Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2023 – 03:37 PM EDT

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
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:

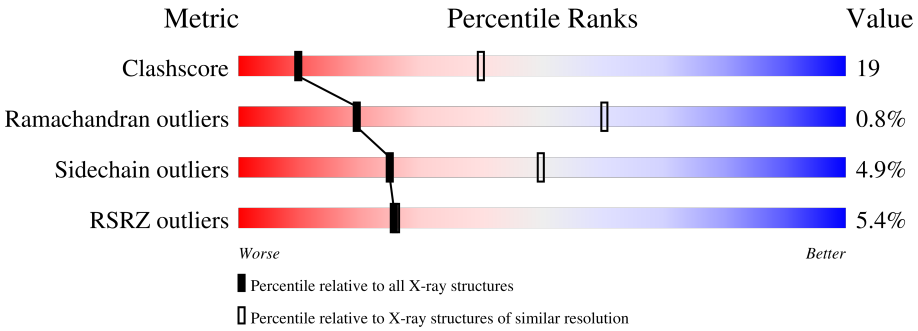
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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 <=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	4% 69% 28%
1	B	269	3% 67% 30%
1	C	269	7% 71% 28%
1	D	269	% 72% 27%
1	E	269	% 66% 30%
1	F	269	7% 69% 29%

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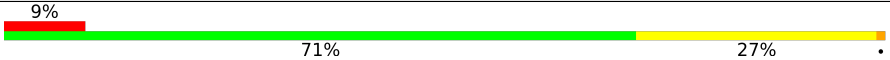
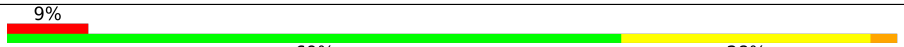
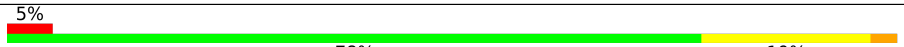
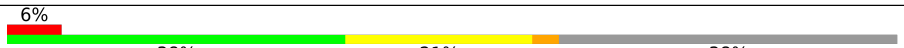
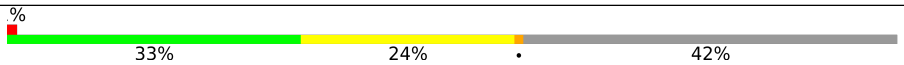
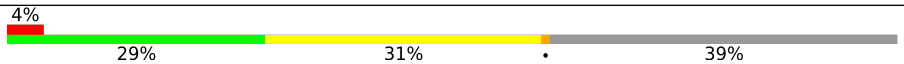
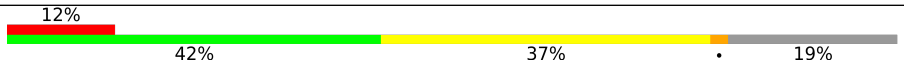
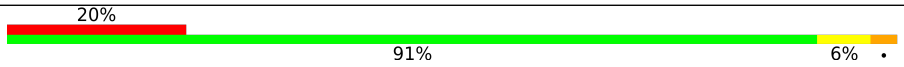
Mol	Chain	Length	Quality of chain
1	G	269	
1	H	269	
1	I	269	
1	J	269	
2	L	335	
3	P	104	
3	Q	104	
3	R	104	
3	S	104	
4	T	127	

2 Entry composition (i)

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).

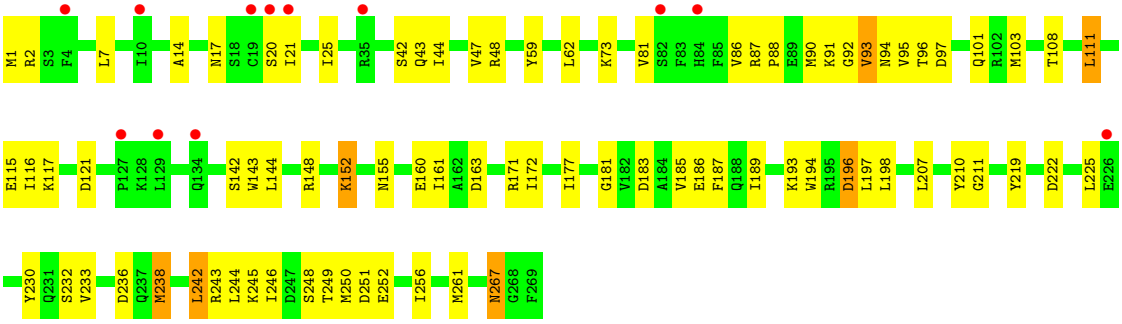
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	E	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		
5	G	1	Total	Ca	0	0
			1	1		
5	H	1	Total	Ca	0	0
			1	1		
5	I	1	Total	Ca	0	0
			1	1		
5	J	1	Total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

