



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:27 PM UTC

PDB ID : 2W0C / pdb_00002w0c
Title : X-ray structure of the entire lipid-containing bacteriophage PM2
Authors : Abrescia, N.G.A.; Grimes, J.M.; Kivela, H.M.; Assenberg, R.; Sutton, G.C.;
Butcher, S.J.; Bamford, J.K.H.; Bamford, D.H.; Stuart, D.I.
Deposited on : 2008-08-13
Resolution : 7.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

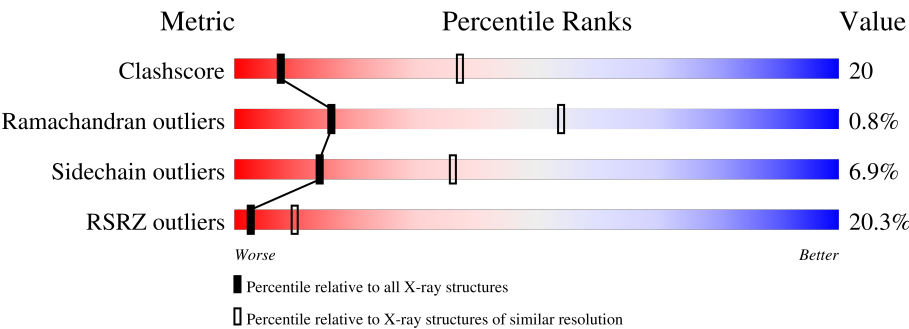
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 7.00 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))
Clashscore	190562	1007 (9.70-4.04)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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

Mol	Chain	Length	Quality of chain
1	A	269	24% 66% 31%
1	B	269	23% 65% 32%
1	C	269	16% 67% 31%
1	D	269	22% 67% 30%
1	E	269	23% 64% 33%
1	F	269	11% 66% 32%
1	G	269	24% 66% 31%

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Mol	Chain	Length	Quality of chain
1	H	269	
1	I	269	
1	J	269	
2	L	335	
3	P	104	
3	Q	104	
3	R	104	
3	S	104	
4	T	127	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26447 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 MAJOR CAPSID PROTEIN P2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	B	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	C	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	D	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	E	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	F	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	G	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	H	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	I	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	J	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			

- Molecule 2 is a protein called PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	335	Total	C	N	O	S	0	0	0
			2634	1660	439	529	6			

- Molecule 3 is a protein called PROTEIN P3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	65	Total	C	N	O	S	0	0	0
			451	275	82	92	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Q	60	Total	C	N	O	S	0	0	0
			432	265	77	89	1			
3	R	63	Total	C	N	O	S	0	0	0
			453	280	80	92	1			
3	S	84	Total	C	N	O	S	0	0	0
			608	386	107	113	2			

- Molecule 4 is a protein called PROTEIN P6.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	T	127	Total	C	N	O	0	0	0
			628	374	127	127			

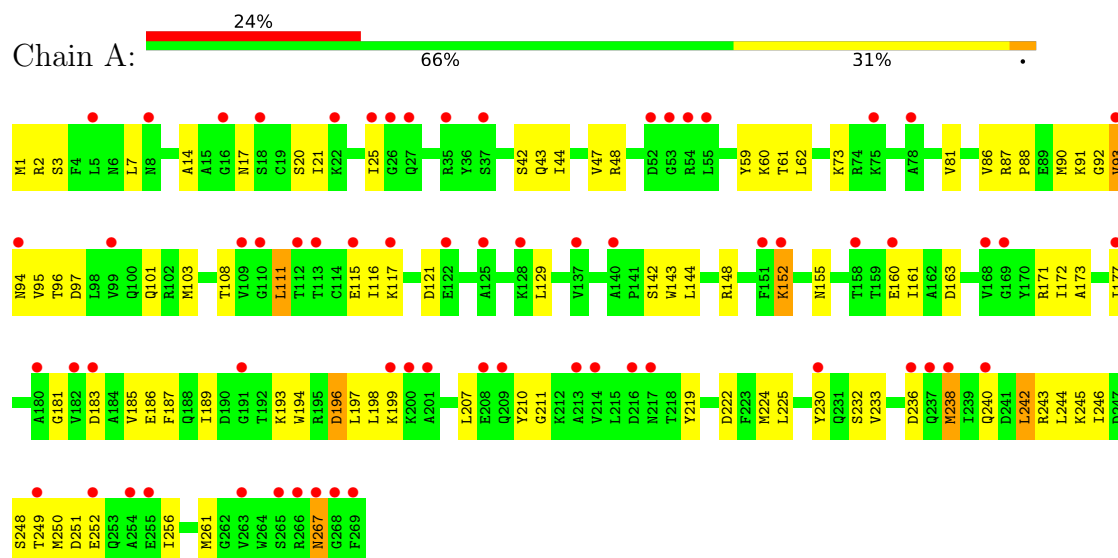
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	E	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		
5	G	1	Total	Ca	0	0
			1	1		
5	H	1	Total	Ca	0	0
			1	1		
5	I	1	Total	Ca	0	0
			1	1		
5	J	1	Total	Ca	0	0
			1	1		
5	L	1	Total	Ca	0	0
			1	1		

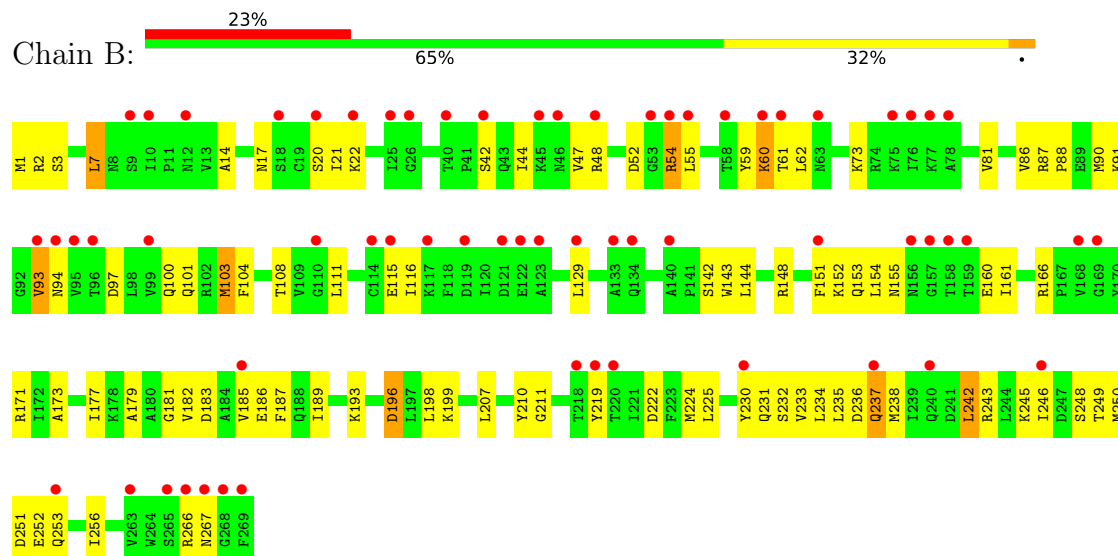
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: MAJOR CAPSID PROTEIN P2

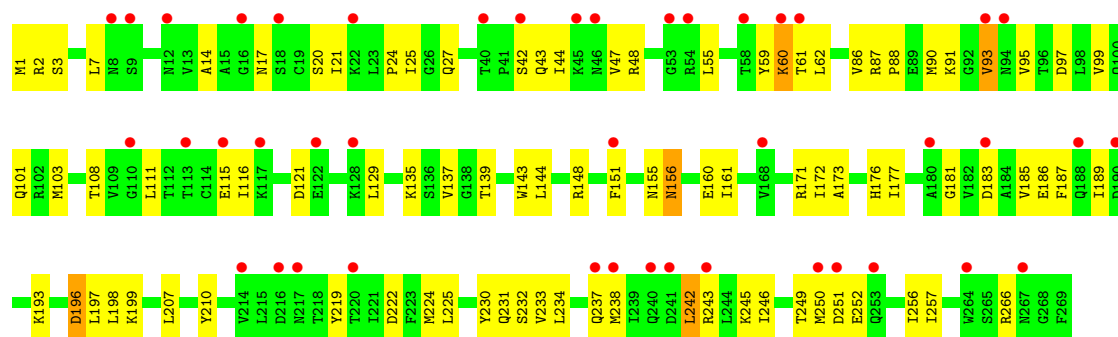


• Molecule 1: MAJOR CAPSID PROTEIN P2

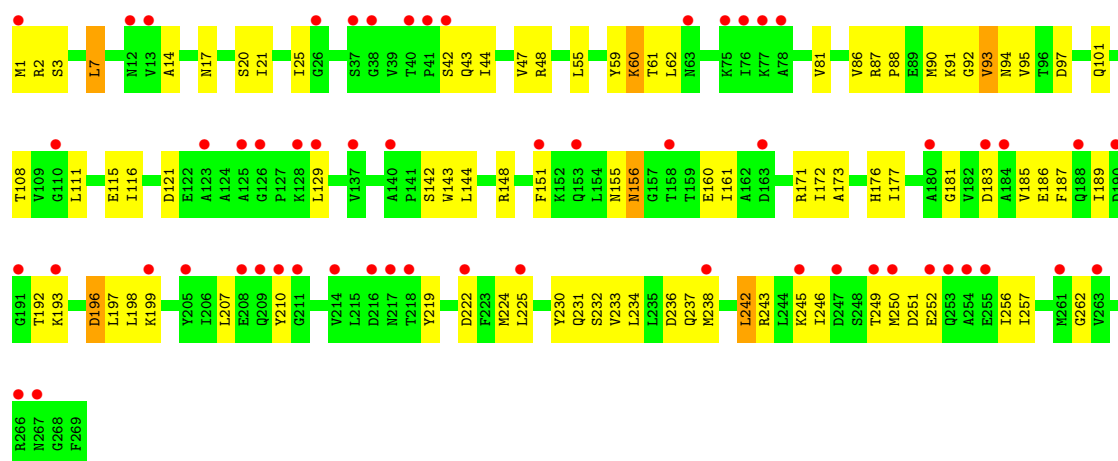


• Molecule 1: MAJOR CAPSID PROTEIN P2

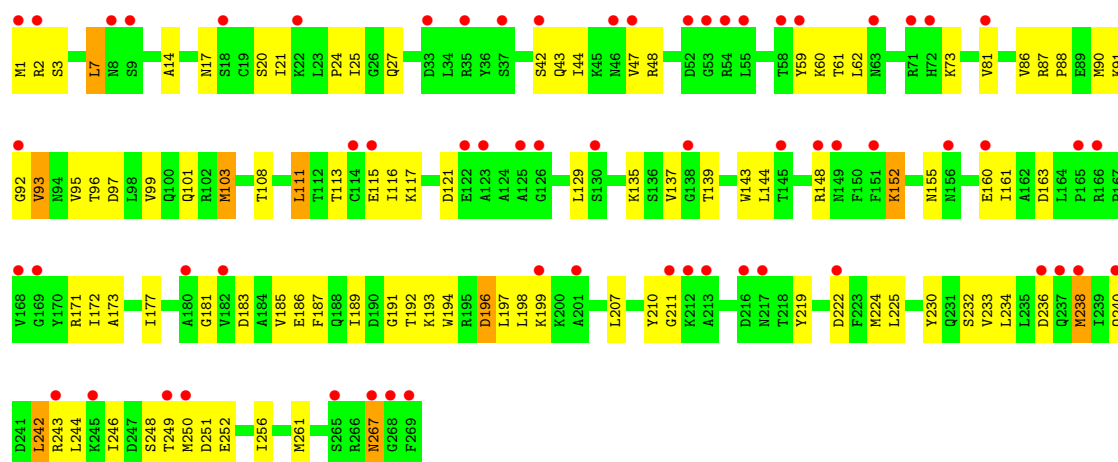




• Molecule 1: MAJOR CAPSID PROTEIN P2

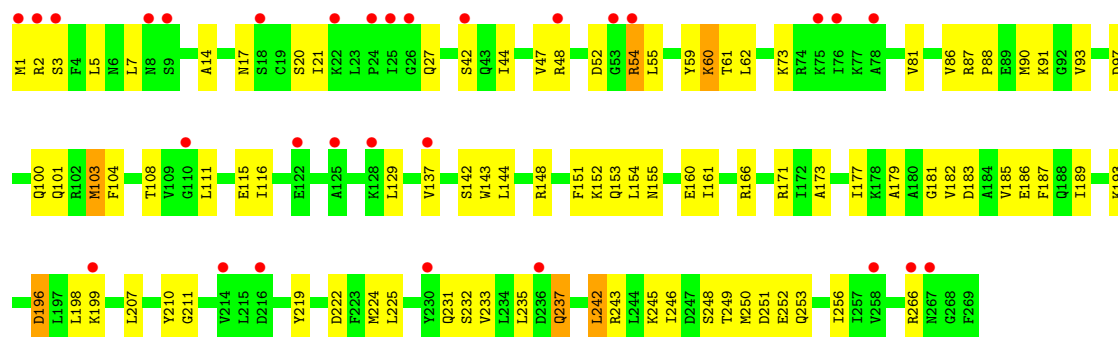


• Molecule 1: MAJOR CAPSID PROTEIN P2

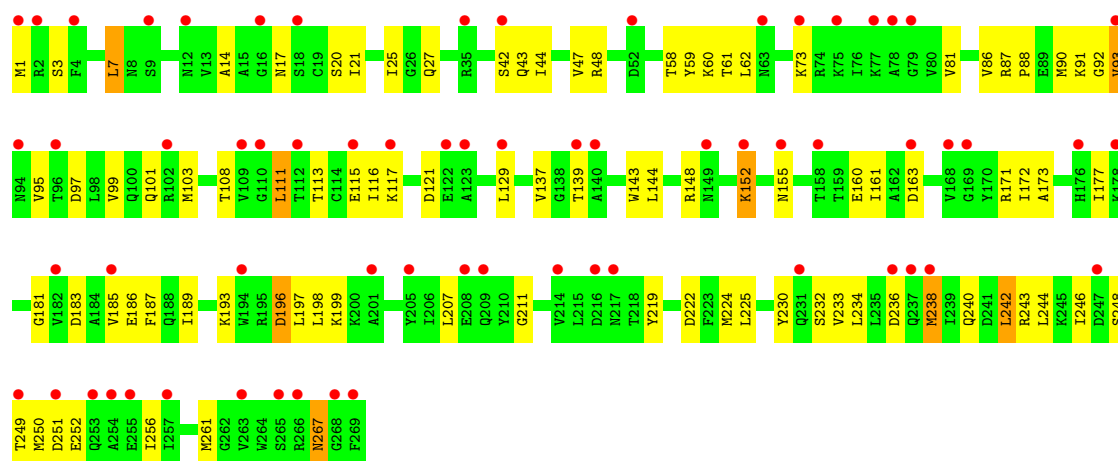


• Molecule 1: MAJOR CAPSID PROTEIN P2

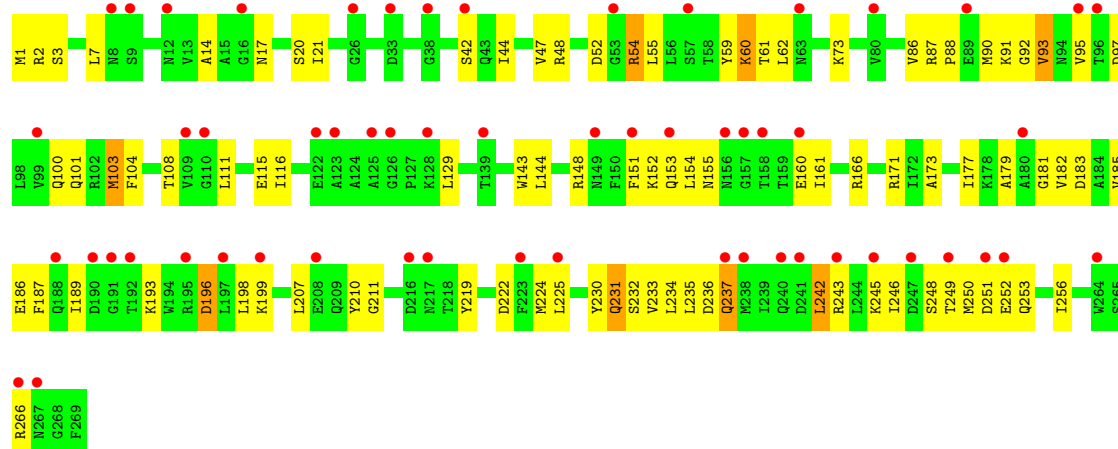




• Molecule 1: MAJOR CAPSID PROTEIN P2

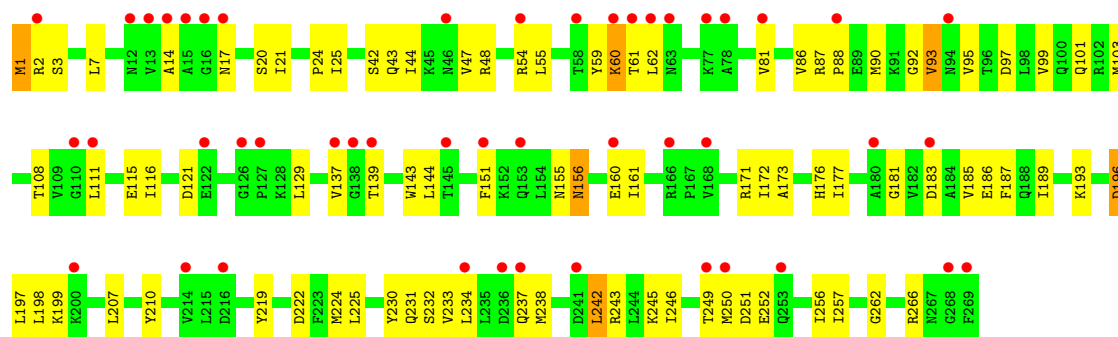


• Molecule 1: MAJOR CAPSID PROTEIN P2

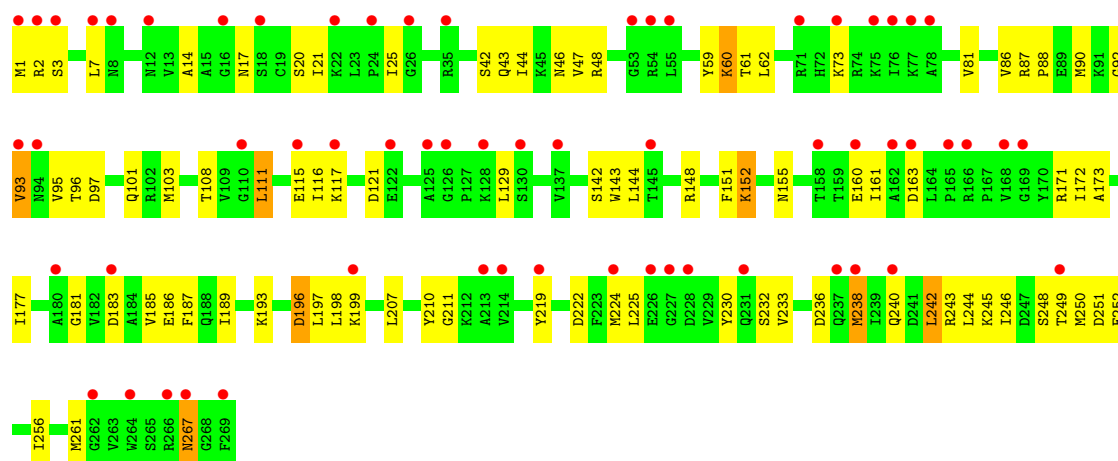


• Molecule 1: MAJOR CAPSID PROTEIN P2

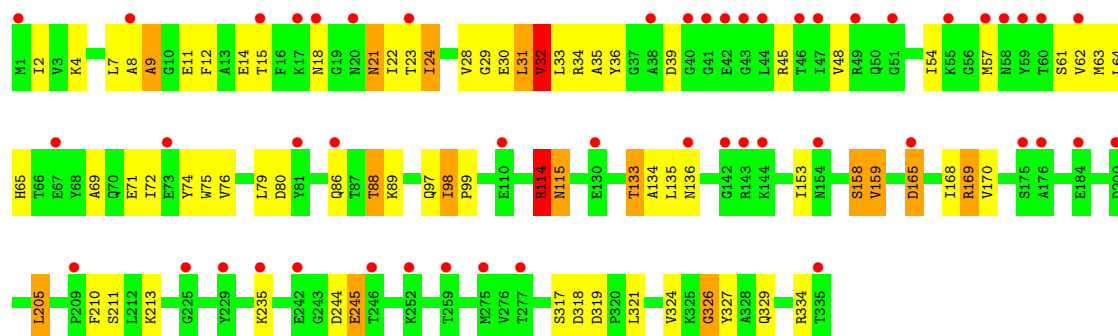
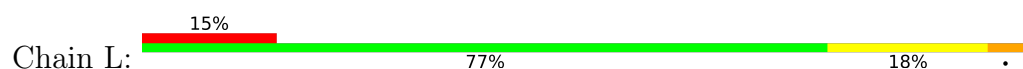




