AU	232	GLU
3	AU	234	VAL
3	AU	258	LEU
3	AU	263	VAL
3	AU	270	ARG
3	AU	291	ILE
3	AV	3	ARG
3	AV	11	LEU
3	AV	12	ASP
3	AV	36	LEU
3	AV	48	ILE
3	AV	54	ARG
3	AV	55	SER
3	AV	66	GLU
3	AV	72	LEU
3	AV	120	LYS
3	AV	196	ILE
3	AV	197	PHE
3	AV	203	LEU
3	AV	227	ILE
3	AV	232	GLU
3	AV	234	VAL
3	AV	240	ILE
3	AV	243	ASP
3	AV	246	ASP
3	AV	258	LEU

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Mol	Chain	Res	Type
3	AV	263	VAL
3	AV	269	TYR
3	AV	291	ILE
3	AW	6	LYS
3	AW	11	LEU
3	AW	26	VAL
3	AW	43	TRP
3	AW	54	ARG
3	AW	55	SER
3	AW	66	GLU
3	AW	72	LEU
3	AW	123	THR
3	AW	196	ILE
3	AW	197	PHE
3	AW	203	LEU
3	AW	228	VAL
3	AW	232	GLU
3	AW	234	VAL
3	AW	258	LEU
3	AW	263	VAL
3	AW	269	TYR
3	AW	270	ARG
3	AW	291	ILE
3	AX	11	LEU
3	AX	26	VAL
3	AX	43	TRP
3	AX	54	ARG
3	AX	66	GLU
3	AX	107	LEU
3	AX	179	TYR
3	AX	196	ILE
3	AX	200	MET
3	AX	203	LEU
3	AX	228	VAL
3	AX	234	VAL
3	AX	243	ASP
3	AX	244	VAL
3	AX	258	LEU
3	AX	263	VAL
3	AX	291	ILE
1	AY	1	MET
1	AY	8	ASP

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Mol	Chain	Res	Type
1	AY	26	LYS
1	AY	40	GLN
1	AY	41	VAL
1	AY	87	LYS
1	AY	88	LYS
1	AY	152	PHE
1	AY	165	ARG
1	AY	192	GLN
1	AY	207	ASN
1	AY	242	ASN
1	AY	243	PHE
1	AY	286	ASP
1	AY	319	VAL
1	AY	340	ILE
1	AY	353	ASP
1	AY	360	ASN
1	AZ	1	MET
1	AZ	2	LEU
1	AZ	8	ASP
1	AZ	26	LYS
1	AZ	39	CYS
1	AZ	40	GLN
1	AZ	41	VAL
1	AZ	88	LYS
1	AZ	151	PHE
1	AZ	165	ARG
1	AZ	207	ASN
1	AZ	238	ARG
1	AZ	286	ASP
1	AZ	320	THR
1	AZ	340	ILE
1	AZ	360	ASN
1	B0	1	MET
1	B0	2	LEU
1	B0	8	ASP
1	B0	40	GLN
1	B0	88	LYS
1	B0	152	PHE
1	B0	165	ARG
1	B0	207	ASN
1	B0	224	ILE
1	B0	238	ARG

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Mol	Chain	Res	Type
1	B0	286	ASP
1	B0	313	ILE
1	B0	360	ASN
2	BA	2	THR
2	BA	7	THR
2	BA	9	PHE
2	BA	18	VAL
2	BA	38	ILE
2	BA	40	ARG
2	BA	79	ASP
2	BA	124	ASP
2	BA	202	ASN
2	BB	38	ILE
2	BB	40	ARG
2	BB	206	THR
2	BB	232	HIS
2	BB	234	ASP
2	BB	252	PRO
2	BC	7	THR
2	BC	38	ILE
2	BC	40	ARG
2	BC	232	HIS
2	BD	9	PHE
2	BD	18	VAL
2	BD	38	ILE
2	BD	40	ARG
2	BD	79	ASP
2	BD	124	ASP
2	BD	202	ASN
2	BE	38	ILE
2	BE	40	ARG
2	BE	206	THR
2	BE	232	HIS
2	BE	234	ASP
2	BE	252	PRO
2	BF	38	ILE
2	BF	40	ARG
2	BF	232	HIS
2	BG	7	THR
2	BG	9	PHE
2	BG	18	VAL
2	BG	38	ILE

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Mol	Chain	Res	Type
2	BG	40	ARG
2	BG	79	ASP
2	BG	124	ASP
2	BG	202	ASN
2	BH	17	PRO
2	BH	38	ILE
2	BH	40	ARG
2	BH	206	THR
2	BH	232	HIS
2	BH	234	ASP
2	BH	252	PRO
2	BI	7	THR
2	BI	38	ILE
2	BI	40	ARG
2	BI	232	HIS
2	BJ	7	THR
2	BJ	9	PHE
2	BJ	18	VAL
2	BJ	38	ILE
2	BJ	40	ARG
2	BJ	79	ASP
2	BJ	124	ASP
2	BJ	202	ASN
2	BK	23	ASP
2	BK	38	ILE
2	BK	40	ARG
2	BK	206	THR
2	BK	232	HIS
2	BK	234	ASP
2	BL	26	LEU
2	BL	38	ILE
2	BL	40	ARG
2	BL	232	HIS
2	BM	7	THR
2	BM	9	PHE
2	BM	18	VAL
2	BM	38	ILE
2	BM	40	ARG
2	BM	79	ASP
2	BM	124	ASP
2	BM	202	ASN
2	BN	23	ASP

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Mol	Chain	Res	Type
2	BN	38	ILE
2	BN	40	ARG
2	BN	206	THR
2	BN	232	HIS
2	BN	234	ASP
2	BO	38	ILE
2	BO	40	ARG
2	BO	232	HIS
2	BP	9	PHE
2	BP	18	VAL
2	BP	38	ILE
2	BP	40	ARG
2	BP	79	ASP
2	BP	124	ASP
2	BP	202	ASN
2	BQ	17	PRO
2	BQ	23	ASP
2	BQ	38	ILE
2	BQ	40	ARG
2	BQ	206	THR
2	BQ	232	HIS
2	BQ	234	ASP
2	BR	7	THR
2	BR	38	ILE
2	BR	40	ARG
2	BR	232	HIS
3	BS	11	LEU
3	BS	12	ASP
3	BS	26	VAL
3	BS	43	TRP
3	BS	54	ARG
3	BS	55	SER
3	BS	66	GLU
3	BS	72	LEU
3	BS	123	THR
3	BS	142	LEU
3	BS	196	ILE
3	BS	197	PHE
3	BS	228	VAL
3	BS	232	GLU
3	BS	234	VAL
3	BS	263	VAL

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Mol	Chain	Res	Type
3	BS	269	TYR
3	BS	270	ARG
3	BS	291	ILE
3	BT	12	ASP
3	BT	26	VAL
3	BT	48	ILE
3	BT	55	SER
3	BT	65	LEU
3	BT	72	LEU
3	BT	123	THR
3	BT	135	LYS
3	BT	159	ILE
3	BT	171	ILE
3	BT	196	ILE
3	BT	203	LEU
3	BT	234	VAL
3	BT	236	ASP
3	BT	243	ASP
3	BT	263	VAL
3	BT	269	TYR
3	BU	3	ARG
3	BU	11	LEU
3	BU	12	ASP
3	BU	26	VAL
3	BU	37	GLN
3	BU	39	THR
3	BU	43	TRP
3	BU	48	ILE
3	BU	53	THR
3	BU	54	ARG
3	BU	55	SER
3	BU	66	GLU
3	BU	72	LEU
3	BU	94	LEU
3	BU	196	ILE
3	BU	200	MET
3	BU	228	VAL
3	BU	232	GLU
3	BU	234	VAL
3	BU	258	LEU
3	BU	263	VAL
3	BU	270	ARG