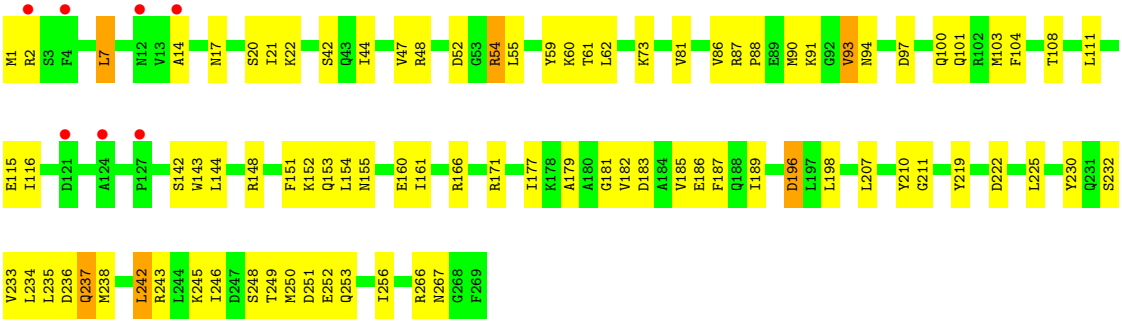
• Molecule 1: MAJOR CAPSID PROTEIN P2

Chain A:



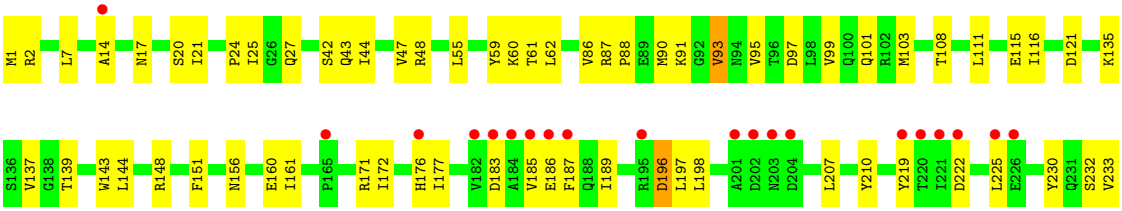
• Molecule 1: MAJOR CAPSID PROTEIN P2

Chain B:



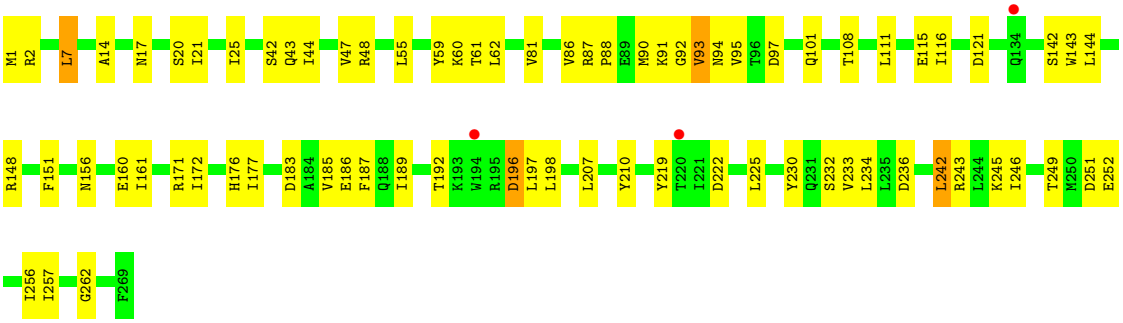
• Molecule 1: MAJOR CAPSID PROTEIN P2

Chain C:



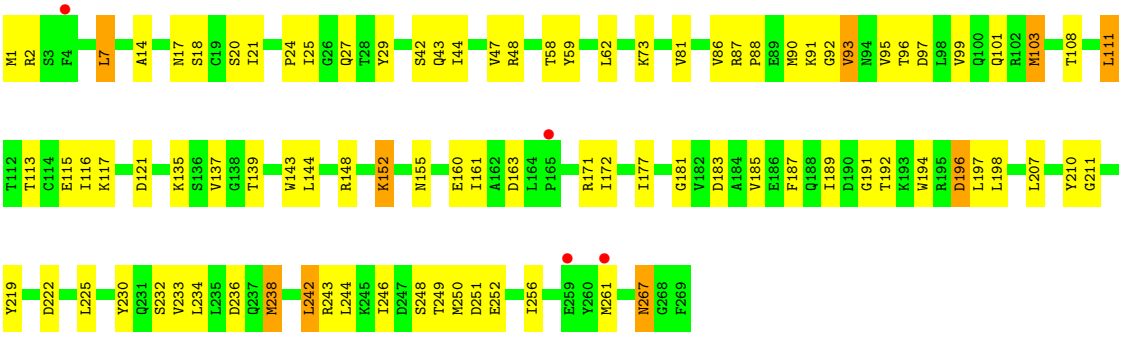
• Molecule 1: MAJOR CAPSID PROTEIN P2

Chain D:



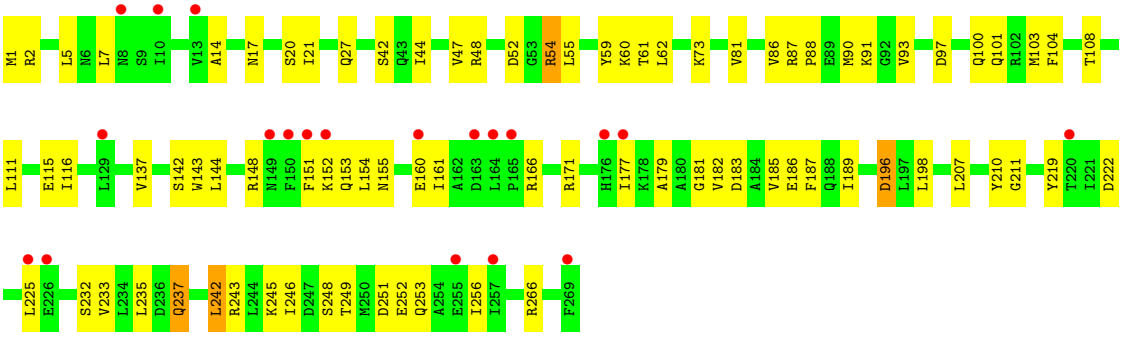
• Molecule 1: MAJOR CAPSID PROTEIN P2

Chain E:



• Molecule 1: MAJOR CAPSID PROTEIN P2

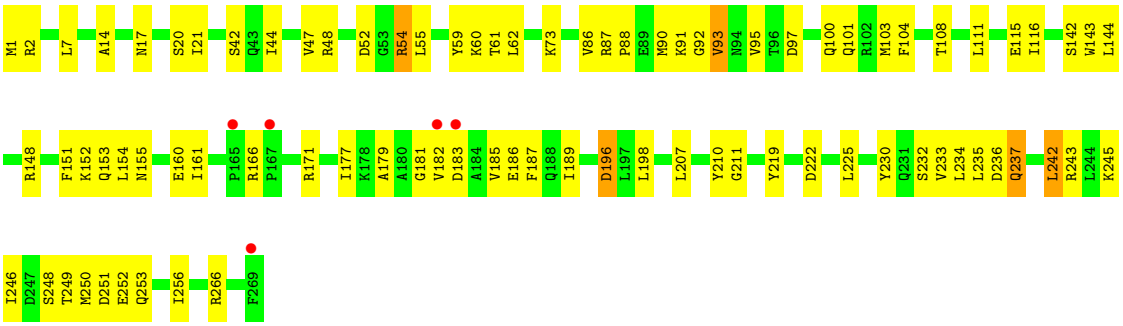
Chain F:



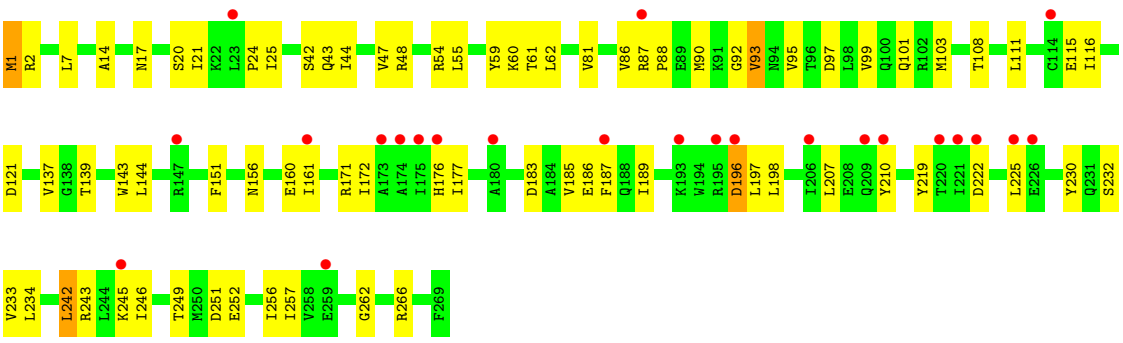
• Molecule 1: MAJOR CAPSID PROTEIN P2

Chain G:

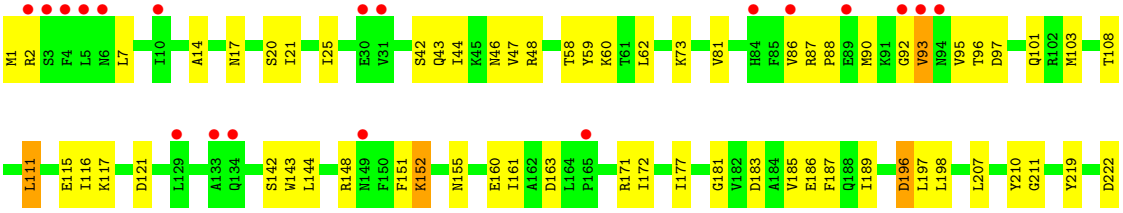
• Molecule 1: MAJOR CAPSID PROTEIN P2

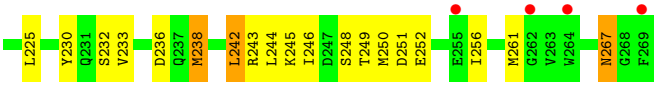


• Molecule 1: MAJOR CAPSID PROTEIN P2

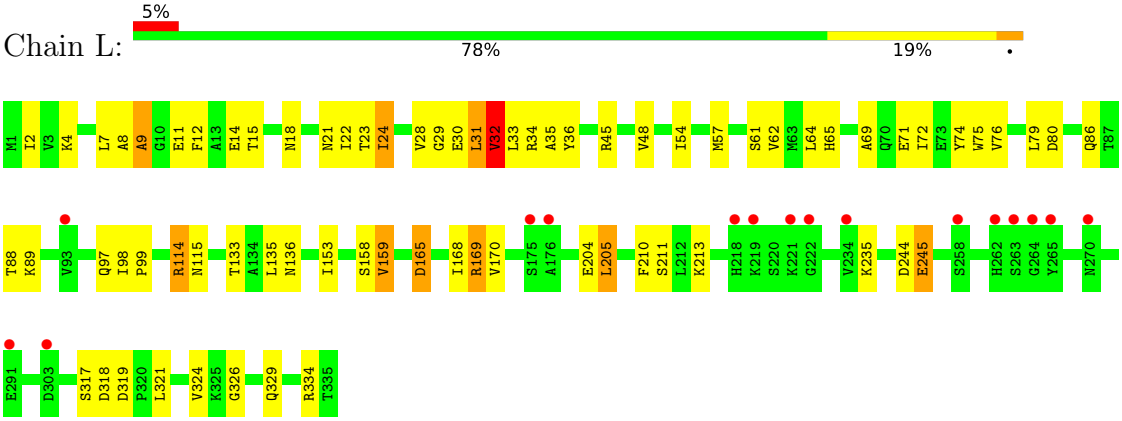


• Molecule 1: MAJOR CAPSID PROTEIN P2

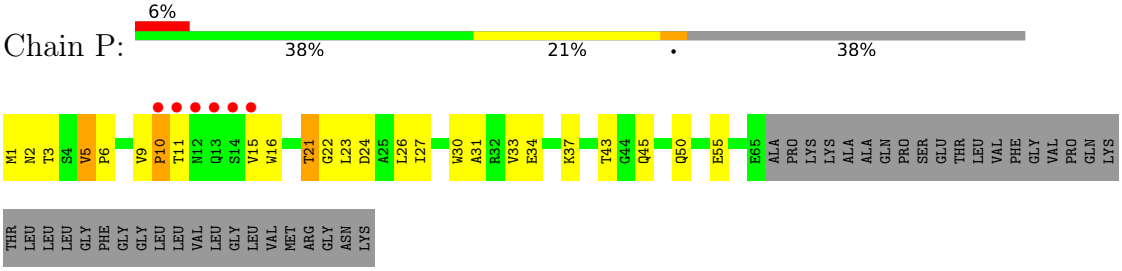




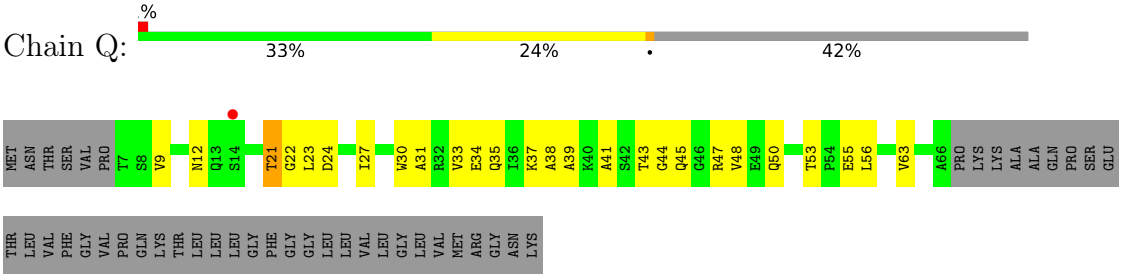
• Molecule 2: PROTEIN 2



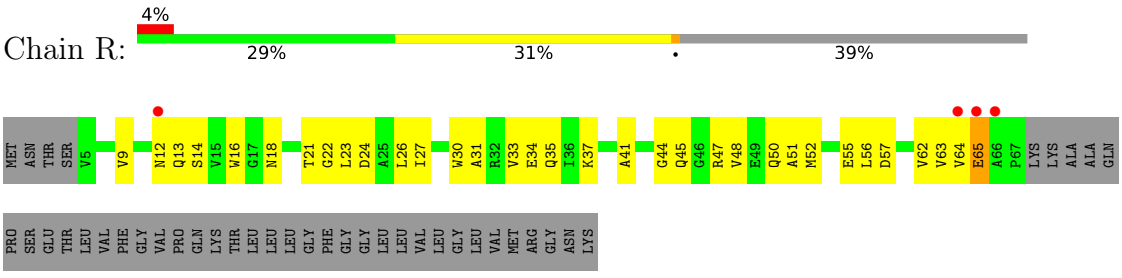
• Molecule 3: PROTEIN P3



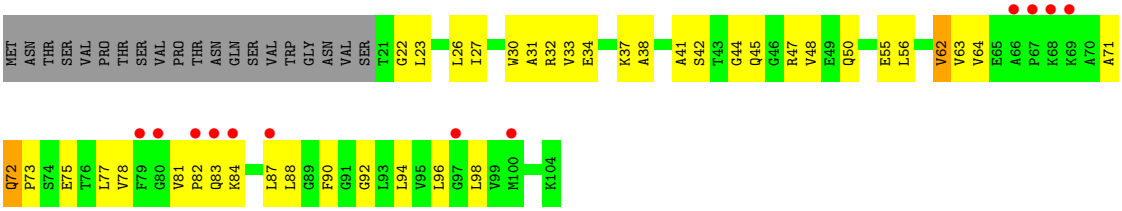
• Molecule 3: PROTEIN P3



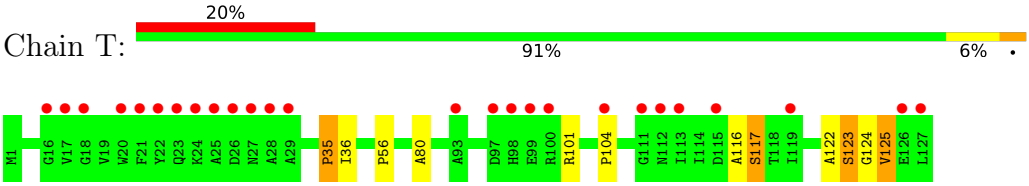
• Molecule 3: PROTEIN P3



• Molecule 3: PROTEIN P3



• Molecule 4: PROTEIN P6



4 Data and refinement statistics (i)

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 96.28 – 7.00	Depositor EDS
% Data completeness (in resolution range)	82.9 (96.00-7.00) 82.9 (96.28-7.00)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 6.73Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.419 , (Not available) 0.352 , (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 , -10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.68	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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: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
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: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: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: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

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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: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: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:B:115:GLU:OE1	3:R:56:LEU:HD23	1.56	1.05
1:C:103:MET:CE	3:Q:30:TRP:C	2.23	1.05
1:C:103:MET:HE2	3:Q:30:TRP:C	1.78	1.04
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: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: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

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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
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
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: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:C:139:THR:HG21	3:Q:37:LYS:HZ3	1.27	0.96
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: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: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:C:103:MET:CE	3:Q:30:TRP:CB	2.44	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

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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: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: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: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: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: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:I:99:VAL:O	3:S:34:GLU:CD	1.98	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: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: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: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
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: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: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: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
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: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: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:A:194:TRP:HH2	3:R:65:GLU:CD	1.84	0.81
1:C:103:MET:HE2	3:Q:30:TRP:HB3	1.62	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:PRO:HB2	3:S:55:GLU:HB3	1.62	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
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:I:143:TRP:N	3:S:30:TRP:CH2	2.53	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: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: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: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: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: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: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: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: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: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