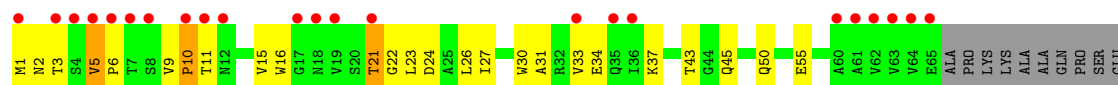
• Molecule 1: MAJOR CAPSID PROTEIN P2



• Molecule 2: PROTEIN 2

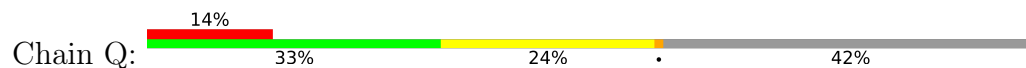


• Molecule 3: PROTEIN P3



THR
LEU
VAL
PHE
SER
GLY
VAL
PRO
GLN
LYS
THR
LEU
LEU
LEU
GLY
GLY
PHE
GLY
GLY
LEU
VAL
LEU
GLY
LEU
VAL
MET
ARG
GLY
ASN
LYS

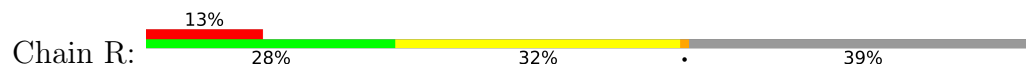
• Molecule 3: PROTEIN P3



MET ASN THR SER VAL PRO T7 S8 V9 P10 T11 N12 W16 G17 N18 T21 G22 L23 D24 I27 S28 PHE G29 W30 A31 R32 V33 E34 Q35 T36 K37 A38 A39 K40 A41 S42 T43 G44 Q45 G46 R47 V48 E49 Q50 T53 P54 E55 L56 D57 N58 G59 A60 V63 V64 E65 A66

PRO LYS LYS ALA ALA PRO SER GLU THR LEU LEU VAL PHE GLY VAL PRO GLN LYS THR LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LYS

• Molecule 3: PROTEIN P3



MET ASN THR SER V5 P6 V9 N12 Q13 S14 W16 G17 N18 V19 S20 T21 G22 L23 D24 A25 L26 I27 S28 G29 W30 A31 R32 V33 E34 Q35 T36 K37 A41 S42 T43 G44 Q45 G46 R47 V48 E49 Q50 A51 M52 E55 L56 D57 A61 V62 V63 V64 E65 A66 P67

LYS LYS ALA ALA PRO SER GLU THR LEU LEU VAL PHE GLY VAL PRO GLN LYS THR LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LYS

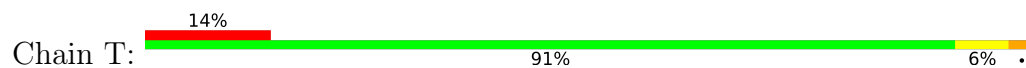
• Molecule 3: PROTEIN P3



MET ASN THR SER VAL PRO THR SER VAL PRO THR VAL THR ASN GLN SER SER TRP GLY ASN VAL SER T21 L23 D24 A25 L26 I27 W30 A31 R32 V33 E34 Q35 T36 K37 A38 A41 S42 T43 G44 Q45 G46 R47 V48 E49 Q50 A51 M52 E55 L56 D57 V62 V63 V64 E65 A66

P67 K68 K69 A70 A71 Q72 P73 S74 E75 T76 L77 V78 W81 P82 Q83 K84 L87 L88 G89 F90 G91 G92 G93 L94 L95 L96 G97 L98 H103 K104

• Molecule 4: PROTEIN P6



W1 A2 N3 K34 P35 I36 A37 D38 F39 P56 N57 D69 D76 A80 H85 E94 I95 L96 D97 H98 E99 R100 R101 P104 A116 S117 T118 A122 S123 G124 V125 E126 L127

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	946.90Å 677.60Å 1067.60Å 90.00° 102.90° 90.00°	Depositor
Resolution (Å)	96.00 – 7.00 96.00 – 7.00	Depositor EDS
% Data completeness (in resolution range)	82.9 (96.00-7.00) 82.9 (96.00-7.00)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 6.73Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.419 , (Not available) 0.466 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	132.6	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.36	EDS
Total number of atoms	26447	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	2/2158 (0.1%)	0.73	1/2917 (0.0%)
1	B	0.29	0/2158	0.73	0/2917
1	C	0.33	1/2158 (0.0%)	0.75	1/2917 (0.0%)
1	D	0.33	1/2158 (0.0%)	0.75	1/2917 (0.0%)
1	E	0.35	2/2158 (0.1%)	0.73	1/2917 (0.0%)
1	F	0.29	0/2158	0.73	0/2917
1	G	0.35	2/2158 (0.1%)	0.73	1/2917 (0.0%)
1	H	0.29	0/2158	0.72	0/2917
1	I	0.33	1/2158 (0.0%)	0.75	1/2917 (0.0%)
1	J	0.35	2/2158 (0.1%)	0.73	1/2917 (0.0%)
2	L	1.21	5/2688 (0.2%)	1.16	19/3646 (0.5%)
3	P	0.46	0/457	0.72	0/624
3	Q	0.42	0/437	0.67	0/596
3	R	0.45	0/460	0.68	0/630
3	S	0.45	0/615	0.73	0/831
4	T	0.49	0/627	0.97	3/872 (0.3%)
All	All	0.50	16/26864 (0.1%)	0.79	29/36369 (0.1%)

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
2	L	0	5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	169	ARG	C-N	49.53	1.94	1.33
2	L	324	VAL	C-N	19.70	1.63	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	111	LEU	CG-CD1	-6.13	1.32	1.52
1	J	111	LEU	CG-CD1	-6.13	1.32	1.52
1	G	111	LEU	CG-CD1	-6.12	1.32	1.52
1	A	111	LEU	CG-CD1	-6.11	1.32	1.52
1	D	155	ASN	C-O	5.74	1.31	1.23
1	I	155	ASN	C-O	5.70	1.31	1.23
1	C	155	ASN	C-O	5.65	1.31	1.23
2	L	134	ALA	CA-CB	-5.52	1.49	1.53
1	G	111	LEU	CG-CD2	-5.30	1.35	1.52
1	A	111	LEU	CG-CD2	-5.29	1.35	1.52
1	J	111	LEU	CG-CD2	-5.29	1.35	1.52
1	E	111	LEU	CG-CD2	-5.28	1.35	1.52
2	L	133	THR	C-O	-5.22	1.17	1.23
2	L	21	ASN	CG-OD1	5.11	1.33	1.23

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	169	ARG	O-C-N	-30.41	87.56	122.84
2	L	115	ASN	N-CA-C	15.31	136.62	111.37
2	L	98	ILE	CA-C-N	14.87	138.43	119.84
2	L	98	ILE	C-N-CA	14.87	138.43	119.84
2	L	169	ARG	CA-C-N	12.43	141.71	122.70
2	L	169	ARG	C-N-CA	12.43	141.71	122.70
2	L	159	VAL	N-CA-C	10.55	124.92	108.89
2	L	324	VAL	O-C-N	-10.45	111.56	122.63
2	L	165	ASP	O-C-N	-10.31	108.89	122.19
2	L	165	ASP	CA-C-N	8.50	133.89	122.84
2	L	165	ASP	C-N-CA	8.50	133.89	122.84
2	L	326	GLY	N-CA-C	-8.20	101.29	112.52
1	A	111	LEU	CD1-CG-CD2	-7.36	94.61	110.80
1	G	111	LEU	CD1-CG-CD2	-7.35	94.62	110.80
1	E	111	LEU	CD1-CG-CD2	-7.35	94.64	110.80
1	J	111	LEU	CD1-CG-CD2	-7.34	94.64	110.80
2	L	114	ARG	CA-C-N	7.12	131.50	120.82
2	L	114	ARG	C-N-CA	7.12	131.50	120.82
4	T	35	PRO	N-CA-CB	6.50	110.08	103.25
4	T	56	PRO	N-CA-CB	6.14	110.32	103.44
4	T	104	PRO	N-CA-CB	6.06	110.23	103.44
2	L	158	SER	N-CA-C	-5.87	101.62	110.24
2	L	327	TYR	N-CA-C	-5.72	97.67	107.23
2	L	88	THR	CB-CA-C	-5.58	109.04	117.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	156	ASN	N-CA-C	-5.44	98.36	107.99
1	I	156	ASN	N-CA-C	-5.42	98.39	107.99
1	D	156	ASN	N-CA-C	-5.41	98.42	107.99
2	L	324	VAL	CA-C-N	5.36	132.65	121.94
2	L	324	VAL	C-N-CA	5.36	132.65	121.94

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	114	ARG	Peptide
2	L	158	SER	Peptide
2	L	165	ASP	Mainchain
2	L	326	GLY	Peptide
2	L	98	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2123	0	2155	99	0
1	B	2123	0	2156	85	0
1	C	2123	0	2155	127	0
1	D	2123	0	2156	71	0
1	E	2123	0	2153	149	0
1	F	2123	0	2156	66	0
1	G	2123	0	2153	105	0
1	H	2123	0	2156	84	0
1	I	2123	0	2154	126	0
1	J	2123	0	2154	58	0
2	L	2634	0	2479	80	0
3	P	451	0	425	94	0
3	Q	432	0	425	114	0
3	R	453	0	443	144	0
3	S	608	0	641	134	0
4	T	628	0	311	4	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
All	All	26447	0	26272	1061	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 20.

