Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 08:07 AM EDT

PDB ID	:	2QI9
Title	:	ABC-transporter BtuCD in complex with its periplasmic binding protein BtuF
Authors	:	Hvorup, R.N.; Goetz, B.A.; Niederer, M.; Hollenstein, K.; Perozo, E.; Locher, K.P.
Deposited on	:	2007-07-03
Resolution	:	2.60 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 (i) symbol.

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

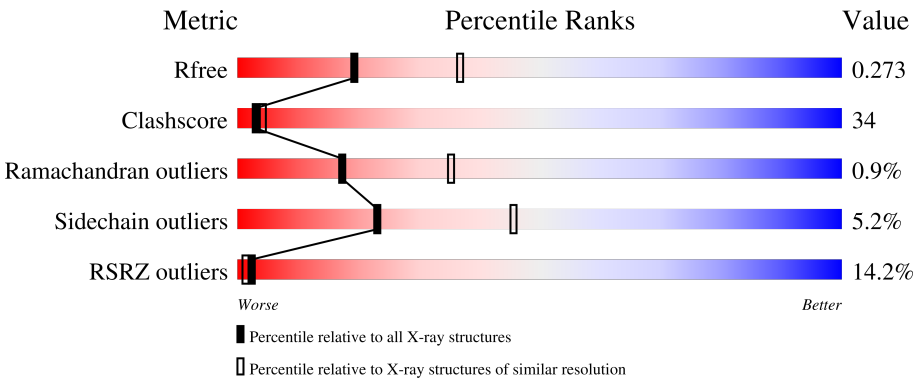
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	326	10% 51% 46% • •
1	B	326	6% 42% 52% 5% •
2	C	249	% 62% 33% 5%
2	D	249	2% 62% 33% •
3	F	245	55% 56% 42% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	1PE	D	800	-	-	-	X
7	PEG	D	500	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10692 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 Vitamin B12 import system permease protein btuC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	324	2441	1611	418	400	1	11	0	0	0
1	B	324	2441	1611	418	400	1	11	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	SER	CYS	engineered mutation	UNP P06609
A	32	SER	CYS	engineered mutation	UNP P06609
A	120	SER	CYS	engineered mutation	UNP P06609
A	156	SER	CYS	engineered mutation	UNP P06609
A	205	SER	CYS	engineered mutation	UNP P06609
A	206	SER	CYS	engineered mutation	UNP P06609
A	267	SER	CYS	engineered mutation	UNP P06609
B	18	SER	CYS	engineered mutation	UNP P06609
B	32	SER	CYS	engineered mutation	UNP P06609
B	120	SER	CYS	engineered mutation	UNP P06609
B	156	SER	CYS	engineered mutation	UNP P06609
B	205	SER	CYS	engineered mutation	UNP P06609
B	206	SER	CYS	engineered mutation	UNP P06609
B	267	SER	CYS	engineered mutation	UNP P06609

- Molecule 2 is a protein called Vitamin B12 import ATP-binding protein btuD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
2	C	248	1893	1184	351	350	8	0	0	0
2	D	248	1893	1184	351	350	8	0	0	0

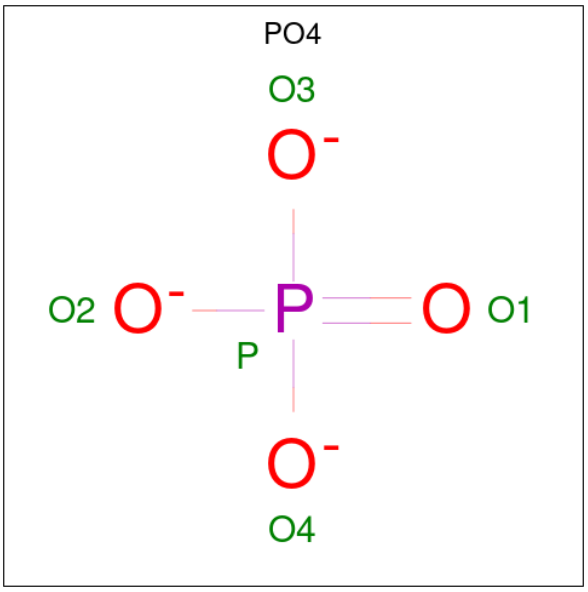
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	180	SER	CYS	engineered mutation	UNP P06611
D	180	SER	CYS	engineered mutation	UNP P06611

- Molecule 3 is a protein called Vitamin B12-binding protein btuF.