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:B:20:SER:OG	1:B:115:GLU:HG2	1.93	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

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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: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: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
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
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:C:20:SER:OG	1:C:115:GLU:HG2	1.96	0.65
1:C:103:MET:HE1	3:Q:30:TRP:C	2.16	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: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: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: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:B:93:VAL:HG21	3:Q:38:ALA:HB2	1.80	0.64
1:C:103:MET:HE1	3:Q:31:ALA:N	2.12	0.64
1:C:135:LYS:NZ	3:Q:55:GLU:OE1	2.21	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
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:I:99:VAL:CG1	3:S:34:GLU:CD	2.64	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: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
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: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

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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: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
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: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: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:C:99:VAL:C	3:Q:34:GLU:OE2	2.42	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: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
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: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

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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: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:H:142:SER:OG	1:H:143:TRP:N	2.37	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: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: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: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: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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:193:LYS:HZ3	1:I:54:ARG:HH22	1.55	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
2:L:76:VAL:O	2:L:76:VAL:HG13	2.09	0.53
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
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: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: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:267:ASN:OD1	3:R:52:MET:HE2	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:108:THR:O	1:I:111:LEU:HB2	2.10	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
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
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: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: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: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:C:171:ARG:HD3	1:C:232:SER:OG	2.11	0.50
1:D:142:SER:OG	1:D:143:TRP:N	2.37	0.50
1:F:52:ASP:OD2	1:F:266:ARG:NE	2.45	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:B:237:GLN:HG3	1:B:237:GLN:O	2.10	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: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: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: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:I:137:VAL:CG2	3:S:50:GLN:CD	2.81	0.49
2:L:32:VAL:CG2	2:L:33:LEU:HD12	2.30	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
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: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
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:113:THR:HG21	3:S:56:LEU:HD11	1.90	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:TYR:CZ	3:R:27:ILE:CD1	2.97	0.48
1:H:171:ARG:NH2	3:S:42:SER:C	2.62	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: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:G:91:LYS:HB3	1:G:91:LYS:HE3	1.76	0.47
2:L:213:LYS:NZ	2:L:318:ASP:OD2	2.44	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:A:194:TRP:CH2	3:R:65:GLU:CD	2.73	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: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: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