All (1061) 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:A:230:TYR:CE1	3:P:1:MET:HG2	1.24	1.70
1:A:230:TYR:CZ	3:P:1:MET:HG2	1.32	1.59
1:E:113:THR:HG21	3:S:56:LEU:CD2	1.37	1.50
1:A:230:TYR:CE1	3:P:1:MET:CG	1.92	1.47
1:D:234:LEU:H	3:R:47:ARG:NH1	1.10	1.47
1:E:113:THR:CG2	3:S:56:LEU:CD2	1.88	1.47
1:C:230:TYR:CE1	3:Q:27:ILE:HD12	1.50	1.46
1:C:230:TYR:CZ	3:Q:27:ILE:HD13	1.53	1.42
1:C:230:TYR:CE1	3:Q:27:ILE:CD1	2.01	1.41
1:C:230:TYR:CZ	3:Q:27:ILE:CD1	2.02	1.41
1:H:233:VAL:HA	3:S:47:ARG:NH1	1.32	1.41
1:B:234:LEU:H	3:Q:47:ARG:NH1	1.06	1.40
1:A:193:LYS:NZ	1:I:54:ARG:HH12	0.92	1.40
1:A:193:LYS:NZ	1:I:54:ARG:NH1	1.67	1.39
1:C:103:MET:HE2	3:Q:30:TRP:CB	1.52	1.39
1:I:139:THR:CG2	3:S:37:LYS:NZ	1.85	1.38
1:A:230:TYR:CZ	3:P:1:MET:CG	2.04	1.38
1:E:171:ARG:HE	3:R:23:LEU:CD2	1.38	1.34
1:A:193:LYS:HZ1	1:I:54:ARG:NH1	1.22	1.32
1:H:234:LEU:HD23	3:S:44:GLY:N	1.41	1.31
1:A:230:TYR:CD1	3:P:1:MET:HE2	1.65	1.30
1:H:233:VAL:CA	3:S:47:ARG:HH12	1.40	1.30
1:E:113:THR:CG2	3:S:56:LEU:HD21	1.57	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:LEU:N	3:R:47:ARG:NH1	1.83	1.27
1:C:139:THR:HG21	3:Q:37:LYS:NZ	1.48	1.26
1:E:113:THR:CG2	3:S:56:LEU:HD22	1.53	1.26
1:B:234:LEU:N	3:Q:47:ARG:HH12	1.30	1.26
1:B:236:ASP:OD2	3:Q:44:GLY:HA3	1.28	1.26
1:I:139:THR:HG21	3:S:37:LYS:NZ	0.95	1.26
1:I:95:VAL:HG11	3:S:31:ALA:CB	1.64	1.25
2:L:169:ARG:C	2:L:170:VAL:N	1.94	1.25
1:A:230:TYR:CE1	3:P:1:MET:SD	2.28	1.25
1:I:230:TYR:OH	3:S:27:ILE:HG21	1.37	1.24
1:C:230:TYR:OH	3:Q:27:ILE:CD1	1.84	1.24
1:E:194:TRP:NE1	3:R:16:TRP:CZ3	1.72	1.23
1:I:99:VAL:O	3:S:34:GLU:OE2	1.54	1.22
1:I:230:TYR:OH	3:S:27:ILE:CG2	1.86	1.21
1:E:143:TRP:N	3:R:30:TRP:CZ2	2.07	1.20
1:C:135:LYS:HZ1	3:Q:55:GLU:CD	1.49	1.20
1:C:135:LYS:NZ	3:Q:55:GLU:OE2	1.74	1.20
1:C:230:TYR:OH	3:Q:27:ILE:HG21	1.41	1.20
1:A:230:TYR:OH	3:P:1:MET:HA	1.42	1.19
1:C:135:LYS:NZ	3:Q:55:GLU:CD	1.98	1.19
1:B:234:LEU:N	3:Q:47:ARG:NH1	1.87	1.18
1:B:238:MET:SD	3:P:16:TRP:HZ2	1.66	1.17
1:E:135:LYS:NZ	3:R:55:GLU:CD	2.03	1.17
1:I:24:PRO:CB	3:S:55:GLU:HB3	1.72	1.17
1:C:103:MET:HE2	3:Q:30:TRP:HB3	1.23	1.16
1:E:171:ARG:NE	3:R:23:LEU:CD2	2.09	1.15
1:E:171:ARG:HE	3:R:23:LEU:HD23	1.06	1.15
1:A:230:TYR:CD1	3:P:1:MET:CE	2.29	1.15
1:C:95:VAL:HG11	3:Q:31:ALA:HB2	1.25	1.15
1:H:230:TYR:CD1	3:S:42:SER:HA	1.80	1.15
1:E:113:THR:HG22	3:S:56:LEU:HD22	1.21	1.14
1:G:171:ARG:HE	3:P:23:LEU:HD23	1.13	1.13
1:D:234:LEU:N	3:R:47:ARG:HH12	1.42	1.12
1:A:193:LYS:HZ1	1:I:54:ARG:CZ	1.60	1.12
1:C:103:MET:CE	3:Q:30:TRP:C	2.23	1.11
1:J:151:PHE:HB3	2:L:11:GLU:OE1	1.49	1.11
1:I:103:MET:HG3	3:S:34:GLU:OE2	1.48	1.10
1:A:230:TYR:CE1	3:P:1:MET:HE2	1.86	1.10
1:C:230:TYR:OH	3:Q:27:ILE:CG2	2.00	1.10
1:A:230:TYR:OH	3:P:1:MET:CB	2.00	1.10
1:A:230:TYR:OH	3:P:1:MET:CA	2.00	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:230:TYR:HD1	3:S:42:SER:HA	1.04	1.09
1:I:24:PRO:HB3	3:S:55:GLU:HB3	1.30	1.09
1:H:171:ARG:NH2	3:S:42:SER:O	1.87	1.08
1:C:24:PRO:HB2	3:Q:55:GLU:HB3	1.29	1.08
1:D:234:LEU:H	3:R:47:ARG:CZ	1.67	1.08
1:E:24:PRO:HB2	3:R:55:GLU:HB3	1.19	1.08
1:A:230:TYR:OH	3:P:1:MET:HG2	1.52	1.07
1:G:95:VAL:HG11	3:P:31:ALA:HB2	1.08	1.07
1:A:230:TYR:CE1	3:P:1:MET:CE	2.38	1.07
1:C:103:MET:HE2	3:Q:30:TRP:C	1.79	1.06
1:G:95:VAL:CG1	3:P:31:ALA:HB2	1.85	1.06
1:B:115:GLU:OE1	3:R:56:LEU:HD23	1.56	1.05
1:B:183:ASP:OD2	1:B:249:THR:CG2	2.07	1.03
1:C:230:TYR:OH	3:Q:27:ILE:CB	2.06	1.03
1:C:95:VAL:HG11	3:Q:31:ALA:CB	1.88	1.03
1:F:183:ASP:OD2	1:F:249:THR:CG2	2.07	1.03
1:C:99:VAL:O	3:Q:34:GLU:OE2	1.77	1.03
1:E:24:PRO:CB	3:R:55:GLU:HB3	1.87	1.03
1:H:183:ASP:OD2	1:H:249:THR:CG2	2.07	1.03
1:I:95:VAL:HG11	3:S:31:ALA:HB1	1.06	1.02
1:H:234:LEU:CD2	3:S:44:GLY:N	2.21	1.02
1:B:94:ASN:HD21	3:Q:35:GLN:HG2	1.24	1.01
1:C:24:PRO:CB	3:Q:55:GLU:HB3	1.90	1.01
1:I:95:VAL:CG1	3:S:31:ALA:HB1	1.90	1.01
1:G:189:ILE:HG12	1:G:242:LEU:HD22	1.43	1.01
1:J:189:ILE:HG12	1:J:242:LEU:HD22	1.42	1.01
1:A:194:TRP:CH2	3:R:65:GLU:OE2	2.14	1.00
1:A:230:TYR:HD1	3:P:1:MET:HE2	1.19	1.00
1:E:135:LYS:HZ1	3:R:55:GLU:CD	1.66	0.99
1:H:93:VAL:HG21	3:S:38:ALA:CB	1.92	0.99
1:C:230:TYR:CZ	3:Q:27:ILE:HD12	1.80	0.99
1:E:171:ARG:NE	3:R:23:LEU:HD22	1.73	0.99
1:B:183:ASP:OD2	1:B:249:THR:HG23	1.62	0.99
1:D:183:ASP:OD2	1:D:249:THR:CG2	2.11	0.99
2:L:32:VAL:HG23	2:L:33:LEU:HD12	1.44	0.99
1:E:24:PRO:HB2	3:R:55:GLU:CB	1.93	0.99
1:G:95:VAL:HG11	3:P:31:ALA:CB	1.91	0.99
1:H:183:ASP:OD2	1:H:249:THR:HG23	1.62	0.99
1:I:139:THR:HG21	3:S:37:LYS:CE	1.92	0.99
1:A:230:TYR:OH	3:P:1:MET:CG	2.05	0.99
1:G:143:TRP:N	3:P:30:TRP:CH2	2.31	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:VAL:HG11	3:R:31:ALA:HB2	1.42	0.99
1:B:238:MET:SD	3:P:16:TRP:CZ2	2.56	0.98
1:C:183:ASP:OD2	1:C:249:THR:CG2	2.11	0.98
1:E:189:ILE:HG12	1:E:242:LEU:HD22	1.43	0.98
1:I:183:ASP:OD2	1:I:249:THR:CG2	2.11	0.98
1:B:267:ASN:OD1	3:R:52:MET:HE2	1.62	0.98
1:C:139:THR:HG21	3:Q:37:LYS:HZ3	1.24	0.98
1:B:189:ILE:HG12	1:B:242:LEU:HD22	1.45	0.98
1:F:183:ASP:OD2	1:F:249:THR:HG23	1.62	0.98
1:E:143:TRP:N	3:R:30:TRP:CH2	2.27	0.97
1:F:189:ILE:HG12	1:F:242:LEU:HD22	1.45	0.97
1:E:194:TRP:HE1	3:R:16:TRP:HZ3	1.04	0.97
1:E:194:TRP:NE1	3:R:16:TRP:HZ3	1.23	0.97
1:E:191:GLY:O	3:R:9:VAL:O	1.83	0.97
1:A:189:ILE:HG12	1:A:242:LEU:HD22	1.43	0.97
1:H:189:ILE:HG12	1:H:242:LEU:HD22	1.45	0.97
1:H:234:LEU:HD23	3:S:44:GLY:CA	1.94	0.96
1:A:230:TYR:CD1	3:P:1:MET:SD	2.56	0.96
1:D:233:VAL:C	3:R:47:ARG:HH12	1.73	0.96
1:I:234:LEU:CD1	3:S:23:LEU:HD22	1.95	0.96
1:I:139:THR:CG2	3:S:37:LYS:CE	2.43	0.96
1:E:99:VAL:O	3:R:34:GLU:OE2	1.82	0.96
1:E:113:THR:CB	3:S:56:LEU:HD21	1.94	0.96
1:I:99:VAL:O	3:S:34:GLU:CD	1.98	0.95
1:E:113:THR:HG22	3:S:56:LEU:CD2	1.77	0.95
1:D:183:ASP:OD2	1:D:249:THR:HG23	1.66	0.95
1:H:230:TYR:CD1	3:S:42:SER:CA	2.49	0.95
1:C:103:MET:HE2	3:Q:30:TRP:CA	1.96	0.95
1:D:94:ASN:HD21	3:R:35:GLN:HG2	1.31	0.95
1:E:135:LYS:NZ	3:R:55:GLU:OE2	1.99	0.95
1:H:236:ASP:OD2	3:S:44:GLY:HA3	1.66	0.95
1:I:183:ASP:OD2	1:I:249:THR:HG23	1.66	0.95
1:G:183:ASP:OD2	1:G:249:THR:CG2	2.15	0.95
1:A:183:ASP:OD2	1:A:249:THR:CG2	2.15	0.94
1:C:183:ASP:OD2	1:C:249:THR:HG23	1.66	0.94
1:D:233:VAL:CA	3:R:47:ARG:HH12	1.79	0.94
1:A:230:TYR:CZ	3:P:1:MET:CB	2.49	0.94
1:C:103:MET:CE	3:Q:30:TRP:CB	2.44	0.94
1:G:143:TRP:H	3:P:30:TRP:HH2	1.07	0.94
1:E:183:ASP:OD2	1:E:249:THR:CG2	2.15	0.94
1:C:139:THR:HG21	3:Q:37:LYS:HZ1	1.26	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:TRP:HD1	3:R:30:TRP:NE1	1.66	0.94
1:E:171:ARG:HE	3:R:23:LEU:HD22	1.25	0.93
1:G:95:VAL:CG1	3:P:31:ALA:CB	2.46	0.93
1:J:183:ASP:OD2	1:J:249:THR:CG2	2.15	0.93
1:E:191:GLY:HA3	3:R:9:VAL:H	1.33	0.93
1:A:183:ASP:OD2	1:A:249:THR:HG23	1.69	0.93
1:D:233:VAL:HA	3:R:47:ARG:NH1	1.84	0.93
1:J:46:ASN:OD1	2:L:45:ARG:NH1	2.01	0.92
1:A:230:TYR:HE1	3:P:1:MET:HG2	1.18	0.92
1:E:194:TRP:CH2	3:R:16:TRP:CG	2.49	0.92
1:E:183:ASP:OD2	1:E:249:THR:HG23	1.69	0.92
1:E:135:LYS:CE	3:R:55:GLU:OE2	2.18	0.92
1:I:139:THR:CG2	3:S:37:LYS:HZ1	1.64	0.92
1:B:94:ASN:ND2	3:Q:35:GLN:HG2	1.84	0.92
1:E:143:TRP:H	3:R:30:TRP:HZ2	1.06	0.92
1:G:99:VAL:HG22	3:P:34:GLU:CB	1.93	0.92
1:I:234:LEU:HD11	3:S:23:LEU:HD22	1.50	0.91
1:G:183:ASP:OD2	1:G:249:THR:HG23	1.69	0.91
1:J:183:ASP:OD2	1:J:249:THR:HG23	1.69	0.91
1:C:103:MET:CE	3:Q:30:TRP:HB3	2.01	0.91
1:B:115:GLU:OE1	3:R:56:LEU:CD2	2.17	0.91
1:E:143:TRP:HZ3	1:E:261:MET:HB3	1.36	0.91
1:D:189:ILE:HG12	1:D:242:LEU:HD22	1.53	0.90
1:F:137:VAL:CG2	3:R:18:ASN:HD21	1.85	0.90
1:E:113:THR:HG21	3:S:56:LEU:CD1	2.02	0.90
1:C:189:ILE:HG12	1:C:242:LEU:HD22	1.53	0.89
1:E:113:THR:HG21	3:S:56:LEU:CG	2.02	0.89
1:F:137:VAL:CG2	3:R:18:ASN:ND2	2.35	0.89
1:E:113:THR:HG21	3:S:56:LEU:HD21	1.21	0.89
1:E:194:TRP:CD1	3:R:16:TRP:CZ3	2.58	0.89
1:G:171:ARG:HE	3:P:23:LEU:CD2	1.84	0.89
1:E:99:VAL:CG1	3:R:34:GLU:OE2	2.08	0.89
1:G:143:TRP:HD1	3:P:30:TRP:CE2	1.89	0.89
1:A:143:TRP:HZ3	1:A:261:MET:HB3	1.36	0.89
1:I:139:THR:CG2	3:S:37:LYS:HZ3	1.59	0.89
1:I:189:ILE:HG12	1:I:242:LEU:HD22	1.53	0.89
1:I:234:LEU:HD11	3:S:23:LEU:CD2	2.03	0.89
1:A:230:TYR:HE1	3:P:1:MET:CG	1.73	0.89
1:I:99:VAL:HG13	3:S:34:GLU:CD	1.93	0.89
1:C:135:LYS:HZ2	3:Q:55:GLU:CD	1.81	0.88
1:F:27:GLN:NE2	3:R:14:SER:O	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:143:TRP:HZ3	1:J:261:MET:HB3	1.36	0.88
1:C:99:VAL:HG22	3:Q:34:GLU:HB3	1.54	0.88
1:A:194:TRP:HH2	3:R:65:GLU:OE2	1.53	0.88
1:C:139:THR:CG2	3:Q:37:LYS:NZ	2.37	0.88
1:E:24:PRO:HB3	3:R:55:GLU:O	1.74	0.88
1:G:99:VAL:O	3:P:34:GLU:OE2	1.92	0.88
1:E:194:TRP:HH2	3:R:16:TRP:HB3	1.38	0.87
1:H:230:TYR:CD1	3:S:42:SER:CB	2.56	0.87
1:E:27:GLN:HB2	3:R:55:GLU:OE2	1.73	0.87
1:D:233:VAL:HA	3:R:47:ARG:HH12	1.37	0.87
1:E:24:PRO:HB3	3:R:55:GLU:C	2.00	0.87
1:B:233:VAL:C	3:Q:47:ARG:HH12	1.83	0.87
2:L:31:LEU:HD12	2:L:74:TYR:CE2	2.09	0.87
1:G:143:TRP:HZ3	1:G:261:MET:HB3	1.36	0.86
1:E:194:TRP:CH2	3:R:16:TRP:HB3	2.10	0.86
1:C:230:TYR:CE1	3:Q:24:ASP:OD1	2.28	0.86
1:F:5:LEU:HD21	3:R:12:ASN:CB	2.06	0.86
1:G:99:VAL:C	3:P:34:GLU:OE2	2.19	0.86
1:I:139:THR:HG21	3:S:37:LYS:HZ3	1.03	0.85
1:B:236:ASP:OD2	3:Q:44:GLY:CA	2.22	0.85
1:H:234:LEU:HD23	3:S:44:GLY:H	1.40	0.85
3:S:30:TRP:O	3:S:33:VAL:HG12	1.75	0.85
1:A:194:TRP:HH2	3:R:65:GLU:CD	1.84	0.85
1:C:230:TYR:OH	3:Q:27:ILE:HD13	1.54	0.85
1:G:99:VAL:HG11	3:P:31:ALA:HA	1.56	0.85
1:E:135:LYS:HZ2	3:R:55:GLU:CD	1.78	0.85
1:F:137:VAL:HB	3:R:18:ASN:ND2	1.91	0.85
1:E:171:ARG:NE	3:R:23:LEU:HD23	1.83	0.84
2:L:32:VAL:HG22	2:L:33:LEU:H	1.43	0.84
2:L:135:LEU:N	2:L:135:LEU:HD12	1.91	0.84
1:H:93:VAL:HG21	3:S:38:ALA:HB1	1.60	0.84
2:L:21:ASN:HA	2:L:24:ILE:HD12	1.59	0.84
1:C:103:MET:HE2	3:Q:30:TRP:HB2	1.58	0.83
1:I:230:TYR:CZ	3:S:27:ILE:HG21	2.12	0.83
1:I:234:LEU:CD1	3:S:23:LEU:CD2	2.56	0.83
1:J:151:PHE:CD1	2:L:11:GLU:OE2	2.31	0.83
1:C:230:TYR:HE1	3:Q:27:ILE:HD12	1.05	0.83
1:F:137:VAL:HG21	3:R:18:ASN:ND2	1.94	0.83
1:C:135:LYS:CE	3:Q:55:GLU:OE2	2.26	0.83
1:E:194:TRP:CH2	3:R:16:TRP:CB	2.62	0.83
1:I:103:MET:CG	3:S:34:GLU:OE2	2.27	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:230:TYR:OH	3:P:27:ILE:HB	1.77	0.83
1:C:103:MET:CE	3:Q:31:ALA:N	2.41	0.82
3:P:21:THR:HB	3:P:26:LEU:HD11	1.61	0.82
1:A:193:LYS:HZ1	1:I:54:ARG:NH2	1.77	0.82
1:G:99:VAL:HG22	3:P:34:GLU:HB3	1.58	0.82
1:H:93:VAL:HG21	3:S:38:ALA:HB2	1.60	0.82
1:B:94:ASN:HD21	3:Q:35:GLN:CG	1.93	0.82
1:C:24:PRO:HB2	3:Q:55:GLU:CB	2.10	0.82
1:E:99:VAL:HG11	3:R:31:ALA:HA	1.62	0.82
1:E:194:TRP:HH2	3:R:16:TRP:CB	1.93	0.82
1:G:99:VAL:CA	3:P:34:GLU:OE2	2.19	0.82
1:I:1:MET:HG3	3:S:47:ARG:CZ	2.11	0.81
1:F:137:VAL:HB	3:R:18:ASN:HD21	1.45	0.81
1:E:99:VAL:HG22	3:R:34:GLU:CB	2.09	0.81
1:E:99:VAL:C	3:R:34:GLU:OE2	2.23	0.81
1:E:234:LEU:HD13	3:R:23:LEU:HD21	1.62	0.80
1:E:95:VAL:HG11	3:R:31:ALA:CB	2.12	0.80
1:F:137:VAL:CB	3:R:18:ASN:HD21	1.95	0.79
1:B:233:VAL:HA	3:Q:47:ARG:HH12	1.48	0.79
1:C:95:VAL:CG1	3:Q:31:ALA:CB	2.60	0.79
1:E:143:TRP:N	3:R:30:TRP:HZ2	1.64	0.79
1:G:171:ARG:NE	3:P:23:LEU:HD23	1.95	0.79
1:H:234:LEU:CD2	3:S:44:GLY:H	1.92	0.79
1:C:230:TYR:OH	3:Q:27:ILE:CG1	2.30	0.79
1:G:160:GLU:OE1	1:G:243:ARG:HD3	1.83	0.79
1:E:171:ARG:CZ	3:R:23:LEU:HD22	2.13	0.79
1:G:171:ARG:HH21	3:P:23:LEU:HD22	1.48	0.79
1:I:24:PRO:HB2	3:S:55:GLU:HB3	1.62	0.79
1:E:191:GLY:C	3:R:9:VAL:O	2.27	0.78
1:H:230:TYR:CE1	3:S:42:SER:CB	2.66	0.78
1:J:160:GLU:OE1	1:J:243:ARG:HD3	1.83	0.78
1:E:160:GLU:OE1	1:E:243:ARG:HD3	1.83	0.78
1:A:193:LYS:NZ	1:I:54:ARG:CZ	2.30	0.78
1:G:143:TRP:N	3:P:30:TRP:HH2	1.75	0.78
1:B:233:VAL:CA	3:Q:47:ARG:HH12	1.97	0.78
1:G:139:THR:HG21	3:P:37:LYS:NZ	1.99	0.78
1:F:137:VAL:CB	3:R:18:ASN:ND2	2.47	0.78
1:A:193:LYS:HZ2	1:I:54:ARG:HH12	0.78	0.77
1:C:230:TYR:CE1	3:Q:24:ASP:CG	2.62	0.77
1:A:193:LYS:NZ	1:I:54:ARG:NH2	2.32	0.77
2:L:32:VAL:HG23	2:L:33:LEU:CD1	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LYS:HZ2	1:I:54:ARG:NH1	1.54	0.77
1:C:99:VAL:HG22	3:Q:34:GLU:CB	2.15	0.77
1:A:160:GLU:OE1	1:A:243:ARG:HD3	1.83	0.77
1:B:160:GLU:OE1	1:B:243:ARG:HD3	1.85	0.77
2:L:32:VAL:HG22	2:L:33:LEU:N	2.00	0.77
1:G:234:LEU:HD13	3:P:23:LEU:HD21	1.67	0.77
1:C:27:GLN:HG3	3:Q:55:GLU:OE2	1.83	0.77
1:F:160:GLU:OE1	1:F:243:ARG:HD3	1.85	0.77
2:L:31:LEU:HD13	2:L:72:ILE:HB	1.67	0.76
1:D:94:ASN:HD21	3:R:35:GLN:CG	1.98	0.76
1:B:181:GLY:CA	1:B:250:MET:HE3	2.16	0.76
1:F:181:GLY:CA	1:F:250:MET:HE3	2.16	0.76
1:I:143:TRP:N	3:S:30:TRP:CH2	2.53	0.76
1:E:99:VAL:CA	3:R:34:GLU:OE2	2.26	0.76
1:E:113:THR:HB	3:S:56:LEU:HD21	1.68	0.76
1:E:234:LEU:HD13	3:R:23:LEU:CD2	2.16	0.76
1:H:181:GLY:CA	1:H:250:MET:HE3	2.16	0.76
1:G:27:GLN:N	3:P:55:GLU:OE2	2.19	0.76
1:I:24:PRO:CB	3:S:55:GLU:CB	2.61	0.76
1:C:27:GLN:CG	3:Q:55:GLU:OE2	2.35	0.75
2:L:30:GLU:OE1	2:L:48:VAL:HG22	1.85	0.75
2:L:62:VAL:HG13	2:L:64:LEU:HD11	1.67	0.75
1:H:160:GLU:OE1	1:H:243:ARG:HD3	1.85	0.74
2:L:135:LEU:H	2:L:135:LEU:CD1	1.99	0.74
1:C:160:GLU:OE1	1:C:243:ARG:HD3	1.87	0.74
1:C:143:TRP:N	3:Q:30:TRP:CH2	2.50	0.74
1:I:139:THR:HG22	3:S:37:LYS:HE2	1.69	0.74
1:D:236:ASP:OD2	3:R:44:GLY:HA3	1.88	0.74
1:I:160:GLU:OE1	1:I:243:ARG:HD3	1.87	0.74
1:D:160:GLU:OE1	1:D:243:ARG:HD3	1.87	0.74
1:A:230:TYR:CZ	3:P:1:MET:HB3	2.22	0.73
2:L:22:ILE:HG23	2:L:57:MET:O	1.87	0.73
2:L:31:LEU:HD12	2:L:74:TYR:CZ	2.22	0.73
1:E:234:LEU:HD11	3:R:23:LEU:HD11	1.70	0.73
1:G:181:GLY:HA3	1:G:250:MET:HE3	1.70	0.73
1:A:181:GLY:HA3	1:A:250:MET:HE3	1.70	0.73
1:E:181:GLY:HA3	1:E:250:MET:HE3	1.70	0.73
1:H:93:VAL:CG2	3:S:38:ALA:CB	2.67	0.73
1:A:93:VAL:HG13	3:P:2:ASN:ND2	2.04	0.73
1:A:193:LYS:NZ	1:I:54:ARG:HH22	1.85	0.73
1:G:143:TRP:CZ3	1:G:261:MET:HB3	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:181:GLY:HA3	1:J:250:MET:HE3	1.70	0.73
1:I:139:THR:CG2	3:S:37:LYS:HE2	2.19	0.72
1:J:143:TRP:CZ3	1:J:261:MET:HB3	2.24	0.72
1:H:230:TYR:CD1	3:S:42:SER:HB3	2.24	0.72
1:C:161:ILE:HD12	1:C:246:ILE:CD1	2.20	0.72
1:I:1:MET:HG3	3:S:47:ARG:NH2	2.05	0.72
2:L:2:ILE:HG22	2:L:75:TRP:CE3	2.25	0.72
2:L:135:LEU:N	2:L:135:LEU:CD1	2.51	0.72
3:P:21:THR:CG2	3:P:26:LEU:HD11	2.19	0.72
1:C:103:MET:HE3	3:Q:30:TRP:C	2.15	0.71
1:G:230:TYR:OH	3:P:27:ILE:CB	2.30	0.71
1:I:230:TYR:HE1	3:S:27:ILE:HD12	1.53	0.71
1:I:234:LEU:HD13	3:S:23:LEU:HD22	1.72	0.71
1:G:143:TRP:HD1	3:P:30:TRP:CZ2	2.09	0.71
1:G:143:TRP:CD1	3:P:30:TRP:CE2	2.77	0.71
1:B:233:VAL:HA	3:Q:47:ARG:NH1	2.05	0.71
1:E:99:VAL:HG22	3:R:34:GLU:HB3	1.73	0.71
1:G:181:GLY:CA	1:G:250:MET:HE3	2.21	0.71
2:L:24:ILE:HG23	2:L:79:LEU:C	2.16	0.71
1:A:95:VAL:HG13	3:P:2:ASN:OD1	1.91	0.71
1:D:161:ILE:HD12	1:D:246:ILE:CD1	2.20	0.71
1:I:99:VAL:CG1	3:S:31:ALA:HA	2.21	0.71
1:I:161:ILE:HD12	1:I:246:ILE:CD1	2.20	0.71
1:A:181:GLY:CA	1:A:250:MET:HE3	2.21	0.70
3:P:5:VAL:HG22	3:P:6:PRO:HD2	1.73	0.70
1:B:22:LYS:NZ	3:R:57:ASP:HB2	2.06	0.70
3:P:21:THR:CB	3:P:26:LEU:HD11	2.20	0.70
1:I:181:GLY:HA3	1:I:250:MET:HE3	1.74	0.70
1:G:113:THR:CG2	3:Q:56:LEU:HD22	2.22	0.70
1:B:181:GLY:HA3	1:B:250:MET:HE3	1.74	0.70
1:D:181:GLY:HA3	1:D:250:MET:HE3	1.74	0.70
1:E:181:GLY:CA	1:E:250:MET:HE3	2.21	0.70
1:H:181:GLY:HA3	1:H:250:MET:HE3	1.74	0.70
1:C:181:GLY:HA3	1:C:250:MET:HE3	1.74	0.70
1:J:181:GLY:CA	1:J:250:MET:HE3	2.21	0.70
1:C:24:PRO:HB3	3:Q:55:GLU:C	2.18	0.69
1:I:230:TYR:OH	3:S:27:ILE:HG22	1.87	0.69
1:C:27:GLN:CD	3:Q:53:THR:HG21	2.17	0.69
1:E:143:TRP:CD1	3:R:30:TRP:NE1	2.57	0.69
1:J:161:ILE:HD12	1:J:246:ILE:CD1	2.23	0.69
1:B:20:SER:OG	1:B:115:GLU:HG2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:TYR:OH	3:Q:27:ILE:HD12	1.77	0.69
1:F:181:GLY:HA3	1:F:250:MET:HE3	1.74	0.69
1:H:230:TYR:CE1	3:S:42:SER:HB2	2.26	0.69
1:I:230:TYR:CE1	3:S:27:ILE:CD1	2.76	0.69
1:I:24:PRO:HB3	3:S:55:GLU:CB	2.17	0.69
2:L:169:ARG:O	2:L:170:VAL:N	2.26	0.69