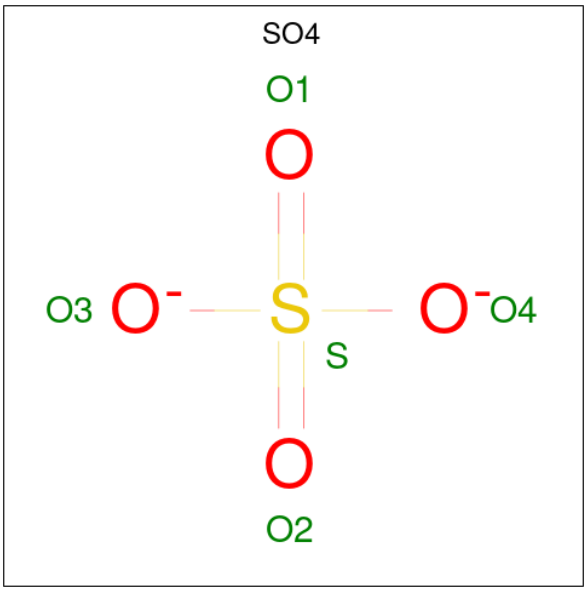
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
3	F	245	1908	1216	332	356	2	2	0	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



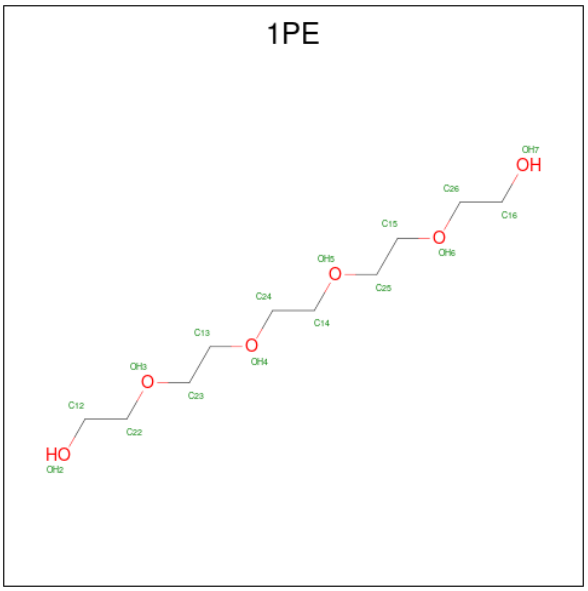
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
4	C	1	5	4	1	0	0
4	D	1	5	4	1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



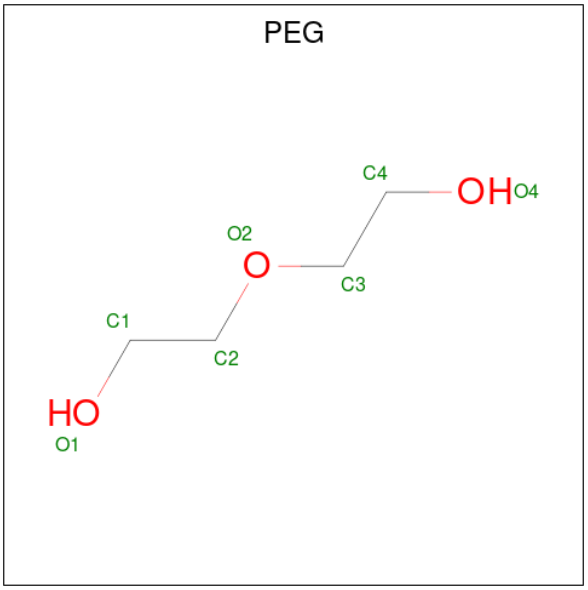
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
5	C	1	5	4	1		0	0
			Total	O	S			
5	C	1	5	4	1		0	0
			Total	O	S			
5	C	1	5	4	1		0	0
			Total	O	S			
5	D	1	5	4	1		0	0
			Total	O	S			
5	D	1	5	4	1		0	0
			Total	O	S			
5	D	1	5	4	1		0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	C	1	16	10	6	0	0
			Total	C	O		
6	D	1	16	10	6	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	C	1	7	4	3	0	0
			Total	C	O		
7	C	1	7	4	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	D	1	7	4	3	0	0
			Total	C	O		
7	D	1	7	4	3	0	0

