Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:43 AM GMT

PDB ID	:	3MUU
Title	:	Crystal structure of the Sindbis virus E2-E1 heterodimer at low pH
Authors	:	Li, L.; Jose, J.; Xiang, Y.; Kuhn, R.J.; Rossmann, M.G.
Deposited on	:	2010-05-03
Resolution	:	3.29 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

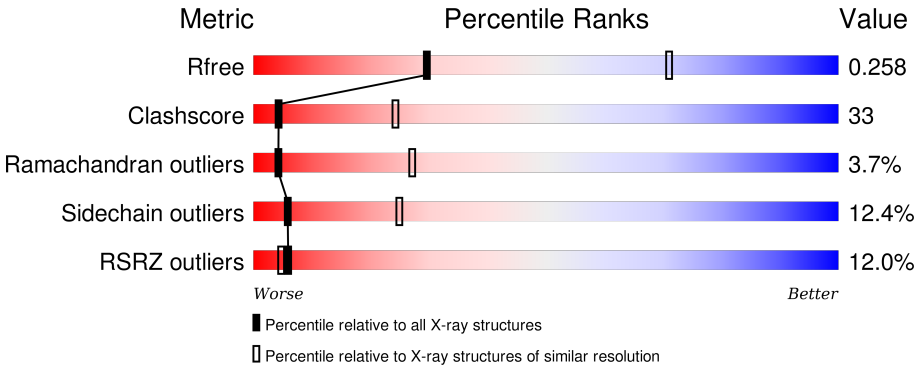
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	750	9% 39% 36% 7% 17%
1	B	750	9% 37% 38% 7% 17%
1	C	750	9% 38% 37% 7% • 17%
1	D	750	11% 39% 36% 8% 17%
1	E	750	10% 40% 35% 7% 17%

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Mol	Chain	Length	Quality of chain
1	F	750	10% 39% 36% 7% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	751	X	-	-	-
2	MAN	B	754	-	-	-	X
2	MAN	E	754	-	-	-	X
2	NAG	F	751	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 29159 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Structural polyprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	623	Total	C	N	O	S	Se	0	0	0
			4767	3015	808	910	24	10			
1	B	622	Total	C	N	O	S	Se	0	0	0
			4761	3013	808	906	24	10			
1	C	622	Total	C	N	O	S	Se	0	0	0
			4761	3012	807	908	24	10			
1	D	622	Total	C	N	O	S	Se	0	0	0
			4760	3009	807	910	24	10			
1	E	623	Total	C	N	O	S	Se	0	0	0
			4761	3012	808	907	24	10			
1	F	618	Total	C	N	O	S	Se	0	0	0
			4727	2990	801	902	24	10			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	345	GLY	-	LINKER	UNP P03316
A	346	GLY	-	LINKER	UNP P03316
A	347	GLY	-	LINKER	UNP P03316
A	348	SER	-	LINKER	UNP P03316
A	349	TRP	-	LINKER	UNP P03316
A	350	SER	-	LINKER	UNP P03316
A	351	HIS	-	LINKER	UNP P03316
A	352	PRO	-	LINKER	UNP P03316
A	353	GLN	-	LINKER	UNP P03316
A	354	PHE	-	LINKER	UNP P03316
A	355	GLU	-	LINKER	UNP P03316
A	356	LYS	-	LINKER	UNP P03316
A	357	GLY	-	LINKER	UNP P03316
A	358	GLY	-	LINKER	UNP P03316
A	359	GLY	-	LINKER	UNP P03316
A	360	GLY	-	LINKER	UNP P03316
A	435	GLY	ASP	ENGINEERED MUTATION	UNP P03316

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Chain	Residue	Modelled	Actual	Comment	Reference
B	345	GLY	-	LINKER	UNP P03316
B	346	GLY	-	LINKER	UNP P03316
B	347	GLY	-	LINKER	UNP P03316
B	348	SER	-	LINKER	UNP P03316
B	349	TRP	-	LINKER	UNP P03316
B	350	SER	-	LINKER	UNP P03316
B	351	HIS	-	LINKER	UNP P03316
B	352	PRO	-	LINKER	UNP P03316
B	353	GLN	-	LINKER	UNP P03316
B	354	PHE	-	LINKER	UNP P03316
B	355	GLU	-	LINKER	UNP P03316
B	356	LYS	-	LINKER	UNP P03316
B	357	GLY	-	LINKER	UNP P03316
B	358	GLY	-	LINKER	UNP P03316
B	359	GLY	-	LINKER	UNP P03316
B	360	GLY	-	LINKER	UNP P03316
B	435	GLY	ASP	ENGINEERED MUTATION	UNP P03316
C	345	GLY	-	LINKER	UNP P03316
C	346	GLY	-	LINKER	UNP P03316
C	347	GLY	-	LINKER	UNP P03316
C	348	SER	-	LINKER	UNP P03316
C	349	TRP	-	LINKER	UNP P03316
C	350	SER	-	LINKER	UNP P03316
C	351	HIS	-	LINKER	UNP P03316
C	352	PRO	-	LINKER	UNP P03316
C	353	GLN	-	LINKER	UNP P03316
C	354	PHE	-	LINKER	UNP P03316
C	355	GLU	-	LINKER	UNP P03316
C	356	LYS	-	LINKER	UNP P03316
C	357	GLY	-	LINKER	UNP P03316
C	358	GLY	-	LINKER	UNP P03316
C	359	GLY	-	LINKER	UNP P03316
C	360	GLY	-	LINKER	UNP P03316
C	435	GLY	ASP	ENGINEERED MUTATION	UNP P03316
D	345	GLY	-	LINKER	UNP P03316
D	346	GLY	-	LINKER	UNP P03316
D	347	GLY	-	LINKER	UNP P03316
D	348	SER	-	LINKER	UNP P03316
D	349	TRP	-	LINKER	UNP P03316
D	350	SER	-	LINKER	UNP P03316
D	351	HIS	-	LINKER	UNP P03316
D	352	PRO	-	LINKER	UNP P03316

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Chain	Residue	Modelled	Actual	Comment	Reference
D	353	GLN	-	LINKER	UNP P03316
D	354	PHE	-	LINKER	UNP P03316
D	355	GLU	-	LINKER	UNP P03316
D	356	LYS	-	LINKER	UNP P03316
D	357	GLY	-	LINKER	UNP P03316
D	358	GLY	-	LINKER	UNP P03316
D	359	GLY	-	LINKER	UNP P03316
D	360	GLY	-	LINKER	UNP P03316
D	435	GLY	ASP	ENGINEERED MUTATION	UNP P03316
E	345	GLY	-	LINKER	UNP P03316
E	346	GLY	-	LINKER	UNP P03316
E	347	GLY	-	LINKER	UNP P03316
E	348	SER	-	LINKER	UNP P03316
E	349	TRP	-	LINKER	UNP P03316
E	350	SER	-	LINKER	UNP P03316
E	351	HIS	-	LINKER	UNP P03316
E	352	PRO	-	LINKER	UNP P03316
E	353	GLN	-	LINKER	UNP P03316
E	354	PHE	-	LINKER	UNP P03316
E	355	GLU	-	LINKER	UNP P03316
E	356	LYS	-	LINKER	UNP P03316
E	357	GLY	-	LINKER	UNP P03316
E	358	GLY	-	LINKER	UNP P03316
E	359	GLY	-	LINKER	UNP P03316
E	360	GLY	-	LINKER	UNP P03316
E	435	GLY	ASP	ENGINEERED MUTATION	UNP P03316
F	345	GLY	-	LINKER	UNP P03316
F	346	GLY	-	LINKER	UNP P03316
F	347	GLY	-	LINKER	UNP P03316
F	348	SER	-	LINKER	UNP P03316
F	349	TRP	-	LINKER	UNP P03316
F	350	SER	-	LINKER	UNP P03316
F	351	HIS	-	LINKER	UNP P03316
F	352	PRO	-	LINKER	UNP P03316
F	353	GLN	-	LINKER	UNP P03316
F	354	PHE	-	LINKER	UNP P03316
F	355	GLU	-	LINKER	UNP P03316
F	356	LYS	-	LINKER	UNP P03316
F	357	GLY	-	LINKER	UNP P03316
F	358	GLY	-	LINKER	UNP P03316
F	359	GLY	-	LINKER	UNP P03316
F	360	GLY	-	LINKER	UNP P03316

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Chain	Residue	Modelled	Actual	Comment	Reference
F	435	GLY	ASP	ENGINEERED MUTATION	UNP P03316

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			50	28	2	20		
2	B	4	Total	C	N	O	0	0
			50	28	2	20		
2	B	4	Total	C	N	O	0	0
			50	28	2	20		
2	C	4	Total	C	N	O	0	0
			50	28	2	20		
2	C	4	Total	C	N	O	0	0
			50	28	2	20		
2	D	4	Total	C	N	O	0	0
			50	28	2	20		
2	E	4	Total	C	N	O	0	0
			50	28	2	20		
2	F	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		
3	E	5	Total	C	N	O	0	0
			61	34	2	25		
3	F	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

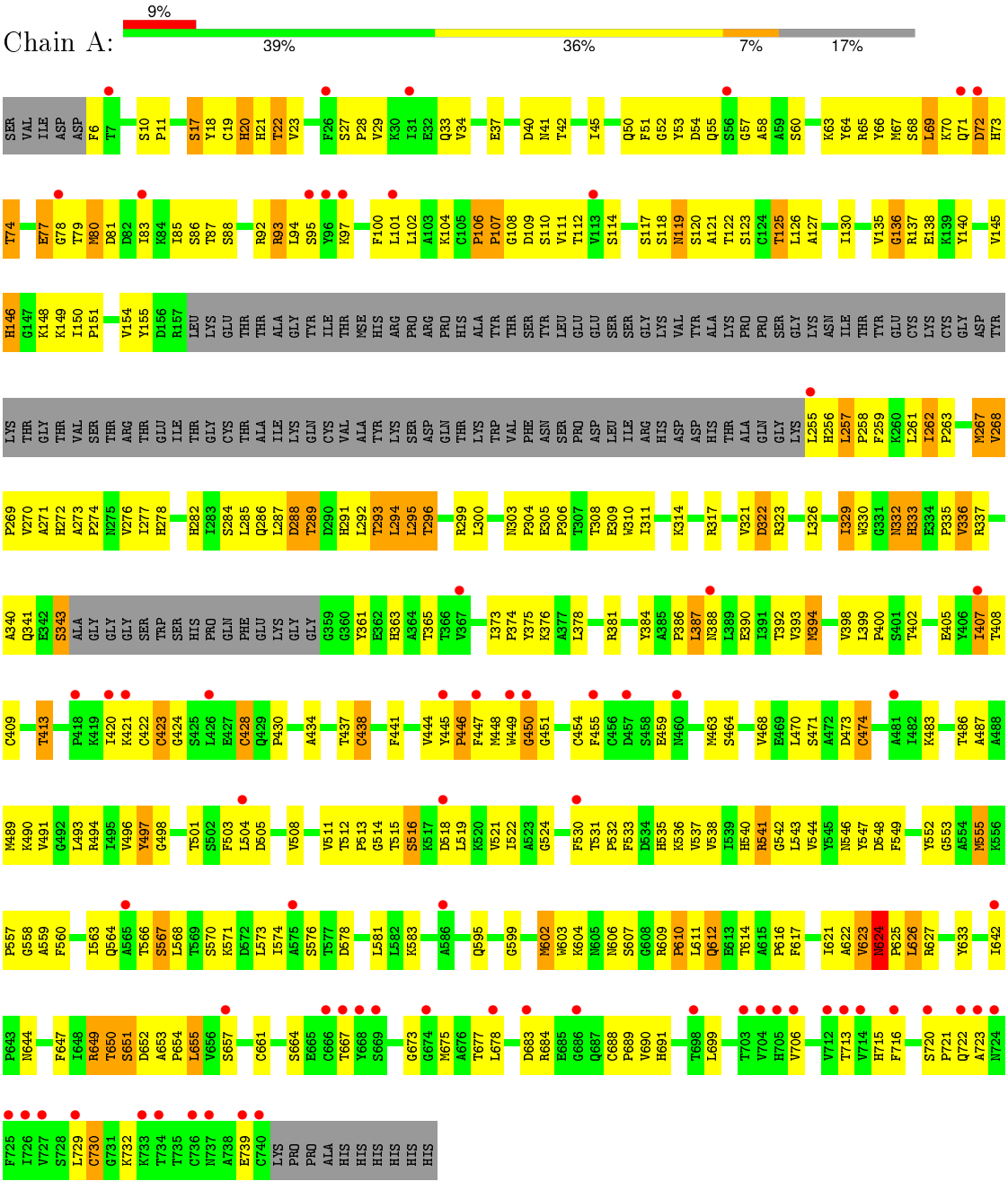
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	3	Total	C	N	O	0	0
			39	22	2	15		

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.

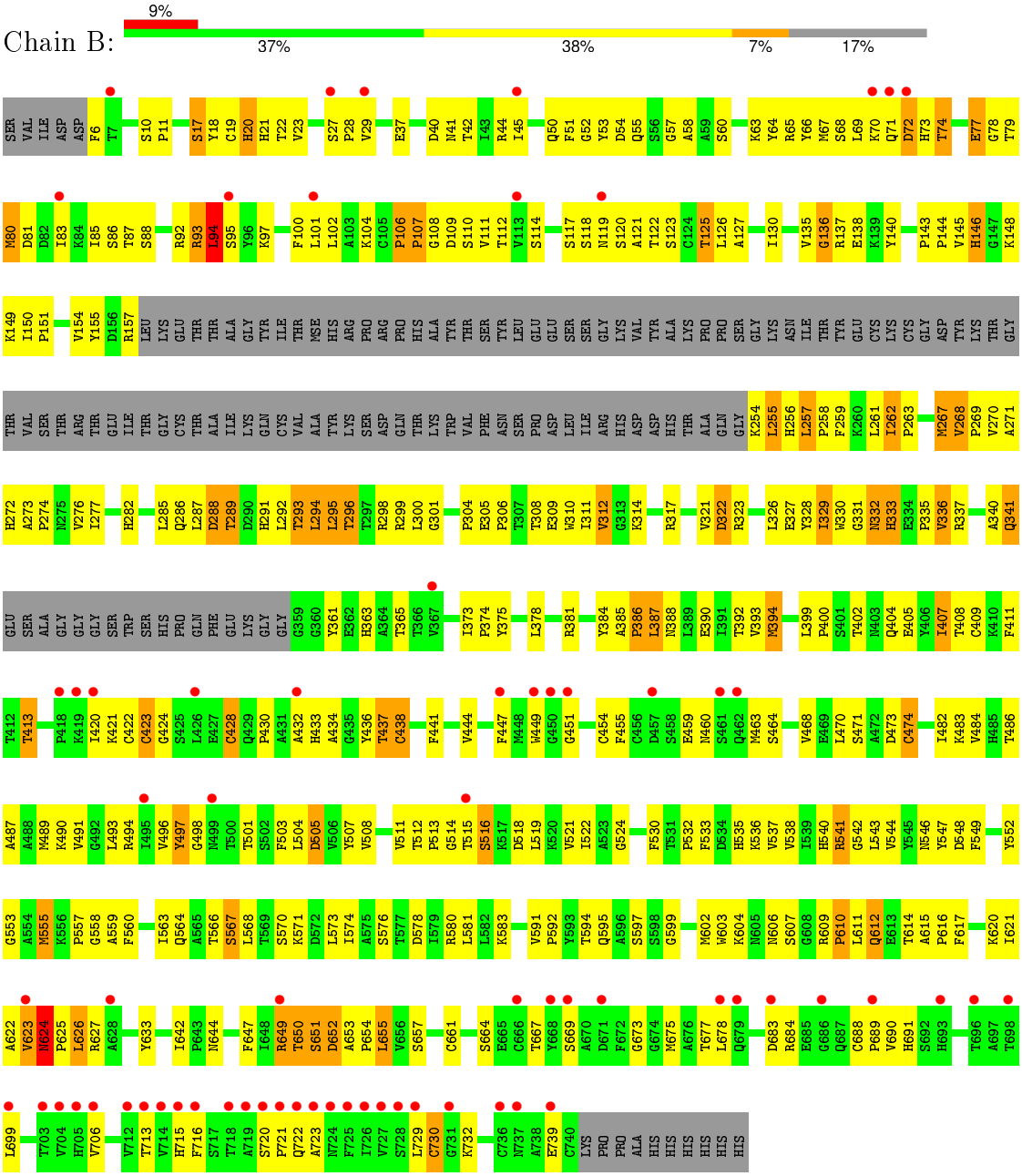
- Molecule 1: Structural polyprotein

Chain A:



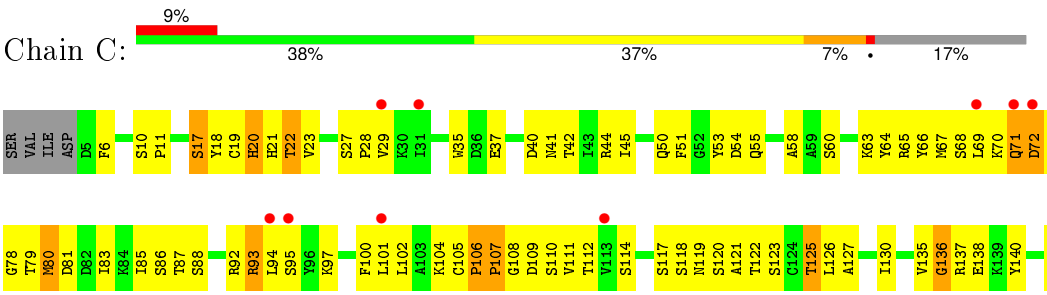
• Molecule 1: Structural polyprotein

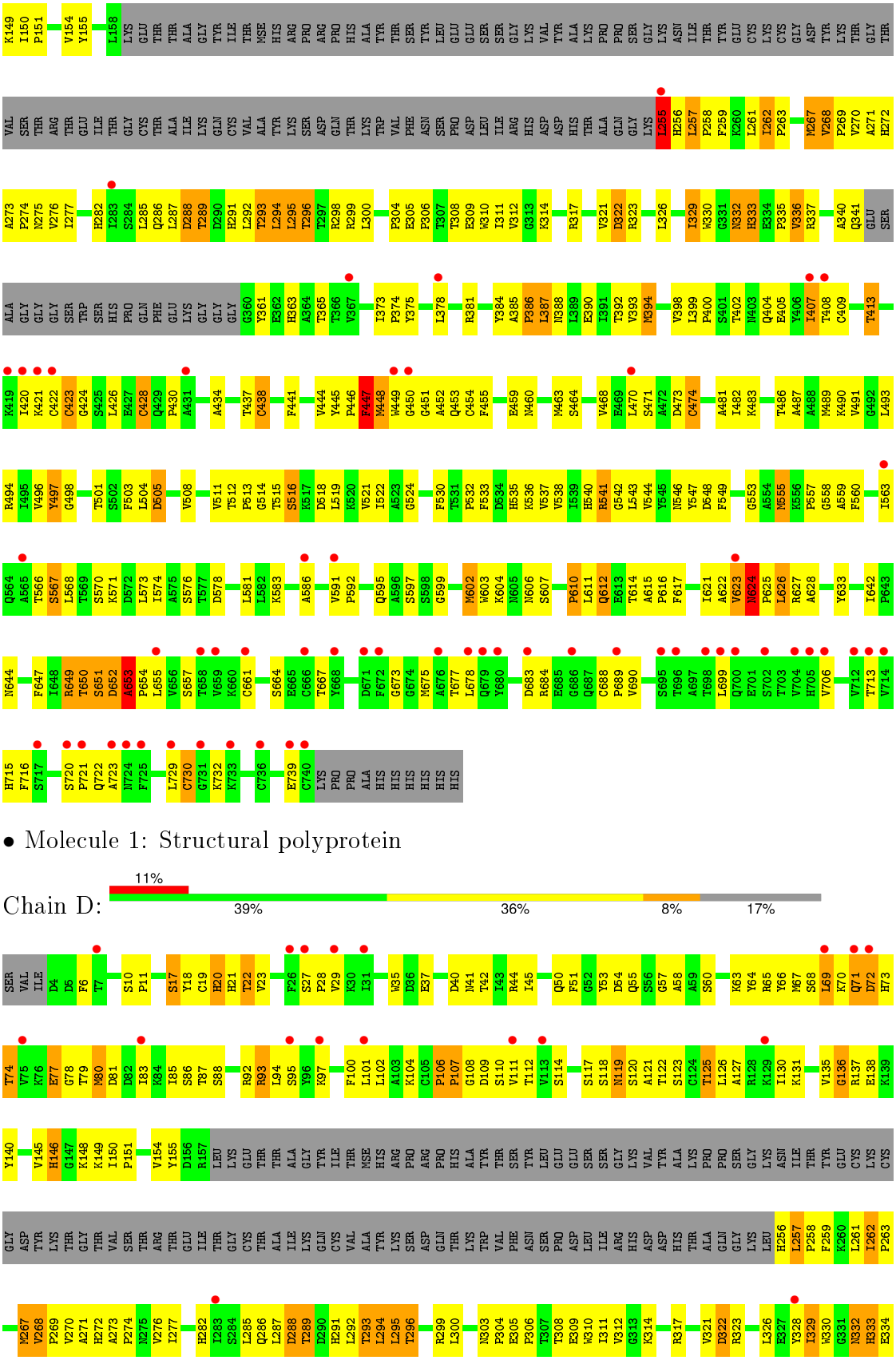
Chain B:



• Molecule 1: Structural polyprotein

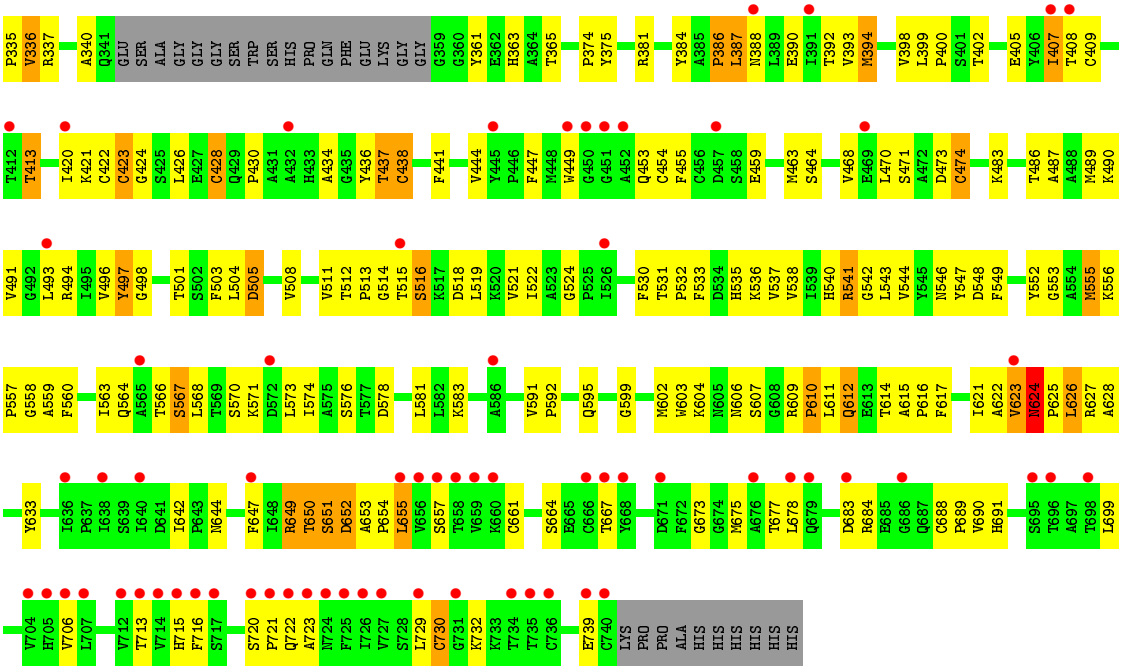
Chain C:





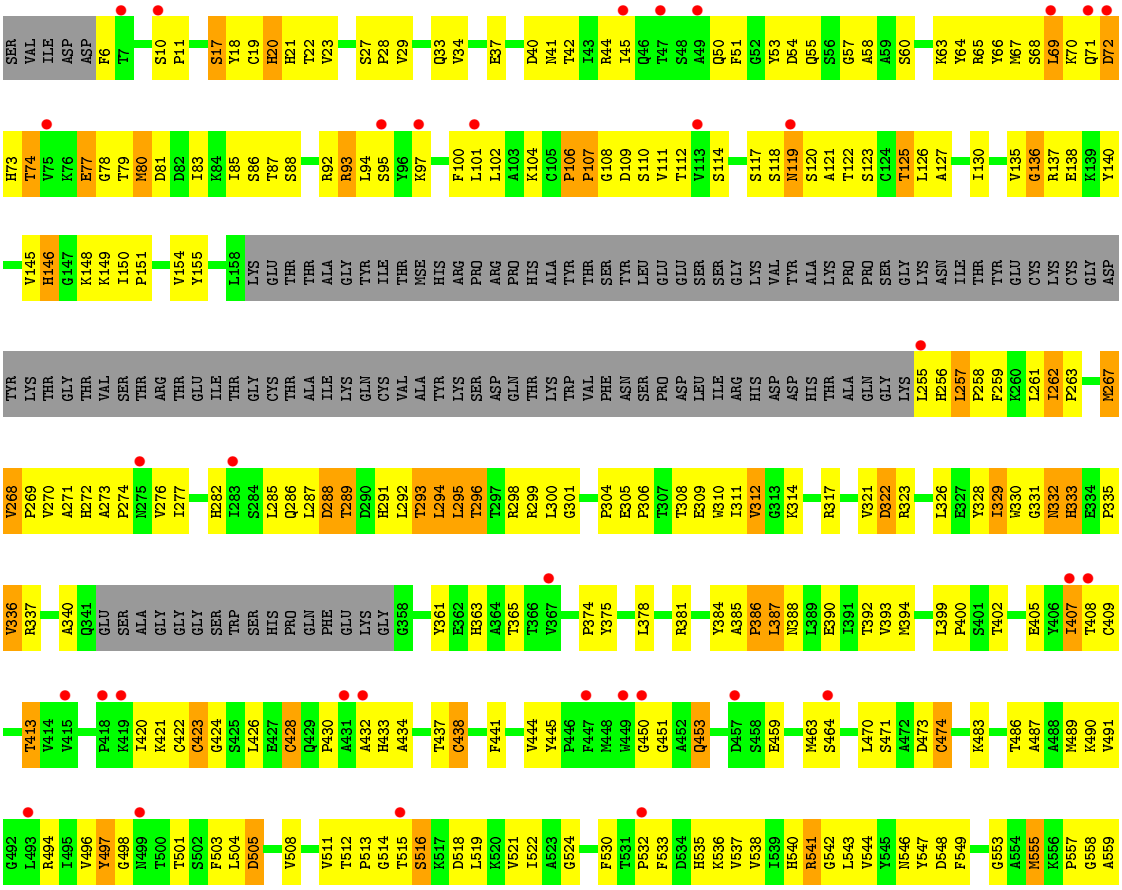
• Molecule 1: Structural polyprotein

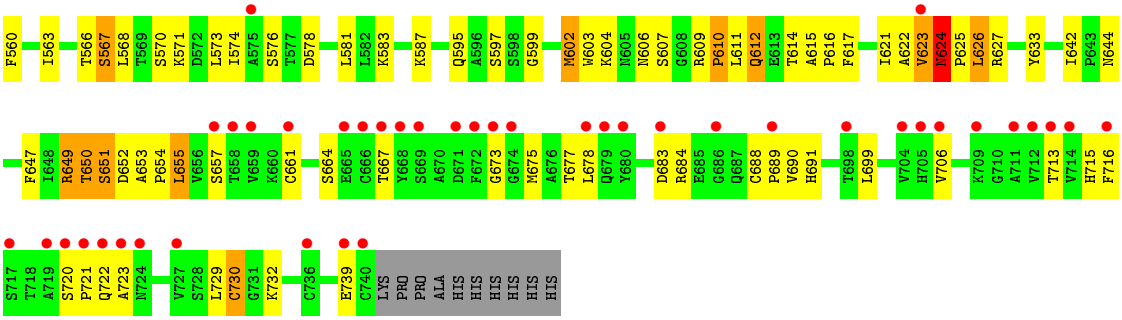
Chain D:

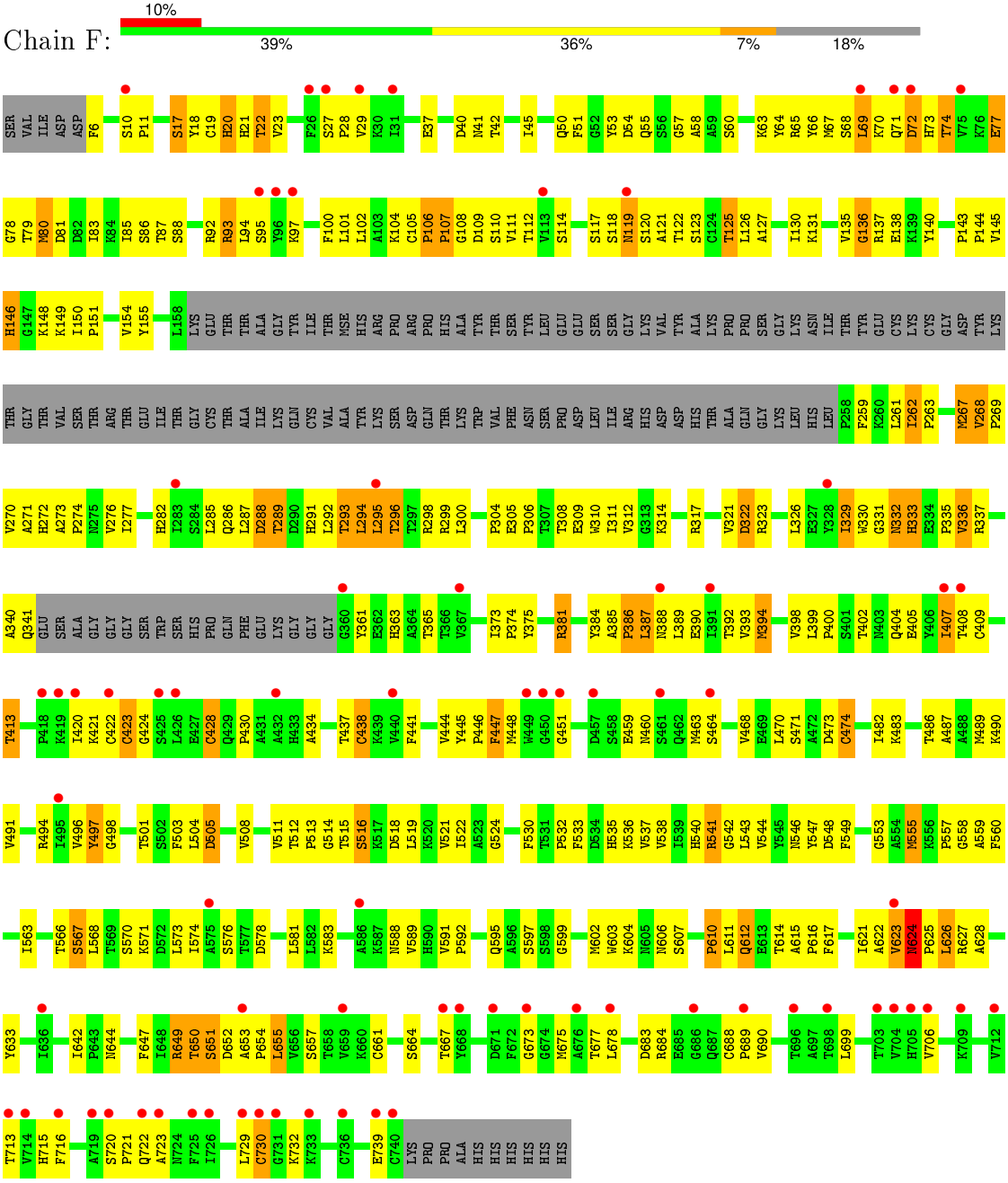


• Molecule 1: Structural polyprotein

Chain E:







• Molecule 1: Structural polyprotein

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.48Å 158.43Å 160.68Å 60.42° 89.80° 89.65°	Depositor
Resolution (Å)	60.72 – 3.29 60.72 – 3.29	Depositor EDS
% Data completeness (in resolution range)	92.4 (60.72-3.29) 77.1 (60.72-3.29)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 3.26Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6_289)	Depositor
R, R_{free}	0.239 , 0.252 0.246 , 0.258	Depositor DCC
R_{free} test set	4173 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	87.2	Xtriage
Anisotropy	0.703	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 97.3	EDS
Estimated twinning fraction	0.033 for h,k-l,k 0.033 for h,l,-k+l 0.297 for h,-l,k-l 0.297 for h,-k+l,-k 0.037 for h,-k,-l 0.408 for -h,k,k-l 0.289 for -h,-l,-k 0.033 for -h,k-l,-l 0.309 for -h,-k+l,l 0.039 for -h,-k,-k+l 0.033 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 82963 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	29159	wwPDB-VP
Average B, all atoms (Å^2)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, NAG, MAN

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	0.35	0/4876	0.58	0/6624
1	B	0.35	0/4870	0.60	1/6615 (0.0%)
1	C	0.38	1/4870 (0.0%)	0.60	1/6617 (0.0%)
1	D	0.35	0/4869	0.58	0/6615
1	E	0.35	0/4870	0.58	0/6616
1	F	0.36	0/4835	0.67	3/6568 (0.0%)
All	All	0.36	1/29190 (0.0%)	0.60	5/39655 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
2	A	1	0
2	F	1	0
All	All	2	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	653	ALA	C-N	7.00	1.47	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	381	ARG	NE-CZ-NH1	-19.90	110.35	120.30
1	F	381	ARG	NE-CZ-NH2	17.34	128.97	120.30
1	B	94	LEU	CA-CB-CG	-7.54	97.95	115.30
1	F	381	ARG	CD-NE-CZ	7.40	133.97	123.60
1	C	255	LEU	CB-CG-CD2	5.25	119.92	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	751	NAG	C1
2	F	751	NAG	C1

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	623	VAL	Peptide
1	A	624	ASN	Peptide
1	B	254	LYS	Peptide
1	B	623	VAL	Peptide
1	B	624	ASN	Peptide
1	C	623	VAL	Peptide
1	C	624	ASN	Peptide
1	D	623	VAL	Peptide
1	D	624	ASN	Peptide
1	E	623	VAL	Peptide
1	E	624	ASN	Peptide
1	F	623	VAL	Peptide
1	F	624	ASN	Peptide

