



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:32 PM GMT

PDB ID : 4XWO  
Title : Structure of Get3 bound to the transmembrane domain of Sec22  
Authors : Mateja, A.; Paduch, M.; Chang, H.-Y.; Szydlowska, A.; Kossiakoff, A.A.; Hegde, R.S.; Keenan, R.J.  
Deposited on : 2015-01-29  
Resolution : 2.75 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](mailto: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.

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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 : rb-20026688  
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

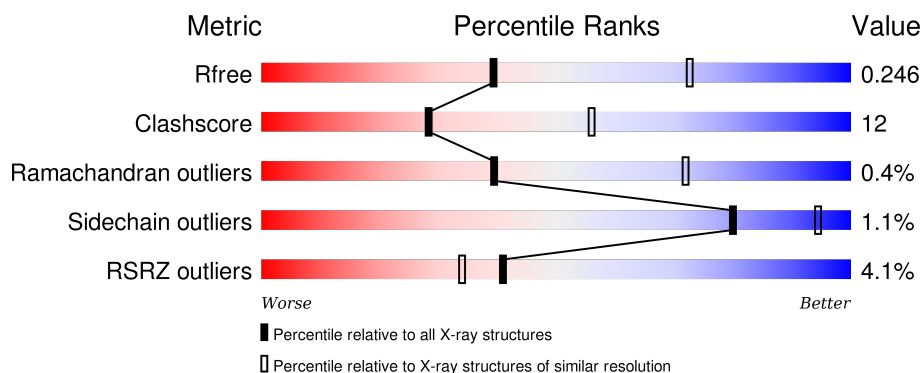
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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  $\geq 3$ , 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	A	354	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>20%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	354	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>22%</div> <div>•</div> <div>16%</div> </div> </div>
1	G	354	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>19%</div> <div>•</div> <div>17%</div> </div> </div>
1	H	354	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>21%</div> <div>•</div> <div>15%</div> </div> </div>
1	M	354	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>21%</div> <div>•</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	N	354	
1	S	354	
1	T	354	
2	C	230	
2	E	230	
2	I	230	
2	K	230	
2	O	230	
2	Q	230	
2	U	230	
2	W	230	
3	D	217	
3	F	217	
3	J	217	
3	L	217	
3	P	217	
3	R	217	
3	V	217	
3	X	217	
4	a	41	
4	g	41	
4	m	41	
4	s	41	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 46697 atoms, of which 184 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 ATPase GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2319	1472	384	446	17			
1	B	297	Total	C	N	O	S	0	0	0
			2336	1483	386	451	16			
1	G	294	Total	C	N	O	S	0	0	0
			2323	1473	386	447	17			
1	H	300	Total	C	N	O	S	0	0	0
			2371	1502	394	459	16			
1	M	304	Total	C	N	O	S	0	0	0
			2405	1521	400	468	16			
1	N	300	Total	C	N	O	S	0	0	0
			2375	1505	393	461	16			
1	S	296	Total	C	N	O	S	0	0	0
			2330	1477	387	450	16			
1	T	306	Total	C	N	O	S	0	0	0
			2402	1523	398	465	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ASN	ASP	engineered mutation	UNP Q12154
B	57	ASN	ASP	engineered mutation	UNP Q12154
G	57	ASN	ASP	engineered mutation	UNP Q12154
H	57	ASN	ASP	engineered mutation	UNP Q12154
M	57	ASN	ASP	engineered mutation	UNP Q12154
N	57	ASN	ASP	engineered mutation	UNP Q12154
S	57	ASN	ASP	engineered mutation	UNP Q12154
T	57	ASN	ASP	engineered mutation	UNP Q12154

- Molecule 2 is a protein called Antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	218	Total	C	N	O	S	0	0	0
			1641	1038	278	319	6			
2	E	222	Total	C	N	O	S	0	0	0
			1664	1050	282	326	6			
2	I	220	Total	C	N	O	S	0	0	0
			1655	1046	279	324	6			
2	K	216	Total	C	N	O	S	0	0	0
			1628	1031	276	315	6			
2	O	218	Total	C	N	O	S	0	0	0
			1635	1034	277	318	6			
2	Q	221	Total	C	N	O	S	0	0	0
			1655	1045	281	323	6			
2	U	214	Total	C	N	O	S	0	0	0
			1616	1024	273	313	6			
2	W	221	Total	C	N	O	S	0	0	0
			1655	1045	281	323	6			

- Molecule 3 is a protein called Antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	216	Total	C	N	O	S	0	0	0
			1658	1038	276	338	6			
3	F	215	Total	C	N	O	S	0	0	0
			1650	1034	275	335	6			
3	J	215	Total	C	N	O	S	0	0	0
			1650	1034	275	335	6			
3	L	215	Total	C	N	O	S	0	0	0
			1650	1034	275	335	6			
3	P	216	Total	C	N	O	S	0	0	0
			1658	1038	276	338	6			
3	R	216	Total	C	N	O	S	0	0	0
			1658	1038	276	338	6			
3	V	215	Total	C	N	O	S	0	0	0
			1650	1034	275	335	6			
3	X	216	Total	C	N	O	S	0	0	0
			1658	1038	276	338	6			

- Molecule 4 is a protein called Sec22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	a	20	Total	C	N	O	0	0	0
			100	60	20	20			
4	g	14	Total	C	N	O	0	0	0
			70	42	14	14			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	m	19	Total	C	N	O	0	0	0
			95	57	19	19			
4	s	21	Total	C	N	O	0	0	0
			105	63	21	21			

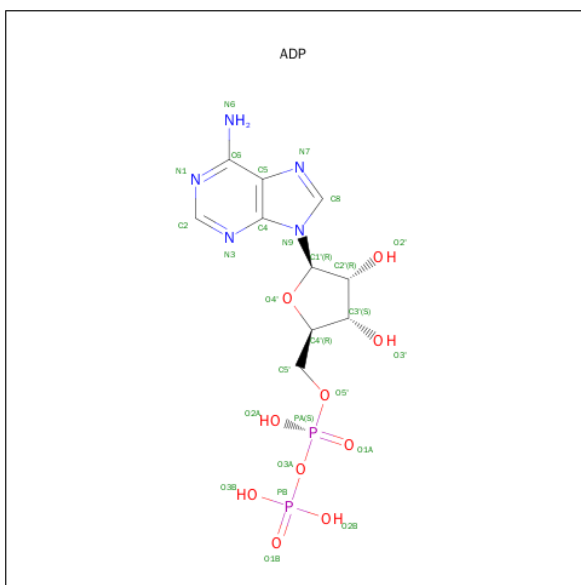
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	T	1	Total	Mg	0	0
			1	1		
5	N	1	Total	Mg	0	0
			1	1		
5	S	1	Total	Mg	0	0
			1	1		
5	M	1	Total	Mg	0	0
			1	1		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

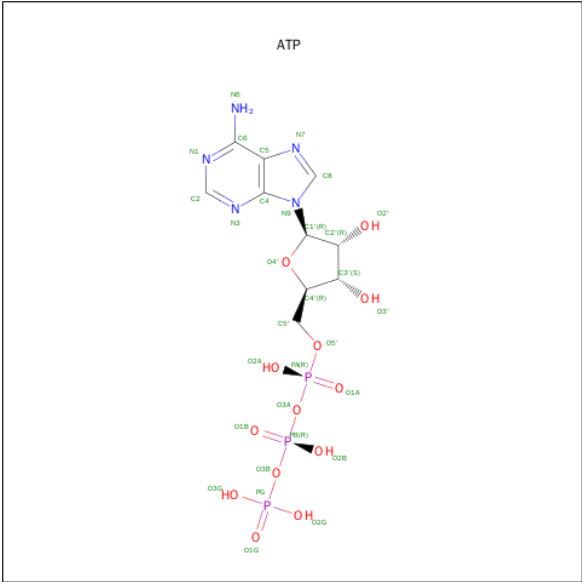
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Zn	0	0
			1	1		
6	A	1	Total	Zn	0	0
			1	1		
6	S	1	Total	Zn	0	0
			1	1		
6	M	1	Total	Zn	0	0
			1	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	1
7	B	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	1
7	G	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	1
7	H	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	1
7	M	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	1
7	N	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	1
7	S	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	1
7	T	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	1

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	P	0	1
			42	10	11	5	13	3		
8	B	1	Total	C	H	N	O	P	0	1
			43	10	12	5	13	3		
8	G	1	Total	C	H	N	O	P	0	1
			42	10	11	5	13	3		
8	H	1	Total	C	H	N	O	P	0	1
			43	10	12	5	13	3		
8	M	1	Total	C	H	N	O	P	0	1
			42	10	11	5	13	3		
8	N	1	Total	C	H	N	O	P	0	1
			43	10	12	5	13	3		
8	S	1	Total	C	H	N	O	P	0	1
			42	10	11	5	13	3		
8	T	1	Total	C	H	N	O	P	0	1
			43	10	12	5	13	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	20	Total	O	0	0
			20	20		
9	B	17	Total	O	0	0
			17	17		
9	C	16	Total	O	0	0
			16	16		
9	D	19	Total	O	0	0
			19	19		

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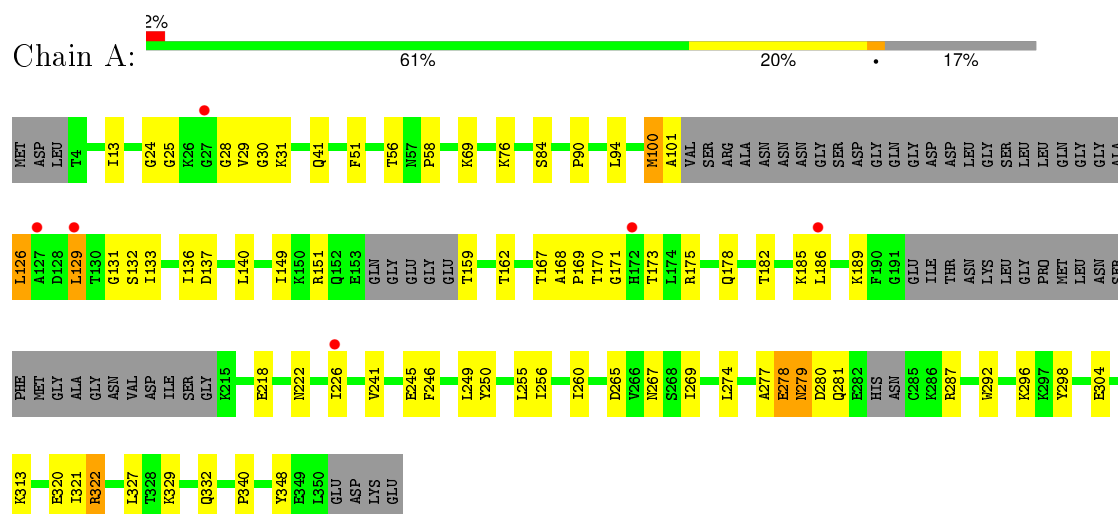
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	14	Total 14	O 14	0	0
9	F	23	Total 23	O 23	0	0
9	G	20	Total 20	O 20	0	0
9	H	25	Total 25	O 25	0	0
9	I	25	Total 25	O 25	0	0
9	J	34	Total 34	O 34	0	0
9	K	15	Total 15	O 15	0	0
9	L	19	Total 19	O 19	0	0
9	M	20	Total 20	O 20	0	0
9	N	29	Total 29	O 29	0	0
9	O	12	Total 12	O 12	0	0
9	P	15	Total 15	O 15	0	0
9	Q	13	Total 13	O 13	0	0
9	R	9	Total 9	O 9	0	0
9	S	16	Total 16	O 16	0	0
9	T	22	Total 22	O 22	0	0
9	U	8	Total 8	O 8	0	0
9	V	9	Total 9	O 9	0	0
9	W	16	Total 16	O 16	0	0
9	X	9	Total 9	O 9	0	0

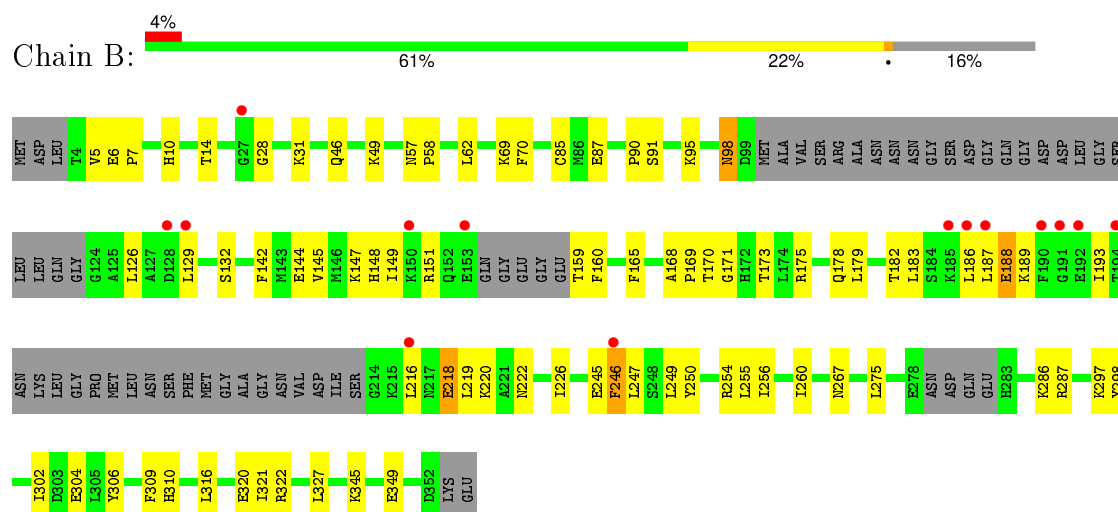
### 3 Residue-property plots [i](#)

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.