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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
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
3:Q:30:TRP:O	3:Q:33:VAL:HG12	2.15	0.46
1:F:54:ARG:CG	1:F:54:ARG:NH1	2.78	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: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:G:236:ASP:C	1:G:238:MET:H	2.19	0.46
1:H:187:PHE:HE1	1:H:242:LEU:HD11	1.81	0.46
1:B:183:ASP:CG	1:B:249:THR:HG23	2.34	0.45
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
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: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:D:148:ARG:HA	1:D:148:ARG:HD3	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:54:ARG:CG	1:B:54:ARG:NH1	2.78	0.45
3:R:30:TRP:O	3:R:33:VAL:HG12	2.16	0.45
1:A:236:ASP:C	1:A:238:MET:H	2.19	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:I:21:ILE:HB	1:I:116:ILE:HB	1.99	0.45
1:J:151:PHE:HB3	2:L:11:GLU:CD	2.32	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:H:230:TYR:HB3	3:S:41:ALA:C	2.37	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:H:183:ASP:CG	1:H:249:THR:HG23	2.34	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:D:93:VAL:C	1:E:96:THR:HG21	2.37	0.44
1:B:207:LEU:HD23	1:B:225:LEU:HD21	1.98	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:C:230:TYR:HH	3:Q:27:ILE:CB	2.21	0.44
1:G:137:VAL:CG2	3:P:50:GLN:CD	2.86	0.44
1:G:171:ARG:NH2	3:P:23:LEU:CD2	2.76	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: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:J:171:ARG:HD3	1:J:232:SER:OG	2.17	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:G:148:ARG:HA	1:G:148:ARG:HD3	1.65	0.44
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
1:J:181:GLY:HA3	1:J:250:MET:HE3	1.99	0.44
1:J:236:ASP:C	1:J:238:MET:H	2.19	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:I:43:GLN:HG2	1:I:121:ASP:HB3	2.00	0.44
1:A:210:TYR:HH	1:B:2:ARG:HH22	1.65	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: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:C:207:LEU:HD23	1:C:225:LEU:HD21	1.99	0.43
1:C:43:GLN:HG2	1:C:121:ASP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ILE:HD12	1:D:246:ILE:HD11	1.99	0.43
1:E:93:VAL:HG11	1:E:230:TYR:CD2	2.52	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
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: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:J:93:VAL:HG11	1:J:230:TYR:CD2	2.52	0.43
1:C:139:THR:CG2	3:Q:37:LYS:HZ1	2.09	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:181:GLY:HA3	1:B:250:MET:HE3	1.99	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: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:H:177:ILE:HG12	1:H:256:ILE:HD12	2.01	0.42
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: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: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
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: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:I:222:ASP:HB3	1:I:225:LEU:HG	2.02	0.42
1:A:181:GLY:HA3	1:A:250:MET:HE3	2.01	0.42
1:G:181:GLY:HA3	1:G:250:MET:HE3	2.02	0.42
1:I:176:HIS:HB2	1:I:257:ILE:HB	2.01	0.42
3:R:55:GLU:C	3:R:56:LEU:HD12	2.39	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:103:MET:CE	3:Q:30:TRP:HB2	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:MET:HE3	3:Q:31:ALA:CA	2.50	0.42
1:C:186:GLU:HB3	1:C:245:LYS:HB2	2.01	0.42
1:E:181:GLY:HA3	1:E:250:MET:HE3	2.00	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:I:137:VAL:HG23	3:S:50:GLN:CD	2.40	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
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: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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:62:LEU:HD21	1:E:81:VAL:HG11	2.02	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
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: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:151:PHE:C	1:B:152:LYS:HG2	2.41	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:H:181:GLY:CA	1:H:250:MET:HE3	2.51	0.40
1:B:60:LYS:HD2	1:B:151:PHE:HZ	1.85	0.40
1:F:183:ASP:CG	1:F:249:THR:HG23	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:151:PHE:C	1:F:152:LYS:HG2	2.41	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
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: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
3:S:55:GLU:C	3:S:56:LEU:HD12	2.41	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
1:H:151:PHE:C	1:H:152:LYS:HG2	2.41	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%)	34 72
1	B	267/269 (99%)	251 (94%)	16 (6%)	0	100 100
1	C	267/269 (99%)	252 (94%)	14 (5%)	1 (0%)	34 72
1	D	267/269 (99%)	251 (94%)	15 (6%)	1 (0%)	34 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	34 72
1	F	267/269 (99%)	251 (94%)	16 (6%)	0	100 100
1	G	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	34 72
1	H	267/269 (99%)	251 (94%)	16 (6%)	0	100 100
1	I	267/269 (99%)	252 (94%)	14 (5%)	1 (0%)	34 72
1	J	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	34 72
2	L	331/335 (99%)	306 (92%)	19 (6%)	6 (2%)	8 40
3	P	63/104 (61%)	56 (89%)	5 (8%)	2 (3%)	4 26
3	Q	58/104 (56%)	51 (88%)	6 (10%)	1 (2%)	9 42
3	R	61/104 (59%)	53 (87%)	6 (10%)	2 (3%)	4 26
3	S	82/104 (79%)	74 (90%)	6 (7%)	2 (2%)	6 33
4	T	125/127 (98%)	112 (90%)	7 (6%)	6 (5%)	2 21
All	All	3390/3568 (95%)	3160 (93%)	204 (6%)	26 (1%)	19 60