5.2 Too-close contacts (i)

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	4767	0	4659	316	0
1	B	4761	0	4661	335	0
1	C	4761	0	4651	329	0
1	D	4760	0	4645	320	0
1	E	4761	0	4653	311	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4727	0	4619	304	0
2	A	50	0	42	2	0
2	B	100	0	86	2	0
2	C	100	0	85	4	0
2	D	50	0	42	1	0
2	E	50	0	42	0	0
2	F	50	0	43	0	0
3	A	61	0	52	3	0
3	E	61	0	52	2	0
3	F	61	0	52	6	0
4	D	39	0	34	2	0
All	All	29159	0	28418	1903	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (1903) 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)
1:D:22:THR:HG21	1:E:104:LYS:HD2	1.29	1.14
1:D:88:SER:HB3	1:D:107:PRO:HG3	1.10	1.09
1:B:507:TYR:CE1	1:D:625:PRO:HG2	1.88	1.09
1:B:255:LEU:HG	1:B:256:HIS:H	1.14	1.08
1:B:88:SER:HB3	1:B:107:PRO:HG3	1.09	1.08
1:E:88:SER:HB3	1:E:107:PRO:HG3	1.09	1.06
1:C:88:SER:HB3	1:C:107:PRO:HG3	1.08	1.06
1:E:255:LEU:HG	1:E:256:HIS:H	1.14	1.05
1:B:311:ILE:HD11	1:B:330:TRP:HE1	1.20	1.05
1:A:255:LEU:HG	1:A:256:HIS:H	1.15	1.05
1:F:88:SER:HB3	1:F:107:PRO:HG3	1.08	1.05
1:A:145:VAL:HG22	1:C:17:SER:HB3	1.35	1.05
1:A:311:ILE:HD11	1:A:330:TRP:HE1	1.21	1.05
1:A:88:SER:HB3	1:A:107:PRO:HG3	1.09	1.05
1:B:22:THR:HG21	1:C:104:LYS:HD2	1.39	1.04
1:E:311:ILE:HD11	1:E:330:TRP:HE1	1.21	1.04
1:D:311:ILE:HD11	1:D:330:TRP:HE1	1.22	1.02
1:A:22:THR:HG21	1:B:104:LYS:HD2	1.38	1.02
1:F:311:ILE:HD11	1:F:330:TRP:HE1	1.20	1.02
1:B:93:ARG:HH11	1:B:93:ARG:H	1.06	1.01
1:B:304:PRO:HG3	1:B:616:PRO:HA	1.39	1.01
1:F:88:SER:HB3	1:F:107:PRO:CG	1.91	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ILE:HD11	1:C:330:TRP:HE1	1.20	1.00
1:E:88:SER:HB3	1:E:107:PRO:CG	1.92	1.00
1:E:22:THR:HG21	1:F:104:LYS:HD2	1.41	1.00
1:B:136:GLY:HA3	1:B:268:VAL:HG21	1.44	1.00
1:C:88:SER:HB3	1:C:107:PRO:CG	1.91	1.00
1:F:93:ARG:HH11	1:F:93:ARG:H	1.08	1.00
1:B:257:LEU:H	1:B:258:PRO:HD3	1.27	0.99
1:A:88:SER:HB3	1:A:107:PRO:CG	1.92	0.99
1:C:93:ARG:H	1:C:93:ARG:HH11	1.09	0.99
1:D:88:SER:HB3	1:D:107:PRO:CG	1.93	0.99
1:B:88:SER:HB3	1:B:107:PRO:CG	1.92	0.99
1:D:93:ARG:HH11	1:D:93:ARG:H	1.07	0.98
1:A:257:LEU:H	1:A:258:PRO:HD3	1.27	0.98
1:F:136:GLY:HA3	1:F:268:VAL:HG21	1.45	0.98
1:A:93:ARG:H	1:A:93:ARG:HH11	1.10	0.97
1:B:289:THR:HG21	1:B:293:THR:HG21	1.47	0.97
1:C:289:THR:HG21	1:C:293:THR:HG21	1.45	0.97
1:C:136:GLY:HA3	1:C:268:VAL:HG21	1.44	0.97
1:A:289:THR:HG21	1:A:293:THR:HG21	1.45	0.97
1:C:257:LEU:H	1:C:258:PRO:HD3	1.27	0.97
1:E:257:LEU:H	1:E:258:PRO:HD3	1.27	0.97
1:D:104:LYS:HD2	1:F:22:THR:HG21	1.46	0.97
1:E:136:GLY:HA3	1:E:268:VAL:HG21	1.44	0.97
1:D:257:LEU:H	1:D:258:PRO:HD3	1.28	0.96
1:D:145:VAL:HG22	1:F:17:SER:HB3	1.43	0.96
1:A:136:GLY:HA3	1:A:268:VAL:HG21	1.46	0.96
1:D:136:GLY:HA3	1:D:268:VAL:HG21	1.45	0.96
1:A:104:LYS:HD2	1:C:22:THR:HG21	1.46	0.96
1:E:93:ARG:H	1:E:93:ARG:HH11	1.07	0.95
1:E:17:SER:HB3	1:F:145:VAL:HG22	1.47	0.95
1:F:289:THR:HG21	1:F:293:THR:HG21	1.44	0.95
1:E:304:PRO:HG3	1:E:616:PRO:HA	1.45	0.95
1:D:304:PRO:HG3	1:D:616:PRO:HA	1.49	0.95
1:D:289:THR:HG21	1:D:293:THR:HG21	1.46	0.95
1:E:289:THR:HG21	1:E:293:THR:HG21	1.46	0.94
1:B:17:SER:HB3	1:C:145:VAL:HG22	1.51	0.93
1:D:17:SER:HB3	1:E:145:VAL:HG22	1.53	0.90
1:C:428:CYS:HB2	1:C:463:MSE:SE	2.24	0.88
1:C:304:PRO:HG3	1:C:616:PRO:HA	1.54	0.87
1:E:428:CYS:HB2	1:E:463:MSE:SE	2.25	0.86
1:D:447:PHE:HD1	1:D:455:PHE:HA	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LEU:HG	1:A:256:HIS:N	1.91	0.85
1:B:428:CYS:HB2	1:B:463:MSE:SE	2.26	0.85
1:A:17:SER:HB3	1:B:145:VAL:HG22	1.58	0.85
1:E:255:LEU:HG	1:E:256:HIS:N	1.90	0.84
1:A:304:PRO:HG3	1:A:616:PRO:HA	1.57	0.84
1:F:304:PRO:HG3	1:F:616:PRO:HA	1.57	0.84
1:B:507:TYR:HE1	1:D:625:PRO:HG2	1.43	0.84
1:B:255:LEU:HG	1:B:256:HIS:N	1.92	0.83
1:D:22:THR:HG21	1:E:104:LYS:CD	2.07	0.83
1:F:428:CYS:HB2	1:F:463:MSE:SE	2.29	0.83
1:C:677:THR:HG22	1:C:713:THR:HG22	1.60	0.83
1:E:677:THR:HG22	1:E:713:THR:HG22	1.61	0.83
1:F:677:THR:HG22	1:F:713:THR:HG22	1.61	0.82
1:B:677:THR:HG22	1:B:713:THR:HG22	1.61	0.82
1:A:677:THR:HG22	1:A:713:THR:HG22	1.60	0.82
1:D:677:THR:HG22	1:D:713:THR:HG22	1.60	0.82
1:A:428:CYS:HB2	1:A:463:MSE:SE	2.29	0.82
1:C:378:LEU:HD21	1:C:689:PRO:HB2	1.63	0.81
1:E:322:ASP:O	1:E:323:ARG:HB3	1.81	0.81
1:C:496:VAL:HG22	1:C:501:THR:HB	1.62	0.81
1:D:496:VAL:HG22	1:D:501:THR:HB	1.63	0.81
1:D:447:PHE:CD1	1:D:455:PHE:HA	2.17	0.80
1:C:322:ASP:O	1:C:323:ARG:HB3	1.81	0.80
1:C:257:LEU:N	1:C:258:PRO:HD3	1.95	0.80
1:A:496:VAL:HG22	1:A:501:THR:HB	1.64	0.80
1:D:322:ASP:O	1:D:323:ARG:HB3	1.81	0.80
1:C:445:TYR:HB3	1:C:451:GLY:HA3	1.62	0.80
1:D:428:CYS:HB2	1:D:463:MSE:SE	2.32	0.80
1:B:257:LEU:N	1:B:258:PRO:HD3	1.96	0.80
1:E:257:LEU:N	1:E:258:PRO:HD3	1.96	0.80
1:A:257:LEU:N	1:A:258:PRO:HD3	1.95	0.80
1:D:257:LEU:N	1:D:258:PRO:HD3	1.96	0.79
1:B:94:LEU:HD22	1:B:157:ARG:HD3	1.64	0.79
1:C:653:ALA:HB1	1:C:684:ARG:HH11	1.47	0.79
1:F:322:ASP:O	1:F:323:ARG:HB3	1.82	0.79
1:A:322:ASP:O	1:A:323:ARG:HB3	1.82	0.79
1:F:114:SER:HB3	1:F:123:SER:CB	2.11	0.79
1:E:114:SER:HB3	1:E:123:SER:CB	2.13	0.79
1:C:114:SER:HB3	1:C:123:SER:CB	2.13	0.79
1:A:255:LEU:CG	1:A:256:HIS:H	1.96	0.79
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.66	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:ARG:NH2	1:D:329:ILE:HB	1.98	0.78
1:A:114:SER:HB3	1:A:123:SER:CB	2.13	0.78
1:F:137:ARG:NH2	1:F:329:ILE:HB	1.98	0.78
1:D:114:SER:HB3	1:D:123:SER:CB	2.12	0.78
1:B:322:ASP:O	1:B:323:ARG:HB3	1.81	0.78
1:B:106:PRO:HB2	1:B:107:PRO:HD3	1.65	0.78
1:E:496:VAL:HG22	1:E:501:THR:HB	1.65	0.78
1:F:88:SER:CB	1:F:107:PRO:HG3	2.04	0.78
1:E:137:ARG:NH2	1:E:329:ILE:HB	1.98	0.78
1:C:106:PRO:HB2	1:C:107:PRO:HD3	1.66	0.78
1:B:114:SER:HB3	1:B:123:SER:CB	2.12	0.78
1:F:496:VAL:HG22	1:F:501:THR:HB	1.64	0.78
1:E:255:LEU:CG	1:E:256:HIS:H	1.95	0.78
1:D:329:ILE:HD13	1:D:335:PRO:HB3	1.66	0.78
1:C:675:MSE:HE2	1:C:715:HIS:HE1	1.49	0.78
1:A:137:ARG:NH2	1:A:329:ILE:HB	1.98	0.78
1:B:496:VAL:HG22	1:B:501:THR:HB	1.65	0.77
1:A:544:VAL:H	1:A:612:GLN:NE2	1.83	0.77
1:B:544:VAL:H	1:B:612:GLN:NE2	1.83	0.77
1:D:544:VAL:H	1:D:612:GLN:NE2	1.83	0.77
3:F:761:NAG:H61	3:F:762:NAG:O7	1.85	0.77
1:D:543:LEU:HA	1:D:612:GLN:NE2	2.00	0.77
1:F:675:MSE:HE2	1:F:715:HIS:HE1	1.50	0.77
1:C:655:LEU:H	1:C:683:ASP:HB2	1.49	0.77
1:D:106:PRO:HB2	1:D:107:PRO:HD3	1.66	0.77
1:D:675:MSE:HE2	1:D:715:HIS:HE1	1.50	0.77
1:A:88:SER:CB	1:A:107:PRO:HG3	2.05	0.76
1:F:114:SER:HB3	1:F:123:SER:HB2	1.68	0.76
3:E:763:BMA:H3	3:F:765:MAN:O3	1.85	0.76
1:C:137:ARG:NH2	1:C:329:ILE:HB	2.00	0.76
1:A:329:ILE:HD13	1:A:335:PRO:HB3	1.67	0.76
1:F:543:LEU:HA	1:F:612:GLN:NE2	2.00	0.76
3:F:762:NAG:H83	3:F:765:MAN:H61	1.66	0.76
1:E:106:PRO:HB2	1:E:107:PRO:HD3	1.66	0.76
3:A:764:MAN:O3	2:C:763:BMA:H5	1.85	0.76
1:B:137:ARG:NH2	1:B:329:ILE:HB	2.01	0.75
1:F:106:PRO:HB2	1:F:107:PRO:HD3	1.66	0.75
1:E:544:VAL:H	1:E:612:GLN:NE2	1.84	0.75
1:B:255:LEU:CG	1:B:256:HIS:H	1.92	0.75
1:F:544:VAL:H	1:F:612:GLN:NE2	1.85	0.75
1:C:114:SER:HB3	1:C:123:SER:HB2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:610:PRO:HB2	1:F:612:GLN:HG2	1.69	0.75
1:B:675:MSE:HE2	1:B:715:HIS:HE1	1.51	0.75
1:A:675:MSE:HE2	1:A:715:HIS:HE1	1.51	0.75
1:A:294:LEU:HG	1:A:310:TRP:CE2	2.22	0.75
1:B:22:THR:HG21	1:C:104:LYS:CD	2.15	0.75
1:E:22:THR:HG21	1:F:104:LYS:CD	2.16	0.75
1:C:329:ILE:HD13	1:C:335:PRO:HB3	1.69	0.74
1:A:543:LEU:HA	1:A:612:GLN:NE2	2.01	0.74
1:A:610:PRO:HB2	1:A:612:GLN:HG2	1.69	0.74
1:E:536:LYS:HG2	1:E:549:PHE:CZ	2.23	0.74
1:A:104:LYS:CD	1:C:22:THR:HG21	2.17	0.74
1:F:294:LEU:HG	1:F:310:TRP:CE2	2.21	0.74
1:C:150:ILE:HG23	1:C:151:PRO:HD2	1.68	0.74
1:E:150:ILE:HG23	1:E:151:PRO:HD2	1.69	0.74
1:F:655:LEU:H	1:F:683:ASP:HB2	1.53	0.74
1:E:675:MSE:HE2	1:E:715:HIS:HE1	1.50	0.74
1:D:114:SER:HB3	1:D:123:SER:HB2	1.69	0.74
1:B:543:LEU:HA	1:B:612:GLN:NE2	2.01	0.74
1:C:544:VAL:H	1:C:612:GLN:NE2	1.85	0.74
1:D:88:SER:CB	1:D:107:PRO:HG3	2.05	0.73
1:C:294:LEU:HG	1:C:310:TRP:CE2	2.23	0.73
1:F:329:ILE:HD13	1:F:335:PRO:HB3	1.68	0.73
1:E:610:PRO:HB2	1:E:612:GLN:HG2	1.70	0.73
1:E:543:LEU:HA	1:E:612:GLN:NE2	2.02	0.73
1:B:114:SER:HB3	1:B:123:SER:HB2	1.69	0.73
1:A:137:ARG:HH22	1:A:329:ILE:HB	1.54	0.73
1:B:447:PHE:CD1	1:B:455:PHE:HA	2.23	0.73
1:B:329:ILE:HD13	1:B:335:PRO:HB3	1.69	0.73
1:C:543:LEU:HA	1:C:612:GLN:NE2	2.02	0.73
1:E:114:SER:HB3	1:E:123:SER:HB2	1.69	0.73
1:B:294:LEU:HG	1:B:310:TRP:CE2	2.24	0.73
1:A:447:PHE:CD1	1:A:455:PHE:HA	2.23	0.73
1:D:150:ILE:HG23	1:D:151:PRO:HD2	1.70	0.73
1:F:361:TYR:HB2	1:F:381:ARG:NH2	2.03	0.73
1:D:610:PRO:HB2	1:D:612:GLN:HG2	1.69	0.73
1:C:610:PRO:HB2	1:C:612:GLN:HG2	1.70	0.73
1:B:655:LEU:H	1:B:683:ASP:HB2	1.53	0.73
1:D:536:LYS:HG2	1:D:549:PHE:CZ	2.24	0.73
2:C:751:NAG:H4	2:C:752:NAG:N2	2.02	0.72
1:C:536:LYS:HG2	1:C:549:PHE:CZ	2.24	0.72
1:B:11:PRO:HD3	1:B:50:GLN:HE21	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:TYR:CE1	1:F:22:THR:HG22	2.25	0.72
1:A:114:SER:HB3	1:A:123:SER:HB2	1.69	0.72
1:C:11:PRO:HD3	1:C:50:GLN:HE21	1.54	0.72
1:F:536:LYS:HG2	1:F:549:PHE:CZ	2.25	0.72
1:B:150:ILE:HG23	1:B:151:PRO:HD2	1.70	0.72
1:A:18:TYR:CE1	1:A:22:THR:HG22	2.24	0.72
1:C:11:PRO:HD3	1:C:50:GLN:NE2	2.04	0.72
1:D:655:LEU:H	1:D:683:ASP:HB2	1.53	0.72
1:D:538:VAL:HG23	1:D:547:TYR:HB3	1.70	0.72
1:D:11:PRO:HD3	1:D:50:GLN:HE21	1.55	0.72
1:E:329:ILE:HD13	1:E:335:PRO:HB3	1.71	0.72
1:E:270:VAL:HG22	1:E:333:HIS:CE1	2.25	0.72
1:E:655:LEU:H	1:E:683:ASP:HB2	1.53	0.72
1:A:95:SER:OG	1:A:259:PHE:CE1	2.41	0.72
1:A:85:ILE:HD11	1:A:101:LEU:HD13	1.71	0.72
1:C:85:ILE:HD11	1:C:101:LEU:HD13	1.72	0.71
1:F:11:PRO:HD3	1:F:50:GLN:HE21	1.53	0.71
1:B:538:VAL:HG23	1:B:547:TYR:HB3	1.71	0.71
1:D:18:TYR:CE1	1:D:22:THR:HG22	2.25	0.71
1:F:11:PRO:HD3	1:F:50:GLN:NE2	2.05	0.71
1:A:655:LEU:H	1:A:683:ASP:HB2	1.54	0.71
1:E:18:TYR:CE1	1:E:22:THR:HG22	2.25	0.71
1:B:11:PRO:HD3	1:B:50:GLN:NE2	2.05	0.71
1:F:150:ILE:HG23	1:F:151:PRO:HD2	1.71	0.71
1:C:18:TYR:CE1	1:C:22:THR:HG22	2.25	0.71
1:A:11:PRO:HD3	1:A:50:GLN:HE21	1.55	0.71
1:B:653:ALA:N	1:B:654:PRO:HD2	2.05	0.71
1:E:11:PRO:HD3	1:E:50:GLN:HE21	1.55	0.71
1:A:536:LYS:HG2	1:A:549:PHE:CZ	2.26	0.71
1:D:270:VAL:HG22	1:D:333:HIS:CE1	2.26	0.71
1:B:18:TYR:CE1	1:B:22:THR:HG22	2.25	0.70
1:A:11:PRO:HD3	1:A:50:GLN:NE2	2.06	0.70
1:A:388:ASN:HB3	1:A:498:GLY:H	1.56	0.70
1:B:287:LEU:HD22	1:B:330:TRP:NE1	2.07	0.70
1:F:270:VAL:HG22	1:F:333:HIS:CE1	2.26	0.70
1:E:294:LEU:HG	1:E:310:TRP:CE2	2.26	0.70
1:A:270:VAL:HG22	1:A:333:HIS:CE1	2.27	0.70
1:E:137:ARG:HH22	1:E:329:ILE:HB	1.54	0.70
1:D:11:PRO:HD3	1:D:50:GLN:NE2	2.05	0.70
1:A:22:THR:HG21	1:B:104:LYS:CD	2.19	0.70
1:A:150:ILE:HG23	1:A:151:PRO:HD2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:VAL:HG23	1:A:547:TYR:HB3	1.72	0.70
1:A:79:THR:C	1:A:81:ASP:H	1.94	0.70
1:A:291:HIS:CD2	1:A:293:THR:HG22	2.27	0.70
1:A:511:VAL:HG23	1:A:512:THR:H	1.57	0.70
1:F:538:VAL:HG23	1:F:547:TYR:HB3	1.72	0.70
1:E:85:ILE:HD11	1:E:101:LEU:HD13	1.73	0.70
1:D:79:THR:C	1:D:81:ASP:H	1.94	0.70
1:D:294:LEU:HG	1:D:310:TRP:CE2	2.27	0.70
1:B:536:LYS:HG2	1:B:549:PHE:CZ	2.26	0.70
1:D:137:ARG:HH22	1:D:329:ILE:HB	1.54	0.70
1:B:85:ILE:HD11	1:B:101:LEU:HD13	1.73	0.70
1:A:650:THR:HG22	1:A:650:THR:O	1.92	0.70
1:A:299:ARG:HB2	1:A:304:PRO:HA	1.74	0.70
1:E:88:SER:CB	1:E:107:PRO:HG3	2.05	0.70
1:F:137:ARG:HH22	1:F:329:ILE:HB	1.54	0.70
1:E:538:VAL:HG23	1:E:547:TYR:HB3	1.72	0.70
1:A:447:PHE:HD1	1:A:454:CYS:O	1.75	0.70
1:E:11:PRO:HD3	1:E:50:GLN:NE2	2.06	0.70
1:A:446:PRO:HD2	1:A:450:GLY:O	1.90	0.70
1:F:511:VAL:HG23	1:F:512:THR:H	1.56	0.70
1:D:85:ILE:HD11	1:D:101:LEU:HD13	1.73	0.69
1:F:85:ILE:HD11	1:F:101:LEU:HD13	1.73	0.69
1:A:447:PHE:CE1	1:A:455:PHE:HD1	2.11	0.69
1:E:79:THR:C	1:E:81:ASP:H	1.95	0.69
1:B:270:VAL:HG22	1:B:333:HIS:CE1	2.26	0.69
1:D:388:ASN:HB3	1:D:498:GLY:H	1.57	0.69
1:C:88:SER:CB	1:C:107:PRO:HG3	2.04	0.69
1:D:653:ALA:N	1:D:654:PRO:HD2	2.08	0.69
1:E:299:ARG:HB2	1:E:304:PRO:HA	1.73	0.69
1:D:291:HIS:CD2	1:D:293:THR:HG22	2.27	0.69
1:E:287:LEU:HD22	1:E:330:TRP:NE1	2.06	0.69
1:B:610:PRO:HB2	1:B:612:GLN:HG2	1.72	0.69
1:C:95:SER:OG	1:C:259:PHE:CE1	2.42	0.69
1:D:108:GLY:HA3	1:D:130:ILE:HB	1.75	0.69
1:D:511:VAL:HG23	1:D:512:THR:H	1.57	0.69
1:C:538:VAL:HG23	1:C:547:TYR:HB3	1.73	0.69
1:D:650:THR:O	1:D:650:THR:HG22	1.93	0.69
1:B:624:ASN:HB3	1:B:625:PRO:CD	2.23	0.68
1:D:299:ARG:HB2	1:D:304:PRO:HA	1.73	0.68
1:F:299:ARG:HB2	1:F:304:PRO:HA	1.75	0.68
1:D:107:PRO:HG2	1:D:108:GLY:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ILE:HD11	1:C:330:TRP:NE1	2.04	0.68
1:C:291:HIS:CD2	1:C:293:THR:HG22	2.28	0.68
1:E:291:HIS:CD2	1:E:293:THR:HG22	2.28	0.68
1:F:79:THR:C	1:F:81:ASP:H	1.95	0.68
1:C:650:THR:O	1:C:650:THR:HG22	1.93	0.68
1:A:287:LEU:HD22	1:A:330:TRP:NE1	2.08	0.68
1:C:270:VAL:HG22	1:C:333:HIS:CE1	2.28	0.68
1:B:511:VAL:HG23	1:B:512:THR:H	1.59	0.68
1:B:79:THR:C	1:B:81:ASP:H	1.96	0.68
1:B:88:SER:CB	1:B:107:PRO:HG3	2.05	0.68
1:C:299:ARG:HB2	1:C:304:PRO:HA	1.75	0.68
1:F:650:THR:O	1:F:650:THR:HG22	1.92	0.68
1:A:445:TYR:HB3	1:A:451:GLY:HA3	1.76	0.68
1:F:388:ASN:HB3	1:F:498:GLY:H	1.58	0.68
1:B:137:ARG:HH22	1:B:329:ILE:HB	1.59	0.68
1:B:386:PRO:HB2	1:B:689:PRO:HG2	1.76	0.68
1:C:79:THR:C	1:C:81:ASP:H	1.96	0.68
1:C:108:GLY:HA3	1:C:130:ILE:HB	1.76	0.67
1:F:287:LEU:HD22	1:F:330:TRP:NE1	2.09	0.67
1:B:299:ARG:HB2	1:B:304:PRO:HA	1.75	0.67
1:F:291:HIS:CD2	1:F:293:THR:HG22	2.29	0.67
1:C:107:PRO:HG2	1:C:108:GLY:H	1.59	0.67
1:E:95:SER:OG	1:E:259:PHE:CE1	2.42	0.67
1:C:287:LEU:HD22	1:C:330:TRP:NE1	2.10	0.67
1:D:530:PHE:HB3	1:D:633:TYR:CE1	2.29	0.67
1:C:511:VAL:HG23	1:C:512:THR:H	1.58	0.67
1:A:108:GLY:HA3	1:A:130:ILE:HB	1.76	0.67
1:B:291:HIS:CD2	1:B:293:THR:HG22	2.30	0.67
1:C:494:ARG:HB2	1:C:503:PHE:HD1	1.59	0.67
1:C:624:ASN:HB3	1:C:625:PRO:CD	2.25	0.67
1:E:108:GLY:HA3	1:E:130:ILE:HB	1.77	0.67
1:C:388:ASN:HB3	1:C:498:GLY:H	1.59	0.67
1:A:107:PRO:HG2	1:A:108:GLY:H	1.58	0.67
1:C:256:HIS:O	1:C:257:LEU:HD13	1.95	0.67
1:C:530:PHE:HB3	1:C:633:TYR:CE1	2.30	0.67
1:F:108:GLY:HA3	1:F:130:ILE:HB	1.77	0.66
1:C:542:GLY:H	1:C:543:LEU:HD12	1.60	0.66
1:E:511:VAL:HG23	1:E:512:THR:H	1.59	0.66
1:B:256:HIS:O	1:B:257:LEU:HD13	1.95	0.66
1:B:108:GLY:HA3	1:B:130:ILE:HB	1.76	0.66
1:E:388:ASN:HB3	1:E:498:GLY:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:624:ASN:HB3	1:F:625:PRO:CD	2.25	0.66
1:B:388:ASN:HB3	1:B:498:GLY:H	1.59	0.66
1:F:107:PRO:HG2	1:F:108:GLY:H	1.59	0.66
1:B:650:THR:HG22	1:B:650:THR:O	1.93	0.66
1:B:107:PRO:HG2	1:B:108:GLY:H	1.60	0.66
1:B:97:LYS:HB2	1:B:259:PHE:CZ	2.31	0.66
1:B:494:ARG:HB2	1:B:503:PHE:HD1	1.61	0.66
1:A:567:SER:HB2	1:A:571:LYS:HD2	1.78	0.66
1:E:107:PRO:HG2	1:E:108:GLY:H	1.59	0.66
1:D:494:ARG:HB2	1:D:503:PHE:HD1	1.61	0.66
1:C:136:GLY:HA3	1:C:268:VAL:CG2	2.25	0.66
1:F:299:ARG:HH12	1:F:305:GLU:CD	1.99	0.66
1:A:256:HIS:O	1:A:257:LEU:HD13	1.96	0.66
1:D:104:LYS:CD	1:F:22:THR:HG21	2.22	0.66
1:F:530:PHE:HB3	1:F:633:TYR:CE1	2.31	0.66
1:C:137:ARG:HH22	1:C:329:ILE:HB	1.59	0.66
1:E:299:ARG:HH12	1:E:305:GLU:CD	2.00	0.66
1:D:542:GLY:H	1:D:543:LEU:HD12	1.61	0.66
1:A:497:TYR:N	1:A:497:TYR:CD2	2.64	0.65
1:B:567:SER:HB2	1:B:571:LYS:HD2	1.78	0.65
1:E:624:ASN:HB3	1:E:625:PRO:CD	2.26	0.65
1:D:287:LEU:HD22	1:D:330:TRP:NE1	2.11	0.65
1:D:256:HIS:O	1:D:257:LEU:HD13	1.95	0.65
1:C:97:LYS:HB2	1:C:259:PHE:CZ	2.31	0.65
1:B:95:SER:OG	1:B:259:PHE:CE1	2.41	0.65
1:E:530:PHE:HB3	1:E:633:TYR:CE1	2.31	0.65
1:D:624:ASN:HB3	1:D:625:PRO:CD	2.27	0.65
1:A:97:LYS:HB2	1:A:259:PHE:CZ	2.31	0.65
1:A:530:PHE:HB3	1:A:633:TYR:CE1	2.31	0.65
1:B:299:ARG:HH12	1:B:305:GLU:CD	2.00	0.65
1:A:299:ARG:HH12	1:A:305:GLU:CD	2.00	0.65
1:A:624:ASN:HB3	1:A:625:PRO:CD	2.26	0.65
1:D:299:ARG:HH12	1:D:305:GLU:CD	2.00	0.65
1:E:536:LYS:HG2	1:E:549:PHE:CE2	2.32	0.65
1:A:106:PRO:HB2	1:A:107:PRO:CD	2.27	0.65
1:D:497:TYR:CD2	1:D:497:TYR:N	2.63	0.65
1:F:97:LYS:HB2	1:F:259:PHE:CZ	2.32	0.65
1:E:256:HIS:O	1:E:257:LEU:HD13	1.96	0.65
1:C:299:ARG:HH12	1:C:305:GLU:CD	1.99	0.65
1:F:494:ARG:HB2	1:F:503:PHE:HD1	1.62	0.65
1:D:108:GLY:HA2	1:D:130:ILE:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLU:OE1	1:B:473:ASP:OD2	2.15	0.64
1:A:494:ARG:HB2	1:A:503:PHE:HD1	1.62	0.64
1:D:384:TYR:HA	1:D:649:ARG:HA	1.79	0.64
1:F:19:CYS:HA	1:F:123:SER:O	1.97	0.64
1:E:19:CYS:HA	1:E:123:SER:O	1.98	0.64
1:A:542:GLY:H	1:A:543:LEU:HD12	1.62	0.64
1:F:542:GLY:H	1:F:543:LEU:HD12	1.60	0.64
1:D:567:SER:HB2	1:D:571:LYS:HD2	1.77	0.64
1:B:530:PHE:HB3	1:B:633:TYR:CE1	2.31	0.64
1:B:289:THR:HG21	1:B:293:THR:CG2	2.26	0.64
1:E:97:LYS:HB2	1:E:259:PHE:CZ	2.32	0.64
1:E:494:ARG:HB2	1:E:503:PHE:HD1	1.61	0.64
1:E:650:THR:HG22	1:E:650:THR:O	1.97	0.64
1:D:558:GLY:O	1:D:599:GLY:HA2	1.97	0.64
1:D:97:LYS:HB2	1:D:259:PHE:CZ	2.31	0.64
1:C:567:SER:HB2	1:C:571:LYS:HD2	1.80	0.64
1:B:108:GLY:HA2	1:B:130:ILE:HD12	1.80	0.64
1:E:567:SER:HB2	1:E:571:LYS:HD2	1.79	0.64
1:E:106:PRO:HB2	1:E:107:PRO:CD	2.27	0.64
1:C:19:CYS:HA	1:C:123:SER:O	1.98	0.64
1:E:542:GLY:H	1:E:543:LEU:HD12	1.62	0.64
1:F:311:ILE:HD11	1:F:330:TRP:NE1	2.04	0.64
1:D:19:CYS:HA	1:D:123:SER:O	1.98	0.64
1:D:624:ASN:HB3	1:D:625:PRO:HD3	1.80	0.64
1:D:106:PRO:HB2	1:D:107:PRO:CD	2.27	0.63
1:F:108:GLY:HA2	1:F:130:ILE:HD12	1.79	0.63
1:B:19:CYS:HA	1:B:123:SER:O	1.97	0.63
1:B:558:GLY:O	1:B:599:GLY:HA2	1.98	0.63
1:A:558:GLY:O	1:A:599:GLY:HA2	1.97	0.63
1:C:289:THR:HG21	1:C:293:THR:CG2	2.25	0.63
1:A:19:CYS:HA	1:A:123:SER:O	1.98	0.63
1:B:653:ALA:HB1	1:B:684:ARG:HD2	1.79	0.63
1:E:384:TYR:HA	1:E:649:ARG:HA	1.80	0.63
1:A:543:LEU:HD23	1:A:610:PRO:HG3	1.81	0.63
1:B:542:GLY:H	1:B:543:LEU:HD12	1.62	0.63
1:B:388:ASN:O	1:B:497:TYR:HA	1.99	0.63
1:C:446:PRO:HG2	1:C:450:GLY:C	2.19	0.63
1:C:108:GLY:HA2	1:C:130:ILE:HD12	1.79	0.63
1:C:448:MSE:HG3	1:C:454:CYS:H	1.63	0.63
1:C:553:GLY:HA2	1:C:574:ILE:HD12	1.81	0.63
1:B:384:TYR:HA	1:B:649:ARG:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:GLY:HA2	1:E:130:ILE:HD12	1.80	0.63
1:A:145:VAL:CG2	1:C:17:SER:HB3	2.21	0.63
1:B:301:GLY:O	1:B:616:PRO:O	2.17	0.63
1:B:652:ASP:C	1:B:654:PRO:HD2	2.19	0.63
1:A:384:TYR:HA	1:A:649:ARG:HA	1.79	0.63
1:A:108:GLY:HA2	1:A:130:ILE:HD12	1.79	0.63
1:E:497:TYR:CD2	1:E:497:TYR:N	2.66	0.63
1:F:413:THR:CG2	1:F:595:GLN:HE22	2.11	0.63
1:F:497:TYR:N	1:F:497:TYR:CD2	2.66	0.63
1:C:384:TYR:HA	1:C:649:ARG:HA	1.80	0.63
1:E:553:GLY:HA2	1:E:574:ILE:HD12	1.81	0.63
1:B:93:ARG:N	1:B:93:ARG:HH11	1.88	0.63
1:E:388:ASN:O	1:E:497:TYR:HA	1.99	0.63
1:C:321:VAL:HG12	1:C:340:ALA:HB2	1.80	0.63
1:F:558:GLY:O	1:F:599:GLY:HA2	1.99	0.63
1:B:106:PRO:HB2	1:B:107:PRO:CD	2.27	0.62
1:D:557:PRO:HB3	1:D:576:SER:O	1.98	0.62
1:B:624:ASN:HB3	1:B:625:PRO:HD3	1.80	0.62
1:C:388:ASN:O	1:C:497:TYR:HA	1.99	0.62
1:E:653:ALA:N	1:E:654:PRO:HD2	2.14	0.62
1:F:388:ASN:O	1:F:497:TYR:HA	1.99	0.62
1:C:497:TYR:CD2	1:C:497:TYR:N	2.67	0.62
1:D:413:THR:CG2	1:D:595:GLN:HE22	2.11	0.62
1:F:567:SER:HB2	1:F:571:LYS:HD2	1.79	0.62
1:E:413:THR:CG2	1:E:595:GLN:HE22	2.13	0.62
1:D:553:GLY:HA2	1:D:574:ILE:HD12	1.81	0.62
1:A:511:VAL:HG23	1:A:512:THR:N	2.14	0.62
1:C:624:ASN:HB3	1:C:625:PRO:HD3	1.81	0.62
1:C:255:LEU:HD22	1:C:256:HIS:H	1.64	0.62
1:C:447:PHE:CE1	1:C:455:PHE:HA	2.34	0.62
1:B:413:THR:CG2	1:B:595:GLN:HE22	2.12	0.62
1:B:553:GLY:HA2	1:B:574:ILE:HD12	1.82	0.62
1:A:271:ALA:HB1	1:A:330:TRP:CH2	2.35	0.62
1:D:497:TYR:HD2	1:D:497:TYR:N	1.96	0.62
1:A:624:ASN:HB3	1:A:625:PRO:HD3	1.82	0.62
1:F:289:THR:HG21	1:F:293:THR:CG2	2.24	0.62
1:D:289:THR:HG21	1:D:293:THR:CG2	2.27	0.62
1:F:11:PRO:HG3	1:F:50:GLN:HB2	1.82	0.62
1:A:497:TYR:HD2	1:A:497:TYR:N	1.97	0.62
1:F:384:TYR:HA	1:F:649:ARG:HA	1.80	0.62
1:C:413:THR:CG2	1:C:595:GLN:HE22	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:ILE:HD11	1:D:330:TRP:NE1	2.05	0.62
1:E:136:GLY:HA3	1:E:268:VAL:CG2	2.26	0.62
1:B:136:GLY:HA3	1:B:268:VAL:CG2	2.26	0.62
1:A:388:ASN:O	1:A:497:TYR:HA	2.00	0.62
1:E:543:LEU:HD23	1:E:610:PRO:HG3	1.81	0.61
1:E:271:ALA:HB1	1:E:330:TRP:CH2	2.35	0.61
1:F:271:ALA:HB1	1:F:330:TRP:CH2	2.36	0.61
1:D:543:LEU:HD23	1:D:610:PRO:HG3	1.80	0.61
1:C:149:LYS:C	1:C:150:ILE:HD12	2.19	0.61
1:B:11:PRO:HG3	1:B:50:GLN:HB2	1.81	0.61
1:B:543:LEU:HD23	1:B:610:PRO:HG3	1.82	0.61
1:B:271:ALA:HB1	1:B:330:TRP:CH2	2.35	0.61
1:D:536:LYS:HG2	1:D:549:PHE:CE2	2.36	0.61
1:E:624:ASN:HB3	1:E:625:PRO:HD3	1.81	0.61
1:F:553:GLY:HA2	1:F:574:ILE:HD12	1.83	0.61
1:D:93:ARG:HH11	1:D:93:ARG:N	1.89	0.61
1:D:388:ASN:O	1:D:497:TYR:HA	2.00	0.61
1:C:537:VAL:HG22	1:C:546:ASN:HD22	1.66	0.61
1:D:271:ALA:HB1	1:D:330:TRP:CH2	2.36	0.61
1:E:289:THR:HG21	1:E:293:THR:CG2	2.25	0.61
1:D:610:PRO:O	1:D:614:THR:HG23	2.01	0.61
1:F:511:VAL:HG23	1:F:512:THR:N	2.15	0.61
1:F:497:TYR:N	1:F:497:TYR:HD2	1.99	0.61
1:A:421:LYS:HE2	1:A:424:GLY:HA3	1.83	0.61
1:A:321:VAL:HG12	1:A:340:ALA:HB2	1.83	0.61
1:C:257:LEU:N	1:C:258:PRO:CD	2.64	0.61
1:F:149:LYS:C	1:F:150:ILE:HD12	2.21	0.61
1:B:497:TYR:CD2	1:B:497:TYR:N	2.67	0.61
1:A:413:THR:CG2	1:A:595:GLN:HE22	2.14	0.61
1:C:536:LYS:HG2	1:C:549:PHE:CE2	2.36	0.61
1:F:536:LYS:HG2	1:F:549:PHE:CE2	2.36	0.61
1:D:511:VAL:HG23	1:D:512:THR:N	2.15	0.61
1:E:497:TYR:HD2	1:E:497:TYR:N	1.99	0.61
1:A:514:GLY:O	1:A:516:SER:N	2.31	0.61
1:F:557:PRO:HB3	1:F:576:SER:O	2.01	0.61
1:D:421:LYS:HE2	1:D:424:GLY:HA3	1.83	0.61
1:A:553:GLY:HA2	1:A:574:ILE:HD12	1.82	0.60
1:C:274:PRO:HD3	1:C:330:TRP:CE3	2.36	0.60
1:E:257:LEU:N	1:E:258:PRO:CD	2.64	0.60
1:A:257:LEU:N	1:A:258:PRO:CD	2.64	0.60
1:E:93:ARG:N	1:E:93:ARG:HH11	1.89	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:PRO:HG3	1:C:50:GLN:HB2	1.83	0.60
1:A:378:LEU:HG	1:A:691:HIS:CD2	2.37	0.60
1:E:149:LYS:C	1:E:150:ILE:HD12	2.22	0.60
1:A:447:PHE:HD1	1:A:455:PHE:HA	1.67	0.60
1:B:126:LEU:HD12	1:B:127:ALA:H	1.67	0.60
1:B:300:LEU:HG	1:B:326:LEU:HA	1.84	0.60
1:B:537:VAL:HG22	1:B:546:ASN:HD22	1.67	0.60
1:A:289:THR:HG21	1:A:293:THR:CG2	2.26	0.60
1:D:496:VAL:HG22	1:D:501:THR:CB	2.32	0.60
1:D:11:PRO:HG3	1:D:50:GLN:HB2	1.83	0.60
1:F:624:ASN:HB3	1:F:625:PRO:HD3	1.84	0.60
1:E:298:ARG:HH12	1:E:615:ALA:HB3	1.66	0.60
1:A:536:LYS:HG2	1:A:549:PHE:CE2	2.37	0.60
1:F:423:CYS:HA	1:F:459:GLU:O	2.02	0.60
1:E:11:PRO:HG3	1:E:50:GLN:HB2	1.83	0.59
1:E:511:VAL:HG23	1:E:512:THR:N	2.17	0.59
1:D:566:THR:OG1	1:D:571:LYS:HB2	2.02	0.59
1:E:537:VAL:HG22	1:E:546:ASN:HD22	1.67	0.59
1:D:257:LEU:N	1:D:258:PRO:CD	2.64	0.59
1:E:566:THR:OG1	1:E:571:LYS:HB2	2.02	0.59
1:C:557:PRO:HB3	1:C:576:SER:O	2.02	0.59
1:F:451:GLY:O	1:F:589:VAL:HG23	2.02	0.59
1:A:496:VAL:HG22	1:A:501:THR:CB	2.33	0.59
1:C:511:VAL:HG23	1:C:512:THR:N	2.17	0.59
1:A:537:VAL:HG22	1:A:546:ASN:HD22	1.67	0.59
1:D:50:GLN:HE22	1:D:65:ARG:NH2	2.01	0.59
1:F:106:PRO:HB2	1:F:107:PRO:CD	2.28	0.59
1:C:271:ALA:HB1	1:C:330:TRP:CH2	2.38	0.59
1:B:149:LYS:C	1:B:150:ILE:HD12	2.22	0.59
1:B:321:VAL:HG12	1:B:340:ALA:HB2	1.85	0.59
1:E:470:LEU:HB3	1:E:474:CYS:SG	2.43	0.59
1:A:126:LEU:HD12	1:A:127:ALA:H	1.67	0.59
1:B:470:LEU:HB3	1:B:474:CYS:SG	2.42	0.59
1:B:257:LEU:H	1:B:258:PRO:CD	2.10	0.59
1:B:311:ILE:HD11	1:B:330:TRP:NE1	2.04	0.59
1:C:257:LEU:H	1:C:258:PRO:CD	2.09	0.59
1:D:136:GLY:HA3	1:D:268:VAL:CG2	2.27	0.59
1:F:496:VAL:HG22	1:F:501:THR:CB	2.33	0.59
1:C:497:TYR:HD2	1:C:497:TYR:N	2.00	0.59
1:F:537:VAL:HG22	1:F:546:ASN:HD22	1.68	0.59
1:F:136:GLY:HA3	1:F:268:VAL:CG2	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:CYS:HA	1:C:459:GLU:O	2.02	0.59
1:A:557:PRO:HB3	1:A:576:SER:O	2.03	0.59
1:B:257:LEU:N	1:B:258:PRO:CD	2.64	0.59
1:C:50:GLN:HE22	1:C:65:ARG:NH2	2.01	0.59
1:D:387:LEU:HD12	1:D:647:PHE:CE1	2.38	0.59
1:B:566:THR:OG1	1:B:571:LYS:HB2	2.03	0.59
1:F:566:THR:OG1	1:F:571:LYS:HB2	2.02	0.59
1:D:126:LEU:HD12	1:D:127:ALA:H	1.68	0.59
1:E:558:GLY:O	1:E:599:GLY:HA2	2.03	0.59
1:E:574:ILE:O	1:E:574:ILE:HG13	2.01	0.59
1:C:514:GLY:O	1:C:516:SER:N	2.30	0.59
1:C:543:LEU:HD23	1:C:610:PRO:HG3	1.84	0.58
1:D:95:SER:OG	1:D:259:PHE:CE1	2.42	0.58
1:F:470:LEU:HB3	1:F:474:CYS:SG	2.43	0.58
1:A:18:TYR:HE1	1:A:22:THR:HG22	1.68	0.58
1:B:511:VAL:HG23	1:B:512:THR:N	2.17	0.58
1:B:497:TYR:HD2	1:B:497:TYR:N	2.00	0.58
1:F:321:VAL:HG12	1:F:340:ALA:HB2	1.86	0.58
1:C:106:PRO:HB2	1:C:107:PRO:CD	2.28	0.58
1:F:274:PRO:HD3	1:F:330:TRP:CE3	2.38	0.58
1:C:386:PRO:HB2	1:C:689:PRO:HG2	1.85	0.58
1:C:496:VAL:HG22	1:C:501:THR:CB	2.30	0.58
3:F:761:NAG:H61	3:F:762:NAG:C7	2.32	0.58
1:F:610:PRO:O	1:F:614:THR:HG23	2.03	0.58
2:C:761:NAG:H62	2:C:762:NAG:O7	2.03	0.58
1:B:361:TYR:HB2	1:B:381:ARG:NH2	2.18	0.58
1:A:566:THR:OG1	1:A:571:LYS:HB2	2.03	0.58
1:D:514:GLY:O	1:D:516:SER:N	2.31	0.58
1:C:300:LEU:HG	1:C:326:LEU:HA	1.85	0.58
1:E:421:LYS:HE2	1:E:424:GLY:HA3	1.85	0.58
1:A:610:PRO:O	1:A:614:THR:HG23	2.03	0.58
1:D:543:LEU:HA	1:D:612:GLN:HE22	1.69	0.58
1:A:447:PHE:CD1	1:A:448:MSE:N	2.69	0.58
1:D:361:TYR:HB2	1:D:381:ARG:NH2	2.19	0.58
1:E:423:CYS:HA	1:E:459:GLU:O	2.04	0.58
1:B:19:CYS:C	1:B:21:HIS:H	2.07	0.58
1:E:675:MSE:HE2	1:E:715:HIS:CE1	2.36	0.58
1:D:149:LYS:C	1:D:150:ILE:HD12	2.22	0.58
1:F:50:GLN:HE22	1:F:65:ARG:NH2	2.02	0.58
1:A:423:CYS:HA	1:A:459:GLU:O	2.04	0.58
1:B:653:ALA:N	1:B:654:PRO:CD	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:537:VAL:HG22	1:D:546:ASN:HD22	1.68	0.58
1:A:729:LEU:O	1:A:730:CYS:C	2.41	0.58
1:E:729:LEU:O	1:E:730:CYS:C	2.42	0.58
1:A:11:PRO:HG3	1:A:50:GLN:HB2	1.84	0.58
1:A:50:GLN:HE22	1:A:65:ARG:NH2	2.02	0.58
1:C:566:THR:OG1	1:C:571:LYS:HB2	2.02	0.58
1:B:421:LYS:HE2	1:B:424:GLY:HA3	1.85	0.58
1:F:126:LEU:HD12	1:F:127:ALA:H	1.69	0.58
1:E:300:LEU:HG	1:E:326:LEU:HA	1.85	0.58
1:C:729:LEU:O	1:C:730:CYS:C	2.42	0.57
1:F:544:VAL:H	1:F:612:GLN:HE22	1.50	0.57
1:C:544:VAL:H	1:C:612:GLN:HE22	1.51	0.57
1:D:497:TYR:HD2	1:D:497:TYR:H	1.52	0.57
1:D:729:LEU:O	1:D:730:CYS:C	2.42	0.57
1:B:274:PRO:HD3	1:B:330:TRP:CE3	2.39	0.57
1:A:19:CYS:C	1:A:21:HIS:H	2.07	0.57
1:E:50:GLN:HE22	1:E:65:ARG:NH2	2.03	0.57
1:E:450:GLY:HA3	1:E:587:LYS:HA	1.85	0.57
1:B:423:CYS:HA	1:B:459:GLU:O	2.03	0.57
1:D:321:VAL:HG12	1:D:340:ALA:HB2	1.85	0.57
1:E:514:GLY:O	1:E:516:SER:N	2.31	0.57
1:D:19:CYS:C	1:D:21:HIS:H	2.07	0.57
1:B:390:GLU:HG2	1:B:496:VAL:HB	1.87	0.57
1:A:387:LEU:HD12	1:A:647:PHE:CE1	2.38	0.57
1:E:450:GLY:HA2	1:E:587:LYS:O	2.04	0.57
1:E:361:TYR:HB2	1:E:381:ARG:NH2	2.20	0.57
1:F:675:MSE:HE2	1:F:715:HIS:CE1	2.37	0.57
1:B:729:LEU:O	1:B:730:CYS:C	2.42	0.57
1:E:387:LEU:HD12	1:E:647:PHE:CE1	2.39	0.57
1:A:300:LEU:HG	1:A:326:LEU:HA	1.86	0.57
1:F:27:SER:HB2	1:F:28:PRO:HD2	1.87	0.57
1:D:399:LEU:O	1:D:487:ALA:HB1	2.03	0.57
1:A:288:ASP:OD1	1:A:314:LYS:HB2	2.05	0.57
1:E:311:ILE:HD11	1:E:330:TRP:NE1	2.05	0.57
1:D:544:VAL:H	1:D:612:GLN:HE22	1.52	0.57
1:D:50:GLN:HE22	1:D:65:ARG:HH21	1.51	0.57
1:B:536:LYS:HG2	1:B:549:PHE:CE2	2.39	0.57
1:F:300:LEU:HG	1:F:326:LEU:HA	1.85	0.57
1:D:300:LEU:HG	1:D:326:LEU:HA	1.85	0.57
1:C:667:THR:OG1	1:C:673:GLY:HA3	2.05	0.57
1:A:399:LEU:O	1:A:487:ALA:HB1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:TYR:HB2	1:C:381:ARG:NH2	2.18	0.57
1:F:18:TYR:HE1	1:F:22:THR:HG22	1.69	0.57
1:C:690:VAL:HG12	1:C:699:LEU:HD13	1.87	0.57
1:E:19:CYS:C	1:E:21:HIS:H	2.07	0.57
1:B:544:VAL:H	1:B:612:GLN:HE22	1.50	0.57
1:B:675:MSE:HE2	1:B:715:HIS:CE1	2.38	0.57
1:A:27:SER:HB2	1:A:28:PRO:HD2	1.87	0.57
1:F:653:ALA:HB1	1:F:684:ARG:HD2	1.87	0.57
1:A:544:VAL:H	1:A:612:GLN:HE22	1.52	0.57
1:F:543:LEU:HD23	1:F:610:PRO:HG3	1.86	0.57
1:B:387:LEU:HD12	1:B:647:PHE:CE1	2.39	0.57
1:F:653:ALA:N	1:F:654:PRO:HD2	2.19	0.57
1:F:421:LYS:HE2	1:F:424:GLY:HA3	1.85	0.57
1:A:92:ARG:HA	1:A:93:ARG:NH1	2.20	0.57
1:A:268:VAL:HG22	1:A:269:PRO:HD2	1.87	0.57
1:C:654:PRO:HB3	1:C:684:ARG:C	2.25	0.57
1:C:399:LEU:O	1:C:487:ALA:HB1	2.05	0.57
1:C:558:GLY:O	1:C:599:GLY:HA2	2.04	0.57
1:A:654:PRO:HB3	1:A:684:ARG:C	2.25	0.57
1:F:514:GLY:O	1:F:516:SER:N	2.30	0.57
1:D:274:PRO:HD3	1:D:330:TRP:CE3	2.40	0.57
1:D:423:CYS:HA	1:D:459:GLU:O	2.04	0.57
1:B:543:LEU:HA	1:B:612:GLN:HE22	1.70	0.57
1:A:622:ALA:HB3	1:A:627:ARG:HG3	1.87	0.57
1:A:361:TYR:HB2	1:A:381:ARG:NH2	2.19	0.57
1:A:274:PRO:HD3	1:A:330:TRP:CE3	2.39	0.57
1:B:298:ARG:HH12	1:B:615:ALA:HB3	1.70	0.57
1:D:390:GLU:HG2	1:D:496:VAL:HB	1.87	0.57
1:E:544:VAL:H	1:E:612:GLN:HE22	1.51	0.57