#### • Molecule 1: ATPase GET3

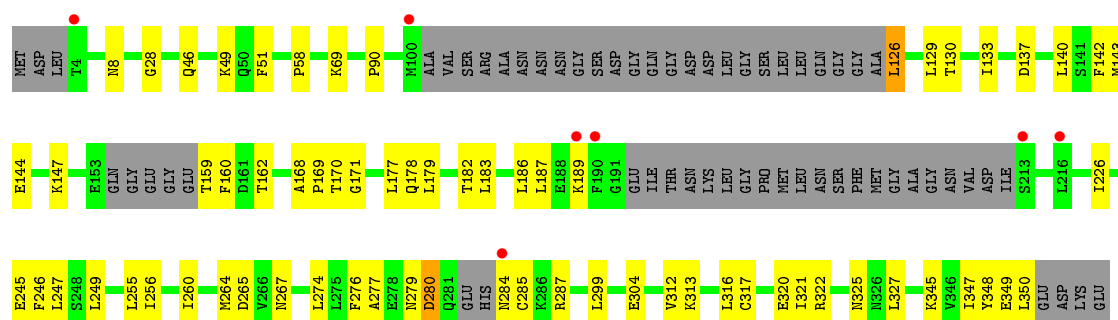


#### • Molecule 1: ATPase GET3

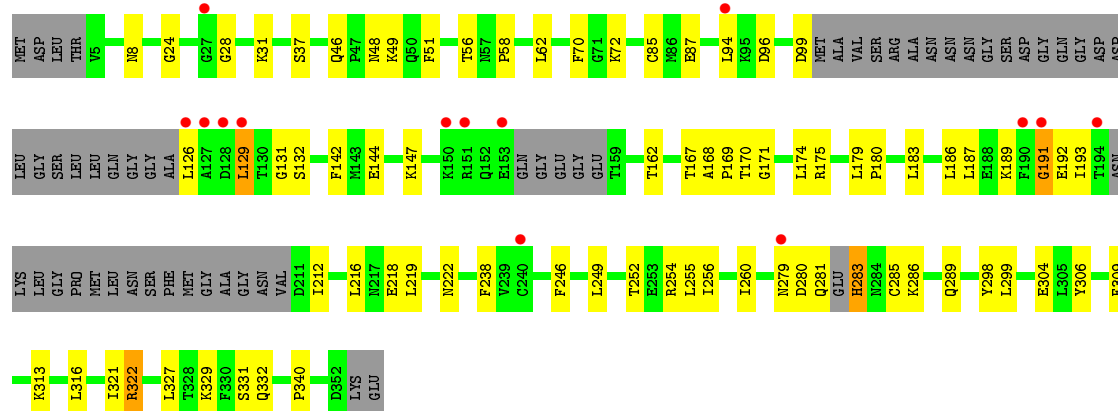


#### • Molecule 1: ATPase GET3

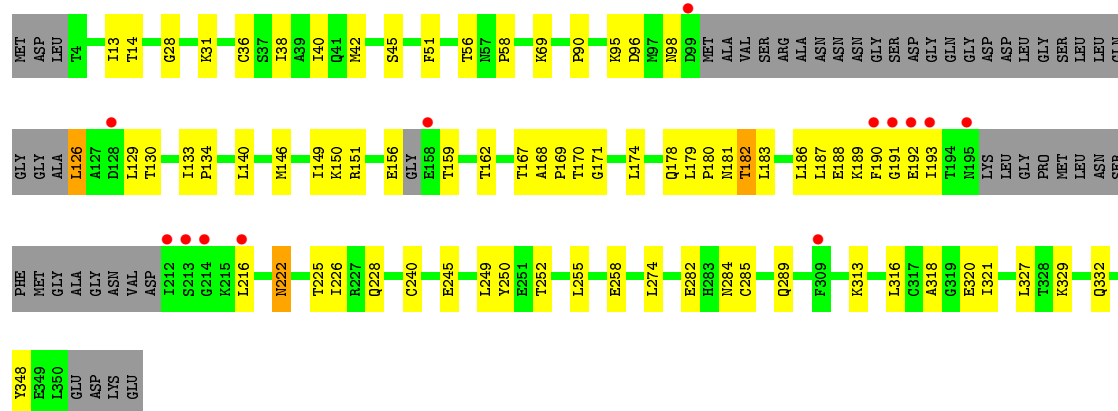




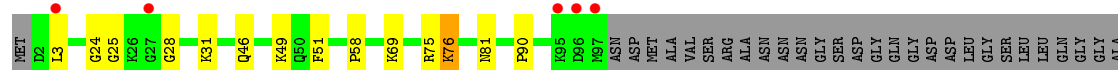
• Molecule 1: ATPase GET3

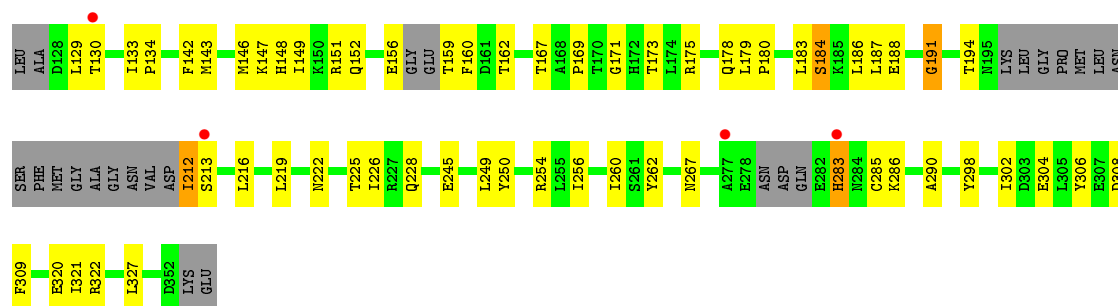


• Molecule 1: ATPase GET3

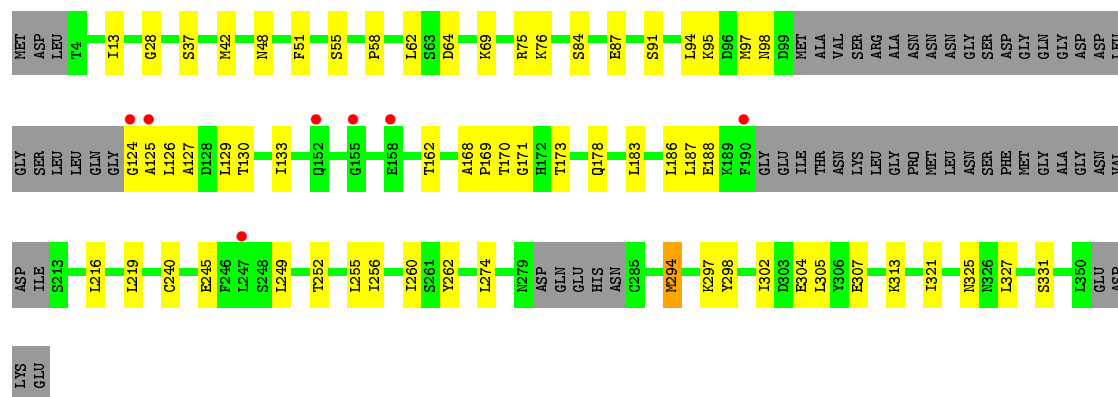


• Molecule 1: ATPase GET3

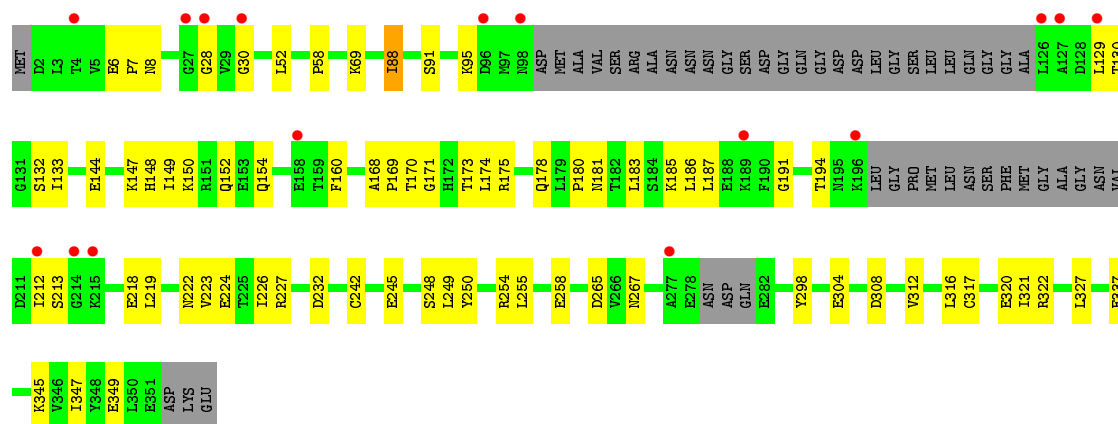




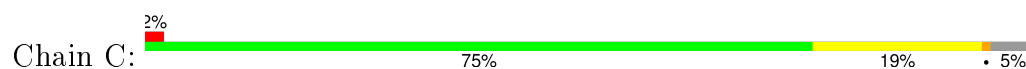
• Molecule 1: ATPase GET3

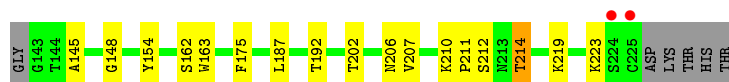


• Molecule 1: ATPase GET3

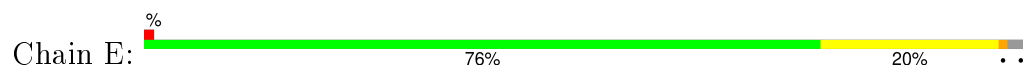


• Molecule 2: Antibody heavy chain

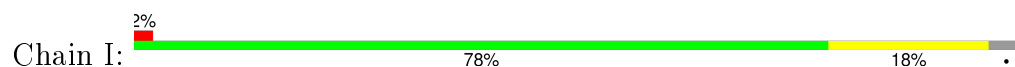




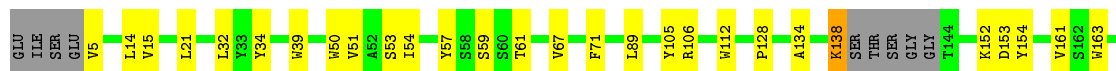
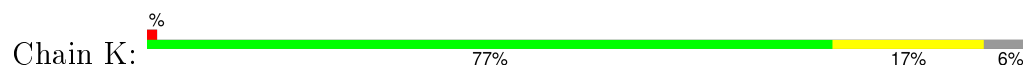
- Molecule 2: Antibody heavy chain



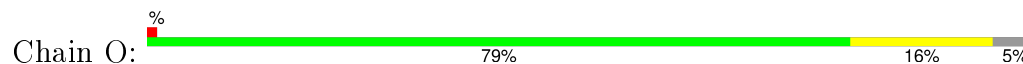
- Molecule 2: Antibody heavy chain



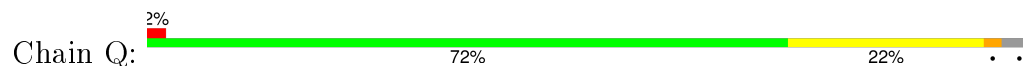
- Molecule 2: Antibody heavy chain

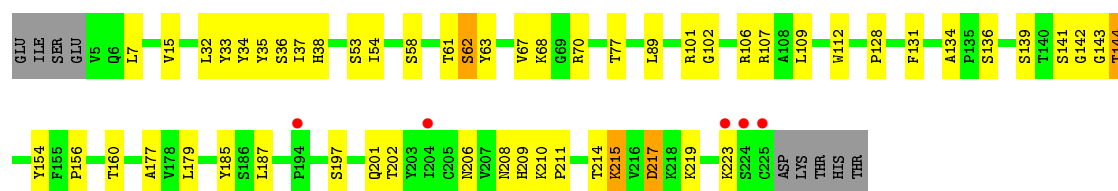


- Molecule 2: Antibody heavy chain

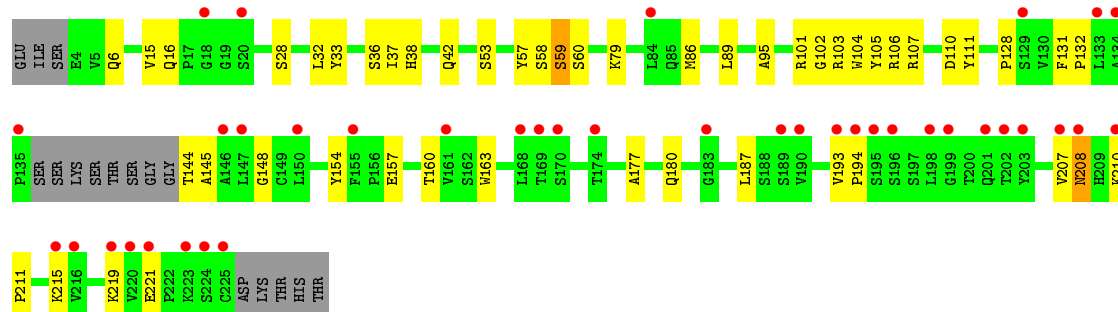


- Molecule 2: Antibody heavy chain

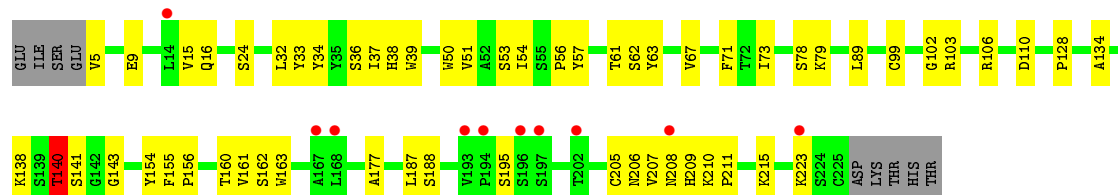




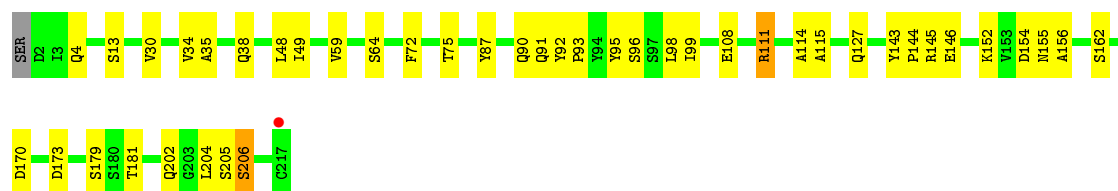
• Molecule 2: Antibody heavy chain



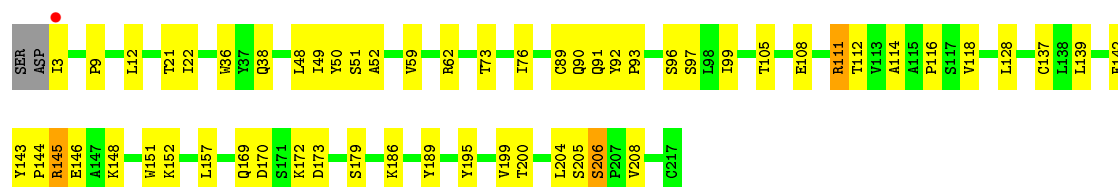
• Molecule 2: Antibody heavy chain



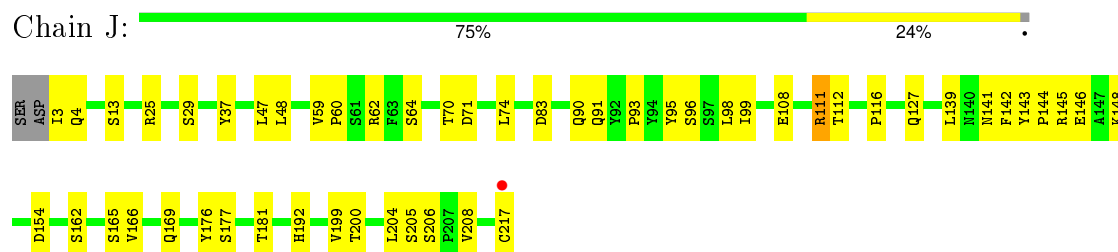
• Molecule 3: Antibody light chain



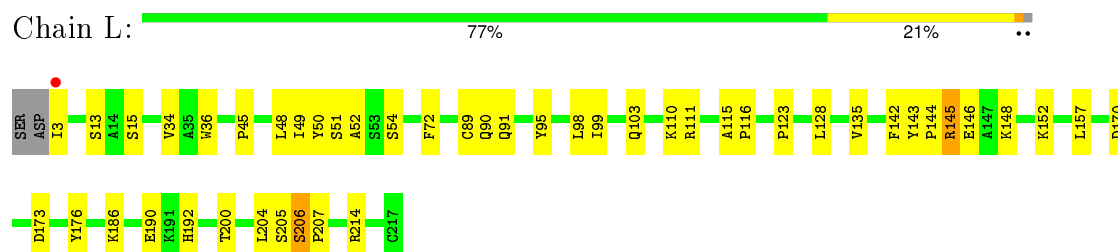
• Molecule 3: Antibody light chain



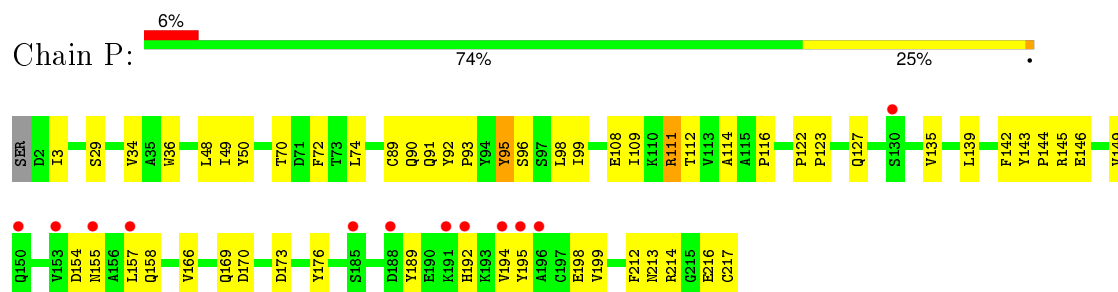
- Molecule 3: Antibody light chain



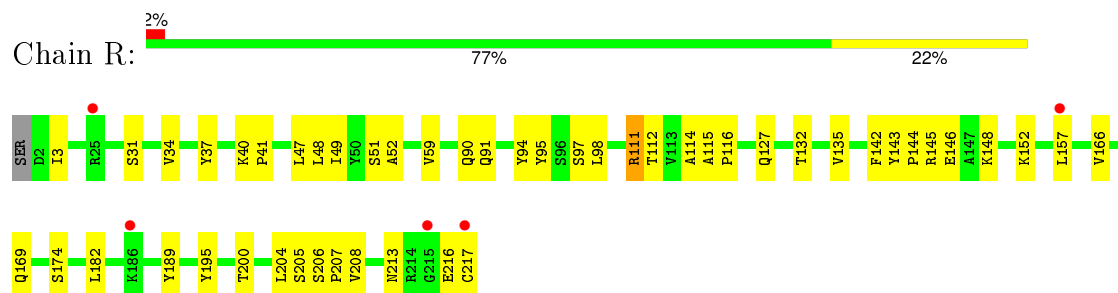
- Molecule 3: Antibody light chain



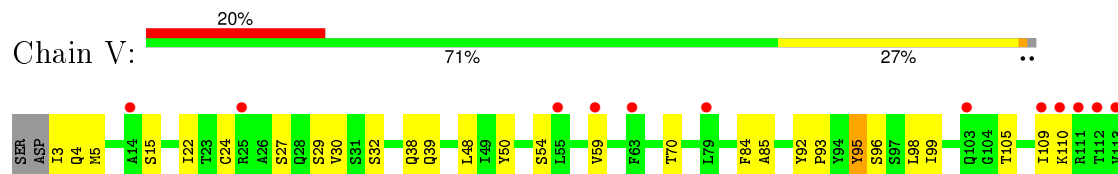
- Molecule 3: Antibody light chain



- Molecule 3: Antibody light chain



- Molecule 3: Antibody light chain







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.58Å 119.45Å 147.57Å 71.89° 89.86° 66.61°	Depositor
Resolution (Å)	39.72 – 2.75 39.72 – 2.75	Depositor EDS
% Data completeness (in resolution range)	90.6 (39.72-2.75) 74.7 (39.72-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 2.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.196 , 0.247 0.196 , 0.246	Depositor DCC
$R_{free}$ test set	7268 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.5	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 156379 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	46697	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.80 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.9625e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: ATP, MG, ZN, ADP

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	A	0.25	0/2356	0.43	0/3175
1	B	0.27	0/2373	0.45	0/3199
1	G	0.27	0/2360	0.44	0/3180
1	H	0.27	0/2409	0.45	0/3247
1	M	0.28	0/2444	0.47	0/3296
1	N	0.28	0/2413	0.46	0/3252
1	S	0.25	0/2368	0.43	0/3192
1	T	0.25	0/2440	0.44	0/3289
2	C	0.28	0/1682	0.47	0/2292
2	E	0.27	0/1706	0.47	0/2326
2	I	0.29	0/1696	0.48	0/2312
2	K	0.26	0/1669	0.46	0/2275
2	O	0.26	0/1676	0.44	0/2285
2	Q	0.26	0/1697	0.48	0/2314
2	U	0.23	0/1657	0.42	0/2260
2	W	0.25	0/1697	0.47	0/2314
3	D	0.27	0/1694	0.47	0/2299
3	F	0.28	0/1686	0.46	0/2288
3	J	0.29	0/1686	0.47	0/2288
3	L	0.26	0/1686	0.46	0/2288
3	P	0.25	0/1694	0.44	0/2299
3	R	0.26	0/1694	0.44	0/2299
3	V	0.23	0/1686	0.41	0/2288
3	X	0.25	0/1694	0.45	0/2299
All	All	0.26	0/46163	0.45	0/62556

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	A	2319	0	2316	77	0
1	B	2336	0	2325	92	0
1	G	2323	0	2319	65	0
1	H	2371	0	2354	66	1
1	M	2405	0	2388	60	1
1	N	2375	0	2362	64	0
1	S	2330	0	2324	65	1
1	T	2402	0	2390	61	0
2	C	1641	0	1604	31	0
2	E	1664	0	1625	38	0
2	I	1655	0	1616	30	0
2	K	1628	0	1595	32	0
2	O	1635	0	1591	33	0
2	Q	1655	0	1619	58	1
2	U	1616	0	1579	40	0
2	W	1655	0	1619	53	2
3	D	1658	0	1611	31	0
3	F	1650	0	1607	44	0
3	J	1650	0	1607	36	0
3	L	1650	0	1607	40	0
3	P	1658	0	1611	46	0
3	R	1658	0	1611	35	0
3	V	1650	0	1608	44	0
3	X	1658	0	1611	39	0
4	a	100	0	22	0	0
4	g	70	0	16	0	0
4	m	95	0	21	0	0
4	s	105	0	23	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	S	1	0	0	0	0
5	T	1	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	1	0	0	0	0
6	M	1	0	0	0	0
6	S	1	0	0	0	0
7	A	27	11	12	0	0
7	B	27	12	12	1	0
7	G	27	11	12	0	0
7	H	27	12	12	1	0
7	M	27	11	9	0	0
7	N	27	12	12	0	0
7	S	27	11	11	0	0
7	T	27	12	12	1	0
8	A	31	11	12	2	0
8	B	31	12	12	2	0
8	G	31	11	12	1	0
8	H	31	12	12	2	0
8	M	31	11	10	1	0
8	N	31	12	12	0	0
8	S	31	11	11	0	0
8	T	31	12	12	2	0
9	A	20	0	0	2	0
9	B	17	0	0	0	0
9	C	16	0	0	0	0
9	D	19	0	0	1	0
9	E	14	0	0	3	0
9	F	23	0	0	1	0
9	G	20	0	0	6	0
9	H	25	0	0	1	0
9	I	25	0	0	2	0
9	J	34	0	0	2	0
9	K	15	0	0	2	0
9	L	19	0	0	1	0
9	M	20	0	0	1	0
9	N	29	0	0	1	0
9	O	12	0	0	0	0
9	P	15	0	0	0	0
9	Q	13	0	0	4	0
9	R	9	0	0	0	0
9	S	16	0	0	3	0
9	T	22	0	0	2	0
9	U	8	0	0	2	0
9	V	9	0	0	1	0
9	W	16	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	X	9	0	0	2	0
All	All	46513	184	44766	1043	3

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 12.