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Mol	Chain	Res	Type
3	BU	291	ILE
3	BV	3	ARG
3	BV	11	LEU
3	BV	12	ASP
3	BV	36	LEU
3	BV	48	ILE
3	BV	54	ARG
3	BV	55	SER
3	BV	66	GLU
3	BV	72	LEU
3	BV	120	LYS
3	BV	196	ILE
3	BV	197	PHE
3	BV	203	LEU
3	BV	227	ILE
3	BV	232	GLU
3	BV	234	VAL
3	BV	240	ILE
3	BV	243	ASP
3	BV	246	ASP
3	BV	258	LEU
3	BV	263	VAL
3	BV	269	TYR
3	BV	291	ILE
3	BW	6	LYS
3	BW	11	LEU
3	BW	26	VAL
3	BW	43	TRP
3	BW	54	ARG
3	BW	55	SER
3	BW	66	GLU
3	BW	72	LEU
3	BW	123	THR
3	BW	196	ILE
3	BW	197	PHE
3	BW	203	LEU
3	BW	228	VAL
3	BW	232	GLU
3	BW	234	VAL
3	BW	258	LEU
3	BW	263	VAL
3	BW	269	TYR

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Mol	Chain	Res	Type
3	BW	270	ARG
3	BW	291	ILE
3	BX	11	LEU
3	BX	26	VAL
3	BX	43	TRP
3	BX	54	ARG
3	BX	66	GLU
3	BX	107	LEU
3	BX	179	TYR
3	BX	196	ILE
3	BX	200	MET
3	BX	203	LEU
3	BX	228	VAL
3	BX	234	VAL
3	BX	243	ASP
3	BX	244	VAL
3	BX	258	LEU
3	BX	263	VAL
3	BX	291	ILE
1	BY	1	MET
1	BY	8	ASP
1	BY	26	LYS
1	BY	40	GLN
1	BY	41	VAL
1	BY	87	LYS
1	BY	88	LYS
1	BY	152	PHE
1	BY	165	ARG
1	BY	192	GLN
1	BY	207	ASN
1	BY	242	ASN
1	BY	243	PHE
1	BY	286	ASP
1	BY	319	VAL
1	BY	340	ILE
1	BY	353	ASP
1	BY	360	ASN
1	BZ	1	MET
1	BZ	2	LEU
1	BZ	8	ASP
1	BZ	26	LYS
1	BZ	39	CYS

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Mol	Chain	Res	Type
1	BZ	40	GLN
1	BZ	41	VAL
1	BZ	88	LYS
1	BZ	151	PHE
1	BZ	165	ARG
1	BZ	207	ASN
1	BZ	238	ARG
1	BZ	286	ASP
1	BZ	320	THR
1	BZ	340	ILE
1	BZ	360	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (169) such sidechains are listed below:

Mol	Chain	Res	Type
1	A0	184	GLN
1	A0	267	ASN
2	AA	5	ASN
2	AA	71	ASN
2	AA	82	ASN
2	AA	172	ASN
2	AA	175	GLN
2	AB	71	ASN
2	AC	172	ASN
2	AD	5	ASN
2	AD	52	ASN
2	AD	71	ASN
2	AD	82	ASN
2	AD	92	GLN
2	AD	172	ASN
2	AD	175	GLN
2	AD	196	ASN
2	AE	54	GLN
2	AE	71	ASN
2	AF	172	ASN
2	AG	71	ASN
2	AG	82	ASN
2	AG	92	GLN
2	AG	172	ASN
2	AG	175	GLN
2	AG	196	ASN
2	AH	71	ASN

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Mol	Chain	Res	Type
2	AI	151	ASN
2	AI	172	ASN
2	AJ	71	ASN
2	AJ	82	ASN
2	AJ	172	ASN
2	AJ	175	GLN
2	AJ	196	ASN
2	AK	54	GLN
2	AK	71	ASN
2	AL	151	ASN
2	AL	172	ASN
2	AM	71	ASN
2	AM	82	ASN
2	AM	172	ASN
2	AM	175	GLN
2	AM	196	ASN
2	AN	54	GLN
2	AN	71	ASN
2	AO	172	ASN
2	AP	5	ASN
2	AP	22	ASN
2	AP	71	ASN
2	AP	82	ASN
2	AP	92	GLN
2	AP	172	ASN
2	AP	175	GLN
2	AP	196	ASN
2	AQ	71	ASN
2	AR	151	ASN
2	AR	172	ASN
3	AS	102	GLN
3	AS	222	ASN
3	AS	250	GLN
3	AT	102	GLN
3	AT	167	ASN
3	AT	235	GLN
3	AU	23	ASN
3	AU	75	ASN
3	AU	250	GLN
3	AV	23	ASN
3	AV	102	GLN
3	AV	121	ASN

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Mol	Chain	Res	Type
3	AV	235	GLN
3	AV	250	GLN
3	AW	102	GLN
3	AW	121	ASN
3	AX	102	GLN
3	AX	121	ASN
3	AX	167	ASN
3	AX	250	GLN
3	AX	278	GLN
1	AY	11	ASN
1	AY	90	ASN
1	AY	143	ASN
1	AZ	143	ASN
1	AZ	184	GLN
1	AZ	192	GLN
1	AZ	212	ASN
1	B0	184	GLN
1	B0	267	ASN
2	BA	5	ASN
2	BA	71	ASN
2	BA	82	ASN
2	BA	172	ASN
2	BA	175	GLN
2	BB	71	ASN
2	BC	172	ASN
2	BD	5	ASN
2	BD	52	ASN
2	BD	71	ASN
2	BD	82	ASN
2	BD	92	GLN
2	BD	172	ASN
2	BD	175	GLN
2	BD	196	ASN
2	BE	54	GLN
2	BE	71	ASN
2	BF	172	ASN
2	BG	71	ASN
2	BG	82	ASN
2	BG	92	GLN
2	BG	172	ASN
2	BG	175	GLN
2	BG	196	ASN

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Mol	Chain	Res	Type
2	BH	71	ASN
2	BI	151	ASN
2	BI	172	ASN
2	BJ	71	ASN
2	BJ	82	ASN
2	BJ	172	ASN
2	BJ	175	GLN
2	BJ	196	ASN
2	BK	71	ASN
2	BL	151	ASN
2	BL	172	ASN
2	BM	71	ASN
2	BM	82	ASN
2	BM	172	ASN
2	BM	175	GLN
2	BM	196	ASN
2	BN	54	GLN
2	BN	71	ASN
2	BO	172	ASN
2	BP	5	ASN
2	BP	22	ASN
2	BP	71	ASN
2	BP	82	ASN
2	BP	92	GLN
2	BP	172	ASN
2	BP	175	GLN
2	BP	196	ASN
2	BQ	54	GLN
2	BQ	71	ASN
2	BR	151	ASN
2	BR	172	ASN
3	BS	102	GLN
3	BS	222	ASN
3	BS	250	GLN
3	BT	102	GLN
3	BT	167	ASN
3	BT	222	ASN
3	BT	235	GLN
3	BU	23	ASN
3	BU	75	ASN
3	BU	250	GLN
3	BV	23	ASN