- Molecule 8 is water.

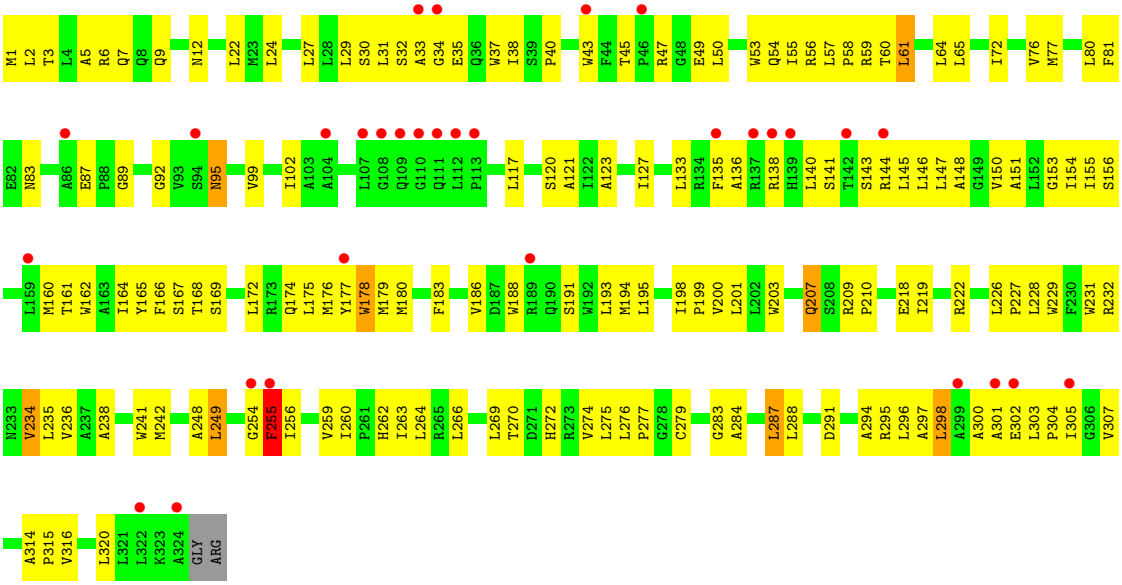
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	C	8	8	8	0	0
			Total	O		
8	D	8	8	8	0	0

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.

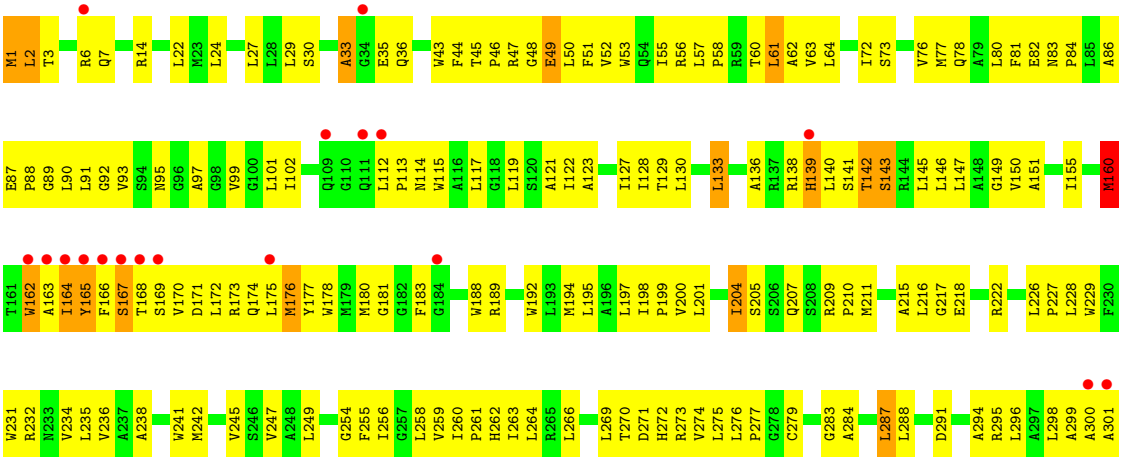
• Molecule 1: Vitamin B12 import system permease protein btuC