All (1043) 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:F:145:ARG:HG2	3:F:145:ARG:HH11	1.20	1.05
2:Q:209:HIS:H	2:Q:215:LYS:HZ1	1.07	1.02
1:G:137:ASP:OD2	1:H:175:ARG:NH1	1.97	0.98
1:N:69:LYS:O	1:N:75:ARG:NH1	1.94	0.98
3:L:145:ARG:HG2	3:L:145:ARG:HH11	1.31	0.94
1:S:129:LEU:HD13	1:T:186:LEU:HD21	1.46	0.94
1:H:31:LYS:NZ	8:H:403[A]:ATP:O1B	2.03	0.92
3:X:123:PRO:HD3	3:X:135:VAL:HG22	1.52	0.92
3:F:204:LEU:HD13	3:F:208:VAL:HG23	1.50	0.91
1:A:149:ILE:HD12	1:A:226:ILE:HG12	1.50	0.91
1:N:149:ILE:HD12	1:N:226:ILE:HG12	1.51	0.90
2:W:140:THR:HG22	2:W:141:SER:HA	1.54	0.89
3:L:152:LYS:HG2	3:L:157:LEU:HD23	1.54	0.89
3:F:111:ARG:HH22	3:F:114:ALA:HB2	1.37	0.88
2:Q:208:ASN:HA	2:Q:215:LYS:NZ	1.88	0.88
2:W:134:ALA:HB3	2:W:223:LYS:NZ	1.88	0.88
2:W:140:THR:CB	2:W:141:SER:HA	2.03	0.88
1:B:149:ILE:HD12	1:B:226:ILE:HG12	1.55	0.88
1:G:170:THR:HG23	1:G:255:LEU:HD13	1.55	0.88
3:L:145:ARG:CG	3:L:145:ARG:HH11	1.87	0.87
1:B:31:LYS:NZ	8:B:403[A]:ATP:O1B	2.08	0.87
3:R:111:ARG:HH22	3:R:114:ALA:HB2	1.40	0.87
2:Q:143:GLY:O	2:Q:144:THR:HG23	1.75	0.86
2:U:128:PRO:HB3	2:U:154:TYR:HB3	1.55	0.86
2:W:140:THR:CG2	2:W:141:SER:HA	2.07	0.84
2:E:32:LEU:HD11	2:E:37:ILE:HG13	1.59	0.84
1:A:151:ARG:HG2	1:A:159:THR:HG22	1.58	0.84
3:R:135:VAL:HG13	3:R:182:LEU:HB3	1.59	0.84
2:W:5:VAL:N	9:W:302:HOH:O	2.11	0.83
1:M:169:PRO:HG2	1:N:169:PRO:HG2	1.60	0.83
2:I:32:LEU:HD11	2:I:37:ILE:HG13	1.60	0.83
1:H:170:THR:HG23	1:H:255:LEU:HD13	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:111:ARG:HH21	3:X:114:ALA:HB2	1.45	0.82
1:H:191:GLY:HA2	1:H:216:LEU:HD21	1.60	0.82
2:Q:214:THR:O	2:Q:215:LYS:NZ	2.12	0.81
3:L:152:LYS:HE2	3:L:157:LEU:HD21	1.59	0.81
2:Q:141:SER:O	2:Q:143:GLY:N	2.11	0.81
1:S:169:PRO:HG2	1:T:169:PRO:HG2	1.63	0.81
1:M:149:ILE:HD12	1:M:226:ILE:HG12	1.63	0.81
1:A:169:PRO:HG2	1:B:169:PRO:HG2	1.61	0.80
2:Q:62:SER:HB3	3:R:97:SER:HB3	1.63	0.79
3:V:192:HIS:O	3:V:214:ARG:NH1	2.15	0.79
2:Q:209:HIS:N	2:Q:215:LYS:HZ1	1.79	0.79
1:B:144:GLU:OE2	1:B:147:LYS:HE2	1.82	0.79
1:A:137:ASP:OD2	1:B:175:ARG:NH1	2.16	0.79
3:X:145:ARG:NH1	9:X:306:HOH:O	2.16	0.78
1:N:159:THR:HG23	1:N:160:PHE:H	1.48	0.78
1:T:7:PRO:HG2	1:T:337:GLU:HG2	1.64	0.78
1:T:69:LYS:NZ	2:U:59:SER:OG	2.14	0.76
1:S:129:LEU:HD12	1:S:130:THR:N	2.01	0.76
1:A:321:ILE:HG22	1:A:327:LEU:HD23	1.67	0.76
1:A:218:GLU:O	1:A:222:ASN:ND2	2.19	0.76
1:S:321:ILE:HG22	1:S:327:LEU:HD23	1.67	0.76
1:S:126:LEU:H	1:S:126:LEU:HD23	1.51	0.75
2:O:70:ARG:NH1	2:O:93:ASP:OD2	2.19	0.75
1:G:169:PRO:HG3	1:H:169:PRO:HG2	1.68	0.75
2:W:128:PRO:HB3	2:W:154:TYR:HB3	1.67	0.75
2:U:58:SER:O	2:U:60:SER:N	2.19	0.74
3:F:145:ARG:CG	3:F:145:ARG:HH11	1.99	0.74
1:B:142:PHE:HB2	1:B:179:LEU:HD23	1.70	0.74
1:N:129:LEU:HD12	1:N:130:THR:N	2.03	0.74
1:A:320:GLU:OE1	1:A:322:ARG:NH1	2.21	0.74
1:A:151:ARG:HG2	1:A:159:THR:CG2	2.18	0.73
1:G:246:PHE:CZ	1:G:247:LEU:HG	2.21	0.73
3:R:145:ARG:HH21	3:R:166:VAL:HG11	1.52	0.73
2:O:208:ASN:HB3	2:O:215:LYS:NZ	2.04	0.73
1:S:129:LEU:HD13	1:T:186:LEU:CD2	2.17	0.73
1:H:187:LEU:HD21	1:H:219:LEU:HD23	1.71	0.73
1:A:129:LEU:HD21	1:B:186:LEU:HD23	1.71	0.73
1:S:187:LEU:HD21	1:S:219:LEU:HD12	1.70	0.73
1:M:284:ASN:OD1	1:N:283:HIS:ND1	2.22	0.73
1:M:187:LEU:HD11	1:M:216:LEU:HD11	1.71	0.72
1:S:124:GLY:O	1:S:127:ALA:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:129:LEU:HD12	1:T:130:THR:N	2.04	0.72
3:P:3:ILE:HG21	3:P:91:GLN:OE1	1.87	0.72
1:B:147:LYS:HE3	1:B:151:ARG:NH2	2.04	0.72
3:P:123:PRO:HD3	3:P:135:VAL:HG22	1.71	0.72
2:Q:208:ASN:HA	2:Q:215:LYS:CE	2.19	0.71
1:H:72:LYS:HE3	1:H:96:ASP:OD2	1.90	0.71
2:Q:136:SER:HB3	2:Q:139:SER:HB3	1.70	0.71
2:K:134:ALA:HB3	2:K:223:LYS:NZ	2.05	0.71
2:Q:202:THR:HG23	2:Q:219:LYS:HD2	1.71	0.71
1:T:187:LEU:HD21	1:T:219:LEU:HD23	1.72	0.71
3:R:135:VAL:CG1	3:R:182:LEU:HB3	2.19	0.71
1:H:280:ASP:OD2	1:H:281:GLN:N	2.24	0.71
2:O:134:ALA:HB3	2:O:223:LYS:NZ	2.06	0.70
1:T:149:ILE:HD12	1:T:226:ILE:HG12	1.73	0.70
2:C:36:SER:O	2:C:102:GLY:HA3	1.92	0.70
1:T:144:GLU:OE2	1:T:147:LYS:HE2	1.91	0.70
3:P:116:PRO:HB3	3:P:142:PHE:HB3	1.74	0.70
1:A:69:LYS:NZ	2:E:59:SER:OG	2.18	0.69
1:S:187:LEU:CD2	1:S:219:LEU:HD12	2.23	0.69
1:T:170:THR:HG23	1:T:255:LEU:HD13	1.74	0.69
3:F:204:LEU:HD13	3:F:208:VAL:CG2	2.22	0.69
2:O:208:ASN:HB3	2:O:215:LYS:HZ2	1.58	0.69
1:N:191:GLY:HA2	1:N:216:LEU:CD2	2.22	0.69
3:V:164:GLU:OE2	3:V:178:LEU:HD11	1.92	0.69
2:Q:62:SER:CB	3:R:97:SER:HB3	2.23	0.69
1:T:154:GLN:OE1	9:T:501:HOH:O	2.10	0.69
1:B:149:ILE:CD1	1:B:226:ILE:HG12	2.22	0.69
1:G:144:GLU:OE2	1:G:147:LYS:HE2	1.93	0.68
3:R:204:LEU:HD13	3:R:208:VAL:HG23	1.76	0.68
1:B:320:GLU:OE1	1:B:322:ARG:NH1	2.26	0.68
3:J:145:ARG:HH11	3:J:166:VAL:HG11	1.58	0.68
2:W:140:THR:HB	2:W:141:SER:HA	1.75	0.68
2:K:128:PRO:HB3	2:K:154:TYR:HB3	1.75	0.68
3:V:109:ILE:HG22	3:V:169:GLN:NE2	2.07	0.68
1:G:304:GLU:OE1	2:I:106:ARG:HD3	1.94	0.68
3:V:15:SER:HB2	3:V:110:LYS:HE2	1.74	0.68
1:G:183:LEU:O	1:G:187:LEU:HD13	1.94	0.67
3:P:213:ASN:HB2	3:P:216:GLU:CD	2.14	0.67
1:B:95:LYS:O	1:B:98:ASN:ND2	2.26	0.67
3:X:108:GLU:HB2	3:X:169:GLN:OE1	1.94	0.67
1:G:321:ILE:CG2	1:G:327:LEU:HD23	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:321:ILE:HG22	1:H:327:LEU:HD23	1.76	0.67
2:K:50:TRP:HE1	2:K:53:SER:HG	1.43	0.67
3:V:146:GLU:OE1	3:V:146:GLU:N	2.28	0.67
1:N:178:GLN:NE2	1:N:262:TYR:OH	2.24	0.66
1:T:224:GLU:OE2	1:T:227:ARG:NH2	2.28	0.66
1:S:178:GLN:HE21	1:T:132:SER:HB3	1.60	0.66
3:X:146:GLU:OE1	3:X:146:GLU:N	2.26	0.66
3:X:145:ARG:NH2	3:X:166:VAL:HG11	2.10	0.66
1:A:321:ILE:CG2	1:A:327:LEU:HD23	2.25	0.66
2:W:134:ALA:HB3	2:W:223:LYS:HZ2	1.58	0.66
1:H:189:LYS:O	1:H:192:GLU:HG2	1.95	0.66
3:P:145:ARG:HH21	3:P:166:VAL:HG11	1.61	0.66
3:P:93:PRO:HG2	3:P:96:SER:OG	1.96	0.66
1:G:321:ILE:HG22	1:G:327:LEU:HD23	1.77	0.65
1:N:187:LEU:HD21	1:N:219:LEU:HD23	1.77	0.65
3:L:170:ASP:HB3	3:L:173:ASP:OD2	1.96	0.65
1:T:148:HIS:O	1:T:152:GLN:HG3	1.97	0.65
1:M:150:LYS:HE3	1:M:222:ASN:OD1	1.97	0.65
1:G:28:GLY:HA3	1:H:28:GLY:HA3	1.79	0.65
2:Q:128:PRO:HB3	2:Q:154:TYR:HB3	1.77	0.65
2:U:103:ARG:NH1	2:U:110:ASP:OD2	2.28	0.65
1:H:281:GLN:HG2	1:H:283:HIS:CD2	2.32	0.65
2:U:160:THR:OG1	9:U:305:HOH:O	2.14	0.65
1:A:90:PRO:HG2	1:B:175:ARG:HH22	1.62	0.65
3:V:109:ILE:HG22	3:V:169:GLN:HE22	1.62	0.65
3:X:111:ARG:NH2	3:X:114:ALA:HB2	2.12	0.64
1:A:149:ILE:CD1	1:A:226:ILE:HG12	2.24	0.64
1:N:191:GLY:HA2	1:N:216:LEU:HD21	1.79	0.64
3:X:158:GLN:OE1	3:X:161:ASN:ND2	2.30	0.64
1:G:129:LEU:HD13	1:H:186:LEU:HD21	1.79	0.64
3:L:146:GLU:OE1	3:L:146:GLU:N	2.30	0.64
2:Q:134:ALA:HB3	2:Q:223:LYS:NZ	2.13	0.64
2:W:50:TRP:HE1	2:W:53:SER:HG	1.45	0.64
3:P:111:ARG:HG3	3:P:112:THR:N	2.11	0.64
1:B:187:LEU:HD11	1:B:216:LEU:HG	1.81	0.63
2:W:36:SER:O	2:W:102:GLY:HA3	1.98	0.63
1:S:75:ARG:NH2	2:W:78:SER:HB3	2.13	0.63
3:P:108:GLU:HB2	3:P:169:GLN:OE1	1.98	0.63
2:I:36:SER:O	2:I:102:GLY:HA3	1.99	0.63
1:S:133:ILE:HD11	1:T:186:LEU:HD11	1.79	0.63
3:X:3:ILE:HG21	3:X:91:GLN:OE1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:111:ARG:HH21	3:X:114:ALA:CB	2.11	0.63
3:L:157:LEU:HD12	1:S:325:ASN:OD1	1.98	0.63
2:I:128:PRO:HB3	2:I:154:TYR:HB3	1.81	0.63
1:S:171:GLY:HA3	1:T:58:PRO:HB2	1.80	0.63
3:V:29:SER:HA	3:V:70:THR:HG22	1.80	0.63
1:N:149:ILE:CD1	1:N:226:ILE:HG12	2.25	0.63
1:B:218:GLU:O	1:B:222:ASN:ND2	2.31	0.63
2:E:54:ILE:HG13	2:E:61:THR:HG22	1.81	0.63
3:L:192:HIS:O	3:L:214:ARG:NH1	2.31	0.62
1:A:279:ASN:OD1	1:A:340:PRO:HB2	2.00	0.62
2:W:33:TYR:HA	2:W:56:PRO:HB2	1.80	0.62
1:T:249:LEU:HD11	1:T:298:TYR:CG	2.34	0.62
2:Q:38:HIS:HD2	9:Q:313:HOH:O	1.82	0.62
2:U:36:SER:O	2:U:102:GLY:HA3	1.99	0.62
2:O:32:LEU:HD11	2:O:37:ILE:HG12	1.80	0.62
2:Q:210:LYS:N	2:Q:211:PRO:HD2	2.14	0.62
2:K:106:ARG:NH1	3:L:50:TYR:CD2	2.68	0.62
1:A:28:GLY:HA3	1:B:28:GLY:HA3	1.81	0.62
3:J:4:GLN:NE2	9:J:301:HOH:O	2.32	0.62
3:R:127:GLN:HE21	3:R:132:THR:HG23	1.64	0.62
1:H:321:ILE:CG2	1:H:327:LEU:HD23	2.29	0.62
1:N:308:ASP:OD2	3:R:31:SER:OG	2.18	0.62
1:B:245:GLU:O	1:B:249:LEU:HG	1.99	0.62
3:J:146:GLU:OE1	3:J:146:GLU:N	2.31	0.62
1:M:187:LEU:HD11	1:M:216:LEU:CD1	2.28	0.62
1:H:218:GLU:O	1:H:222:ASN:ND2	2.30	0.62
3:F:145:ARG:HG2	3:F:145:ARG:NH1	2.00	0.61
2:Q:208:ASN:HA	2:Q:215:LYS:HZ1	1.63	0.61
1:B:187:LEU:CD2	1:B:220:LYS:HA	2.30	0.61
3:P:146:GLU:N	3:P:146:GLU:OE1	2.32	0.61
1:N:129:LEU:HD12	1:N:130:THR:H	1.66	0.61
1:T:227:ARG:HH11	1:T:227:ARG:HG2	1.63	0.61
1:S:313:LYS:O	9:S:501:HOH:O	2.16	0.61
2:E:160:THR:N	9:E:302:HOH:O	2.22	0.61
2:I:103:ARG:CZ	2:I:106:ARG:HH11	2.14	0.61
3:F:111:ARG:HG3	3:F:112:THR:N	2.15	0.61
2:O:4:GLU:N	2:O:4:GLU:OE1	2.34	0.61
2:I:58:SER:O	2:I:60:SER:N	2.34	0.61
3:V:123:PRO:HD3	3:V:135:VAL:HG22	1.83	0.61
3:V:38:GLN:HB2	3:V:48:LEU:HD11	1.83	0.61
1:G:140:LEU:HD23	1:G:143:MET:SD	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:134:ALA:HB3	2:W:223:LYS:HZ1	1.64	0.60
1:M:149:ILE:CD1	1:M:226:ILE:HG12	2.30	0.60
1:A:178:GLN:HE21	1:B:132:SER:HB3	1.66	0.60
3:L:152:LYS:HG2	3:L:157:LEU:CD2	2.31	0.60
2:U:208:ASN:HB3	2:U:215:LYS:NZ	2.17	0.60
3:V:93:PRO:HG2	3:V:96:SER:OG	2.01	0.60
1:S:75:ARG:HH22	2:W:78:SER:HB3	1.66	0.60
1:T:218:GLU:O	1:T:222:ASN:ND2	2.27	0.60
2:E:32:LEU:HD11	2:E:37:ILE:CG1	2.31	0.60
1:N:146:MET:HG2	1:N:222:ASN:ND2	2.17	0.60
1:H:279:ASN:ND2	1:H:340:PRO:O	2.35	0.60
1:G:129:LEU:CD1	1:H:186:LEU:HD21	2.32	0.60
1:G:348:TYR:CE1	1:H:286:LYS:HG2	2.37	0.60
1:A:186:LEU:HD22	1:B:129:LEU:HD21	1.83	0.60
1:M:51:PHE:CD1	1:M:162:THR:HB	2.37	0.59
3:L:3:ILE:HG21	3:L:91:GLN:OE1	2.02	0.59
3:D:146:GLU:OE1	3:D:146:GLU:N	2.35	0.59
2:Q:15:VAL:HG21	2:Q:89:LEU:HD13	1.84	0.59
2:U:101:ARG:NH1	2:U:111:TYR:CD2	2.71	0.59
1:H:254:ARG:NH1	2:K:57:TYR:O	2.34	0.59
1:T:175:ARG:NH1	1:T:178:GLN:OE1	2.35	0.59
3:F:137:CYS:HB2	3:F:151:TRP:CH2	2.37	0.59
2:W:50:TRP:NE1	2:W:53:SER:OG	2.32	0.59
3:F:93:PRO:HG2	3:F:96:SER:OG	2.03	0.59
3:P:90:GLN:HE21	3:P:99:ILE:HG23	1.67	0.59
1:T:308:ASP:OD2	3:X:31:SER:OG	2.16	0.59
2:K:106:ARG:HH11	2:K:106:ARG:HG3	1.68	0.59
2:E:106:ARG:HG3	2:E:106:ARG:HH11	1.67	0.59
3:D:93:PRO:HG2	3:D:96:SER:OG	2.02	0.59
1:G:159:THR:OG1	1:G:160:PHE:N	2.33	0.59
1:M:245:GLU:O	1:M:249:LEU:HG	2.03	0.59
1:S:28:GLY:HA3	1:T:28:GLY:HA3	1.85	0.59
1:M:129:LEU:HD12	1:M:130:THR:N	2.17	0.58
2:E:210:LYS:N	2:E:211:PRO:HD2	2.18	0.58
1:T:227:ARG:HG2	1:T:227:ARG:NH1	2.17	0.58
3:R:111:ARG:HG3	3:R:112:THR:N	2.17	0.58
3:L:123:PRO:HD3	3:L:135:VAL:HG22	1.84	0.58
1:N:320:GLU:OE1	1:N:322:ARG:NH1	2.37	0.58
3:P:108:GLU:OE1	3:P:176:TYR:OH	2.20	0.58
1:T:245:GLU:O	1:T:249:LEU:HG	2.03	0.58
3:R:204:LEU:HD13	3:R:208:VAL:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:321:ILE:HG22	1:T:327:LEU:HD23	1.85	0.58
3:J:205:SER:O	3:J:206:SER:OG	2.19	0.58
2:U:107:ARG:NH1	9:U:304:HOH:O	2.35	0.58
1:G:287:ARG:NH1	9:G:504:HOH:O	2.37	0.58
1:G:169:PRO:CG	1:H:169:PRO:HG2	2.34	0.57
2:I:16:GLN:HG2	9:I:323:HOH:O	2.03	0.57
1:A:185:LYS:HB2	1:B:129:LEU:HD11	1.86	0.57
3:F:146:GLU:OE1	3:F:146:GLU:N	2.34	0.57
2:E:106:ARG:NH1	3:F:50:TYR:CE2	2.72	0.57
1:S:245:GLU:O	1:S:249:LEU:HG	2.04	0.57
3:P:192:HIS:O	3:P:214:ARG:NH1	2.37	0.57
1:A:31:LYS:HE2	9:A:518:HOH:O	2.04	0.57
1:S:91:SER:O	1:S:95:LYS:HG3	2.04	0.57
1:A:320:GLU:HB2	1:B:246:PHE:CZ	2.40	0.57
2:Q:209:HIS:H	2:Q:215:LYS:NZ	1.92	0.57
2:K:210:LYS:N	2:K:211:PRO:HD2	2.20	0.57
2:K:106:ARG:NH1	3:L:50:TYR:CE2	2.73	0.57
1:G:129:LEU:HD12	1:G:130:THR:N	2.19	0.57
1:B:62:LEU:HB2	1:B:87:GLU:OE2	2.05	0.57
2:K:134:ALA:HB3	2:K:223:LYS:HZ2	1.68	0.56
3:F:170:ASP:HB3	3:F:173:ASP:OD2	2.05	0.56
3:R:205:SER:O	3:R:206:SER:OG	2.16	0.56
2:Q:38:HIS:ND1	2:Q:53:SER:HB2	2.20	0.56
2:I:208:ASN:ND2	2:I:215:LYS:HE3	2.19	0.56
2:O:32:LEU:CD1	2:O:37:ILE:HD11	2.35	0.56
1:A:132:SER:HB3	1:B:178:GLN:HE21	1.70	0.56
1:S:294:MET:HE2	1:S:297:LYS:HE2	1.86	0.56
1:A:100:MET:HG3	1:A:101:ALA:N	2.20	0.56
1:B:321:ILE:HG22	1:B:327:LEU:HD23	1.87	0.56
1:H:304:GLU:OE1	2:K:106:ARG:NH1	2.38	0.56
1:M:170:THR:HG23	1:M:255:LEU:HD13	1.88	0.56
3:P:154:ASP:HA	3:P:194:VAL:HB	1.86	0.56
1:S:186:LEU:HD12	1:T:129:LEU:HD13	1.88	0.56
3:J:145:ARG:HH11	3:J:166:VAL:CG1	2.17	0.56
3:P:145:ARG:HB2	3:P:176:TYR:CZ	2.41	0.56
3:V:148:LYS:HB3	3:V:200:THR:HB	1.87	0.56
2:E:134:ALA:HB3	2:E:223:LYS:NZ	2.21	0.56
3:D:111:ARG:NH2	3:D:114:ALA:HB2	2.20	0.56
1:G:126:LEU:O	1:G:129:LEU:HG	2.05	0.56
1:H:256:ILE:O	1:H:260:ILE:HG13	2.05	0.56
3:L:115:ALA:HB1	3:L:204:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLY:HA2	1:A:31:LYS:HD2	1.88	0.56
3:L:115:ALA:HB1	3:L:204:LEU:CD2	2.36	0.56
2:I:144:THR:HG22	2:I:145:ALA:N	2.21	0.56
1:N:148:HIS:O	1:N:152:GLN:HG3	2.05	0.56
1:M:151:ARG:HG2	1:M:159:THR:HG22	1.88	0.56
1:A:256:ILE:CD1	1:A:269:ILE:HD11	2.36	0.56
3:P:157:LEU:HD23	3:P:158:GLN:N	2.20	0.56
2:O:134:ALA:HB3	2:O:223:LYS:HZ2	1.67	0.55
1:S:168:ALA:O	1:S:173:THR:OG1	2.22	0.55
1:B:246:PHE:CD1	1:B:247:LEU:HD13	2.41	0.55
3:V:84:PHE:HB2	9:V:308:HOH:O	2.05	0.55
2:C:128:PRO:HB3	2:C:154:TYR:HB3	1.88	0.55
1:B:187:LEU:HD23	1:B:220:LYS:HA	1.89	0.55
2:O:134:ALA:CB	2:O:223:LYS:HZ2	2.19	0.55
2:C:101:ARG:O	2:C:109:LEU:HA	2.06	0.55
1:M:285:CYS:O	1:M:289:GLN:HB2	2.07	0.55
1:M:187:LEU:CD1	1:M:216:LEU:HD11	2.36	0.55
3:J:111:ARG:HD3	3:J:112:THR:O	2.07	0.55
1:G:46:GLN:OE1	1:G:49:LYS:HD3	2.05	0.55
3:F:36:TRP:CZ3	3:F:89:CYS:HB3	2.42	0.55
1:B:159:THR:HG23	1:B:160:PHE:H	1.71	0.55
3:P:111:ARG:HH22	3:P:114:ALA:CB	2.20	0.55
2:W:210:LYS:N	2:W:211:PRO:HD2	2.21	0.55
1:T:52:LEU:HB2	1:T:160:PHE:CG	2.41	0.55
2:W:208:ASN:OD1	2:W:215:LYS:HD3	2.06	0.55
1:G:178:GLN:HE21	1:H:132:SER:HB3	1.70	0.55
1:B:345:LYS:HG3	1:B:349:GLU:OE2	2.06	0.55
2:O:210:LYS:N	2:O:211:PRO:HD2	2.22	0.54
3:X:13:SER:OG	3:X:143:TYR:OH	2.19	0.54
1:M:321:ILE:HG22	1:M:327:LEU:HD23	1.87	0.54
1:A:13:ILE:HD13	1:A:41:GLN:HB3	1.89	0.54
2:I:39:TRP:O	2:I:51:VAL:HG22	2.07	0.54
2:C:50:TRP:HE1	2:C:53:SER:HG	1.53	0.54
1:S:171:GLY:CA	1:T:58:PRO:HB2	2.37	0.54
1:M:151:ARG:HG2	1:M:159:THR:CG2	2.38	0.54
2:K:152:LYS:NZ	2:K:180:GLN:OE1	2.40	0.54
1:A:189:LYS:HZ2	1:B:126:LEU:HD13	1.72	0.54
1:B:297:LYS:HE3	1:B:298:TYR:CE1	2.43	0.54
1:G:345:LYS:HG3	1:G:349:GLU:OE2	2.08	0.54
2:I:87:ASN:ND2	9:I:306:HOH:O	2.40	0.54
1:A:126:LEU:O	1:A:126:LEU:HD22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:GLU:OE1	2:E:106:ARG:NH1	2.40	0.54
2:C:50:TRP:NE1	2:C:53:SER:OG	2.39	0.54
2:U:210:LYS:N	2:U:211:PRO:HD2	2.23	0.54
1:N:143:MET:O	1:N:147:LYS:HG3	2.06	0.54
1:M:188:GLU:HG3	1:M:189:LYS:HG3	1.90	0.54
2:Q:32:LEU:CD1	2:Q:37:ILE:HD11	2.38	0.54
1:G:256:ILE:O	1:G:260:ILE:HG13	2.08	0.54
2:W:54:ILE:HG13	2:W:61:THR:HG22	1.88	0.54
1:G:90:PRO:HA	1:G:140:LEU:CD1	2.38	0.54
3:F:139:LEU:HD21	3:F:199:VAL:HG13	1.90	0.54
3:R:94:TYR:O	3:R:95:TYR:HB2	2.08	0.54
1:A:129:LEU:HD12	1:B:182:THR:HG23	1.89	0.53
2:E:136:SER:HB2	2:E:139:SER:OG	2.08	0.53
1:S:178:GLN:NE2	1:T:132:SER:HB3	2.23	0.53
2:U:208:ASN:HA	2:U:215:LYS:HD2	1.91	0.53
3:F:116:PRO:HB3	3:F:142:PHE:HB3	1.89	0.53
1:A:56:THR:OG1	1:A:167:THR:HA	2.08	0.53
3:L:145:ARG:CG	3:L:145:ARG:NH1	2.57	0.53
3:D:38:GLN:HB2	3:D:87:TYR:CE2	2.44	0.53
2:W:32:LEU:CD1	2:W:37:ILE:HD11	2.39	0.53
3:J:108:GLU:OE1	3:J:176:TYR:OH	2.18	0.53
1:H:46:GLN:OE1	1:H:49:LYS:HD3	2.08	0.53
2:C:107:ARG:NH2	3:D:96:SER:O	2.42	0.53
1:N:25:GLY:N	1:N:31:LYS:HD3	2.24	0.53
1:S:321:ILE:CG2	1:S:327:LEU:HD23	2.36	0.53
1:H:142:PHE:HB2	1:H:179:LEU:HD23	1.90	0.53
2:Q:101:ARG:O	2:Q:109:LEU:HA	2.09	0.53
2:Q:179:LEU:HD13	2:Q:185:TYR:CZ	2.44	0.53
2:W:163:TRP:CH2	2:W:205:CYS:HB3	2.43	0.53
1:S:129:LEU:O	1:S:133:ILE:HG13	2.08	0.52
1:B:144:GLU:CD	1:B:147:LYS:HE2	2.30	0.52
2:C:134:ALA:HB3	2:C:223:LYS:NZ	2.24	0.52
2:Q:32:LEU:HD11	2:Q:37:ILE:CD1	2.40	0.52
1:H:283:HIS:HB2	1:H:289:GLN:OE1	2.09	0.52
1:M:189:LYS:O	1:M:193:ILE:HG12	2.09	0.52
1:B:170:THR:HG23	1:B:255:LEU:HD13	1.90	0.52
3:R:152:LYS:HG2	3:R:157:LEU:HD23	1.91	0.52
3:D:143:TYR:CG	3:D:144:PRO:HA	2.44	0.52
2:Q:214:THR:C	2:Q:215:LYS:HD2	2.30	0.52
3:L:48:LEU:CB	3:L:49:ILE:HD12	2.39	0.52
1:N:156:GLU:N	1:N:156:GLU:OE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:62:LEU:HB2	1:H:87:GLU:OE2	2.09	0.52
1:M:31:LYS:HE2	9:M:515:HOH:O	2.09	0.52
3:L:148:LYS:HB3	3:L:200:THR:HB	1.91	0.52
2:C:54:ILE:HG13	2:C:61:THR:HG22	1.92	0.52
2:Q:160:THR:OG1	2:Q:208:ASN:HB2	2.10	0.52
2:Q:209:HIS:NE2	2:Q:211:PRO:HG2	2.24	0.52
2:O:76:ASP:OD1	2:O:78:SER:OG	2.21	0.52
1:A:281:GLN:OE1	1:B:286:LYS:HE3	2.09	0.52
2:E:141:SER:HB3	3:F:118:VAL:O	2.10	0.52
1:A:287:ARG:NH2	1:B:275:LEU:HD22	2.25	0.52
3:R:146:GLU:OE1	3:R:146:GLU:N	2.37	0.52
2:Q:156:PRO:HD2	2:Q:211:PRO:HB2	1.91	0.52
1:H:321:ILE:HG22	1:H:327:LEU:CD2	2.40	0.52
1:G:245:GLU:O	1:G:249:LEU:HG	2.10	0.52
1:T:320:GLU:CD	1:T:322:ARG:HH12	2.13	0.52
1:B:5:VAL:HG13	1:B:310:HIS:CE1	2.45	0.52
3:X:206:SER:HB2	3:X:207:PRO:HD2	1.92	0.52
2:K:153:ASP:OD1	9:K:303:HOH:O	2.19	0.52
2:I:32:LEU:HD11	2:I:37:ILE:CG1	2.35	0.52
1:H:191:GLY:HA2	1:H:216:LEU:CD2	2.36	0.52
2:K:209:HIS:NE2	2:K:211:PRO:HG2	2.24	0.52
3:J:204:LEU:HD13	3:J:208:VAL:HG23	1.92	0.52
2:E:5:VAL:HG11	2:E:111:TYR:CD2	2.45	0.52
2:W:140:THR:HG22	2:W:141:SER:CA	2.36	0.52
1:M:156:GLU:O	1:M:156:GLU:HG2	2.10	0.52
1:T:168:ALA:O	1:T:173:THR:OG1	2.21	0.51
1:G:321:ILE:HG22	1:G:327:LEU:CD2	2.40	0.51
2:Q:36:SER:O	2:Q:102:GLY:HA3	2.10	0.51
3:J:108:GLU:HB2	3:J:169:GLN:OE1	2.10	0.51
2:E:107:ARG:HB3	3:F:92:TYR:HB2	1.92	0.51
2:E:38:HIS:HD1	2:E:53:SER:HB3	1.75	0.51
2:E:50:TRP:HE1	2:E:53:SER:HB3	1.76	0.51
2:K:15:VAL:HG11	2:K:21:LEU:HB2	1.91	0.51
2:Q:208:ASN:HA	2:Q:215:LYS:HE3	1.91	0.51
3:X:108:GLU:HG2	9:X:304:HOH:O	2.10	0.51
1:G:126:LEU:HG	1:G:129:LEU:HD21	1.92	0.51
2:Q:35:TYR:CD1	2:Q:101:ARG:HD2	2.45	0.51
3:D:48:LEU:CB	3:D:49:ILE:HD12	2.39	0.51
3:X:204:LEU:HD13	3:X:208:VAL:HG23	1.91	0.51
2:Q:215:LYS:HA	2:Q:215:LYS:NZ	2.25	0.51
2:E:159:VAL:HG13	9:E:302:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:32:LEU:HD11	2:W:37:ILE:HG12	1.92	0.51
1:A:249:LEU:HD11	1:A:298:TYR:CG	2.46	0.51
2:I:210:LYS:N	2:I:211:PRO:HD2	2.26	0.51
3:V:116:PRO:HB3	3:V:142:PHE:HB3	1.92	0.51
2:W:143:GLY:O	2:W:195:SER:N	2.25	0.51
1:S:307:GLU:OE2	3:V:32:SER:HB2	2.11	0.51
1:N:191:GLY:CA	1:N:216:LEU:HD21	2.40	0.51
1:A:189:LYS:NZ	1:B:126:LEU:HD13	2.26	0.51
3:J:139:LEU:HD21	3:J:199:VAL:HG13	1.91	0.51
1:S:75:ARG:NH1	9:S:508:HOH:O	2.41	0.51
2:E:106:ARG:NH1	3:F:50:TYR:CD2	2.78	0.51
1:N:304:GLU:OE1	2:Q:106:ARG:HD3	2.10	0.51
3:L:145:ARG:HD2	3:L:176:TYR:CE2	2.46	0.51
2:Q:109:LEU:HD22	9:Q:313:HOH:O	2.10	0.51
1:M:129:LEU:HD13	1:N:186:LEU:HD21	1.91	0.51
2:U:38:HIS:HD1	2:U:53:SER:HB3	1.76	0.51
3:R:145:ARG:NH2	3:R:166:VAL:HG11	2.21	0.51
1:S:187:LEU:HD11	1:S:216:LEU:CD1	2.41	0.51
1:G:129:LEU:HD13	1:H:186:LEU:CD2	2.41	0.51
3:V:204:LEU:HD13	3:V:208:VAL:HG23	1.93	0.51
2:I:223:LYS:HD2	3:J:217:CYS:O	2.11	0.51
3:J:93:PRO:HG2	3:J:96:SER:HB3	1.91	0.51
3:J:25:ARG:HG3	3:J:71:ASP:OD1	2.10	0.51
1:H:187:LEU:CD2	1:H:219:LEU:HD23	2.41	0.51
1:A:178:GLN:NE2	1:B:132:SER:HB3	2.25	0.51
3:F:148:LYS:HB3	3:F:200:THR:HB	1.92	0.51
3:R:143:TYR:CG	3:R:144:PRO:HA	2.46	0.51
1:A:304:GLU:OE1	2:C:106:ARG:HD3	2.11	0.51
3:D:48:LEU:HB3	3:D:49:ILE:HD12	1.93	0.51
1:B:256:ILE:O	1:B:260:ILE:HG13	2.10	0.51
3:R:48:LEU:HA	3:R:59:VAL:HG21	1.92	0.50
1:G:277:ALA:O	1:G:280:ASP:HB2	2.11	0.50
3:R:148:LYS:HB3	3:R:200:THR:HB	1.92	0.50
1:A:185:LYS:HB2	1:B:129:LEU:CD1	2.40	0.50
2:W:209:HIS:NE2	2:W:211:PRO:HG2	2.26	0.50
2:Q:177:ALA:HA	2:Q:187:LEU:HB3	1.92	0.50
2:E:177:ALA:HA	2:E:187:LEU:HB3	1.93	0.50
1:B:148:HIS:HA	1:B:151:ARG:HD2	1.93	0.50
2:E:39:TRP:O	2:E:51:VAL:HG22	2.11	0.50
1:H:329:LYS:O	1:H:332:GLN:HG2	2.10	0.50
1:M:320:GLU:OE1	1:N:298:TYR:OH	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:168:ALA:HB1	1:G:169:PRO:HD2	1.93	0.50
1:M:129:LEU:HD13	1:N:186:LEU:CD2	2.41	0.50
1:N:159:THR:HG23	1:N:160:PHE:N	2.20	0.50
1:B:159:THR:HG23	1:B:160:PHE:N	2.27	0.50
1:M:348:TYR:OH	1:N:286:LYS:HB2	2.12	0.50
1:A:90:PRO:HA	1:A:140:LEU:CD1	2.42	0.50
1:B:246:PHE:N	1:B:246:PHE:CD2	2.72	0.50
1:S:274:LEU:HD12	1:S:313:LYS:HB3	1.93	0.50
2:O:209:HIS:NE2	2:O:211:PRO:HG2	2.27	0.50
2:W:134:ALA:CB	2:W:223:LYS:HZ2	2.24	0.50
2:E:128:PRO:HB3	2:E:154:TYR:HB3	1.94	0.50
1:B:145:VAL:HG22	1:B:165:PHE:HZ	1.75	0.50
1:A:250:TYR:OH	2:C:34:TYR:HB3	2.12	0.50
3:D:154:ASP:O	3:D:155:ASN:HB2	2.12	0.50
2:K:50:TRP:NE1	2:K:53:SER:OG	2.36	0.50
2:U:144:THR:HG22	2:U:145:ALA:N	2.26	0.50
1:B:91:SER:O	1:B:95:LYS:HG3	2.12	0.50
3:F:143:TYR:CG	3:F:144:PRO:HA	2.47	0.49
1:S:170:THR:HG23	1:S:255:LEU:HD13	1.94	0.49
1:N:245:GLU:O	1:N:249:LEU:HG	2.12	0.49
3:J:141:ASN:ND2	9:J:332:HOH:O	2.45	0.49
1:B:147:LYS:O	1:B:151:ARG:HG3	2.12	0.49
1:A:321:ILE:HG22	1:A:327:LEU:CD2	2.38	0.49
2:I:94:THR:HG23	2:I:119:THR:HA	1.93	0.49
2:U:6:GLN:HG2	2:U:28:SER:OG	2.12	0.49
2:E:209:HIS:NE2	2:E:211:PRO:HG2	2.26	0.49
1:A:280:ASP:OD2	1:B:287:ARG:NH2	2.46	0.49
1:S:76:LYS:HD2	1:S:84:SER:OG	2.12	0.49
1:N:256:ILE:O	1:N:260:ILE:HG13	2.12	0.49
1:H:142:PHE:CE2	1:H:183:LEU:HD12	2.47	0.49
1:T:149:ILE:CD1	1:T:226:ILE:HG12	2.42	0.49
3:P:109:ILE:HG23	3:P:169:GLN:NE2	2.28	0.49
1:M:129:LEU:CD1	1:N:186:LEU:HD21	2.42	0.49
1:A:24:GLY:HA2	1:A:31:LYS:CD	2.43	0.49
1:H:94:LEU:HD12	1:H:131:GLY:HA2	1.95	0.49
3:X:137:CYS:HB2	3:X:151:TRP:CZ2	2.48	0.49
3:X:158:GLN:OE1	3:X:182:LEU:HD11	2.13	0.49
3:X:115:ALA:HB1	3:X:204:LEU:HD21	1.94	0.49
1:N:90:PRO:HB2	9:N:517:HOH:O	2.12	0.49
3:J:116:PRO:HB3	3:J:142:PHE:HB3	1.94	0.49
2:W:103:ARG:NH1	2:W:110:ASP:OD2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:265:ASP:OD2	1:T:267:ASN:ND2	2.45	0.49
2:I:161:VAL:HG21	2:I:189:SER:HB2	1.95	0.49
3:D:152:LYS:HA	3:D:156:ALA:O	2.13	0.49
2:U:180:GLN:HG2	3:V:163:GLN:OE1	2.13	0.49
2:C:103:ARG:NH1	2:C:110:ASP:OD2	2.44	0.49
2:U:219:LYS:HZ1	2:U:221:GLU:CD	2.16	0.49
3:J:37:TYR:CE1	3:J:47:LEU:HD13	2.47	0.49
1:G:144:GLU:CD	1:G:147:LYS:HE2	2.33	0.49
3:V:93:PRO:HB2	3:V:95:TYR:CE2	2.47	0.49
3:X:137:CYS:HB2	3:X:151:TRP:CH2	2.48	0.49
1:H:183:LEU:O	1:H:187:LEU:HB2	2.13	0.49
3:V:164:GLU:CD	3:V:178:LEU:HD11	2.33	0.49
1:T:8:ASN:HA	1:T:312:VAL:HG22	1.93	0.49
3:J:64:SER:O	3:J:74:LEU:HD12	2.13	0.49
3:F:48:LEU:CB	3:F:49:ILE:HD12	2.43	0.49
1:G:316:LEU:HD12	8:G:404[A]:ATP:C2	2.48	0.49
1:S:69:LYS:HD3	2:W:33:TYR:CE1	2.48	0.49
2:K:112:TRP:CE3	3:L:45:PRO:HD2	2.48	0.49
1:M:274:LEU:HD12	1:M:313:LYS:HB3	1.95	0.49
1:S:304:GLU:OE1	2:U:106:ARG:HD3	2.12	0.49
2:K:134:ALA:HB3	2:K:223:LYS:HZ1	1.76	0.48
3:J:145:ARG:NH1	3:J:166:VAL:HG11	2.25	0.48
1:M:188:GLU:HG3	1:M:189:LYS:N	2.28	0.48
3:X:170:ASP:HB3	3:X:173:ASP:OD1	2.12	0.48
3:R:3:ILE:HG21	3:R:91:GLN:OE1	2.13	0.48
2:C:134:ALA:HB3	2:C:223:LYS:HZ2	1.78	0.48
2:E:15:VAL:HG11	2:E:21:LEU:HB2	1.96	0.48
1:A:296:LYS:HG2	9:A:507:HOH:O	2.13	0.48
2:U:32:LEU:CD1	2:U:37:ILE:HD11	2.43	0.48
3:J:48:LEU:HA	3:J:59:VAL:HG21	1.95	0.48
1:M:171:GLY:HA3	1:N:58:PRO:HB2	1.95	0.48
1:T:88:ILE:H	1:T:88:ILE:HG13	1.35	0.48
2:U:148:GLY:HA2	2:U:163:TRP:CH2	2.48	0.48
2:O:141:SER:N	2:O:144:THR:O	2.46	0.48
3:V:39:GLN:O	3:V:85:ALA:HB1	2.13	0.48
2:U:42:GLN:C	2:U:95:ALA:HB1	2.34	0.48
3:P:3:ILE:HG21	3:P:91:GLN:CD	2.34	0.48
