



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:08 AM GMT

PDB ID : 2W0C
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

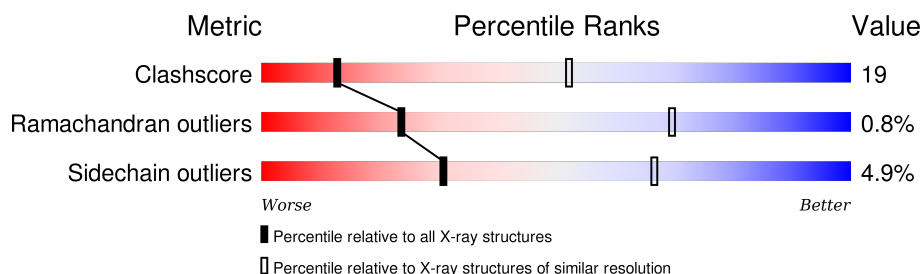
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)





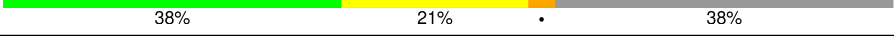
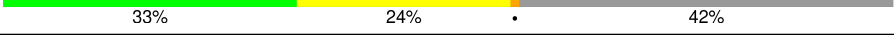
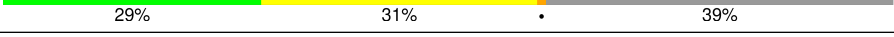


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	269	
1	B	269	
1	C	269	
1	D	269	
1	E	269	
1	F	269	
1	G	269	

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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 (three-letter code: CA) (formula: Ca).

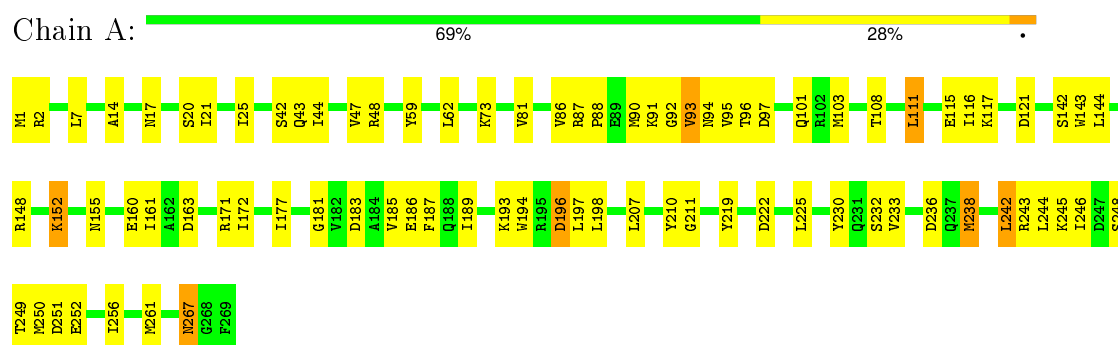
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Ca	0	0
			1	1		
5	J	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	E	1	Total	Ca	0	0
			1	1		
5	H	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	I	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		
5	A	1	Total	Ca	0	0
			1	1		
5	L	1	Total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

3 Residue-property plots [i](#)

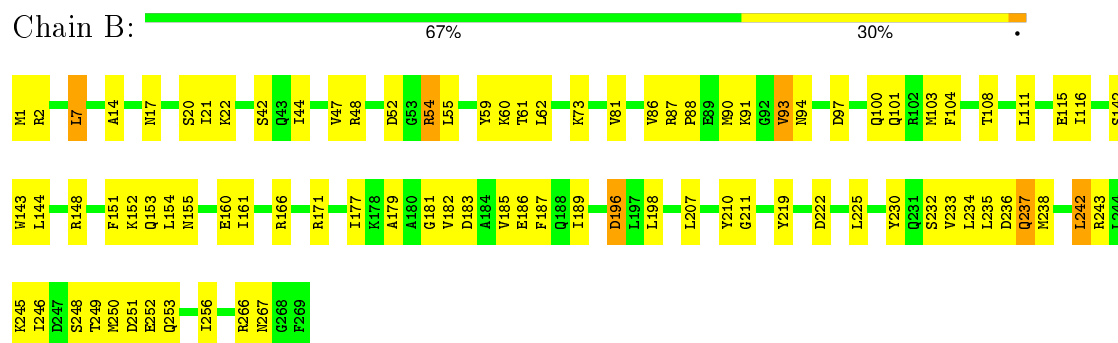
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS failed to run properly.