1:F:387:LEU:HD12	1:F:647:PHE:CE1	2.40	0.57
1:E:690:VAL:HG12	1:E:699:LEU:HD13	1.86	0.57
1:E:557:PRO:HB3	1:E:576:SER:O	2.05	0.57
1:C:93:ARG:HH11	1:C:93:ARG:N	1.91	0.56
1:D:454:CYS:SG	1:D:455:PHE:N	2.75	0.56
1:E:390:GLU:HG2	1:E:496:VAL:HB	1.86	0.56
1:B:496:VAL:HG22	1:B:501:THR:CB	2.33	0.56
1:A:149:LYS:C	1:A:150:ILE:HD12	2.25	0.56
1:E:654:PRO:HB3	1:E:684:ARG:C	2.25	0.56
1:F:654:PRO:HB3	1:F:684:ARG:C	2.25	0.56
1:D:667:THR:OG1	1:D:673:GLY:HA3	2.05	0.56
1:F:729:LEU:O	1:F:730:CYS:C	2.42	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:HIS:HB3	1:A:343:SER:HB3	1.87	0.56
1:F:667:THR:OG1	1:F:673:GLY:HA3	2.05	0.56
1:F:399:LEU:O	1:F:487:ALA:HB1	2.05	0.56
1:C:19:CYS:C	1:C:21:HIS:H	2.07	0.56
1:D:654:PRO:HB3	1:D:684:ARG:C	2.25	0.56
1:B:530:PHE:CZ	1:B:617:PHE:HD1	2.23	0.56
1:C:288:ASP:OD1	1:C:314:LYS:HB2	2.04	0.56
1:D:622:ALA:HB3	1:D:627:ARG:HG3	1.87	0.56
1:E:18:TYR:HE1	1:E:22:THR:HG22	1.69	0.56
1:B:690:VAL:HG12	1:B:699:LEU:HD13	1.86	0.56
1:D:470:LEU:HB3	1:D:474:CYS:SG	2.46	0.56
1:B:557:PRO:HB3	1:B:576:SER:O	2.05	0.56
1:C:27:SER:HB2	1:C:28:PRO:HD2	1.87	0.56
1:D:118:SER:O	1:D:119:ASN:HB2	2.05	0.56
1:A:390:GLU:HG2	1:A:496:VAL:HB	1.86	0.56
1:B:50:GLN:HE22	1:B:65:ARG:NH2	2.02	0.56
1:E:37:GLU:OE1	1:E:473:ASP:OD2	2.24	0.56
1:E:441:PHE:CD1	1:E:583:LYS:HG2	2.41	0.56
1:C:470:LEU:HB3	1:C:474:CYS:SG	2.46	0.56
1:E:622:ALA:HB3	1:E:627:ARG:HG3	1.87	0.56
1:C:421:LYS:HE2	1:C:424:GLY:HA3	1.87	0.56
1:A:138:GLU:OE2	1:A:271:ALA:HB2	2.05	0.56
1:E:496:VAL:HG22	1:E:501:THR:CB	2.33	0.56
1:D:675:MSE:HE2	1:D:715:HIS:CE1	2.37	0.56
1:E:50:GLN:HE22	1:E:65:ARG:HH21	1.52	0.56
1:C:51:PHE:HB3	1:C:80:MSE:SE	2.55	0.56
1:B:574:ILE:HG13	1:B:574:ILE:O	2.06	0.56
1:E:321:VAL:HG12	1:E:340:ALA:HB2	1.86	0.56
1:E:667:THR:OG1	1:E:673:GLY:HA3	2.05	0.56
1:B:374:PRO:HA	1:B:392:THR:HG22	1.88	0.56
2:B:763:BMA:C2	2:B:764:MAN:O5	2.53	0.56
1:B:654:PRO:HB3	1:B:684:ARG:C	2.26	0.56
1:A:690:VAL:HG12	1:A:699:LEU:HD13	1.87	0.56
1:D:321:VAL:HG22	1:D:326:LEU:HD23	1.87	0.56
1:F:66:TYR:CD2	1:F:67:MSE:O	2.59	0.56
1:A:470:LEU:HB3	1:A:474:CYS:SG	2.46	0.56
1:F:288:ASP:OD1	1:F:314:LYS:HB2	2.05	0.56
1:F:93:ARG:HH11	1:F:93:ARG:N	1.90	0.56
1:D:257:LEU:H	1:D:258:PRO:CD	2.10	0.56
1:E:655:LEU:HB2	1:E:683:ASP:OD2	2.06	0.56
1:F:50:GLN:HE22	1:F:65:ARG:HH21	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:ILE:HG13	1:A:574:ILE:O	2.06	0.56
1:C:66:TYR:CD2	1:C:67:MSE:O	2.59	0.56
1:B:27:SER:HB2	1:B:28:PRO:HD2	1.86	0.56
1:B:87:THR:OG1	1:B:107:PRO:HD2	2.06	0.56
1:E:274:PRO:HD3	1:E:330:TRP:CE3	2.41	0.56
1:C:622:ALA:HB3	1:C:627:ARG:HG3	1.88	0.56
1:A:311:ILE:HD11	1:A:330:TRP:NE1	2.05	0.56
1:A:93:ARG:N	1:A:93:ARG:HH11	1.91	0.56
1:B:50:GLN:HE22	1:B:65:ARG:HH21	1.52	0.56
1:A:50:GLN:HE22	1:A:65:ARG:HH21	1.52	0.56
1:C:387:LEU:HD12	1:C:647:PHE:CE1	2.41	0.56
1:D:690:VAL:HG12	1:D:699:LEU:HD13	1.87	0.56
1:E:27:SER:HB2	1:E:28:PRO:HD2	1.88	0.56
1:E:288:ASP:OD1	1:E:314:LYS:HB2	2.06	0.56
1:E:87:THR:OG1	1:E:107:PRO:HD2	2.06	0.55
1:A:87:THR:OG1	1:A:107:PRO:HD2	2.06	0.55
1:C:18:TYR:HE1	1:C:22:THR:HG22	1.68	0.55
1:B:138:GLU:OE2	1:B:271:ALA:HB2	2.07	0.55
1:F:390:GLU:HG2	1:F:496:VAL:HB	1.86	0.55
1:C:50:GLN:HE22	1:C:65:ARG:HH21	1.52	0.55
1:C:441:PHE:CD1	1:C:583:LYS:HG2	2.42	0.55
1:B:514:GLY:O	1:B:516:SER:N	2.31	0.55
1:F:135:VAL:HG12	1:F:140:TYR:OH	2.06	0.55
1:C:126:LEU:HD12	1:C:127:ALA:H	1.71	0.55
1:D:393:VAL:HG23	1:D:491:VAL:HG13	1.89	0.55
1:E:126:LEU:HD12	1:E:127:ALA:H	1.71	0.55
1:F:19:CYS:C	1:F:21:HIS:H	2.08	0.55
1:D:574:ILE:HG13	1:D:574:ILE:O	2.06	0.55
1:F:451:GLY:HA2	1:F:588:ASN:HA	1.88	0.55
1:A:135:VAL:HG12	1:A:140:TYR:OH	2.07	0.55
1:D:27:SER:HB2	1:D:28:PRO:HD2	1.88	0.55
1:B:288:ASP:OD1	1:B:314:LYS:HB2	2.07	0.55
1:D:92:ARG:HA	1:D:93:ARG:NH1	2.21	0.55
1:B:51:PHE:HB3	1:B:80:MSE:SE	2.55	0.55
1:E:374:PRO:HA	1:E:392:THR:HG22	1.88	0.55
1:B:667:THR:OG1	1:B:673:GLY:HA3	2.06	0.55
1:F:441:PHE:CD1	1:F:583:LYS:HG2	2.42	0.55
1:A:114:SER:HB3	1:A:123:SER:HB3	1.88	0.55
1:C:655:LEU:HB2	1:C:683:ASP:OD2	2.06	0.55
1:A:292:LEU:HD22	1:A:310:TRP:HB3	1.88	0.55
1:E:530:PHE:CZ	1:E:617:PHE:HD1	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:GLU:HG2	1:C:496:VAL:HB	1.87	0.55
1:C:675:MSE:HE2	1:C:715:HIS:CE1	2.35	0.55
1:B:610:PRO:O	1:B:614:THR:HG23	2.06	0.55
1:D:655:LEU:HB2	1:D:683:ASP:OD2	2.06	0.55
1:F:51:PHE:HB3	1:F:80:MSE:SE	2.57	0.55
1:D:288:ASP:OD1	1:D:314:LYS:HB2	2.05	0.55
1:D:135:VAL:HG12	1:D:140:TYR:OH	2.07	0.55
1:D:87:THR:OG1	1:D:107:PRO:HD2	2.07	0.55
1:C:135:VAL:HG12	1:C:140:TYR:OH	2.06	0.55
1:E:66:TYR:CD2	1:E:67:MSE:O	2.60	0.55
1:D:18:TYR:HE1	1:D:22:THR:HG22	1.70	0.55
1:B:298:ARG:NH1	1:B:615:ALA:HB3	2.22	0.55
1:D:268:VAL:HG22	1:D:269:PRO:HD2	1.88	0.55
1:F:655:LEU:HB2	1:F:683:ASP:OD2	2.07	0.55
1:A:497:TYR:HD2	1:A:497:TYR:H	1.54	0.55
1:B:114:SER:HB3	1:B:123:SER:HB3	1.88	0.55
1:F:690:VAL:HG12	1:F:699:LEU:HD13	1.87	0.55
1:F:118:SER:O	1:F:119:ASN:HB2	2.07	0.55
1:A:257:LEU:H	1:A:258:PRO:CD	2.09	0.54
1:D:138:GLU:OE2	1:D:271:ALA:HB2	2.07	0.54
1:F:92:ARG:HA	1:F:93:ARG:NH1	2.22	0.54
1:E:114:SER:HB3	1:E:123:SER:HB3	1.88	0.54
1:C:393:VAL:HG23	1:C:491:VAL:HG13	1.90	0.54
1:A:667:THR:OG1	1:A:673:GLY:HA3	2.05	0.54
1:E:298:ARG:NH1	1:E:615:ALA:HB3	2.22	0.54
1:E:610:PRO:O	1:E:614:THR:HG23	2.06	0.54
1:A:118:SER:O	1:A:119:ASN:HB2	2.07	0.54
1:A:393:VAL:HG23	1:A:491:VAL:HG13	1.88	0.54
1:B:441:PHE:CD1	1:B:583:LYS:HG2	2.42	0.54
1:B:92:ARG:HA	1:B:93:ARG:NH1	2.22	0.54
1:C:610:PRO:O	1:C:614:THR:HG23	2.08	0.54
1:E:292:LEU:HD22	1:E:310:TRP:HB3	1.88	0.54
1:A:79:THR:C	1:A:81:ASP:N	2.60	0.54
1:D:51:PHE:HB3	1:D:80:MSE:SE	2.58	0.54
1:D:622:ALA:HB3	1:D:627:ARG:CG	2.38	0.54
1:C:92:ARG:HA	1:C:93:ARG:NH1	2.22	0.54
1:F:268:VAL:HG11	1:F:332:ASN:ND2	2.22	0.54
1:B:655:LEU:HB2	1:B:683:ASP:OD2	2.06	0.54
1:B:79:THR:C	1:B:81:ASP:N	2.61	0.54
1:D:66:TYR:CD2	1:D:67:MSE:O	2.60	0.54
1:C:87:THR:OG1	1:C:107:PRO:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:THR:C	1:D:81:ASP:N	2.60	0.54
1:D:374:PRO:HA	1:D:392:THR:HG22	1.89	0.54
1:F:374:PRO:HA	1:F:392:THR:HG22	1.89	0.54
1:E:399:LEU:O	1:E:487:ALA:HB1	2.07	0.54
1:A:441:PHE:CD1	1:A:583:LYS:HG2	2.42	0.54
1:F:295:LEU:HG	1:F:330:TRP:HD1	1.73	0.54
1:C:114:SER:HB3	1:C:123:SER:HB3	1.90	0.54
1:A:321:VAL:HG22	1:A:326:LEU:HD23	1.88	0.54
1:B:135:VAL:HG12	1:B:140:TYR:OH	2.07	0.54
1:B:399:LEU:O	1:B:487:ALA:HB1	2.07	0.54
1:F:87:THR:OG1	1:F:107:PRO:HD2	2.07	0.54
1:E:295:LEU:HG	1:E:330:TRP:HD1	1.72	0.54
1:C:136:GLY:CA	1:C:268:VAL:HG21	2.29	0.54
1:E:268:VAL:HG22	1:E:269:PRO:HD2	1.90	0.54
1:E:92:ARG:HA	1:E:93:ARG:NH1	2.22	0.54
1:C:445:TYR:CD2	1:C:452:ALA:HB3	2.43	0.54
1:B:292:LEU:HD22	1:B:310:TRP:HB3	1.88	0.54
1:A:655:LEU:HB2	1:A:683:ASP:OD2	2.07	0.54
1:C:574:ILE:O	1:C:574:ILE:HG13	2.07	0.54
1:C:374:PRO:HA	1:C:392:THR:HG22	1.90	0.54
1:C:445:TYR:HB3	1:C:451:GLY:CA	2.33	0.54
1:D:79:THR:HG23	1:D:81:ASP:HB3	1.90	0.54
1:F:508:VAL:HG13	1:F:524:GLY:O	2.08	0.54
1:E:138:GLU:OE2	1:E:271:ALA:HB2	2.07	0.54
1:F:114:SER:HB3	1:F:123:SER:HB3	1.87	0.54
1:A:543:LEU:HA	1:A:612:GLN:HE22	1.72	0.54
1:E:20:HIS:NE2	1:E:121:ALA:HB1	2.23	0.54
1:F:530:PHE:CZ	1:F:617:PHE:HD1	2.26	0.54
1:E:622:ALA:HB3	1:E:627:ARG:CG	2.38	0.54
1:F:393:VAL:HG23	1:F:491:VAL:HG13	1.90	0.53
1:B:66:TYR:CD2	1:B:67:MSE:O	2.61	0.53
1:A:374:PRO:HA	1:A:392:THR:HG22	1.88	0.53
1:E:257:LEU:H	1:E:258:PRO:CD	2.10	0.53
1:A:295:LEU:HG	1:A:330:TRP:HD1	1.73	0.53
1:F:287:LEU:HD13	1:F:311:ILE:HD13	1.90	0.53
1:C:445:TYR:HB3	1:C:452:ALA:N	2.23	0.53
1:D:114:SER:HB3	1:D:123:SER:HB3	1.88	0.53
1:E:393:VAL:HG23	1:E:491:VAL:HG13	1.90	0.53
1:F:543:LEU:HA	1:F:612:GLN:HE22	1.69	0.53
1:E:51:PHE:HB3	1:E:80:MSE:SE	2.58	0.53
1:D:300:LEU:HD11	1:D:337:ARG:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:TYR:HD2	1:E:58:ALA:O	1.91	0.53
1:C:262:ILE:HG13	1:C:263:PRO:N	2.23	0.53
1:A:66:TYR:CD2	1:A:67:MSE:O	2.61	0.53
1:F:29:VAL:HG12	1:F:29:VAL:O	2.08	0.53
1:C:42:THR:HG22	1:C:104:LYS:HG3	1.91	0.53
1:F:95:SER:OG	1:F:259:PHE:CE1	2.42	0.53
1:C:454:CYS:SG	1:C:455:PHE:N	2.81	0.53
1:B:20:HIS:NE2	1:B:121:ALA:HB1	2.24	0.53
1:D:441:PHE:CD1	1:D:583:LYS:HG2	2.43	0.53
1:E:532:PRO:HD2	1:E:533:PHE:CD1	2.43	0.53
1:A:136:GLY:HA3	1:A:268:VAL:CG2	2.27	0.53
1:C:652:ASP:C	1:C:654:PRO:HD2	2.29	0.53
1:C:79:THR:C	1:C:81:ASP:N	2.61	0.53
1:C:508:VAL:HG13	1:C:524:GLY:O	2.08	0.53
1:B:532:PRO:HD2	1:B:533:PHE:CD1	2.44	0.53
1:D:532:PRO:HD2	1:D:533:PHE:CD1	2.44	0.53
1:C:497:TYR:HD2	1:C:497:TYR:H	1.57	0.53
1:D:508:VAL:HG13	1:D:524:GLY:O	2.09	0.53
1:E:118:SER:O	1:E:119:ASN:HB2	2.09	0.53
1:E:29:VAL:HG12	1:E:29:VAL:O	2.09	0.53
1:E:301:GLY:O	1:E:616:PRO:O	2.27	0.53
1:D:447:PHE:HB2	1:D:455:PHE:O	2.09	0.53
1:D:292:LEU:HD22	1:D:310:TRP:HB3	1.90	0.53
1:A:622:ALA:HB3	1:A:627:ARG:CG	2.38	0.53
1:A:20:HIS:NE2	1:A:121:ALA:HB1	2.23	0.53
1:A:29:VAL:HG12	1:A:29:VAL:O	2.09	0.53
1:B:18:TYR:HE1	1:B:22:THR:HG22	1.70	0.53
1:C:20:HIS:NE2	1:C:121:ALA:HB1	2.23	0.53
1:D:131:LYS:NZ	4:D:761:NAG:H81	2.24	0.53
1:C:29:VAL:O	1:C:29:VAL:HG12	2.09	0.53
1:B:93:ARG:H	1:B:93:ARG:NH1	1.90	0.53
1:F:268:VAL:HG22	1:F:269:PRO:HD2	1.91	0.53
1:C:292:LEU:HD22	1:C:310:TRP:HB3	1.90	0.53
1:F:361:TYR:HB2	1:F:381:ARG:HH21	1.74	0.53
1:C:85:ILE:HG22	1:C:86:SER:N	2.24	0.53
1:D:20:HIS:NE2	1:D:121:ALA:HB1	2.23	0.53
1:B:29:VAL:HG12	1:B:29:VAL:O	2.09	0.53
1:B:295:LEU:HG	1:B:330:TRP:HD1	1.73	0.52
1:B:321:VAL:HG22	1:B:326:LEU:HD23	1.91	0.52
1:B:393:VAL:HG23	1:B:491:VAL:HG13	1.91	0.52
1:F:53:TYR:HD2	1:F:58:ALA:O	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:508:VAL:HG13	1:E:524:GLY:O	2.09	0.52
1:B:118:SER:O	1:B:119:ASN:HB2	2.10	0.52
1:C:53:TYR:HD2	1:C:58:ALA:O	1.91	0.52
1:D:107:PRO:CG	1:D:108:GLY:H	2.22	0.52
1:F:497:TYR:H	1:F:497:TYR:HD2	1.55	0.52
1:A:530:PHE:CZ	1:A:617:PHE:HD1	2.27	0.52
1:E:135:VAL:HG12	1:E:140:TYR:OH	2.08	0.52
1:E:603:TRP:O	1:E:607:SER:N	2.43	0.52
1:F:138:GLU:OE2	1:F:271:ALA:HB2	2.10	0.52
1:B:137:ARG:NH1	1:B:296:THR:OG1	2.42	0.52
1:D:42:THR:HG22	1:D:104:LYS:HG3	1.91	0.52
1:C:150:ILE:HG23	1:C:151:PRO:CD	2.39	0.52
1:C:447:PHE:HE1	1:C:455:PHE:HA	1.72	0.52
1:A:287:LEU:HD13	1:A:311:ILE:HD13	1.92	0.52
1:D:295:LEU:HG	1:D:330:TRP:HD1	1.74	0.52
1:F:544:VAL:HG12	1:F:623:VAL:HG21	1.92	0.52
1:F:292:LEU:HD22	1:F:310:TRP:HB3	1.90	0.52
1:C:530:PHE:CZ	1:C:617:PHE:HD1	2.27	0.52
1:F:413:THR:HG23	1:F:595:GLN:HE22	1.75	0.52
1:E:321:VAL:HG22	1:E:326:LEU:HD23	1.91	0.52
1:F:532:PRO:HD2	1:F:533:PHE:CD1	2.44	0.52
1:F:37:GLU:OE1	1:F:473:ASP:OD2	2.27	0.52
1:D:93:ARG:NH1	1:D:93:ARG:H	1.91	0.52
1:A:51:PHE:HB3	1:A:80:MSE:SE	2.60	0.52
1:B:622:ALA:HB3	1:B:627:ARG:HG3	1.91	0.52
1:F:79:THR:C	1:F:81:ASP:N	2.61	0.52
1:B:413:THR:HG23	1:B:595:GLN:HE22	1.75	0.52
1:D:438:CYS:HA	1:D:464:SER:O	2.09	0.52
1:B:438:CYS:HA	1:B:464:SER:O	2.10	0.52
1:F:20:HIS:NE2	1:F:121:ALA:HB1	2.23	0.52
1:A:483:LYS:HD3	1:A:535:HIS:NE2	2.25	0.52
1:D:287:LEU:HD13	1:D:311:ILE:HD13	1.92	0.52
1:B:268:VAL:HG22	1:B:269:PRO:HD2	1.92	0.52
1:A:79:THR:HG23	1:A:81:ASP:HB3	1.91	0.52
1:B:85:ILE:HG22	1:B:86:SER:N	2.25	0.52
1:E:79:THR:HG23	1:E:81:ASP:HB3	1.91	0.52
1:F:321:VAL:HG22	1:F:326:LEU:HD23	1.91	0.52
1:D:689:PRO:HD2	1:D:730:CYS:HA	1.92	0.52
1:E:112:THR:OG1	1:E:125:THR:HB	2.10	0.52
1:A:53:TYR:HD2	1:A:58:ALA:O	1.93	0.52
1:A:555:MSE:H	1:A:555:MSE:HE2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:294:LEU:HG	1:F:310:TRP:NE1	2.25	0.52
1:C:294:LEU:HD23	1:C:309:GLU:O	2.10	0.52
1:B:341:GLN:O	1:B:669:SER:O	2.27	0.52
1:F:438:CYS:HA	1:F:464:SER:O	2.10	0.52
1:D:72:ASP:HB2	1:D:74:THR:OG1	2.10	0.52
1:A:112:THR:OG1	1:A:125:THR:HB	2.10	0.52
1:D:29:VAL:HG12	1:D:29:VAL:O	2.09	0.52
1:C:295:LEU:HG	1:C:330:TRP:HD1	1.75	0.52
1:A:137:ARG:NH1	1:A:296:THR:OG1	2.43	0.52
1:B:544:VAL:HG12	1:B:623:VAL:HG21	1.92	0.52
1:B:79:THR:HG23	1:B:81:ASP:HB3	1.92	0.52
1:A:496:VAL:HG13	1:A:501:THR:HG22	1.92	0.52
1:E:496:VAL:HG13	1:E:501:THR:HG22	1.92	0.52
1:B:496:VAL:HG13	1:B:501:THR:HG22	1.92	0.52
1:E:85:ILE:HG22	1:E:86:SER:N	2.25	0.51
1:A:508:VAL:HG13	1:A:524:GLY:O	2.10	0.51
1:F:262:ILE:HG13	1:F:263:PRO:O	2.10	0.51
1:C:438:CYS:HA	1:C:464:SER:O	2.10	0.51
1:C:543:LEU:HA	1:C:612:GLN:HE22	1.71	0.51
1:E:45:ILE:HB	1:E:101:LEU:HB2	1.93	0.51
1:C:448:MSE:C	1:C:450:GLY:H	2.13	0.51
1:E:136:GLY:CA	1:E:268:VAL:HG21	2.30	0.51
1:A:675:MSE:HE2	1:A:715:HIS:CE1	2.38	0.51
1:A:79:THR:O	1:A:81:ASP:N	2.43	0.51
1:D:79:THR:O	1:D:81:ASP:N	2.43	0.51
1:F:79:THR:HG23	1:F:81:ASP:HB3	1.92	0.51
1:F:276:VAL:HG22	1:F:285:LEU:HD23	1.91	0.51
1:A:540:HIS:HD2	1:A:541:ARG:HB2	1.76	0.51
1:D:603:TRP:O	1:D:607:SER:N	2.44	0.51
1:A:72:ASP:HB2	1:A:74:THR:OG1	2.10	0.51
1:C:390:GLU:HG3	1:C:390:GLU:O	2.10	0.51
1:D:496:VAL:HG13	1:D:501:THR:HG22	1.92	0.51
1:E:544:VAL:HG12	1:E:623:VAL:HG21	1.91	0.51
1:C:544:VAL:HG12	1:C:623:VAL:HG21	1.92	0.51
1:B:497:TYR:HD2	1:B:497:TYR:H	1.58	0.51
1:C:483:LYS:HD3	1:C:535:HIS:CE1	2.45	0.51
1:F:483:LYS:HD3	1:F:535:HIS:CE1	2.45	0.51
1:B:483:LYS:HD3	1:B:535:HIS:CE1	2.45	0.51
1:E:483:LYS:HD3	1:E:535:HIS:CE1	2.44	0.51
1:A:689:PRO:HD2	1:A:730:CYS:HA	1.92	0.51
1:F:262:ILE:HG13	1:F:263:PRO:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:LYS:HD3	1:B:535:HIS:NE2	2.26	0.51
1:F:603:TRP:O	1:F:607:SER:N	2.44	0.51
1:C:496:VAL:HG13	1:C:501:THR:HG22	1.93	0.51
1:F:85:ILE:HG22	1:F:86:SER:N	2.26	0.51
1:E:413:THR:HG23	1:E:595:GLN:HE22	1.75	0.51
1:C:413:THR:HG23	1:C:595:GLN:HE22	1.76	0.51
1:F:622:ALA:HB3	1:F:627:ARG:CG	2.40	0.51
1:D:483:LYS:HD3	1:D:535:HIS:CE1	2.46	0.51
1:A:438:CYS:HA	1:A:464:SER:O	2.10	0.51
1:B:53:TYR:HD2	1:B:58:ALA:O	1.92	0.51
1:E:262:ILE:HG13	1:E:263:PRO:O	2.10	0.51
1:B:42:THR:HG22	1:B:104:LYS:HG3	1.93	0.51
1:E:137:ARG:NH1	1:E:296:THR:OG1	2.43	0.51
1:A:42:THR:HG22	1:A:104:LYS:HG3	1.92	0.51
1:D:544:VAL:HG12	1:D:623:VAL:HG21	1.93	0.51
1:D:85:ILE:HG22	1:D:86:SER:N	2.25	0.51
1:B:689:PRO:HD2	1:B:730:CYS:HA	1.92	0.51
1:D:530:PHE:CZ	1:D:617:PHE:HD1	2.27	0.51
1:F:483:LYS:HD3	1:F:535:HIS:NE2	2.26	0.51
1:B:508:VAL:HG13	1:B:524:GLY:O	2.10	0.51
1:B:540:HIS:HD2	1:B:541:ARG:HB2	1.76	0.51
1:C:287:LEU:HD13	1:C:311:ILE:HD13	1.93	0.51
1:A:390:GLU:HG3	1:A:390:GLU:O	2.10	0.51
1:C:649:ARG:O	1:C:651:SER:N	2.44	0.51
1:C:603:TRP:O	1:C:607:SER:N	2.44	0.51
1:E:287:LEU:HD13	1:E:311:ILE:HD13	1.93	0.51
1:C:274:PRO:HD3	1:C:330:TRP:CZ3	2.46	0.51
1:B:94:LEU:HD22	1:B:157:ARG:CD	2.38	0.51
1:E:294:LEU:HD23	1:E:309:GLU:O	2.11	0.51
1:F:649:ARG:O	1:F:651:SER:N	2.44	0.51
1:E:689:PRO:HD2	1:E:730:CYS:HA	1.92	0.51
1:C:483:LYS:HD3	1:C:535:HIS:NE2	2.26	0.51
1:D:483:LYS:HD3	1:D:535:HIS:NE2	2.25	0.51
1:B:603:TRP:O	1:B:607:SER:N	2.43	0.51
1:D:540:HIS:HD2	1:D:541:ARG:HB2	1.76	0.51
1:C:581:LEU:HD22	1:C:581:LEU:N	2.26	0.51
1:E:555:MSE:H	1:E:555:MSE:HE2	1.75	0.51
1:E:42:THR:HG22	1:E:104:LYS:HG3	1.92	0.51
1:B:287:LEU:HD13	1:B:311:ILE:HD13	1.93	0.51
1:C:137:ARG:NH1	1:C:296:THR:OG1	2.42	0.51
1:F:390:GLU:O	1:F:390:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ILE:HB	1:B:101:LEU:HB2	1.93	0.51
1:F:622:ALA:HB3	1:F:627:ARG:HG3	1.92	0.51
1:E:107:PRO:CG	1:E:108:GLY:H	2.23	0.50
1:C:268:VAL:HG22	1:C:269:PRO:HD2	1.92	0.50
1:F:496:VAL:HG13	1:F:501:THR:HG22	1.93	0.50
1:A:447:PHE:CZ	1:A:448:MSE:HG2	2.46	0.50
1:E:483:LYS:HD3	1:E:535:HIS:NE2	2.26	0.50
1:C:118:SER:O	1:C:119:ASN:HB2	2.10	0.50
1:B:262:ILE:HG13	1:B:263:PRO:O	2.11	0.50
1:E:438:CYS:HA	1:E:464:SER:O	2.11	0.50
1:B:94:LEU:CD2	1:B:157:ARG:HD3	2.38	0.50
1:C:653:ALA:O	1:C:684:ARG:HD2	2.11	0.50
1:E:79:THR:C	1:E:81:ASP:N	2.61	0.50
1:E:79:THR:O	1:E:81:ASP:N	2.44	0.50
1:C:321:VAL:HG22	1:C:326:LEU:HD23	1.94	0.50
1:D:413:THR:HG23	1:D:595:GLN:HE22	1.75	0.50
1:A:504:LEU:HD21	1:A:521:VAL:HB	1.93	0.50
1:D:390:GLU:HG3	1:D:390:GLU:O	2.11	0.50
1:A:85:ILE:HG22	1:A:86:SER:N	2.27	0.50
1:E:80:MSE:HE3	1:E:80:MSE:CA	2.41	0.50
1:A:400:PRO:CA	1:A:487:ALA:HB2	2.41	0.50
1:D:262:ILE:HG13	1:D:263:PRO:N	2.25	0.50
1:C:689:PRO:HD2	1:C:730:CYS:HA	1.92	0.50
1:F:79:THR:O	1:F:81:ASP:N	2.44	0.50
1:C:79:THR:HG23	1:C:81:ASP:HB3	1.92	0.50
1:D:262:ILE:HG13	1:D:263:PRO:O	2.11	0.50
1:A:262:ILE:HG13	1:A:263:PRO:N	2.25	0.50
1:A:262:ILE:HG13	1:A:263:PRO:O	2.11	0.50
1:E:504:LEU:HD21	1:E:521:VAL:HB	1.94	0.50
1:A:447:PHE:CD1	1:A:454:CYS:O	2.61	0.50
1:C:138:GLU:OE2	1:C:271:ALA:HB2	2.12	0.50
1:F:42:THR:HG22	1:F:104:LYS:HG3	1.92	0.50
1:F:80:MSE:HA	1:F:80:MSE:HE3	1.94	0.50
1:C:622:ALA:HB3	1:C:627:ARG:CG	2.42	0.50
1:A:400:PRO:HD2	1:A:626:LEU:O	2.12	0.50
1:A:278:HIS:CB	1:A:343:SER:HB3	2.41	0.50
1:D:581:LEU:HD22	1:D:581:LEU:N	2.26	0.50
1:A:544:VAL:HG12	1:A:623:VAL:HG21	1.93	0.50
1:B:294:LEU:HG	1:B:310:TRP:NE1	2.26	0.50
1:F:689:PRO:HD2	1:F:730:CYS:HA	1.92	0.50
1:C:262:ILE:HG13	1:C:263:PRO:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:LYS:HD3	1:A:535:HIS:CE1	2.47	0.50
1:B:722:GLN:HG2	1:B:739:GLU:HG2	1.94	0.50
1:C:277:ILE:HD12	1:C:286:GLN:NE2	2.27	0.50
1:C:420:ILE:O	1:C:420:ILE:HD12	2.12	0.50
1:B:622:ALA:HB3	1:B:627:ARG:CG	2.41	0.50
1:B:690:VAL:HG12	1:B:699:LEU:CD1	2.42	0.50
1:A:300:LEU:HD11	1:A:337:ARG:HD3	1.93	0.50
1:A:690:VAL:HG12	1:A:699:LEU:CD1	2.42	0.50
1:D:400:PRO:HD2	1:D:626:LEU:O	2.12	0.50
1:B:374:PRO:CA	1:B:392:THR:HG22	2.42	0.50
1:E:400:PRO:HD2	1:E:626:LEU:O	2.12	0.50
1:E:276:VAL:HG22	1:E:285:LEU:HD23	1.94	0.50
1:A:276:VAL:HG12	1:A:277:ILE:N	2.26	0.50
1:F:112:THR:OG1	1:F:125:THR:HB	2.12	0.50
1:C:532:PRO:HD2	1:C:533:PHE:CD1	2.47	0.50
1:A:581:LEU:N	1:A:581:LEU:HD22	2.26	0.50
1:A:45:ILE:HB	1:A:101:LEU:HB2	1.94	0.50
1:D:504:LEU:HD21	1:D:521:VAL:HB	1.94	0.50
1:E:540:HIS:HD2	1:E:541:ARG:HB2	1.77	0.50
1:F:555:MSE:HE2	1:F:555:MSE:H	1.76	0.50
1:F:106:PRO:CB	1:F:107:PRO:HD3	2.41	0.49
1:F:45:ILE:HB	1:F:101:LEU:HB2	1.93	0.49
1:C:112:THR:OG1	1:C:125:THR:HB	2.11	0.49
1:A:722:GLN:HG2	1:A:739:GLU:HG2	1.94	0.49
1:C:722:GLN:HG2	1:C:739:GLU:HG2	1.94	0.49
1:C:255:LEU:HD22	1:C:256:HIS:CD2	2.47	0.49
1:C:652:ASP:HB3	1:C:654:PRO:HD2	1.95	0.49
1:C:45:ILE:HB	1:C:101:LEU:HB2	1.93	0.49
1:A:80:MSE:CA	1:A:80:MSE:HE3	2.42	0.49
1:D:654:PRO:HB3	1:D:684:ARG:O	2.12	0.49
1:E:497:TYR:HD2	1:E:497:TYR:H	1.56	0.49
1:F:574:ILE:HG13	1:F:574:ILE:O	2.11	0.49
1:E:262:ILE:HG13	1:E:263:PRO:N	2.25	0.49
1:A:603:TRP:O	1:A:607:SER:N	2.45	0.49
1:B:79:THR:O	1:B:81:ASP:N	2.45	0.49
1:D:649:ARG:O	1:D:651:SER:N	2.45	0.49
1:B:504:LEU:HD21	1:B:521:VAL:HB	1.94	0.49
1:F:581:LEU:HD22	1:F:581:LEU:N	2.27	0.49
1:B:138:GLU:OE2	1:B:271:ALA:N	2.46	0.49
1:B:262:ILE:HG13	1:B:263:PRO:N	2.27	0.49
1:A:532:PRO:HD2	1:A:533:PHE:CD1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:LEU:CG	1:B:256:HIS:N	2.65	0.49
1:D:63:LYS:C	1:D:80:MSE:HG2	2.33	0.49
1:E:63:LYS:C	1:E:80:MSE:HG2	2.32	0.49
1:C:79:THR:O	1:C:81:ASP:N	2.45	0.49
1:E:690:VAL:HG12	1:E:699:LEU:CD1	2.42	0.49
1:E:374:PRO:CA	1:E:392:THR:HG22	2.42	0.49
1:D:374:PRO:CA	1:D:392:THR:HG22	2.42	0.49
1:C:276:VAL:HG22	1:C:285:LEU:HD23	1.93	0.49
1:C:72:ASP:HB2	1:C:74:THR:OG1	2.12	0.49
1:A:154:VAL:HG22	1:A:155:TYR:N	2.28	0.49
1:D:112:THR:OG1	1:D:125:THR:HB	2.12	0.49
1:E:72:ASP:HB2	1:E:74:THR:OG1	2.13	0.49
1:D:625:PRO:HD2	1:D:627:ARG:HH12	1.78	0.49
1:D:45:ILE:HB	1:D:101:LEU:HB2	1.94	0.49
1:C:63:LYS:C	1:C:80:MSE:HG2	2.33	0.49
1:C:644:ASN:HA	1:C:647:PHE:CD2	2.48	0.49
1:E:654:PRO:HB3	1:E:684:ARG:O	2.12	0.49
1:A:336:VAL:CG2	1:A:337:ARG:N	2.76	0.49
1:C:400:PRO:HD2	1:C:626:LEU:O	2.13	0.49
1:A:374:PRO:CA	1:A:392:THR:HG22	2.42	0.49
1:A:276:VAL:HG22	1:A:285:LEU:HD23	1.94	0.49
1:D:268:VAL:HG11	1:D:332:ASN:ND2	2.27	0.49
1:E:543:LEU:HA	1:E:612:GLN:HE22	1.72	0.49
1:A:294:LEU:HG	1:A:310:TRP:NE1	2.26	0.49
1:B:654:PRO:HB3	1:B:684:ARG:O	2.13	0.49
1:D:80:MSE:HA	1:D:80:MSE:HE3	1.94	0.49
1:F:63:LYS:C	1:F:80:MSE:HG2	2.33	0.49
1:B:649:ARG:O	1:B:651:SER:N	2.45	0.49
1:A:400:PRO:HA	1:A:487:ALA:CB	2.43	0.49
1:E:276:VAL:HG12	1:E:277:ILE:N	2.28	0.49
1:F:504:LEU:HD21	1:F:521:VAL:HB	1.95	0.49
1:C:508:VAL:HG12	1:C:508:VAL:O	2.13	0.49
1:C:504:LEU:HD21	1:C:521:VAL:HB	1.95	0.49
1:B:112:THR:OG1	1:B:125:THR:HB	2.12	0.49
1:E:138:GLU:OE2	1:E:271:ALA:N	2.46	0.49
1:A:63:LYS:C	1:A:80:MSE:HG2	2.33	0.49
1:C:80:MSE:HE3	1:C:80:MSE:HA	1.95	0.49
1:E:649:ARG:O	1:E:651:SER:N	2.46	0.49
1:E:300:LEU:HD11	1:E:337:ARG:HD3	1.95	0.49
1:F:276:VAL:HG12	1:F:277:ILE:N	2.28	0.49
1:E:722:GLN:HG2	1:E:739:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:GLU:O	1:B:390:GLU:HG3	2.13	0.49
1:C:80:MSE:HE3	1:C:80:MSE:CA	2.43	0.49
1:D:400:PRO:CA	1:D:487:ALA:HB2	2.42	0.49
1:F:508:VAL:HG12	1:F:508:VAL:O	2.12	0.49
1:D:276:VAL:HG22	1:D:285:LEU:HD23	1.95	0.49
1:F:407:ILE:HG21	1:F:568:LEU:HD13	1.95	0.49
1:E:77:GLU:HG2	1:E:78:GLY:N	2.28	0.49
1:B:555:MSE:HE2	1:B:555:MSE:H	1.77	0.49
1:D:137:ARG:NH1	1:D:296:THR:OG1	2.46	0.48
1:D:653:ALA:N	1:D:654:PRO:CD	2.74	0.48
1:F:722:GLN:HG2	1:F:739:GLU:HG2	1.94	0.48
1:D:722:GLN:HG2	1:D:739:GLU:HG2	1.94	0.48
1:B:92:ARG:HA	1:B:93:ARG:HH12	1.79	0.48
1:B:268:VAL:HG11	1:B:332:ASN:ND2	2.28	0.48
1:F:93:ARG:H	1:F:93:ARG:NH1	1.92	0.48
1:F:644:ASN:HA	1:F:647:PHE:CD2	2.48	0.48
1:E:644:ASN:HA	1:E:647:PHE:CD2	2.49	0.48
1:C:77:GLU:HG2	1:C:78:GLY:N	2.28	0.48
1:F:77:GLU:HG2	1:F:78:GLY:N	2.28	0.48
1:B:72:ASP:HB2	1:B:74:THR:OG1	2.12	0.48
1:B:136:GLY:CA	1:B:268:VAL:HG21	2.30	0.48
1:F:80:MSE:CA	1:F:80:MSE:HE3	2.43	0.48
1:F:446:PRO:O	1:F:447:PHE:CB	2.61	0.48
1:B:688:CYS:SG	1:B:706:VAL:HG21	2.53	0.48
1:E:688:CYS:SG	1:E:706:VAL:HG21	2.53	0.48
1:F:274:PRO:HD3	1:F:330:TRP:CZ3	2.48	0.48
1:C:690:VAL:HG12	1:C:699:LEU:CD1	2.42	0.48
1:D:80:MSE:HE3	1:D:80:MSE:CA	2.43	0.48
1:D:644:ASN:HA	1:D:647:PHE:CD2	2.48	0.48
1:A:649:ARG:O	1:A:651:SER:N	2.45	0.48
1:E:537:VAL:HG22	1:E:546:ASN:ND2	2.28	0.48
1:A:653:ALA:N	1:A:654:PRO:HD2	2.28	0.48
1:F:690:VAL:HG12	1:F:699:LEU:CD1	2.43	0.48
1:D:154:VAL:HG22	1:D:155:TYR:N	2.28	0.48
1:D:92:ARG:HA	1:D:93:ARG:HH12	1.78	0.48
1:C:321:VAL:CG1	1:C:340:ALA:HB2	2.44	0.48
1:B:399:LEU:HD12	1:B:399:LEU:N	2.28	0.48
1:F:688:CYS:SG	1:F:706:VAL:HG21	2.54	0.48
1:A:272:HIS:O	1:A:273:ALA:C	2.51	0.48
1:F:420:ILE:HD12	1:F:420:ILE:O	2.13	0.48
1:B:420:ILE:HD12	1:B:420:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:ARG:HA	1:F:93:ARG:HH12	1.79	0.48
1:F:150:ILE:HG23	1:F:151:PRO:CD	2.42	0.48
1:A:644:ASN:HA	1:A:647:PHE:CD2	2.48	0.48
1:B:644:ASN:HA	1:B:647:PHE:CD2	2.48	0.48
1:C:537:VAL:HG22	1:C:546:ASN:ND2	2.27	0.48
1:D:276:VAL:HG12	1:D:277:ILE:N	2.27	0.48
1:D:277:ILE:HD12	1:D:286:GLN:NE2	2.28	0.48
1:D:53:TYR:HD2	1:D:58:ALA:O	1.97	0.48
1:A:64:TYR:CG	1:A:83:ILE:HD11	2.49	0.48
1:A:106:PRO:CB	1:A:107:PRO:HD3	2.40	0.48
1:E:92:ARG:HA	1:E:93:ARG:HH12	1.79	0.48
1:D:652:ASP:C	1:D:654:PRO:HD2	2.34	0.48
1:C:336:VAL:CG2	1:C:337:ARG:N	2.76	0.48
1:A:537:VAL:HG22	1:A:546:ASN:ND2	2.28	0.48
1:F:336:VAL:CG2	1:F:337:ARG:N	2.77	0.48
1:D:400:PRO:HA	1:D:487:ALA:CB	2.44	0.48
1:F:400:PRO:HD2	1:F:626:LEU:O	2.13	0.48
1:F:72:ASP:HB2	1:F:74:THR:OG1	2.13	0.48
1:E:420:ILE:O	1:E:420:ILE:HD12	2.13	0.48
1:F:154:VAL:HG22	1:F:155:TYR:N	2.28	0.48
1:A:107:PRO:CG	1:A:108:GLY:H	2.22	0.48
1:C:445:TYR:CB	1:C:451:GLY:HA3	2.37	0.48
1:A:413:THR:HG23	1:A:595:GLN:HE22	1.77	0.48
1:F:374:PRO:CA	1:F:392:THR:HG22	2.44	0.48
1:E:400:PRO:CA	1:E:487:ALA:HB2	2.44	0.48
1:B:594:THR:HG21	1:C:272:HIS:HA	1.95	0.48
1:B:274:PRO:HD3	1:B:330:TRP:CZ3	2.49	0.48
1:A:262:ILE:HD12	1:A:263:PRO:HD2	1.96	0.48
1:E:504:LEU:O	1:E:504:LEU:HD12	2.14	0.48
1:D:106:PRO:CB	1:D:107:PRO:HD3	2.40	0.48
1:E:329:ILE:HG12	1:E:329:ILE:H	1.49	0.48
1:E:93:ARG:NH1	1:E:93:ARG:H	1.91	0.48
1:F:137:ARG:NH1	1:F:296:THR:OG1	2.45	0.48
1:E:80:MSE:HE3	1:E:80:MSE:HA	1.94	0.48
1:A:449:TRP:O	1:A:451:GLY:N	2.46	0.48
1:F:400:PRO:CA	1:F:487:ALA:HB2	2.44	0.48
1:C:688:CYS:SG	1:C:706:VAL:HG21	2.53	0.48
1:B:394:MSE:HE2	1:B:394:MSE:HB3	1.91	0.48
1:D:555:MSE:HE2	1:D:555:MSE:H	1.78	0.48
1:F:329:ILE:HG12	1:F:329:ILE:H	1.50	0.47
1:B:336:VAL:CG2	1:B:337:ARG:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:690:VAL:HG12	1:D:699:LEU:CD1	2.43	0.47
1:E:400:PRO:HA	1:E:487:ALA:CB	2.44	0.47
1:D:106:PRO:CB	1:D:107:PRO:CD	2.92	0.47
1:F:138:GLU:OE2	1:F:271:ALA:N	2.47	0.47
1:C:92:ARG:HA	1:C:93:ARG:HH12	1.80	0.47
1:A:294:LEU:HD23	1:A:309:GLU:O	2.14	0.47
1:A:80:MSE:HA	1:A:80:MSE:HE3	1.95	0.47
1:C:300:LEU:HD11	1:C:337:ARG:HD3	1.95	0.47
1:B:537:VAL:HG22	1:B:546:ASN:ND2	2.28	0.47
1:C:374:PRO:CA	1:C:392:THR:HG22	2.43	0.47
1:F:148:LYS:O	1:F:267:MSE:HA	2.15	0.47
1:F:64:TYR:CG	1:F:83:ILE:HD11	2.49	0.47
1:B:106:PRO:CB	1:B:107:PRO:CD	2.92	0.47
1:E:106:PRO:CB	1:E:107:PRO:CD	2.92	0.47
1:D:145:VAL:CG2	1:F:17:SER:HB3	2.30	0.47
1:D:336:VAL:CG2	1:D:337:ARG:N	2.78	0.47
1:F:654:PRO:HB3	1:F:684:ARG:O	2.14	0.47
1:B:400:PRO:HD2	1:B:626:LEU:O	2.14	0.47
1:F:277:ILE:HD12	1:F:286:GLN:NE2	2.30	0.47
1:B:508:VAL:O	1:B:508:VAL:HG12	2.15	0.47
1:F:540:HIS:HD2	1:F:541:ARG:HB2	1.79	0.47
1:D:77:GLU:HG2	1:D:78:GLY:N	2.29	0.47
1:C:540:HIS:HD2	1:C:541:ARG:HB2	1.79	0.47
1:B:106:PRO:CB	1:B:107:PRO:HD3	2.40	0.47
1:D:615:ALA:HA	1:D:616:PRO:HD3	1.55	0.47
1:E:390:GLU:O	1:E:390:GLU:HG3	2.13	0.47
1:C:294:LEU:HG	1:C:310:TRP:NE1	2.28	0.47
1:B:80:MSE:HA	1:B:80:MSE:HE3	1.95	0.47
1:B:400:PRO:HA	1:B:487:ALA:CB	2.44	0.47
1:D:661:CYS:HA	1:D:678:LEU:HD23	1.97	0.47
1:E:154:VAL:HG22	1:E:155:TYR:N	2.29	0.47
1:E:137:ARG:H	1:E:332:ASN:HD22	1.63	0.47
1:F:400:PRO:HA	1:F:487:ALA:CB	2.45	0.47
1:B:148:LYS:O	1:B:267:MSE:HA	2.14	0.47
1:B:276:VAL:HG22	1:B:285:LEU:HD23	1.95	0.47
1:A:420:ILE:HD12	1:A:420:ILE:O	2.13	0.47
1:B:294:LEU:HD23	1:B:309:GLU:O	2.14	0.47
1:B:80:MSE:CA	1:B:80:MSE:HE3	2.45	0.47
1:F:272:HIS:O	1:F:273:ALA:C	2.53	0.47
1:E:148:LYS:O	1:E:267:MSE:HA	2.15	0.47
1:D:493:LEU:HD23	1:D:493:LEU:HA	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:PRO:CB	1:C:107:PRO:CD	2.93	0.47
1:C:268:VAL:HG11	1:C:332:ASN:ND2	2.29	0.47
1:A:268:VAL:HG22	1:A:269:PRO:CD	2.44	0.47
1:E:305:GLU:N	1:E:306:PRO:HD3	2.30	0.47
1:C:375:TYR:O	1:C:390:GLU:HA	2.14	0.47
1:D:375:TYR:O	1:D:390:GLU:HA	2.15	0.47
1:F:375:TYR:O	1:F:390:GLU:HA	2.14	0.47
1:B:63:LYS:C	1:B:80:MSE:HG2	2.35	0.47
1:B:300:LEU:HD11	1:B:337:ARG:HD3	1.96	0.47
1:E:378:LEU:HG	1:E:691:HIS:CG	2.49	0.47
1:E:336:VAL:CG2	1:E:337:ARG:N	2.77	0.47
1:B:505:ASP:OD1	1:D:505:ASP:OD1	2.32	0.47
1:D:508:VAL:O	1:D:508:VAL:HG12	2.15	0.47
1:D:262:ILE:HD12	1:D:263:PRO:HD2	1.97	0.47
1:B:504:LEU:O	1:B:504:LEU:HD12	2.13	0.47
1:F:621:ILE:H	1:F:621:ILE:CD1	2.27	0.47
1:F:394:MSE:HB3	1:F:394:MSE:HE2	1.92	0.47
1:A:268:VAL:HG11	1:A:332:ASN:ND2	2.29	0.47
1:B:375:TYR:O	1:B:390:GLU:HA	2.15	0.47
1:D:294:LEU:HD23	1:D:309:GLU:O	2.15	0.47
1:B:661:CYS:HA	1:B:678:LEU:HD23	1.97	0.47
1:B:77:GLU:HG2	1:B:78:GLY:N	2.29	0.47
1:D:537:VAL:HG22	1:D:546:ASN:ND2	2.29	0.47
1:D:688:CYS:SG	1:D:706:VAL:HG21	2.54	0.47
1:B:400:PRO:CA	1:B:487:ALA:HB2	2.45	0.47
1:A:688:CYS:SG	1:A:706:VAL:HG21	2.55	0.47
1:B:154:VAL:HG22	1:B:155:TYR:N	2.29	0.47
1:C:148:LYS:O	1:C:267:MSE:HA	2.14	0.47
1:A:407:ILE:HG21	1:A:568:LEU:HD13	1.96	0.47
1:C:720:SER:OG	1:C:723:ALA:HB2	2.15	0.47
1:B:305:GLU:N	1:B:306:PRO:HD3	2.30	0.47
1:A:305:GLU:N	1:A:306:PRO:HD3	2.30	0.47
1:C:451:GLY:HA2	1:C:586:ALA:HB1	1.95	0.47
1:A:60:SER:HB2	1:A:63:LYS:HB2	1.97	0.47
1:A:445:TYR:CG	1:A:451:GLY:HA3	2.51	0.47
1:D:504:LEU:HD21	1:D:521:VAL:CG2	2.45	0.47
1:C:400:PRO:CA	1:C:487:ALA:HB2	2.45	0.47
1:F:262:ILE:HD12	1:F:263:PRO:HD2	1.96	0.47
1:A:504:LEU:HD21	1:A:521:VAL:CG2	2.45	0.47
1:C:272:HIS:O	1:C:273:ALA:C	2.53	0.47
1:C:154:VAL:HG22	1:C:155:TYR:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:ASP:CG	1:D:55:GLN:H	2.18	0.47
1:A:661:CYS:HA	1:A:678:LEU:HD23	1.97	0.47
1:A:375:TYR:O	1:A:390:GLU:HA	2.15	0.46
1:E:375:TYR:O	1:E:390:GLU:HA	2.15	0.46
1:A:277:ILE:HD12	1:A:286:GLN:NE2	2.29	0.46
1:F:504:LEU:HD21	1:F:521:VAL:CG2	2.45	0.46
1:F:720:SER:OG	1:F:723:ALA:HB2	2.15	0.46
1:D:449:TRP:HD1	1:D:453:GLN:HG3	1.80	0.46
1:C:107:PRO:CG	1:C:108:GLY:H	2.23	0.46
1:A:145:VAL:HG22	1:C:17:SER:CB	2.25	0.46
1:B:150:ILE:HG23	1:B:151:PRO:CD	2.41	0.46
1:A:97:LYS:HB3	1:A:100:PHE:HB2	1.97	0.46
1:E:294:LEU:HG	1:E:310:TRP:NE1	2.30	0.46
1:A:321:VAL:CG1	1:A:340:ALA:HB2	2.45	0.46