1:C:230:TYR:OH	3:Q:27:ILE:HB	1.90	0.69
1:E:27:GLN:CB	3:R:55:GLU:OE2	2.40	0.69
1:F:20:SER:OG	1:F:115:GLU:HG2	1.93	0.69
1:G:161:ILE:HD12	1:G:246:ILE:CD1	2.23	0.69
1:G:230:TYR:CE1	3:P:24:ASP:OD1	2.46	0.69
1:C:181:GLY:CA	1:C:250:MET:HE3	2.23	0.68
1:I:181:GLY:CA	1:I:250:MET:HE3	2.23	0.68
1:C:234:LEU:HD13	3:Q:23:LEU:HD22	1.74	0.68
1:D:181:GLY:CA	1:D:250:MET:HE3	2.23	0.68
1:C:103:MET:HE1	3:Q:31:ALA:N	2.08	0.68
1:H:20:SER:OG	1:H:115:GLU:HG2	1.93	0.68
1:A:143:TRP:CZ3	1:A:261:MET:HB3	2.23	0.68
1:E:135:LYS:HE3	3:R:55:GLU:OE2	1.92	0.68
1:C:230:TYR:CE1	3:Q:27:ILE:HD11	2.25	0.68
1:D:94:ASN:ND2	3:R:35:GLN:HG2	2.05	0.68
2:L:24:ILE:HG23	2:L:79:LEU:O	1.94	0.68
1:I:139:THR:HG23	3:S:37:LYS:HZ3	1.57	0.68
1:J:151:PHE:CB	2:L:11:GLU:OE1	2.37	0.68
1:A:161:ILE:HD12	1:A:246:ILE:CD1	2.23	0.67
1:I:99:VAL:CG1	3:S:34:GLU:CD	2.64	0.67
1:G:113:THR:HG21	3:Q:56:LEU:HD22	1.76	0.67
2:L:24:ILE:HD13	2:L:80:ASP:N	2.10	0.67
1:E:161:ILE:HD12	1:E:246:ILE:CD1	2.23	0.67
1:G:143:TRP:HD1	3:P:30:TRP:NE1	1.90	0.67
1:E:143:TRP:HB2	3:R:30:TRP:CZ2	2.30	0.67
1:G:171:ARG:NE	3:P:23:LEU:CD2	2.55	0.67
1:G:143:TRP:HB2	3:P:30:TRP:CH2	2.30	0.67
1:E:143:TRP:CZ3	1:E:261:MET:HB3	2.24	0.67
1:I:99:VAL:HG22	3:S:34:GLU:CB	2.25	0.66
1:I:230:TYR:CE1	3:S:27:ILE:HD12	2.29	0.66
1:I:139:THR:HG22	3:S:37:LYS:CE	2.22	0.66
1:G:113:THR:HG21	3:Q:56:LEU:CD2	2.25	0.66
1:J:152:LYS:NZ	1:J:163:ASP:OD1	2.29	0.66
1:E:152:LYS:NZ	1:E:163:ASP:OD1	2.29	0.66
1:A:230:TYR:HH	3:P:1:MET:HA	1.56	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:ARG:CZ	3:Q:63:VAL:HG11	2.26	0.65
4:T:124:GLY:O	4:T:125:VAL:CB	2.43	0.65
1:G:143:TRP:N	3:P:30:TRP:CZ2	2.58	0.65
1:E:99:VAL:HG13	3:R:34:GLU:OE2	1.48	0.65
1:I:137:VAL:HG23	3:S:50:GLN:HG2	1.78	0.65
1:G:143:TRP:CD1	3:P:30:TRP:CZ2	2.84	0.65
1:A:152:LYS:NZ	1:A:163:ASP:OD1	2.29	0.65
1:I:20:SER:OG	1:I:115:GLU:HG2	1.96	0.65
1:C:20:SER:OG	1:C:115:GLU:HG2	1.96	0.65
1:D:233:VAL:HA	3:R:47:ARG:CZ	2.27	0.65
1:F:161:ILE:HD12	1:F:246:ILE:CD1	2.27	0.65
1:A:230:TYR:HE1	3:P:1:MET:CE	2.08	0.65
1:H:161:ILE:HD12	1:H:246:ILE:CD1	2.27	0.65
1:A:230:TYR:HD1	3:P:1:MET:CE	1.90	0.65
1:B:234:LEU:HD23	3:Q:44:GLY:N	2.11	0.65
1:G:20:SER:OG	1:G:115:GLU:HG2	1.97	0.65
1:G:152:LYS:NZ	1:G:163:ASP:OD1	2.29	0.65
1:B:161:ILE:HD12	1:B:246:ILE:CD1	2.27	0.64
1:C:99:VAL:HG11	3:Q:31:ALA:HA	1.79	0.64
2:L:2:ILE:HG22	2:L:75:TRP:HE3	1.62	0.64
1:G:139:THR:HG21	3:P:37:LYS:HZ3	1.59	0.64
1:C:27:GLN:OE1	3:Q:53:THR:HG21	1.98	0.64
1:D:20:SER:OG	1:D:115:GLU:HG2	1.96	0.64
1:B:93:VAL:HG21	3:Q:38:ALA:HB2	1.80	0.64
1:A:20:SER:OG	1:A:115:GLU:HG2	1.97	0.64
1:E:171:ARG:NH2	3:R:23:LEU:HD22	2.12	0.64
1:H:93:VAL:CG2	3:S:38:ALA:HB2	2.28	0.64
1:J:20:SER:OG	1:J:115:GLU:HG2	1.97	0.64
1:C:139:THR:CG2	3:Q:37:LYS:HZ3	2.07	0.63
2:L:32:VAL:CG2	2:L:33:LEU:N	2.62	0.63
1:C:95:VAL:CG1	3:Q:31:ALA:HB1	2.27	0.63
1:H:210:TYR:OH	1:I:2:ARG:NH2	2.29	0.63
1:C:27:GLN:HB2	3:Q:55:GLU:OE2	1.99	0.63
1:G:171:ARG:NH2	3:P:23:LEU:HD22	2.12	0.63
1:G:95:VAL:HG12	3:P:31:ALA:CB	2.27	0.63
1:C:103:MET:HG3	3:Q:34:GLU:OE2	1.98	0.63
1:E:20:SER:OG	1:E:115:GLU:HG2	1.97	0.63
1:I:24:PRO:HB2	3:S:55:GLU:CG	2.29	0.62
2:L:7:LEU:HD11	2:L:34:ARG:NH2	2.14	0.62
1:C:230:TYR:HH	3:Q:27:ILE:CG2	2.12	0.62
1:E:194:TRP:CD1	3:R:16:TRP:CH2	2.87	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:PRO:HG2	3:S:55:GLU:OE1	1.99	0.62
1:J:155:ASN:O	1:J:248:SER:HB3	2.00	0.62
3:R:62:VAL:HG23	3:S:63:VAL:HG13	1.81	0.62
1:F:137:VAL:HG21	3:R:18:ASN:HD22	1.65	0.62
1:E:155:ASN:O	1:E:248:SER:HB3	2.00	0.62
1:H:230:TYR:CE1	3:S:42:SER:HB3	2.34	0.62
1:E:87:ARG:HB2	1:E:90:MET:HG2	1.82	0.62
1:G:171:ARG:HH21	3:P:23:LEU:CD2	2.13	0.61
1:G:230:TYR:OH	3:P:24:ASP:HA	2.00	0.61
1:C:99:VAL:C	3:Q:34:GLU:OE2	2.42	0.61
2:L:31:LEU:CD1	2:L:72:ILE:HB	2.31	0.61
1:A:87:ARG:HB2	1:A:90:MET:HG2	1.82	0.61
1:I:230:TYR:OH	3:S:27:ILE:CB	2.49	0.61
1:A:155:ASN:O	1:A:248:SER:HB3	2.00	0.61
1:C:230:TYR:CD1	3:Q:24:ASP:OD1	2.53	0.61
1:D:2:ARG:NH2	1:F:210:TYR:OH	2.29	0.61
1:J:87:ARG:HB2	1:J:90:MET:HG2	1.82	0.61
1:B:210:TYR:OH	1:C:2:ARG:NH2	2.29	0.61
1:E:24:PRO:CB	3:R:55:GLU:CB	2.66	0.61
1:C:87:ARG:HB2	1:C:90:MET:HG2	1.83	0.61
1:G:155:ASN:O	1:G:248:SER:HB3	2.00	0.61
1:I:24:PRO:HB2	3:S:55:GLU:CB	2.26	0.61
1:C:143:TRP:N	3:Q:30:TRP:CZ2	2.68	0.60
1:F:153:GLN:OE1	1:F:253:GLN:NE2	2.33	0.60
3:P:22:GLY:O	3:P:26:LEU:HD13	2.01	0.60
1:E:95:VAL:CG1	3:R:31:ALA:CB	2.79	0.60
1:D:87:ARG:HB2	1:D:90:MET:HG2	1.83	0.60
1:H:153:GLN:OE1	1:H:253:GLN:NE2	2.33	0.60
1:G:230:TYR:HE1	3:P:24:ASP:OD1	1.84	0.60
1:E:139:THR:HG21	3:R:37:LYS:NZ	2.16	0.60
2:L:31:LEU:HD22	2:L:72:ILE:HD13	1.83	0.60
1:G:113:THR:HG21	3:Q:56:LEU:CD1	2.32	0.60
1:I:87:ARG:HB2	1:I:90:MET:HG2	1.83	0.60
1:B:153:GLN:OE1	1:B:253:GLN:NE2	2.33	0.60
1:G:87:ARG:HB2	1:G:90:MET:HG2	1.82	0.60
2:L:97:GLN:HE21	2:L:329:GLN:HE22	1.50	0.60
1:I:234:LEU:HD13	3:S:23:LEU:CD2	2.31	0.59
1:E:143:TRP:HD1	3:R:30:TRP:CE2	2.19	0.59
1:I:99:VAL:HG22	3:S:34:GLU:HB3	1.84	0.59
1:G:113:THR:HG21	3:Q:56:LEU:HD13	1.84	0.59
1:I:230:TYR:CE1	3:S:27:ILE:HD13	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:ARG:HB2	1:F:90:MET:HG2	1.85	0.59
1:B:22:LYS:HZ2	3:R:57:ASP:CG	2.11	0.58
1:D:234:LEU:N	3:R:47:ARG:CZ	2.43	0.58
1:D:14:ALA:O	1:D:17:ASN:HB2	2.02	0.58
1:G:143:TRP:CD1	3:P:30:TRP:NE1	2.70	0.58
1:B:87:ARG:HB2	1:B:90:MET:HG2	1.85	0.58
2:L:35:ALA:HB3	2:L:65:HIS:HB2	1.84	0.58
1:D:48:ARG:NH2	1:D:55:LEU:HB2	2.19	0.58
1:E:113:THR:HG21	3:S:56:LEU:HD22	1.32	0.58
1:E:192:THR:HG23	3:R:13:GLN:CG	2.33	0.58
3:P:5:VAL:HG22	3:P:6:PRO:CD	2.33	0.58
1:I:14:ALA:O	1:I:17:ASN:HB2	2.02	0.58
1:H:236:ASP:OD2	3:S:44:GLY:CA	2.48	0.58
2:L:12:PHE:O	2:L:64:LEU:HD13	2.03	0.58
1:I:99:VAL:HG13	3:S:34:GLU:HB2	1.85	0.58
1:C:14:ALA:O	1:C:17:ASN:HB2	2.03	0.58
1:H:230:TYR:HD1	3:S:42:SER:CA	1.91	0.58
2:L:21:ASN:HB3	2:L:24:ILE:HG21	1.86	0.58
1:B:142:SER:OG	1:B:143:TRP:N	2.37	0.57
1:C:48:ARG:NH2	1:C:55:LEU:HB2	2.19	0.57
1:C:27:GLN:CB	3:Q:55:GLU:OE2	2.53	0.57
1:I:48:ARG:NH2	1:I:55:LEU:HB2	2.18	0.57
1:E:230:TYR:OH	3:R:24:ASP:HA	2.04	0.57
1:C:230:TYR:HE1	3:Q:27:ILE:CD1	1.77	0.57
1:H:87:ARG:HB2	1:H:90:MET:HG2	1.85	0.57
1:E:143:TRP:HD1	3:R:30:TRP:HE1	1.47	0.57
1:E:192:THR:HA	3:R:13:GLN:HG3	1.86	0.57
3:S:75:GLU:HA	3:S:78:VAL:HG12	1.87	0.57
1:E:173:ALA:HB1	1:E:224:MET:HE2	1.87	0.57
1:G:14:ALA:O	1:G:17:ASN:HB2	2.05	0.57
1:G:99:VAL:CG2	3:P:34:GLU:CB	2.74	0.57
1:I:139:THR:HG21	3:S:37:LYS:HZ1	0.74	0.57
2:L:205:LEU:HG	2:L:321:LEU:CD1	2.34	0.57
1:E:48:ARG:HH21	1:E:117:LYS:HB3	1.70	0.56
1:I:99:VAL:HG22	3:S:34:GLU:HB2	1.86	0.56
2:L:31:LEU:CD2	2:L:72:ILE:HD13	2.34	0.56
1:G:173:ALA:HB1	1:G:224:MET:HE2	1.87	0.56
1:A:48:ARG:HH21	1:A:117:LYS:HB3	1.70	0.56
1:H:234:LEU:H	3:S:47:ARG:NH1	2.02	0.56
2:L:31:LEU:HD22	2:L:72:ILE:CD1	2.34	0.56
1:D:161:ILE:HD12	1:D:246:ILE:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:VAL:HB	1:H:59:TYR:HB2	1.88	0.56
1:I:1:MET:CG	3:S:47:ARG:CZ	2.83	0.56
1:A:173:ALA:HB1	1:A:224:MET:HE2	1.87	0.56
1:E:234:LEU:CD1	3:R:23:LEU:HD11	2.36	0.56
1:A:14:ALA:O	1:A:17:ASN:HB2	2.05	0.56
1:B:22:LYS:HZ3	3:R:57:ASP:HB2	1.70	0.56
1:D:237:GLN:HG2	1:D:238:MET:HE2	1.88	0.56
1:I:1:MET:HB2	3:S:47:ARG:NE	2.21	0.56
1:B:47:VAL:HB	1:B:59:TYR:HB2	1.88	0.56
1:C:24:PRO:CB	3:Q:55:GLU:CB	2.74	0.56
1:E:99:VAL:CG1	3:R:31:ALA:HA	2.34	0.56
1:C:103:MET:HE3	3:Q:30:TRP:O	2.06	0.56
1:C:139:THR:CG2	3:Q:37:LYS:CE	2.84	0.55
1:J:14:ALA:O	1:J:17:ASN:HB2	2.05	0.55
1:D:233:VAL:CA	3:R:47:ARG:NH1	2.51	0.55
1:I:161:ILE:HD12	1:I:246:ILE:HD13	1.88	0.55
1:I:237:GLN:HG2	1:I:238:MET:HE2	1.88	0.55
1:D:86:VAL:O	1:D:88:PRO:HD3	2.06	0.55
1:E:14:ALA:O	1:E:17:ASN:HB2	2.05	0.55
1:F:47:VAL:HB	1:F:59:TYR:HB2	1.88	0.55
1:G:25:ILE:N	3:P:55:GLU:HB3	2.21	0.55
1:I:173:ALA:HB1	1:I:224:MET:HE2	1.89	0.55
1:A:189:ILE:HG12	1:A:242:LEU:CD2	2.28	0.55
1:J:173:ALA:HB1	1:J:224:MET:HE2	1.87	0.55
1:C:161:ILE:HD12	1:C:246:ILE:HD13	1.87	0.55
1:G:48:ARG:HH21	1:G:117:LYS:HB3	1.70	0.55
1:D:173:ALA:HB1	1:D:224:MET:HE2	1.89	0.55
1:E:27:GLN:CG	3:R:55:GLU:OE2	2.55	0.55
1:I:234:LEU:HD11	3:S:23:LEU:HD21	1.85	0.55
1:J:48:ARG:HH21	1:J:117:LYS:HB3	1.70	0.55
1:J:161:ILE:HD12	1:J:246:ILE:HD13	1.89	0.55
1:G:189:ILE:HG12	1:G:242:LEU:CD2	2.28	0.55
1:H:14:ALA:O	1:H:17:ASN:HB2	2.07	0.55
1:J:151:PHE:HD1	2:L:11:GLU:OE2	1.89	0.55
1:F:14:ALA:O	1:F:17:ASN:HB2	2.07	0.54
1:I:86:VAL:O	1:I:88:PRO:HD3	2.06	0.54
1:C:86:VAL:O	1:C:88:PRO:HD3	2.06	0.54
1:J:86:VAL:O	1:J:88:PRO:HD3	2.08	0.54
1:A:230:TYR:HH	3:P:1:MET:HG2	1.70	0.54
1:C:27:GLN:CD	3:Q:53:THR:CG2	2.80	0.54
1:D:94:ASN:HD21	3:R:35:GLN:CD	2.14	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:VAL:O	1:G:88:PRO:HD3	2.08	0.54
1:I:137:VAL:CG2	3:S:50:GLN:CD	2.81	0.54
1:A:161:ILE:HD12	1:A:246:ILE:HD13	1.89	0.54
1:B:86:VAL:O	1:B:88:PRO:HD3	2.08	0.54
1:C:237:GLN:HG2	1:C:238:MET:HE2	1.88	0.54
3:R:64:VAL:O	3:R:65:GLU:HB2	2.07	0.54
1:G:161:ILE:HD12	1:G:246:ILE:HD13	1.89	0.54
1:D:236:ASP:CG	3:R:44:GLY:HA3	2.33	0.54
1:E:161:ILE:HD12	1:E:246:ILE:HD13	1.89	0.54
1:H:86:VAL:O	1:H:88:PRO:HD3	2.08	0.54
1:I:266:ARG:NE	3:S:63:VAL:HG11	2.22	0.54
3:S:83:GLN:O	3:S:87:LEU:HD13	2.08	0.54
1:E:230:TYR:CZ	3:R:27:ILE:HD12	2.43	0.54
1:F:173:ALA:HB1	1:F:224:MET:HE2	1.90	0.54
3:P:21:THR:HG22	3:P:26:LEU:HD11	1.89	0.54
1:B:14:ALA:O	1:B:17:ASN:HB2	2.07	0.53
1:F:142:SER:OG	1:F:143:TRP:N	2.37	0.53
1:J:108:THR:O	1:J:111:LEU:HB2	2.08	0.53
1:A:86:VAL:O	1:A:88:PRO:HD3	2.08	0.53
1:F:86:VAL:O	1:F:88:PRO:HD3	2.08	0.53
1:E:143:TRP:N	3:R:30:TRP:HH2	2.01	0.53
3:S:81:VAL:HG13	3:S:82:PRO:HD3	1.90	0.53
1:B:22:LYS:HZ2	3:R:57:ASP:HB2	1.72	0.53
1:C:173:ALA:HB1	1:C:224:MET:HE2	1.89	0.53
1:A:193:LYS:HZ3	1:I:54:ARG:HH22	1.55	0.53
1:H:173:ALA:HB1	1:H:224:MET:HE2	1.90	0.53
1:C:60:LYS:HD2	1:C:151:PHE:HZ	1.74	0.53
1:D:210:TYR:OH	1:E:2:ARG:NH2	2.39	0.53
1:E:86:VAL:O	1:E:88:PRO:HD3	2.08	0.53
1:E:108:THR:O	1:E:111:LEU:HB2	2.08	0.53
1:G:108:THR:O	1:G:111:LEU:HB2	2.08	0.53
1:A:108:THR:O	1:A:111:LEU:HB2	2.08	0.53
1:A:194:TRP:CH2	3:R:65:GLU:CD	2.73	0.53
2:L:76:VAL:O	2:L:76:VAL:HG13	2.09	0.53
1:H:171:ARG:NH2	3:S:42:SER:C	2.62	0.52
1:I:60:LYS:HD2	1:I:151:PHE:HZ	1.74	0.52
2:L:21:ASN:HA	2:L:24:ILE:CD1	2.34	0.52
1:A:210:TYR:OH	1:B:2:ARG:NH2	2.39	0.52
1:F:54:ARG:CG	1:F:54:ARG:HH11	2.22	0.52
3:P:30:TRP:O	3:P:33:VAL:HG12	2.10	0.52
1:G:267:ASN:N	1:G:267:ASN:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:54:ARG:CG	1:H:54:ARG:HH11	2.22	0.52
2:L:97:GLN:HE21	2:L:329:GLN:NE2	2.08	0.52
1:D:47:VAL:HB	1:D:59:TYR:HB2	1.91	0.52
3:S:71:ALA:O	3:S:72:GLN:HB2	2.10	0.52
1:B:173:ALA:HB1	1:B:224:MET:HE2	1.90	0.52
1:J:47:VAL:HB	1:J:59:TYR:HB2	1.91	0.52
1:B:54:ARG:HH11	1:B:54:ARG:CG	2.22	0.52
1:E:47:VAL:HB	1:E:59:TYR:HB2	1.91	0.52
1:E:267:ASN:N	1:E:267:ASN:OD1	2.42	0.52
1:E:191:GLY:CA	3:R:9:VAL:O	2.58	0.52
1:G:143:TRP:HB2	3:P:30:TRP:CZ2	2.45	0.52
1:J:142:SER:OG	1:J:143:TRP:N	2.43	0.52
1:A:142:SER:OG	1:A:143:TRP:N	2.43	0.52
1:D:108:THR:O	1:D:111:LEU:HB2	2.10	0.52
1:G:234:LEU:HD13	3:P:23:LEU:CD2	2.37	0.52
1:I:143:TRP:N	3:S:30:TRP:CZ2	2.78	0.52
4:T:122:ALA:O	4:T:123:SER:CB	2.58	0.52
1:A:267:ASN:OD1	1:A:267:ASN:N	2.42	0.52
1:C:47:VAL:HB	1:C:59:TYR:HB2	1.91	0.52
1:G:47:VAL:HB	1:G:59:TYR:HB2	1.91	0.52
1:H:237:GLN:O	1:H:237:GLN:HG3	2.10	0.52
1:A:47:VAL:HB	1:A:59:TYR:HB2	1.91	0.51
1:B:155:ASN:O	1:B:248:SER:HB3	2.11	0.51
1:I:47:VAL:HB	1:I:59:TYR:HB2	1.91	0.51
1:C:24:PRO:HB3	3:Q:55:GLU:HB3	1.88	0.51
1:H:183:ASP:CG	1:H:249:THR:HG23	2.34	0.51
1:I:108:THR:O	1:I:111:LEU:HB2	2.10	0.51
1:I:137:VAL:HB	3:S:50:GLN:CD	2.36	0.51
1:D:60:LYS:HD2	1:D:151:PHE:HZ	1.74	0.51
1:H:155:ASN:O	1:H:248:SER:HB3	2.11	0.51
1:I:99:VAL:HG11	3:S:31:ALA:HA	1.90	0.51
3:S:90:PHE:O	3:S:94:LEU:HD13	2.09	0.51
4:T:116:ALA:O	4:T:117:SER:CB	2.58	0.51
1:D:192:THR:OG1	3:R:51:ALA:HB1	2.10	0.51
1:F:155:ASN:O	1:F:248:SER:HB3	2.11	0.51
1:C:103:MET:CE	3:Q:30:TRP:HB2	2.27	0.51
1:I:103:MET:HG2	3:S:30:TRP:HB3	1.91	0.51
1:F:183:ASP:CG	1:F:249:THR:HG23	2.34	0.51
1:G:113:THR:CG2	3:Q:56:LEU:CD2	2.86	0.51
1:I:137:VAL:HG23	3:S:50:GLN:CG	2.40	0.51
3:P:43:THR:HG22	3:P:45:GLN:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:THR:O	1:C:111:LEU:HB2	2.10	0.51
1:J:267:ASN:N	1:J:267:ASN:OD1	2.42	0.51
1:E:236:ASP:C	1:E:238:MET:H	2.19	0.50
1:B:22:LYS:NZ	3:R:57:ASP:CB	2.74	0.50
1:D:171:ARG:HD3	1:D:232:SER:OG	2.11	0.50
1:F:161:ILE:HD12	1:F:246:ILE:HD13	1.94	0.50
1:H:161:ILE:HD12	1:H:246:ILE:HD13	1.94	0.50
1:J:236:ASP:C	1:J:238:MET:H	2.19	0.50
1:B:183:ASP:CG	1:B:249:THR:HG23	2.34	0.50
2:L:21:ASN:HD22	2:L:24:ILE:HD12	1.77	0.50
1:C:171:ARG:HD3	1:C:232:SER:OG	2.11	0.50
1:F:52:ASP:OD2	1:F:266:ARG:NE	2.45	0.50
1:G:236:ASP:C	1:G:238:MET:H	2.19	0.50
1:H:234:LEU:HD23	3:S:43:THR:C	2.28	0.50
1:A:194:TRP:CZ3	3:R:65:GLU:OE2	2.65	0.50
1:C:103:MET:HG2	3:Q:30:TRP:HB3	1.94	0.50
1:E:24:PRO:CB	3:R:55:GLU:O	2.53	0.50
1:E:189:ILE:HG12	1:E:242:LEU:CD2	2.28	0.50
1:F:237:GLN:O	1:F:237:GLN:HG3	2.10	0.50
2:L:168:ILE:HB	2:L:317:SER:O	2.12	0.50
1:E:143:TRP:CB	3:R:30:TRP:CZ2	2.94	0.50
1:A:96:THR:HG21	1:C:93:VAL:C	2.37	0.49
1:B:237:GLN:O	1:B:237:GLN:HG3	2.10	0.49
1:C:234:LEU:CD1	3:Q:23:LEU:HD22	2.41	0.49
1:D:233:VAL:HA	3:R:47:ARG:NH2	2.27	0.49
1:B:108:THR:O	1:B:111:LEU:HB2	2.12	0.49
1:F:5:LEU:HD21	3:R:12:ASN:HB3	1.88	0.49
1:F:108:THR:O	1:F:111:LEU:HB2	2.12	0.49
1:H:230:TYR:HB3	3:S:41:ALA:C	2.37	0.49
1:A:236:ASP:C	1:A:238:MET:H	2.19	0.49
1:H:108:THR:O	1:H:111:LEU:HB2	2.12	0.49
1:H:233:VAL:HA	3:S:47:ARG:HH12	0.49	0.49
1:J:151:PHE:HB3	2:L:11:GLU:CD	2.32	0.49
2:L:32:VAL:CG2	2:L:33:LEU:HD12	2.30	0.49
1:A:177:ILE:HG12	1:A:256:ILE:HD12	1.95	0.49
1:E:177:ILE:HG12	1:E:256:ILE:HD12	1.95	0.49
1:I:171:ARG:HD3	1:I:232:SER:OG	2.11	0.49
1:G:137:VAL:CG2	3:P:50:GLN:CD	2.86	0.49
2:L:210:PHE:HB3	2:L:319:ASP:OD2	2.13	0.49
1:D:93:VAL:C	1:E:96:THR:HG21	2.37	0.49
2:L:21:ASN:CA	2:L:24:ILE:HD12	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:244:ASP:HB2	2:L:245:GLU:OE2	2.13	0.49
3:Q:43:THR:HG22	3:Q:45:GLN:H	1.78	0.49
1:B:93:VAL:HG21	3:Q:38:ALA:CB	2.42	0.49
1:H:2:ARG:NH2	1:J:210:TYR:OH	2.39	0.48
1:I:93:VAL:C	1:J:96:THR:HG21	2.37	0.48
1:B:22:LYS:HZ2	3:R:57:ASP:CB	2.26	0.48
1:C:230:TYR:CZ	3:Q:27:ILE:HG21	2.41	0.48
1:C:230:TYR:HH	3:Q:27:ILE:HB	1.77	0.48
1:J:189:ILE:HG12	1:J:242:LEU:CD2	2.28	0.48
1:D:142:SER:OG	1:D:143:TRP:N	2.37	0.48
2:L:133:THR:HB	2:L:135:LEU:CD1	2.43	0.48
1:A:73:LYS:HG3	1:A:211:GLY:O	2.14	0.48
1:E:192:THR:HG23	3:R:13:GLN:HG3	1.96	0.48
1:G:73:LYS:HG3	1:G:211:GLY:O	2.13	0.48
1:I:99:VAL:HG13	3:S:34:GLU:CG	2.42	0.48
1:I:171:ARG:HA	1:I:233:VAL:O	2.14	0.48
1:C:139:THR:HG22	3:Q:37:LYS:HE2	1.95	0.48
1:E:143:TRP:CD1	3:R:30:TRP:CE2	3.00	0.48
1:J:177:ILE:HG12	1:J:256:ILE:HD12	1.94	0.48
3:S:81:VAL:CG1	3:S:82:PRO:HD3	2.44	0.48
1:B:52:ASP:OD2	1:B:266:ARG:NE	2.45	0.48
1:C:137:VAL:HG23	3:Q:50:GLN:HG2	1.96	0.48
2:L:34:ARG:NH1	2:L:36:TYR:OH	2.44	0.48
2:L:211:SER:HB3	2:L:318:ASP:OD1	2.13	0.48
1:B:230:TYR:HB3	3:Q:41:ALA:HB1	1.96	0.48
1:D:171:ARG:HA	1:D:233:VAL:O	2.14	0.48
1:E:27:GLN:HG3	1:E:135:LYS:HZ1	1.79	0.48
1:E:113:THR:HG21	3:S:56:LEU:HD11	1.90	0.48
1:E:230:TYR:CZ	3:R:27:ILE:CD1	2.97	0.48
1:H:234:LEU:N	3:S:47:ARG:NH1	2.62	0.48
1:A:94:ASN:HB3	3:P:3:THR:N	2.28	0.47
1:J:148:ARG:HA	1:J:148:ARG:HD3	1.65	0.47
1:E:73:LYS:HG3	1:E:211:GLY:O	2.13	0.47
1:E:171:ARG:HH21	3:R:23:LEU:HD22	1.76	0.47
3:S:92:GLY:O	3:S:96:LEU:HD13	2.15	0.47
1:B:267:ASN:CG	3:R:52:MET:HE2	2.37	0.47
1:F:166:ARG:HA	1:F:235:LEU:HD13	1.96	0.47
1:B:161:ILE:HD12	1:B:246:ILE:HD13	1.94	0.47
1:B:166:ARG:HA	1:B:235:LEU:HD13	1.96	0.47
1:E:192:THR:C	3:R:16:TRP:HH2	2.21	0.47