3:P:109:ILE:HG23	3:P:169:GLN:HE22	1.78	0.48
2:W:39:TRP:O	2:W:51:VAL:HG22	2.14	0.48
1:G:137:ASP:CG	1:H:175:ARG:HH12	2.13	0.48
1:G:189:LYS:NZ	1:H:129:LEU:HD11	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:3:ILE:HG21	3:J:91:GLN:OE1	2.14	0.48
3:V:143:TYR:CG	3:V:144:PRO:HA	2.48	0.48
1:M:318:ALA:HB1	1:N:290:ALA:HB3	1.96	0.48
1:M:90:PRO:HA	1:M:140:LEU:CD1	2.44	0.48
2:C:9:GLU:OE2	2:C:113:GLY:HA3	2.13	0.48
2:W:162:SER:O	2:W:205:CYS:HA	2.14	0.48
3:F:108:GLU:HB3	3:F:169:GLN:OE1	2.14	0.48
1:T:321:ILE:CG2	1:T:327:LEU:HD23	2.43	0.47
3:D:170:ASP:HB3	3:D:173:ASP:OD1	2.14	0.47
3:J:93:PRO:HB2	3:J:95:TYR:CE2	2.49	0.47
3:L:186:LYS:HE3	3:L:190:GLU:OE2	2.14	0.47
3:D:115:ALA:HB1	3:D:204:LEU:CD2	2.44	0.47
1:M:174:LEU:HD22	1:M:258:GLU:HG2	1.95	0.47
3:D:90:GLN:HE21	3:D:99:ILE:HG23	1.78	0.47
3:L:206:SER:HB2	3:L:207:PRO:HD2	1.94	0.47
1:H:31:LYS:HB2	7:H:402[B]:ADP:O1B	2.14	0.47
3:P:93:PRO:HB2	3:P:95:TYR:CE1	2.49	0.47
2:Q:131:PHE:CE1	3:R:127:GLN:HA	2.49	0.47
1:G:159:THR:N	9:G:515:HOH:O	2.47	0.47
2:E:162:SER:HB2	2:E:206:ASN:HB2	1.95	0.47
3:P:170:ASP:HB3	3:P:173:ASP:OD1	2.13	0.47
3:P:98:LEU:HD12	3:P:98:LEU:N	2.29	0.47
1:S:129:LEU:CD1	1:T:186:LEU:HD21	2.32	0.47
1:B:183:LEU:O	1:B:187:LEU:HB2	2.14	0.47
3:V:5:MET:CE	3:V:24:CYS:SG	3.02	0.47
1:B:142:PHE:CE2	1:B:183:LEU:HD12	2.49	0.47
1:N:148:HIS:ND1	1:N:159:THR:HG21	2.30	0.47
2:W:128:PRO:CB	2:W:154:TYR:HB3	2.42	0.47
3:J:145:ARG:O	3:J:145:ARG:HG2	2.13	0.47
1:H:189:LYS:O	1:H:193:ILE:HG12	2.14	0.47
1:H:94:LEU:HD12	1:H:131:GLY:CA	2.44	0.47
3:F:38:GLN:HB2	3:F:48:LEU:HD11	1.97	0.47
1:H:56:THR:OG1	1:H:167:THR:HA	2.15	0.47
3:V:109:ILE:HG22	3:V:169:GLN:CD	2.34	0.47
1:A:277:ALA:O	1:A:280:ASP:HB2	2.14	0.47
1:A:246:PHE:CZ	1:B:322:ARG:NH2	2.83	0.47
1:S:178:GLN:OE1	1:S:262:TYR:OH	2.17	0.47
2:U:208:ASN:HB3	2:U:215:LYS:HZ1	1.78	0.47
1:A:186:LEU:HD22	1:B:129:LEU:CG	2.44	0.47
3:D:93:PRO:HB2	3:D:95:TYR:CE2	2.50	0.47
1:B:302:ILE:HG23	1:B:306:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:39:TRP:O	2:K:51:VAL:HG22	2.14	0.47
3:L:90:GLN:HE21	3:L:99:ILE:HG23	1.80	0.47
1:B:250:TYR:O	1:B:254:ARG:HB2	2.15	0.47
2:I:38:HIS:HD1	2:I:53:SER:HB3	1.80	0.47
1:H:8:ASN:O	9:H:513:HOH:O	2.20	0.47
3:V:98:LEU:N	3:V:98:LEU:HD12	2.29	0.47
1:N:142:PHE:HB2	1:N:179:LEU:HD23	1.96	0.47
1:B:321:ILE:CG2	1:B:327:LEU:HD23	2.44	0.47
2:O:106:ARG:NH1	3:P:50:TYR:CE2	2.83	0.47
2:Q:107:ARG:NE	9:Q:309:HOH:O	2.46	0.47
1:G:246:PHE:CE2	1:G:247:LEU:HG	2.49	0.47
1:N:187:LEU:CD2	1:N:219:LEU:HD23	2.44	0.47
2:W:63:TYR:OH	2:W:73:ILE:HG22	2.14	0.47
1:T:30:GLY:HA2	8:T:403[A]:ATP:PA	2.55	0.47
1:T:232:ASP:OD2	9:T:502:HOH:O	2.19	0.47
3:D:205:SER:O	3:D:206:SER:CB	2.62	0.47
2:O:134:ALA:CB	2:O:223:LYS:NZ	2.76	0.47
2:U:107:ARG:NH2	3:V:96:SER:O	2.48	0.47
3:X:143:TYR:CG	3:X:144:PRO:HA	2.50	0.47
1:G:142:PHE:HB2	1:G:179:LEU:HD23	1.96	0.47
1:A:76:LYS:HD2	1:A:84:SER:OG	2.15	0.47
2:I:15:VAL:HG11	2:I:89:LEU:HD13	1.96	0.47
3:P:143:TYR:CG	3:P:144:PRO:HA	2.49	0.47
3:X:128:LEU:O	3:X:186:LYS:HD2	2.14	0.47
1:A:171:GLY:HA3	1:B:58:PRO:HB2	1.95	0.47
2:Q:179:LEU:HD13	2:Q:185:TYR:CE1	2.50	0.46
3:R:37:TYR:CE1	3:R:47:LEU:HD13	2.51	0.46
1:M:146:MET:HA	1:M:226:ILE:HD11	1.97	0.46
1:N:24:GLY:HA2	1:N:31:LYS:CD	2.44	0.46
2:C:187:LEU:HD12	2:C:187:LEU:C	2.36	0.46
1:S:126:LEU:CD2	1:S:126:LEU:H	2.24	0.46
1:G:129:LEU:HD12	1:G:129:LEU:C	2.36	0.46
3:V:30:VAL:HA	3:V:95:TYR:OH	2.16	0.46
3:L:15:SER:OG	3:L:110:LYS:HG2	2.16	0.46
3:V:205:SER:O	3:V:206:SER:CB	2.63	0.46
1:G:274:LEU:HD12	1:G:313:LYS:HB3	1.97	0.46
1:G:8:ASN:HA	1:G:312:VAL:HG22	1.97	0.46
3:D:98:LEU:N	3:D:98:LEU:HD12	2.30	0.46
1:S:126:LEU:HA	1:S:129:LEU:HG	1.98	0.46
2:I:144:THR:HG21	2:I:192:THR:HB	1.96	0.46
2:E:15:VAL:HG21	2:E:89:LEU:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:ALA:O	2:C:192:THR:HA	2.15	0.46
3:R:98:LEU:N	3:R:98:LEU:HD22	2.30	0.46
1:G:246:PHE:CE1	1:H:322:ARG:HB3	2.51	0.46
1:N:191:GLY:O	1:N:194:THR:HG22	2.16	0.46
2:K:5:VAL:N	9:K:310:HOH:O	2.49	0.46
3:R:189:TYR:HA	3:R:195:TYR:OH	2.16	0.46
2:C:148:GLY:HA2	2:C:163:TRP:CH2	2.51	0.46
3:L:205:SER:O	3:L:206:SER:CB	2.64	0.46
3:L:103:GLN:HB2	9:L:318:HOH:O	2.14	0.46
1:A:94:LEU:HD12	1:A:131:GLY:CA	2.45	0.46
3:P:111:ARG:HH22	3:P:114:ALA:HB2	1.80	0.46
1:S:64:ASP:HA	2:W:34:TYR:OH	2.16	0.46
1:N:24:GLY:HA2	1:N:31:LYS:HD2	1.97	0.46
3:X:205:SER:O	3:X:206:SER:CB	2.63	0.46
3:P:189:TYR:O	3:P:195:TYR:OH	2.33	0.46
3:D:30:VAL:HG11	3:D:91:GLN:NE2	2.30	0.46
1:A:186:LEU:HD22	1:B:129:LEU:CD2	2.46	0.46
2:O:107:ARG:HB3	3:P:92:TYR:HB2	1.98	0.46
3:J:13:SER:OG	3:J:108:GLU:OE2	2.33	0.46
3:D:64:SER:OG	3:D:75:THR:HB	2.15	0.46
1:N:254:ARG:HD3	2:Q:58:SER:HA	1.98	0.46
1:G:159:THR:HG22	9:G:515:HOH:O	2.16	0.46
2:O:103:ARG:NH1	2:O:110:ASP:OD2	2.44	0.46
3:L:13:SER:HG	3:L:143:TYR:HH	1.58	0.46
3:D:162:SER:HA	3:D:181:THR:O	2.16	0.46
3:V:22:ILE:HG12	3:V:105:THR:HG21	1.98	0.46
1:T:181:ASN:O	1:T:185:LYS:HG2	2.16	0.46
1:N:46:GLN:OE1	1:N:49:LYS:HD3	2.15	0.46
3:P:48:LEU:CB	3:P:49:ILE:HD12	2.46	0.46
3:L:145:ARG:NH1	3:L:145:ARG:HG2	2.11	0.45
1:S:126:LEU:O	1:S:129:LEU:HG	2.16	0.45
3:P:3:ILE:CG2	3:P:91:GLN:HE22	2.29	0.45
2:Q:134:ALA:HB3	2:Q:223:LYS:HZ2	1.81	0.45
2:E:208:ASN:O	9:E:302:HOH:O	2.20	0.45
1:A:132:SER:HB3	1:B:178:GLN:NE2	2.31	0.45
3:L:48:LEU:HB3	3:L:49:ILE:HD12	1.97	0.45
3:F:3:ILE:HG21	3:F:91:GLN:OE1	2.16	0.45
1:N:184:SER:O	1:N:188:GLU:HG3	2.16	0.45
1:S:294:MET:HE1	1:S:297:LYS:NZ	2.32	0.45
1:M:156:GLU:OE1	1:M:156:GLU:N	2.49	0.45
2:U:86:MET:HB3	2:U:89:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:250:TYR:O	1:T:254:ARG:HB2	2.16	0.45
3:V:154:ASP:HA	3:V:194:VAL:HB	1.98	0.45
1:H:70:PHE:CE1	1:H:85:CYS:HB2	2.51	0.45
3:F:145:ARG:CG	3:F:145:ARG:NH1	2.64	0.45
1:B:142:PHE:CB	1:B:179:LEU:HD23	2.45	0.45
3:V:206:SER:HB2	3:V:207:PRO:HD2	1.98	0.45
1:M:178:GLN:O	1:M:182:THR:OG1	2.29	0.45
1:N:146:MET:HG2	1:N:222:ASN:HD22	1.82	0.45
3:R:169:GLN:HG2	3:R:174:SER:HA	1.97	0.45
2:C:131:PHE:CE1	3:D:127:GLN:HA	2.51	0.45
1:H:51:PHE:CD1	1:H:162:THR:HB	2.52	0.45
3:J:143:TYR:CG	3:J:144:PRO:HA	2.51	0.45
1:S:168:ALA:HB1	1:S:169:PRO:HD2	1.98	0.45
9:S:503:HOH:O	1:T:175:ARG:NE	2.49	0.45
3:R:48:LEU:CB	3:R:49:ILE:HD12	2.46	0.45
3:V:205:SER:O	3:V:206:SER:OG	2.34	0.45
1:G:325:ASN:ND2	9:G:509:HOH:O	2.35	0.45
2:W:9:GLU:HA	2:W:24:SER:O	2.16	0.45
1:M:13:ILE:HA	1:M:42:MET:HG2	1.99	0.45
1:N:51:PHE:CD1	1:N:162:THR:HB	2.51	0.45
2:C:107:ARG:HB3	3:D:92:TYR:HB2	1.99	0.45
1:G:51:PHE:CD1	1:G:162:THR:HB	2.52	0.45
1:B:149:ILE:HD12	1:B:226:ILE:CG1	2.37	0.45
1:B:246:PHE:CE1	1:B:247:LEU:HD13	2.52	0.45
3:J:166:VAL:HG23	3:J:177:SER:O	2.17	0.45
2:E:154:TYR:CE2	2:E:159:VAL:HG23	2.52	0.45
1:H:252:THR:O	1:H:256:ILE:HG13	2.17	0.45
3:V:50:TYR:O	3:V:54:SER:HB2	2.17	0.45
1:A:329:LYS:O	1:A:332:GLN:HG2	2.17	0.45
2:O:94:THR:HG23	2:O:119:THR:HA	1.98	0.45
2:C:42:GLN:C	2:C:95:ALA:HB1	2.37	0.45
1:G:171:GLY:HA3	1:H:58:PRO:HB2	1.98	0.45
2:I:9:GLU:HA	2:I:24:SER:O	2.17	0.45
3:P:139:LEU:HD21	3:P:199:VAL:HG13	1.99	0.45
3:V:204:LEU:HD13	3:V:208:VAL:CG2	2.47	0.45
3:P:49:ILE:HD13	3:P:74:LEU:HD13	1.99	0.45
1:M:38:ILE:O	1:M:42:MET:HG3	2.17	0.45
1:H:144:GLU:CD	1:H:147:LYS:HE2	2.37	0.45
3:V:213:ASN:HB2	3:V:216:GLU:OE1	2.17	0.45
3:X:118:VAL:CG2	3:X:199:VAL:HG21	2.47	0.45
1:H:316:LEU:HD12	8:H:403[A]:ATP:C2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:187:LEU:HD11	1:S:216:LEU:HD11	1.97	0.45
1:S:219:LEU:HD13	1:S:219:LEU:C	2.37	0.45
1:M:129:LEU:HD12	1:M:129:LEU:C	2.37	0.45
2:U:157:GLU:OE1	2:U:177:ALA:HB3	2.16	0.45
1:S:219:LEU:HD13	1:S:219:LEU:O	2.17	0.45
2:O:107:ARG:HG2	3:P:99:ILE:HD11	1.98	0.45
3:D:4:GLN:NE2	9:D:301:HOH:O	2.50	0.45
1:T:174:LEU:HD22	1:T:258:GLU:HG2	1.99	0.45
3:F:205:SER:O	3:F:206:SER:CB	2.65	0.45
1:H:249:LEU:HD11	1:H:298:TYR:CG	2.52	0.45
1:G:133:ILE:HD11	1:H:186:LEU:HD11	1.97	0.44
2:Q:15:VAL:HG21	2:Q:89:LEU:CD1	2.46	0.44
1:T:317:CYS:HA	1:T:347:ILE:HB	1.97	0.44
2:C:76:ASP:OD1	2:C:78:SER:OG	2.24	0.44
2:Q:63:TYR:HB2	2:Q:68:LYS:HG3	1.98	0.44
2:O:128:PRO:HB3	2:O:154:TYR:HB3	1.99	0.44
3:J:98:LEU:N	3:J:98:LEU:HD12	2.32	0.44
1:B:188:GLU:HG3	1:B:188:GLU:H	1.39	0.44
1:B:69:LYS:NZ	2:C:59:SER:OG	2.20	0.44
1:B:267:ASN:O	1:B:310:HIS:N	2.43	0.44
2:E:62:SER:HB3	3:F:97:SER:HB2	2.00	0.44
1:S:55:SER:HB2	1:S:62:LEU:CD1	2.47	0.44
2:O:32:LEU:HD11	2:O:37:ILE:CG1	2.48	0.44
1:A:126:LEU:HD13	1:A:126:LEU:C	2.38	0.44
3:R:34:VAL:HA	3:R:90:GLN:O	2.17	0.44
2:O:15:VAL:HG22	2:O:16:GLN:N	2.33	0.44
3:V:3:ILE:HA	3:V:27:SER:OG	2.17	0.44
1:T:30:GLY:HA2	7:T:402[B]:ADP:PA	2.57	0.44
2:K:181:SER:HB2	1:S:48:ASN:ND2	2.32	0.44
1:S:94:LEU:HD23	1:S:97:MET:HE2	1.98	0.44
2:E:175:PHE:CE1	3:F:179:SER:HB3	2.53	0.44
3:P:3:ILE:HG21	3:P:91:GLN:NE2	2.31	0.44
2:U:32:LEU:HD11	2:U:37:ILE:HG12	1.98	0.44
1:T:316:LEU:HD12	8:T:403[A]:ATP:C2	2.53	0.44
2:O:15:VAL:HG11	2:O:89:LEU:HD13	1.99	0.44
1:G:182:THR:O	1:G:186:LEU:HD13	2.17	0.44
1:A:168:ALA:HB1	1:A:169:PRO:HD2	2.00	0.44
2:U:107:ARG:HG2	3:V:99:ILE:HD11	2.00	0.44
3:F:137:CYS:HB2	3:F:151:TRP:CZ2	2.53	0.44
3:V:4:GLN:H	3:V:27:SER:HB3	1.83	0.44
2:U:33:TYR:CZ	2:U:57:TYR:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:135:PRO:HB3	2:E:147:LEU:HB3	1.99	0.44
3:F:111:ARG:HG3	3:F:112:THR:H	1.82	0.44
1:S:95:LYS:O	1:S:98:ASN:HB3	2.17	0.44
2:W:67:VAL:HB	2:W:71:PHE:CG	2.53	0.44
1:M:28:GLY:HA3	1:N:28:GLY:HA3	2.00	0.44
2:O:4:GLU:O	2:O:4:GLU:HG2	2.18	0.44
3:V:48:LEU:HA	3:V:59:VAL:HG21	1.98	0.44
2:W:160:THR:OG1	2:W:208:ASN:HB2	2.18	0.44
1:A:189:LYS:NZ	1:B:126:LEU:CD1	2.81	0.44
3:R:48:LEU:HB3	3:R:49:ILE:HD12	1.99	0.44
1:N:302:ILE:HG23	1:N:306:TYR:CD2	2.52	0.44
2:K:163:TRP:CH2	2:K:205:CYS:HB3	2.52	0.44
3:X:38:GLN:HB2	3:X:48:LEU:HD11	2.00	0.44
2:C:14:LEU:HD23	2:C:14:LEU:C	2.38	0.44
1:A:30:GLY:HA2	8:A:404[A]:ATP:PA	2.57	0.44
1:G:246:PHE:CZ	1:H:322:ARG:HB3	2.53	0.44
1:N:147:LYS:O	1:N:151:ARG:HB2	2.18	0.44
1:M:348:TYR:CZ	1:N:286:LYS:HB2	2.53	0.44
1:N:225:THR:O	1:N:228:GLN:HG2	2.17	0.44
2:E:67:VAL:HB	2:E:71:PHE:CG	2.53	0.44
1:G:58:PRO:HB2	1:H:171:GLY:HA3	1.98	0.44
2:E:209:HIS:CE1	2:E:211:PRO:HG2	2.53	0.43
2:Q:32:LEU:HD11	2:Q:37:ILE:HD11	1.99	0.43
2:Q:177:ALA:HB2	2:Q:187:LEU:HD23	2.00	0.43
2:Q:141:SER:C	2:Q:143:GLY:N	2.71	0.43
2:K:15:VAL:HG21	2:K:89:LEU:HD13	2.00	0.43
1:A:245:GLU:O	1:A:249:LEU:HG	2.18	0.43
1:G:325:ASN:HB2	9:G:510:HOH:O	2.18	0.43
2:O:157:GLU:CB	2:O:158:PRO:HA	2.47	0.43
3:J:148:LYS:HB3	3:J:200:THR:HB	1.99	0.43
1:S:51:PHE:CD1	1:S:162:THR:HB	2.53	0.43
3:D:13:SER:HA	3:D:108:GLU:HG3	2.00	0.43
2:U:128:PRO:CB	2:U:154:TYR:HB3	2.38	0.43
3:F:139:LEU:HD12	3:F:139:LEU:N	2.33	0.43
3:D:143:TYR:CD1	3:D:144:PRO:HA	2.54	0.43
3:P:34:VAL:HG21	3:P:72:PHE:CE1	2.52	0.43
1:B:10:HIS:CE1	1:B:14:THR:HG21	2.53	0.43
3:J:90:GLN:HE21	3:J:99:ILE:HG23	1.82	0.43
2:E:202:THR:HG23	2:E:219:LYS:HD2	2.00	0.43
1:H:306:TYR:HB3	1:H:309:PHE:HB2	1.99	0.43
3:X:145:ARG:HH21	3:X:166:VAL:HG11	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:183:LEU:O	1:M:187:LEU:HB2	2.17	0.43
2:Q:109:LEU:HD12	2:Q:112:TRP:CZ2	2.53	0.43
3:X:40:LYS:HB3	3:X:41:PRO:HD2	1.99	0.43
2:W:62:SER:HB3	3:X:97:SER:HB3	2.01	0.43
1:B:187:LEU:HD21	1:B:219:LEU:HD23	2.00	0.43
1:A:168:ALA:O	1:A:173:THR:OG1	2.33	0.43
3:V:189:TYR:CZ	3:V:214:ARG:HG3	2.53	0.43
2:O:32:LEU:CD1	2:O:37:ILE:CD1	2.97	0.43
2:U:131:PHE:HA	2:U:132:PRO:HD3	1.88	0.43
3:L:34:VAL:HG21	3:L:72:PHE:CZ	2.54	0.43
2:K:54:ILE:HG13	2:K:61:THR:HG22	2.00	0.43
2:Q:206:ASN:ND2	2:Q:217:ASP:OD2	2.48	0.43
1:H:37:SER:HB3	1:H:331:SER:CB	2.48	0.43
1:M:95:LYS:O	1:M:98:ASN:HB3	2.18	0.43
1:S:321:ILE:H	1:S:321:ILE:HD12	1.82	0.43
3:X:30:VAL:HG11	3:X:91:GLN:NE2	2.33	0.43
3:D:111:ARG:HD2	3:D:173:ASP:O	2.19	0.43
1:A:348:TYR:CE1	1:B:286:LYS:HG2	2.54	0.43
1:N:298:TYR:O	1:N:302:ILE:HG13	2.19	0.43
2:W:15:VAL:HG11	2:W:89:LEU:HD13	2.01	0.43
1:H:246:PHE:HE2	2:K:34:TYR:CE1	2.37	0.43
2:E:33:TYR:O	2:E:57:TYR:HB3	2.17	0.43
2:C:175:PHE:CE1	3:D:179:SER:HB3	2.53	0.43
2:O:39:TRP:O	2:O:51:VAL:HG22	2.19	0.43
1:N:212:ILE:HG23	1:N:213:SER:N	2.34	0.43
1:N:222:ASN:O	1:N:226:ILE:HG13	2.18	0.43
1:B:186:LEU:O	1:B:186:LEU:HD13	2.18	0.43
1:S:256:ILE:O	1:S:260:ILE:HG13	2.19	0.43
1:H:24:GLY:HA3	1:H:238:PHE:CZ	2.54	0.43
1:A:265:ASP:OD1	1:A:267:ASN:ND2	2.51	0.43
2:Q:197:SER:HB2	2:Q:201:GLN:CG	2.49	0.43
2:K:67:VAL:HB	2:K:71:PHE:CG	2.53	0.43
1:N:267:ASN:HA	1:N:309:PHE:CD1	2.54	0.43
1:B:46:GLN:OE1	1:B:49:LYS:HD2	2.19	0.43
2:C:32:LEU:CD1	2:C:37:ILE:HD11	2.49	0.43
1:N:183:LEU:HD23	1:N:183:LEU:HA	1.86	0.43
1:G:246:PHE:CG	1:G:247:LEU:N	2.87	0.43
2:W:33:TYR:HD2	2:W:34:TYR:CE1	2.36	0.43
1:M:51:PHE:CE1	1:M:162:THR:HB	2.54	0.43
2:I:144:THR:CG2	2:I:192:THR:HB	2.49	0.43
2:I:51:VAL:HG23	2:I:52:ALA:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:PHE:CZ	1:G:226:ILE:HD12	2.53	0.43
2:W:38:HIS:O	2:W:99:CYS:HA	2.18	0.43
1:N:167:THR:HB	1:N:173:THR:OG1	2.19	0.43
3:J:162:SER:HA	3:J:181:THR:O	2.19	0.43
1:M:58:PRO:HB2	1:N:171:GLY:HA3	2.01	0.43
1:T:180:PRO:HA	1:T:223:VAL:HG13	2.01	0.43
2:C:162:SER:HB2	2:C:206:ASN:HB2	2.00	0.43
2:I:176:PRO:HD2	3:J:165:SER:OG	2.19	0.43
1:M:225:THR:O	1:M:228:GLN:HG2	2.19	0.43
1:S:321:ILE:HG22	1:S:327:LEU:CD2	2.44	0.43
1:H:168:ALA:HB1	1:H:169:PRO:HD2	2.01	0.43
1:A:186:LEU:CD2	1:B:129:LEU:HG	2.48	0.43
3:R:206:SER:HB2	3:R:207:PRO:HD2	2.00	0.43
2:C:210:LYS:HB2	2:C:211:PRO:HD3	2.00	0.43
2:C:212:SER:OG	2:C:214:THR:OG1	2.33	0.43
2:O:177:ALA:HA	2:O:187:LEU:HB3	2.01	0.43
2:K:105:TYR:H	2:K:105:TYR:HD1	1.67	0.43
1:A:136:ILE:CG2	1:B:175:ARG:NH1	2.82	0.42
2:U:58:SER:O	2:U:58:SER:OG	2.20	0.42
3:P:213:ASN:HB2	3:P:216:GLU:CG	2.49	0.42
3:P:145:ARG:HH21	3:P:166:VAL:CG1	2.27	0.42
1:B:267:ASN:HA	1:B:309:PHE:CD1	2.54	0.42
1:N:76:LYS:HE2	1:N:81:ASN:O	2.18	0.42
2:U:193:VAL:HB	2:U:194:PRO:HD2	2.01	0.42
2:K:14:LEU:HD23	2:K:14:LEU:C	2.38	0.42
1:T:130:THR:HA	1:T:133:ILE:HG13	2.01	0.42
1:M:186:LEU:HD11	1:N:133:ILE:HD11	2.01	0.42
2:U:79:LYS:HE2	2:U:79:LYS:HB3	1.80	0.42
3:F:152:LYS:HE2	3:F:157:LEU:HD21	2.01	0.42
3:F:111:ARG:CG	3:F:112:THR:N	2.81	0.42
1:B:187:LEU:HD21	1:B:220:LYS:HA	2.01	0.42
2:C:36:SER:OG	2:C:102:GLY:HA2	2.19	0.42
2:I:16:GLN:OE1	2:I:122:SER:HA	2.20	0.42
2:O:187:LEU:HD12	2:O:187:LEU:C	2.40	0.42
2:W:177:ALA:HA	2:W:187:LEU:HB3	2.02	0.42
3:P:149:VAL:HA	3:P:198:GLU:O	2.19	0.42
3:R:116:PRO:HB3	3:R:142:PHE:HB3	2.01	0.42
1:S:298:TYR:O	1:S:302:ILE:HG13	2.19	0.42
3:D:145:ARG:HG2	3:D:145:ARG:O	2.19	0.42
2:W:140:THR:HB	2:W:141:SER:CA	2.47	0.42
1:B:187:LEU:HD11	1:B:216:LEU:CG	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:222:ASN:O	1:M:226:ILE:HG13	2.19	0.42
3:J:145:ARG:HH21	3:J:145:ARG:HG2	1.84	0.42
1:T:91:SER:O	1:T:95:LYS:HG3	2.18	0.42
1:T:345:LYS:HG3	1:T:349:GLU:OE2	2.19	0.42
2:U:15:VAL:HG22	2:U:16:GLN:N	2.34	0.42
2:C:15:VAL:HG22	2:C:16:GLN:N	2.33	0.42
2:O:79:LYS:HE2	2:O:79:LYS:HB3	1.87	0.42
1:B:246:PHE:CD1	1:B:247:LEU:CD1	3.02	0.42
1:A:129:LEU:O	1:A:133:ILE:HG13	2.20	0.42
2:W:54:ILE:HB	2:W:73:ILE:HD13	2.01	0.42
2:W:37:ILE:HD12	2:W:37:ILE:N	2.35	0.42
1:B:70:PHE:CE1	1:B:85:CYS:HB2	2.54	0.42
3:F:172:LYS:NZ	9:F:317:HOH:O	2.34	0.42
1:A:175:ARG:HH21	1:B:90:PRO:HG2	1.85	0.42
3:P:36:TRP:CZ3	3:P:89:CYS:HB3	2.55	0.42
3:L:51:SER:O	3:L:52:ALA:HB3	2.20	0.42
1:G:90:PRO:HG2	1:H:175:ARG:HH22	1.83	0.42
3:L:157:LEU:CD1	1:S:325:ASN:HD21	2.33	0.42
2:I:103:ARG:NH1	2:I:110:ASP:OD2	2.46	0.42
3:F:36:TRP:CH2	3:F:89:CYS:HB3	2.55	0.42
1:S:13:ILE:HA	1:S:42:MET:HG2	2.02	0.42
1:G:350:LEU:O	9:G:502:HOH:O	2.21	0.42
3:F:21:THR:HG23	3:F:73:THR:HG23	2.01	0.42
1:B:168:ALA:O	1:B:173:THR:OG1	2.32	0.42
1:A:185:LYS:HD2	1:B:129:LEU:HD13	2.02	0.42
2:W:209:HIS:CE1	2:W:211:PRO:HG2	2.54	0.42
2:E:15:VAL:HG21	2:E:89:LEU:HD13	2.01	0.42
1:G:299:LEU:HD21	1:G:313:LYS:HD3	2.01	0.42
1:N:212:ILE:C	1:N:212:ILE:HD13	2.39	0.42
1:G:317:CYS:HA	1:G:347:ILE:HB	2.02	0.42
1:M:168:ALA:HB1	1:M:169:PRO:HD2	2.02	0.42
3:D:48:LEU:HA	3:D:59:VAL:HG21	2.02	0.42
2:W:188:SER:OG	9:W:311:HOH:O	2.21	0.42
3:F:9:PRO:HG2	3:F:12:LEU:HB3	2.02	0.42
1:T:242:CYS:HB2	1:T:248:SER:OG	2.20	0.42
2:K:138:LYS:HB2	2:K:138:LYS:HE2	1.70	0.42
2:U:58:SER:C	2:U:60:SER:N	2.72	0.42
2:Q:101:ARG:HA	2:Q:102:GLY:HA3	1.80	0.42
1:A:256:ILE:O	1:A:260:ILE:HG13	2.20	0.42
2:W:63:TYR:CZ	2:W:73:ILE:HG22	2.55	0.42
1:G:320:GLU:OE1	1:G:322:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:131:PHE:CE1	3:P:127:GLN:HA	2.55	0.42
1:M:179:LEU:HB3	1:M:180:PRO:HD3	2.01	0.42
3:R:213:ASN:HB2	3:R:216:GLU:CD	2.39	0.42
3:X:15:SER:OG	3:X:110:LYS:HG2	2.20	0.42
1:N:149:ILE:HD12	1:N:226:ILE:CG1	2.38	0.42
1:H:174:LEU:HD21	1:H:255:LEU:HD12	2.02	0.42
1:B:147:LYS:HE3	1:B:151:ARG:HH21	1.81	0.42
1:S:187:LEU:CD1	1:S:216:LEU:HD11	2.50	0.42
1:T:144:GLU:CD	1:T:147:LYS:HE2	2.40	0.42
1:T:321:ILE:HG22	1:T:327:LEU:CD2	2.47	0.42
1:S:249:LEU:HD13	2:U:104:TRP:CZ2	2.55	0.42
1:M:189:LYS:O	1:M:192:GLU:HG2	2.19	0.42
1:M:329:LYS:O	1:M:332:GLN:HG2	2.19	0.42
3:V:122:PRO:HB3	3:V:212:PHE:CE1	2.55	0.42
1:B:31:LYS:HB2	7:B:402[B]:ADP:O1B	2.20	0.41
2:U:180:GLN:HA	3:V:163:GLN:HE22	1.85	0.41
1:G:322:ARG:NH2	1:H:246:PHE:CZ	2.88	0.41
2:Q:33:TYR:HD2	2:Q:34:TYR:CD1	2.38	0.41
2:E:163:TRP:CH2	2:E:205:CYS:HB3	2.55	0.41
1:S:58:PRO:HB2	1:T:171:GLY:HA3	2.02	0.41
3:X:122:PRO:HB3	3:X:212:PHE:CE1	2.54	0.41
1:T:8:ASN:CA	1:T:312:VAL:HG22	2.50	0.41
3:X:14:ALA:HA	3:X:110:LYS:HE3	2.02	0.41
2:K:177:ALA:HA	2:K:187:LEU:HB3	2.02	0.41
3:L:36:TRP:CZ3	3:L:89:CYS:HB3	2.55	0.41
3:P:29:SER:HA	3:P:70:THR:HG22	2.03	0.41
3:V:170:ASP:HB3	3:V:173:ASP:OD1	2.20	0.41
2:I:36:SER:OG	2:I:102:GLY:HA2	2.20	0.41
3:L:128:LEU:O	3:L:186:LYS:HD2	2.20	0.41
1:A:30:GLY:HA2	8:A:404[A]:ATP:O3A	2.20	0.41
3:X:51:SER:O	3:X:52:ALA:HB3	2.21	0.41
3:F:51:SER:O	3:F:52:ALA:HB3	2.20	0.41
3:X:93:PRO:HG2	3:X:96:SER:OG	2.20	0.41
1:H:299:LEU:HD21	1:H:313:LYS:HD3	2.03	0.41
1:T:212:ILE:HG23	1:T:213:SER:N	2.36	0.41
2:Q:215:LYS:N	2:Q:215:LYS:HD2	2.34	0.41
1:A:151:ARG:CG	1:A:159:THR:HG22	2.40	0.41
1:B:159:THR:OG1	1:B:160:PHE:N	2.53	0.41
3:L:34:VAL:HG21	3:L:72:PHE:CE1	2.55	0.41
2:C:202:THR:HG23	2:C:219:LYS:HD2	2.01	0.41
2:W:155:PHE:CG	2:W:156:PRO:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:HD12	1:A:313:LYS:HB3	2.03	0.41
2:Q:210:LYS:N	2:Q:211:PRO:CD	2.81	0.41
1:H:187:LEU:HD13	1:H:187:LEU:O	2.21	0.41
3:P:213:ASN:HB2	3:P:216:GLU:HG3	2.02	0.41
1:N:321:ILE:HG22	1:N:327:LEU:HD23	2.02	0.41
1:A:170:THR:HG23	1:A:255:LEU:HD13	2.02	0.41
3:R:51:SER:O	3:R:52:ALA:HB3	2.20	0.41
3:X:20:VAL:O	3:X:75:THR:HA	2.20	0.41
3:F:62:ARG:O	3:F:76:ILE:HA	2.20	0.41
2:O:208:ASN:HB3	2:O:215:LYS:HZ1	1.83	0.41
3:P:3:ILE:HG21	3:P:91:GLN:HE22	1.84	0.41
3:R:115:ALA:HB1	3:R:204:LEU:CD2	2.51	0.41
3:D:34:VAL:HG21	3:D:72:PHE:CZ	2.55	0.41
1:G:177:LEU:HD13	1:G:264:MET:HE3	2.03	0.41
2:K:161:VAL:HA	2:K:206:ASN:O	2.21	0.41
1:G:285:CYS:HB2	1:H:285:CYS:SG	2.60	0.41
1:B:142:PHE:CZ	1:B:226:ILE:HD12	2.55	0.41
1:A:320:GLU:CB	1:B:246:PHE:CZ	3.03	0.41
3:J:59:VAL:HA	3:J:60:PRO:HD3	1.97	0.41
1:N:250:TYR:O	1:N:254:ARG:HB2	2.21	0.41
2:W:155:PHE:HA	2:W:156:PRO:HA	1.84	0.41
1:A:29:VAL:HG21	1:A:241:VAL:O	2.21	0.41
3:F:128:LEU:O	3:F:186:LYS:HD2	2.20	0.41
1:G:69:LYS:NZ	2:K:59:SER:OG	2.33	0.41
1:A:278:GLU:HG2	1:A:292:TRP:CD1	2.56	0.41
1:S:305:LEU:HD22	2:U:105:TYR:HA	2.03	0.41
3:L:111:ARG:HD2	3:L:173:ASP:O	2.20	0.41
1:B:302:ILE:HG23	1:B:306:TYR:HD2	1.86	0.41
1:G:276:PHE:O	1:G:279:ASN:HB2	2.21	0.41
1:M:126:LEU:N	1:M:126:LEU:CD1	2.84	0.41
1:B:316:LEU:HD12	8:B:403[A]:ATP:C2	2.54	0.41
1:T:6:GLU:HA	1:T:7:PRO:HD3	1.95	0.41
1:T:183:LEU:O	1:T:187:LEU:HG	2.20	0.41
1:G:183:LEU:HD23	1:G:183:LEU:HA	1.95	0.41
1:G:321:ILE:HD12	1:G:321:ILE:H	1.84	0.41
2:U:101:ARG:HA	2:U:102:GLY:HA3	1.85	0.41
2:U:107:ARG:HB3	3:V:92:TYR:HB2	2.01	0.41
1:T:150:LYS:HE3	1:T:222:ASN:OD1	2.21	0.41
1:A:25:GLY:N	1:A:31:LYS:HD3	2.35	0.41
3:L:143:TYR:CG	3:L:144:PRO:HA	2.56	0.41
2:E:57:TYR:CD1	2:E:58:SER:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:304:GLU:OE1	2:W:106:ARG:HD3	2.20	0.41
3:F:189:TYR:HA	3:F:195:TYR:OH	2.20	0.41
3:F:22:ILE:HG12	3:F:105:THR:HG21	2.02	0.41
1:M:69:LYS:HB3	2:Q:77:THR:OG1	2.20	0.41
2:K:32:LEU:C	2:K:32:LEU:HD12	2.40	0.41
2:C:79:LYS:HB3	2:C:79:LYS:HE2	1.86	0.41
1:M:56:THR:OG1	1:M:167:THR:HA	2.21	0.41
2:W:161:VAL:HA	2:W:206:ASN:O	2.20	0.41
1:M:316:LEU:HA	8:M:404[A]:ATP:N1	2.36	0.41
1:A:51:PHE:CD1	1:A:162:THR:HB	2.55	0.41
1:T:168:ALA:HB1	1:T:169:PRO:HD2	2.03	0.41
1:A:320:GLU:OE2	1:B:246:PHE:CD2	2.73	0.41
3:D:35:ALA:HA	3:D:49:ILE:O	2.21	0.41
1:S:240:CYS:SG	1:S:252:THR:HG23	2.61	0.41
2:Q:54:ILE:HG13	2:Q:61:THR:HG22	2.03	0.41
1:H:179:LEU:N	1:H:180:PRO:CD	2.84	0.40
2:W:50:TRP:CG	3:X:99:ILE:HB	2.56	0.40
3:L:50:TYR:O	3:L:54:SER:HB2	2.21	0.40
3:F:48:LEU:HA	3:F:59:VAL:HG21	2.03	0.40
3:D:13:SER:HB2	3:D:108:GLU:OE2	2.21	0.40
1:M:250:TYR:HD1	2:O:57:TYR:CD1	2.39	0.40
3:R:40:LYS:HB3	3:R:41:PRO:HD2	2.03	0.40
3:P:122:PRO:HA	3:P:212:PHE:CZ	2.56	0.40
1:G:265:ASP:OD1	1:G:267:ASN:ND2	2.54	0.40
3:J:62:ARG:NE	3:J:83:ASP:OD2	2.43	0.40
1:A:58:PRO:HB2	1:B:171:GLY:HA3	2.03	0.40
1:S:183:LEU:HA	1:S:183:LEU:HD23	1.95	0.40
2:Q:208:ASN:CA	2:Q:215:LYS:HZ1	2.33	0.40
2:E:106:ARG:NH1	2:E:106:ARG:HG3	2.35	0.40
3:X:115:ALA:HB1	3:X:204:LEU:CD2	2.51	0.40
3:R:143:TYR:CD1	3:R:144:PRO:HA	2.57	0.40
2:I:161:VAL:HG22	2:I:174:THR:HG21	2.03	0.40
1:M:90:PRO:HG2	1:N:175:ARG:HH21	1.86	0.40
3:X:118:VAL:HA	3:X:138:LEU:O	2.21	0.40
2:Q:197:SER:HB2	2:Q:201:GLN:HG3	2.03	0.40
1:B:57:ASN:HA	1:B:168:ALA:HB2	2.04	0.40
2:Q:67:VAL:HG12	2:Q:70:ARG:NH2	2.36	0.40
1:M:133:ILE:HA	1:M:134:PRO:HD3	1.92	0.40
2:I:79:LYS:HB3	2:I:79:LYS:HE2	1.81	0.40
2:I:187:LEU:C	2:I:187:LEU:HD12	2.42	0.40
3:J:29:SER:HA	3:J:70:THR:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:154:ASP:OD1	3:J:192:HIS:HB3	2.22	0.40
3:L:157:LEU:HD13	1:S:325:ASN:HD21	1.85	0.40
2:Q:106:ARG:HD3	2:Q:106:ARG:HH21	1.79	0.40
1:H:94:LEU:CD1	1:H:131:GLY:HA2	2.52	0.40
1:N:180:PRO:O	1:N:184:SER:HB2	2.21	0.40
3:V:154:ASP:O	3:V:155:ASN:HB2	2.20	0.40
1:S:62:LEU:HB2	1:S:87:GLU:OE2	2.22	0.40
1:S:37:SER:HB3	1:S:331:SER:CB	2.51	0.40
3:X:162:SER:HA	3:X:181:THR:O	2.21	0.40
1:M:14:THR:HG22	1:M:45:SER:OG	2.22	0.40
2:U:187:LEU:HD12	2:U:187:LEU:C	2.41	0.40
1:B:193:ILE:HG22	1:B:193:ILE:O	2.21	0.40
3:F:90:GLN:HE21	3:F:99:ILE:HG23	1.86	0.40
3:P:111:ARG:HH22	3:P:114:ALA:HB3	1.85	0.40
1:A:182:THR:O	1:A:186:LEU:HD23	2.21	0.40
3:P:154:ASP:O	3:P:155:ASN:HB2	2.20	0.40
3:P:48:LEU:HB3	3:P:49:ILE:HD12	2.03	0.40
2:W:15:VAL:HG22	2:W:16:GLN:N	2.36	0.40
1:N:133:ILE:HA	1:N:134:PRO:HD3	1.94	0.40
3:L:116:PRO:HB3	3:L:142:PHE:HB3	2.03	0.40
2:Q:7:LEU:O	9:Q:302:HOH:O	2.22	0.40
2:I:131:PHE:CE1	3:J:127:GLN:HA	2.57	0.40
1:M:240:CYS:SG	1:M:252:THR:HG23	2.62	0.40
3:V:128:LEU:O	3:V:186:LYS:HD2	2.22	0.40
1:M:36:CYS:O	1:M:40:ILE:HG13	2.21	0.40
1:B:6:GLU:HA	1:B:7:PRO:HD3	1.86	0.40
2:W:79:LYS:HE2	2:W:79:LYS:HB3	1.88	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:141:SER:OG	1:S:188:GLU:OE2[1_564]	1.82	0.38
1:H:48:ASN:OD1	2:W:24:SER:OG[1_455]	2.13	0.07
1:M:188:GLU:OE1	2:W:138:LYS:NZ[1_455]	2.15	0.05