1:D:399:LEU:N	1:D:399:LEU:HD12	2.30	0.46
1:C:64:TYR:CG	1:C:83:ILE:HD11	2.50	0.46
1:A:621:ILE:CD1	1:A:621:ILE:H	2.28	0.46
1:C:621:ILE:CD1	1:C:621:ILE:H	2.28	0.46
1:C:305:GLU:N	1:C:306:PRO:HD3	2.30	0.46
1:D:422:CYS:SG	1:D:455:PHE:N	2.88	0.46
1:F:294:LEU:HD23	1:F:309:GLU:O	2.16	0.46
1:C:262:ILE:HD12	1:C:263:PRO:HD2	1.97	0.46
1:D:407:ILE:HG21	1:D:568:LEU:HD13	1.96	0.46
1:F:106:PRO:CB	1:F:107:PRO:CD	2.93	0.46
1:A:274:PRO:HD3	1:A:330:TRP:CZ3	2.51	0.46
1:E:268:VAL:HG11	1:E:332:ASN:ND2	2.30	0.46
1:F:655:LEU:N	1:F:683:ASP:HB2	2.27	0.46
1:E:60:SER:HB2	1:E:63:LYS:HB2	1.98	0.46
1:E:378:LEU:HG	1:E:691:HIS:CD2	2.51	0.46
1:D:400:PRO:HA	1:D:487:ALA:HB2	1.98	0.46
1:A:399:LEU:N	1:A:399:LEU:HD12	2.30	0.46
1:A:77:GLU:HG2	1:A:78:GLY:N	2.28	0.46
1:D:64:TYR:CG	1:D:83:ILE:HD11	2.51	0.46
1:E:64:TYR:CG	1:E:83:ILE:HD11	2.50	0.46
1:D:97:LYS:HB3	1:D:100:PHE:HB2	1.98	0.46
1:A:400:PRO:HA	1:A:487:ALA:HB2	1.97	0.46
1:E:399:LEU:N	1:E:399:LEU:HD12	2.31	0.46
1:B:486:THR:HG22	1:B:487:ALA:H	1.81	0.46
1:D:720:SER:OG	1:D:723:ALA:HB2	2.15	0.46
1:C:37:GLU:OE1	1:C:473:ASP:OD2	2.33	0.46
2:C:751:NAG:C4	2:C:752:NAG:N2	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:LEU:C	1:A:487:ALA:HB1	2.36	0.46
1:A:489:MSE:HG3	1:A:508:VAL:HB	1.98	0.46
1:F:504:LEU:HD12	1:F:504:LEU:O	2.16	0.46
1:A:148:LYS:O	1:A:267:MSE:HA	2.16	0.46
1:F:661:CYS:HA	1:F:678:LEU:HD23	1.97	0.46
1:C:106:PRO:CB	1:C:107:PRO:HD3	2.41	0.46
1:D:268:VAL:HG22	1:D:269:PRO:CD	2.45	0.46
1:D:150:ILE:HG23	1:D:151:PRO:CD	2.41	0.46
1:F:513:PRO:HA	1:F:522:ILE:HG12	1.98	0.46
1:B:97:LYS:HB3	1:B:100:PHE:HB2	1.98	0.46
1:E:494:ARG:HB2	1:E:503:PHE:CD1	2.47	0.46
1:E:555:MSE:HE3	1:E:555:MSE:HB2	1.75	0.46
1:B:276:VAL:HG12	1:B:277:ILE:N	2.29	0.46
1:E:720:SER:OG	1:E:723:ALA:HB2	2.16	0.46
1:C:661:CYS:HA	1:C:678:LEU:HD23	1.97	0.46
1:A:363:HIS:NE2	1:A:365:THR:HG23	2.30	0.46
1:B:449:TRP:C	1:B:451:GLY:H	2.19	0.46
1:B:64:TYR:CG	1:B:83:ILE:HD11	2.50	0.46
1:C:555:MSE:HB2	1:C:555:MSE:HE3	1.70	0.46
1:B:146:HIS:H	1:B:146:HIS:CD2	2.34	0.46
1:C:407:ILE:HG21	1:C:568:LEU:HD13	1.95	0.46
1:A:295:LEU:HG	1:A:330:TRP:CD1	2.51	0.46
1:F:559:ALA:O	1:F:599:GLY:HA3	2.16	0.46
1:C:504:LEU:HD21	1:C:521:VAL:CG2	2.46	0.46
1:C:40:ASP:OD1	1:C:41:ASN:N	2.48	0.46
1:E:150:ILE:HG23	1:E:151:PRO:CD	2.40	0.46
1:B:60:SER:HB2	1:B:63:LYS:HB2	1.98	0.46
1:A:654:PRO:HB3	1:A:684:ARG:O	2.16	0.46
1:C:53:TYR:CD2	1:C:58:ALA:O	2.69	0.46
1:F:581:LEU:HD22	1:F:581:LEU:H	1.81	0.46
1:B:277:ILE:HD12	1:B:286:GLN:NE2	2.31	0.46
1:F:54:ASP:CG	1:F:55:GLN:H	2.19	0.46
1:B:720:SER:OG	1:B:723:ALA:HB2	2.16	0.46
1:D:295:LEU:HG	1:D:330:TRP:CD1	2.51	0.46
1:E:97:LYS:HB3	1:E:100:PHE:HB2	1.98	0.46
1:C:494:ARG:HB2	1:C:503:PHE:CD1	2.45	0.46
1:F:494:ARG:HB2	1:F:503:PHE:CD1	2.47	0.46
1:C:400:PRO:HA	1:C:487:ALA:CB	2.46	0.46
1:E:54:ASP:CG	1:E:55:GLN:H	2.19	0.46
1:A:54:ASP:CG	1:A:55:GLN:H	2.19	0.46
1:E:655:LEU:N	1:E:683:ASP:HB2	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:LYS:HD3	1:C:79:THR:HA	1.98	0.45
1:F:413:THR:HG21	1:F:595:GLN:NE2	2.31	0.45
1:E:262:ILE:HD12	1:E:263:PRO:HD2	1.98	0.45
1:E:363:HIS:NE2	1:E:365:THR:HG23	2.32	0.45
1:A:37:GLU:OE1	1:A:473:ASP:OD2	2.33	0.45
1:A:146:HIS:H	1:A:146:HIS:CD2	2.34	0.45
1:A:138:GLU:OE2	1:A:271:ALA:N	2.48	0.45
1:B:268:VAL:HG22	1:B:269:PRO:CD	2.46	0.45
1:A:92:ARG:HA	1:A:93:ARG:HH12	1.79	0.45
3:F:761:NAG:H61	3:F:762:NAG:N2	2.30	0.45
1:C:10:SER:HA	1:C:50:GLN:NE2	2.32	0.45
1:A:650:THR:CG2	1:A:650:THR:O	2.64	0.45
1:B:262:ILE:HD12	1:B:263:PRO:HD2	1.97	0.45
1:E:106:PRO:CB	1:E:107:PRO:HD3	2.41	0.45
1:C:45:ILE:HD12	1:C:85:ILE:HD13	1.99	0.45
1:B:63:LYS:HD3	1:B:79:THR:HA	1.98	0.45
1:C:60:SER:HB2	1:C:63:LYS:HB2	1.99	0.45
1:C:497:TYR:CD1	1:C:642:ILE:HG23	2.51	0.45
1:C:446:PRO:O	1:C:447:PHE:O	2.34	0.45
1:A:508:VAL:O	1:A:508:VAL:HG12	2.15	0.45
1:A:40:ASP:OD1	1:A:41:ASN:N	2.50	0.45
1:E:268:VAL:HG22	1:E:269:PRO:CD	2.46	0.45
1:D:45:ILE:HD12	1:D:85:ILE:HD13	1.99	0.45
1:C:97:LYS:HB3	1:C:100:PHE:HB2	1.98	0.45
1:C:413:THR:HG21	1:C:595:GLN:NE2	2.32	0.45
1:A:110:SER:HB2	1:A:126:LEU:O	2.16	0.45
1:F:537:VAL:HG22	1:F:546:ASN:ND2	2.29	0.45
1:F:653:ALA:N	1:F:654:PRO:CD	2.79	0.45
1:C:399:LEU:N	1:C:399:LEU:HD12	2.32	0.45
1:E:508:VAL:HG12	1:E:508:VAL:O	2.15	0.45
1:D:581:LEU:HD22	1:D:581:LEU:H	1.80	0.45
1:A:581:LEU:H	1:A:581:LEU:HD22	1.81	0.45
1:F:621:ILE:N	1:F:621:ILE:HD12	2.31	0.45
1:D:363:HIS:NE2	1:D:365:THR:HG23	2.31	0.45
1:E:604:LYS:C	1:E:606:ASN:H	2.20	0.45
1:E:581:LEU:HD22	1:E:581:LEU:N	2.31	0.45
1:E:274:PRO:HD3	1:E:330:TRP:CZ3	2.52	0.45
1:D:136:GLY:CA	1:D:268:VAL:HG21	2.33	0.45
1:A:497:TYR:CD1	1:A:642:ILE:HG23	2.51	0.45
1:D:399:LEU:C	1:D:487:ALA:HB1	2.37	0.45
1:E:277:ILE:HD12	1:E:286:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:LEU:O	1:C:504:LEU:HD12	2.17	0.45
1:F:40:ASP:OD1	1:F:41:ASN:N	2.50	0.45
1:C:137:ARG:H	1:C:332:ASN:HD22	1.64	0.45
1:B:497:TYR:CD1	1:B:642:ILE:HG23	2.52	0.45
1:F:97:LYS:HB3	1:F:100:PHE:HB2	1.99	0.45
1:D:413:THR:HG21	1:D:595:GLN:NE2	2.31	0.45
1:D:110:SER:HB2	1:D:126:LEU:O	2.17	0.45
1:D:321:VAL:HG12	1:D:321:VAL:O	2.16	0.45
1:F:400:PRO:HA	1:F:487:ALA:HB2	1.99	0.45
1:B:604:LYS:C	1:B:606:ASN:H	2.19	0.45
1:F:107:PRO:CG	1:F:108:GLY:H	2.23	0.45
1:D:274:PRO:HD3	1:D:330:TRP:CZ3	2.51	0.45
1:F:305:GLU:N	1:F:306:PRO:HD3	2.32	0.45
1:D:148:LYS:O	1:D:267:MSE:HA	2.16	0.45
1:D:292:LEU:HD23	1:D:312:VAL:HG22	1.99	0.45
1:B:45:ILE:HD12	1:B:85:ILE:HD13	1.98	0.45
1:C:513:PRO:HA	1:C:522:ILE:HG12	1.99	0.45
1:A:625:PRO:HD2	1:A:627:ARG:HH12	1.81	0.45
1:C:321:VAL:HG12	1:C:321:VAL:O	2.16	0.45
1:B:110:SER:HB2	1:B:126:LEU:O	2.17	0.45
1:D:486:THR:HG22	1:D:487:ALA:H	1.81	0.45
1:C:591:VAL:HA	1:C:592:PRO:HD3	1.79	0.45
1:F:363:HIS:NE2	1:F:365:THR:HG23	2.32	0.45
1:A:720:SER:OG	1:A:723:ALA:HB2	2.16	0.45
1:B:272:HIS:O	1:B:273:ALA:C	2.55	0.45
1:C:363:HIS:NE2	1:C:365:THR:HG23	2.32	0.45
1:B:581:LEU:HD22	1:B:581:LEU:N	2.32	0.45
1:B:295:LEU:HG	1:B:330:TRP:CD1	2.52	0.45
1:D:138:GLU:OE2	1:D:271:ALA:N	2.50	0.45
1:C:655:LEU:N	1:C:683:ASP:HB2	2.25	0.45
1:D:294:LEU:HG	1:D:310:TRP:NE1	2.32	0.45
1:F:497:TYR:CD1	1:F:642:ILE:HG23	2.52	0.45
1:B:642:ILE:HB	1:B:647:PHE:HZ	1.82	0.45
1:B:321:VAL:O	1:B:321:VAL:HG12	2.16	0.45
1:F:321:VAL:HG12	1:F:321:VAL:O	2.17	0.45
1:E:321:VAL:HG12	1:E:321:VAL:O	2.17	0.45
1:B:407:ILE:HG21	1:B:568:LEU:HD13	1.97	0.45
1:E:661:CYS:HA	1:E:678:LEU:HD23	1.97	0.45
1:C:604:LYS:C	1:C:606:ASN:H	2.20	0.45
1:C:268:VAL:HG22	1:C:269:PRO:CD	2.47	0.45
1:E:63:LYS:HD3	1:E:79:THR:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:497:TYR:CD1	1:D:642:ILE:HG23	2.51	0.45
1:A:445:TYR:CB	1:A:451:GLY:HA3	2.47	0.45
1:E:486:THR:HG22	1:E:487:ALA:H	1.82	0.45
1:E:53:TYR:CD2	1:E:58:ALA:O	2.69	0.45
1:A:53:TYR:CD2	1:A:58:ALA:O	2.70	0.45
1:C:621:ILE:N	1:C:621:ILE:HD12	2.32	0.45
1:C:568:LEU:C	1:C:570:SER:H	2.20	0.45
1:A:602:MSE:HB3	1:A:602:MSE:HE3	1.58	0.45
1:D:420:ILE:HD12	1:D:420:ILE:O	2.16	0.45
1:A:87:THR:OG1	1:A:106:PRO:HD2	2.17	0.45
1:A:45:ILE:HD12	1:A:85:ILE:HD13	1.99	0.45
1:A:150:ILE:HG23	1:A:151:PRO:CD	2.45	0.45
1:E:45:ILE:HD12	1:E:85:ILE:HD13	1.98	0.45
1:B:642:ILE:HB	1:B:647:PHE:CZ	2.52	0.45
1:E:400:PRO:HA	1:E:487:ALA:HB2	1.99	0.45
1:E:504:LEU:HD21	1:E:521:VAL:CG2	2.47	0.45
1:D:272:HIS:O	1:D:273:ALA:C	2.56	0.45
1:D:305:GLU:N	1:D:306:PRO:HD3	2.33	0.44
1:A:63:LYS:HD3	1:A:79:THR:HA	1.99	0.44
1:D:63:LYS:HD3	1:D:79:THR:HA	1.99	0.44
1:E:497:TYR:CD1	1:E:642:ILE:HG23	2.52	0.44
1:D:494:ARG:HB2	1:D:503:PHE:CD1	2.47	0.44
1:B:559:ALA:O	1:B:599:GLY:HA3	2.17	0.44
1:F:110:SER:HB2	1:F:126:LEU:O	2.18	0.44
1:C:399:LEU:C	1:C:487:ALA:HB1	2.37	0.44
1:D:489:MSE:HG3	1:D:508:VAL:HB	1.99	0.44
1:C:581:LEU:HD22	1:C:581:LEU:H	1.81	0.44
1:F:568:LEU:C	1:F:570:SER:H	2.20	0.44
1:F:298:ARG:HH12	1:F:615:ALA:HB3	1.81	0.44
1:A:284:SER:HB3	2:A:751:NAG:O5	2.17	0.44
1:B:621:ILE:H	1:B:621:ILE:CD1	2.30	0.44
1:B:580:ARG:NH2	1:C:275:ASN:HB2	2.32	0.44
1:C:54:ASP:CG	1:C:55:GLN:H	2.19	0.44
1:B:287:LEU:CD2	1:B:330:TRP:NE1	2.80	0.44
1:F:10:SER:HA	1:F:50:GLN:NE2	2.32	0.44
1:C:446:PRO:HG2	1:C:450:GLY:O	2.16	0.44
1:B:649:ARG:HG3	1:B:649:ARG:H	1.51	0.44
1:A:321:VAL:O	1:A:321:VAL:HG12	2.16	0.44
1:F:300:LEU:HD11	1:F:337:ARG:HD3	1.98	0.44
1:A:486:THR:HG22	1:A:487:ALA:H	1.82	0.44
1:F:399:LEU:C	1:F:487:ALA:HB1	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:486:THR:HG22	1:F:487:ALA:H	1.82	0.44
1:F:53:TYR:CD2	1:F:58:ALA:O	2.70	0.44
1:C:138:GLU:OE2	1:C:271:ALA:N	2.50	0.44
1:C:93:ARG:H	1:C:93:ARG:NH1	1.93	0.44
1:A:642:ILE:HB	1:A:647:PHE:HZ	1.83	0.44
1:C:486:THR:HG22	1:C:487:ALA:H	1.81	0.44
1:F:399:LEU:HD12	1:F:399:LEU:N	2.32	0.44
1:E:407:ILE:HG22	1:E:408:THR:N	2.32	0.44
1:A:106:PRO:CB	1:A:107:PRO:CD	2.92	0.44
1:E:271:ALA:CB	1:E:330:TRP:CZ3	3.00	0.44
1:F:21:HIS:O	1:F:23:VAL:N	2.51	0.44
1:B:454:CYS:SG	1:B:460:ASN:OD1	2.76	0.44
1:F:45:ILE:HD12	1:F:85:ILE:HD13	1.99	0.44
1:D:642:ILE:HB	1:D:647:PHE:HZ	1.83	0.44
1:D:699:LEU:HD23	1:D:716:PHE:HB3	2.00	0.44
1:C:276:VAL:HG12	1:C:277:ILE:N	2.33	0.44
1:B:504:LEU:HD21	1:B:521:VAL:CG2	2.46	0.44
1:D:40:ASP:OD1	1:D:41:ASN:N	2.49	0.44
1:B:108:GLY:CA	1:B:130:ILE:HB	2.47	0.44
1:F:295:LEU:HG	1:F:330:TRP:CD1	2.51	0.44
1:F:268:VAL:HG22	1:F:269:PRO:CD	2.47	0.44
1:E:21:HIS:O	1:E:23:VAL:N	2.51	0.44
1:E:287:LEU:CD2	1:E:330:TRP:NE1	2.77	0.44
1:A:642:ILE:HB	1:A:647:PHE:CZ	2.52	0.44
1:D:60:SER:HB2	1:D:63:LYS:HB2	2.00	0.44
1:D:642:ILE:HB	1:D:647:PHE:CZ	2.52	0.44
1:E:642:ILE:HB	1:E:647:PHE:CZ	2.52	0.44
1:E:399:LEU:C	1:E:487:ALA:HB1	2.37	0.44
1:D:112:THR:HG23	1:D:125:THR:HG22	1.99	0.44
1:A:621:ILE:N	1:A:621:ILE:HD12	2.33	0.44
1:E:407:ILE:HG21	1:E:568:LEU:HD13	1.99	0.44
1:E:568:LEU:C	1:E:570:SER:H	2.21	0.44
1:B:54:ASP:CG	1:B:55:GLN:H	2.21	0.44
1:D:394:MSE:HB3	1:D:394:MSE:HE2	1.91	0.44
1:E:146:HIS:CD2	1:E:146:HIS:H	2.34	0.44
1:A:394:MSE:HE2	1:A:394:MSE:HB3	1.92	0.44
1:F:604:LYS:C	1:F:606:ASN:H	2.21	0.44
1:E:270:VAL:HG22	1:E:333:HIS:HE1	1.80	0.44
1:B:568:LEU:C	1:B:570:SER:H	2.21	0.44
1:E:40:ASP:OD1	1:E:41:ASN:N	2.49	0.44
1:F:385:ALA:HA	1:F:386:PRO:HD2	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ASP:OD1	1:B:41:ASN:N	2.50	0.44
1:E:137:ARG:HH21	1:E:331:GLY:H	1.66	0.44
1:C:21:HIS:O	1:C:23:VAL:N	2.50	0.44
1:A:494:ARG:HB2	1:A:503:PHE:CD1	2.47	0.44
1:A:112:THR:HG23	1:A:125:THR:HG22	2.00	0.44
1:A:102:LEU:HD11	1:A:155:TYR:CB	2.48	0.44
1:B:363:HIS:NE2	1:B:365:THR:HG23	2.32	0.44
1:E:621:ILE:N	1:E:621:ILE:HD12	2.33	0.44
1:D:146:HIS:H	1:D:146:HIS:CD2	2.35	0.44
1:A:108:GLY:CA	1:A:130:ILE:HB	2.47	0.44
1:E:295:LEU:HG	1:E:330:TRP:CD1	2.51	0.44
1:F:131:LYS:NZ	3:F:761:NAG:H81	2.33	0.44
1:D:10:SER:HA	1:D:50:GLN:NE2	2.32	0.44
1:F:512:THR:HA	1:F:513:PRO:HD3	1.75	0.44
1:E:559:ALA:O	1:E:599:GLY:HA3	2.18	0.44
1:A:72:ASP:O	1:A:73:HIS:HB2	2.17	0.44
1:F:72:ASP:O	1:F:73:HIS:HB2	2.18	0.44
1:A:513:PRO:HA	1:A:522:ILE:HG12	2.00	0.44
1:B:513:PRO:HA	1:B:522:ILE:HG12	1.99	0.44
1:D:604:LYS:C	1:D:606:ASN:H	2.22	0.44
1:F:87:THR:OG1	1:F:106:PRO:HD2	2.18	0.43
1:F:63:LYS:HD3	1:F:79:THR:HA	1.99	0.43
1:E:653:ALA:N	1:E:654:PRO:CD	2.79	0.43
1:E:385:ALA:HA	1:E:386:PRO:HD2	1.78	0.43
1:E:386:PRO:HG3	1:E:730:CYS:O	2.18	0.43
2:B:763:BMA:O2	2:B:764:MAN:O5	2.32	0.43
1:B:399:LEU:C	1:B:487:ALA:HB1	2.38	0.43
1:A:504:LEU:HD12	1:A:504:LEU:O	2.17	0.43
1:A:102:LEU:HD11	1:A:155:TYR:HB3	2.00	0.43
1:E:407:ILE:CG2	1:E:408:THR:N	2.81	0.43
1:F:60:SER:HB2	1:F:63:LYS:HB2	1.99	0.43
1:F:649:ARG:O	1:F:650:THR:C	2.56	0.43
1:F:642:ILE:HB	1:F:647:PHE:CZ	2.53	0.43
1:A:559:ALA:O	1:A:599:GLY:HA3	2.18	0.43
1:A:699:LEU:HD23	1:A:716:PHE:HB3	2.00	0.43
1:C:559:ALA:O	1:C:599:GLY:HA3	2.18	0.43
1:E:489:MSE:HG3	1:E:508:VAL:HB	2.00	0.43
1:F:112:THR:HG23	1:F:125:THR:HG22	2.01	0.43
1:B:112:THR:HG23	1:B:125:THR:HG22	2.00	0.43
1:A:287:LEU:CD2	1:A:330:TRP:NE1	2.80	0.43
1:A:21:HIS:O	1:A:23:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:642:ILE:HB	1:E:647:PHE:HZ	1.83	0.43
1:E:625:PRO:HD2	1:E:627:ARG:HH12	1.82	0.43
1:B:530:PHE:CE2	1:B:617:PHE:HD1	2.36	0.43
1:D:504:LEU:HD12	1:D:504:LEU:O	2.17	0.43
1:A:653:ALA:O	1:A:654:PRO:C	2.56	0.43
1:B:493:LEU:HD23	1:B:493:LEU:HA	1.60	0.43
1:D:87:THR:OG1	1:D:106:PRO:HD2	2.18	0.43
1:B:107:PRO:CG	1:B:108:GLY:H	2.23	0.43
1:A:271:ALA:CB	1:A:330:TRP:CZ3	3.02	0.43
1:C:445:TYR:O	1:C:460:ASN:ND2	2.51	0.43
1:B:494:ARG:HB2	1:B:503:PHE:CD1	2.47	0.43
1:F:321:VAL:CG1	1:F:340:ALA:HB2	2.48	0.43
1:B:400:PRO:HA	1:B:487:ALA:HB2	1.99	0.43
1:B:621:ILE:N	1:B:621:ILE:HD12	2.33	0.43
1:E:621:ILE:CD1	1:E:621:ILE:H	2.31	0.43
1:E:272:HIS:O	1:E:273:ALA:C	2.57	0.43
1:D:69:LEU:HA	1:D:69:LEU:HD22	1.84	0.43
1:E:19:CYS:C	1:E:21:HIS:N	2.72	0.43
1:C:664:SER:OG	1:C:675:MSE:HB3	2.19	0.43
1:E:612:GLN:H	1:E:612:GLN:HG2	1.53	0.43
1:B:10:SER:HA	1:B:50:GLN:NE2	2.33	0.43
1:E:292:LEU:HD23	1:E:312:VAL:HG22	2.00	0.43
1:A:445:TYR:CD1	1:A:451:GLY:HA3	2.53	0.43
1:C:447:PHE:CD1	1:C:455:PHE:HA	2.53	0.43
1:F:398:VAL:HB	1:F:628:ALA:HB3	1.99	0.43
1:B:53:TYR:CD2	1:B:58:ALA:O	2.70	0.43
1:F:555:MSE:HB2	1:F:555:MSE:HE3	1.69	0.43
1:E:6:PHE:HA	1:E:57:GLY:O	2.18	0.43
1:F:146:HIS:H	1:F:146:HIS:CD2	2.35	0.43
1:E:602:MSE:HB3	1:E:602:MSE:HE3	1.68	0.43
1:E:615:ALA:HA	1:E:616:PRO:HD3	1.57	0.43
1:D:21:HIS:O	1:D:23:VAL:N	2.52	0.43
1:A:447:PHE:CG	1:A:448:MSE:N	2.86	0.43
1:C:642:ILE:HB	1:C:647:PHE:CZ	2.53	0.43
1:D:72:ASP:O	1:D:73:HIS:HB2	2.19	0.43
1:D:102:LEU:HD11	1:D:155:TYR:HB3	2.01	0.43
1:E:102:LEU:HD11	1:E:155:TYR:CB	2.49	0.43
1:D:568:LEU:C	1:D:570:SER:H	2.21	0.43
1:C:146:HIS:CD2	1:C:146:HIS:H	2.36	0.43
1:A:271:ALA:HB3	1:A:330:TRP:CZ3	2.54	0.43
1:F:287:LEU:HD13	1:F:311:ILE:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:LEU:HG	1:C:330:TRP:CD1	2.53	0.43
1:C:298:ARG:HH12	1:C:615:ALA:HB3	1.83	0.43
1:B:21:HIS:O	1:B:23:VAL:N	2.52	0.43
1:E:664:SER:OG	1:E:675:MSE:HB3	2.19	0.43
1:D:513:PRO:HA	1:D:522:ILE:HG12	2.00	0.43
1:B:52:GLY:N	1:B:63:LYS:O	2.51	0.43
1:A:449:TRP:HA	1:A:449:TRP:CE3	2.52	0.43
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.77	0.43
1:B:413:THR:HG21	1:B:595:GLN:NE2	2.34	0.43
1:E:112:THR:HG23	1:E:125:THR:HG22	2.01	0.43
1:C:102:LEU:HD11	1:C:155:TYR:CB	2.49	0.43
1:C:394:MSE:HB3	1:C:394:MSE:HE2	1.90	0.43
1:B:271:ALA:CB	1:B:330:TRP:CZ3	3.02	0.43
1:B:137:ARG:HH21	1:B:331:GLY:H	1.65	0.43
1:F:136:GLY:CA	1:F:268:VAL:HG21	2.31	0.43
1:E:17:SER:HB3	1:F:145:VAL:CG2	2.33	0.43
1:A:655:LEU:N	1:A:683:ASP:HB2	2.28	0.43
1:B:699:LEU:HD23	1:B:716:PHE:HB3	2.01	0.43
1:E:512:THR:HA	1:E:513:PRO:HD3	1.74	0.43
1:E:503:PHE:C	1:E:503:PHE:CD2	2.92	0.43
1:C:398:VAL:HB	1:C:628:ALA:HB3	2.00	0.43
1:F:690:VAL:HG22	1:F:729:LEU:HD23	2.01	0.43
1:C:489:MSE:HB2	1:C:489:MSE:HE3	1.90	0.43
1:F:111:VAL:O	1:F:125:THR:HA	2.19	0.43
1:A:104:LYS:HD2	1:C:22:THR:CG2	2.34	0.43
1:B:547:TYR:OH	1:B:560:PHE:HB3	2.19	0.43
1:A:10:SER:HA	1:A:50:GLN:NE2	2.33	0.43
1:B:340:ALA:C	1:B:341:GLN:HG2	2.39	0.43
1:D:690:VAL:HG22	1:D:729:LEU:HD23	2.01	0.43
1:F:699:LEU:HD23	1:F:716:PHE:HB3	2.00	0.43
1:E:110:SER:HB2	1:E:126:LEU:O	2.18	0.43
1:E:657:SER:HA	1:E:732:LYS:HE3	2.01	0.43
1:A:69:LEU:HA	1:A:69:LEU:HD22	1.84	0.43
1:D:621:ILE:CD1	1:D:621:ILE:H	2.31	0.43
1:D:621:ILE:N	1:D:621:ILE:HD12	2.33	0.43
1:A:136:GLY:CA	1:A:268:VAL:HG21	2.33	0.43
1:C:699:LEU:HD23	1:C:716:PHE:HB3	2.01	0.43
1:F:664:SER:OG	1:F:675:MSE:HB3	2.19	0.43
1:D:664:SER:OG	1:D:675:MSE:HB3	2.19	0.43
1:B:292:LEU:HD23	1:B:312:VAL:HG22	2.00	0.43
1:D:559:ALA:O	1:D:599:GLY:HA3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:THR:HG23	1:B:468:VAL:HG12	2.01	0.43
1:A:690:VAL:HG22	1:A:729:LEU:HD23	2.01	0.43
1:E:699:LEU:HD23	1:E:716:PHE:HB3	2.01	0.43
1:C:112:THR:HG23	1:C:125:THR:HG22	2.00	0.43
1:A:568:LEU:C	1:A:570:SER:H	2.22	0.43
1:C:102:LEU:HD11	1:C:155:TYR:HB3	2.01	0.43
1:A:493:LEU:HA	1:A:493:LEU:HD23	1.60	0.43
1:B:287:LEU:HD22	1:B:330:TRP:CE2	2.54	0.42
1:B:137:ARG:H	1:B:332:ASN:HD22	1.67	0.42
1:C:642:ILE:HB	1:C:647:PHE:HZ	1.83	0.42
1:E:422:CYS:O	1:E:423:CYS:HB2	2.19	0.42
1:C:400:PRO:HA	1:C:487:ALA:HB2	2.01	0.42
1:C:110:SER:HB2	1:C:126:LEU:O	2.19	0.42
1:B:491:VAL:O	1:B:505:ASP:HA	2.19	0.42
1:B:102:LEU:HD11	1:B:155:TYR:CB	2.48	0.42
1:F:445:TYR:O	1:F:460:ASN:ND2	2.52	0.42
1:B:328:TYR:O	1:B:328:TYR:CD1	2.72	0.42
1:E:328:TYR:O	1:E:328:TYR:CD1	2.71	0.42
1:E:445:TYR:CG	1:E:451:GLY:HA3	2.53	0.42
1:E:87:THR:OG1	1:E:106:PRO:HD2	2.19	0.42
1:C:108:GLY:CA	1:C:130:ILE:HB	2.47	0.42
1:D:137:ARG:H	1:D:332:ASN:HD22	1.66	0.42
1:D:303:ASN:HA	1:D:304:PRO:HD3	1.83	0.42
1:F:292:LEU:HD23	1:F:312:VAL:HG22	2.01	0.42
1:E:10:SER:HA	1:E:50:GLN:NE2	2.33	0.42
1:D:512:THR:HA	1:D:513:PRO:HD3	1.75	0.42
1:F:642:ILE:HB	1:F:647:PHE:HZ	1.84	0.42
1:F:503:PHE:CD2	1:F:503:PHE:C	2.91	0.42
1:B:471:SER:C	1:B:473:ASP:N	2.72	0.42
1:B:6:PHE:HA	1:B:57:GLY:O	2.19	0.42
1:B:271:ALA:HB3	1:B:330:TRP:CZ3	2.55	0.42
1:B:655:LEU:N	1:B:683:ASP:HB2	2.27	0.42
1:B:95:SER:OG	1:B:259:PHE:CZ	2.67	0.42
1:D:300:LEU:CD1	1:D:337:ARG:HD3	2.49	0.42
1:F:398:VAL:O	1:F:400:PRO:HD3	2.19	0.42
1:D:531:THR:HA	1:D:532:PRO:HD3	1.89	0.42
1:E:489:MSE:HE3	1:E:489:MSE:HB2	1.92	0.42
1:A:531:THR:HA	1:A:532:PRO:HD3	1.89	0.42
1:E:72:ASP:O	1:E:73:HIS:HB2	2.19	0.42
1:B:102:LEU:HD11	1:B:155:TYR:HB3	2.00	0.42
1:B:404:GLN:HA	1:B:482:ILE:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:PHE:HA	1:B:454:CYS:O	2.20	0.42
1:B:385:ALA:HA	1:B:386:PRO:HD2	1.78	0.42
1:A:413:THR:HG21	1:A:595:GLN:NE2	2.34	0.42
1:B:422:CYS:O	1:B:423:CYS:HB2	2.19	0.42
1:F:102:LEU:HD11	1:F:155:TYR:CB	2.49	0.42
1:E:102:LEU:HD11	1:E:155:TYR:HB3	2.00	0.42
1:C:407:ILE:HG22	1:C:408:THR:N	2.34	0.42
1:B:407:ILE:HG22	1:B:408:THR:N	2.34	0.42
1:D:145:VAL:HG22	1:F:17:SER:CB	2.31	0.42
1:C:385:ALA:HA	1:C:386:PRO:HD2	1.79	0.42
1:C:452:ALA:O	1:C:453:GLN:C	2.58	0.42
1:A:19:CYS:C	1:A:21:HIS:N	2.72	0.42
1:A:664:SER:OG	1:A:675:MSE:HB3	2.19	0.42
1:E:547:TYR:OH	1:E:560:PHE:HB3	2.20	0.42
1:E:649:ARG:H	1:E:649:ARG:HG3	1.52	0.42
1:C:422:CYS:O	1:C:423:CYS:HB2	2.20	0.42
2:A:753:BMA:O3	2:A:754:MAN:C4	2.63	0.42
1:F:389:LEU:HD12	1:F:389:LEU:HA	1.86	0.42
1:B:287:LEU:HD13	1:B:311:ILE:CD1	2.49	0.42
1:F:649:ARG:O	1:F:651:SER:HB2	2.20	0.42
1:F:471:SER:C	1:F:473:ASP:N	2.72	0.42
1:D:407:ILE:HG22	1:D:408:THR:N	2.34	0.42
3:A:763:BMA:H61	3:A:765:MAN:H2	1.32	0.42
1:F:271:ALA:HB3	1:F:330:TRP:CZ3	2.54	0.42
1:C:287:LEU:HD13	1:C:311:ILE:CD1	2.50	0.42
1:C:690:VAL:HG22	1:C:729:LEU:HD23	2.01	0.42
1:F:19:CYS:C	1:F:21:HIS:N	2.73	0.42
1:B:625:PRO:HD2	1:B:627:ARG:HH12	1.84	0.42
1:C:489:MSE:HG3	1:C:508:VAL:HB	2.00	0.42
1:C:111:VAL:O	1:C:125:THR:HA	2.20	0.42
1:C:72:ASP:O	1:C:73:HIS:HB2	2.18	0.42
1:B:555:MSE:HB2	1:B:555:MSE:HE3	1.65	0.42
1:B:72:ASP:O	1:B:73:HIS:HB2	2.19	0.42
1:C:404:GLN:HA	1:C:482:ILE:HG12	2.02	0.42
1:F:657:SER:HA	1:F:732:LYS:HE3	2.01	0.42
1:D:591:VAL:HA	1:D:592:PRO:HD3	1.79	0.42
1:B:87:THR:OG1	1:B:106:PRO:HD2	2.20	0.42
1:C:87:THR:OG1	1:C:106:PRO:HD2	2.19	0.42
1:E:271:ALA:HB3	1:E:330:TRP:CZ3	2.54	0.42
1:B:378:LEU:HG	1:B:691:HIS:CB	2.50	0.42
1:B:471:SER:C	1:B:473:ASP:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:413:THR:HG21	1:E:595:GLN:NE2	2.35	0.42
1:C:413:THR:HG23	1:C:468:VAL:HG12	2.02	0.42
1:A:413:THR:HG23	1:A:468:VAL:HG12	2.01	0.42
1:E:378:LEU:HD23	1:E:378:LEU:HA	1.77	0.42
1:D:688:CYS:HA	1:D:689:PRO:HD3	1.93	0.42
1:F:102:LEU:HD11	1:F:155:TYR:HB3	2.01	0.42
1:A:604:LYS:C	1:A:606:ASN:H	2.22	0.42
1:D:37:GLU:OE1	1:D:473:ASP:OD2	2.37	0.42
1:E:287:LEU:HD22	1:E:311:ILE:HD11	2.01	0.42
1:F:287:LEU:HD22	1:F:311:ILE:HD11	2.02	0.42
1:F:271:ALA:CB	1:F:330:TRP:CZ3	3.03	0.42
1:D:329:ILE:H	1:D:329:ILE:HG12	1.53	0.42
1:D:422:CYS:O	1:D:423:CYS:HB2	2.20	0.42
1:A:503:PHE:CD2	1:A:503:PHE:C	2.93	0.42
1:F:471:SER:C	1:F:473:ASP:H	2.23	0.42
1:A:471:SER:C	1:A:473:ASP:N	2.72	0.42
1:D:471:SER:C	1:D:473:ASP:H	2.23	0.42
1:B:436:TYR:O	1:B:437:THR:HG23	2.20	0.42
2:D:752:NAG:O3	2:D:752:NAG:H83	2.20	0.42
1:D:271:ALA:CB	1:D:330:TRP:CZ3	3.03	0.42
1:B:664:SER:OG	1:B:675:MSE:HB3	2.19	0.42
1:A:60:SER:CB	1:A:63:LYS:HB2	2.50	0.42
1:B:386:PRO:HG3	1:B:730:CYS:O	2.20	0.42
1:C:512:THR:HA	1:C:513:PRO:HD3	1.76	0.42
1:B:503:PHE:C	1:B:503:PHE:CD2	2.92	0.42
1:D:503:PHE:CD2	1:D:503:PHE:C	2.94	0.42
1:D:413:THR:HG23	1:D:468:VAL:HG12	2.02	0.42
1:D:398:VAL:O	1:D:400:PRO:HD3	2.20	0.42
1:A:398:VAL:O	1:A:400:PRO:HD3	2.20	0.42
1:F:491:VAL:O	1:F:505:ASP:HA	2.20	0.42
1:C:471:SER:C	1:C:473:ASP:N	2.73	0.42
1:E:33:GLN:O	1:E:34:VAL:HG23	2.19	0.42
1:F:69:LEU:HA	1:F:69:LEU:HD22	1.84	0.42
1:C:445:TYR:CB	1:C:452:ALA:H	2.32	0.41
1:A:52:GLY:N	1:A:63:LYS:O	2.51	0.41
1:C:625:PRO:HD2	1:C:627:ARG:HH12	1.84	0.41
1:E:513:PRO:HA	1:E:522:ILE:HG12	2.01	0.41
1:B:591:VAL:HA	1:B:592:PRO:HD3	1.80	0.41
1:D:436:TYR:O	1:D:437:THR:HG23	2.20	0.41
1:D:287:LEU:HD13	1:D:311:ILE:CD1	2.50	0.41
1:B:615:ALA:HA	1:B:616:PRO:HD3	1.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:PHE:C	1:C:503:PHE:CD2	2.94	0.41
1:F:413:THR:HG23	1:F:468:VAL:HG12	2.02	0.41
1:A:376:LYS:O	1:A:691:HIS:HE1	2.03	0.41
1:D:491:VAL:O	1:D:505:ASP:HA	2.20	0.41
1:B:489:MSE:HG3	1:B:508:VAL:HB	2.02	0.41
1:A:407:ILE:HG22	1:A:408:THR:N	2.34	0.41
1:C:555:MSE:H	1:C:555:MSE:HE2	1.84	0.41
1:B:657:SER:HA	1:B:732:LYS:HE3	2.01	0.41
1:C:426:LEU:HA	1:C:426:LEU:HD23	1.87	0.41
1:A:271:ALA:O	1:A:333:HIS:HE1	2.03	0.41
1:C:271:ALA:O	1:C:333:HIS:HE1	2.02	0.41
1:D:19:CYS:C	1:D:21:HIS:N	2.72	0.41
1:F:547:TYR:OH	1:F:560:PHE:HB3	2.19	0.41
1:A:373:ILE:HA	1:A:374:PRO:HD2	1.91	0.41
1:E:111:VAL:O	1:E:125:THR:HA	2.20	0.41
1:A:657:SER:HA	1:A:732:LYS:HE3	2.01	0.41
1:A:6:PHE:HA	1:A:57:GLY:O	2.19	0.41
1:E:453:GLN:CD	1:E:453:GLN:H	2.23	0.41
1:D:328:TYR:O	1:D:328:TYR:CD1	2.73	0.41
1:E:426:LEU:HD23	1:E:426:LEU:HA	1.88	0.41
1:A:287:LEU:HD13	1:A:311:ILE:CD1	2.49	0.41
1:D:271:ALA:HB3	1:D:330:TRP:CZ3	2.55	0.41
1:D:334:GLU:HA	1:D:335:PRO:HD3	1.85	0.41
1:B:19:CYS:C	1:B:21:HIS:N	2.72	0.41
1:D:150:ILE:HG22	1:D:151:PRO:O	2.20	0.41
1:C:51:PHE:CD2	1:C:80:MSE:SE	3.23	0.41
1:C:413:THR:HG21	1:C:595:GLN:HE22	1.83	0.41
1:A:300:LEU:CD1	1:A:337:ARG:HD3	2.50	0.41
1:D:504:LEU:HB3	1:D:516:SER:HB2	2.03	0.41
1:E:691:HIS:HA	1:E:699:LEU:HD12	2.02	0.41
1:D:691:HIS:HA	1:D:699:LEU:HD12	2.02	0.41
1:D:321:VAL:CG1	1:D:340:ALA:HB2	2.50	0.41
1:D:102:LEU:HD11	1:D:155:TYR:CB	2.49	0.41
1:B:329:ILE:H	1:B:329:ILE:HG12	1.50	0.41
1:D:653:ALA:HB1	1:D:684:ARG:HD2	2.02	0.41
1:C:649:ARG:HG3	1:C:649:ARG:H	1.52	0.41
1:E:690:VAL:HG22	1:E:729:LEU:HD23	2.01	0.41
1:D:386:PRO:HG3	1:D:730:CYS:O	2.21	0.41
1:B:407:ILE:CG2	1:B:408:THR:N	2.84	0.41
3:A:762:NAG:O3	3:A:763:BMA:H5	2.20	0.41
1:A:552:TYR:HA	1:A:564:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:LEU:HD23	1:C:493:LEU:HA	1.61	0.41
1:A:287:LEU:HD22	1:A:330:TRP:CE2	2.55	0.41
1:E:287:LEU:HD22	1:E:330:TRP:CE2	2.56	0.41
1:D:271:ALA:O	1:D:333:HIS:HE1	2.02	0.41
1:C:386:PRO:HB2	1:C:689:PRO:CG	2.50	0.41
1:D:292:LEU:CD2	1:D:312:VAL:HG22	2.51	0.41
1:B:690:VAL:HG22	1:B:729:LEU:HD23	2.01	0.41
1:F:652:ASP:C	1:F:654:PRO:HD2	2.40	0.41
1:E:491:VAL:O	1:E:505:ASP:HA	2.20	0.41
1:D:489:MSE:HE3	1:D:489:MSE:HB2	1.89	0.41
1:B:111:VAL:O	1:B:125:THR:HA	2.21	0.41
1:C:407:ILE:CG2	1:C:408:THR:N	2.84	0.41
1:F:6:PHE:HA	1:F:57:GLY:O	2.21	0.41
1:F:287:LEU:CD2	1:F:330:TRP:NE1	2.80	0.41
1:B:327:GLU:HA	1:B:337:ARG:HB3	2.03	0.41
1:C:398:VAL:O	1:C:400:PRO:HD3	2.20	0.41
1:F:489:MSE:HG3	1:F:508:VAL:HB	2.03	0.41
4:D:761:NAG:O3	4:D:762:NAG:C7	2.69	0.41
1:A:407:ILE:CG2	1:A:408:THR:N	2.84	0.41
1:F:404:GLN:HA	1:F:482:ILE:HG12	2.02	0.41
1:D:657:SER:HA	1:D:732:LYS:HE3	2.01	0.41
1:C:42:THR:CG2	1:C:104:LYS:HG3	2.51	0.41
1:C:271:ALA:HB3	1:C:330:TRP:CZ3	2.56	0.41
1:B:612:GLN:HG2	1:B:612:GLN:H	1.50	0.41
1:E:51:PHE:CD2	1:E:80:MSE:SE	3.23	0.41
1:B:413:THR:HG21	1:B:595:GLN:HE22	1.86	0.41
1:B:373:ILE:HA	1:B:374:PRO:HD2	1.90	0.41
1:C:602:MSE:HE3	1:C:602:MSE:HB3	1.60	0.41
1:D:426:LEU:HA	1:D:426:LEU:HD23	1.89	0.41
1:D:108:GLY:CA	1:D:130:ILE:HB	2.46	0.41
1:B:44:ARG:NH1	1:B:258:PRO:HB2	2.36	0.41
1:E:44:ARG:NH1	1:E:258:PRO:HB2	2.35	0.41
1:D:287:LEU:CD2	1:D:330:TRP:NE1	2.83	0.41
1:F:271:ALA:O	1:F:333:HIS:HE1	2.04	0.41
1:C:287:LEU:HD22	1:C:311:ILE:HD11	2.03	0.41
1:C:19:CYS:C	1:C:21:HIS:N	2.73	0.41
1:B:544:VAL:N	1:B:612:GLN:HE22	2.18	0.41
1:E:150:ILE:HG22	1:E:151:PRO:O	2.21	0.41
1:D:655:LEU:N	1:D:683:ASP:HB2	2.27	0.41
1:D:547:TYR:OH	1:D:560:PHE:HB3	2.21	0.41
1:B:691:HIS:HA	1:B:699:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:LYS:HA	1:D:557:PRO:HD3	1.90	0.41
1:F:373:ILE:HA	1:F:374:PRO:HD2	1.91	0.41
1:D:111:VAL:O	1:D:125:THR:HA	2.21	0.41
1:E:568:LEU:HD22	1:E:568:LEU:H	1.85	0.41
1:C:35:TRP:HB2	1:C:44:ARG:HB3	2.02	0.41
1:C:6:PHE:CD2	1:C:6:PHE:N	2.88	0.41
3:E:762:NAG:H83	3:E:762:NAG:H2	1.94	0.41
1:D:552:TYR:HA	1:D:564:GLN:OE1	2.21	0.41
1:B:411:PHE:C	1:B:411:PHE:CD1	2.93	0.41
1:B:287:LEU:CD2	1:B:330:TRP:CE2	3.04	0.41
1:E:287:LEU:HD13	1:E:311:ILE:CD1	2.50	0.41
1:E:287:LEU:CD2	1:E:330:TRP:CE2	3.03	0.41
1:C:287:LEU:CD2	1:C:330:TRP:NE1	2.82	0.41
1:D:44:ARG:NH1	1:D:258:PRO:HB2	2.36	0.41
1:C:615:ALA:HA	1:C:616:PRO:HD3	1.55	0.41
1:D:148:LYS:HB3	1:D:150:ILE:CD1	2.51	0.41
1:C:547:TYR:OH	1:C:560:PHE:HB3	2.21	0.41
1:F:80:MSE:HE2	1:F:80:MSE:HB3	1.93	0.41
1:F:422:CYS:O	1:F:423:CYS:HB2	2.20	0.41
1:E:471:SER:C	1:E:473:ASP:H	2.24	0.41
1:A:471:SER:C	1:A:473:ASP:H	2.24	0.41
1:A:33:GLN:O	1:A:34:VAL:HG23	2.21	0.41
1:C:657:SER:HA	1:C:732:LYS:HE3	2.02	0.41
1:F:107:PRO:CG	1:F:108:GLY:N	2.85	0.40
1:A:107:PRO:CG	1:A:108:GLY:N	2.84	0.40
1:F:292:LEU:CD2	1:F:312:VAL:HG22	2.52	0.40
1:C:481:ALA:HB1	1:C:549:PHE:CE1	2.57	0.40
1:A:150:ILE:HG22	1:A:151:PRO:O	2.21	0.40
1:A:413:THR:HG21	1:A:595:GLN:HE22	1.86	0.40
1:A:422:CYS:O	1:A:423:CYS:HB2	2.20	0.40
1:D:407:ILE:CG2	1:D:408:THR:N	2.83	0.40
1:F:143:PRO:HA	1:F:144:PRO:HD3	1.96	0.40
1:E:69:LEU:HD22	1:E:69:LEU:HA	1.85	0.40
1:D:107:PRO:CG	1:D:108:GLY:N	2.84	0.40
1:F:287:LEU:HD22	1:F:330:TRP:CE2	2.56	0.40
1:D:35:TRP:HB2	1:D:44:ARG:HB3	2.02	0.40
1:F:137:ARG:HH21	1:F:331:GLY:H	1.69	0.40
1:B:337:ARG:NH2	1:B:620:LYS:HE2	2.36	0.40
1:D:361:TYR:HB2	1:D:381:ARG:HH21	1.86	0.40
1:E:300:LEU:CD1	1:E:337:ARG:HD3	2.50	0.40
1:B:400:PRO:HB2	1:B:484:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:SER:C	1:D:473:ASP:N	2.72	0.40
1:F:591:VAL:HA	1:F:592:PRO:HD3	1.80	0.40
1:F:287:LEU:CD2	1:F:330:TRP:CE2	3.04	0.40
1:C:654:PRO:HB3	1:C:684:ARG:H	1.87	0.40
1:D:544:VAL:N	1:D:612:GLN:HE22	2.19	0.40
1:B:447:PHE:CE1	1:B:455:PHE:HA	2.54	0.40
1:B:51:PHE:CD2	1:B:80:MSE:SE	3.25	0.40
1:B:60:SER:CB	1:B:63:LYS:HB2	2.51	0.40
1:C:373:ILE:HA	1:C:374:PRO:HD2	1.91	0.40
1:F:407:ILE:CG2	1:F:408:THR:N	2.85	0.40
1:A:146:HIS:N	1:A:146:HIS:CD2	2.89	0.40
1:B:568:LEU:H	1:B:568:LEU:HD22	1.87	0.40
1:B:143:PRO:HA	1:B:144:PRO:HD3	1.95	0.40
1:B:432:ALA:O	1:B:433:HIS:HB3	2.22	0.40
1:B:552:TYR:HA	1:B:564:GLN:OE1	2.20	0.40
1:C:105:CYS:HA	1:C:106:PRO:HD3	1.89	0.40
1:F:108:GLY:CA	1:F:130:ILE:HB	2.48	0.40
1:F:92:ARG:HD3	1:F:92:ARG:HA	1.92	0.40
1:C:292:LEU:CD2	1:C:312:VAL:HG22	2.51	0.40
1:C:300:LEU:CD1	1:C:337:ARG:HD3	2.51	0.40
1:B:300:LEU:CD1	1:B:337:ARG:HD3	2.52	0.40
1:B:399:LEU:H	1:B:399:LEU:HD12	1.85	0.40
1:F:489:MSE:HB2	1:F:489:MSE:HE3	1.91	0.40
1:D:71:GLN:C	1:D:73:HIS:H	2.24	0.40
1:A:111:VAL:O	1:A:125:THR:HA	2.20	0.40
1:C:71:GLN:C	1:C:73:HIS:H	2.25	0.40
1:F:105:CYS:HA	1:F:106:PRO:HD3	1.89	0.40
1:A:303:ASN:HA	1:A:304:PRO:HD3	1.84	0.40
1:A:547:TYR:OH	1:A:560:PHE:HB3	2.21	0.40
1:C:530:PHE:CE2	1:C:617:PHE:HD1	2.40	0.40
1:E:530:PHE:CE2	1:E:617:PHE:HD1	2.38	0.40
1:D:398:VAL:HB	1:D:628:ALA:HB3	2.03	0.40
1:E:471:SER:C	1:E:473:ASP:N	2.73	0.40
1:C:491:VAL:O	1:C:505:ASP:HA	2.21	0.40
1:D:6:PHE:HA	1:D:57:GLY:O	2.22	0.40
1:E:432:ALA:O	1:E:433:HIS:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	617/750 (82%)	501 (81%)	92 (15%)	24 (4%)	4	25
1	B	616/750 (82%)	499 (81%)	96 (16%)	21 (3%)	5	29
1	C	616/750 (82%)	500 (81%)	92 (15%)	24 (4%)	4	25
1	D	616/750 (82%)	502 (82%)	92 (15%)	22 (4%)	4	28
1	E	617/750 (82%)	505 (82%)	90 (15%)	22 (4%)	4	28
1	F	612/750 (82%)	503 (82%)	87 (14%)	22 (4%)	4	28
All	All	3694/4500 (82%)	3010 (82%)	549 (15%)	135 (4%)	4	27