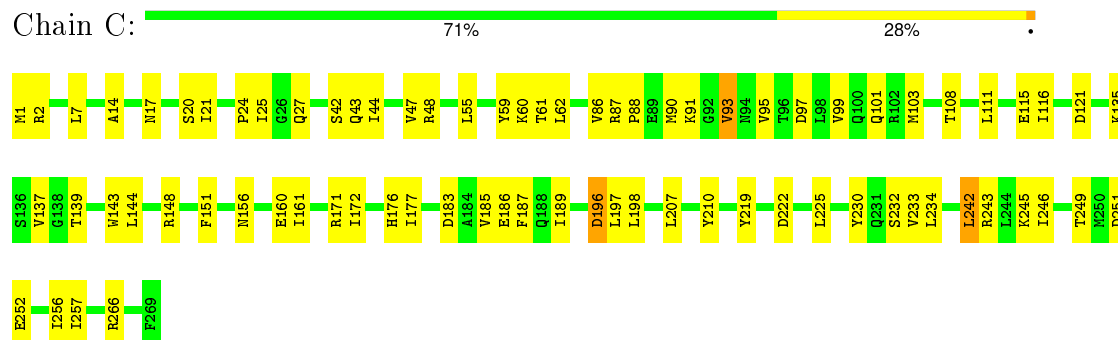
• Molecule 1: MAJOR CAPSID PROTEIN P2



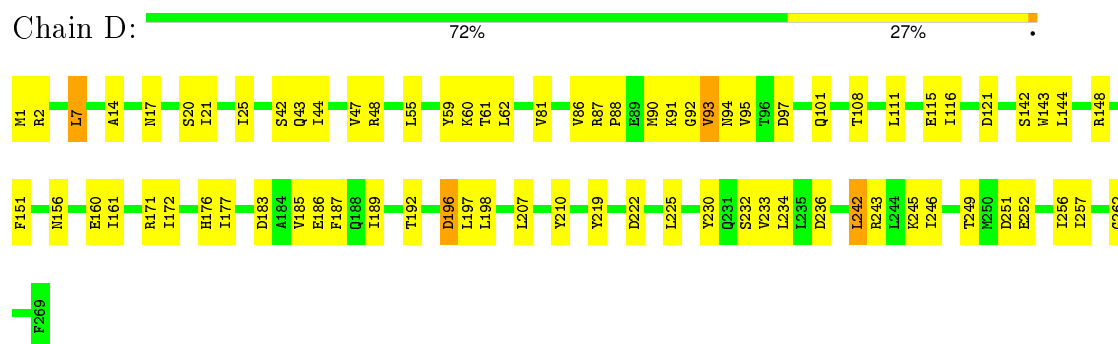
• Molecule 1: MAJOR CAPSID PROTEIN P2



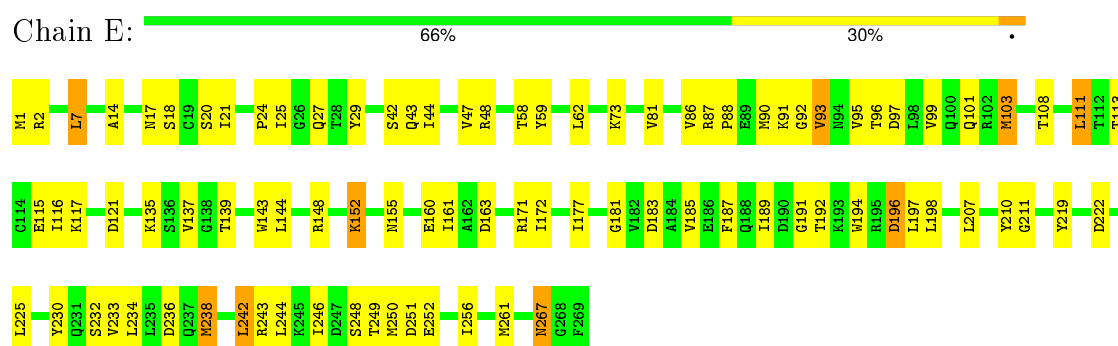
• Molecule 1: MAJOR CAPSID PROTEIN P2



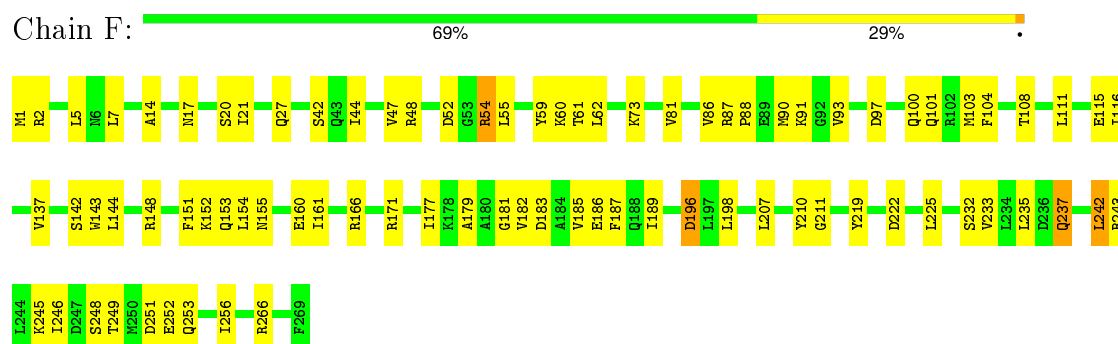
• Molecule 1: MAJOR CAPSID PROTEIN P2



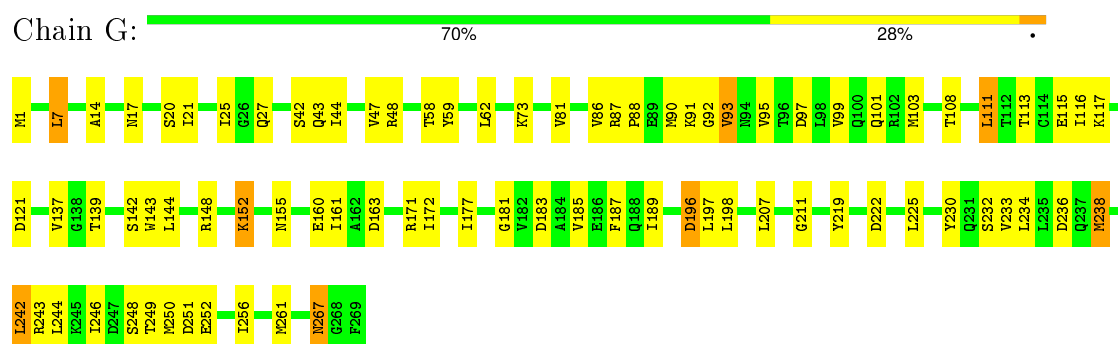
• Molecule 1: MAJOR CAPSID PROTEIN P2



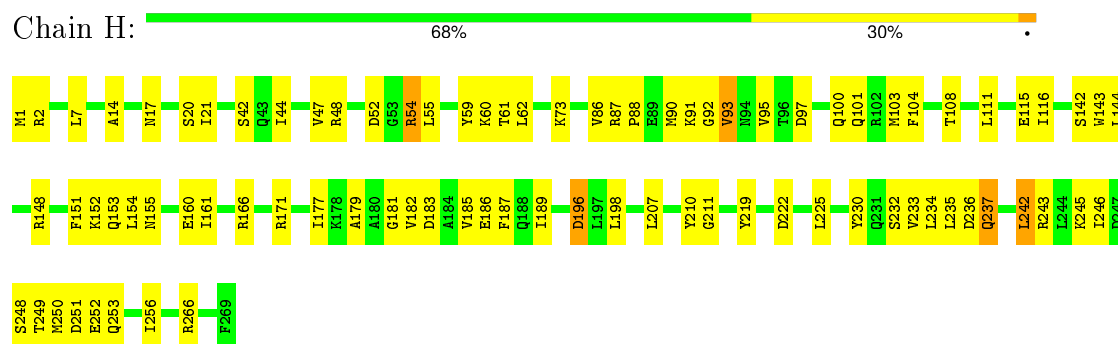
• Molecule 1: MAJOR CAPSID PROTEIN P2



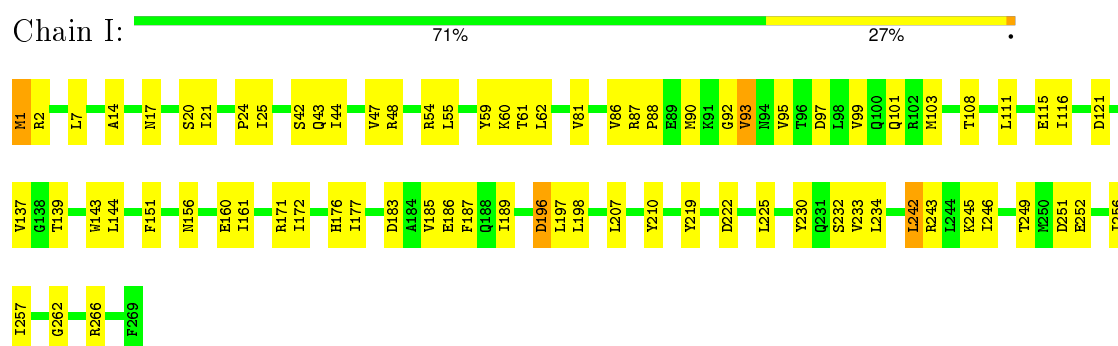
• Molecule 1: MAJOR CAPSID PROTEIN P2



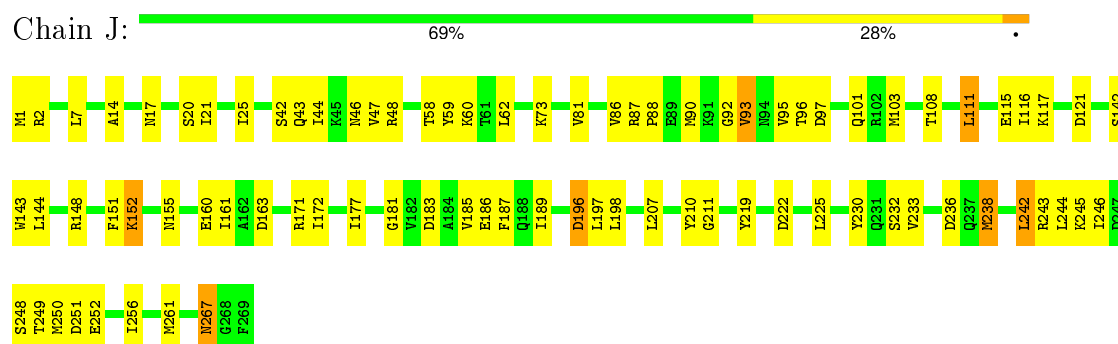
- Molecule 1: MAJOR CAPSID PROTEIN P2



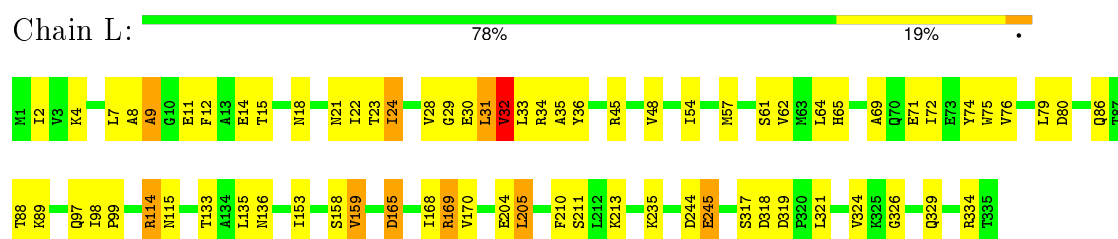
- Molecule 1: MAJOR CAPSID PROTEIN P2



- Molecule 1: MAJOR CAPSID PROTEIN P2

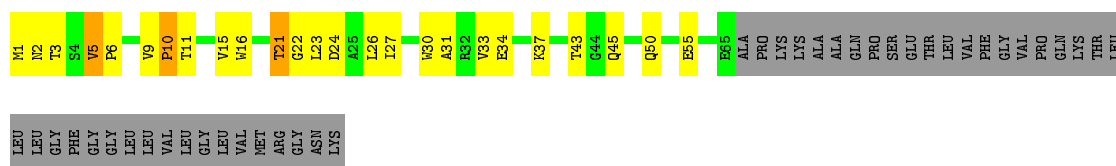


- Molecule 2: PROTEIN 2

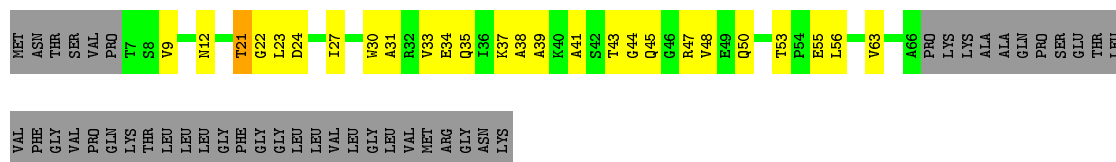
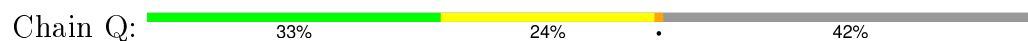


- Molecule 3: PROTEIN P3

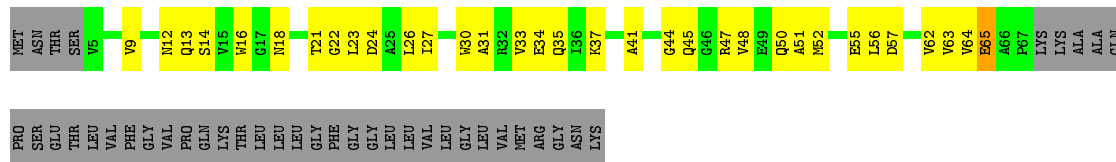
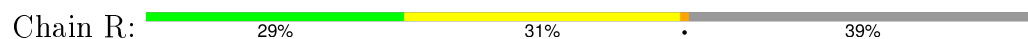