## 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	A	283/354 (80%)	277 (98%)	6 (2%)	0	100	100
1	B	287/354 (81%)	280 (98%)	7 (2%)	0	100	100
1	G	284/354 (80%)	278 (98%)	5 (2%)	1 (0%)	39	72
1	H	290/354 (82%)	285 (98%)	4 (1%)	1 (0%)	46	77
1	M	296/354 (84%)	289 (98%)	6 (2%)	1 (0%)	46	77
1	N	290/354 (82%)	282 (97%)	4 (1%)	4 (1%)	14	38
1	S	288/354 (81%)	284 (99%)	3 (1%)	1 (0%)	46	77
1	T	298/354 (84%)	293 (98%)	4 (1%)	1 (0%)	46	77
2	C	214/230 (93%)	204 (95%)	9 (4%)	1 (0%)	34	67
2	E	220/230 (96%)	207 (94%)	12 (6%)	1 (0%)	34	67
2	I	216/230 (94%)	207 (96%)	8 (4%)	1 (0%)	34	67
2	K	212/230 (92%)	205 (97%)	7 (3%)	0	100	100
2	O	214/230 (93%)	204 (95%)	10 (5%)	0	100	100
2	Q	219/230 (95%)	205 (94%)	12 (6%)	2 (1%)	21	52
2	U	210/230 (91%)	199 (95%)	9 (4%)	2 (1%)	19	48
2	W	219/230 (95%)	206 (94%)	12 (6%)	1 (0%)	34	67
3	D	214/217 (99%)	209 (98%)	4 (2%)	1 (0%)	34	67
3	F	213/217 (98%)	207 (97%)	5 (2%)	1 (0%)	34	67
3	J	213/217 (98%)	208 (98%)	5 (2%)	0	100	100
3	L	213/217 (98%)	206 (97%)	5 (2%)	2 (1%)	21	52
3	P	214/217 (99%)	208 (97%)	5 (2%)	1 (0%)	34	67
3	R	214/217 (99%)	208 (97%)	6 (3%)	0	100	100
3	V	213/217 (98%)	205 (96%)	6 (3%)	2 (1%)	21	52
3	X	214/217 (99%)	208 (97%)	5 (2%)	1 (0%)	34	67
All	All	5748/6408 (90%)	5564 (97%)	159 (3%)	25 (0%)	39	72