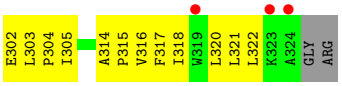
Chain A:



• Molecule 1: Vitamin B12 import system permease protein btuC

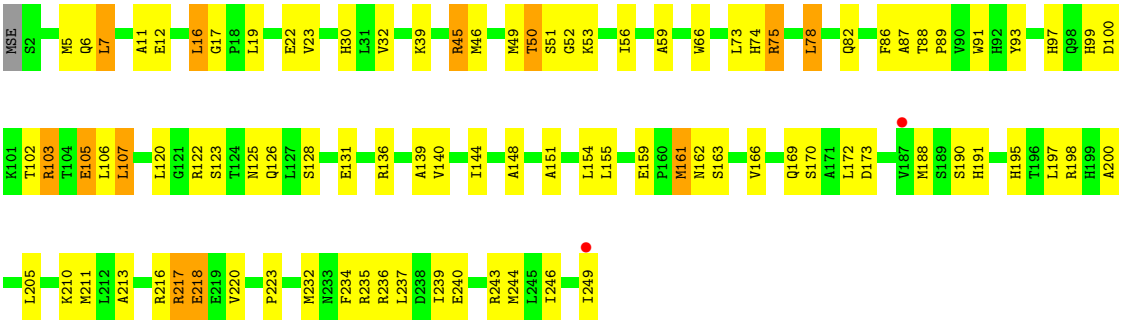
Chain B:





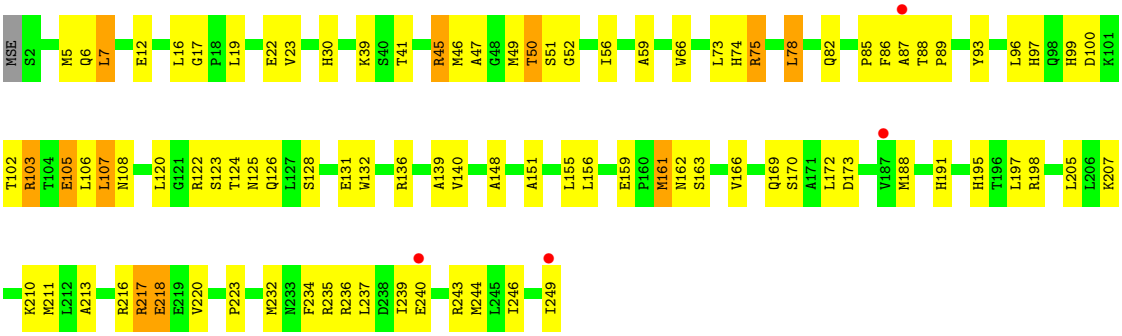
• Molecule 2: Vitamin B12 import ATP-binding protein btuD

Chain C:



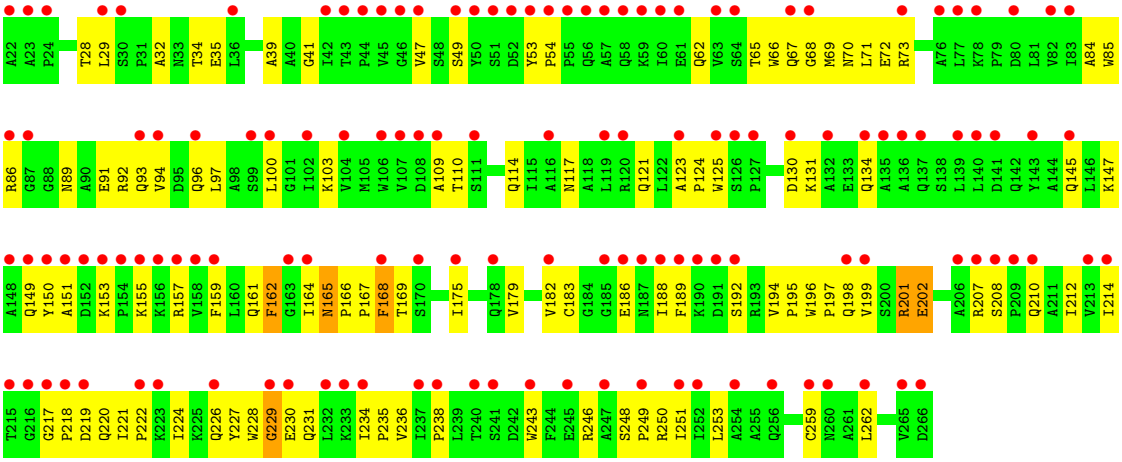
• Molecule 2: Vitamin B12 import ATP-binding protein btuD

Chain D:



• Molecule 3: Vitamin B12-binding protein btuF

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	213.58Å 127.40Å 97.55Å 90.00° 112.76° 90.00°	Depositor
Resolution (Å)	29.81 – 2.60 29.81 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.81-2.60) 99.2 (29.81-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 2.61Å)	Xtriage
Refinement program	REFMAC, CNS	Depositor
R, R_{free}	0.262 , 0.280 0.259 , 0.273	Depositor DCC
R_{free} test set	3738 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	59.3	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 72.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10692	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 1PE, PO4, PEG

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	0.42	1/2485 (0.0%)	0.66	2/3378 (0.1%)
1	B	0.50	5/2485 (0.2%)	0.80	5/3378 (0.1%)
2	C	0.40	0/1919	0.63	0/2587
2	D	0.39	0/1919	0.65	0/2587
3	F	0.30	0/1950	0.57	0/2655
All	All	0.42	6/10758 (0.1%)	0.67	7/14585 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	PHE	C-N	-9.62	1.11	1.34
1	B	167	SER	C-N	6.62	1.49	1.34
1	B	164	ILE	C-N	6.21	1.48	1.34
1	B	143	SER	CB-OG	-6.21	1.34	1.42
1	B	296	LEU	C-N	-5.78	1.20	1.34
1	B	160	MSE	C-N	-5.33	1.21	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	296	LEU	O-C-N	-14.87	98.91	122.70
1	B	296	LEU	CA-C-N	10.55	140.42	117.20
1	B	160	MSE	O-C-N	-9.32	107.79	122.70
1	B	296	LEU	C-N-CA	8.95	144.06	121.70
1	A	255	PHE	O-C-N	-8.61	108.92	122.70
1	B	167	SER	C-N-CA	5.80	136.19	121.70
1	A	255	PHE	C-N-CA	5.25	134.81	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	PHE	Peptide
1	B	160	MSE	Mainchain

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	2441	0	2605	225	0
1	B	2441	0	2604	270	0
2	C	1893	0	1925	100	0
2	D	1893	0	1925	106	0
3	F	1908	0	1924	156	0
4	C	5	0	0	1	0
4	D	5	0	0	1	0
5	C	15	0	0	0	0
5	D	15	0	0	0	0
6	C	16	0	22	6	0
6	D	16	0	22	5	0
7	C	14	0	20	0	0
7	D	14	0	20	1	0
8	C	8	0	0	1	0
8	D	8	0	0	1	0
All	All	10692	0	11067	743	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 34.