1:G:91:LYS:HB3	1:G:91:LYS:HE3	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:213:LYS:NZ	2:L:318:ASP:OD2	2.44	0.47
1:A:94:ASN:ND2	3:P:2:ASN:C	2.69	0.47
1:D:172:ILE:HB	1:D:233:VAL:HB	1.96	0.47
1:G:177:ILE:HG12	1:G:256:ILE:HD12	1.95	0.47
3:R:64:VAL:O	3:R:65:GLU:CB	2.62	0.47
3:S:45:GLN:O	3:S:48:VAL:HG12	2.14	0.47
1:I:172:ILE:HB	1:I:233:VAL:HB	1.96	0.47
1:C:139:THR:CG2	3:Q:37:LYS:HE2	2.44	0.47
1:C:171:ARG:HA	1:C:233:VAL:O	2.14	0.47
1:F:148:ARG:HA	1:F:148:ARG:HD3	1.64	0.47
1:H:48:ARG:NH2	1:H:55:LEU:HB2	2.30	0.47
1:I:97:ASP:O	1:I:101:GLN:HG3	2.15	0.47
3:Q:9:VAL:O	4:T:80:ALA:HB2	2.14	0.47
1:D:97:ASP:O	1:D:101:GLN:HG3	2.14	0.47
1:J:97:ASP:O	1:J:101:GLN:HG3	2.15	0.47
1:C:172:ILE:HB	1:C:233:VAL:HB	1.96	0.47
1:H:166:ARG:HA	1:H:235:LEU:HD13	1.96	0.47
1:H:233:VAL:CA	3:S:47:ARG:NH1	2.24	0.47
1:E:97:ASP:O	1:E:101:GLN:HG3	2.15	0.47
2:L:22:ILE:HG22	2:L:23:THR:N	2.29	0.47
3:S:84:LYS:O	3:S:88:LEU:HD13	2.15	0.47
1:A:97:ASP:O	1:A:101:GLN:HG3	2.15	0.46
1:B:189:ILE:HG12	1:B:242:LEU:CD2	2.32	0.46
1:C:97:ASP:O	1:C:101:GLN:HG3	2.15	0.46
1:C:103:MET:SD	3:Q:30:TRP:HB3	2.55	0.46
1:I:137:VAL:HG23	3:S:50:GLN:CD	2.40	0.46
2:L:205:LEU:HG	2:L:321:LEU:HD13	1.97	0.46
3:R:55:GLU:C	3:R:56:LEU:HD12	2.39	0.46
1:F:48:ARG:NH2	1:F:55:LEU:HB2	2.30	0.46
1:J:73:LYS:HG3	1:J:211:GLY:O	2.14	0.46
1:E:148:ARG:HD3	1:E:148:ARG:HA	1.65	0.46
1:F:5:LEU:HD21	3:R:12:ASN:HB2	1.91	0.46
1:G:97:ASP:O	1:G:101:GLN:HG3	2.15	0.46
1:I:266:ARG:CZ	3:S:63:VAL:HG11	2.46	0.46
2:L:9:ALA:HA	2:L:69:ALA:CB	2.46	0.46
3:P:21:THR:HG22	3:P:26:LEU:CD1	2.46	0.46
3:S:94:LEU:O	3:S:98:LEU:HD13	2.16	0.46
1:A:2:ARG:NH2	1:C:210:TYR:OH	2.39	0.46
1:C:148:ARG:HA	1:C:148:ARG:HD3	1.64	0.46
1:H:52:ASP:OD2	1:H:266:ARG:NE	2.45	0.46
2:L:12:PHE:HB2	2:L:64:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:30:TRP:O	3:Q:33:VAL:HG12	2.15	0.46
1:B:151:PHE:C	1:B:152:LYS:HG2	2.41	0.46
3:S:55:GLU:C	3:S:56:LEU:HD12	2.41	0.46
1:F:54:ARG:CG	1:F:54:ARG:NH1	2.78	0.46
1:F:151:PHE:C	1:F:152:LYS:HG2	2.41	0.46
2:L:15:THR:HG23	2:L:61:SER:HB3	1.98	0.46
2:L:135:LEU:H	2:L:135:LEU:HD13	1.78	0.46
3:P:15:VAL:HG13	3:P:15:VAL:O	2.15	0.46
1:B:48:ARG:NH2	1:B:55:LEU:HB2	2.30	0.46
1:I:185:VAL:HB	1:I:219:TYR:CE2	2.51	0.46
1:I:210:TYR:OH	1:J:2:ARG:NH2	2.39	0.46
1:C:99:VAL:C	3:Q:34:GLU:CD	2.80	0.46
1:F:189:ILE:HG12	1:F:242:LEU:CD2	2.32	0.46
1:H:151:PHE:C	1:H:152:LYS:HG2	2.41	0.46
1:H:187:PHE:HE1	1:H:242:LEU:HD11	1.81	0.46
1:D:185:VAL:HB	1:D:219:TYR:CE2	2.51	0.45
1:H:44:ILE:HB	1:H:62:LEU:HB2	1.98	0.45
1:H:148:ARG:HA	1:H:148:ARG:HD3	1.63	0.45
3:P:10:PRO:CG	3:Q:39:ALA:HB1	2.46	0.45
1:D:207:LEU:HD23	1:D:225:LEU:HD21	1.99	0.45
1:H:185:VAL:HB	1:H:219:TYR:CE2	2.52	0.45
1:I:207:LEU:HD23	1:I:225:LEU:HD21	1.99	0.45
2:L:39:ASP:OD2	2:L:63:MET:HE3	2.16	0.45
1:B:44:ILE:HB	1:B:62:LEU:HB2	1.98	0.45
1:B:185:VAL:HB	1:B:219:TYR:CE2	2.52	0.45
2:L:24:ILE:HG12	2:L:80:ASP:HA	1.98	0.45
3:R:22:GLY:O	3:R:26:LEU:HD13	2.16	0.45
1:A:185:VAL:HB	1:A:219:TYR:CE2	2.52	0.45
2:L:153:ILE:HG21	2:L:159:VAL:HG21	1.98	0.45
1:C:95:VAL:HG12	3:Q:31:ALA:HB1	1.95	0.45
1:D:148:ARG:HA	1:D:148:ARG:HD3	1.64	0.45
1:F:187:PHE:HE1	1:F:242:LEU:HD11	1.81	0.45
1:G:185:VAL:HB	1:G:219:TYR:CE2	2.52	0.45
1:C:21:ILE:HB	1:C:116:ILE:HB	1.99	0.45
1:C:185:VAL:HB	1:C:219:TYR:CE2	2.51	0.45
1:E:210:TYR:OH	1:F:2:ARG:NH2	2.39	0.45
1:G:99:VAL:CG1	3:P:31:ALA:HA	2.37	0.45
1:H:230:TYR:O	3:S:41:ALA:HB1	2.17	0.45
1:D:21:ILE:HB	1:D:116:ILE:HB	1.99	0.45
1:F:185:VAL:HB	1:F:219:TYR:CE2	2.52	0.45
1:B:54:ARG:CG	1:B:54:ARG:NH1	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:GLY:HA2	1:B:250:MET:HE3	1.98	0.45
3:R:30:TRP:O	3:R:33:VAL:HG12	2.16	0.45
1:G:95:VAL:CG1	3:P:31:ALA:HB1	2.43	0.45
1:I:21:ILE:HB	1:I:116:ILE:HB	1.99	0.45
1:C:27:GLN:HG3	1:C:135:LYS:HZ1	1.82	0.45
1:D:233:VAL:CA	3:R:47:ARG:NH2	2.80	0.45
1:H:91:LYS:HE3	1:H:91:LYS:HB3	1.79	0.45
1:I:137:VAL:HB	3:S:50:GLN:NE2	2.31	0.45
1:B:21:ILE:HB	1:B:116:ILE:HB	1.99	0.44
1:D:234:LEU:N	3:R:47:ARG:NH2	2.65	0.44
1:E:91:LYS:HB3	1:E:91:LYS:HE3	1.77	0.44
2:L:114:ARG:HA	2:L:334:ARG:HG2	2.00	0.44
1:B:181:GLY:O	1:B:249:THR:N	2.50	0.44
1:B:187:PHE:HE1	1:B:242:LEU:HD11	1.81	0.44
1:F:44:ILE:HB	1:F:62:LEU:HB2	1.98	0.44
1:H:73:LYS:HG3	1:H:211:GLY:O	2.18	0.44
1:I:99:VAL:HG13	3:S:34:GLU:CB	2.47	0.44
1:J:207:LEU:HD23	1:J:225:LEU:HD21	1.99	0.44
2:L:213:LYS:CE	2:L:318:ASP:OD2	2.66	0.44
1:A:93:VAL:HG11	1:A:230:TYR:CD2	2.52	0.44
1:A:171:ARG:HD3	1:A:232:SER:OG	2.17	0.44
1:B:148:ARG:HA	1:B:148:ARG:HD3	1.64	0.44
1:H:186:GLU:CD	1:H:193:LYS:HD3	2.43	0.44
1:B:207:LEU:HD23	1:B:225:LEU:HD21	1.98	0.44
1:C:230:TYR:HH	3:Q:27:ILE:CB	2.21	0.44
1:G:171:ARG:NH2	3:P:23:LEU:CD2	2.76	0.44
1:G:186:GLU:CD	1:G:193:LYS:HD3	2.43	0.44
3:S:22:GLY:O	3:S:26:LEU:HD13	2.18	0.44
1:E:137:VAL:HG23	3:R:50:GLN:HG2	2.00	0.44
1:E:171:ARG:HD3	1:E:232:SER:OG	2.17	0.44
1:F:207:LEU:HD23	1:F:225:LEU:HD21	1.99	0.44
1:F:222:ASP:HB3	1:F:225:LEU:HG	2.00	0.44
1:G:21:ILE:HB	1:G:116:ILE:HB	2.00	0.44
1:J:21:ILE:HB	1:J:116:ILE:HB	2.00	0.44
1:J:171:ARG:HD3	1:J:232:SER:OG	2.17	0.44
1:J:186:GLU:CD	1:J:193:LYS:HD3	2.43	0.44
1:B:91:LYS:HB3	1:B:91:LYS:HE3	1.79	0.44
1:J:185:VAL:HB	1:J:219:TYR:CE2	2.52	0.44
1:E:21:ILE:HB	1:E:116:ILE:HB	2.00	0.44
1:E:186:GLU:CD	1:E:193:LYS:HD3	2.43	0.44
1:G:148:ARG:HA	1:G:148:ARG:HD3	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:ARG:HD3	1:G:232:SER:OG	2.17	0.44
1:H:21:ILE:HB	1:H:116:ILE:HB	1.99	0.44
2:L:32:VAL:HG13	2:L:71:GLU:CG	2.47	0.44
1:A:91:LYS:HB3	1:A:91:LYS:HE3	1.76	0.44
1:D:7:LEU:HD12	1:D:7:LEU:HA	1.79	0.44
1:F:73:LYS:HG3	1:F:211:GLY:O	2.18	0.44
1:F:186:GLU:CD	1:F:193:LYS:HD3	2.43	0.44
1:I:43:GLN:HG2	1:I:121:ASP:HB3	2.00	0.44
1:B:73:LYS:HG3	1:B:211:GLY:O	2.17	0.44
1:H:207:LEU:HD23	1:H:225:LEU:HD21	1.98	0.44
1:J:187:PHE:HE1	1:J:242:LEU:HD11	1.83	0.44
2:L:88:THR:HB	2:L:89:LYS:HG3	1.98	0.44
2:L:205:LEU:HG	2:L:321:LEU:HD12	1.99	0.44
1:E:185:VAL:HB	1:E:219:TYR:CE2	2.52	0.43
1:F:103:MET:HE2	1:F:143:TRP:CG	2.53	0.43
1:G:7:LEU:HD12	1:G:7:LEU:HA	1.81	0.43
1:G:187:PHE:HE1	1:G:242:LEU:HD11	1.83	0.43
1:H:181:GLY:O	1:H:249:THR:N	2.50	0.43
1:H:222:ASP:HB3	1:H:225:LEU:HG	2.00	0.43
1:I:177:ILE:HG12	1:I:256:ILE:HD12	2.00	0.43
3:Q:21:THR:HG22	3:Q:22:GLY:H	1.82	0.43
1:A:222:ASP:HB3	1:A:225:LEU:HG	2.01	0.43
1:B:186:GLU:CD	1:B:193:LYS:HD3	2.43	0.43
1:C:207:LEU:HD23	1:C:225:LEU:HD21	1.99	0.43
1:F:181:GLY:HA2	1:F:250:MET:HE3	1.98	0.43
1:B:103:MET:HE2	1:B:143:TRP:CG	2.53	0.43
1:C:43:GLN:HG2	1:C:121:ASP:HB3	2.00	0.43
1:D:161:ILE:HD12	1:D:246:ILE:HD11	1.99	0.43
1:D:186:GLU:CD	1:D:193:LYS:HD3	2.44	0.43
1:E:93:VAL:HG11	1:E:230:TYR:CD2	2.52	0.43
1:E:135:LYS:HZ1	3:R:55:GLU:CG	2.29	0.43
1:E:207:LEU:HD23	1:E:225:LEU:HD21	1.99	0.43
1:E:222:ASP:HB3	1:E:225:LEU:HG	2.01	0.43
1:F:181:GLY:O	1:F:249:THR:N	2.50	0.43
1:G:93:VAL:HG11	1:G:230:TYR:CD2	2.52	0.43
1:I:93:VAL:O	1:J:96:THR:HG21	2.19	0.43
1:I:137:VAL:CG2	3:S:50:GLN:HG2	2.46	0.43
1:J:60:LYS:HA	2:L:45:ARG:HH22	1.83	0.43
1:A:207:LEU:HD23	1:A:225:LEU:HD21	1.99	0.43
1:B:222:ASP:HB3	1:B:225:LEU:HG	2.00	0.43
1:C:24:PRO:HB3	3:Q:55:GLU:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ILE:HG12	1:C:256:ILE:HD12	2.00	0.43
1:D:177:ILE:HG12	1:D:256:ILE:HD12	2.00	0.43
1:G:171:ARG:HA	1:G:233:VAL:O	2.18	0.43
1:J:172:ILE:HB	1:J:233:VAL:HB	2.00	0.43
2:L:29:GLY:HA3	2:L:74:TYR:CD1	2.54	0.43
1:A:21:ILE:HB	1:A:116:ILE:HB	2.00	0.43
1:A:171:ARG:HA	1:A:233:VAL:O	2.18	0.43
1:A:187:PHE:HE1	1:A:242:LEU:HD11	1.82	0.43
1:G:137:VAL:HG23	3:P:50:GLN:HG2	1.99	0.43
1:I:186:GLU:CD	1:I:193:LYS:HD3	2.44	0.43
1:I:186:GLU:HB3	1:I:245:LYS:HB2	2.01	0.43
2:L:135:LEU:O	2:L:136:ASN:HB2	2.18	0.43
3:Q:45:GLN:O	3:Q:48:VAL:HG12	2.18	0.43
1:H:231:GLN:C	3:S:47:ARG:NH2	2.76	0.43
1:J:93:VAL:HG11	1:J:230:TYR:CD2	2.52	0.43
1:D:176:HIS:HB2	1:D:257:ILE:HB	2.01	0.43
1:E:171:ARG:HA	1:E:233:VAL:O	2.19	0.43
1:E:172:ILE:HB	1:E:233:VAL:HB	2.00	0.43
1:G:43:GLN:HG2	1:G:121:ASP:HB3	2.01	0.43
1:J:43:GLN:HG2	1:J:121:ASP:HB3	2.01	0.43
1:C:183:ASP:CG	1:C:249:THR:HG23	2.41	0.43
1:F:137:VAL:HG23	3:R:18:ASN:HD21	1.76	0.43
2:L:9:ALA:HA	2:L:69:ALA:HB1	2.00	0.43
1:A:172:ILE:HB	1:A:233:VAL:HB	2.00	0.43
1:A:193:LYS:HZ3	1:I:54:ARG:NH2	2.14	0.43
1:F:21:ILE:HB	1:F:116:ILE:HB	1.99	0.43
1:F:91:LYS:HB3	1:F:91:LYS:HE3	1.78	0.43
1:G:196:ASP:O	1:G:198:LEU:N	2.52	0.43
1:G:207:LEU:HD23	1:G:225:LEU:HD21	1.99	0.43
1:H:103:MET:HE2	1:H:143:TRP:CG	2.53	0.43
1:I:161:ILE:HD12	1:I:246:ILE:HD11	1.99	0.43
1:J:196:ASP:O	1:J:198:LEU:N	2.52	0.43
1:E:135:LYS:CE	3:R:55:GLU:CD	2.78	0.43
1:E:196:ASP:O	1:E:198:LEU:N	2.52	0.43
2:L:4:LYS:HG2	2:L:75:TRP:CZ2	2.54	0.43
1:B:7:LEU:HD12	1:B:7:LEU:HA	1.81	0.42
1:B:186:GLU:HB3	1:B:245:LYS:HB2	2.01	0.42
1:C:44:ILE:HB	1:C:62:LEU:HB2	2.02	0.42
1:E:187:PHE:HE1	1:E:242:LEU:HD11	1.83	0.42
1:G:95:VAL:HG12	3:P:31:ALA:HB1	2.00	0.42
1:H:177:ILE:HG12	1:H:256:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:7:LEU:CD2	2:L:71:GLU:HB2	2.49	0.42
2:L:72:ILE:HD12	2:L:72:ILE:N	2.33	0.42
1:A:186:GLU:CD	1:A:193:LYS:HD3	2.43	0.42
1:F:177:ILE:HG12	1:F:256:ILE:HD12	2.01	0.42
1:G:172:ILE:HB	1:G:233:VAL:HB	2.00	0.42
1:H:181:GLY:HA2	1:H:250:MET:HE3	1.98	0.42
1:J:171:ARG:HA	1:J:233:VAL:O	2.18	0.42
1:A:43:GLN:HG2	1:A:121:ASP:HB3	2.01	0.42
1:D:93:VAL:O	1:E:96:THR:HG21	2.19	0.42
1:E:44:ILE:HB	1:E:62:LEU:HB2	2.01	0.42
1:E:103:MET:O	3:R:30:TRP:CZ3	2.71	0.42
2:L:63:MET:C	2:L:64:LEU:HD12	2.44	0.42
1:A:96:THR:HG21	1:C:93:VAL:O	2.19	0.42
1:C:176:HIS:HB2	1:C:257:ILE:HB	2.01	0.42
1:C:186:GLU:CD	1:C:193:LYS:HD3	2.44	0.42
1:D:44:ILE:HB	1:D:62:LEU:HB2	2.01	0.42
1:J:222:ASP:HB3	1:J:225:LEU:HG	2.01	0.42
3:S:71:ALA:O	3:S:72:GLN:CB	2.67	0.42
1:B:97:ASP:O	1:B:101:GLN:HG3	2.20	0.42
1:E:27:GLN:HG3	3:R:55:GLU:OE2	2.18	0.42
1:G:236:ASP:C	1:G:238:MET:N	2.78	0.42
1:I:222:ASP:HB3	1:I:225:LEU:HG	2.02	0.42
2:L:71:GLU:C	2:L:72:ILE:HD12	2.45	0.42
1:I:176:HIS:HB2	1:I:257:ILE:HB	2.01	0.42
3:R:63:VAL:O	3:S:64:VAL:HG23	2.19	0.42
1:A:25:ILE:HD12	1:A:25:ILE:N	2.35	0.42
1:E:43:GLN:HG2	1:E:121:ASP:HB3	2.01	0.42
1:F:186:GLU:HB3	1:F:245:LYS:HB2	2.01	0.42
2:L:135:LEU:HD12	2:L:135:LEU:H	1.61	0.42
1:A:148:ARG:HA	1:A:148:ARG:HD3	1.65	0.42
1:A:196:ASP:O	1:A:198:LEU:N	2.52	0.42
1:B:171:ARG:HD3	1:B:232:SER:OG	2.20	0.42
1:B:171:ARG:HA	1:B:233:VAL:O	2.20	0.42
1:C:186:GLU:HB3	1:C:245:LYS:HB2	2.01	0.42
1:F:97:ASP:O	1:F:101:GLN:HG3	2.20	0.42
1:G:44:ILE:HB	1:G:62:LEU:HB2	2.01	0.42
1:G:113:THR:HG22	3:Q:56:LEU:HD22	2.00	0.42
1:G:222:ASP:HB3	1:G:225:LEU:HG	2.01	0.42
1:H:97:ASP:O	1:H:101:GLN:HG3	2.20	0.42
1:A:62:LEU:HD21	1:A:81:VAL:HG11	2.02	0.42
1:D:43:GLN:HG2	1:D:121:ASP:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:LEU:HD12	1:E:7:LEU:HA	1.81	0.42
1:E:143:TRP:HB2	3:R:30:TRP:CH2	2.54	0.42
1:F:171:ARG:HA	1:F:233:VAL:O	2.20	0.42
1:G:25:ILE:N	1:G:25:ILE:HD12	2.35	0.42
1:H:104:PHE:CE1	1:H:143:TRP:CD1	3.08	0.42
3:R:45:GLN:O	3:R:48:VAL:HG12	2.20	0.42
1:B:62:LEU:HD21	1:B:81:VAL:HG11	2.02	0.42
1:H:54:ARG:CG	1:H:54:ARG:NH1	2.78	0.42
1:I:99:VAL:HG11	3:S:31:ALA:CA	2.50	0.42
1:J:236:ASP:C	1:J:238:MET:N	2.78	0.42
1:D:186:GLU:HB3	1:D:245:LYS:HB2	2.01	0.41
1:D:230:TYR:O	3:R:41:ALA:HB1	2.20	0.41
1:E:160:GLU:HA	1:E:244:LEU:O	2.20	0.41
1:F:60:LYS:HD2	1:F:151:PHE:HZ	1.85	0.41
1:F:171:ARG:HD3	1:F:232:SER:OG	2.20	0.41
1:F:196:ASP:O	1:F:198:LEU:N	2.53	0.41
1:J:62:LEU:HD21	1:J:81:VAL:HG11	2.02	0.41
3:S:62:VAL:O	3:S:62:VAL:HG13	2.20	0.41
1:D:234:LEU:HD23	3:R:43:THR:C	2.45	0.41
1:J:160:GLU:HA	1:J:244:LEU:O	2.20	0.41
1:B:104:PHE:CE1	1:B:143:TRP:CD1	3.08	0.41
1:B:177:ILE:HG12	1:B:256:ILE:HD12	2.01	0.41
1:E:25:ILE:N	1:E:25:ILE:HD12	2.35	0.41
3:S:73:PRO:O	3:S:77:LEU:HD13	2.20	0.41
1:E:236:ASP:C	1:E:238:MET:N	2.78	0.41
1:F:104:PHE:CE1	1:F:143:TRP:CD1	3.08	0.41
1:G:160:GLU:HA	1:G:244:LEU:O	2.20	0.41
1:H:186:GLU:HB3	1:H:245:LYS:HB2	2.01	0.41
1:I:25:ILE:N	1:I:25:ILE:HD12	2.35	0.41
1:I:92:GLY:HA3	1:I:95:VAL:O	2.21	0.41
1:A:44:ILE:HB	1:A:62:LEU:HB2	2.01	0.41
1:D:25:ILE:HD12	1:D:25:ILE:N	2.35	0.41
1:I:143:TRP:CZ3	1:I:262:GLY:HA2	2.56	0.41
1:J:44:ILE:HB	1:J:62:LEU:HB2	2.01	0.41
1:B:100:GLN:OE1	1:B:103:MET:SD	2.79	0.41
1:C:25:ILE:HD12	1:C:25:ILE:N	2.35	0.41
1:C:196:ASP:O	1:C:198:LEU:N	2.54	0.41
1:D:143:TRP:CZ3	1:D:262:GLY:HA2	2.56	0.41
1:D:196:ASP:O	1:D:198:LEU:N	2.54	0.41
1:C:91:LYS:HE3	1:C:91:LYS:HB3	1.79	0.41
1:C:222:ASP:HB3	1:C:225:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:LEU:HD21	1:E:81:VAL:HG11	2.02	0.41
1:A:94:ASN:HB3	3:P:2:ASN:C	2.07	0.41
1:A:236:ASP:C	1:A:238:MET:N	2.78	0.41
1:D:92:GLY:HA3	1:D:95:VAL:O	2.21	0.41
1:E:92:GLY:HA3	1:E:95:VAL:O	2.21	0.41
1:E:95:VAL:CG1	3:R:31:ALA:HB2	2.28	0.41
1:E:108:THR:HA	1:E:111:LEU:HD12	2.03	0.41
1:H:171:ARG:HA	1:H:233:VAL:O	2.20	0.41
1:H:171:ARG:HD3	1:H:232:SER:OG	2.20	0.41
1:H:196:ASP:O	1:H:198:LEU:N	2.53	0.41
1:I:62:LEU:HD21	1:I:81:VAL:HG11	2.03	0.41
1:I:183:ASP:CG	1:I:249:THR:HG23	2.41	0.41
2:L:28:VAL:HG11	2:L:54:ILE:HD11	2.02	0.41
1:B:171:ARG:HH12	3:Q:47:ARG:NH2	2.19	0.41
1:B:267:ASN:OD1	3:R:52:MET:CE	2.51	0.41
1:D:187:PHE:HE1	1:D:242:LEU:HD11	1.86	0.41
1:D:222:ASP:HB3	1:D:225:LEU:HG	2.02	0.41
1:G:108:THR:HA	1:G:111:LEU:HD12	2.03	0.41
1:H:60:LYS:HD2	1:H:151:PHE:HZ	1.85	0.41
1:H:100:GLN:OE1	1:H:103:MET:SD	2.79	0.41
1:I:44:ILE:HB	1:I:62:LEU:HB2	2.01	0.41
1:I:196:ASP:O	1:I:198:LEU:N	2.54	0.41
1:B:22:LYS:NZ	3:R:57:ASP:CG	2.78	0.41
1:B:196:ASP:O	1:B:198:LEU:N	2.53	0.41
1:G:137:VAL:HB	3:P:50:GLN:OE1	2.21	0.41
1:J:92:GLY:HA3	1:J:95:VAL:O	2.21	0.41
2:L:14:GLU:O	2:L:62:VAL:HG12	2.20	0.41
3:P:9:VAL:O	3:P:9:VAL:HG13	2.20	0.41
1:A:92:GLY:HA3	1:A:95:VAL:O	2.21	0.40
1:D:91:LYS:HE3	1:D:91:LYS:HB3	1.79	0.40
1:H:179:ALA:HB3	1:H:182:VAL:HG23	2.03	0.40
1:B:60:LYS:HD2	1:B:151:PHE:HZ	1.85	0.40
1:G:92:GLY:HA3	1:G:95:VAL:O	2.21	0.40
1:I:187:PHE:HE1	1:I:242:LEU:HD11	1.86	0.40
1:D:62:LEU:HD21	1:D:81:VAL:HG11	2.03	0.40
1:D:236:ASP:OD2	3:R:44:GLY:CA	2.63	0.40
1:F:62:LEU:HD21	1:F:81:VAL:HG11	2.02	0.40
1:F:100:GLN:OE1	1:F:103:MET:SD	2.79	0.40
1:G:62:LEU:HD21	1:G:81:VAL:HG11	2.02	0.40
1:J:25:ILE:N	1:J:25:ILE:HD12	2.35	0.40
1:J:186:GLU:HB3	1:J:245:LYS:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:24:ILE:HD13	2:L:79:LEU:C	2.46	0.40
2:L:32:VAL:CG1	2:L:71:GLU:HG2	2.52	0.40
2:L:64:LEU:HD12	2:L:64:LEU:N	2.36	0.40
1:A:186:GLU:HB3	1:A:245:LYS:HB2	2.03	0.40
1:C:139:THR:CG2	3:Q:37:LYS:HZ1	2.11	0.40
1:C:187:PHE:HE1	1:C:242:LEU:HD11	1.86	0.40
1:G:99:VAL:CG2	3:P:34:GLU:HB3	2.40	0.40
1:H:92:GLY:HA3	1:H:95:VAL:O	2.22	0.40
1:A:108:THR:HA	1:A:111:LEU:HD12	2.03	0.40
1:A:160:GLU:HA	1:A:244:LEU:O	2.20	0.40
1:B:179:ALA:HB3	1:B:182:VAL:HG23	2.03	0.40
1:E:87:ARG:HA	1:E:88:PRO:HD3	1.89	0.40
1:F:179:ALA:HB3	1:F:182:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	30	67
1	B	267/269 (99%)	251 (94%)	16 (6%)	0	100	100
1	C	267/269 (99%)	252 (94%)	14 (5%)	1 (0%)	30	67
1	D	267/269 (99%)	251 (94%)	15 (6%)	1 (0%)	30	67
1	E	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	30	67
1	F	267/269 (99%)	251 (94%)	16 (6%)	0	100	100
1	G	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	30	67
1	H	267/269 (99%)	251 (94%)	16 (6%)	0	100	100
1	I	267/269 (99%)	252 (94%)	14 (5%)	1 (0%)	30	67
1	J	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	331/335 (99%)	306 (92%)	19 (6%)	6 (2%)	6	34
3	P	63/104 (61%)	56 (89%)	5 (8%)	2 (3%)	3	21
3	Q	58/104 (56%)	51 (88%)	6 (10%)	1 (2%)	7	36
3	R	61/104 (59%)	53 (87%)	6 (10%)	2 (3%)	3	21
3	S	82/104 (79%)	74 (90%)	6 (7%)	2 (2%)	4	27
4	T	125/127 (98%)	112 (90%)	7 (6%)	6 (5%)	2	16
All	All	3390/3568 (95%)	3160 (93%)	204 (6%)	26 (1%)	16	54