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	206	SER
3	F	206	SER
2	I	59	SER
3	L	206	SER
1	N	283	HIS
3	P	95	TYR
2	Q	142	GLY
2	U	59	SER
2	U	208	ASN
3	V	95	TYR
3	V	206	SER
3	X	206	SER
1	H	191	GLY
3	L	95	TYR
1	N	285	CYS
1	S	125	ALA
2	C	59	SER
2	E	141	SER
1	T	191	GLY
1	G	280	ASP
1	N	191	GLY
1	N	3	LEU
2	Q	144	THR
2	W	140	THR
1	M	191	GLY

### 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	A	263/309 (85%)	257 (98%)	6 (2%)	58	87
1	B	263/309 (85%)	258 (98%)	5 (2%)	65	89
1	G	264/309 (85%)	262 (99%)	2 (1%)	86	96
1	H	269/309 (87%)	263 (98%)	6 (2%)	60	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	273/309 (88%)	266 (97%)	7 (3%)	54	84
1	N	270/309 (87%)	267 (99%)	3 (1%)	80	94
1	S	263/309 (85%)	262 (100%)	1 (0%)	93	98
1	T	270/309 (87%)	268 (99%)	2 (1%)	88	97
2	C	182/193 (94%)	180 (99%)	2 (1%)	80	94
2	E	185/193 (96%)	184 (100%)	1 (0%)	92	97
2	I	184/193 (95%)	184 (100%)	0	100	100
2	K	181/193 (94%)	179 (99%)	2 (1%)	80	94
2	O	180/193 (93%)	178 (99%)	2 (1%)	80	94
2	Q	184/193 (95%)	181 (98%)	3 (2%)	70	91
2	U	179/193 (93%)	178 (99%)	1 (1%)	90	97
2	W	184/193 (95%)	181 (98%)	3 (2%)	70	91
3	D	191/192 (100%)	189 (99%)	2 (1%)	82	95
3	F	190/192 (99%)	188 (99%)	2 (1%)	80	94
3	J	190/192 (99%)	189 (100%)	1 (0%)	92	97
3	L	190/192 (99%)	188 (99%)	2 (1%)	80	94
3	P	191/192 (100%)	189 (99%)	2 (1%)	82	95
3	R	191/192 (100%)	189 (99%)	2 (1%)	82	95
3	V	190/192 (99%)	190 (100%)	0	100	100
3	X	191/192 (100%)	190 (100%)	1 (0%)	92	97
All	All	5118/5552 (92%)	5060 (99%)	58 (1%)	80	94