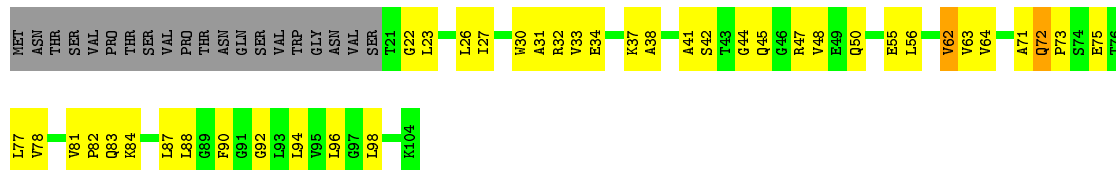
- Molecule 3: PROTEIN P3



- Molecule 3: PROTEIN P3



- Molecule 3: PROTEIN P3



- Molecule 4: PROTEIN P6



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

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	Depositor
% Data completeness (in resolution range)	82.9 (96.00-7.00)	Depositor
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)	Depositor
Wilson B-factor (Å ²)	132.6	Xtriage
Anisotropy	0.244	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	0 of 851677 reflections	Xtriage
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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.29	1/2158 (0.0%)	0.45	1/2917 (0.0%)
1	B	0.24	0/2158	0.45	0/2917
1	C	0.27	0/2158	0.46	0/2917
1	D	0.27	0/2158	0.46	0/2917
1	E	0.29	1/2158 (0.0%)	0.45	1/2917 (0.0%)
1	F	0.24	0/2158	0.45	0/2917
1	G	0.29	1/2158 (0.0%)	0.45	1/2917 (0.0%)
1	H	0.24	0/2158	0.45	0/2917
1	I	0.27	0/2158	0.46	0/2917
1	J	0.29	1/2158 (0.0%)	0.45	1/2917 (0.0%)
2	L	0.77	3/2688 (0.1%)	0.82	8/3646 (0.2%)
3	P	0.28	0/457	0.38	0/624
3	Q	0.28	0/437	0.36	0/596
3	R	0.29	0/460	0.38	0/630
3	S	0.30	0/615	0.39	0/831
4	T	0.34	0/627	0.48	3/872 (0.3%)
All	All	0.35	7/26864 (0.0%)	0.50	15/36369 (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
2	L	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	169	ARG	C-N	26.31	1.94	1.34
2	L	324	VAL	C-N	12.83	1.63	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	111	LEU	CG-CD1	-5.28	1.32	1.51
1	J	111	LEU	CG-CD1	-5.28	1.32	1.51
1	G	111	LEU	CG-CD1	-5.27	1.32	1.51
1	A	111	LEU	CG-CD1	-5.26	1.32	1.51
2	L	204	GLU	CD-OE2	5.16	1.31	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	169	ARG	O-C-N	-21.96	87.56	122.70
2	L	169	ARG	CA-C-N	9.86	138.88	117.20
2	L	115	ASN	N-CA-C	9.49	136.62	111.00
2	L	165	ASP	O-C-N	-8.63	108.89	122.70
2	L	169	ARG	C-N-CA	8.01	141.71	121.70
2	L	324	VAL	O-C-N	-6.96	111.56	122.70
4	T	56	PRO	N-CA-CB	5.85	110.32	103.30
4	T	104	PRO	N-CA-CB	5.78	110.23	103.30
4	T	35	PRO	N-CA-CB	5.65	110.08	103.30
2	L	165	ASP	CA-C-N	5.32	128.91	117.20
1	A	111	LEU	CD1-CG-CD2	-5.29	94.61	110.50
1	G	111	LEU	CD1-CG-CD2	-5.29	94.62	110.50
1	E	111	LEU	CD1-CG-CD2	-5.29	94.64	110.50
1	J	111	LEU	CD1-CG-CD2	-5.29	94.64	110.50
2	L	159	VAL	N-CA-C	5.16	124.92	111.00

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	96	0
1	B	2123	0	2156	79	0
1	C	2123	0	2155	126	0
1	D	2123	0	2156	65	0
1	E	2123	0	2153	145	0
1	F	2123	0	2156	60	0
1	G	2123	0	2153	102	0
1	H	2123	0	2156	79	0
1	I	2123	0	2154	120	0
1	J	2123	0	2154	54	0
2	L	2634	0	2479	76	0
3	P	451	0	425	94	0
3	Q	432	0	425	119	0
3	R	453	0	443	141	0
3	S	608	0	641	132	0
4	T	628	0	311	4	0
5	A	1	0	0	0	0
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	1012	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 19.