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Mol	Chain	Res	Type
3	BV	102	GLN
3	BV	121	ASN
3	BV	235	GLN
3	BV	250	GLN
3	BW	102	GLN
3	BW	121	ASN
3	BX	102	GLN
3	BX	121	ASN
3	BX	167	ASN
3	BX	250	GLN
1	BY	90	ASN
1	BY	143	ASN
1	BZ	143	ASN
1	BZ	184	GLN
1	BZ	192	GLN
1	BZ	212	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A0	372/372 (100%)	0.60	49 (13%) 4 8	351, 388, 435, 523	0
1	AY	372/372 (100%)	0.42	42 (11%) 7 10	359, 396, 449, 555	0
1	AZ	372/372 (100%)	0.48	41 (11%) 7 10	364, 394, 445, 557	0
1	B0	372/372 (100%)	0.48	33 (8%) 12 14	337, 377, 425, 485	0
1	BY	372/372 (100%)	0.19	18 (4%) 34 31	331, 361, 429, 557	0
1	BZ	372/372 (100%)	0.37	31 (8%) 14 16	332, 360, 422, 502	0
2	AA	263/263 (100%)	0.11	9 (3%) 49 44	248, 312, 407, 435	0
2	AB	263/263 (100%)	0.19	18 (6%) 20 20	284, 350, 440, 481	0
2	AC	263/263 (100%)	-0.07	13 (4%) 33 31	257, 345, 417, 473	0
2	AD	263/263 (100%)	0.27	18 (6%) 20 20	258, 320, 441, 485	0
2	AE	263/263 (100%)	0.00	12 (4%) 36 33	277, 344, 466, 480	0
2	AF	263/263 (100%)	0.17	17 (6%) 22 21	265, 367, 471, 497	0
2	AG	263/263 (100%)	0.32	25 (9%) 10 13	265, 348, 500, 556	0
2	AH	263/263 (100%)	-0.04	11 (4%) 40 36	315, 402, 524, 572	0
2	AI	263/263 (100%)	0.20	21 (7%) 15 17	282, 416, 532, 576	0
2	AJ	263/263 (100%)	0.05	15 (5%) 27 26	264, 342, 429, 539	0
2	AK	263/263 (100%)	0.05	12 (4%) 36 33	255, 301, 456, 521	0
2	AL	263/263 (100%)	0.23	20 (7%) 17 18	277, 345, 485, 575	0
2	AM	263/263 (100%)	0.23	23 (8%) 13 15	266, 358, 425, 467	0
2	AN	263/263 (100%)	0.26	17 (6%) 22 21	252, 313, 386, 420	0
2	AO	263/263 (100%)	0.18	14 (5%) 30 29	276, 347, 419, 449	0
2	AP	263/263 (100%)	0.26	20 (7%) 17 18	267, 341, 556, 576	0
2	AQ	263/263 (100%)	0.37	29 (11%) 7 10	295, 397, 566, 605	0
2	AR	263/263 (100%)	0.25	23 (8%) 13 15	298, 417, 541, 571	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	BA	263/263 (100%)	0.13	13 (4%) 33 31	259, 312, 430, 466	0
2	BB	263/263 (100%)	0.10	15 (5%) 27 26	282, 346, 455, 506	0
2	BC	263/263 (100%)	0.02	15 (5%) 27 26	273, 344, 419, 481	0
2	BD	263/263 (100%)	0.22	19 (7%) 18 19	252, 316, 445, 484	0
2	BE	263/263 (100%)	0.04	12 (4%) 36 33	274, 342, 448, 477	0
2	BF	263/263 (100%)	0.41	23 (8%) 13 15	258, 361, 457, 487	0
2	BG	263/263 (100%)	0.33	26 (9%) 9 12	252, 346, 496, 557	0
2	BH	263/263 (100%)	0.21	24 (9%) 11 14	314, 408, 514, 559	0
2	BI	263/263 (100%)	0.05	12 (4%) 36 33	276, 420, 541, 584	0
2	BJ	263/263 (100%)	-0.13	7 (2%) 58 53	268, 345, 419, 521	0
2	BK	263/263 (100%)	0.15	20 (7%) 17 18	256, 305, 435, 496	0
2	BL	263/263 (100%)	0.25	23 (8%) 13 15	283, 341, 452, 534	0
2	BM	263/263 (100%)	0.44	30 (11%) 7 10	264, 357, 438, 484	0
2	BN	263/263 (100%)	0.23	19 (7%) 18 19	255, 316, 388, 433	0
2	BO	263/263 (100%)	0.12	17 (6%) 22 21	276, 348, 418, 453	0
2	BP	263/263 (100%)	0.37	32 (12%) 5 9	261, 365, 541, 549	0
2	BQ	263/263 (100%)	0.24	24 (9%) 11 14	312, 413, 547, 559	0
2	BR	263/263 (100%)	0.35	29 (11%) 7 10	308, 418, 537, 556	0
3	AS	298/298 (100%)	0.36	17 (5%) 27 26	219, 262, 346, 379	0
3	AT	298/298 (100%)	0.33	17 (5%) 27 26	230, 260, 318, 344	0
3	AU	298/298 (100%)	0.22	10 (3%) 49 44	228, 269, 334, 364	0
3	AV	298/298 (100%)	0.27	18 (6%) 25 24	229, 264, 317, 332	0
3	AW	298/298 (100%)	0.23	11 (3%) 45 40	213, 254, 317, 347	0
3	AX	298/298 (100%)	0.16	15 (5%) 32 30	216, 255, 347, 401	0
3	BS	298/298 (100%)	0.26	14 (4%) 35 33	222, 256, 339, 388	0
3	BT	298/298 (100%)	0.25	12 (4%) 42 38	218, 265, 316, 343	0
3	BU	298/298 (100%)	0.14	11 (3%) 45 40	228, 262, 338, 382	0
3	BV	298/298 (100%)	0.35	20 (6%) 21 21	218, 260, 305, 324	0
3	BW	298/298 (100%)	0.13	10 (3%) 49 44	215, 256, 341, 403	0
3	BX	298/298 (100%)	0.15	14 (4%) 35 33	228, 272, 370, 407	0
All	All	15276/15276 (100%)	0.23	1060 (6%) 20 20	213, 344, 468, 605	0

All (1060) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	AQ	221	VAL	17.3
2	AQ	220	LEU	16.4
2	BN	260	SER	9.8
2	BO	260	SER	9.8
1	A0	32	LEU	9.7
2	BF	260	SER	9.6
2	BM	259	GLY	9.6
1	A0	198	THR	9.4
2	BF	259	GLY	9.3
2	BB	260	SER	9.0
2	BH	259	GLY	8.9
2	BH	260	SER	8.8
2	BP	192	GLY	8.8
2	BO	259	GLY	8.7
2	BR	30	LEU	8.7
1	B0	164	ASN	8.7
2	BR	221	VAL	8.5
1	BZ	209	ALA	8.5
2	BI	259	GLY	8.5
2	BC	260	SER	8.4
2	AF	260	SER	8.4
2	AO	260	SER	8.2
2	AR	222	GLY	8.0
2	AM	176	LEU	8.0
1	BY	1	MET	7.9
1	AZ	367	GLU	7.8
2	AR	221	VAL	7.8
2	BM	258	ASN	7.8
1	A0	202	ASN	7.7
2	BG	254	ALA	7.7
1	A0	164	ASN	7.6
2	AD	258	ASN	7.6
2	BM	174	LEU	7.5
2	BE	258	ASN	7.5
3	AS	298	VAL	7.4
2	AQ	222	GLY	7.4
2	BQ	221	VAL	7.3
1	A0	195	PRO	7.3
2	BG	221	VAL	7.3
2	BQ	230	SER	7.2
2	AL	221	VAL	7.0
1	AZ	164	ASN	7.0