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	PRO
1	A	117	SER
1	A	434	ALA
1	A	650	THR
1	A	730	CYS
1	B	106	PRO
1	B	117	SER
1	B	434	ALA
1	B	650	THR
1	B	730	CYS
1	C	106	PRO
1	C	117	SER
1	C	434	ALA
1	C	447	PHE
1	C	650	THR
1	C	730	CYS
1	D	106	PRO
1	D	117	SER
1	D	434	ALA
1	D	650	THR

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Mol	Chain	Res	Type
1	D	730	CYS
1	E	106	PRO
1	E	117	SER
1	E	434	ALA
1	E	650	THR
1	E	730	CYS
1	F	106	PRO
1	F	117	SER
1	F	434	ALA
1	F	447	PHE
1	F	650	THR
1	F	730	CYS
1	A	80	MSE
1	A	107	PRO
1	A	446	PRO
1	A	450	GLY
1	A	515	THR
1	B	80	MSE
1	B	107	PRO
1	B	515	THR
1	C	80	MSE
1	C	107	PRO
1	C	515	THR
1	D	80	MSE
1	D	107	PRO
1	D	515	THR
1	E	80	MSE
1	E	107	PRO
1	E	515	THR
1	F	80	MSE
1	F	107	PRO
1	F	515	THR
1	A	257	LEU
1	A	624	ASN
1	B	255	LEU
1	B	257	LEU
1	B	624	ASN
1	C	257	LEU
1	C	624	ASN
1	D	257	LEU
1	D	624	ASN
1	E	257	LEU