All (1012) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:236:ASP:OD2	3:Q:44:GLY:HA3	1.28	1.26
1:B:234:LEU:N	3:Q:47:ARG:HH12	1.30	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
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
2:L:169:ARG:C	2:L:170:VAL:N	1.94	1.21
1:E:143:TRP:N	3:R:30:TRP:CZ2	2.07	1.20
1:C:230:TYR:OH	3:Q:27:ILE:HG21	1.41	1.20
1:C:135:LYS:NZ	3:Q:55:GLU:OE2	1.74	1.20
1:A:230:TYR:OH	3:P:1:MET:HA	1.42	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:I:24:PRO:CB	3:S:55:GLU:HB3	1.72	1.17
1:E:171:ARG:NE	3:R:23:LEU:CD2	2.09	1.15
1:C:135:LYS:HZ1	3:Q:55:GLU:CD	1.49	1.15
1:A:230:TYR:CD1	3:P:1:MET:CE	2.29	1.15
1:E:171:ARG:HE	3:R:23:LEU:HD23	1.06	1.15
1:H:230:TYR:CD1	3:S:42:SER:HA	1.80	1.15
1:C:95:VAL:HG11	3:Q:31:ALA:HB2	1.25	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LYS:NZ	3:Q:55:GLU:CD	1.98	1.14
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:E:135:LYS:NZ	3:R:55:GLU:CD	2.03	1.12
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: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
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:D:234:LEU:H	3:R:47:ARG:CZ	1.67	1.08
1:C:24:PRO:HB2	3:Q:55:GLU:HB3	1.29	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:E:135:LYS:HZ1	3:R:55:GLU:CD	1.56	1.06
1:G:95:VAL:CG1	3:P:31:ALA:HB2	1.85	1.06
1:C:103:MET:CE	3:Q:30:TRP:C	2.23	1.05
1:B:115:GLU:OE1	3:R:56:LEU:HD23	1.56	1.05
1:C:103:MET:HE2	3:Q:30:TRP:C	1.78	1.04
1:C:230:TYR:OH	3:Q:27:ILE:CB	2.06	1.03
1:B:183:ASP:OD2	1:B:249:THR:CG2	2.07	1.03
1:A:230:TYR:CE1	3:P:1:MET:HE2	1.92	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:I:95:VAL:CG1	3:S:31:ALA:HB1	1.90	1.01
1:C:24:PRO:CB	3:Q:55:GLU:HB3	1.90	1.01
1:B:94:ASN:HD21	3:Q:35:GLN:HG2	1.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:32:VAL:HG23	2:L:33:LEU:HD12	1.44	0.99
1:D:183:ASP:OD2	1:D:249:THR:CG2	2.11	0.99
1:I:139:THR:HG21	3:S:37:LYS:CE	1.92	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: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
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: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:C:183:ASP:OD2	1:C:249:THR:CG2	2.11	0.98
1:F:183:ASP:OD2	1:F:249:THR:HG23	1.62	0.98
1:B:189:ILE:HG12	1:B:242:LEU:HD22	1.45	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:C:139:THR:HG21	3:Q:37:LYS:HZ3	1.27	0.96
1:A:230:TYR:CD1	3:P:1:MET:SD	2.56	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:113:THR:CB	3:S:56:LEU:HD21	1.94	0.96
1:E:99:VAL:O	3:R:34:GLU:OE2	1.82	0.96
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:D:94:ASN:HD21	3:R:35:GLN:HG2	1.31	0.95
1:H:236:ASP:OD2	3:S:44:GLY:HA3	1.66	0.95
1:C:103:MET:CE	3:Q:30:TRP:CB	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ASP:OD2	1:A:249:THR:CG2	2.15	0.94
1:C:139:THR:HG21	3:Q:37:LYS:HZ1	1.23	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: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: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:D:233:VAL:HA	3:R:47:ARG:NH1	1.84	0.93
1:A:183:ASP:OD2	1:A:249:THR:HG23	1.69	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:I:139:THR:CG2	3:S:37:LYS:HZ1	1.64	0.92
1:E:135:LYS:NZ	3:R:55:GLU:OE2	1.99	0.92
1:E:135:LYS:CE	3:R:55:GLU:OE2	2.18	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:D:233:VAL:C	3:R:47:ARG:HH12	1.73	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:I:99:VAL:O	3:S:34:GLU:CD	1.98	0.91
1:E:143:TRP:HZ3	1:E:261:MET:HB3	1.36	0.91
1:B:115:GLU:OE1	3:R:56:LEU:CD2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:139:THR:CG2	3:S:37:LYS:HZ3	1.59	0.89
1:I:234:LEU:HD11	3:S:23:LEU:CD2	2.03	0.89
1:A:143:TRP:HZ3	1:A:261:MET:HB3	1.36	0.89
1:I:189:ILE:HG12	1:I:242:LEU:HD22	1.53	0.89
1:A:230:TYR:HE1	3:P:1:MET:CG	1.73	0.89
1:C:103:MET:HE1	3:Q:30:TRP:CB	2.04	0.88
1:F:27:GLN:NE2	3:R:14:SER:O	2.06	0.88
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: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:A:194:TRP:HH2	3:R:65:GLU:OE2	1.53	0.88
1:H:230:TYR:CD1	3:S:42:SER:CB	2.56	0.87
1:E:194:TRP:HH2	3:R:16:TRP:HB3	1.38	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
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:I:99:VAL:HG13	3:S:34:GLU:CD	1.93	0.86
1:F:5:LEU:HD21	3:R:12:ASN:CB	2.06	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: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: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
1:C:103:MET:HE1	3:Q:30:TRP:HB2	1.58	0.84
2:L:135:LEU:HD12	2:L:135:LEU:N	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:A:230:TYR:HE1	3:P:1:MET:HE2	1.42	0.84
1:C:135:LYS:HZ2	3:Q:55:GLU:CD	1.81	0.84
1:A:230:TYR:HD1	3:P:1:MET:CE	1.90	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:103:MET:CG	3:S:34:GLU:OE2	2.27	0.83
1:E:194:TRP:CH2	3:R:16:TRP:CB	2.62	0.83
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:E:24:PRO:HB3	3:R:55:GLU:C	2.00	0.82
1:B:233:VAL:C	3:Q:47:ARG:HH12	1.83	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:C:24:PRO:HB2	3:Q:55:GLU:CB	2.10	0.82
1:B:94:ASN:HD21	3:Q:35:GLN:CG	1.93	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:G:99:VAL:C	3:P:34:GLU:OE2	2.19	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:C:103:MET:HE2	3:Q:30:TRP:HB3	1.62	0.81
1:A:194:TRP:HH2	3:R:65:GLU:CD	1.84	0.81
1:E:234:LEU:HD13	3:R:23:LEU:HD21	1.62	0.80
1:C:143:TRP:N	3:Q:30:TRP:CH2	2.50	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:E:143:TRP:N	3:R:30:TRP:HZ2	1.64	0.79
1:C:95:VAL:CG1	3:Q:31:ALA:CB	2.60	0.79
1:G:171:ARG:NE	3:P:23:LEU:HD23	1.95	0.79
1:A:230:TYR:CD1	3:P:1:MET:HE1	2.16	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:I:24:PRO:HB2	3:S:55:GLU:HB3	1.62	0.79
1:E:171:ARG:CZ	3:R:23:LEU:HD22	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:ARG:HH21	3:P:23:LEU:HD22	1.48	0.79
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: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
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
2:L:32:VAL:HG22	2:L:33:LEU:N	2.00	0.77
1:B:160:GLU:OE1	1:B:243:ARG:HD3	1.85	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:I:143:TRP:N	3:S:30:TRP:CH2	2.53	0.76
1:E:113:THR:HB	3:S:56:LEU:HD21	1.68	0.76
1:C:103:MET:HE2	3:Q:30:TRP:O	1.85	0.76
1:E:99:VAL:C	3:R:34:GLU:OE2	2.23	0.76
1:E:99:VAL:CA	3:R:34:GLU:OE2	2.26	0.76
1:E:234:LEU:HD13	3:R:23:LEU:CD2	2.16	0.76
1:I:24:PRO:CB	3:S:55:GLU:CB	2.61	0.76
1:G:27:GLN:N	3:P:55:GLU:OE2	2.19	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
2:L:135:LEU:CD1	2:L:135:LEU:H	1.99	0.74
1:H:160:GLU:OE1	1:H:243:ARG:HD3	1.85	0.74
1:C:160:GLU:OE1	1:C:243:ARG:HD3	1.87	0.74
1:I:139:THR:HG22	3:S:37:LYS:HE2	1.69	0.74
1:I:160:GLU:OE1	1:I:243:ARG:HD3	1.87	0.74
1:D:236:ASP:OD2	3:R:44:GLY:HA3	1.88	0.74
1:D:160:GLU:OE1	1:D:243:ARG:HD3	1.87	0.74
1:E:191:GLY:C	3:R:9:VAL:O	2.27	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:TYR:CZ	3:P:1:MET:HB3	2.22	0.73
2:L:31:LEU:HD12	2:L:74:TYR:CZ	2.22	0.73
2:L:22:ILE:HG23	2:L:57:MET:O	1.87	0.73
1:E:234:LEU:HD11	3:R:23:LEU:HD11	1.70	0.73
1:A:230:TYR:CD1	3:P:1:MET:HE2	2.08	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:C:230:TYR:CE1	3:Q:24:ASP:CG	2.62	0.73
1:G:143:TRP:CZ3	1:G:261:MET:HB3	2.24	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:E:135:LYS:HZ2	3:R:55:GLU:CD	1.88	0.72
1:I:1:MET:HG3	3:S:47:ARG:NH2	2.05	0.72
1:C:161:ILE:HD12	1:C:246:ILE:CD1	2.20	0.72
2:L:135:LEU:CD1	2:L:135:LEU:N	2.51	0.72
2:L:2:ILE:HG22	2:L:75:TRP:CE3	2.25	0.72
3:P:21:THR:CG2	3:P:26:LEU:HD11	2.19	0.72
1:I:230:TYR:HE1	3:S:27:ILE:HD12	1.53	0.71
1:G:230:TYR:OH	3:P:27:ILE:CB	2.30	0.71
1:I:234:LEU:HD13	3:S:23:LEU:HD22	1.72	0.71
1:G:143:TRP:CD1	3:P:30:TRP:CE2	2.77	0.71
1:G:143:TRP:HD1	3:P:30:TRP:CZ2	2.09	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:A:95:VAL:HG13	3:P:2:ASN:OD1	1.91	0.71
1:I:99:VAL:CG1	3:S:31:ALA:HA	2.21	0.71
1:D:161:ILE:HD12	1:D:246:ILE:CD1	2.20	0.71
1:I:161:ILE:HD12	1:I:246:ILE:CD1	2.20	0.71
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:G:113:THR:CG2	3:Q:56:LEU:HD22	2.22	0.70