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/232 (100%)	219 (94%)	13 (6%)	21	46
1	B	232/232 (100%)	219 (94%)	13 (6%)	21	46
1	C	232/232 (100%)	221 (95%)	11 (5%)	26	51
1	D	232/232 (100%)	221 (95%)	11 (5%)	26	51
1	E	232/232 (100%)	217 (94%)	15 (6%)	17	42
1	F	232/232 (100%)	219 (94%)	13 (6%)	21	46
1	G	232/232 (100%)	218 (94%)	14 (6%)	19	44
1	H	232/232 (100%)	219 (94%)	13 (6%)	21	46
1	I	232/232 (100%)	221 (95%)	11 (5%)	26	51
1	J	232/232 (100%)	218 (94%)	14 (6%)	19	44
2	L	272/285 (95%)	266 (98%)	6 (2%)	52	71
3	P	44/81 (54%)	42 (96%)	2 (4%)	27	52
3	Q	45/81 (56%)	44 (98%)	1 (2%)	52	71
3	R	48/81 (59%)	48 (100%)	0	100	100
3	S	62/81 (76%)	61 (98%)	1 (2%)	62	79
All	All	2791/2929 (95%)	2653 (95%)	138 (5%)	25	50

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

Sometimes 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 monosaccharides 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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	269/269 (100%)	0.08	12 (4%) 33 31	40, 40, 40, 40	0
1	B	269/269 (100%)	0.07	7 (2%) 56 49	40, 40, 40, 40	0
1	C	269/269 (100%)	0.24	20 (7%) 14 15	40, 40, 40, 40	0
1	D	269/269 (100%)	-0.08	3 (1%) 80 73	40, 40, 40, 40	0
1	E	269/269 (100%)	-0.13	4 (1%) 73 65	40, 40, 40, 40	0
1	F	269/269 (100%)	0.24	20 (7%) 14 15	40, 40, 40, 40	0
1	G	269/269 (100%)	-0.11	1 (0%) 92 87	40, 40, 40, 40	0
1	H	269/269 (100%)	-0.05	5 (1%) 66 59	40, 40, 40, 40	0
1	I	269/269 (100%)	0.45	24 (8%) 9 12	40, 40, 40, 40	0
1	J	269/269 (100%)	0.36	23 (8%) 10 13	40, 40, 40, 40	0
2	L	335/335 (100%)	0.33	16 (4%) 30 29	40, 40, 40, 40	0
3	P	65/104 (62%)	0.26	6 (9%) 9 11	40, 40, 40, 40	0
3	Q	60/104 (57%)	-0.15	1 (1%) 70 62	40, 40, 40, 40	0
3	R	63/104 (60%)	0.07	4 (6%) 20 19	40, 40, 40, 40	0
3	S	84/104 (80%)	0.69	12 (14%) 2 6	40, 40, 40, 40	0
4	T	127/127 (100%)	1.06	26 (20%) 1 3	40, 40, 40, 40	0
All	All	3424/3568 (95%)	0.18	184 (5%) 25 26	40, 40, 40, 40	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	4	PHE	5.9
3	P	14	SER	5.7
1	F	165	PRO	5.0
1	I	196	ASP	4.9
3	S	68	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
4	T	24	LYS	4.9
4	T	127	LEU	4.9
1	H	269	PHE	4.8
1	J	134	GLN	4.8
1	I	222	ASP	4.8
1	C	222	ASP	4.7
2	L	263	SER	4.7
3	P	13	GLN	4.6
4	T	23	GLN	4.5
3	P	10	PRO	4.3
1	I	195	ARG	4.3
2	L	175	SER	4.3
3	P	11	THR	4.2
4	T	27	ASN	4.1
3	S	83	GLN	4.0
4	T	26	ASP	4.0
3	P	12	ASN	4.0
3	S	67	PRO	3.9
4	T	126	GLU	3.8
1	I	193	LYS	3.8
1	C	202	ASP	3.8
1	I	220	THR	3.7
4	T	25	ALA	3.7
3	S	66	ALA	3.6
3	R	65	GLU	3.6
1	F	226	GLU	3.6
1	F	220	THR	3.6
1	F	149	ASN	3.6
1	F	13	VAL	3.5
1	H	167	PRO	3.5
1	I	114	CYS	3.5
1	J	133	ALA	3.5
1	F	10	ILE	3.5
2	L	264	GLY	3.4
1	I	221	ILE	3.4
4	T	99	GLU	3.4
4	T	98	HIS	3.4
1	J	149	ASN	3.3
1	B	124	ALA	3.3
1	F	257	ILE	3.3
1	I	210	TYR	3.3
2	L	176	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	20	SER	3.2