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	32	VAL
2	L	99	PRO
3	R	65	GLU
3	S	72	GLN
4	T	35	PRO
4	T	125	VAL
2	L	18	ASN
3	R	21	THR
4	T	117	SER
4	T	123	SER
2	L	9	ALA
4	T	36	ILE
4	T	101	ARG
2	L	8	ALA
3	P	11	THR
3	Q	12	ASN
1	A	197	LEU
1	E	197	LEU
1	G	197	LEU
1	J	197	LEU
2	L	86	GLN
1	C	197	LEU
1	D	197	LEU
1	I	197	LEU
3	S	62	VAL
3	P	10	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/232 (100%)	213 (92%)	19 (8%)	10	30
1	B	232/232 (100%)	213 (92%)	19 (8%)	10	30
1	C	232/232 (100%)	216 (93%)	16 (7%)	14	36
1	D	232/232 (100%)	216 (93%)	16 (7%)	14	36
1	E	232/232 (100%)	213 (92%)	19 (8%)	10	30
1	F	232/232 (100%)	213 (92%)	19 (8%)	10	30
1	G	232/232 (100%)	212 (91%)	20 (9%)	10	29
1	H	232/232 (100%)	213 (92%)	19 (8%)	10	30
1	I	232/232 (100%)	216 (93%)	16 (7%)	14	36
1	J	232/232 (100%)	213 (92%)	19 (8%)	10	30
2	L	272/285 (95%)	265 (97%)	7 (3%)	40	62
3	P	44/81 (54%)	42 (96%)	2 (4%)	24	46
3	Q	45/81 (56%)	44 (98%)	1 (2%)	45	64
3	R	48/81 (59%)	48 (100%)	0	100	100
3	S	62/81 (76%)	61 (98%)	1 (2%)	55	70
All	All	2791/2929 (95%)	2598 (93%)	193 (7%)	14	36