1:I:230:TYR:OH	3:S:27:ILE:HG22	1.87	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:C:230:TYR:OH	3:Q:27:ILE:HD12	1.77	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: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: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:G:230:TYR:CE1	3:P:24:ASP:OD1	2.46	0.69
1:G:161:ILE:HD12	1:G:246:ILE:CD1	2.23	0.69
1:F:20:SER:OG	1:F:115:GLU:HG2	1.93	0.69
1:C:234:LEU:HD13	3:Q:23:LEU:HD22	1.74	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:C:103:MET:HE2	3:Q:30:TRP:CB	2.19	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
2:L:24:ILE:HD13	2:L:80:ASP:N	2.10	0.67
1:G:113:THR:HG21	3:Q:56:LEU:HD22	1.76	0.67
1:G:143:TRP:HD1	3:P:30:TRP:NE1	1.90	0.67
1:E:161:ILE:HD12	1:E:246:ILE:CD1	2.23	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
2:L:24:ILE:HG23	2:L:79:LEU:C	2.16	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	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:20:SER:OG	1:I:115:GLU:HG2	1.96	0.65
1:A:230:TYR:HD1	3:P:1:MET:HE1	1.51	0.65
1:D:233:VAL:HA	3:R:47:ARG:CZ	2.27	0.65
1:C:103:MET:HE1	3:Q:30:TRP:C	2.16	0.65
1:F:161:ILE:HD12	1:F:246:ILE:CD1	2.27	0.65
1:C:20:SER:OG	1:C:115:GLU:HG2	1.96	0.65
1:C:24:PRO:HB3	3:Q:55:GLU:C	2.18	0.65
1:H:161:ILE:HD12	1:H:246:ILE:CD1	2.27	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: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:B:161:ILE:HD12	1:B:246:ILE:CD1	2.27	0.64
1:C:27:GLN:CD	3:Q:53:THR:HG21	2.17	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:G:152:LYS:NZ	1:G:163:ASP:OD1	2.29	0.64
1:C:135:LYS:NZ	3:Q:55:GLU:OE1	2.21	0.64
1:C:103:MET:HE1	3:Q:31:ALA:N	2.12	0.64
1:B:93:VAL:HG21	3:Q:38:ALA:HB2	1.80	0.64
1:E:171:ARG:NH2	3:R:23:LEU:HD22	2.12	0.64
1:A:20:SER:OG	1:A:115:GLU:HG2	1.97	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
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:I:99:VAL:CG1	3:S:34:GLU:CD	2.64	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:31:LEU:CD1	2:L:72:ILE:HB	2.31	0.61
1:I:230:TYR:OH	3:S:27:ILE:CB	2.49	0.61
1:A:87:ARG:HB2	1:A:90:MET:HG2	1.82	0.61
1:C:230:TYR:CD1	3:Q:24:ASP:OD1	2.53	0.61
1:A:155:ASN:O	1:A:248:SER:HB3	2.00	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:E:24:PRO:CB	3:R:55:GLU:CB	2.66	0.61
1:B:210:TYR:OH	1:C:2:ARG:NH2	2.29	0.61
1:I:24:PRO:HB2	3:S:55:GLU:CB	2.26	0.61
1:G:155:ASN:O	1:G:248:SER:HB3	2.00	0.61
1:C:87:ARG:HB2	1:C:90:MET:HG2	1.83	0.61
1:C:143:TRP:N	3:Q:30:TRP:CZ2	2.68	0.60
3:P:22:GLY:O	3:P:26:LEU:HD13	2.01	0.60
1:F:153:GLN:OE1	1:F:253:GLN:NE2	2.33	0.60
1:E:95:VAL:CG1	3:R:31:ALA:CB	2.79	0.60
1:H:153:GLN:OE1	1:H:253:GLN:NE2	2.33	0.60
1:D:87:ARG:HB2	1:D:90:MET:HG2	1.83	0.60
1:G:230:TYR:HE1	3:P:24:ASP:OD1	1.84	0.60
2:L:31:LEU:HD22	2:L:72:ILE:HD13	1.83	0.60
1:E:139:THR:HG21	3:R:37:LYS:NZ	2.16	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
2:L:97:GLN:HE21	2:L:329:GLN:HE22	1.50	0.60
1:G:87:ARG:HB2	1:G:90:MET:HG2	1.82	0.60
1:I:234:LEU:HD13	3:S:23:LEU:CD2	2.31	0.59
1:I:99:VAL:HG22	3:S:34:GLU:HB3	1.84	0.59
1:E:143:TRP:HD1	3:R:30:TRP:CE2	2.19	0.59
1:I:230:TYR:CE1	3:S:27:ILE:HD13	2.38	0.59
1:G:113:THR:HG21	3:Q:56:LEU:HD13	1.84	0.59
1:F:87:ARG:HB2	1:F:90:MET:HG2	1.85	0.59
1:D:234:LEU:N	3:R:47:ARG:CZ	2.43	0.58
1:G:143:TRP:CD1	3:P:30:TRP:NE1	2.70	0.58
1:D:14:ALA:O	1:D:17:ASN:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:267:ASN:OD1	3:R:52:MET:CE	2.51	0.58
1:D:48:ARG:NH2	1:D:55:LEU:HB2	2.19	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: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:C:14:ALA:O	1:C:17:ASN:HB2	2.03	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:E:29:TYR:OH	3:R:55:GLU:OE1	2.10	0.57
1:H:87:ARG:HB2	1:H:90:MET:HG2	1.85	0.57
1:E:192:THR:HA	3:R:13:GLN:HG3	1.86	0.57
1:E:143:TRP:HD1	3:R:30:TRP:HE1	1.47	0.57
3:S:75:GLU:HA	3:S:78:VAL:HG12	1.87	0.57
1:I:139:THR:HG21	3:S:37:LYS:HZ1	0.74	0.57
1:C:99:VAL:C	3:Q:34:GLU:OE2	2.42	0.57
1:G:99:VAL:CG2	3:P:34:GLU:CB	2.74	0.57
1:G:14:ALA:O	1:G:17:ASN:HB2	2.05	0.57
2:L:205:LEU:HG	2:L:321:LEU:CD1	2.34	0.57
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:E:48:ARG:HH21	1:E: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:A:48:ARG:HH21	1:A:117:LYS:HB3	1.70	0.56
1:D:161:ILE:HD12	1:D:246:ILE:HD13	1.88	0.56
1:I:1:MET:CG	3:S:47:ARG:CZ	2.83	0.56
1:H:47:VAL:HB	1:H:59:TYR:HB2	1.88	0.56
1:E:234:LEU:CD1	3:R:23:LEU:HD11	2.36	0.56
1:I:1:MET:HB2	3:S:47:ARG:NE	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LYS:HZ3	3:R:57:ASP:HB2	1.70	0.56
1:A:14:ALA:O	1:A:17:ASN:HB2	2.05	0.56
1:H:142:SER:OG	1:H:143:TRP:N	2.37	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: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:G:25:ILE:N	3:P:55:GLU:HB3	2.21	0.55
1:D:86:VAL:O	1:D:88:PRO:HD3	2.06	0.55
1:F:47:VAL:HB	1:F:59:TYR:HB2	1.88	0.55
1:E:14:ALA:O	1:E:17:ASN:HB2	2.05	0.55
1:A:189:ILE:HG12	1:A:242:LEU:CD2	2.28	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: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:161:ILE:HD12	1:J:246:ILE:HD13	1.89	0.55
1:J:48:ARG:HH21	1:J:117:LYS:HB3	1.70	0.55
1:J:151:PHE:HD1	2:L:11:GLU:OE2	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: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:A:230:TYR:HH	3:P:1:MET:HG2	1.70	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:G:86:VAL:O	1:G:88:PRO:HD3	2.08	0.54
1:C:103:MET:CE	3:Q:30:TRP:CA	2.85	0.54
3:R:64:VAL:O	3:R:65:GLU:HB2	2.07	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:B:22:LYS:HZ2	3:R:57:ASP:CG	2.11	0.54
1:G:161:ILE:HD12	1:G:246:ILE:HD13	1.89	0.54
1:E:161:ILE:HD12	1:E:246:ILE:HD13	1.89	0.54
1:I:266:ARG:NE	3:S:63:VAL:HG11	2.22	0.54
1:H:86:VAL:O	1:H:88:PRO:HD3	2.08	0.54
3:S:83:GLN:O	3:S:87:LEU:HD13	2.08	0.54
3:P:21:THR:HG22	3:P:26:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:TYR:CZ	3:R:27:ILE:HD12	2.43	0.54
1:J:108:THR:O	1:J:111:LEU:HB2	2.08	0.53
1:F:142:SER:OG	1:F:143:TRP:N	2.37	0.53
1:B:14:ALA:O	1:B:17:ASN:HB2	2.07	0.53
1:F:86:VAL:O	1:F:88:PRO:HD3	2.08	0.53
1:A:86:VAL:O	1:A: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:A:193:LYS:HZ3	1:I:54:ARG:HH22	1.55	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:D:210:TYR:OH	1:E:2:ARG:NH2	2.39	0.53
1:G:108:THR:O	1:G:111:LEU:HB2	2.08	0.53
1:C:60:LYS:HD2	1:C:151:PHE:HZ	1.74	0.53
1:A:108:THR:O	1:A:111:LEU:HB2	2.08	0.53
2:L:76:VAL:HG13	2:L:76:VAL:O	2.09	0.53
2:L:21:ASN:HA	2:L:24:ILE:CD1	2.34	0.52
1:I:60:LYS:HD2	1:I:151:PHE:HZ	1.74	0.52
3:P:30:TRP:O	3:P:33:VAL:HG12	2.10	0.52
1:A:210:TYR:OH	1:B:2:ARG:NH2	2.39	0.52
1:F:54:ARG:HH11	1:F:54:ARG:CG	2.22	0.52
2:L:97:GLN:HE21	2:L:329:GLN:NE2	2.08	0.52
1:G:267:ASN:N	1:G:267:ASN:OD1	2.42	0.52
1:H:54:ARG:HH11	1:H:54:ARG:CG	2.22	0.52
3:S:71:ALA:O	3:S:72:GLN:HB2	2.10	0.52
1:D:47:VAL:HB	1:D:59:TYR:HB2	1.91	0.52
1:J:47:VAL:HB	1:J:59:TYR:HB2	1.91	0.52
1:C:103:MET:HE2	3:Q:30:TRP:CA	2.39	0.52
1:E:47:VAL:HB	1:E:59:TYR:HB2	1.91	0.52
1:B:54:ARG:HH11	1:B:54:ARG:CG	2.22	0.52
1:B:267:ASN:OD1	3:R:52:MET:HE2	2.08	0.52
1:E:267:ASN:OD1	1:E:267:ASN:N	2.42	0.52
1:G:143:TRP:HB2	3:P:30:TRP:CZ2	2.45	0.52
1:E:191:GLY:CA	3:R:9:VAL:O	2.58	0.52
1:J:142:SER:OG	1:J:143:TRP:N	2.43	0.52
1:I:143:TRP:N	3:S:30:TRP:CZ2	2.78	0.52
1:G:234:LEU:HD13	3:P:23:LEU:CD2	2.37	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
4:T:122:ALA:O	4:T:123:SER:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:VAL:HB	1:G:59:TYR:HB2	1.91	0.52
1:H:237:GLN:HG3	1:H:237:GLN:O	2.10	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: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:I:108:THR:O	1:I:111:LEU:HB2	2.10	0.51
1:I:99:VAL:HG11	3:S:31:ALA:HA	1.90	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
4:T:116:ALA:O	4:T:117:SER:CB	2.58	0.51
1:J:267:ASN:N	1:J:267:ASN:OD1	2.42	0.51
3:S:90:PHE:O	3:S:94:LEU:HD13	2.09	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:I:103:MET:HG2	3:S:30:TRP:HB3	1.91	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
1:C:108:THR:O	1:C:111:LEU:HB2	2.10	0.51
1:D:171:ARG:HD3	1:D:232:SER:OG	2.11	0.50
1:B:22:LYS:NZ	3:R:57:ASP:CB	2.74	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:E:135:LYS:HZ1	3:R:55:GLU:CG	2.23	0.50
2:L:21:ASN:HD22	2:L:24:ILE:HD12	1.77	0.50
1:F:52:ASP:OD2	1:F:266:ARG:NE	2.45	0.50