All (743) 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:B:164:ILE:HG23	1:B:175:LEU:CD1	1.55	1.33
1:A:35:GLU:CD	3:F:72:GLU:HG3	1.47	1.33
1:B:162:TRP:O	1:B:165:TYR:HD2	1.27	1.18
2:D:86:PHE:CA	2:D:125:ASN:HD21	1.60	1.15
1:A:307:VAL:CG1	1:B:162:TRP:HE3	1.62	1.12
1:A:35:GLU:CB	3:F:72:GLU:CB	2.28	1.11
2:D:86:PHE:HA	2:D:125:ASN:ND2	1.63	1.10
2:D:86:PHE:HA	2:D:125:ASN:HD21	1.10	1.10
1:B:90:LEU:HG	1:B:258:LEU:HD11	1.32	1.09
1:B:164:ILE:HG12	1:B:175:LEU:HD13	1.19	1.08
1:B:167:SER:HB2	1:B:171:ASP:HB2	1.38	1.05
1:A:35:GLU:HG2	3:F:72:GLU:HB2	1.33	1.04
1:B:61:LEU:HB3	1:B:194:MSE:HE1	1.39	1.03
1:B:164:ILE:CG2	1:B:175:LEU:CD1	2.37	1.03
1:A:35:GLU:CG	3:F:72:GLU:HB2	1.87	1.03
1:B:164:ILE:CG1	1:B:175:LEU:HD13	1.90	1.02
2:C:5:MSE:HE3	2:C:46:MSE:HE2	1.41	1.02
1:B:164:ILE:HG23	1:B:175:LEU:HD12	1.38	1.01
1:A:35:GLU:OE1	3:F:72:GLU:HG3	1.59	1.01
2:D:5:MSE:HE3	2:D:46:MSE:HE2	1.42	0.99
1:B:162:TRP:O	1:B:165:TYR:CD2	2.14	0.99
1:B:83:ASN:HD22	1:B:145:LEU:HD23	1.24	0.99
1:A:35:GLU:CB	3:F:72:GLU:HB2	1.91	0.99
1:A:146:LEU:HD21	1:B:147:LEU:HD11	1.45	0.99
2:C:86:PHE:HA	2:C:125:ASN:HD21	1.27	0.98
1:A:301:ALA:HB3	3:F:70:ASN:HA	1.42	0.97
1:A:302:GLU:HG2	3:F:68:GLY:HA3	1.46	0.97
1:A:55:ILE:HD11	3:F:100:LEU:HD11	1.49	0.95
1:B:298:LEU:HB2	1:B:301:ALA:HB3	1.47	0.94
1:A:35:GLU:CG	3:F:72:GLU:HG3	1.97	0.93
2:C:87:ALA:H	2:C:125:ASN:ND2	1.64	0.93
1:A:146:LEU:HD23	1:B:143:SER:HB3	1.52	0.92
2:D:159:GLU:HA	6:D:800:1PE:H261	1.53	0.91
1:A:30:SER:HB2	1:A:295:ARG:HH22	1.35	0.90
1:A:35:GLU:CD	3:F:72:GLU:CG	2.39	0.90
1:A:35:GLU:CG	3:F:72:GLU:CB	2.49	0.90
1:A:302:GLU:CB	3:F:68:GLY:HA3	2.03	0.89
1:A:35:GLU:CB	3:F:72:GLU:HB3	2.01	0.89
1:A:180:MSE:HE2	1:A:304:PRO:HG3	1.52	0.89
1:A:307:VAL:CG1	1:B:162:TRP:CE3	2.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASN:N	1:A:95:ASN:HD22	1.72	0.88
1:A:138:ARG:HH12	1:B:322:LEU:HD22	1.37	0.88
1:B:262:HIS:HD2	1:B:320:LEU:HD11	1.40	0.87
1:A:302:GLU:CG	3:F:68:GLY:HA3	2.04	0.86
2:C:86:PHE:HA	2:C:125:ASN:ND2	1.89	0.86
3:F:243:TRP:HE1	3:F:250:ARG:HH21	1.23	0.86