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	MET
1	A	126	LEU
1	A	129	LEU
1	A	278	GLU
1	A	279	ASN
1	A	322	ARG
1	B	98	ASN
1	B	188	GLU
1	B	189	LYS
1	B	218	GLU

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Mol	Chain	Res	Type
1	B	246	PHE
2	C	207	VAL
2	C	214	THR
3	D	111	ARG
3	D	202	GLN
2	E	57	TYR
3	F	111	ARG
3	F	145	ARG
1	G	126	LEU
1	G	284	ASN
1	H	99	ASP
1	H	126	LEU
1	H	129	LEU
1	H	212	ILE
1	H	283	HIS
1	H	322	ARG
3	J	111	ARG
2	K	138	LYS
2	K	207	VAL
3	L	98	LEU
3	L	145	ARG
1	M	96	ASP
1	M	126	LEU
1	M	181	ASN
1	M	182	THR
1	M	190	PHE
1	M	222	ASN
1	M	282	GLU
1	N	76	LYS
1	N	184	SER
1	N	212	ILE
2	O	101	ARG
2	O	106	ARG
3	P	111	ARG
3	P	217	CYS
2	Q	62	SER
2	Q	215	LYS
2	Q	217	ASP
3	R	111	ARG
3	R	217	CYS
1	S	294	MET
1	T	88	ILE

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Mol	Chain	Res	Type
1	T	194	THR
2	U	207	VAL
2	W	57	TYR
2	W	140	THR
2	W	207	VAL
3	X	111	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	148	HIS
1	H	61	ASN
1	H	98	ASN
1	H	279	ASN
1	M	152	GLN
1	N	222	ASN
1	N	301	GLN
2	Q	173	HIS
3	R	127	GLN
3	R	140	ASN
1	S	41	GLN
1	S	48	ASN
1	S	98	ASN
1	S	148	HIS
1	T	154	GLN
3	V	38	GLN
2	W	173	HIS
3	X	140	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 28 ligands modelled in this entry, 12 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	ADP	A	403[B]	5	22,29,29	4.05	7 (31%)	27,45,45	2.72	3 (11%)
8	ATP	A	404[A]	5	24,33,33	2.27	9 (37%)	31,52,52	2.20	7 (22%)
7	ADP	B	402[B]	1,5	22,29,29	4.07	8 (36%)	27,45,45	2.80	4 (14%)
8	ATP	B	403[A]	5	24,33,33	2.28	9 (37%)	31,52,52	2.21	6 (19%)
7	ADP	G	403[B]	5	22,29,29	4.04	6 (27%)	27,45,45	2.81	4 (14%)
8	ATP	G	404[A]	5	24,33,33	2.25	9 (37%)	31,52,52	2.33	8 (25%)
7	ADP	H	402[B]	1,5	22,29,29	4.06	8 (36%)	27,45,45	2.81	4 (14%)
8	ATP	H	403[A]	5	24,33,33	2.25	9 (37%)	31,52,52	2.22	7 (22%)
7	ADP	M	403[B]	1,5	22,29,29	4.14	5 (22%)	27,45,45	2.99	5 (18%)
8	ATP	M	404[A]	1,5	24,33,33	2.45	8 (33%)	31,52,52	2.44	12 (38%)
7	ADP	N	402[B]	5	22,29,29	4.08	7 (31%)	27,45,45	2.79	3 (11%)
8	ATP	N	403[A]	5	24,33,33	2.29	9 (37%)	31,52,52	2.26	7 (22%)
7	ADP	S	403[B]	5	22,29,29	4.05	7 (31%)	27,45,45	2.79	4 (14%)
8	ATP	S	404[A]	5	24,33,33	2.31	9 (37%)	31,52,52	2.26	10 (32%)
7	ADP	T	402[B]	1,5	22,29,29	4.09	7 (31%)	27,45,45	2.75	3 (11%)
8	ATP	T	403[A]	1,5	24,33,33	2.28	9 (37%)	31,52,52	2.23	11 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	A	403[B]	5	-	0/12/32/32	0/3/3/3
8	ATP	A	404[A]	5	-	0/18/38/38	0/3/3/3
7	ADP	B	402[B]	1,5	-	0/12/32/32	0/3/3/3
8	ATP	B	403[A]	5	-	0/18/38/38	0/3/3/3
7	ADP	G	403[B]	5	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ATP	G	404[A]	5	-	0/18/38/38	0/3/3/3
7	ADP	H	402[B]	1,5	-	0/12/32/32	0/3/3/3
8	ATP	H	403[A]	5	-	0/18/38/38	0/3/3/3
7	ADP	M	403[B]	1,5	-	0/12/32/32	0/3/3/3
8	ATP	M	404[A]	1,5	-	0/18/38/38	0/3/3/3
7	ADP	N	402[B]	5	-	0/12/32/32	0/3/3/3
8	ATP	N	403[A]	5	-	0/18/38/38	0/3/3/3
7	ADP	S	403[B]	5	-	0/12/32/32	0/3/3/3
8	ATP	S	404[A]	5	-	0/18/38/38	0/3/3/3
7	ADP	T	402[B]	1,5	-	0/12/32/32	0/3/3/3
8	ATP	T	403[A]	1,5	-	0/18/38/38	0/3/3/3

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	403[B]	ADP	O4'-C4'	-5.60	1.32	1.45
7	N	402[B]	ADP	O4'-C4'	-5.55	1.32	1.45
7	A	403[B]	ADP	O4'-C4'	-5.53	1.32	1.45
7	T	402[B]	ADP	O4'-C4'	-5.52	1.32	1.45
7	S	403[B]	ADP	O4'-C4'	-5.51	1.32	1.45
7	M	403[B]	ADP	O4'-C4'	-5.43	1.32	1.45
7	H	402[B]	ADP	O4'-C4'	-5.41	1.32	1.45
7	B	402[B]	ADP	O4'-C4'	-5.39	1.32	1.45
8	S	404[A]	ATP	C2-N1	-5.21	1.24	1.33
8	B	403[A]	ATP	C2-N1	-5.20	1.24	1.33
8	N	403[A]	ATP	C2-N1	-5.16	1.24	1.33
8	G	404[A]	ATP	C2-N1	-5.14	1.24	1.33
8	M	404[A]	ATP	C2-N1	-5.09	1.24	1.33
8	H	403[A]	ATP	C2-N1	-5.07	1.24	1.33
8	T	403[A]	ATP	C2-N1	-5.04	1.24	1.33
8	A	404[A]	ATP	C2-N1	-5.00	1.24	1.33
8	M	404[A]	ATP	C6-N1	-2.52	1.25	1.37
8	N	403[A]	ATP	C6-N1	-2.50	1.25	1.37
8	A	404[A]	ATP	C6-N1	-2.48	1.25	1.37
8	H	403[A]	ATP	C6-N1	-2.47	1.25	1.37
8	B	403[A]	ATP	C6-N1	-2.47	1.25	1.37
7	G	403[B]	ADP	C5-C4	-2.47	1.34	1.40
8	G	404[A]	ATP	C6-N1	-2.46	1.25	1.37
8	S	404[A]	ATP	C6-N1	-2.45	1.25	1.37
8	T	403[A]	ATP	C6-N1	-2.45	1.25	1.37
7	B	402[B]	ADP	C5-C4	-2.43	1.35	1.40
7	S	403[B]	ADP	C5-C4	-2.42	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	402[B]	ADP	C5-C4	-2.40	1.35	1.40
7	N	402[B]	ADP	C5-C4	-2.40	1.35	1.40
7	H	402[B]	ADP	C5-C4	-2.39	1.35	1.40
7	A	403[B]	ADP	C5-C4	-2.37	1.35	1.40
8	S	404[A]	ATP	C2'-C3'	-2.25	1.47	1.53
8	A	404[A]	ATP	C2'-C3'	-2.22	1.47	1.53
8	G	404[A]	ATP	C2'-C3'	-2.20	1.47	1.53
8	N	403[A]	ATP	C2'-C3'	-2.11	1.47	1.53
8	H	403[A]	ATP	PG-O2G	-2.11	1.47	1.54
8	M	404[A]	ATP	PG-O2G	-2.11	1.47	1.54
8	B	403[A]	ATP	C2'-C3'	-2.10	1.47	1.53
8	B	403[A]	ATP	PG-O2G	-2.10	1.47	1.54
8	T	403[A]	ATP	PG-O2G	-2.10	1.47	1.54
8	T	403[A]	ATP	C2'-C3'	-2.10	1.47	1.53
8	G	404[A]	ATP	PG-O2G	-2.10	1.47	1.54
8	A	404[A]	ATP	PG-O2G	-2.10	1.47	1.54
8	S	404[A]	ATP	PG-O2G	-2.09	1.47	1.54
8	N	403[A]	ATP	PG-O2G	-2.07	1.47	1.54
8	H	403[A]	ATP	C2'-C3'	-2.05	1.47	1.53
7	N	402[B]	ADP	O3'-C3'	-2.03	1.38	1.43
7	B	402[B]	ADP	PA-O5'	2.00	1.68	1.59
7	N	402[B]	ADP	C2-N1	2.01	1.37	1.33
7	S	403[B]	ADP	C2-N1	2.02	1.37	1.33
7	S	403[B]	ADP	C2-N3	2.02	1.35	1.32
7	T	402[B]	ADP	C2-N3	2.02	1.35	1.32
7	B	402[B]	ADP	C2-N1	2.04	1.37	1.33
7	G	403[B]	ADP	C2-N1	2.06	1.37	1.33
7	H	402[B]	ADP	C2-N3	2.06	1.35	1.32
7	A	403[B]	ADP	C2-N3	2.08	1.35	1.32
7	M	403[B]	ADP	C2-N1	2.08	1.37	1.33
7	B	402[B]	ADP	C2-N3	2.10	1.35	1.32
7	H	402[B]	ADP	C2-N1	2.12	1.37	1.33
7	T	402[B]	ADP	C2-N1	2.13	1.38	1.33
7	H	402[B]	ADP	PA-O5'	2.15	1.68	1.59
7	A	403[B]	ADP	C2-N1	2.16	1.38	1.33
8	T	403[A]	ATP	C6-N6	2.86	1.43	1.34
8	A	404[A]	ATP	C6-N6	2.86	1.43	1.34
8	N	403[A]	ATP	C6-N6	2.86	1.43	1.34
8	S	404[A]	ATP	C6-N6	2.87	1.43	1.34
8	G	404[A]	ATP	C6-N6	2.88	1.43	1.34
8	H	403[A]	ATP	C6-N6	2.93	1.44	1.34
8	B	403[A]	ATP	C6-N6	2.96	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	403[B]	ADP	O2'-C2'	3.18	1.50	1.43
7	S	403[B]	ADP	O2'-C2'	3.20	1.50	1.43
7	A	403[B]	ADP	O2'-C2'	3.24	1.50	1.43
7	G	403[B]	ADP	O2'-C2'	3.27	1.50	1.43
7	N	402[B]	ADP	O2'-C2'	3.30	1.50	1.43
7	T	402[B]	ADP	O2'-C2'	3.31	1.50	1.43
7	B	402[B]	ADP	O2'-C2'	3.32	1.50	1.43
8	G	404[A]	ATP	C5-C4	3.34	1.48	1.40
8	B	403[A]	ATP	C5-C4	3.37	1.48	1.40
8	H	403[A]	ATP	C5-C4	3.41	1.48	1.40
7	H	402[B]	ADP	O2'-C2'	3.45	1.51	1.43
8	N	403[A]	ATP	C5-C4	3.47	1.48	1.40
8	A	404[A]	ATP	C5-C4	3.49	1.48	1.40
8	S	404[A]	ATP	C5-C4	3.50	1.48	1.40
8	T	403[A]	ATP	C5-C4	3.50	1.48	1.40
8	G	404[A]	ATP	C4-N3	3.70	1.41	1.35
8	H	403[A]	ATP	C8-N7	3.71	1.41	1.34
8	T	403[A]	ATP	C8-N7	3.73	1.41	1.34
8	B	403[A]	ATP	C8-N7	3.76	1.41	1.34
8	N	403[A]	ATP	C8-N7	3.77	1.41	1.34
8	A	404[A]	ATP	C8-N7	3.80	1.41	1.34
8	M	404[A]	ATP	C4-N3	3.80	1.41	1.35
8	S	404[A]	ATP	C8-N7	3.82	1.41	1.34
8	G	404[A]	ATP	C8-N7	3.84	1.42	1.34
8	B	403[A]	ATP	C4-N3	3.84	1.41	1.35
8	M	404[A]	ATP	C6-N6	3.87	1.46	1.34
8	H	403[A]	ATP	C4-N3	3.91	1.41	1.35
8	N	403[A]	ATP	C4-N3	3.91	1.41	1.35
8	G	404[A]	ATP	O4'-C1'	3.95	1.46	1.41
8	T	403[A]	ATP	C4-N3	3.99	1.41	1.35
8	A	404[A]	ATP	C4-N3	4.00	1.41	1.35
8	S	404[A]	ATP	C4-N3	4.03	1.41	1.35
8	H	403[A]	ATP	O4'-C1'	4.07	1.46	1.41
8	A	404[A]	ATP	O4'-C1'	4.09	1.46	1.41
8	M	404[A]	ATP	C5-C4	4.17	1.49	1.40
8	B	403[A]	ATP	O4'-C1'	4.18	1.46	1.41
8	N	403[A]	ATP	O4'-C1'	4.25	1.46	1.41
8	S	404[A]	ATP	O4'-C1'	4.25	1.46	1.41
8	M	404[A]	ATP	C8-N7	4.30	1.42	1.34
8	T	403[A]	ATP	O4'-C1'	4.37	1.46	1.41
8	M	404[A]	ATP	O4'-C1'	4.57	1.47	1.41
7	A	403[B]	ADP	C6-N6	5.05	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	402[B]	ADP	C6-N6	5.07	1.50	1.34
7	S	403[B]	ADP	C6-N6	5.07	1.50	1.34
7	G	403[B]	ADP	C6-N6	5.08	1.50	1.34
7	N	402[B]	ADP	C6-N6	5.08	1.50	1.34
7	H	402[B]	ADP	C6-N6	5.11	1.50	1.34
7	B	402[B]	ADP	C6-N6	5.12	1.50	1.34
7	M	403[B]	ADP	C6-N6	5.99	1.53	1.34
7	G	403[B]	ADP	O4'-C1'	16.11	1.61	1.41
7	A	403[B]	ADP	O4'-C1'	16.17	1.61	1.41
7	H	402[B]	ADP	O4'-C1'	16.18	1.61	1.41
7	S	403[B]	ADP	O4'-C1'	16.25	1.61	1.41
7	B	402[B]	ADP	O4'-C1'	16.28	1.61	1.41
7	N	402[B]	ADP	O4'-C1'	16.37	1.61	1.41
7	T	402[B]	ADP	O4'-C1'	16.38	1.61	1.41
7	M	403[B]	ADP	O4'-C1'	16.53	1.62	1.41