1:D:142:SER:OG	1:D:143:TRP:N	2.37	0.50
1:C:171:ARG:HD3	1:C:232:SER:OG	2.11	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:HG3	1:F:237:GLN:O	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:D:233:VAL:HA	3:R:47:ARG:NH2	2.27	0.49
1:C:103:MET:HE3	3:Q:31:ALA:N	2.25	0.49
1:C:234:LEU:CD1	3:Q:23:LEU:HD22	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:GLN:O	1:B:237:GLN:HG3	2.10	0.49
1:D:94:ASN:HD21	3:R:35:GLN:CD	2.14	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:B:108:THR:O	1:B:111:LEU:HB2	2.12	0.49
1:H:233:VAL:HA	3:S:47:ARG:HH12	0.49	0.49
2:L:32:VAL:CG2	2:L:33:LEU:HD12	2.30	0.49
1:I:137:VAL:CG2	3:S:50:GLN:CD	2.81	0.49
1:H:108:THR:O	1:H:111:LEU:HB2	2.12	0.49
1:C:27:GLN:CD	3:Q:53:THR:CG2	2.80	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:D:236:ASP:CG	3:R:44:GLY:HA3	2.33	0.49
2:L:210:PHE:HB3	2:L:319:ASP:OD2	2.13	0.49
2:L:21:ASN:CA	2:L:24:ILE:HD12	2.38	0.49
3:Q:43:THR:HG22	3:Q:45:GLN:H	1.78	0.49
2:L:244:ASP:HB2	2:L:245:GLU:OE2	2.13	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:C:230:TYR:HH	3:Q:27:ILE:HB	1.77	0.48
1:C:230:TYR:CZ	3:Q:27:ILE:HG21	2.41	0.48
1:J:189:ILE:HG12	1:J:242:LEU:CD2	2.28	0.48
1:B:22:LYS:HZ2	3:R:57:ASP:CB	2.26	0.48
2:L:133:THR:HB	2:L:135:LEU:CD1	2.43	0.48
1:I:99:VAL:HG13	3:S:34:GLU:CG	2.42	0.48
1:E:192:THR:HG23	3:R:13:GLN:HG3	1.96	0.48
1:I:171:ARG:HA	1:I:233:VAL:O	2.14	0.48
1:A:73:LYS:HG3	1:A:211:GLY:O	2.14	0.48
1:G:73:LYS:HG3	1:G:211:GLY:O	2.13	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
3:S:81:VAL:CG1	3:S:82:PRO:HD3	2.44	0.48
1:J:177:ILE:HG12	1:J:256:ILE:HD12	1.94	0.48
2:L:34:ARG:NH1	2:L:36:TYR:OH	2.44	0.48
1:C:137:VAL:HG23	3:Q:50:GLN:HG2	1.96	0.48
2:L:211:SER:HB3	2:L:318:ASP:OD1	2.13	0.48
1:B:52:ASP:OD2	1:B:266:ARG:NE	2.45	0.48
1:E:113:THR:HG21	3:S:56:LEU:HD11	1.90	0.48
1:D:171:ARG:HA	1:D:233:VAL:O	2.14	0.48
1:H:171:ARG:NH2	3:S:42:SER:C	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:234:LEU:N	3:S:47:ARG:NH1	2.62	0.48
1:E:230:TYR:CZ	3:R:27:ILE:CD1	2.97	0.48
1:B:230:TYR:HB3	3:Q:41:ALA:HB1	1.96	0.48
1:A:94:ASN:HB3	3:P:3:THR:N	2.28	0.47
1:J:148:ARG:HD3	1:J:148:ARG:HA	1.65	0.47
1:E:171:ARG:HH21	3:R:23:LEU:HD22	1.76	0.47
1:E:73:LYS:HG3	1:E:211:GLY:O	2.13	0.47
3:S:92:GLY:O	3:S:96:LEU:HD13	2.15	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
2:L:213:LYS:NZ	2:L:318:ASP:OD2	2.44	0.47
1:B:166:ARG:HA	1:B:235:LEU:HD13	1.96	0.47
1:G:91:LYS:HE3	1:G:91:LYS:HB3	1.76	0.47
1:D:172:ILE:HB	1:D:233:VAL:HB	1.96	0.47
3:R:64:VAL:O	3:R:65:GLU:CB	2.62	0.47
1:G:177:ILE:HG12	1:G:256:ILE:HD12	1.95	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: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
1:F:148:ARG:HD3	1:F:148:ARG:HA	1.64	0.47
3:Q:9:VAL:O	4:T:80:ALA:HB2	2.14	0.47
1:J:97:ASP:O	1:J:101:GLN:HG3	2.15	0.47
1:D:97:ASP:O	1:D:101:GLN:HG3	2.14	0.47
1:H:233:VAL:CA	3:S:47:ARG:NH1	2.24	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:A:194:TRP:CH2	3:R:65:GLU:CD	2.73	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:E:97:ASP:O	1:E:101:GLN:HG3	2.15	0.47
1:C:103:MET:SD	3:Q:30:TRP:HB3	2.55	0.46
1:B:189:ILE:HG12	1:B:242:LEU:CD2	2.32	0.46
1:I:137:VAL:HB	3:S:50:GLN:CD	2.36	0.46
2:L:205:LEU:HG	2:L:321:LEU:HD13	1.97	0.46
1:C:97:ASP:O	1:C:101:GLN:HG3	2.15	0.46
1:A:97:ASP:O	1:A:101:GLN:HG3	2.15	0.46
1:J:73:LYS:HG3	1:J:211:GLY:O	2.14	0.46
1:F:48:ARG:NH2	1:F:55:LEU:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:P:21:THR:HG22	3:P:26:LEU:CD1	2.46	0.46
1:I:266:ARG:CZ	3:S:63:VAL:HG11	2.46	0.46
3:S:94:LEU:O	3:S:98:LEU:HD13	2.16	0.46
2:L:9:ALA:HA	2:L:69:ALA:CB	2.46	0.46
1:G:97:ASP:O	1:G:101:GLN:HG3	2.15	0.46
2:L:12:PHE:HB2	2:L:64:LEU:HD22	1.98	0.46
1:A:2:ARG:NH2	1:C:210:TYR:OH	2.39	0.46
1:H:52:ASP:OD2	1:H:266:ARG:NE	2.45	0.46
1:C:148:ARG:HD3	1:C:148:ARG:HA	1.64	0.46
3:Q:30:TRP:O	3:Q:33:VAL:HG12	2.15	0.46
2:L:135:LEU:H	2:L:135:LEU:HD13	1.78	0.46
1:F:54:ARG:NH1	1:F:54:ARG:CG	2.78	0.46
2:L:15:THR:HG23	2:L:61:SER:HB3	1.98	0.46
3:P:15:VAL:O	3:P:15:VAL:HG13	2.15	0.46
1:I:210:TYR:OH	1:J:2:ARG:NH2	2.39	0.46
1:I:185:VAL:HB	1:I:219:TYR:CE2	2.51	0.46
1:B:48:ARG:NH2	1:B:55:LEU:HB2	2.30	0.46
1:C:139:THR:CG2	3:Q:37:LYS:HZ3	2.10	0.46
1:F:189:ILE:HG12	1:F:242:LEU:CD2	2.32	0.46
1:H:187:PHE:HE1	1:H:242:LEU:HD11	1.81	0.46
1:G:236:ASP:C	1:G:238:MET:H	2.19	0.46
1:B:183:ASP:CG	1:B:249:THR:HG23	2.34	0.45
1:H:44:ILE:HB	1:H:62:LEU:HB2	1.98	0.45
3:P:10:PRO:CG	3:Q:39:ALA:HB1	2.46	0.45
1:D:185:VAL:HB	1:D:219:TYR:CE2	2.51	0.45
1:H:148:ARG:HD3	1:H:148:ARG:HA	1.63	0.45
1:I:207:LEU:HD23	1:I:225:LEU:HD21	1.99	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
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: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
1:A:94:ASN:ND2	3:P:2:ASN:C	2.69	0.45
1:A:185:VAL:HB	1:A:219:TYR:CE2	2.52	0.45
1:E:236:ASP:C	1:E:238:MET:H	2.19	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:F:187:PHE:HE1	1:F:242:LEU:HD11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:185:VAL:HB	1:G:219:TYR:CE2	2.52	0.45
1:D:148:ARG:HD3	1:D:148:ARG:HA	1.64	0.45
1:H:230:TYR:O	3:S:41:ALA:HB1	2.17	0.45
1:G:99:VAL:CG1	3:P:31:ALA:HA	2.37	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:F:185:VAL:HB	1:F:219:TYR:CE2	2.52	0.45
1:I:93:VAL:C	1:J:96:THR:HG21	2.37	0.45
1:A:96:THR:HG21	1:C:93:VAL:C	2.37	0.45
1:D:21:ILE:HB	1:D:116:ILE:HB	1.99	0.45
3:R:30:TRP:O	3:R:33:VAL:HG12	2.16	0.45
1:B:54:ARG:CG	1:B:54:ARG:NH1	2.78	0.45
1:J:151:PHE:HB3	2:L:11:GLU:CD	2.32	0.45
1:G:95:VAL:CG1	3:P:31:ALA:HB1	2.43	0.45
1:G:142:SER:OG	1:G:143:TRP:N	2.43	0.45
1:A:236:ASP:C	1:A:238:MET:H	2.19	0.45
1:I:21:ILE:HB	1:I:116:ILE:HB	1.99	0.45
1:D:233:VAL:CA	3:R:47:ARG:NH2	2.80	0.45
1:H:230:TYR:HB3	3:S:41:ALA:C	2.37	0.45
1:C:27:GLN:HG3	1:C:135:LYS:HZ1	1.82	0.45
1:I:137:VAL:HB	3:S:50:GLN:NE2	2.31	0.45
1:H:91:LYS:HE3	1:H:91:LYS:HB3	1.79	0.45
1:D:234:LEU:N	3:R:47:ARG:NH2	2.65	0.44
2:L:114:ARG:HA	2:L:334:ARG:HG2	2.00	0.44
1:E:91:LYS:HB3	1:E:91:LYS:HE3	1.77	0.44
1:B:21:ILE:HB	1:B:116:ILE:HB	1.99	0.44
1:I:99:VAL:HG13	3:S:34:GLU:CB	2.47	0.44
1:B:181:GLY:O	1:B:249:THR:N	2.50	0.44
1:H:183:ASP:CG	1:H:249:THR:HG23	2.34	0.44
1:B:187:PHE:HE1	1:B:242:LEU:HD11	1.81	0.44
2:L:213:LYS:CE	2:L:318:ASP:OD2	2.66	0.44
1:J:207:LEU:HD23	1:J:225:LEU:HD21	1.99	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: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:D:93:VAL:C	1:E:96:THR:HG21	2.37	0.44
1:B:148:ARG:HD3	1:B:148:ARG:HA	1.64	0.44
1:C:230:TYR:HH	3:Q:27:ILE:CB	2.21	0.44
1:C:103:MET:HE1	3:Q:30:TRP:CA	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:ARG:NH2	3:P:23:LEU:CD2	2.76	0.44
1:G:137:VAL:CG2	3:P:50:GLN:CD	2.86	0.44
1:B:207:LEU:HD23	1:B:225:LEU:HD21	1.98	0.44
3:S:22:GLY:O	3:S:26:LEU:HD13	2.18	0.44
1:E:171:ARG:HD3	1:E:232:SER:OG	2.17	0.44
1:H:181:GLY:HA3	1:H:250:MET:HE3	1.99	0.44
1:J:21:ILE:HB	1:J:116:ILE:HB	2.00	0.44
1:E:137:VAL:HG23	3:R:50:GLN:HG2	2.00	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:171:ARG:HD3	1:J:232:SER:OG	2.17	0.44
1:J:185:VAL:HB	1:J:219:TYR:CE2	2.52	0.44
1:B:91:LYS:HE3	1:B:91:LYS:HB3	1.79	0.44
1:G:171:ARG:HD3	1:G:232:SER:OG	2.17	0.44
2:L:32:VAL:HG13	2:L:71:GLU:CG	2.47	0.44
1:J:236:ASP:C	1:J:238:MET:H	2.19	0.44
1:J:181:GLY:HA3	1:J:250:MET:HE3	1.99	0.44
1:H:21:ILE:HB	1:H:116:ILE:HB	1.99	0.44
1:G:148:ARG:HA	1:G:148:ARG:HD3	1.65	0.44
1:E:21:ILE:HB	1:E:116:ILE:HB	2.00	0.44
1:I:43:GLN:HG2	1:I:121:ASP:HB3	2.00	0.44
1:F:73:LYS:HG3	1:F:211:GLY:O	2.18	0.44
1:A:91:LYS:HB3	1:A:91:LYS:HE3	1.76	0.44
1:D:7:LEU:HA	1:D:7:LEU:HD12	1.79	0.44
1:J:187:PHE:HE1	1:J:242:LEU:HD11	1.83	0.44
2:L:205:LEU:HG	2:L:321:LEU:HD12	1.99	0.44
1:A:210:TYR:HH	1:B:2:ARG:HH22	1.65	0.44
1:H:207:LEU:HD23	1:H:225:LEU:HD21	1.98	0.44
2:L:88:THR:HB	2:L:89:LYS:HG3	1.98	0.44
1:B:73:LYS:HG3	1:B:211:GLY:O	2.17	0.44
1:H:181:GLY:O	1:H:249:THR:N	2.50	0.43
1:G:187:PHE:HE1	1:G:242:LEU:HD11	1.83	0.43
1:H:222:ASP:HB3	1:H:225:LEU:HG	2.00	0.43
1:E:185:VAL:HB	1:E:219:TYR:CE2	2.52	0.43
1:I:177:ILE:HG12	1:I:256:ILE:HD12	2.00	0.43
1:G:7:LEU:HA	1:G:7:LEU:HD12	1.81	0.43
3:Q:21:THR:HG22	3:Q:22:GLY:H	1.82	0.43
1:C:207:LEU:HD23	1:C:225:LEU:HD21	1.99	0.43