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Mol	Chain	Res	Type	RSRZ
2	BM	257	GLY	6.9
2	AF	259	GLY	6.9
2	AO	259	GLY	6.8
1	BZ	208	PHE	6.8
2	AG	192	GLY	6.8
2	BB	221	VAL	6.8
2	AM	221	VAL	6.7
2	BP	193	SER	6.7
2	BN	259	GLY	6.7
2	BQ	222	GLY	6.6
2	AF	62	ALA	6.6
2	BR	3	ILE	6.5
2	BL	252	PRO	6.5
1	AZ	215	ARG	6.4
2	BI	260	SER	6.4
2	AR	31	THR	6.4
1	AY	128	THR	6.4
1	AY	217	ARG	6.3
1	A0	196	SER	6.3
2	AP	222	GLY	6.2
2	BA	221	VAL	6.2
2	BF	221	VAL	6.2
2	AM	260	SER	6.1
2	AG	225	ALA	6.1
3	BX	298	VAL	6.0
1	B0	162	THR	6.0
1	BY	215	ARG	6.0
1	A0	197	GLU	6.0
2	BQ	231	PHE	6.0
2	BQ	233	ILE	6.0
2	AM	175	GLN	5.9
2	AE	221	VAL	5.9
1	AY	164	ASN	5.8
2	AP	117	GLY	5.7
2	AD	221	VAL	5.7
2	BR	31	THR	5.7
2	BM	188	VAL	5.7
2	BH	261	TYR	5.7
1	B0	195	PRO	5.6
2	AR	258	ASN	5.6
1	BZ	207	ASN	5.6
2	BM	260	SER	5.5

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Mol	Chain	Res	Type	RSRZ
2	AQ	260	SER	5.5
1	A0	327	ASN	5.5
2	AG	254	ALA	5.5
2	AK	221	VAL	5.4
1	A0	326	GLN	5.4
2	BF	63	GLY	5.4
2	AI	36	ARG	5.4
2	AG	211	PRO	5.4
2	AQ	219	SER	5.4
2	AI	35	TYR	5.4
2	BA	130	GLY	5.3
2	BA	260	SER	5.3
2	BA	222	GLY	5.3
1	AY	129	THR	5.3
2	BO	157	GLY	5.3
2	AM	174	LEU	5.3
1	A0	68	ILE	5.2
2	BM	176	LEU	5.2
2	AD	260	SER	5.2
2	AH	260	SER	5.2
1	B0	209	ALA	5.2
2	BK	30	LEU	5.2
2	BH	222	GLY	5.2
2	AO	221	VAL	5.1
3	BV	296	ASP	5.1
2	BO	219	SER	5.0
2	AP	254	ALA	5.0
2	AQ	63	GLY	5.0
2	AG	221	VAL	5.0
2	AD	161	VAL	4.9
1	AY	1	MET	4.9
1	AY	372	PRO	4.9
2	BR	126	VAL	4.9
1	AZ	1	MET	4.9
2	BM	168	VAL	4.9
2	AF	220	LEU	4.9
2	BQ	2	THR	4.8
2	AN	259	GLY	4.8
2	AN	260	SER	4.8
3	AT	298	VAL	4.8
2	AE	257	GLY	4.8
2	BM	167	THR	4.8