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	SER
1	A	7	LEU
1	A	42	SER
1	A	60	LYS
1	A	61	THR
1	A	93	VAL
1	A	103	MET
1	A	129	LEU
1	A	144	LEU

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Mol	Chain	Res	Type
1	A	152	LYS
1	A	196	ASP
1	A	199	LYS
1	A	238	MET
1	A	240	GLN
1	A	242	LEU
1	A	251	ASP
1	A	252	GLU
1	A	267	ASN
1	B	1	MET
1	B	3	SER
1	B	7	LEU
1	B	42	SER
1	B	54	ARG
1	B	60	LYS
1	B	61	THR
1	B	93	VAL
1	B	103	MET
1	B	129	LEU
1	B	144	LEU
1	B	154	LEU
1	B	196	ASP
1	B	199	LYS
1	B	231	GLN
1	B	237	GLN
1	B	242	LEU
1	B	251	ASP
1	B	252	GLU
1	C	1	MET
1	C	3	SER
1	C	7	LEU
1	C	42	SER
1	C	60	LYS
1	C	61	THR
1	C	93	VAL
1	C	129	LEU
1	C	144	LEU
1	C	156	ASN
1	C	196	ASP
1	C	199	LYS
1	C	231	GLN
1	C	242	LEU

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Mol	Chain	Res	Type
1	C	251	ASP
1	C	252	GLU
1	D	1	MET
1	D	3	SER
1	D	7	LEU
1	D	42	SER
1	D	60	LYS
1	D	61	THR
1	D	93	VAL
1	D	129	LEU
1	D	144	LEU
1	D	156	ASN
1	D	196	ASP
1	D	199	LYS
1	D	231	GLN
1	D	242	LEU
1	D	251	ASP
1	D	252	GLU
1	E	1	MET
1	E	3	SER
1	E	7	LEU
1	E	42	SER
1	E	60	LYS
1	E	61	THR
1	E	93	VAL
1	E	103	MET
1	E	129	LEU
1	E	144	LEU
1	E	152	LYS
1	E	196	ASP
1	E	199	LYS
1	E	238	MET
1	E	240	GLN
1	E	242	LEU
1	E	251	ASP
1	E	252	GLU
1	E	267	ASN
1	F	1	MET
1	F	3	SER
1	F	7	LEU
1	F	42	SER
1	F	54	ARG

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Mol	Chain	Res	Type
1	F	60	LYS
1	F	61	THR
1	F	93	VAL
1	F	103	MET
1	F	129	LEU
1	F	144	LEU
1	F	154	LEU
1	F	196	ASP
1	F	199	LYS
1	F	231	GLN
1	F	237	GLN
1	F	242	LEU
1	F	251	ASP
1	F	252	GLU
1	G	1	MET
1	G	3	SER
1	G	7	LEU
1	G	42	SER
1	G	58	THR
1	G	60	LYS
1	G	61	THR
1	G	93	VAL
1	G	103	MET
1	G	129	LEU
1	G	144	LEU
1	G	152	LYS
1	G	196	ASP
1	G	199	LYS
1	G	238	MET
1	G	240	GLN
1	G	242	LEU
1	G	251	ASP
1	G	252	GLU
1	G	267	ASN
1	H	1	MET
1	H	3	SER
1	H	7	LEU
1	H	42	SER
1	H	54	ARG
1	H	60	LYS
1	H	61	THR
1	H	93	VAL

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Mol	Chain	Res	Type
1	H	103	MET
1	H	129	LEU
1	H	144	LEU
1	H	154	LEU
1	H	196	ASP
1	H	199	LYS
1	H	231	GLN
1	H	237	GLN
1	H	242	LEU
1	H	251	ASP
1	H	252	GLU
1	I	1	MET
1	I	3	SER
1	I	7	LEU
1	I	42	SER
1	I	60	LYS
1	I	61	THR
1	I	93	VAL
1	I	129	LEU
1	I	144	LEU
1	I	156	ASN
1	I	196	ASP
1	I	199	LYS
1	I	231	GLN
1	I	242	LEU
1	I	251	ASP
1	I	252	GLU
1	J	1	MET
1	J	3	SER
1	J	7	LEU
1	J	42	SER
1	J	60	LYS
1	J	61	THR
1	J	93	VAL
1	J	103	MET
1	J	129	LEU
1	J	144	LEU
1	J	152	LYS
1	J	196	ASP
1	J	199	LYS
1	J	238	MET
1	J	240	GLN

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Mol	Chain	Res	Type
1	J	242	LEU
1	J	251	ASP
1	J	252	GLU
1	J	267	ASN
2	L	24	ILE
2	L	31	LEU
2	L	32	VAL
2	L	115	ASN
2	L	205	LEU
2	L	235	LYS
2	L	245	GLU
3	P	5	VAL
3	P	21	THR
3	Q	21	THR
3	S	32	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	B	27	GLN
1	B	94	ASN
1	B	100	GLN
1	B	156	ASN
1	B	217	ASN
1	B	237	GLN
1	C	27	GLN
1	C	156	ASN
1	D	94	ASN
1	D	156	ASN
1	E	240	GLN
1	E	253	GLN
1	F	27	GLN
1	F	100	GLN
1	F	237	GLN
1	G	27	GLN
1	G	155	ASN
1	H	27	GLN
1	H	237	GLN
1	I	156	ASN
1	J	27	GLN
2	L	97	GLN

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Mol	Chain	Res	Type
2	L	115	ASN
2	L	152	GLN
3	R	18	ASN
3	S	50	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	L	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	88:THR	C	89:LYS	N	2.88
1	L	169:ARG	C	170:VAL	N	1.94
1	L	324:VAL	C	325:LYS	N	1.63

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	269/269 (100%)	1.12	65 (24%) 2 9	40, 40, 40, 40	0
1	B	269/269 (100%)	1.33	63 (23%) 2 9	40, 40, 40, 40	0
1	C	269/269 (100%)	0.67	43 (15%) 5 12	40, 40, 40, 40	0
1	D	269/269 (100%)	0.97	58 (21%) 2 9	40, 40, 40, 40	0
1	E	269/269 (100%)	1.23	63 (23%) 2 9	40, 40, 40, 40	0
1	F	269/269 (100%)	0.44	30 (11%) 10 18	40, 40, 40, 40	0
1	G	269/269 (100%)	1.09	65 (24%) 2 9	40, 40, 40, 40	0
1	H	269/269 (100%)	0.99	57 (21%) 2 10	40, 40, 40, 40	0
1	I	269/269 (100%)	0.88	47 (17%) 4 12	40, 40, 40, 40	0
1	J	269/269 (100%)	1.16	61 (22%) 2 9	40, 40, 40, 40	0
2	L	335/335 (100%)	0.69	50 (14%) 5 14	40, 40, 40, 40	0
3	P	65/104 (62%)	1.94	23 (35%) 1 6	40, 40, 40, 40	0
3	Q	60/104 (57%)	1.55	15 (25%) 2 8	40, 40, 40, 40	0
3	R	63/104 (60%)	1.58	14 (22%) 2 9	40, 40, 40, 40	0
3	S	84/104 (80%)	1.64	23 (27%) 1 8	40, 40, 40, 40	0
4	T	127/127 (100%)	0.78	18 (14%) 6 15	40, 40, 40, 40	0
All	All	3424/3568 (95%)	1.01	695 (20%) 3 10	40, 40, 40, 40	0

All (695) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	S	21	THR	19.1
1	E	237	GLN	16.6
3	P	64	VAL	14.8
2	L	42	GLU	13.0
1	J	78	ALA	12.5

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Mol	Chain	Res	Type	RSRZ
2	L	41	GLY	11.6
1	D	216	ASP	11.2
2	L	58	ASN	11.1
1	G	78	ALA	10.8
3	R	18	ASN	10.6
1	J	237	GLN	10.2
1	J	18	SER	10.0
1	B	75	LYS	9.9
1	H	237	GLN	9.3
1	E	168	VAL	9.2
3	R	15	VAL	9.2
1	B	42	SER	9.1
1	A	267	ASN	9.1
1	G	122	GLU	8.8
1	J	77	LYS	8.8
1	E	269	PHE	8.7
1	B	122	GLU	8.7
1	I	60	LYS	8.7
1	A	237	GLN	8.4
1	I	78	ALA	8.3
2	L	17	LYS	8.3
3	R	17	GLY	8.1
1	G	216	ASP	8.0
3	P	4	SER	8.0
1	B	237	GLN	7.8
4	T	98	HIS	7.7
1	B	110	GLY	7.5
3	P	17	GLY	7.5
1	D	183	ASP	7.5
1	J	267	ASN	7.4
1	A	240	GLN	7.4
1	D	217	ASN	7.4
1	G	237	GLN	7.3
1	D	125	ALA	7.3
3	Q	18	ASN	7.2
1	H	240	GLN	7.2
3	P	3	THR	7.1
3	R	19	VAL	7.1
1	B	78	ALA	7.0
1	E	8	ASN	7.0
1	C	60	LYS	7.0
1	A	168	VAL	7.0

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Mol	Chain	Res	Type	RSRZ
2	L	57	MET	6.9
3	P	65	GLU	6.9
3	S	24	ASP	6.9
1	B	77	LYS	6.9
1	H	191	GLY	6.9
1	B	269	PHE	6.8
1	J	75	LYS	6.8
4	T	97	ASP	6.8
1	E	53	GLY	6.8
2	L	209	PRO	6.7
1	E	268	GLY	6.7
1	C	8	ASN	6.6
1	B	60	LYS	6.6
3	R	45	GLN	6.6
1	C	216	ASP	6.5
1	J	1	MET	6.4
1	A	18	SER	6.4
1	E	267	ASN	6.4
1	C	237	GLN	6.4
1	B	55	LEU	6.4
1	B	267	ASN	6.3
3	P	5	VAL	6.3
1	J	168	VAL	6.3
2	L	60	THR	6.3
1	E	238	MET	6.2
1	B	268	GLY	6.2
3	P	10	PRO	6.2
1	G	140	ALA	6.1
3	S	104	LYS	6.1
1	A	8	ASN	6.1
1	J	2	ARG	6.1
3	Q	57	ASP	6.1
4	T	1	MET	6.1
3	S	23	LEU	6.1
1	D	78	ALA	6.0
1	H	190	ASP	6.0
1	B	45	LYS	6.0
1	G	77	LYS	6.0
1	E	54	ARG	5.9
1	C	42	SER	5.9
1	E	55	LEU	5.9
1	F	9	SER	5.7