1	C	221	ILE	3.2
2	L	93	VAL	3.2
4	T	22	TYR	3.2
4	T	112	ASN	3.1
1	J	269	PHE	3.1
3	R	12	ASN	3.1
1	F	151	PHE	3.1
1	I	259	GLU	3.0
1	F	255	GLU	3.0
1	J	165	PRO	3.0
3	R	64	VAL	3.0
1	J	5	LEU	3.0
1	C	183	ASP	2.9
1	F	164	LEU	2.9
1	J	93	VAL	2.9
4	T	21	PHE	2.9
1	F	129	LEU	2.9
4	T	20	TRP	2.9
1	I	176	HIS	2.9
3	Q	14	SER	2.9
1	A	4	PHE	2.9
1	C	195	ARG	2.9
1	D	194	TRP	2.9
1	J	262	GLY	2.8
4	T	100	ARG	2.8
1	I	187	PHE	2.8
1	H	183	ASP	2.8
1	I	209	GLN	2.8
1	J	10	ILE	2.8
1	F	269	PHE	2.8
4	T	104	PRO	2.8
1	C	187	PHE	2.8
1	J	255	GLU	2.8
1	A	134	GLN	2.8
1	J	6	ASN	2.7
2	L	218	HIS	2.7
1	A	19	CYS	2.7
1	D	134	GLN	2.7
1	C	220	THR	2.7
1	F	150	PHE	2.7
1	A	129	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	175	ILE	2.7
4	T	97	ASP	2.6
1	J	2	ARG	2.6
1	C	182	VAL	2.6
1	I	174	ALA	2.6
3	S	79	PHE	2.6
1	A	226	GLU	2.6
1	J	94	ASN	2.5
3	P	15	VAL	2.5
1	H	165	PRO	2.5
1	F	163	ASP	2.5
4	T	119	ILE	2.5
1	C	176	HIS	2.5
2	L	258	SER	2.5
1	E	261	MET	2.5
3	S	87	LEU	2.5
4	T	16	GLY	2.5
1	E	4	PHE	2.4
2	L	219	LYS	2.4
1	I	225	LEU	2.4
2	L	262	HIS	2.4
1	D	220	THR	2.4
1	C	184	ALA	2.4
2	L	265	TYR	2.4
1	B	2	ARG	2.4
2	L	270	ASN	2.4
1	B	14	ALA	2.4
4	T	17	VAL	2.4
1	F	152	LYS	2.4
1	J	264	TRP	2.4
2	L	303	ASP	2.4
3	S	80	GLY	2.4
1	J	3	SER	2.4
1	C	165	PRO	2.3
2	L	291	GLU	2.3
4	T	111	GLY	2.3
1	H	182	VAL	2.3
1	F	8	ASN	2.3
2	L	221	LYS	2.3
3	S	84	LYS	2.3
1	C	226	GLU	2.3
1	C	201	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	84	HIS	2.3
1	J	30	GLU	2.3
1	E	165	PRO	2.3
3	S	69	LYS	2.3
1	I	206	ILE	2.3
1	A	82	SER	2.2
1	G	165	PRO	2.2
1	F	176	HIS	2.2
1	E	259	GLU	2.2
1	C	203	ASN	2.2
3	S	97	GLY	2.2
1	A	127	PRO	2.2
4	T	28	ALA	2.2
1	C	219	TYR	2.2
2	L	234	VAL	2.2
1	J	31	VAL	2.2
1	B	121	ASP	2.2
1	I	161	ILE	2.2
3	S	100	MET	2.2
1	I	23	LEU	2.1
4	T	93	ALA	2.1
1	A	21	ILE	2.1
1	F	160	GLU	2.1
3	S	82	PRO	2.1
1	B	4	PHE	2.1
1	C	225	LEU	2.1
1	A	35	ARG	2.1
1	F	225	LEU	2.1
1	I	147	ARG	2.1
1	C	14	ALA	2.1
1	J	86	VAL	2.1
1	I	87	ARG	2.1
1	J	89	GLU	2.1
2	L	222	GLY	2.1
4	T	18	GLY	2.1
4	T	29	ALA	2.1
4	T	115	ASP	2.1
1	F	177	ILE	2.1
1	I	180	ALA	2.1
1	J	92	GLY	2.0
4	T	113	ILE	2.0
1	C	186	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	226	GLU	2.0
3	R	66	ALA	2.0
1	I	173	ALA	2.0
1	B	12	ASN	2.0
1	I	245	LYS	2.0
1	B	127	PRO	2.0
1	J	129	LEU	2.0
1	J	84	HIS	2.0
1	C	204	ASP	2.0
1	C	185	VAL	2.0
1	A	10	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	B	1270	1/1	0.64	0.17	40,40,40,40	0
5	CA	C	1270	1/1	0.68	0.11	40,40,40,40	0
5	CA	H	1270	1/1	0.69	0.13	40,40,40,40	0
5	CA	E	1270	1/1	0.72	0.18	40,40,40,40	0
5	CA	F	1270	1/1	0.87	0.10	40,40,40,40	0
5	CA	G	1270	1/1	0.87	0.09	40,40,40,40	0
5	CA	D	1270	1/1	0.87	0.18	40,40,40,40	0
5	CA	J	1270	1/1	0.88	0.33	40,40,40,40	0
5	CA	A	1270	1/1	0.91	0.14	40,40,40,40	0
5	CA	L	400	1/1	0.92	0.62	40,40,40,40	0
5	CA	I	1270	1/1	0.98	0.10	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.