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Mol	Chain	Res	Type	RSRZ
3	AT	288	GLU	4.8
3	BS	212	ALA	4.8
2	BG	260	SER	4.8
1	AZ	210	SER	4.7
2	BI	188	VAL	4.7
2	AN	258	ASN	4.7
1	BY	372	PRO	4.7
2	BB	259	GLY	4.6
3	AT	287	ALA	4.6
2	AQ	259	GLY	4.6
2	AQ	94	ALA	4.6
3	AT	240	ILE	4.6
2	AA	31	THR	4.6
2	BG	220	LEU	4.6
1	BY	162	THR	4.5
2	BE	259	GLY	4.5
2	BD	260	SER	4.5
2	BP	176	LEU	4.5
1	A0	356	LYS	4.5
2	BE	257	GLY	4.5
2	BN	185	LEU	4.5
2	BD	264	LYS	4.5
2	AM	62	ALA	4.5
2	BH	221	VAL	4.5
2	BM	190	PHE	4.5
2	BK	64	GLY	4.5
2	AL	254	ALA	4.5
2	BR	29	MET	4.5
2	BC	247	ASN	4.5
1	AY	158	ALA	4.4
2	BR	228	ASP	4.4
2	AB	222	GLY	4.4
2	BQ	62	ALA	4.4
2	BP	254	ALA	4.4
2	BQ	215	ALA	4.4
1	A0	151	PHE	4.4
2	AL	62	ALA	4.4
2	BB	222	GLY	4.4
3	BX	99	GLU	4.4
2	BR	260	SER	4.4
3	AU	158	LYS	4.4
2	AD	38	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
2	AG	256	ARG	4.4
2	BP	61	ILE	4.3
2	AF	63	GLY	4.3
2	BK	27	TYR	4.3
1	A0	332	LEU	4.3
1	A0	31	GLY	4.3
2	AL	63	GLY	4.3
2	BF	220	LEU	4.3
2	BP	211	PRO	4.3
2	AE	258	ASN	4.3
1	AZ	233	GLU	4.3
1	A0	265	ALA	4.3
2	AR	99	LEU	4.3
1	AZ	52	LEU	4.3
2	BO	30	LEU	4.3
3	BV	247	GLU	4.3
2	BF	174	LEU	4.3
1	B0	292	THR	4.2
1	AY	315	PRO	4.2
2	AL	222	GLY	4.2
2	BK	168	VAL	4.2
3	BT	247	GLU	4.2
2	AH	258	ASN	4.2
2	BM	221	VAL	4.2
2	BI	221	VAL	4.2
3	BV	298	VAL	4.2
2	AP	221	VAL	4.2
2	AP	223	HIS	4.2
2	AI	188	VAL	4.2
2	BP	175	GLN	4.1
1	B0	280	ASP	4.1
2	BD	257	GLY	4.1
2	BH	253	ILE	4.1
1	A0	199	ASP	4.1
1	A0	162	THR	4.1
2	AM	258	ASN	4.1
2	BE	260	SER	4.1
2	AM	188	VAL	4.1
3	AT	202	ILE	4.1
1	AY	162	THR	4.1
3	AT	34	LEU	4.1
1	B0	125	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
2	BF	99	LEU	4.1
2	BP	253	ILE	4.1
2	BN	221	VAL	4.1
2	AQ	95	ASN	4.1
1	AZ	299	ASP	4.1
3	AV	287	ALA	4.1
2	BO	221	VAL	4.1
2	BH	116	SER	4.1
2	BO	159	ILE	4.1
2	AD	18	VAL	4.1
3	BT	158	LYS	4.1
2	AQ	27	TYR	4.0
2	BJ	260	SER	4.0
2	BM	261	TYR	4.0
2	AN	221	VAL	4.0
2	AG	190	PHE	4.0
2	AA	30	LEU	4.0
2	AC	184	ASP	4.0
2	AQ	253	ILE	4.0
2	BP	62	ALA	4.0
2	BH	258	ASN	4.0
2	BQ	38	ILE	4.0
2	BD	221	VAL	4.0
3	BU	158	LYS	4.0
2	BR	197	ILE	4.0
3	AU	203	LEU	4.0
2	AJ	26	LEU	4.0
2	BL	43	TRP	4.0
1	BZ	264	ILE	4.0
2	AJ	261	TYR	4.0
2	AF	219	SER	4.0
2	BM	153	MET	3.9
2	AM	259	GLY	3.9
1	AZ	136	TYR	3.9
1	AZ	166	LYS	3.9
2	AL	188	VAL	3.9
2	BE	221	VAL	3.9
2	BD	181	LYS	3.9
2	AH	222	GLY	3.9
2	AG	226	GLY	3.9
1	A0	200	PRO	3.9
2	AC	183	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
3	AT	2	VAL	3.9
2	BA	259	GLY	3.9
2	BN	186	VAL	3.9
2	AQ	30	LEU	3.9
2	BL	194	VAL	3.8
1	BY	271	VAL	3.8
2	AG	23	ASP	3.8
2	AR	30	LEU	3.8
2	BP	252	PRO	3.8
2	BL	197	ILE	3.8
2	AG	167	THR	3.8
1	AZ	209	ALA	3.8
3	BV	249	TYR	3.8
2	AD	259	GLY	3.8
2	AC	260	SER	3.8
2	AB	69	LEU	3.8
1	AZ	368	SER	3.8
2	BL	221	VAL	3.8
2	AL	219	SER	3.8
2	AQ	62	ALA	3.8
2	BG	175	GLN	3.7
1	AY	126	THR	3.7
2	AJ	260	SER	3.7
2	BF	262	PHE	3.7
2	BP	216	ALA	3.7
1	B0	328	GLU	3.7
1	BZ	76	VAL	3.7
2	AN	181	LYS	3.7
2	BP	38	ILE	3.7
2	AD	99	LEU	3.7
2	BF	222	GLY	3.7
3	AV	289	PHE	3.7
2	BH	252	PRO	3.7
1	A0	66	GLY	3.7
2	BQ	220	LEU	3.7
3	BX	296	ASP	3.7
2	BC	258	ASN	3.7
2	BM	220	LEU	3.7
1	BZ	142	LYS	3.7
2	AG	27	TYR	3.7
2	AP	30	LEU	3.7
2	AE	222	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
2	BF	64	GLY	3.7
2	BG	27	TYR	3.7
2	AG	175	GLN	3.6
3	BS	34	LEU	3.6
2	AL	258	ASN	3.6
2	BF	144	THR	3.6
1	AY	233	GLU	3.6
2	AD	211	PRO	3.6
2	BF	176	LEU	3.6
2	BP	31	THR	3.6
1	AY	159	GLY	3.6
2	AQ	215	ALA	3.6
1	B0	163	ILE	3.6
2	BO	158	SER	3.6
2	AN	23	ASP	3.6
3	AT	212	ALA	3.6
1	AY	314	SER	3.6
2	BL	188	VAL	3.6
2	BC	259	GLY	3.6
2	AD	220	LEU	3.6
3	BS	213	GLY	3.6
2	BK	31	THR	3.5
3	AS	287	ALA	3.5
1	A0	314	SER	3.5
2	BL	202	ASN	3.5
2	BB	30	LEU	3.5
2	AN	213	ARG	3.5
1	AY	337	LEU	3.5
2	AM	27	TYR	3.5
2	AI	75	ALA	3.5
1	AY	36	LYS	3.5
2	BB	261	TYR	3.5
2	BG	192	GLY	3.5
2	BR	222	GLY	3.5
3	AU	238	ILE	3.5
1	A0	194	ALA	3.5
2	AK	62	ALA	3.5
2	BH	257	GLY	3.5
3	AX	200	MET	3.5
1	A0	315	PRO	3.5
1	AZ	230	MET	3.5
3	AW	281	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
2	BR	220	LEU	3.5
3	BW	279	MET	3.4
2	AM	177	GLN	3.4
2	AQ	233	ILE	3.4
2	BL	251	THR	3.4
1	B0	127	LYS	3.4
2	BB	48	ASN	3.4
1	AZ	201	ARG	3.4
1	A0	9	ASN	3.4
1	BY	335	ASN	3.4
2	AG	191	PHE	3.4
2	AG	220	LEU	3.4
2	BA	220	LEU	3.4
3	BU	287	ALA	3.4
3	AU	154	ALA	3.4
1	AZ	315	PRO	3.4
2	AA	3	ILE	3.4
3	BX	100	ILE	3.4
1	AZ	319	VAL	3.4
1	BZ	372	PRO	3.4
2	AJ	27	TYR	3.4
2	AO	220	LEU	3.4
3	BV	139	TYR	3.4
3	AS	212	ALA	3.4
1	AZ	278	HIS	3.4
2	AI	259	GLY	3.4
2	BN	261	TYR	3.4
2	AM	61	ILE	3.4
3	AT	72	LEU	3.4
3	BX	281	LEU	3.4
2	BI	27	TYR	3.4