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Mol	Chain	Res	Type
1	E	423	CYS
1	E	624	ASN
1	F	624	ASN
1	A	70	LYS
1	A	322	ASP
1	A	386	PRO
1	A	423	CYS
1	A	721	PRO
1	B	322	ASP
1	B	332	ASN
1	B	423	CYS
1	B	721	PRO
1	C	22	THR
1	C	136	GLY
1	C	322	ASP
1	C	423	CYS
1	C	721	PRO
1	D	322	ASP
1	D	332	ASN
1	D	423	CYS
1	D	721	PRO
1	E	322	ASP
1	E	453	GLN
1	E	721	PRO
1	F	22	THR
1	F	136	GLY
1	F	322	ASP
1	F	332	ASN
1	F	423	CYS
1	F	721	PRO
1	A	22	THR
1	A	332	ASN
1	A	430	PRO
1	B	70	LYS
1	B	136	GLY
1	B	386	PRO
1	B	430	PRO
1	C	70	LYS
1	C	386	PRO
1	C	430	PRO
1	D	70	LYS
1	D	386	PRO

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Mol	Chain	Res	Type
1	D	430	PRO
1	E	70	LYS
1	E	136	GLY
1	E	332	ASN
1	E	386	PRO
1	E	430	PRO
1	F	70	LYS
1	F	386	PRO
1	F	430	PRO
1	A	119	ASN
1	A	136	GLY
1	B	444	VAL
1	C	332	ASN
1	C	449	TRP
1	C	653	ALA
1	D	22	THR
1	D	119	ASN
1	D	136	GLY
1	E	119	ASN
1	F	119	ASN
1	F	444	VAL
1	A	444	VAL
1	C	444	VAL
1	D	444	VAL
1	E	444	VAL
1	F	610	PRO
1	E	610	PRO
1	A	610	PRO
1	C	610	PRO
1	D	610	PRO
1	B	610	PRO

5.3.2 Protein sidechains (i)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	534/630 (85%)	468 (88%)	66 (12%)	6 25
1	B	533/630 (85%)	466 (87%)	67 (13%)	5 24
1	C	533/630 (85%)	466 (87%)	67 (13%)	5 24
1	D	533/630 (85%)	469 (88%)	64 (12%)	6 27
1	E	532/630 (84%)	466 (88%)	66 (12%)	6 25
1	F	529/630 (84%)	464 (88%)	65 (12%)	6 25
All	All	3194/3780 (84%)	2799 (88%)	395 (12%)	6 25

All (395) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	20	HIS
1	A	68	SER
1	A	69	LEU
1	A	71	GLN
1	A	72	ASP
1	A	74	THR
1	A	77	GLU
1	A	93	ARG
1	A	94	LEU
1	A	109	ASP
1	A	120	SER
1	A	122	THR
1	A	125	THR
1	A	146	HIS
1	A	261	LEU
1	A	262	ILE
1	A	267	MSE
1	A	268	VAL
1	A	282	HIS
1	A	288	ASP
1	A	289	THR
1	A	293	THR
1	A	294	LEU
1	A	295	LEU
1	A	296	THR
1	A	308	THR

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Mol	Chain	Res	Type
1	A	317	ARG
1	A	329	ILE
1	A	333	HIS
1	A	336	VAL
1	A	341	GLN
1	A	343	SER
1	A	387	LEU
1	A	394	MSE
1	A	402	THR
1	A	405	GLU
1	A	407	ILE
1	A	409	CYS
1	A	413	THR
1	A	428	CYS
1	A	437	THR
1	A	438	CYS
1	A	474	CYS
1	A	490	LYS
1	A	497	TYR
1	A	505	ASP
1	A	516	SER
1	A	518	ASP
1	A	519	LEU
1	A	541	ARG
1	A	548	ASP
1	A	555	MSE
1	A	563	ILE
1	A	567	SER
1	A	573	LEU
1	A	578	ASP
1	A	602	MSE
1	A	609	ARG
1	A	611	LEU
1	A	612	GLN
1	A	626	LEU
1	A	649	ARG
1	A	651	SER
1	A	652	ASP
1	A	655	LEU
1	B	17	SER
1	B	20	HIS
1	B	68	SER

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Mol	Chain	Res	Type
1	B	69	LEU
1	B	71	GLN
1	B	72	ASP
1	B	74	THR
1	B	77	GLU
1	B	93	ARG
1	B	94	LEU
1	B	109	ASP
1	B	120	SER
1	B	122	THR
1	B	125	THR
1	B	146	HIS
1	B	261	LEU
1	B	262	ILE
1	B	267	MSE
1	B	268	VAL
1	B	282	HIS
1	B	288	ASP
1	B	289	THR
1	B	293	THR
1	B	294	LEU
1	B	295	LEU
1	B	296	THR
1	B	308	THR
1	B	312	VAL
1	B	317	ARG
1	B	329	ILE
1	B	333	HIS
1	B	336	VAL
1	B	341	GLN
1	B	387	LEU
1	B	394	MSE
1	B	402	THR
1	B	405	GLU
1	B	407	ILE
1	B	409	CYS
1	B	413	THR
1	B	428	CYS
1	B	437	THR
1	B	438	CYS
1	B	474	CYS
1	B	490	LYS

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Mol	Chain	Res	Type
1	B	497	TYR
1	B	505	ASP
1	B	516	SER
1	B	518	ASP
1	B	519	LEU
1	B	541	ARG
1	B	548	ASP
1	B	555	MSE
1	B	563	ILE
1	B	567	SER
1	B	573	LEU
1	B	578	ASP
1	B	597	SER
1	B	602	MSE
1	B	609	ARG
1	B	611	LEU
1	B	612	GLN
1	B	626	LEU
1	B	649	ARG
1	B	651	SER
1	B	652	ASP
1	B	655	LEU
1	C	17	SER
1	C	20	HIS
1	C	68	SER
1	C	69	LEU
1	C	71	GLN
1	C	72	ASP
1	C	74	THR
1	C	77	GLU
1	C	93	ARG
1	C	94	LEU
1	C	109	ASP
1	C	120	SER
1	C	122	THR
1	C	125	THR
1	C	146	HIS
1	C	255	LEU
1	C	261	LEU
1	C	262	ILE
1	C	267	MSE
1	C	268	VAL

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Mol	Chain	Res	Type
1	C	282	HIS
1	C	288	ASP
1	C	289	THR
1	C	293	THR
1	C	294	LEU
1	C	295	LEU
1	C	296	THR
1	C	308	THR
1	C	317	ARG
1	C	329	ILE
1	C	333	HIS
1	C	336	VAL
1	C	341	GLN
1	C	387	LEU
1	C	394	MSE
1	C	402	THR
1	C	405	GLU
1	C	407	ILE
1	C	409	CYS
1	C	413	THR
1	C	428	CYS
1	C	437	THR
1	C	438	CYS
1	C	447	PHE
1	C	448	MSE
1	C	474	CYS
1	C	490	LYS
1	C	497	TYR
1	C	505	ASP
1	C	516	SER
1	C	518	ASP
1	C	519	LEU
1	C	541	ARG
1	C	548	ASP
1	C	555	MSE
1	C	563	ILE
1	C	567	SER
1	C	573	LEU
1	C	578	ASP
1	C	597	SER
1	C	602	MSE
1	C	611	LEU

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Mol	Chain	Res	Type
1	C	612	GLN
1	C	626	LEU
1	C	649	ARG
1	C	651	SER
1	C	652	ASP
1	D	17	SER
1	D	20	HIS
1	D	68	SER
1	D	69	LEU
1	D	71	GLN
1	D	72	ASP
1	D	74	THR
1	D	77	GLU
1	D	93	ARG
1	D	94	LEU
1	D	109	ASP
1	D	120	SER
1	D	122	THR
1	D	125	THR
1	D	146	HIS
1	D	261	LEU
1	D	262	ILE
1	D	267	MSE
1	D	268	VAL
1	D	282	HIS
1	D	288	ASP
1	D	289	THR
1	D	293	THR
1	D	294	LEU
1	D	295	LEU
1	D	296	THR
1	D	308	THR
1	D	317	ARG
1	D	329	ILE
1	D	333	HIS
1	D	336	VAL
1	D	387	LEU
1	D	394	MSE
1	D	402	THR
1	D	405	GLU
1	D	407	ILE
1	D	409	CYS

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Mol	Chain	Res	Type
1	D	413	THR
1	D	428	CYS
1	D	437	THR
1	D	438	CYS
1	D	474	CYS
1	D	490	LYS
1	D	497	TYR
1	D	505	ASP
1	D	516	SER
1	D	518	ASP
1	D	519	LEU
1	D	541	ARG
1	D	548	ASP
1	D	555	MSE
1	D	563	ILE
1	D	567	SER
1	D	573	LEU
1	D	578	ASP
1	D	602	MSE
1	D	609	ARG
1	D	611	LEU
1	D	612	GLN
1	D	626	LEU
1	D	649	ARG
1	D	651	SER
1	D	652	ASP
1	D	655	LEU
1	E	17	SER
1	E	20	HIS
1	E	68	SER
1	E	69	LEU
1	E	71	GLN
1	E	72	ASP
1	E	74	THR
1	E	77	GLU
1	E	93	ARG
1	E	94	LEU
1	E	109	ASP
1	E	120	SER
1	E	122	THR
1	E	125	THR
1	E	146	HIS

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Mol	Chain	Res	Type
1	E	261	LEU
1	E	262	ILE
1	E	267	MSE
1	E	268	VAL
1	E	282	HIS
1	E	288	ASP
1	E	289	THR
1	E	293	THR
1	E	294	LEU
1	E	295	LEU
1	E	296	THR
1	E	308	THR
1	E	312	VAL
1	E	317	ARG
1	E	329	ILE
1	E	333	HIS
1	E	336	VAL
1	E	387	LEU
1	E	394	MSE
1	E	402	THR
1	E	405	GLU
1	E	407	ILE
1	E	409	CYS
1	E	413	THR
1	E	428	CYS
1	E	437	THR
1	E	438	CYS
1	E	474	CYS
1	E	490	LYS
1	E	497	TYR
1	E	505	ASP
1	E	516	SER
1	E	518	ASP
1	E	519	LEU
1	E	541	ARG
1	E	548	ASP
1	E	555	MSE
1	E	563	ILE
1	E	567	SER
1	E	573	LEU
1	E	578	ASP
1	E	597	SER

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Mol	Chain	Res	Type
1	E	602	MSE
1	E	609	ARG
1	E	611	LEU
1	E	612	GLN
1	E	626	LEU
1	E	649	ARG
1	E	651	SER
1	E	652	ASP
1	E	655	LEU
1	F	17	SER
1	F	20	HIS
1	F	68	SER
1	F	69	LEU
1	F	71	GLN
1	F	72	ASP
1	F	74	THR
1	F	77	GLU
1	F	93	ARG
1	F	94	LEU
1	F	109	ASP
1	F	120	SER
1	F	122	THR
1	F	125	THR
1	F	146	HIS
1	F	261	LEU
1	F	262	ILE
1	F	267	MSE
1	F	268	VAL
1	F	282	HIS
1	F	288	ASP
1	F	289	THR
1	F	293	THR
1	F	294	LEU
1	F	295	LEU
1	F	296	THR
1	F	308	THR
1	F	317	ARG
1	F	329	ILE
1	F	333	HIS
1	F	336	VAL
1	F	341	GLN
1	F	387	LEU

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Mol	Chain	Res	Type
1	F	394	MSE
1	F	402	THR
1	F	405	GLU
1	F	407	ILE
1	F	409	CYS
1	F	413	THR
1	F	428	CYS
1	F	437	THR
1	F	438	CYS
1	F	448	MSE
1	F	474	CYS
1	F	490	LYS
1	F	497	TYR
1	F	505	ASP
1	F	516	SER
1	F	518	ASP
1	F	519	LEU
1	F	541	ARG
1	F	548	ASP
1	F	555	MSE
1	F	563	ILE
1	F	567	SER
1	F	573	LEU
1	F	578	ASP
1	F	597	SER
1	F	602	MSE
1	F	611	LEU
1	F	612	GLN
1	F	626	LEU
1	F	649	ARG
1	F	651	SER
1	F	655	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	50	GLN
1	A	62	ASN
1	A	146	HIS
1	A	291	HIS
1	A	332	ASN

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Mol	Chain	Res	Type
1	A	333	HIS
1	A	453	GLN
1	A	540	HIS
1	A	546	ASN
1	A	595	GLN
1	A	612	GLN
1	A	691	HIS
1	A	715	HIS
1	B	46	GLN
1	B	50	GLN
1	B	62	ASN
1	B	146	HIS
1	B	291	HIS
1	B	332	ASN
1	B	333	HIS
1	B	460	ASN
1	B	540	HIS
1	B	546	ASN
1	B	595	GLN
1	B	612	GLN
1	B	715	HIS
1	C	46	GLN
1	C	50	GLN
1	C	62	ASN
1	C	146	HIS
1	C	256	HIS
1	C	291	HIS
1	C	332	ASN
1	C	333	HIS
1	C	540	HIS
1	C	546	ASN
1	C	595	GLN
1	C	612	GLN
1	C	691	HIS
1	C	715	HIS
1	D	46	GLN
1	D	50	GLN
1	D	62	ASN
1	D	146	HIS
1	D	291	HIS
1	D	332	ASN
1	D	333	HIS

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Mol	Chain	Res	Type
1	D	453	GLN
1	D	540	HIS
1	D	546	ASN
1	D	595	GLN
1	D	612	GLN
1	D	691	HIS
1	D	715	HIS
1	E	46	GLN
1	E	50	GLN
1	E	62	ASN
1	E	146	HIS
1	E	291	HIS
1	E	332	ASN
1	E	333	HIS
1	E	540	HIS
1	E	546	ASN
1	E	595	GLN
1	E	612	GLN
1	E	691	HIS
1	E	715	HIS
1	F	46	GLN
1	F	50	GLN
1	F	62	ASN
1	F	146	HIS
1	F	291	HIS
1	F	332	ASN
1	F	333	HIS
1	F	540	HIS
1	F	546	ASN
1	F	595	GLN
1	F	612	GLN
1	F	691	HIS
1	F	715	HIS

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 (i)

50 carbohydrates are modelled in this entry.

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	$\#\|Z\| > 2$
2	NAG	A	751	1,2	14,14,15	0.39	0	15,19,21	2.19	1 (6%)
2	NAG	A	752	2	14,14,15	0.52	0	15,19,21	2.01	2 (13%)
2	BMA	A	753	2	11,11,12	1.75	3 (27%)	14,15,17	4.36	12 (85%)
2	MAN	A	754	2	11,11,12	0.87	1 (9%)	14,15,17	2.39	4 (28%)
3	NAG	A	761	1,3	14,14,15	0.67	0	15,19,21	1.37	2 (13%)
3	NAG	A	762	3	14,14,15	0.46	0	15,19,21	1.22	1 (6%)
3	BMA	A	763	3	11,11,12	2.15	4 (36%)	14,15,17	3.27	9 (64%)
3	MAN	A	764	3	11,11,12	0.41	0	14,15,17	1.65	2 (14%)
3	MAN	A	765	3	11,11,12	0.49	0	14,15,17	1.52	1 (7%)
2	NAG	B	751	1,2	14,14,15	0.73	0	15,19,21	0.99	0
2	NAG	B	752	2	14,14,15	0.81	0	15,19,21	1.67	2 (13%)
2	BMA	B	753	2	11,11,12	2.25	5 (45%)	14,15,17	3.10	9 (64%)
2	MAN	B	754	2	11,11,12	0.52	0	14,15,17	1.17	2 (14%)
2	NAG	B	761	1,2	14,14,15	0.53	0	15,19,21	1.20	1 (6%)
2	NAG	B	762	2	14,14,15	0.57	0	15,19,21	1.50	3 (20%)
2	BMA	B	763	2	11,11,12	1.85	4 (36%)	14,15,17	3.79	9 (64%)
2	MAN	B	764	2	11,11,12	0.59	0	14,15,17	0.77	0
2	NAG	C	751	1,2	14,14,15	0.66	0	15,19,21	0.78	0
2	NAG	C	752	2	14,14,15	0.61	0	15,19,21	0.81	1 (6%)
2	BMA	C	753	2	11,11,12	2.13	4 (36%)	14,15,17	3.82	9 (64%)
2	MAN	C	754	2	11,11,12	0.77	1 (9%)	14,15,17	1.81	5 (35%)
2	NAG	C	761	1,2	14,14,15	0.44	0	15,19,21	2.02	2 (13%)
2	NAG	C	762	2	14,14,15	0.47	0	15,19,21	3.08	4 (26%)
2	BMA	C	763	2	11,11,12	1.85	3 (27%)	14,15,17	3.48	9 (64%)
2	MAN	C	764	2	11,11,12	0.44	0	14,15,17	1.90	2 (14%)
2	NAG	D	751	1,2	14,14,15	0.74	0	15,19,21	2.30	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	D	752	2	14,14,15	0.56	0	15,19,21	1.65	3 (20%)
2	BMA	D	753	2	11,11,12	1.95	4 (36%)	14,15,17	3.40	11 (78%)
2	MAN	D	754	2	11,11,12	0.54	0	14,15,17	1.05	1 (7%)
4	NAG	D	761	1,4	14,14,15	0.37	0	15,19,21	2.23	1 (6%)
4	NAG	D	762	4	14,14,15	0.49	0	15,19,21	1.07	1 (6%)
4	BMA	D	763	4	11,11,12	2.05	4 (36%)	14,15,17	3.48	10 (71%)
2	NAG	E	751	1,2	14,14,15	0.60	0	15,19,21	1.05	1 (6%)
2	NAG	E	752	2	14,14,15	0.66	0	15,19,21	1.71	3 (20%)
2	BMA	E	753	2	11,11,12	2.01	4 (36%)	14,15,17	3.86	10 (71%)
2	MAN	E	754	2	11,11,12	0.63	0	14,15,17	0.78	0
3	NAG	E	761	1,3	14,14,15	0.49	0	15,19,21	2.39	4 (26%)
3	NAG	E	762	3	14,14,15	0.63	1 (7%)	15,19,21	2.62	4 (26%)
3	BMA	E	763	3	11,11,12	1.86	3 (27%)	14,15,17	3.97	8 (57%)
3	MAN	E	764	3	11,11,12	0.56	0	14,15,17	1.18	1 (7%)
3	MAN	E	765	3	11,11,12	0.59	0	14,15,17	0.58	0
2	NAG	F	751	1,2	14,14,15	0.66	0	15,19,21	1.92	2 (13%)
2	NAG	F	752	2	14,14,15	0.47	0	15,19,21	3.35	4 (26%)
2	BMA	F	753	2	11,11,12	2.09	4 (36%)	14,15,17	4.54	10 (71%)
2	MAN	F	754	2	11,11,12	0.49	0	14,15,17	1.43	2 (14%)
3	NAG	F	761	1,3	14,14,15	0.41	0	15,19,21	2.01	3 (20%)
3	NAG	F	762	3	14,14,15	0.43	0	15,19,21	2.24	2 (13%)
3	BMA	F	763	3	11,11,12	2.15	4 (36%)	14,15,17	2.19	7 (50%)
3	MAN	F	764	3	11,11,12	0.59	0	14,15,17	0.74	0
3	MAN	F	765	3	11,11,12	0.46	0	14,15,17	1.64	4 (28%)

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
2	NAG	A	751	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	752	2	-	0/6/23/26	0/1/1/1
2	BMA	A	753	2	-	0/2/19/22	0/1/1/1
2	MAN	A	754	2	-	0/2/19/22	0/1/1/1
3	NAG	A	761	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	762	3	-	0/6/23/26	0/1/1/1
3	BMA	A	763	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	A	764	3	-	0/2/19/22	0/1/1/1
3	MAN	A	765	3	-	0/2/19/22	1/1/1/1
2	NAG	B	751	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	752	2	-	0/6/23/26	0/1/1/1
2	BMA	B	753	2	-	0/2/19/22	0/1/1/1
2	MAN	B	754	2	-	0/2/19/22	0/1/1/1
2	NAG	B	761	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	762	2	-	0/6/23/26	0/1/1/1
2	BMA	B	763	2	-	0/2/19/22	0/1/1/1
2	MAN	B	764	2	-	0/2/19/22	0/1/1/1
2	NAG	C	751	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	752	2	-	0/6/23/26	0/1/1/1
2	BMA	C	753	2	-	0/2/19/22	0/1/1/1
2	MAN	C	754	2	-	0/2/19/22	0/1/1/1
2	NAG	C	761	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	762	2	-	0/6/23/26	0/1/1/1
2	BMA	C	763	2	-	0/2/19/22	0/1/1/1
2	MAN	C	764	2	-	0/2/19/22	1/1/1/1
2	NAG	D	751	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	752	2	-	0/6/23/26	0/1/1/1
2	BMA	D	753	2	-	0/2/19/22	0/1/1/1
2	MAN	D	754	2	-	0/2/19/22	0/1/1/1
4	NAG	D	761	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	762	4	-	0/6/23/26	0/1/1/1
4	BMA	D	763	4	-	0/2/19/22	0/1/1/1
2	NAG	E	751	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	752	2	-	2/6/23/26	0/1/1/1
2	BMA	E	753	2	-	0/2/19/22	0/1/1/1
2	MAN	E	754	2	-	0/2/19/22	0/1/1/1
3	NAG	E	761	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	762	3	-	0/6/23/26	0/1/1/1
3	BMA	E	763	3	-	0/2/19/22	0/1/1/1
3	MAN	E	764	3	-	0/2/19/22	1/1/1/1
3	MAN	E	765	3	-	0/2/19/22	0/1/1/1
2	NAG	F	751	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	F	752	2	-	1/6/23/26	0/1/1/1
2	BMA	F	753	2	-	0/2/19/22	0/1/1/1
2	MAN	F	754	2	-	0/2/19/22	1/1/1/1
3	NAG	F	761	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	762	3	-	0/6/23/26	0/1/1/1
3	BMA	F	763	3	-	0/2/19/22	0/1/1/1
3	MAN	F	764	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	F	765	3	-	0/2/19/22	1/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	753	BMA	C2-C3	-4.19	1.46	1.52
2	B	753	BMA	C2-C3	-3.40	1.47	1.52
3	F	763	BMA	C2-C3	-3.40	1.47	1.52
2	D	753	BMA	C2-C3	-3.13	1.48	1.52
2	E	753	BMA	C2-C3	-3.10	1.48	1.52
3	E	763	BMA	C2-C3	-3.03	1.48	1.52
3	A	763	BMA	C2-C3	-3.01	1.48	1.52
4	D	763	BMA	C2-C3	-3.00	1.48	1.52
2	F	753	BMA	C2-C3	-2.34	1.49	1.52
2	A	754	MAN	O5-C1	-2.29	1.39	1.43
2	A	753	BMA	C2-C3	-2.18	1.49	1.52
2	C	754	MAN	O5-C1	-2.12	1.40	1.43
2	B	763	BMA	C2-C3	-2.12	1.49	1.52
2	B	753	BMA	C1-C2	-2.10	1.47	1.52
2	C	753	BMA	C4-C3	2.15	1.58	1.52
3	E	762	NAG	C1-C2	2.17	1.55	1.52
2	D	753	BMA	C4-C3	2.19	1.58	1.52
4	D	763	BMA	C4-C3	2.22	1.58	1.52
2	B	763	BMA	C4-C3	2.30	1.58	1.52
2	E	753	BMA	C4-C3	2.33	1.58	1.52
3	F	763	BMA	C4-C3	2.33	1.58	1.52
2	C	763	BMA	C4-C3	2.44	1.58	1.52
2	F	753	BMA	C4-C3	2.67	1.59	1.52
3	A	763	BMA	C4-C3	2.72	1.59	1.52
2	B	753	BMA	C4-C3	2.86	1.59	1.52
2	A	753	BMA	C4-C5	3.10	1.59	1.53
3	E	763	BMA	C4-C5	3.21	1.59	1.53
2	C	763	BMA	C4-C5	3.36	1.60	1.53
2	B	753	BMA	O4-C4	3.38	1.51	1.43
2	C	753	BMA	C4-C5	3.38	1.60	1.53
2	D	753	BMA	C4-C5	3.38	1.60	1.53
2	B	763	BMA	C4-C5	3.44	1.60	1.53
3	A	763	BMA	O4-C4	3.46	1.51	1.43
2	E	753	BMA	O4-C4	3.46	1.51	1.43
3	F	763	BMA	O4-C4	3.51	1.51	1.43
2	E	753	BMA	C4-C5	3.51	1.60	1.53
2	D	753	BMA	O4-C4	3.53	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	753	BMA	O4-C4	3.54	1.51	1.43
3	E	763	BMA	O4-C4	3.59	1.51	1.43
4	D	763	BMA	O4-C4	3.64	1.51	1.43
2	B	763	BMA	O4-C4	3.67	1.51	1.43
2	A	753	BMA	O4-C4	3.69	1.51	1.43
2	F	753	BMA	O4-C4	3.74	1.51	1.43
2	C	763	BMA	O4-C4	3.76	1.52	1.43
3	F	763	BMA	C4-C5	3.87	1.61	1.53
4	D	763	BMA	C4-C5	3.98	1.61	1.53
3	A	763	BMA	C4-C5	4.08	1.61	1.53
2	B	753	BMA	C4-C5	4.24	1.62	1.53
2	F	753	BMA	C4-C5	4.31	1.62	1.53