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	403[B]	ADP	N3-C2-N1	-11.83	119.83	128.89
7	N	402[B]	ADP	N3-C2-N1	-11.75	119.90	128.89
7	S	403[B]	ADP	N3-C2-N1	-11.72	119.92	128.89
7	T	402[B]	ADP	N3-C2-N1	-11.72	119.92	128.89
7	H	402[B]	ADP	N3-C2-N1	-11.56	120.04	128.89
7	A	403[B]	ADP	N3-C2-N1	-11.39	120.17	128.89
7	M	403[B]	ADP	N3-C2-N1	-11.38	120.18	128.89
7	B	402[B]	ADP	N3-C2-N1	-11.36	120.19	128.89
8	G	404[A]	ATP	N3-C2-N1	-8.43	122.44	128.89
8	N	403[A]	ATP	N3-C2-N1	-8.29	122.55	128.89
8	S	404[A]	ATP	N3-C2-N1	-8.25	122.58	128.89
7	M	403[B]	ADP	N6-C6-N1	-8.19	101.64	119.20
8	T	403[A]	ATP	N3-C2-N1	-8.18	122.63	128.89
8	H	403[A]	ATP	N3-C2-N1	-8.12	122.68	128.89
8	B	403[A]	ATP	N3-C2-N1	-7.91	122.84	128.89
8	A	404[A]	ATP	N3-C2-N1	-7.90	122.85	128.89
8	M	404[A]	ATP	N3-C2-N1	-7.83	122.90	128.89
7	N	402[B]	ADP	N6-C6-N1	-6.96	104.26	119.20
7	T	402[B]	ADP	N6-C6-N1	-6.94	104.31	119.20
7	S	403[B]	ADP	N6-C6-N1	-6.87	104.45	119.20
7	A	403[B]	ADP	N6-C6-N1	-6.87	104.46	119.20
7	B	402[B]	ADP	N6-C6-N1	-6.83	104.54	119.20
7	G	403[B]	ADP	N6-C6-N1	-6.82	104.56	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	402[B]	ADP	N6-C6-N1	-6.60	105.03	119.20
7	M	403[B]	ADP	C4-C5-N7	-3.77	106.01	109.48
8	M	404[A]	ATP	PA-O3A-PB	-3.61	122.60	132.73
8	G	404[A]	ATP	PA-O3A-PB	-3.59	122.64	132.73
8	B	403[A]	ATP	PA-O3A-PB	-3.47	123.00	132.73
8	N	403[A]	ATP	PA-O3A-PB	-3.45	123.05	132.73
7	B	402[B]	ADP	PA-O3A-PB	-3.29	121.62	132.67
7	M	403[B]	ADP	PA-O3A-PB	-3.23	121.82	132.67
7	H	402[B]	ADP	PA-O3A-PB	-3.23	121.84	132.67
8	S	404[A]	ATP	PA-O3A-PB	-3.23	123.67	132.73
8	H	403[A]	ATP	PA-O3A-PB	-3.14	123.92	132.73
7	G	403[B]	ADP	PA-O3A-PB	-2.89	122.98	132.67
8	T	403[A]	ATP	PA-O3A-PB	-2.87	124.67	132.73
7	N	402[B]	ADP	PA-O3A-PB	-2.87	123.05	132.67
8	A	404[A]	ATP	PB-O3B-PG	-2.85	123.09	132.67
8	A	404[A]	ATP	PA-O3A-PB	-2.82	124.81	132.73
7	S	403[B]	ADP	PA-O3A-PB	-2.78	123.35	132.67
8	G	404[A]	ATP	PB-O3B-PG	-2.77	123.38	132.67
8	M	404[A]	ATP	C4-C5-N7	-2.68	107.01	109.48
8	S	404[A]	ATP	PB-O3B-PG	-2.60	123.94	132.67
8	N	403[A]	ATP	PB-O3B-PG	-2.55	124.11	132.67
8	T	403[A]	ATP	PB-O3B-PG	-2.51	124.26	132.67
7	A	403[B]	ADP	PA-O3A-PB	-2.45	124.45	132.67
8	M	404[A]	ATP	PB-O3B-PG	-2.44	124.49	132.67
7	T	402[B]	ADP	PA-O3A-PB	-2.35	124.78	132.67
8	T	403[A]	ATP	O3G-PG-O1G	-2.18	103.58	110.58
8	B	403[A]	ATP	PB-O3B-PG	-2.16	125.43	132.67
8	B	403[A]	ATP	O2B-PB-O1B	-2.12	101.02	112.53
8	T	403[A]	ATP	O2A-PA-O1A	-2.11	101.07	112.53
8	M	404[A]	ATP	C1'-N9-C4	-2.10	123.77	126.94
8	S	404[A]	ATP	O2A-PA-O1A	-2.09	101.22	112.53
8	S	404[A]	ATP	O2G-PG-O1G	-2.09	103.87	110.58
8	S	404[A]	ATP	O2B-PB-O1B	-2.08	101.26	112.53
8	G	404[A]	ATP	C1'-N9-C4	-2.06	123.83	126.94
8	H	403[A]	ATP	O2B-PB-O1B	-2.06	101.36	112.53
8	M	404[A]	ATP	O2B-PB-O1B	-2.06	101.38	112.53
8	G	404[A]	ATP	O2A-PA-O1A	-2.06	101.39	112.53
8	N	403[A]	ATP	O3G-PG-O1G	-2.05	104.00	110.58
8	M	404[A]	ATP	O2A-PA-O1A	-2.04	101.45	112.53
8	A	404[A]	ATP	O2A-PA-O1A	-2.04	101.45	112.53
8	H	403[A]	ATP	O2G-PG-O1G	-2.03	104.04	110.58
8	T	403[A]	ATP	O2B-PB-O1B	-2.01	101.62	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	403[A]	ATP	O2A-PA-O1A	-2.01	101.64	112.53
8	T	403[A]	ATP	O2G-PG-O1G	-2.01	104.12	110.58
8	A	404[A]	ATP	O2B-PB-O1B	-2.01	101.64	112.53
8	T	403[A]	ATP	O3G-PG-O3B	2.01	114.23	105.09
8	G	404[A]	ATP	O3G-PG-O3B	2.02	114.24	105.09
8	N	403[A]	ATP	O2G-PG-O3B	2.03	114.29	105.09
8	A	404[A]	ATP	O3G-PG-O3B	2.03	114.31	105.09
8	N	403[A]	ATP	O3G-PG-O3B	2.03	114.32	105.09
8	M	404[A]	ATP	O2G-PG-O3B	2.05	114.38	105.09
8	S	404[A]	ATP	O3G-PG-O3B	2.06	114.43	105.09
8	S	404[A]	ATP	O2G-PG-O3B	2.07	114.48	105.09
7	G	403[B]	ADP	O3A-PA-O5'	2.07	108.43	102.94
8	H	403[A]	ATP	O3G-PG-O3B	2.10	114.62	105.09
8	M	404[A]	ATP	O3G-PG-O3B	2.10	114.63	105.09
8	B	403[A]	ATP	O3G-PG-O3B	2.12	114.72	105.09
8	T	403[A]	ATP	O2G-PG-O3B	2.13	114.74	105.09
7	S	403[B]	ADP	O3A-PA-O5'	2.17	108.69	102.94
8	S	404[A]	ATP	O3A-PA-O5'	2.21	108.80	102.94
8	G	404[A]	ATP	O3A-PA-O5'	2.26	108.93	102.94
7	M	403[B]	ADP	O3A-PA-O5'	2.44	109.42	102.94
8	T	403[A]	ATP	O3A-PA-O5'	2.47	109.48	102.94
8	M	404[A]	ATP	O3A-PA-O5'	2.66	110.00	102.94
8	M	404[A]	ATP	C2'-C1'-N9	2.87	118.67	114.29
7	B	402[B]	ADP	O3A-PA-O5'	3.33	111.78	102.94
7	H	402[B]	ADP	O3A-PA-O5'	3.56	112.38	102.94
8	B	403[A]	ATP	C2-N1-C6	4.94	127.60	118.77
8	H	403[A]	ATP	C2-N1-C6	5.03	127.75	118.77
8	A	404[A]	ATP	C2-N1-C6	5.05	127.79	118.77
8	S	404[A]	ATP	C2-N1-C6	5.06	127.81	118.77
8	T	403[A]	ATP	C2-N1-C6	5.06	127.82	118.77
8	N	403[A]	ATP	C2-N1-C6	5.19	128.04	118.77
8	G	404[A]	ATP	C2-N1-C6	5.24	128.13	118.77
8	M	404[A]	ATP	C2-N1-C6	6.29	130.01	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	404[A]	ATP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	402[B]	ADP	1	0
8	B	403[A]	ATP	2	0
8	G	404[A]	ATP	1	0
7	H	402[B]	ADP	1	0
8	H	403[A]	ATP	2	0
8	M	404[A]	ATP	1	0
7	T	402[B]	ADP	1	0
8	T	403[A]	ATP	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	293/354 (82%)	-0.02	6 (2%) 68 63	39, 68, 136, 194	0
1	B	297/354 (83%)	0.08	14 (4%) 35 28	29, 56, 148, 213	0
1	G	294/354 (83%)	-0.10	7 (2%) 62 56	28, 56, 134, 178	0
1	H	300/354 (84%)	0.04	14 (4%) 35 28	30, 59, 143, 244	0
1	M	304/354 (85%)	-0.05	13 (4%) 39 32	32, 57, 152, 226	0
1	N	300/354 (84%)	-0.02	9 (3%) 54 47	28, 52, 136, 183	0
1	S	296/354 (83%)	-0.01	7 (2%) 62 56	48, 77, 141, 197	0
1	T	306/354 (86%)	0.07	16 (5%) 31 24	43, 64, 139, 201	0
2	C	218/230 (94%)	-0.44	5 (2%) 64 57	32, 55, 96, 150	0
2	E	222/230 (96%)	-0.52	3 (1%) 78 73	33, 53, 98, 150	0
2	I	220/230 (95%)	-0.49	4 (1%) 71 66	28, 49, 95, 190	0
2	K	216/230 (93%)	-0.38	2 (0%) 85 82	42, 62, 119, 165	0
2	O	218/230 (94%)	-0.27	3 (1%) 78 73	36, 64, 142, 199	0
2	Q	221/230 (96%)	-0.29	5 (2%) 64 57	35, 63, 132, 223	0
2	U	214/230 (93%)	0.92	39 (18%) 2 1	55, 112, 204, 273	0
2	W	221/230 (96%)	0.11	10 (4%) 37 30	50, 82, 133, 172	0
3	D	216/217 (99%)	-0.41	1 (0%) 91 90	39, 62, 91, 165	0
3	F	215/217 (99%)	-0.52	1 (0%) 91 90	35, 52, 78, 129	0
3	J	215/217 (99%)	-0.47	1 (0%) 91 90	29, 50, 81, 178	0
3	L	215/217 (99%)	-0.42	1 (0%) 91 90	42, 71, 100, 182	0
3	P	216/217 (99%)	-0.02	12 (5%) 28 21	42, 88, 149, 231	0
3	R	216/217 (99%)	-0.25	5 (2%) 64 57	42, 69, 108, 167	0
3	V	215/217 (99%)	0.99	43 (20%) 1 1	74, 141, 202, 241	0
3	X	216/217 (99%)	0.33	18 (8%) 14 9	53, 86, 166, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
4	a	0/41	-	-	-	-
4	g	0/41	-	-	-	-
4	m	0/41	-	-	-	-
4	s	0/41	-	-	-	-
All	All	5864/6572 (89%)	-0.08	239 (4%) 41 34	28, 65, 151, 273	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	U	225	CYS	17.4
1	M	214	GLY	12.6
3	V	157	LEU	11.6
2	U	207	VAL	10.9
3	V	156	ALA	9.6
2	U	220	VAL	9.2
2	U	193	VAL	8.9
1	G	4	THR	8.4
3	V	153	VAL	7.9
3	V	110	LYS	7.8
2	O	224	SER	7.7
2	U	194	PRO	7.1
3	V	211	SER	6.8
2	O	225	CYS	6.7
2	C	138	LYS	6.7
1	B	190	PHE	6.6
1	M	193	ILE	6.6
3	V	196	ALA	6.3
3	J	217	CYS	6.3
1	N	277	ALA	6.2
3	V	195	TYR	6.1
1	M	190	PHE	6.1
2	U	133	LEU	6.0
3	V	155	ASN	5.9
2	U	161	VAL	5.9
2	U	202	THR	5.8
3	V	152	LYS	5.7
3	P	188	ASP	5.7
3	D	217	CYS	5.5
3	V	120	ILE	5.5
3	X	154	ASP	5.4
1	S	124	GLY	5.4
1	H	190	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
2	C	137	SER	5.3
1	T	129	LEU	5.3
2	W	194	PRO	5.2
3	X	195	TYR	5.1
2	I	225	CYS	5.1
2	U	219	LYS	5.0
1	M	158	GLU	4.9
2	U	203	TYR	4.9
1	A	129	LEU	4.9
2	U	223	LYS	4.8
2	Q	223	LYS	4.8
2	U	224	SER	4.7
3	V	217	CYS	4.7
2	Q	225	CYS	4.7
2	U	201	GLN	4.7
3	X	190	GLU	4.7
2	U	155	PHE	4.7
3	X	153	VAL	4.6
1	M	213	SER	4.5
2	U	198	LEU	4.5
2	U	134	ALA	4.4
3	V	112	THR	4.4
3	V	14	ALA	4.4
1	N	283	HIS	4.3
3	P	153	VAL	4.3
1	H	151	ARG	4.2
1	G	100	MET	4.2
2	U	150	LEU	4.1
1	H	127	ALA	4.1
1	M	128	ASP	4.1
3	V	213	ASN	4.0
1	T	126	LEU	4.0
1	A	127	ALA	4.0
3	X	213	ASN	3.9
2	C	136	SER	3.9
2	U	195	SER	3.9
2	U	189	SER	3.9
2	K	200	THR	3.9
2	U	170	SER	3.9
3	V	212	PHE	3.9
1	T	158	GLU	3.8
1	A	186	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	N	130	THR	3.8
1	H	128	ASP	3.7
2	W	167	ALA	3.7
3	X	209	THR	3.7
1	G	190	PHE	3.7
2	W	197	SER	3.7
3	X	155	ASN	3.7
2	U	221	GLU	3.7
3	V	202	GLN	3.7
2	I	2	ILE	3.7
2	U	169	THR	3.7
3	V	113	VAL	3.6
3	F	3	ILE	3.6
3	V	208	VAL	3.6
2	U	199	GLY	3.6
1	B	27	GLY	3.6
3	P	130	SER	3.6
3	V	111	ARG	3.5
3	V	184	LEU	3.5
3	P	155	ASN	3.5
3	P	196	ALA	3.5
2	C	225	CYS	3.4
2	U	135	PRO	3.4
3	X	188	ASP	3.4
2	Q	224	SER	3.3
3	V	130	SER	3.3
3	R	157	LEU	3.3
1	T	189	LYS	3.2
2	U	147	LEU	3.2
1	T	196	LYS	3.2
3	V	154	ASP	3.2
1	N	97	MET	3.2
1	T	214	GLY	3.2
2	E	138	LYS	3.2
3	V	59	VAL	3.1
3	L	3	ILE	3.1
2	C	224	SER	3.1
1	M	191	GLY	3.1
2	E	141	SER	3.1
1	M	212	ILE	3.1
3	X	212	PHE	3.0
3	P	157	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	W	196	SER	3.0
2	U	183	GLY	3.0
2	O	193	VAL	3.0
3	V	200	THR	3.0
3	V	193	LYS	3.0
1	T	30	GLY	3.0
1	H	279	ASN	3.0
3	V	192	HIS	2.9
1	M	216	LEU	2.9
1	A	27	GLY	2.9
1	B	216	LEU	2.9
3	V	209	THR	2.9
2	U	18	GLY	2.9
1	B	191	GLY	2.9
1	B	128	ASP	2.8
1	H	129	LEU	2.8
2	I	137	SER	2.8
1	S	152	GLN	2.8
2	U	174	THR	2.8
3	V	143	TYR	2.8
3	R	215	GLY	2.8
3	X	156	ALA	2.8
3	X	172	LYS	2.7
1	T	215	LYS	2.7
1	B	194	THR	2.7
1	T	96	ASP	2.7
3	P	150	GLN	2.7
1	H	150	LYS	2.7
3	R	186	LYS	2.7
1	T	28	GLY	2.6
3	P	194	VAL	2.6
2	I	224	SER	2.6
2	U	196	SER	2.6
1	G	189	LYS	2.6
1	H	27	GLY	2.6
2	W	223	LYS	2.6
1	H	240	CYS	2.6
3	V	151	TRP	2.6
3	V	129	LYS	2.6
1	B	246	PHE	2.6
2	Q	204	ILE	2.6
2	W	14	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	S	155	GLY	2.5
1	S	190	PHE	2.5
3	V	79	LEU	2.5
2	E	223	LYS	2.5
2	W	202	THR	2.5
3	X	189	TYR	2.5
2	U	20	SER	2.5
1	T	98	ASN	2.5
2	U	168	LEU	2.5
1	G	216	LEU	2.4
2	U	84	LEU	2.4
1	M	192	GLU	2.4
1	T	212	ILE	2.4
1	T	4	THR	2.4
3	P	192	HIS	2.4
2	Q	194	PRO	2.4
1	N	95	LYS	2.4
3	V	103	GLN	2.4
1	G	213	SER	2.4
1	S	125	ALA	2.3
2	U	216	VAL	2.3
2	W	193	VAL	2.3
3	V	204	LEU	2.3
2	U	146	ALA	2.3
1	B	185	LYS	2.3
3	P	191	LYS	2.3
1	T	27	GLY	2.3
1	B	187	LEU	2.3
1	B	150	LYS	2.3
1	B	153	GLU	2.3
1	H	194	THR	2.3
3	R	25	ARG	2.3
1	S	158	GLU	2.3
1	M	195	ASN	2.3
3	X	191	LYS	2.3
1	N	3	LEU	2.3
2	U	215	LYS	2.3
3	V	55	LEU	2.3
2	W	208	ASN	2.3
2	W	168	LEU	2.2
1	B	129	LEU	2.2
1	H	94	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	S	247	LEU	2.2
2	U	208	ASN	2.2
3	V	158	GLN	2.2
3	V	198	GLU	2.2
3	V	216	GLU	2.2
1	A	172	HIS	2.2
2	U	210	LYS	2.2
1	H	126	LEU	2.2
3	P	195	TYR	2.2
3	V	25	ARG	2.2
3	V	115	ALA	2.2
2	U	190	VAL	2.2
1	B	192	GLU	2.2
1	T	127	ALA	2.2
2	U	129	SER	2.1
1	M	99	ASP	2.1
3	V	63	PHE	2.1
3	V	191	LYS	2.1
1	N	27	GLY	2.1
1	N	213	SER	2.1
3	V	109	ILE	2.1
1	T	277	ALA	2.1
1	G	284	ASN	2.1
1	M	309	PHE	2.1
3	R	217	CYS	2.1
2	K	223	LYS	2.1
1	H	191	GLY	2.1
3	X	148	LYS	2.1
1	N	96	ASP	2.0
3	V	205	SER	2.0
3	P	185	SER	2.0
1	B	186	LEU	2.0
3	X	187	ALA	2.0
3	X	196	ALA	2.0
3	X	111	ARG	2.0
1	A	226	ILE	2.0
3	X	171	SER	2.0
1	H	153	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	ADP	N	402[B]	27/27	0.96	0.23	0.38	41,49,61,64	39
8	ATP	N	403[A]	31/31	0.96	0.23	0.23	41,49,60,64	43
5	MG	H	401	1/1	0.93	0.23	-0.11	43,43,43,43	0
8	ATP	M	404[A]	31/31	0.95	0.18	-0.12	34,42,49,52	42
7	ADP	M	403[B]	27/27	0.95	0.17	-0.17	34,42,49,52	38
8	ATP	A	404[A]	31/31	0.96	0.19	-0.18	44,50,59,60	42
7	ADP	G	403[B]	27/27	0.97	0.17	-0.21	38,45,56,60	38
7	ADP	A	403[B]	27/27	0.96	0.18	-0.24	44,50,60,60	38
8	ATP	G	404[A]	31/31	0.97	0.17	-0.25	36,44,54,60	42
8	ATP	H	403[A]	31/31	0.97	0.19	-0.29	35,46,57,62	43
7	ADP	B	402[B]	27/27	0.96	0.18	-0.30	34,42,55,62	39
8	ATP	B	403[A]	31/31	0.96	0.19	-0.31	34,42,53,62	43
8	ATP	S	404[A]	31/31	0.95	0.18	-0.36	49,57,68,72	42
7	ADP	H	402[B]	27/27	0.97	0.18	-0.39	36,45,62,62	39
7	ADP	S	403[B]	27/27	0.96	0.17	-0.42	49,57,69,71	38
8	ATP	T	403[A]	31/31	0.96	0.19	-0.46	48,56,68,73	43
7	ADP	T	402[B]	27/27	0.96	0.17	-0.66	48,56,70,73	39
6	ZN	G	402	1/1	0.99	0.06	-	67,67,67,67	0
5	MG	T	401	1/1	0.98	0.23	-	55,55,55,55	0
5	MG	G	401	1/1	0.96	0.18	-	32,32,32,32	0
5	MG	B	401	1/1	0.96	0.24	-	54,54,54,54	0
5	MG	S	401	1/1	0.90	0.15	-	53,53,53,53	0
6	ZN	M	402	1/1	0.94	0.06	-	72,72,72,72	0
5	MG	M	401	1/1	0.98	0.07	-	50,50,50,50	0
6	ZN	S	402	1/1	0.97	0.05	-	97,97,97,97	0
6	ZN	A	402	1/1	0.97	0.04	-	65,65,65,65	0
5	MG	A	401	1/1	0.93	0.18	-	57,57,57,57	0
5	MG	N	401	1/1	0.97	0.15	-	50,50,50,50	0

## 6.5 Other polymers

There are no such residues in this entry.