3	BU	1	MET	3.3
2	AF	221	VAL	3.3
1	AY	371	LYS	3.3
2	AN	27	TYR	3.3
3	AW	158	LYS	3.3
2	BK	69	LEU	3.3
2	BM	166	LEU	3.3
3	BU	203	LEU	3.3
2	AH	221	VAL	3.3
2	BD	27	TYR	3.3
2	BH	99	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	AY	87	LYS	3.3
1	AZ	126	THR	3.3
2	BD	258	ASN	3.3
3	AV	201	GLY	3.3
2	AL	220	LEU	3.3
2	BF	261	TYR	3.3
3	AT	1	MET	3.3
2	AI	64	GLY	3.3
2	BH	188	VAL	3.3
3	AT	296	ASP	3.3
2	AF	258	ASN	3.3
1	BZ	356	LYS	3.3
2	AL	227	ARG	3.3
2	BR	233	ILE	3.2
1	B0	126	THR	3.2
2	BP	223	HIS	3.2
3	AV	213	GLY	3.2
3	BS	249	TYR	3.2
2	BG	99	LEU	3.2
2	BR	4	LYS	3.2
2	BG	235	ILE	3.2
2	AP	116	SER	3.2
2	BB	220	LEU	3.2
2	BK	26	LEU	3.2
1	A0	163	ILE	3.2
2	BP	66	TYR	3.2
1	AY	88	LYS	3.2
2	AN	187	ILE	3.2
2	AL	161	VAL	3.2
2	BO	188	VAL	3.2
2	AK	27	TYR	3.2
1	AY	132	ALA	3.2
3	BU	12	ASP	3.2
3	AV	190	TRP	3.2
2	BM	189	ARG	3.2
2	AI	260	SER	3.2
2	AO	27	TYR	3.2
2	BH	215	ALA	3.2
2	BB	97	VAL	3.2
2	BN	206	THR	3.1
1	AZ	320	THR	3.1
2	BK	221	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B0	208	PHE	3.1
2	AN	208	VAL	3.1
1	BZ	244	ALA	3.1
2	BD	184	ASP	3.1
2	AR	125	ILE	3.1
3	AU	289	PHE	3.1
3	AV	200	MET	3.1
2	BF	62	ALA	3.1
1	BZ	263	TYR	3.1
2	BO	220	LEU	3.1
2	BP	215	ALA	3.1
1	AZ	65	VAL	3.1
1	A0	203	LEU	3.1
2	BP	67	PHE	3.1
1	A0	67	ASP	3.1
2	BE	99	LEU	3.1
2	AJ	262	PHE	3.1
2	BM	263	ILE	3.1
2	AI	63	GLY	3.1
2	AI	114	ASN	3.1
1	A0	207	ASN	3.1
2	BM	142	THR	3.1
2	AQ	216	ALA	3.0
2	BN	97	VAL	3.0
1	AZ	165	ARG	3.0
2	BP	256	ARG	3.0
1	BY	371	LYS	3.0
2	BJ	185	LEU	3.0
2	BL	66	TYR	3.0
2	AJ	212	PHE	3.0
2	BG	176	LEU	3.0
2	AF	262	PHE	3.0
2	BH	251	THR	3.0
3	AV	269	TYR	3.0
2	AC	99	LEU	3.0
2	BB	258	ASN	3.0
1	B0	329	LEU	3.0
2	BL	176	LEU	3.0
1	AZ	232	THR	3.0
2	AH	259	GLY	3.0
2	BQ	246	ALA	3.0
3	AV	214	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	BB	53	VAL	3.0
3	AX	1	MET	3.0
1	AY	182	LYS	3.0
2	BK	99	LEU	3.0
2	AH	99	LEU	3.0
2	BD	99	LEU	3.0
3	BS	227	ILE	3.0
2	BG	259	GLY	3.0
3	BV	142	LEU	3.0
2	BE	222	GLY	3.0
2	BL	222	GLY	3.0
1	AZ	162	THR	3.0
2	BG	167	THR	3.0
2	BP	30	LEU	3.0
3	AX	187	LEU	3.0
1	AY	370	ASP	3.0
2	AR	257	GLY	3.0
2	BD	259	GLY	3.0
2	BC	185	LEU	3.0
1	BZ	210	SER	3.0
3	AS	204	TYR	3.0
1	B0	235	ILE	3.0
2	BL	196	ASN	3.0
1	AY	184	GLN	3.0
1	AY	348	SER	3.0
2	AK	67	PHE	3.0
2	AB	88	ILE	3.0
2	AL	160	ASP	3.0
3	AX	272	ARG	2.9
2	AR	27	TYR	2.9
2	BB	27	TYR	2.9
2	AQ	97	VAL	2.9
2	AM	86	ALA	2.9
2	AB	27	TYR	2.9
2	AI	27	TYR	2.9
2	AK	97	VAL	2.9
2	AD	62	ALA	2.9
2	BK	67	PHE	2.9
2	BO	27	TYR	2.9
2	BQ	63	GLY	2.9
2	BQ	232	HIS	2.9
1	B0	160	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	BY	160	LYS	2.9
2	BK	62	ALA	2.9
2	BF	143	SER	2.9
3	AW	122	GLY	2.9
2	AR	231	PHE	2.9
2	AO	185	LEU	2.9
2	AG	193	SER	2.9
2	AP	26	LEU	2.9
3	BT	248	THR	2.9
3	BW	158	LYS	2.9
2	AG	30	LEU	2.9
3	BT	143	THR	2.9
3	AX	118	TYR	2.9
2	AO	103	THR	2.9
1	BY	78	PRO	2.9
2	AI	99	LEU	2.9
2	BR	232	HIS	2.9
2	BP	221	VAL	2.9
2	BQ	168	VAL	2.9
2	BQ	208	VAL	2.9
1	AY	339	ASP	2.9
1	AY	2	LEU	2.9
2	AM	30	LEU	2.9
2	AN	185	LEU	2.9
2	AJ	220	LEU	2.8
2	AP	145	LEU	2.8
2	BQ	99	LEU	2.8
2	AQ	237	PRO	2.8
2	BA	18	VAL	2.8
2	BO	97	VAL	2.8
2	AL	253	ILE	2.8
1	B0	183	VAL	2.8
2	AM	99	LEU	2.8
2	BR	139	ILE	2.8
1	A0	148	TYR	2.8
2	AF	176	LEU	2.8
2	AI	34	ASP	2.8
2	BD	182	ASN	2.8
2	BL	253	ILE	2.8
2	BJ	262	PHE	2.8
2	AG	255	THR	2.8
2	BC	262	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	AC	264	LYS	2.8
2	BC	218	GLN	2.8
2	AR	124	ASP	2.8
2	BG	185	LEU	2.8
3	AS	213	GLY	2.8
3	AW	1	MET	2.8
1	B0	87	LYS	2.8
2	AJ	81	VAL	2.8
2	BA	30	LEU	2.8
1	BZ	120	ASP	2.8
2	BF	258	ASN	2.8
3	BX	288	GLU	2.8
2	BI	258	ASN	2.8
2	AL	259	GLY	2.8
2	AQ	258	ASN	2.8
2	BL	259	GLY	2.8
3	AT	201	GLY	2.8
1	AZ	228	VAL	2.8
2	BJ	3	ILE	2.8
3	AT	289	PHE	2.8
2	AB	110	VAL	2.8
1	BZ	271	VAL	2.8
2	AB	190	PHE	2.8
2	BN	153	MET	2.7
1	B0	136	TYR	2.7
2	AF	188	VAL	2.7
1	B0	207	ASN	2.7
2	AG	214	PRO	2.7
2	BP	255	THR	2.7
3	BU	90	LYS	2.7
1	BY	332	LEU	2.7
2	AA	124	ASP	2.7
2	BL	203	MET	2.7
3	BS	125	SER	2.7
1	AZ	163	ILE	2.7
2	AP	225	ALA	2.7
1	A0	328	GLU	2.7
2	BC	261	TYR	2.7
2	BG	159	ILE	2.7
2	AE	256	ARG	2.7
1	B0	138	ILE	2.7
2	AF	218	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	BZ	137	LEU	2.7
3	AV	142	LEU	2.7
2	BK	187	ILE	2.7
2	BQ	115	GLY	2.7
3	AX	280	GLU	2.7
1	A0	87	LYS	2.7
1	AY	19	ASP	2.7
1	B0	335	ASN	2.7
2	BL	248	ILE	2.7
2	AO	258	ASN	2.7
2	BI	167	THR	2.7
3	AS	250	GLN	2.7
2	BO	31	THR	2.7
2	BL	116	SER	2.7
2	BC	184	ASP	2.7
3	AV	144	PHE	2.7
3	BV	119	GLY	2.7
2	AC	185	LEU	2.7
1	BY	125	ILE	2.7
2	AK	199	LYS	2.7
2	BI	261	TYR	2.7
2	BK	63	GLY	2.7
2	AB	68	GLU	2.7