1:A:222:ASP:HB3	1:A:225:LEU:HG	2.01	0.43
1:F:181:GLY:O	1:F:249:THR:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:60:LYS:HA	2:L:45:ARG:HH22	1.83	0.43
1:G:93:VAL:HG11	1:G:230:TYR:CD2	2.52	0.43
1:D:161:ILE:HD12	1:D:246:ILE:HD11	1.99	0.43
1:I:137:VAL:CG2	3:S:50:GLN:HG2	2.46	0.43
1:E:93:VAL:HG11	1:E:230:TYR:CD2	2.52	0.43
1:I:93:VAL:O	1:J:96:THR:HG21	2.19	0.43
1:C:43:GLN:HG2	1:C:121:ASP:HB3	2.00	0.43
1:E:222:ASP:HB3	1:E:225:LEU:HG	2.01	0.43
1:E:207:LEU:HD23	1:E:225:LEU:HD21	1.99	0.43
1:C:24:PRO:HB3	3:Q:55:GLU:O	2.17	0.43
1:G:171:ARG:HA	1:G:233:VAL:O	2.18	0.43
2:L:29:GLY:HA3	2:L:74:TYR:CD1	2.54	0.43
1:B:222:ASP:HB3	1:B:225:LEU:HG	2.00	0.43
1:J:172:ILE:HB	1:J:233:VAL:HB	2.00	0.43
1:A:207:LEU:HD23	1:A:225:LEU:HD21	1.99	0.43
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:A:187:PHE:HE1	1:A:242:LEU:HD11	1.82	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:A:171:ARG:HA	1:A:233:VAL:O	2.18	0.43
1:G:137:VAL:HG23	3:P:50:GLN:HG2	1.99	0.43
1:I:186:GLU:HB3	1:I:245:LYS:HB2	2.01	0.43
1:A:21:ILE:HB	1:A:116:ILE:HB	2.00	0.43
1:J:93:VAL:HG11	1:J:230:TYR:CD2	2.52	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:C:139:THR:CG2	3:Q:37:LYS:HZ1	2.09	0.43
1:J:43:GLN:HG2	1:J:121:ASP:HB3	2.01	0.43
1:G:43:GLN:HG2	1:G:121:ASP:HB3	2.01	0.43
1:D:176:HIS:HB2	1:D:257:ILE:HB	2.01	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:193:LYS:HZ3	1:I:54:ARG:NH2	2.14	0.43
1:I:161:ILE:HD12	1:I:246:ILE:HD11	1.99	0.43
1:A:172:ILE:HB	1:A:233:VAL:HB	2.00	0.43
1:G:196:ASP:O	1:G:198:LEU:N	2.52	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:207:LEU:HD23	1:G:225:LEU:HD21	1.99	0.43
1:J:196:ASP:O	1:J:198:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:4:LYS:HG2	2:L:75:TRP:CZ2	2.54	0.43
1:E:196:ASP:O	1:E:198:LEU:N	2.52	0.43
1:E:192:THR:C	3:R:16:TRP:HH2	2.21	0.42
1:G:95:VAL:HG12	3:P:31:ALA:HB1	2.00	0.42
1:B:181:GLY:HA3	1:B:250:MET:HE3	1.99	0.42
2:L:7:LEU:CD2	2:L:71:GLU:HB2	2.49	0.42
1:E:187:PHE:HE1	1:E:242:LEU:HD11	1.83	0.42
2:L:72:ILE:N	2:L:72:ILE:HD12	2.33	0.42
1:C:44:ILE:HB	1:C:62:LEU:HB2	2.02	0.42
1:B:186:GLU:HB3	1:B:245:LYS:HB2	2.01	0.42
1:H:177:ILE:HG12	1:H:256:ILE:HD12	2.01	0.42
1:B:7:LEU:HA	1:B:7:LEU:HD12	1.81	0.42
1:G:172:ILE:HB	1:G:233:VAL:HB	2.00	0.42
1:J:171:ARG:HA	1:J:233:VAL:O	2.18	0.42
1:F:177:ILE:HG12	1:F:256:ILE:HD12	2.01	0.42
1:E:103:MET:O	3:R:30:TRP:CZ3	2.71	0.42
1:D:93:VAL:O	1:E:96:THR:HG21	2.19	0.42
1:A:43:GLN:HG2	1:A:121:ASP:HB3	2.01	0.42
1:E:44:ILE:HB	1:E:62:LEU:HB2	2.01	0.42
3:S:71:ALA:O	3:S:72:GLN:CB	2.67	0.42
1:A:96:THR:HG21	1:C:93:VAL:O	2.19	0.42
1:J:222:ASP:HB3	1:J:225:LEU:HG	2.01	0.42
1:D:44:ILE:HB	1:D:62:LEU:HB2	2.01	0.42
1:C:176:HIS:HB2	1:C:257:ILE:HB	2.01	0.42
1:E:27:GLN:HG3	3:R:55:GLU:OE2	2.18	0.42
1:I:222:ASP:HB3	1:I:225:LEU:HG	2.02	0.42
1:B:97:ASP:O	1:B:101:GLN:HG3	2.20	0.42
3:R:55:GLU:C	3:R:56:LEU:HD12	2.39	0.42
1:G:181:GLY:HA3	1:G:250:MET:HE3	2.02	0.42
1:A:181:GLY:HA3	1:A:250:MET:HE3	2.01	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
2:L:135:LEU:HD12	2:L:135:LEU:H	1.61	0.42
1:E:43:GLN:HG2	1:E:121:ASP:HB3	2.01	0.42
1:A:25:ILE:HD12	1:A:25:ILE:N	2.35	0.42
1:F:186:GLU:HB3	1:F:245:LYS:HB2	2.01	0.42
1:B:171:ARG:HA	1:B:233:VAL:O	2.20	0.42
1:B:171:ARG:HD3	1:B:232:SER:OG	2.20	0.42
1:C:103:MET:HE3	3:Q:31:ALA:CA	2.50	0.42
1:C:103:MET:CE	3:Q:30:TRP:HB2	2.27	0.42
1:G:113:THR:HG22	3:Q:56:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:137:VAL:HG23	3:S:50:GLN:CD	2.40	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:E:181:GLY:HA3	1:E:250:MET:HE3	2.00	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:A:196:ASP:O	1:A:198:LEU:N	2.52	0.42
1:G:44:ILE:HB	1:G:62:LEU:HB2	2.01	0.42
1:A:148:ARG:HD3	1:A:148:ARG:HA	1.65	0.42
1:E:143:TRP:HB2	3:R:30:TRP:CH2	2.54	0.42
1:G:25:ILE:HD12	1:G:25:ILE:N	2.35	0.42
1:H:104:PHE:CE1	1:H:143:TRP:CD1	3.08	0.42
1:F:171:ARG:HA	1:F:233:VAL:O	2.20	0.42
3:R:45:GLN:O	3:R:48:VAL:HG12	2.20	0.42
1:D:43:GLN:HG2	1:D:121:ASP:HB3	2.00	0.42
1:A:62:LEU:HD21	1:A:81:VAL:HG11	2.02	0.42
1:E:7:LEU:HD12	1:E:7:LEU:HA	1.81	0.42
1:I:99:VAL:HG11	3:S:31:ALA:CA	2.50	0.42
1:H:54:ARG:CG	1:H:54:ARG:NH1	2.78	0.42
1:B:62:LEU:HD21	1:B:81:VAL:HG11	2.02	0.42
1:E:27:GLN:HG3	1:E:135:LYS:HZ1	1.85	0.41
1:E:160:GLU:HA	1:E:244:LEU:O	2.20	0.41
1:F:171:ARG:HD3	1:F:232:SER:OG	2.20	0.41
1:J:62:LEU:HD21	1:J:81:VAL:HG11	2.02	0.41
1:D:230:TYR:O	3:R:41:ALA:HB1	2.20	0.41
1:F:196:ASP:O	1:F:198:LEU:N	2.53	0.41
1:F:60:LYS:HD2	1:F:151:PHE:HZ	1.85	0.41
1:D:186:GLU:HB3	1:D:245:LYS:HB2	2.01	0.41
3:S:62:VAL:O	3:S:62:VAL:HG13	2.20	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
3:S:73:PRO:O	3:S:77:LEU:HD13	2.20	0.41
1:E:25:ILE:HD12	1:E:25:ILE:N	2.35	0.41
1:I:92:GLY:HA3	1:I:95:VAL:O	2.21	0.41
1:G:160:GLU:HA	1:G:244:LEU:O	2.20	0.41
1:F:104:PHE:CE1	1:F:143:TRP:CD1	3.08	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:143:TRP:CZ3	1:I:262:GLY:HA2	2.56	0.41
1:A:44:ILE:HB	1:A:62:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:44:ILE:HB	1:J:62:LEU:HB2	2.01	0.41
1:D:25:ILE:N	1:D:25:ILE:HD12	2.35	0.41
1:D:143:TRP:CZ3	1:D:262:GLY:HA2	2.56	0.41
1:C:196:ASP:O	1:C:198:LEU:N	2.54	0.41
1:C:25:ILE:HD12	1:C:25:ILE:N	2.35	0.41
1:B:100:GLN:OE1	1:B:103:MET:SD	2.79	0.41
1:D:196:ASP:O	1:D:198:LEU:N	2.54	0.41
1:C:222:ASP:HB3	1:C:225:LEU:HG	2.02	0.41
1:E:62:LEU:HD21	1:E:81:VAL:HG11	2.02	0.41
1:C:91:LYS:HB3	1:C:91:LYS:HE3	1.79	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: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
2:L:28:VAL:HG11	2:L:54:ILE:HD11	2.02	0.41
1:D:92:GLY:HA3	1:D:95:VAL:O	2.21	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:B:171:ARG:HH12	3:Q:47:ARG:NH2	2.19	0.41
1:D:187:PHE:HE1	1:D:242:LEU:HD11	1.86	0.41
1:G:108:THR:HA	1:G:111:LEU:HD12	2.03	0.41
1:D:222:ASP:HB3	1:D:225:LEU:HG	2.02	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: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
2:L:14:GLU:O	2:L:62:VAL:HG12	2.20	0.41
1:G:137:VAL:HB	3:P:50:GLN:OE1	2.21	0.41
1:B:151:PHE:C	1:B:152:LYS:HG2	2.41	0.41
1:J:92:GLY:HA3	1:J:95:VAL:O	2.21	0.41
1:B:196:ASP:O	1:B:198:LEU:N	2.53	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:H:181:GLY:CA	1:H:250:MET:HE3	2.51	0.40
1:H:179:ALA:HB3	1:H:182:VAL:HG23	2.03	0.40
1:D:91:LYS:HE3	1:D:91:LYS:HB3	1.79	0.40
1:G:92:GLY:HA3	1:G:95:VAL:O	2.21	0.40
1:F:183:ASP:CG	1:F:249:THR:HG23	2.34	0.40
1:I:187:PHE:HE1	1:I:242:LEU:HD11	1.86	0.40
1:B:60:LYS:HD2	1:B:151:PHE:HZ	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:62:LEU:HD21	1:D:81:VAL:HG11	2.03	0.40
1:G:62:LEU:HD21	1:G:81:VAL:HG11	2.02	0.40
1:F:151:PHE:C	1:F:152:LYS:HG2	2.41	0.40
1:F:100:GLN:OE1	1:F:103:MET:SD	2.79	0.40
1:J:186:GLU:HB3	1:J:245:LYS:HB2	2.04	0.40
1:J:25:ILE:N	1:J:25:ILE:HD12	2.35	0.40
3:S:55:GLU:C	3:S:56:LEU:HD12	2.41	0.40
1:G:99:VAL:CG2	3:P:34:GLU:HB3	2.40	0.40
1:C:187:PHE:HE1	1:C:242:LEU:HD11	1.86	0.40
1:H:92:GLY:HA3	1:H:95:VAL:O	2.22	0.40
1:A:186:GLU:HB3	1:A:245:LYS:HB2	2.03	0.40
1:A:160:GLU:HA	1:A:244:LEU:O	2.20	0.40
1:E:87:ARG:HA	1:E:88:PRO:HD3	1.89	0.40
1:A:108:THR:HA	1:A:111:LEU:HD12	2.03	0.40
1:H:151:PHE:C	1:H:152:LYS:HG2	2.41	0.40
1:F:179:ALA:HB3	1:F:182:VAL:HG23	2.03	0.40
1:B:179:ALA:HB3	1:B:182:VAL:HG23	2.03	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	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	39	80
1	B	267/269 (99%)	251 (94%)	16 (6%)	0	100	100
1	C	267/269 (99%)	252 (94%)	14 (5%)	1 (0%)	39	80
1	D	267/269 (99%)	251 (94%)	15 (6%)	1 (0%)	39	80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	39	80
1	F	267/269 (99%)	251 (94%)	16 (6%)	0	100	100
1	G	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	39	80
1	H	267/269 (99%)	251 (94%)	16 (6%)	0	100	100
1	I	267/269 (99%)	252 (94%)	14 (5%)	1 (0%)	39	80
1	J	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	39	80
2	L	331/335 (99%)	306 (92%)	19 (6%)	6 (2%)	11	53
3	P	63/104 (61%)	56 (89%)	5 (8%)	2 (3%)	5	41
3	Q	58/104 (56%)	51 (88%)	6 (10%)	1 (2%)	11	55
3	R	61/104 (59%)	53 (87%)	6 (10%)	2 (3%)	5	40
3	S	82/104 (79%)	74 (90%)	6 (7%)	2 (2%)	7	47
4	T	125/127 (98%)	112 (90%)	7 (6%)	6 (5%)	3	32
All	All	3390/3568 (95%)	3160 (93%)	204 (6%)	26 (1%)	24	69