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Mol	Chain	Res	Type	RSRZ
2	L	23	THR	5.7
1	J	238	MET	5.7
1	J	94	ASN	5.6
3	S	51	ALA	5.6
1	B	54	ARG	5.6
1	J	122	GLU	5.6
1	A	214	VAL	5.6
1	B	46	ASN	5.6
2	L	51	GLY	5.5
1	H	122	GLU	5.5
1	B	263	VAL	5.5
1	F	8	ASN	5.5
1	A	238	MET	5.4
1	H	245	LYS	5.3
1	A	93	VAL	5.3
3	P	11	THR	5.3
1	J	8	ASN	5.3
1	J	53	GLY	5.3
1	E	236	ASP	5.2
1	H	160	GLU	5.2
1	I	122	GLU	5.2
1	D	42	SER	5.2
1	H	158	THR	5.1
3	R	14	SER	5.1
1	B	123	ALA	5.1
1	A	112	THR	5.1
1	G	269	PHE	5.0
3	Q	59	GLY	5.0
1	A	249	THR	5.0
1	B	63	ASN	5.0
1	I	46	ASN	5.0
1	I	216	ASP	5.0
3	Q	60	ALA	5.0
3	P	63	VAL	4.9
3	Q	17	GLY	4.9
3	S	22	GLY	4.9
1	D	126	GLY	4.9
1	D	153	GLN	4.8
1	E	182	VAL	4.8
1	B	12	ASN	4.8
1	D	12	ASN	4.8
1	B	53	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	58	THR	4.8
1	G	110	GLY	4.8
1	G	112	THR	4.8
4	T	76	ASP	4.7
4	T	69	ASP	4.7
3	P	19	VAL	4.7
4	T	99	GLU	4.7
1	I	145	THR	4.7
1	J	128	LYS	4.7
1	E	9	SER	4.6
1	D	222	ASP	4.6
1	I	237	GLN	4.6
1	B	156	ASN	4.6
1	G	208	GLU	4.6
3	P	62	VAL	4.6
1	B	99	VAL	4.6
1	E	122	GLU	4.6
1	D	209	GLN	4.6
1	I	12	ASN	4.6
1	G	18	SER	4.6
2	L	175	SER	4.6
1	G	266	ARG	4.5
3	S	32	ARG	4.5
3	Q	8	SER	4.5
1	H	125	ALA	4.5
1	A	26	GLY	4.5
1	A	53	GLY	4.5
1	G	75	LYS	4.5
3	P	1	MET	4.5
1	B	168	VAL	4.5
1	G	205	TYR	4.5
1	I	138	GLY	4.5
2	L	259	THR	4.5
3	S	64	VAL	4.5
1	G	12	ASN	4.5
1	H	156	ASN	4.5
1	C	94	ASN	4.4
1	D	158	THR	4.4
1	A	122	GLU	4.4
3	Q	29	GLY	4.4
1	B	96	THR	4.4
1	D	63	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
3	Q	54	PRO	4.4
2	L	43	GLY	4.3
1	J	26	GLY	4.3
1	H	9	SER	4.3
1	I	269	PHE	4.3
3	R	21	THR	4.3
1	H	195	ARG	4.3
1	E	212	LYS	4.3
1	G	73	LYS	4.3
1	B	18	SER	4.3
3	Q	7	THR	4.3
2	L	242	GLU	4.2
1	H	267	ASN	4.2
1	A	183	ASP	4.2
1	D	180	ALA	4.1
1	J	55	LEU	4.1
1	H	251	ASP	4.1
2	L	40	GLY	4.1
1	G	123	ALA	4.1
1	B	9	SER	4.1
1	A	16	GLY	4.1
1	G	109	VAL	4.0
3	S	52	MET	4.0
4	T	37	ALA	4.0
1	F	54	ARG	4.0
2	L	55	LYS	4.0
1	G	255	GLU	4.0
1	J	76	ILE	4.0
1	C	168	VAL	4.0
1	H	238	MET	4.0
1	J	227	GLY	4.0
1	C	220	THR	4.0
2	L	136	ASN	4.0
1	A	158	THR	4.0
3	Q	65	GLU	3.9
1	H	241	ASP	3.9
1	H	123	ALA	3.9
1	G	94	ASN	3.9
1	A	110	GLY	3.9
1	D	123	ALA	3.9
1	E	123	ALA	3.9
1	H	216	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	I	180	ALA	3.9
2	L	275	MET	3.9
1	E	18	SER	3.9
4	T	96	LEU	3.9
1	A	255	GLU	3.9
1	A	54	ARG	3.9
1	J	158	THR	3.9
3	S	54	PRO	3.9
1	A	94	ASN	3.9
1	H	199	LYS	3.8
1	G	169	GLY	3.8
1	A	266	ARG	3.8
1	B	266	ARG	3.8
1	A	78	ALA	3.8
1	E	166	ARG	3.8
1	H	243	ARG	3.8
1	I	236	ASP	3.8
1	I	14	ALA	3.8
2	L	184	GLU	3.8
1	J	231	GLN	3.8
1	J	137	VAL	3.8
2	L	47	ILE	3.8
1	J	226	GLU	3.8
1	C	267	ASN	3.7
1	G	209	GLN	3.7
1	B	121	ASP	3.7
1	G	2	ARG	3.7
1	B	94	ASN	3.7
1	C	180	ALA	3.7
1	F	53	GLY	3.7
1	D	267	ASN	3.7
1	A	254	ALA	3.7
1	I	13	VAL	3.7
1	D	255	GLU	3.7
3	Q	16	TRP	3.7
1	C	22	LYS	3.7
1	C	12	ASN	3.7
1	A	99	VAL	3.7
4	T	3	ASN	3.6
1	F	110	GLY	3.6
1	F	122	GLU	3.6
1	B	20	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	I	63	ASN	3.6
1	G	139	THR	3.6
1	D	245	LYS	3.6
1	J	160	GLU	3.6
1	G	182	VAL	3.6
1	D	1	MET	3.6
1	G	1	MET	3.6
1	I	183	ASP	3.6
1	F	199	LYS	3.6
1	J	24	PRO	3.6
3	S	70	ALA	3.6
1	H	223	PHE	3.6
1	D	238	MET	3.6
2	L	200	ASP	3.6
1	G	152	LYS	3.6
1	G	263	VAL	3.6
1	B	76	ILE	3.6
1	C	253	GLN	3.6
1	G	253	GLN	3.6
1	D	76	ILE	3.6
1	E	217	ASN	3.6
1	F	267	ASN	3.6
1	H	109	VAL	3.6
1	C	58	THR	3.6
1	G	129	LEU	3.5
1	J	266	ARG	3.5
1	B	240	GLN	3.5
2	L	62	VAL	3.5
1	E	114	CYS	3.5
1	J	199	LYS	3.5
3	P	7	THR	3.5
1	D	38	GLY	3.5
1	E	216	ASP	3.5
1	A	160	GLU	3.5
1	D	40	THR	3.5
1	I	54	ARG	3.5
1	B	219	TYR	3.5
1	I	16	GLY	3.5
1	D	110	GLY	3.5
1	E	71	ARG	3.4
1	J	110	GLY	3.4
1	J	117	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	201	ALA	3.4
1	C	240	GLN	3.4
1	G	35	ARG	3.4
1	J	54	ARG	3.4
3	R	56	LEU	3.4
1	J	22	LYS	3.4
1	E	52	ASP	3.4
1	G	201	ALA	3.4
1	D	191	GLY	3.4
1	H	26	GLY	3.4
1	H	126	GLY	3.4
3	S	55	GLU	3.3
1	C	110	GLY	3.3
1	I	62	LEU	3.3
3	R	29	GLY	3.3
1	E	115	GLU	3.3
1	G	251	ASP	3.3
1	D	249	THR	3.3
1	A	125	ALA	3.3
1	D	254	ALA	3.3
2	L	8	ALA	3.3
1	G	115	GLU	3.3
1	A	169	GLY	3.3
3	S	35	GLN	3.3
1	J	269	PHE	3.3
1	I	58	THR	3.3
1	D	250	MET	3.3
1	J	262	GLY	3.3
1	A	55	LEU	3.3
1	B	25	ILE	3.3
1	C	217	ASN	3.3
1	I	200	LYS	3.3
1	I	168	VAL	3.3
3	P	18	ASN	3.2
1	B	115	GLU	3.2
3	S	69	LYS	3.2
1	G	42	SER	3.2
1	H	110	GLY	3.2
1	D	266	ARG	3.2
1	F	1	MET	3.2
1	D	199	LYS	3.2
4	T	2	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	26	GLY	3.2
1	D	140	ALA	3.2
1	A	75	LYS	3.2
1	E	72	HIS	3.2
1	C	18	SER	3.2
1	C	214	VAL	3.2
1	A	209	GLN	3.2
1	F	24	PRO	3.2
1	I	127	PRO	3.2
1	A	180	ALA	3.2
1	F	125	ALA	3.2
1	E	63	ASN	3.2
1	B	230	TYR	3.2
1	B	58	THR	3.1
1	B	159	THR	3.1
1	H	192	THR	3.1
1	D	253	GLN	3.1
1	D	77	LYS	3.1
4	T	34	LYS	3.1
3	P	6	PRO	3.1
3	S	103	ASN	3.1
1	I	214	VAL	3.1
1	G	254	ALA	3.1
3	P	61	ALA	3.1
1	F	42	SER	3.1
1	A	137	VAL	3.1
1	I	166	ARG	3.1
1	H	128	LYS	3.1
1	E	169	GLY	3.1
1	J	16	GLY	3.1
1	B	185	VAL	3.1
2	L	143	ARG	3.1
1	G	194	TRP	3.1
1	C	45	LYS	3.1
1	C	16	GLY	3.0
1	B	218	THR	3.0
1	E	42	SER	3.0
1	A	22	LYS	3.0
1	F	214	VAL	3.0
1	J	166	ARG	3.0
1	I	15	ALA	3.0
1	H	197	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	268	GLY	3.0
1	G	249	THR	3.0
2	L	15	THR	3.0
1	H	266	ARG	3.0
3	P	21	THR	3.0
1	G	238	MET	3.0
1	E	35	ARG	3.0
1	C	241	ASP	3.0
2	L	252	LYS	3.0
1	C	264	TRP	3.0
1	I	234	LEU	3.0
1	B	265	SER	2.9
1	E	138	GLY	2.9
3	Q	10	PRO	2.9
1	A	208	GLU	2.9
1	D	252	GLU	2.9
1	F	76	ILE	2.9
1	I	2	ARG	2.9
1	B	119	ASP	2.9
1	C	61	THR	2.9
1	E	130	SER	2.9
1	I	88	PRO	2.9
1	F	266	ARG	2.9
1	G	155	ASN	2.9
2	L	18	ASN	2.9
1	I	253	GLN	2.9
1	F	22	LYS	2.9
1	B	93	VAL	2.9
1	G	178	LYS	2.9
1	J	126	GLY	2.9
1	A	263	VAL	2.9
1	D	37	SER	2.9
1	E	213	ALA	2.9
1	G	163	ASP	2.9
1	E	156	ASN	2.9
1	G	149	ASN	2.9
1	B	246	ILE	2.9
4	T	39	PHE	2.9
1	B	220	THR	2.9
1	G	265	SER	2.9
1	I	249	THR	2.9
1	I	137	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	165	PRO	2.8
3	S	25	ALA	2.8
1	B	158	THR	2.8
1	E	245	LYS	2.8
2	L	144	LYS	2.8
1	A	216	ASP	2.8
1	G	4	PHE	2.8
1	E	160	GLU	2.8
1	A	230	TYR	2.8
1	C	117	LYS	2.8
3	Q	45	GLN	2.8
3	R	63	VAL	2.8
1	D	218	THR	2.8
1	F	137	VAL	2.8
1	B	169	GLY	2.8
1	D	214	VAL	2.8
1	C	122	GLU	2.8
1	F	75	LYS	2.8
1	J	228	ASP	2.8
1	F	236	ASP	2.8
1	D	151	PHE	2.8
1	A	152	LYS	2.7
1	A	199	LYS	2.7
1	E	145	THR	2.7
1	J	249	THR	2.7
2	L	86	GLN	2.7
1	D	163	ASP	2.7
1	A	217	ASN	2.7
1	G	63	ASN	2.7
2	L	20	ASN	2.7
2	L	38	ALA	2.7
2	L	229	TYR	2.7
1	E	265	SER	2.7
1	A	52	ASP	2.7
1	A	236	ASP	2.7
1	E	33	ASP	2.7
1	B	117	LYS	2.7
1	C	128	LYS	2.7
1	I	126	GLY	2.7
2	L	67	GLU	2.7
1	D	211	GLY	2.7
1	H	38	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	162	ALA	2.7
1	G	214	VAL	2.7
3	Q	9	VAL	2.7
3	S	90	PHE	2.7
1	I	139	THR	2.7
1	H	252	GLU	2.7
1	B	61	THR	2.7
1	F	18	SER	2.7
1	I	110	GLY	2.7
1	H	80	VAL	2.6
3	R	6	PRO	2.6
1	D	225	LEU	2.6
1	A	27	GLN	2.6
1	J	163	ASP	2.6
1	E	250	MET	2.6
1	G	217	ASN	2.6
1	B	114	CYS	2.6
1	C	190	ASP	2.6
1	J	125	ALA	2.6
2	L	73	GLU	2.6
3	R	35	GLN	2.6
1	H	53	GLY	2.6
1	E	125	ALA	2.6
1	C	243	ARG	2.6
1	J	93	VAL	2.6
1	E	37	SER	2.6
1	H	151	PHE	2.6
1	G	16	GLY	2.6
1	H	208	GLU	2.6
1	H	12	ASN	2.6
1	J	180	ALA	2.6
1	D	128	LYS	2.6
1	F	216	ASP	2.6
1	A	182	VAL	2.6
1	B	140	ALA	2.6
1	H	63	ASN	2.6
3	P	33	VAL	2.6
1	E	1	MET	2.6
1	A	151	PHE	2.5
1	G	176	HIS	2.5
1	I	77	LYS	2.5
1	D	190	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	188	GLN	2.5
1	I	17	ASN	2.5
1	I	111	LEU	2.5
1	D	263	VAL	2.5
2	L	1	MET	2.5
1	B	10	ILE	2.5
1	J	7	LEU	2.5
1	B	157	GLY	2.5
1	H	157	GLY	2.5
3	S	48	VAL	2.5
1	E	201	ALA	2.5
1	J	213	ALA	2.5
1	J	224	MET	2.5
1	H	153	GLN	2.5
1	D	210	TYR	2.5
1	D	41	PRO	2.5
1	A	109	VAL	2.5
1	A	5	LEU	2.5
1	C	238	MET	2.5
1	A	265	SER	2.5
1	A	117	LYS	2.5
1	A	269	PHE	2.5
1	E	151	PHE	2.5
2	L	154	ASN	2.5
1	J	145	THR	2.5
1	D	137	VAL	2.5
1	F	26	GLY	2.5
2	L	225	GLY	2.5
1	H	225	LEU	2.4
1	H	89	GLU	2.4
2	L	176	ALA	2.4
1	B	48	ARG	2.4
1	I	241	ASP	2.4
1	H	264	TRP	2.4
2	L	59	TYR	2.4
4	T	94	GLU	2.4
1	E	22	LYS	2.4
1	J	169	GLY	2.4
1	F	78	ALA	2.4
2	L	44	LEU	2.4
3	S	56	LEU	2.4
4	T	127	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	12	ASN	2.4
1	I	81	VAL	2.4
1	B	134	GLN	2.4
1	C	250	MET	2.4
1	J	73	LYS	2.4
3	Q	37	LYS	2.4
1	E	222	ASP	2.4
1	G	102	ARG	2.4
1	G	117	LYS	2.4
2	L	277	THR	2.4
1	E	126	GLY	2.4
1	H	42	SER	2.4
4	T	85	HIS	2.4
1	B	40	THR	2.4
1	C	115	GLU	2.4
1	E	59	TYR	2.4
1	E	148	ARG	2.4
1	A	200	LYS	2.4
1	E	46	ASN	2.4
1	H	217	ASN	2.4
1	A	115	GLU	2.3
1	A	213	ALA	2.3
1	I	250	MET	2.3
3	S	73	PRO	2.3
1	E	240	GLN	2.3
1	G	268	GLY	2.3
2	L	130	GLU	2.3
1	C	113	THR	2.3
1	G	168	VAL	2.3
1	H	16	GLY	2.3
3	R	61	ALA	2.3
1	G	93	VAL	2.3
1	J	264	TRP	2.3
1	B	151	PHE	2.3
1	C	188	GLN	2.3
1	C	93	VAL	2.3
1	D	261	MET	2.3
1	C	9	SER	2.3
1	A	25	ILE	2.3
1	G	257	ILE	2.3
1	G	231	GLN	2.3
3	S	68	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	251	ASP	2.3
1	G	52	ASP	2.3
1	B	253	GLN	2.3
1	J	115	GLU	2.3
1	A	113	THR	2.3
1	E	249	THR	2.3
2	L	335	THR	2.3
1	D	75	LYS	2.2
1	J	35	ARG	2.2
1	F	25	ILE	2.2
1	A	128	LYS	2.2
1	B	22	LYS	2.2
1	B	129	LEU	2.2
1	G	96	THR	2.2
1	J	3	SER	2.2
1	A	177	ILE	2.2
1	D	205	TYR	2.2
2	L	81	TYR	2.2
1	B	133	ALA	2.2
1	E	211	GLY	2.2
1	E	2	ARG	2.2
1	D	188	GLN	2.2
1	I	151	PHE	2.2
1	J	183	ASP	2.2
1	E	149	ASN	2.2
3	R	25	ALA	2.2
4	T	57	ASN	2.2
4	T	118	THR	2.2
1	F	3	SER	2.2
1	F	128	LYS	2.2
1	I	160	GLU	2.2
1	E	81	VAL	2.2
1	A	140	ALA	2.2
1	A	191	GLY	2.2
1	B	26	GLY	2.2
3	S	38	ALA	2.2
1	A	252	GLU	2.2
1	C	54	ARG	2.2
3	P	60	ALA	2.2
1	E	199	LYS	2.2
1	H	249	THR	2.2
1	A	37	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	57	SER	2.2
1	D	208	GLU	2.2
1	H	95	VAL	2.2
1	F	2	ARG	2.2
1	H	247	ASP	2.1
1	H	8	ASN	2.1
2	L	235	LYS	2.1
1	C	40	THR	2.1
1	I	61	THR	2.1
1	B	95	VAL	2.1
1	A	35	ARG	2.1
1	F	230	TYR	2.1
1	H	99	VAL	2.1
2	L	49	ARG	2.1
1	D	184	ALA	2.1
2	L	165	ASP	2.1
1	D	129	LEU	2.1
1	D	13	VAL	2.1
1	G	185	VAL	2.1
1	E	243	ARG	2.1
1	G	158	THR	2.1
1	H	139	THR	2.1
1	J	71	ARG	2.1
1	J	130	SER	2.1
1	D	193	LYS	2.1
1	J	165	PRO	2.1
1	J	214	VAL	2.1
1	I	94	ASN	2.1
1	H	96	THR	2.1
2	L	246	THR	2.1
3	P	35	GLN	2.1
1	D	247	ASP	2.1
1	C	46	ASN	2.1
3	P	12	ASN	2.1
1	C	151	PHE	2.1
2	L	142	GLY	2.1
1	E	47	VAL	2.1
1	H	33	ASP	2.1
1	C	53	GLY	2.1
1	E	180	ALA	2.1
1	H	149	ASN	2.1
1	J	240	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	183	ASP	2.0
1	A	268	GLY	2.0
1	G	79	GLY	2.0
1	H	180	ALA	2.0
3	P	36	ILE	2.0
3	S	66	ALA	2.0
1	I	153	GLN	2.0
2	L	110	GLU	2.0
1	F	48	ARG	2.0
1	G	236	ASP	2.0
2	L	46	THR	2.0
1	G	9	SER	2.0
3	P	8	SER	2.0
1	J	219	TYR	2.0
1	E	92	GLY	2.0
4	T	116	ALA	2.0
1	G	247	ASP	2.0
1	F	258	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	J	1270	1/1	0.93	0.32	40,40,40,40	0
5	CA	D	1270	1/1	0.99	0.04	40,40,40,40	0
5	CA	G	1270	1/1	0.99	0.05	40,40,40,40	0
5	CA	H	1270	1/1	0.99	0.09	40,40,40,40	0
5	CA	C	1270	1/1	0.99	0.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	L	400	1/1	0.99	0.07	40,40,40,40	0
5	CA	A	1270	1/1	1.00	0.09	40,40,40,40	0
5	CA	B	1270	1/1	1.00	0.10	40,40,40,40	0
5	CA	I	1270	1/1	1.00	0.06	40,40,40,40	0
5	CA	E	1270	1/1	1.00	0.20	40,40,40,40	0
5	CA	F	1270	1/1	1.00	0.11	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.