2	AM	218	GLN	2.7
2	AP	253	ILE	2.7
2	BM	169	GLU	2.7
2	BI	69	LEU	2.7
2	BN	53	VAL	2.7
2	BP	225	ALA	2.7
2	AM	220	LEU	2.7
3	AS	203	LEU	2.7
1	A0	357	THR	2.7
2	AE	37	THR	2.7
3	BX	287	ALA	2.6
3	BV	294	LYS	2.6
1	B0	9	ASN	2.6
2	BP	191	PHE	2.6
2	AG	235	ILE	2.6
3	AS	61	ILE	2.6
2	AC	40	ARG	2.6
2	AI	109	GLY	2.6
2	BK	176	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	BQ	206	THR	2.6
1	BZ	116	ILE	2.6
2	AQ	218	GLN	2.6
2	BM	64	GLY	2.6
3	BW	298	VAL	2.6
1	BZ	186	GLN	2.6
2	AF	99	LEU	2.6
2	AP	260	SER	2.6
1	BZ	138	ILE	2.6
2	BP	60	ILE	2.6
3	AS	249	TYR	2.6
1	A0	300	HIS	2.6
2	AF	253	ILE	2.6
2	AI	30	LEU	2.6
2	BP	39	ARG	2.6
3	AS	281	LEU	2.6
3	BS	114	LYS	2.6
1	AZ	199	ASP	2.6
2	AM	31	THR	2.6
2	BI	222	GLY	2.6
2	BH	27	TYR	2.6
2	BC	183	ASN	2.6
2	BG	105	ASN	2.6
2	BF	175	GLN	2.6
3	AS	238	ILE	2.6
3	AX	90	LYS	2.6
1	AY	65	VAL	2.6
3	AS	214	VAL	2.6
3	BX	1	MET	2.6
2	AC	211	PRO	2.6
2	AD	63	GLY	2.6
2	AO	3	ILE	2.6
2	BA	76	LEU	2.6
2	BH	26	LEU	2.6
2	BC	254	ALA	2.6
1	A0	69	VAL	2.6
2	AB	176	LEU	2.6
2	BE	62	ALA	2.6
2	BE	146	ASP	2.6
2	AR	190	PHE	2.5
3	AV	240	ILE	2.5
2	BP	27	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
3	AV	249	TYR	2.5
3	BS	287	ALA	2.5
2	BG	23	ASP	2.5
3	BW	68	PHE	2.5
1	BY	331	PRO	2.5
2	AK	220	LEU	2.5
2	BK	169	GLU	2.5
2	AC	123	PHE	2.5
2	AD	61	ILE	2.5
2	AP	97	VAL	2.5
2	AL	27	TYR	2.5
1	AZ	167	ALA	2.5
3	AV	202	ILE	2.5
2	BR	77	LYS	2.5
2	AN	188	VAL	2.5
2	AR	69	LEU	2.5
1	BZ	318	ILE	2.5
3	AS	156	MET	2.5
2	AC	30	LEU	2.5
2	AD	30	LEU	2.5
1	A0	167	ALA	2.5
3	BU	55	SER	2.5
2	AL	217	VAL	2.5
2	AP	220	LEU	2.5
2	BH	30	LEU	2.5
2	BK	25	LYS	2.5
2	AJ	138	PRO	2.5
2	AM	262	PHE	2.5
1	AY	366	VAL	2.5
2	AC	212	PHE	2.5
2	AL	251	THR	2.5
1	AY	160	LYS	2.5
1	AZ	14	TYR	2.5
3	AW	280	GLU	2.5
3	BX	82	PHE	2.5
2	AC	263	ILE	2.5
3	AW	107	LEU	2.5
3	BS	250	GLN	2.5
3	AX	290	LYS	2.5
2	AK	60	ILE	2.5
3	AT	3	ARG	2.5
3	BW	288	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	AD	101	ALA	2.5
2	BM	264	LYS	2.5
3	BV	289	PHE	2.5
1	AZ	316	SER	2.5
1	AY	216	LYS	2.5
2	AE	62	ALA	2.5
3	AX	297	PHE	2.5
2	BM	251	THR	2.5
2	AP	90	LEU	2.5
2	AQ	37	THR	2.5
1	B0	137	LEU	2.5
2	BG	103	THR	2.5
2	BD	123	PHE	2.5
2	BR	198	GLN	2.5
2	AO	161	VAL	2.4
2	BK	258	ASN	2.4
3	AW	34	LEU	2.4
1	A0	320	THR	2.4
1	B0	185	PHE	2.4
2	BA	231	PHE	2.4
2	BM	173	GLY	2.4
1	BZ	119	LEU	2.4
2	BD	3	ILE	2.4
3	BT	142	LEU	2.4
2	BG	67	PHE	2.4
2	AC	3	ILE	2.4
3	BT	152	VAL	2.4
2	BL	48	ASN	2.4
1	A0	36	LYS	2.4
2	BL	190	PHE	2.4
1	A0	147	SER	2.4
2	AG	260	SER	2.4
2	BD	179	THR	2.4
2	AF	216	ALA	2.4
2	AB	97	VAL	2.4
2	AL	159	ILE	2.4
2	BJ	60	ILE	2.4
2	BO	74	VAL	2.4
1	AZ	229	THR	2.4
1	AY	161	ALA	2.4
3	BT	157	SER	2.4
2	BA	131	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	BV	30	GLN	2.4
2	AJ	137	LYS	2.4
2	BR	2	THR	2.4
2	AH	261	TYR	2.4
1	BY	359	PHE	2.4
2	BN	27	TYR	2.4
2	AI	221	VAL	2.4
2	BN	208	VAL	2.4
1	AZ	300	HIS	2.4
2	BL	249	ASP	2.4
2	BR	185	LEU	2.4
1	AZ	369	GLY	2.4
2	BJ	30	LEU	2.4
3	AS	31	PRO	2.4
2	BN	184	ASP	2.4
3	AX	141	ASN	2.4
2	AH	215	ALA	2.4
1	AY	215	ARG	2.4
1	B0	356	LYS	2.4
1	BZ	247	PHE	2.4
2	AB	188	VAL	2.4
2	AR	26	LEU	2.4
2	AH	204	SER	2.4
2	BP	88	ILE	2.4
2	AG	176	LEU	2.4
2	AF	139	ILE	2.3
2	BD	126	VAL	2.3
3	BU	200	MET	2.3
2	AQ	209	ASP	2.3
1	AY	328	GLU	2.3
2	BE	27	TYR	2.3
2	BE	159	ILE	2.3
2	BR	123	PHE	2.3
2	AO	257	GLY	2.3
2	BL	3	ILE	2.3
2	BK	29	MET	2.3
1	BY	137	LEU	2.3
2	AG	222	GLY	2.3
2	AP	192	GLY	2.3
3	AX	289	PHE	2.3
2	AJ	223	HIS	2.3
1	BZ	246	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B0	295	TYR	2.3
2	BL	46	PRO	2.3
2	BN	205	GLY	2.3
3	BV	158	LYS	2.3
1	AZ	8	ASP	2.3
3	BX	214	VAL	2.3
2	AL	181	LYS	2.3
2	AO	188	VAL	2.3
2	AI	67	PHE	2.3
1	AZ	202	ASN	2.3
2	BF	185	LEU	2.3
2	BG	219	SER	2.3
3	AW	212	ALA	2.3
2	AN	64	GLY	2.3
1	B0	178	ARG	2.3
2	BN	18	VAL	2.3
2	BP	99	LEU	2.3
1	BZ	141	ASN	2.3
2	AQ	2	THR	2.3
2	BC	187	ILE	2.3
2	AP	169	GLU	2.3
2	AM	219	SER	2.3
2	BN	78	GLY	2.3
3	AV	59	PRO	2.3
1	AY	214	ASN	2.3
2	AG	144	THR	2.3
2	AQ	235	ILE	2.3
2	BR	82	ASN	2.3
2	AR	74	VAL	2.3
3	AX	2	VAL	2.3
1	BZ	352	ALA	2.3
2	AB	62	ALA	2.3
2	AO	162	PRO	2.3
2	BF	168	VAL	2.3
2	AK	61	ILE	2.3
2	AM	64	GLY	2.3
2	BP	169	GLU	2.3
2	BQ	131	THR	2.3
2	BR	70	LEU	2.3
3	BX	297	PHE	2.3
1	AZ	304	PRO	2.3
2	BI	3	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
3	BS	61	ILE	2.3
2	BN	23	ASP	2.3
2	BM	69	LEU	2.2
3	AT	279	MET	2.2
1	BZ	125	ILE	2.2
2	BO	261	TYR	2.2
3	AW	118	TYR	2.2
1	BZ	79	ILE	2.2
1	AY	259	PRO	2.2
2	AB	99	LEU	2.2
2	BB	185	LEU	2.2
3	BS	199	PHE	2.2
1	AZ	142	LYS	2.2
2	AA	235	ILE	2.2
1	B0	188	THR	2.2
3	AS	286	LYS	2.2