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

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Mol	Chain	Res	Type
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%)	219 (94%)	13 (6%)	26	62
1	B	232/232 (100%)	219 (94%)	13 (6%)	26	62
1	C	232/232 (100%)	221 (95%)	11 (5%)	32	68
1	D	232/232 (100%)	221 (95%)	11 (5%)	32	68
1	E	232/232 (100%)	217 (94%)	15 (6%)	21	58
1	F	232/232 (100%)	219 (94%)	13 (6%)	26	62
1	G	232/232 (100%)	218 (94%)	14 (6%)	24	60
1	H	232/232 (100%)	219 (94%)	13 (6%)	26	62
1	I	232/232 (100%)	221 (95%)	11 (5%)	32	68
1	J	232/232 (100%)	218 (94%)	14 (6%)	24	60
2	L	272/285 (95%)	266 (98%)	6 (2%)	60	83
3	P	44/81 (54%)	42 (96%)	2 (4%)	34	69
3	Q	45/81 (56%)	44 (98%)	1 (2%)	60	83
3	R	48/81 (59%)	48 (100%)	0	100	100
3	S	62/81 (76%)	61 (98%)	1 (2%)	70	88
All	All	2791/2929 (95%)	2653 (95%)	138 (5%)	31	66

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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

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Mol	Chain	Res	Type
1	D	156	ASN
1	D	196	ASP
1	D	242	LEU
1	D	251	ASP
1	D	252	GLU
1	E	1	MET
1	E	7	LEU
1	E	18	SER
1	E	42	SER
1	E	58	THR
1	E	93	VAL
1	E	103	MET
1	E	144	LEU
1	E	152	LYS
1	E	196	ASP
1	E	238	MET
1	E	242	LEU
1	E	251	ASP
1	E	252	GLU
1	E	267	ASN
1	F	1	MET
1	F	7	LEU
1	F	42	SER
1	F	54	ARG
1	F	61	THR
1	F	93	VAL
1	F	144	LEU
1	F	154	LEU
1	F	196	ASP
1	F	237	GLN
1	F	242	LEU
1	F	251	ASP
1	F	252	GLU
1	G	1	MET
1	G	7	LEU
1	G	42	SER
1	G	58	THR
1	G	93	VAL
1	G	103	MET
1	G	144	LEU
1	G	152	LYS
1	G	196	ASP

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Mol	Chain	Res	Type
1	G	238	MET
1	G	242	LEU
1	G	251	ASP
1	G	252	GLU
1	G	267	ASN
1	H	1	MET
1	H	7	LEU
1	H	42	SER
1	H	54	ARG
1	H	61	THR
1	H	93	VAL
1	H	144	LEU
1	H	154	LEU
1	H	196	ASP
1	H	237	GLN
1	H	242	LEU
1	H	251	ASP
1	H	252	GLU
1	I	1	MET
1	I	7	LEU
1	I	42	SER
1	I	61	THR
1	I	93	VAL
1	I	144	LEU
1	I	156	ASN
1	I	196	ASP
1	I	242	LEU
1	I	251	ASP
1	I	252	GLU
1	J	1	MET
1	J	7	LEU
1	J	42	SER
1	J	58	THR
1	J	93	VAL
1	J	103	MET
1	J	144	LEU
1	J	152	LYS
1	J	196	ASP
1	J	238	MET
1	J	242	LEU
1	J	251	ASP
1	J	252	GLU

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Mol	Chain	Res	Type
1	J	267	ASN
2	L	24	ILE
2	L	31	LEU
2	L	32	VAL
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	155	ASN
1	B	94	ASN
1	D	94	ASN
1	D	253	GLN
1	E	253	GLN
1	F	27	GLN
1	G	155	ASN
1	G	253	GLN
2	L	115	ASN
2	L	152	GLN
2	L	329	GLN
3	R	18	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.