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	753	BMA	C1-O5-C5	-10.24	99.26	112.25
2	F	752	NAG	C4-C3-C2	-9.80	96.00	111.23
3	A	763	BMA	C1-O5-C5	-8.62	101.31	112.25
2	E	753	BMA	C1-O5-C5	-8.25	101.78	112.25
2	B	753	BMA	C1-O5-C5	-7.11	103.23	112.25
2	F	753	BMA	C1-C2-C3	-6.32	102.07	109.54
4	D	763	BMA	C1-O5-C5	-6.21	104.37	112.25
2	C	762	NAG	C4-C3-C2	-5.88	102.09	111.23
2	C	753	BMA	C2-C3-C4	-5.80	101.19	111.04
2	C	763	BMA	C1-O5-C5	-5.40	105.39	112.25
2	A	753	BMA	C3-C4-C5	-5.39	100.80	110.20
2	A	754	MAN	O5-C1-C2	-5.33	102.21	110.86
2	F	752	NAG	C2-N2-C7	-5.12	116.46	123.04
3	E	762	NAG	C4-C3-C2	-4.87	103.65	111.23
3	E	763	BMA	C2-C3-C4	-4.27	103.79	111.04
2	E	752	NAG	C2-N2-C7	-4.23	117.61	123.04
2	D	752	NAG	C1-O5-C5	-4.13	107.01	112.25
2	A	753	BMA	C2-C3-C4	-4.10	104.08	111.04
2	B	763	BMA	C2-C3-C4	-3.82	104.55	111.04
3	E	763	BMA	C1-O5-C5	-3.70	107.55	112.25
2	E	752	NAG	C4-C3-C2	-3.66	105.54	111.23
3	E	761	NAG	C4-C3-C2	-3.59	105.65	111.23
2	B	752	NAG	C2-N2-C7	-3.45	118.60	123.04
3	F	763	BMA	O5-C1-C2	-3.44	105.28	110.86
2	A	754	MAN	C1-C2-C3	-3.37	105.56	109.54
2	A	754	MAN	C1-O5-C5	-3.36	107.98	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	753	BMA	C1-C2-C3	-3.30	105.64	109.54
2	D	751	NAG	C3-C4-C5	-3.29	104.47	110.20
2	C	753	BMA	C3-C4-C5	-3.28	104.48	110.20
2	D	753	BMA	C1-O5-C5	-3.25	108.12	112.25
2	B	762	NAG	C1-O5-C5	-3.25	108.13	112.25
3	F	761	NAG	C4-C3-C2	-3.22	106.23	111.23
2	D	751	NAG	C2-N2-C7	-3.06	119.11	123.04
2	C	762	NAG	C2-N2-C7	-3.04	119.14	123.04
2	B	763	BMA	C3-C4-C5	-3.02	104.93	110.20
3	A	764	MAN	C2-C3-C4	-3.02	105.91	111.04
2	D	751	NAG	C4-C3-C2	-2.90	106.72	111.23
2	D	753	BMA	C2-C3-C4	-2.86	106.18	111.04
3	E	763	BMA	C3-C4-C5	-2.80	105.32	110.20
4	D	763	BMA	C2-C3-C4	-2.72	106.42	111.04
2	C	754	MAN	C6-C5-C4	-2.63	106.53	113.02
2	D	752	NAG	C2-N2-C7	-2.60	119.70	123.04
2	C	754	MAN	O5-C1-C2	-2.53	106.75	110.86
3	F	765	MAN	C3-C4-C5	-2.51	105.82	110.20
2	C	761	NAG	C2-N2-C7	-2.41	119.94	123.04
3	F	765	MAN	C2-C3-C4	-2.38	107.00	111.04
3	E	761	NAG	C2-N2-C7	-2.30	120.08	123.04
2	C	754	MAN	C1-C2-C3	-2.30	106.82	109.54
2	E	751	NAG	C3-C2-N2	-2.29	105.08	110.56
2	D	753	BMA	C3-C4-C5	-2.23	106.31	110.20
2	C	752	NAG	C3-C2-N2	-2.17	105.37	110.56
2	D	754	MAN	C2-C3-C4	-2.15	107.39	111.04
3	F	761	NAG	C2-N2-C7	-2.06	120.39	123.04
2	B	754	MAN	C2-C3-C4	-2.02	107.61	111.04
2	A	753	BMA	O2-C2-C1	2.01	113.23	109.21
2	B	753	BMA	O4-C4-C3	2.01	114.86	110.34
2	F	754	MAN	O5-C5-C6	2.04	111.76	107.35
2	C	763	BMA	O3-C3-C4	2.05	114.96	110.34
2	B	753	BMA	O2-C2-C1	2.08	113.37	109.21
3	E	762	NAG	O4-C4-C5	2.09	114.78	109.24
3	F	765	MAN	O5-C5-C6	2.10	111.90	107.35
2	F	753	BMA	C6-C5-C4	2.14	118.30	113.02
2	D	753	BMA	O2-C2-C3	2.15	114.43	110.12
2	F	753	BMA	O3-C3-C4	2.15	115.17	110.34
3	A	763	BMA	C6-C5-C4	2.18	118.40	113.02
3	F	763	BMA	O2-C2-C1	2.19	113.60	109.21
4	D	763	BMA	O2-C2-C1	2.22	113.66	109.21
4	D	762	NAG	C3-C4-C5	2.25	114.12	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	763	BMA	O2-C2-C3	2.26	114.67	110.12
2	A	753	BMA	O5-C1-C2	2.28	114.56	110.86
3	F	762	NAG	C3-C4-C5	2.30	114.20	110.20
3	A	763	BMA	C3-C4-C5	2.30	114.21	110.20
2	B	762	NAG	C4-C3-C2	2.35	114.88	111.23
2	D	753	BMA	O2-C2-C1	2.36	113.94	109.21
2	B	754	MAN	C1-O5-C5	2.37	115.25	112.25
2	A	753	BMA	O2-C2-C3	2.39	114.92	110.12
2	F	752	NAG	O3-C3-C4	2.39	115.72	110.34
2	C	764	MAN	C1-C2-C3	2.41	112.39	109.54
2	E	752	NAG	C3-C4-C5	2.42	114.41	110.20
3	F	763	BMA	O4-C4-C3	2.42	115.78	110.34
3	A	763	BMA	O4-C4-C3	2.43	115.82	110.34
2	C	763	BMA	C6-C5-C4	2.44	119.05	113.02
2	B	753	BMA	O3-C3-C2	2.46	114.44	110.00
2	C	754	MAN	C1-O5-C5	2.51	115.44	112.25
2	C	763	BMA	O2-C2-C3	2.52	115.19	110.12
2	A	753	BMA	C1-C2-C3	2.55	112.55	109.54
2	B	763	BMA	C6-C5-C4	2.56	119.34	113.02
3	F	763	BMA	O3-C3-C2	2.57	114.64	110.00
2	D	753	BMA	C6-C5-C4	2.61	119.45	113.02
2	B	763	BMA	O2-C2-C3	2.64	115.44	110.12
3	A	761	NAG	C3-C4-C5	2.64	114.81	110.20
2	B	762	NAG	C3-C4-C5	2.66	114.84	110.20
2	C	763	BMA	O2-C2-C1	2.68	114.58	109.21
2	B	753	BMA	O4-C4-C5	2.71	116.41	109.24
2	E	753	BMA	O2-C2-C1	2.72	114.66	109.21
3	A	763	BMA	O3-C3-C2	2.74	114.95	110.00
2	B	753	BMA	O3-C3-C4	2.77	116.58	110.34
2	B	761	NAG	C1-O5-C5	2.77	115.77	112.25
2	A	753	BMA	C6-C5-C4	2.80	119.92	113.02
3	A	763	BMA	O2-C2-C3	2.83	115.80	110.12
2	E	753	BMA	O2-C2-C3	2.84	115.82	110.12
3	E	762	NAG	O4-C4-C3	2.86	116.78	110.34
2	D	752	NAG	C3-C4-C5	2.91	115.28	110.20
3	A	763	BMA	O3-C3-C4	2.92	116.91	110.34
4	D	763	BMA	C6-C5-C4	2.92	120.22	113.02
2	C	753	BMA	C6-C5-C4	2.94	120.27	113.02
3	A	762	NAG	C1-O5-C5	2.95	116.00	112.25
2	B	753	BMA	O2-C2-C3	3.04	116.24	110.12
3	A	763	BMA	O4-C4-C5	3.05	117.33	109.24
3	E	761	NAG	O4-C4-C3	3.07	117.26	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	764	MAN	C1-O5-C5	3.10	116.18	112.25
2	E	753	BMA	C6-C5-C4	3.11	120.68	113.02
2	F	753	BMA	O4-C4-C3	3.12	117.36	110.34
3	F	763	BMA	C3-C4-C5	3.17	115.72	110.20
2	F	751	NAG	O4-C4-C3	3.19	117.51	110.34
3	A	761	NAG	C4-C3-C2	3.22	116.23	111.23
2	D	751	NAG	C1-O5-C5	3.22	116.33	112.25
2	A	753	BMA	O3-C3-C4	3.24	117.64	110.34
3	F	763	BMA	O5-C5-C6	3.25	114.38	107.35
3	E	763	BMA	C1-C2-C3	3.26	113.40	109.54
2	F	753	BMA	O2-C2-C3	3.32	116.79	110.12
2	C	762	NAG	O4-C4-C3	3.33	117.84	110.34
3	F	763	BMA	O4-C4-C5	3.36	118.15	109.24
2	C	753	BMA	O2-C2-C1	3.37	115.97	109.21
4	D	763	BMA	O3-C3-C4	3.38	117.94	110.34
2	E	753	BMA	O3-C3-C4	3.50	118.22	110.34
2	A	752	NAG	C3-C4-C5	3.59	116.46	110.20
2	C	753	BMA	O3-C3-C2	3.67	116.62	110.00
2	D	753	BMA	O3-C3-C4	3.73	118.74	110.34
2	F	753	BMA	O2-C2-C1	3.78	116.78	109.21
2	B	752	NAG	C3-C4-C5	3.80	116.82	110.20
2	C	754	MAN	C3-C4-C5	3.83	116.87	110.20
2	B	763	BMA	O3-C3-C4	3.86	119.03	110.34
2	B	753	BMA	C3-C4-C5	3.86	116.93	110.20
3	F	765	MAN	C1-O5-C5	4.04	117.37	112.25
4	D	763	BMA	O4-C4-C3	4.08	119.52	110.34
3	A	763	BMA	O5-C5-C6	4.14	116.32	107.35
2	E	753	BMA	O3-C3-C2	4.23	117.64	110.00
2	D	753	BMA	O3-C3-C2	4.28	117.73	110.00
2	E	753	BMA	O4-C4-C3	4.32	120.06	110.34
2	F	754	MAN	C1-O5-C5	4.33	117.74	112.25
2	B	753	BMA	O5-C5-C6	4.40	116.88	107.35
2	F	753	BMA	O4-C4-C5	4.44	121.00	109.24
3	A	764	MAN	C1-O5-C5	4.56	118.04	112.25
2	A	754	MAN	C3-C4-C5	4.57	118.16	110.20
2	C	763	BMA	O4-C4-C3	4.69	120.89	110.34
2	E	753	BMA	O4-C4-C5	4.69	121.66	109.24
4	D	763	BMA	O5-C5-C6	4.78	117.69	107.35
2	B	763	BMA	O5-C5-C6	4.88	117.91	107.35
2	C	763	BMA	O4-C4-C5	4.91	122.25	109.24
3	E	763	BMA	O4-C4-C3	4.91	121.40	110.34
3	A	765	MAN	C1-O5-C5	4.96	118.54	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	763	BMA	O3-C3-C2	4.97	118.97	110.00
2	B	763	BMA	O4-C4-C5	5.04	122.60	109.24
2	D	753	BMA	O4-C4-C5	5.07	122.69	109.24
2	D	753	BMA	O4-C4-C3	5.10	121.82	110.34
2	C	753	BMA	O3-C3-C4	5.19	122.02	110.34
4	D	763	BMA	O4-C4-C5	5.21	123.03	109.24
3	E	763	BMA	O4-C4-C5	5.39	123.52	109.24
2	F	751	NAG	C1-O5-C5	5.40	119.10	112.25
2	F	752	NAG	O4-C4-C3	5.42	122.54	110.34
2	C	753	BMA	O4-C4-C5	5.45	123.68	109.24
2	C	763	BMA	O5-C5-C6	5.47	119.18	107.35
2	E	753	BMA	O5-C5-C6	5.54	119.34	107.35
2	C	753	BMA	O5-C5-C6	5.56	119.39	107.35
2	B	763	BMA	O4-C4-C3	5.63	123.01	110.34
2	A	752	NAG	C1-O5-C5	5.72	119.51	112.25
2	F	753	BMA	O5-C5-C6	5.76	119.83	107.35
2	C	763	BMA	O3-C3-C2	5.84	120.55	110.00
2	D	753	BMA	O5-C5-C6	5.85	120.02	107.35
2	D	751	NAG	O4-C4-C3	5.87	123.55	110.34
3	F	761	NAG	C1-O5-C5	5.91	119.75	112.25
2	C	753	BMA	O4-C4-C3	5.95	123.73	110.34
2	C	764	MAN	C1-O5-C5	6.03	119.90	112.25
2	A	753	BMA	O4-C4-C3	6.04	123.93	110.34
2	A	753	BMA	O4-C4-C5	6.27	125.87	109.24
2	A	753	BMA	O5-C5-C6	6.31	121.01	107.35
2	F	753	BMA	O3-C3-C2	6.43	121.61	110.00
2	C	761	NAG	C1-O5-C5	6.61	120.64	112.25
3	E	763	BMA	O5-C5-C6	6.65	121.75	107.35
3	E	761	NAG	C1-O5-C5	6.94	121.06	112.25
3	E	762	NAG	C1-O5-C5	7.25	121.45	112.25
2	A	751	NAG	C1-O5-C5	7.62	121.92	112.25
3	E	763	BMA	O3-C3-C2	7.90	124.27	110.00
3	F	762	NAG	C1-O5-C5	7.93	122.31	112.25
2	B	763	BMA	O3-C3-C2	7.97	124.40	110.00
2	A	753	BMA	O3-C3-C2	8.00	124.44	110.00
4	D	761	NAG	C1-O5-C5	8.01	122.42	112.25
2	C	762	NAG	C1-O5-C5	8.76	123.36	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	751	NAG	C1

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Mol	Chain	Res	Type	Atom
2	F	751	NAG	C1

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	752	NAG	C8-C7-N2-C2
2	F	752	NAG	O7-C7-N2-C2
2	E	752	NAG	O7-C7-N2-C2

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	764	MAN	C1-C2-C3-C4-C5-O5
2	C	764	MAN	C1-C2-C3-C4-C5-O5
3	F	765	MAN	C1-C2-C3-C4-C5-O5
3	A	765	MAN	C1-C2-C3-C4-C5-O5
2	F	754	MAN	C1-C2-C3-C4-C5-O5

22 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	751	NAG	1	0
2	A	753	BMA	1	0
2	A	754	MAN	1	0
3	A	762	NAG	1	0
3	A	763	BMA	2	0
3	A	764	MAN	1	0
3	A	765	MAN	1	0
2	B	763	BMA	2	0
2	B	764	MAN	2	0
2	C	751	NAG	2	0
2	C	752	NAG	2	0
2	C	761	NAG	1	0
2	C	762	NAG	1	0
2	C	763	BMA	1	0
2	D	752	NAG	1	0
4	D	761	NAG	2	0
4	D	762	NAG	1	0
3	E	762	NAG	1	0
3	E	763	BMA	1	0
3	F	761	NAG	4	0
3	F	762	NAG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	765	MAN	2	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	613/750 (81%)	0.75	68 (11%)	7 6	52, 123, 277, 384	0
1	B	612/750 (81%)	0.78	69 (11%)	7 5	53, 123, 278, 384	0
1	C	612/750 (81%)	0.76	67 (10%)	7 6	53, 123, 276, 384	0
1	D	612/750 (81%)	0.81	86 (14%)	4 3	52, 123, 275, 384	0
1	E	613/750 (81%)	0.74	76 (12%)	5 4	52, 123, 278, 384	0
1	F	608/750 (81%)	0.77	76 (12%)	5 4	52, 122, 277, 377	0
All	All	3670/4500 (81%)	0.77	442 (12%)	6 5	52, 123, 278, 384	0

All (442) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	706	VAL	14.3
1	D	706	VAL	13.7
1	B	720	SER	13.7
1	C	705	HIS	13.5
1	F	705	HIS	11.9
1	E	666	CYS	11.4
1	A	705	HIS	10.9
1	A	706	VAL	10.9
1	F	714	VAL	10.7
1	D	714	VAL	10.3
1	D	705	HIS	10.2
1	D	683	ASP	10.1
1	B	706	VAL	10.0
1	E	683	ASP	9.9
1	C	698	THR	9.3
1	E	705	HIS	8.9
1	C	686	GLY	8.5
1	F	449	TRP	8.3
1	E	720	SER	8.2

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Mol	Chain	Res	Type	RSRZ
1	A	736	CYS	8.1
1	F	704	VAL	8.0
1	A	704	VAL	7.8
1	E	449	TRP	7.8
1	C	696	THR	7.6
1	E	704	VAL	7.5
1	C	689	PRO	7.3
1	E	667	THR	7.2
1	C	704	VAL	7.2
1	D	686	GLY	7.0
1	C	736	CYS	7.0
1	A	723	ALA	6.9
1	D	723	ALA	6.8
1	B	705	HIS	6.7
1	B	719	ALA	6.7
1	B	666	CYS	6.6
1	D	736	CYS	6.5
1	B	714	VAL	6.4
1	D	655	LEU	6.4
1	B	725	PHE	6.3
1	D	449	TRP	6.3
1	F	71	GLN	6.2
1	A	667	THR	6.1
1	A	686	GLY	6.1
1	D	704	VAL	6.0
1	A	727	VAL	6.0
1	F	723	ALA	5.9
1	E	706	VAL	5.9
1	B	712	VAL	5.9
1	E	71	GLN	5.8
1	B	669	SER	5.8
1	D	724	ASN	5.8
1	D	667	THR	5.7
1	B	713	THR	5.7
1	A	725	PHE	5.7
1	D	727	VAL	5.7
1	F	451	GLY	5.6
1	C	723	ALA	5.6
1	E	722	GLN	5.5
1	D	659	VAL	5.4
1	F	420	ILE	5.4
1	E	712	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	420	ILE	5.3
1	E	714	VAL	5.3
1	A	666	CYS	5.3
1	B	727	VAL	5.3
1	C	714	VAL	5.2
1	C	695	SER	5.1
1	F	667	THR	5.1
1	E	713	THR	5.0
1	B	420	ILE	5.0
1	A	740	CYS	5.0
1	F	706	VAL	5.0
1	D	451	GLY	4.9
1	C	676	ALA	4.9
1	E	716	PHE	4.8
1	C	449	TRP	4.8
1	B	726	ILE	4.7
1	E	659	VAL	4.7
1	A	420	ILE	4.7
1	E	709	LYS	4.6
1	B	683	ASP	4.5
1	A	720	SER	4.5
1	D	457	ASP	4.5
1	C	101	LEU	4.5
1	B	724	ASN	4.5
1	B	723	ALA	4.5
1	B	450	GLY	4.5
1	D	666	CYS	4.5
1	C	71	GLN	4.4
1	F	713	THR	4.4
1	E	740	CYS	4.4
1	E	658	THR	4.4
1	E	72	ASP	4.4
1	C	720	SER	4.3
1	B	716	PHE	4.3
1	C	659	VAL	4.3
1	F	668	TYR	4.3
1	F	689	PRO	4.3
1	F	676	ALA	4.2
1	B	686	GLY	4.2
1	C	671	ASP	4.2
1	F	722	GLN	4.2
1	F	712	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	696	THR	4.2
1	D	676	ALA	4.1
1	F	720	SER	4.1
1	D	739	GLU	4.1
1	A	726	ILE	4.1
1	E	255	LEU	4.0
1	F	731	GLY	4.0
1	B	668	TYR	4.0
1	C	717	SER	4.0
1	E	739	GLU	4.0
1	B	671	ASP	4.0
1	D	725	PHE	4.0
1	F	461	SER	4.0
1	E	668	TYR	4.0
1	B	721	PRO	4.0
1	E	719	ALA	4.0
1	E	724	ASN	3.9
1	D	679	GLN	3.9
1	E	723	ALA	3.9
1	A	101	LEU	3.9
1	F	432	ALA	3.9
1	F	450	GLY	3.9
1	F	673	GLY	3.9
1	F	740	CYS	3.8
1	D	713	THR	3.8
1	C	72	ASP	3.8
1	B	689	PRO	3.8
1	A	457	ASP	3.8
1	A	669	SER	3.8
1	A	713	THR	3.8
1	C	739	GLU	3.7
1	A	72	ASP	3.7
1	F	730	CYS	3.7
1	A	714	VAL	3.7
1	A	56	SER	3.7
1	D	95	SER	3.7
1	F	72	ASP	3.7
1	D	586	ALA	3.6
1	A	71	GLN	3.6
1	C	683	ASP	3.6
1	D	720	SER	3.6
1	E	717	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	715	HIS	3.6
1	D	716	PHE	3.6
1	F	426	LEU	3.5
1	A	95	SER	3.5
1	A	255	LEU	3.5
1	C	668	TYR	3.5
1	D	712	VAL	3.5
1	C	740	CYS	3.5
1	D	740	CYS	3.5
1	F	696	THR	3.5
1	B	447	PHE	3.5
1	D	671	ASP	3.5
1	C	702	SER	3.5
1	E	698	THR	3.4
1	F	678	LEU	3.5
1	E	432	ALA	3.4
1	B	739	GLU	3.4
1	F	425	SER	3.4
1	B	499	ASN	3.4
1	E	515	THR	3.4
1	F	586	ALA	3.4
1	F	736	CYS	3.4
1	C	721	PRO	3.3
1	E	113	VAL	3.3
1	D	721	PRO	3.3
1	C	731	GLY	3.3
1	F	367	VAL	3.3
1	C	419	LYS	3.3
1	A	447	PHE	3.3
1	D	469	GLU	3.3
1	C	661	CYS	3.3
1	D	722	GLN	3.2
1	A	668	TYR	3.2
1	D	69	LEU	3.2
1	F	698	THR	3.2
1	F	725	PHE	3.2
1	C	658	THR	3.2
1	E	75	VAL	3.2
1	B	704	VAL	3.2
1	B	72	ASP	3.2
1	E	727	VAL	3.2
1	C	450	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	729	LEU	3.2
1	E	457	ASP	3.1
1	B	432	ALA	3.1
1	C	679	GLN	3.1
1	A	698	THR	3.1
1	C	408	THR	3.1
1	B	426	LEU	3.1
1	C	699	LEU	3.1
1	C	725	PHE	3.1
1	D	515	THR	3.1
1	D	707	LEU	3.1
1	B	419	LYS	3.0
1	F	659	VAL	3.0
1	A	504	LEU	3.0
1	B	113	VAL	3.0
1	D	450	GLY	3.0
1	D	432	ALA	3.0
1	D	726	ILE	3.0
1	F	360	GLY	3.0
1	A	113	VAL	3.0
1	B	698	THR	3.0
1	B	29	VAL	2.9
1	B	71	GLN	2.9
1	C	724	ASN	2.9
1	C	666	CYS	2.9
1	E	669	SER	2.9
1	D	445	TYR	2.9
1	E	450	GLY	2.9
1	B	462	GLN	2.9
1	F	95	SER	2.9
1	A	449	TRP	2.9
1	C	591	VAL	2.9
1	F	29	VAL	2.9
1	D	97	LYS	2.8
1	C	69	LEU	2.8
1	E	418	PRO	2.8
1	D	29	VAL	2.8
1	F	31	ILE	2.8
1	A	421	LYS	2.8
1	B	45	ILE	2.8
1	B	83	ILE	2.8
1	D	735	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	96	TYR	2.8
1	B	70	LYS	2.8
1	E	673	GLY	2.8
1	F	575	ALA	2.8
1	E	119	ASN	2.8
1	A	575	ALA	2.8
1	F	739	GLU	2.8
1	C	367	VAL	2.8
1	E	671	ASP	2.8
1	D	715	HIS	2.8
1	C	713	THR	2.8
1	B	27	SER	2.8
1	E	674	GLY	2.7
1	B	367	VAL	2.7
1	A	739	GLU	2.7
1	A	734	THR	2.7
1	F	719	ALA	2.7
1	B	737	ASN	2.7
1	D	493	LEU	2.7
1	C	283	ILE	2.7
1	E	736	CYS	2.7
1	F	27	SER	2.7
1	F	671	ASP	2.7
1	E	679	GLN	2.7
1	A	724	ASN	2.7
1	C	422	CYS	2.7
1	F	457	ASP	2.7
1	B	101	LEU	2.7
1	E	408	THR	2.7
1	D	388	ASN	2.7
1	C	407	ILE	2.6
1	B	649	ARG	2.6
1	B	718	THR	2.6
1	C	655	LEU	2.6
1	E	493	LEU	2.6
1	E	672	PHE	2.6
1	A	683	ASP	2.6
1	B	722	GLN	2.6
1	F	75	VAL	2.6
1	D	113	VAL	2.6
1	B	679	GLN	2.6
1	B	457	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	716	PHE	2.6
1	B	736	CYS	2.6
1	B	461	SER	2.6
1	A	31	ILE	2.6
1	D	734	THR	2.6
1	F	636	ILE	2.6
1	D	640	ILE	2.6
1	D	668	TYR	2.6
1	E	431	ALA	2.6
1	D	678	LEU	2.5
1	A	97	LYS	2.5
1	F	97	LYS	2.5
1	F	26	PHE	2.5
1	B	703	THR	2.5
1	B	451	GLY	2.5
1	A	712	VAL	2.5
1	E	721	PRO	2.5
1	D	452	ALA	2.5
1	C	421	LYS	2.5
1	A	737	ASN	2.5
1	E	407	ILE	2.5
1	B	728	SER	2.5
1	E	689	PRO	2.5
1	D	565	ALA	2.5
1	E	101	LEU	2.5
1	A	674	GLY	2.5
1	C	563	ILE	2.5
1	D	657	SER	2.5
1	F	119	ASN	2.5
1	F	283	ILE	2.5
1	A	678	LEU	2.5
1	B	418	PRO	2.5
1	E	661	CYS	2.5
1	D	636	ILE	2.4
1	D	698	THR	2.4
1	A	455	PHE	2.4
1	C	672	PHE	2.4
1	F	388	ASN	2.4
1	E	419	LYS	2.4
1	C	678	LEU	2.4
1	F	10	SER	2.4
1	D	695	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	283	ILE	2.4
1	E	45	ILE	2.4
1	E	686	GLY	2.4
1	D	731	GLY	2.4
1	D	129	LYS	2.4
1	F	418	PRO	2.4
1	B	628	ALA	2.4
1	B	7	THR	2.4
1	E	680	TYR	2.4
1	E	678	LEU	2.4
1	A	418	PRO	2.4
1	D	328	TYR	2.4
1	F	464	SER	2.4
1	F	419	LYS	2.4
1	A	445	TYR	2.4
1	D	71	GLN	2.4
1	A	450	GLY	2.3
1	D	75	VAL	2.3
1	E	97	LYS	2.3
1	E	575	ALA	2.3
1	F	408	THR	2.3
1	C	29	VAL	2.3
1	F	113	VAL	2.3
1	B	495	ILE	2.3
1	E	49	ALA	2.3
1	B	95	SER	2.3
1	B	693	HIS	2.3
1	F	686	GLY	2.3
1	A	367	VAL	2.3
1	D	391	ILE	2.3
1	E	447	PHE	2.3
1	A	657	SER	2.3
1	A	388	ASN	2.3
1	D	83	ILE	2.3
1	D	101	LEU	2.3
1	D	647	PHE	2.3
1	D	696	THR	2.3
1	E	10	SER	2.3
1	D	526	ILE	2.3
1	D	72	ASP	2.3
1	B	515	THR	2.3
1	B	731	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	420	ILE	2.3
1	D	656	VAL	2.3
1	D	7	THR	2.3
1	A	733	LYS	2.3
1	F	653	ALA	2.3
1	D	26	PHE	2.3
1	C	94	LEU	2.2
1	F	703	THR	2.2
1	C	680	TYR	2.2
1	A	722	GLN	2.2
1	F	733	LYS	2.2
1	B	699	LEU	2.2
1	E	623	VAL	2.2
1	E	47	THR	2.2
1	F	716	PHE	2.2
1	A	96	TYR	2.2
1	A	78	GLY	2.2
1	B	119	ASN	2.2
1	E	711	ALA	2.2
1	C	378	LEU	2.2
1	E	657	SER	2.2
1	C	113	VAL	2.2
1	D	412	THR	2.2
1	C	586	ALA	2.2
1	F	69	LEU	2.2
1	F	623	VAL	2.2
1	E	275	ASN	2.2
1	E	665	GLU	2.2
1	F	407	ILE	2.2
1	F	495	ILE	2.2
1	D	658	THR	2.2
1	E	499	ASN	2.2
1	C	623	VAL	2.2
1	F	328	TYR	2.2
1	C	470	LEU	2.2
1	D	717	SER	2.2
1	D	31	ILE	2.2
1	D	407	ILE	2.2
1	F	391	ILE	2.2
1	A	26	PHE	2.1
1	A	83	ILE	2.1
1	D	623	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	407	ILE	2.1
1	C	712	VAL	2.1
1	E	464	SER	2.1
1	C	733	LYS	2.1
1	C	431	ALA	2.1
1	E	7	THR	2.1
1	A	586	ALA	2.1
1	D	660	LYS	2.1
1	C	95	SER	2.1
1	D	408	THR	2.1
1	C	565	ALA	2.1
1	F	709	LYS	2.1
1	C	31	ILE	2.1
1	A	7	THR	2.1
1	A	565	ALA	2.1
1	D	572	ASP	2.1
1	A	642	ILE	2.1
1	E	367	VAL	2.1
1	E	283	ILE	2.1
1	F	422	CYS	2.1
1	A	518	ASP	2.1
1	A	703	THR	2.1
1	B	449	TRP	2.1
1	C	700	GLN	2.1
1	D	111	VAL	2.1
1	F	729	LEU	2.1
1	D	638	ILE	2.1
1	A	426	LEU	2.1
1	E	69	LEU	2.0
1	A	481	ALA	2.0
1	E	415	VAL	2.0
1	F	440	VAL	2.0
1	F	726	ILE	2.0
1	E	532	PRO	2.0
1	A	729	LEU	2.0
1	C	255	LEU	2.0
1	F	295	LEU	2.0
1	D	27	SER	2.0
1	B	623	VAL	2.0
1	B	678	LEU	2.0
1	B	729	LEU	2.0
1	C	729	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	95	SER	2.0
1	A	460	ASN	2.0
1	A	530	PHE	2.0

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

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

6.3 Carbohydrates (i)

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MAN	B	754	11/12	0.72	0.59	2.08	164,189,195,195	0
2	MAN	E	754	11/12	0.89	0.52	1.75	191,196,204,207	0
2	MAN	D	754	11/12	0.83	0.38	0.57	176,185,193,194	0
2	MAN	A	754	11/12	0.70	0.31	0.17	225,228,240,247	0
2	MAN	C	754	11/12	0.76	0.31	-0.09	177,187,197,202	0
2	MAN	F	754	11/12	0.85	0.21	-0.71	185,192,197,199	0
2	NAG	F	751	14/15	0.88	0.18	-1.23	78,105,124,134	0
2	NAG	D	751	14/15	0.91	0.17	-1.42	92,103,130,136	0
2	NAG	C	751	14/15	0.90	0.18	-1.61	92,108,127,134	0
2	NAG	B	751	14/15	0.92	0.18	-1.63	91,98,122,133	0
2	NAG	A	751	14/15	0.92	0.15	-2.10	77,100,126,131	0
2	NAG	E	751	14/15	0.90	0.14	-2.28	93,108,125,132	0
3	NAG	F	762	14/15	0.77	0.14	-	199,205,211,212	0
3	MAN	E	765	11/12	0.71	0.26	-	193,208,213,216	0
3	NAG	E	762	14/15	0.75	0.18	-	189,205,217,222	0
3	MAN	A	764	11/12	0.57	0.48	-	176,202,226,228	0
2	NAG	C	761	14/15	0.84	0.17	-	127,150,176,205	0
2	BMA	D	753	11/12	0.80	0.23	-	176,190,223,224	0
2	NAG	B	752	14/15	0.86	0.23	-	113,130,175,175	0
3	BMA	F	763	11/12	0.77	0.17	-	195,209,234,236	0
2	BMA	B	753	11/12	0.83	0.20	-	185,193,201,201	0
2	BMA	C	763	11/12	0.53	0.22	-	138,178,231,243	0
3	BMA	E	763	11/12	0.70	0.18	-	195,214,225,225	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	BMA	D	763	11/12	0.75	0.21	-	176,193,202,203	0
3	MAN	A	765	11/12	0.67	0.31	-	174,195,201,207	0
2	NAG	B	762	14/15	0.74	0.20	-	165,190,204,219	0
2	MAN	C	764	11/12	0.59	0.26	-	248,250,254,260	0
2	MAN	B	764	11/12	0.64	0.34	-	244,259,266,268	0
2	BMA	C	753	11/12	0.87	0.13	-	159,180,190,193	0
2	NAG	A	752	14/15	0.84	0.21	-	113,136,144,151	0
3	MAN	F	764	11/12	0.76	0.30	-	241,253,263,265	0
3	MAN	E	764	11/12	0.83	0.29	-	114,174,187,188	0
2	BMA	A	753	11/12	0.89	0.21	-	165,169,197,213	0
3	MAN	F	765	11/12	0.39	0.31	-	209,236,246,247	0
2	NAG	C	752	14/15	0.82	0.33	-	124,164,186,188	0
2	NAG	C	762	14/15	0.70	0.23	-	218,236,246,251	0
2	NAG	B	761	14/15	0.82	0.21	-	144,161,170,183	0
3	NAG	A	761	14/15	0.91	0.19	-	138,164,178,204	0
4	NAG	D	762	14/15	0.84	0.18	-	184,194,201,202	0
2	NAG	F	752	14/15	0.87	0.24	-	98,134,160,166	0
3	NAG	F	761	14/15	0.87	0.16	-	129,152,172,190	0
4	NAG	D	761	14/15	0.82	0.20	-	154,177,186,194	0
2	NAG	D	752	14/15	0.86	0.25	-	110,131,162,178	0
2	BMA	F	753	11/12	0.84	0.19	-	137,172,188,193	0
3	BMA	A	763	11/12	0.63	0.24	-	194,229,252,253	0
3	NAG	A	762	14/15	0.59	0.25	-	218,228,238,243	0
2	NAG	E	752	14/15	0.93	0.18	-	113,124,164,165	0
2	BMA	E	753	11/12	0.84	0.14	-	173,180,196,200	0
3	NAG	E	761	14/15	0.75	0.24	-	144,163,174,188	0
2	BMA	B	763	11/12	0.80	0.18	-	234,243,255,256	0

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.