2	BF	214	PRO	2.2
2	BQ	176	LEU	2.2
3	BU	178	TYR	2.2
2	BH	249	ASP	2.2
1	BZ	206	ILE	2.2
2	AI	233	ILE	2.2
2	AQ	246	ALA	2.2
1	A0	367	GLU	2.2
1	BZ	148	TYR	2.2
3	AT	118	TYR	2.2
2	BH	23	ASP	2.2
2	BK	23	ASP	2.2
2	BR	125	ILE	2.2
3	AX	76	TYR	2.2
3	BS	228	VAL	2.2
2	AE	38	ILE	2.2
3	AU	227	ILE	2.2
3	BV	200	MET	2.2
2	BR	26	LEU	2.2
2	AI	33	MET	2.2
3	BT	238	ILE	2.2
1	A0	166	LYS	2.2
2	AI	222	GLY	2.2
2	AQ	230	SER	2.2
2	AJ	30	LEU	2.2
1	AZ	158	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	BY	235	ILE	2.2
3	BX	227	ILE	2.2
2	AA	27	TYR	2.2
1	AY	336	ASP	2.2
2	AD	257	GLY	2.2
2	AR	33	MET	2.2
3	BV	272	ARG	2.2
2	AB	255	THR	2.2
2	AI	131	THR	2.2
2	AN	179	THR	2.2
2	AO	261	TYR	2.2
2	BQ	27	TYR	2.2
3	AT	76	TYR	2.2
1	AY	286	ASP	2.2
1	BZ	10	PHE	2.2
2	AB	116	SER	2.2
2	BG	86	ALA	2.2
2	BR	27	TYR	2.2
2	AB	221	VAL	2.2
2	AE	145	LEU	2.2
2	BD	86	ALA	2.2
2	BG	64	GLY	2.2
2	BP	123	PHE	2.2
3	BT	296	ASP	2.2
3	BV	250	GLN	2.2
2	BC	199	LYS	2.2
2	AR	260	SER	2.2
3	BW	212	ALA	2.2
2	AK	79	ASP	2.2
2	AQ	187	ILE	2.2
2	AA	136	THR	2.2
3	BT	298	VAL	2.2
2	BP	210	ARG	2.2
1	AY	133	ILE	2.2
2	AJ	42	ASP	2.2
2	AK	159	ILE	2.2
3	BW	25	LYS	2.2
2	AI	197	ILE	2.2
2	BD	185	LEU	2.2
2	BI	30	LEU	2.2
3	BV	260	LEU	2.2
1	A0	276	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	AQ	93	THR	2.1
2	BH	68	GLU	2.1
3	AV	143	THR	2.1
2	AR	148	ILE	2.1
2	BG	60	ILE	2.1
3	AV	61	ILE	2.1
3	BV	34	LEU	2.1
1	A0	165	ARG	2.1
1	BZ	245	VAL	2.1
2	AM	222	GLY	2.1
1	B0	265	ALA	2.1
1	BY	330	LEU	2.1
2	BE	145	LEU	2.1
2	BG	18	VAL	2.1
1	B0	221	ARG	2.1
2	BQ	209	ASP	2.1
3	BV	48	ILE	2.1
2	BB	262	PHE	2.1
3	AS	62	GLU	2.1
2	BM	81	VAL	2.1
2	AP	175	GLN	2.1
1	B0	247	PHE	2.1
2	BF	65	ARG	2.1
1	BZ	274	TYR	2.1
2	AL	252	PRO	2.1
2	AP	27	TYR	2.1
2	AR	29	MET	2.1
2	BJ	211	PRO	2.1
2	AA	208	VAL	2.1
2	AR	185	LEU	2.1
2	BH	171	GLY	2.1
3	BW	144	PHE	2.1
1	AZ	214	ASN	2.1
3	BV	31	PRO	2.1
2	BN	30	LEU	2.1
2	BK	181	LYS	2.1
3	BT	76	TYR	2.1
1	A0	278	HIS	2.1
3	AW	279	MET	2.1
1	A0	264	ILE	2.1
1	A0	333	TYR	2.1
2	AN	186	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	BA	27	TYR	2.1
3	AU	214	VAL	2.1
3	BT	34	LEU	2.1
2	AF	3	ILE	2.1
2	BR	71	ASN	2.1
2	BG	225	ALA	2.1
2	BP	69	LEU	2.1
2	BC	212	PHE	2.1
2	AD	64	GLY	2.1
3	BW	5	TYR	2.1
3	BW	120	LYS	2.1
2	BM	187	ILE	2.1
2	BL	112	ILE	2.1
2	AE	97	VAL	2.1
2	AG	257	GLY	2.1
2	BM	170	ALA	2.1
3	AS	297	PHE	2.1
2	BH	161	VAL	2.1
2	BR	36	ARG	2.1
2	AQ	232	HIS	2.1
3	AX	12	ASP	2.1
1	AZ	225	LYS	2.1
2	AN	257	GLY	2.1
2	BO	99	LEU	2.1
1	AZ	125	ILE	2.1
2	AJ	125	ILE	2.1
2	BQ	229	THR	2.1
2	AD	185	LEU	2.1
2	BM	218	GLN	2.1
3	AU	142	LEU	2.1
1	A0	208	PHE	2.1
2	AH	257	GLY	2.1
2	BB	31	THR	2.1
2	BM	178	LEU	2.1
2	AB	72	GLU	2.1
2	AB	243	TRP	2.1
2	AK	63	GLY	2.1
1	B0	124	ALA	2.1
2	AM	189	ARG	2.1
1	B0	309	ILE	2.1
1	BY	136	TYR	2.1
2	AN	209	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
3	BS	279	MET	2.1
2	BN	222	GLY	2.1
3	BU	116	GLU	2.1
3	BU	288	GLU	2.1
3	BX	213	GLY	2.1
2	AP	123	PHE	2.0
2	BQ	258	ASN	2.0
1	AY	127	LYS	2.0
1	A0	201	ARG	2.0
2	AJ	69	LEU	2.0
2	AE	155	VAL	2.0
1	AY	136	TYR	2.0
3	AV	141	ASN	2.0
2	BG	53	VAL	2.0
1	AY	130	ASN	2.0
2	AE	88	ILE	2.0
2	AR	228	ASP	2.0
1	A0	331	PRO	2.0
2	BF	188	VAL	2.0
1	A0	329	LEU	2.0
2	AH	264	LYS	2.0
2	BH	220	LEU	2.0
2	AR	256	ARG	2.0
2	BO	256	ARG	2.0
3	AW	141	ASN	2.0
1	BY	216	LYS	2.0
2	BA	190	PHE	2.0
2	BF	190	PHE	2.0
2	BR	57	ASN	2.0
3	AU	288	GLU	2.0
2	BG	184	ASP	2.0
2	AB	90	LEU	2.0
3	BX	258	LEU	2.0
1	AZ	51	TYR	2.0
1	BZ	134	ILE	2.0
3	BV	291	ILE	2.0
2	BM	256	ARG	2.0
3	BV	195	GLU	2.0
2	AA	77	LYS	2.0
2	BR	32	GLY	2.0
3	BS	214	VAL	2.0
1	AY	368	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	BC	159	ILE	2.0
3	AU	202	ILE	2.0
3	AV	281	LEU	2.0
2	AR	137	LYS	2.0
1	A0	6	VAL	2.0
2	BD	188	VAL	2.0
2	BH	97	VAL	2.0
3	AX	199	PHE	2.0
2	AG	99	LEU	2.0
2	BD	187	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CA	BS	301	1/1	0.80	0.34	1.06	267,267,267,267	0
4	CA	AS	301	1/1	0.82	0.33	0.69	281,281,281,281	0
4	CA	AV	301	1/1	0.89	0.36	0.40	276,276,276,276	0
4	CA	AW	301	1/1	0.80	0.29	-0.32	266,266,266,266	0
4	CA	BT	301	1/1	0.85	0.35	-0.40	279,279,279,279	0
4	CA	AX	301	1/1	0.92	0.29	-0.47	275,275,275,275	0
4	CA	BW	301	1/1	0.81	0.26	-0.56	268,268,268,268	0
4	CA	AT	301	1/1	0.94	0.25	-0.58	275,275,275,275	0
4	CA	BV	301	1/1	0.80	0.27	-0.88	272,272,272,272	0
4	CA	BX	301	1/1	0.79	0.26	-1.03	287,287,287,287	0
4	CA	AU	301	1/1	0.88	0.35	-	275,275,275,275	0
4	CA	BU	301	1/1	0.83	0.32	-	269,269,269,269	0

6.5 Other polymers [i](#)

There are no such residues in this entry.