2:C:161:MSE:HG3	2:C:169:GLN:HG2	1.56	0.86
1:B:171:ASP:O	1:B:175:LEU:HG	1.76	0.85
1:B:298:LEU:HD12	1:B:301:ALA:HB1	1.57	0.85
2:C:86:PHE:CA	2:C:125:ASN:HD21	1.89	0.85
2:D:161:MSE:HG3	2:D:169:GLN:HG2	1.59	0.85
1:A:35:GLU:HB3	3:F:72:GLU:CB	2.03	0.85
1:A:35:GLU:HB3	3:F:72:GLU:HB2	1.58	0.85
1:B:87:GLU:HG2	1:B:89:GLY:H	1.41	0.85
1:A:35:GLU:CG	3:F:72:GLU:CG	2.55	0.84
1:B:164:ILE:HG23	1:B:175:LEU:HD11	1.59	0.84
1:A:147:LEU:HD13	1:B:321:LEU:HD22	1.60	0.84
1:A:161:THR:HG22	1:B:180:MSE:HE3	1.59	0.84
1:B:298:LEU:HD12	1:B:301:ALA:CB	2.08	0.84
1:B:80:LEU:HD21	1:B:236:VAL:CG2	2.08	0.83
1:B:167:SER:HB2	1:B:171:ASP:CB	2.08	0.83
2:D:86:PHE:HA	2:D:125:ASN:CG	1.98	0.83
1:A:35:GLU:HG2	3:F:72:GLU:CB	2.07	0.83
1:A:35:GLU:HB2	3:F:72:GLU:CB	2.09	0.83
1:B:30:SER:HB2	1:B:295:ARG:HH22	1.43	0.83
3:F:165:ASN:O	3:F:167:PRO:HD3	1.78	0.83
1:B:163:ALA:O	1:B:166:PHE:CD2	2.31	0.82
1:B:270:THR:HG23	2:D:87:ALA:O	1.80	0.82
2:D:191:HIS:HB3	6:D:800:1PE:OH6	1.79	0.82
2:C:159:GLU:HA	6:C:800:1PE:H261	1.62	0.82
2:C:191:HIS:HB3	6:C:800:1PE:OH6	1.78	0.82
1:B:139:HIS:O	1:B:140:LEU:HG	1.80	0.82
1:A:35:GLU:HB2	3:F:72:GLU:HB3	1.61	0.81
1:A:12:ASN:HB3	1:A:274:VAL:HG11	1.60	0.81
1:A:298:LEU:HD13	3:F:67:GLN:NE2	1.96	0.81
3:F:165:ASN:HB3	3:F:166:PRO:CD	2.10	0.81
1:A:207:GLN:HE21	1:A:207:GLN:HA	1.46	0.81
1:A:302:GLU:CD	3:F:93:GLN:NE2	2.34	0.81
1:A:307:VAL:HG12	1:B:162:TRP:HE3	1.44	0.81
1:B:1:MSE:HE2	1:B:2:LEU:HA	1.62	0.79
2:C:87:ALA:H	2:C:125:ASN:HD21	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ILE:HG23	1:B:175:LEU:HD13	1.62	0.79
3:F:159:PHE:CE2	3:F:161:GLN:HB2	2.18	0.79
1:A:193:LEU:HB3	1:A:249:LEU:CD2	2.13	0.79
1:A:95:ASN:HD22	1:A:95:ASN:H	1.31	0.78
1:A:307:VAL:HG13	1:B:162:TRP:HB2	1.65	0.78
1:A:302:GLU:OE1	3:F:93:GLN:NE2	2.17	0.78
1:B:160:MSE:O	1:B:164:ILE:HG13	1.83	0.78
3:F:53:TYR:CD2	3:F:250:ARG:HD2	2.19	0.78
1:A:256:ILE:HG23	1:A:260:ILE:HD12	1.65	0.77
3:F:86:ARG:HG2	3:F:86:ARG:HH11	1.49	0.77
1:B:1:MSE:HG3	2:D:120:LEU:HD13	1.66	0.77
1:A:298:LEU:HD13	3:F:67:GLN:HE22	1.50	0.76
3:F:123:ALA:HB3	3:F:124:PRO:HD3	1.67	0.76
1:A:264:LEU:HD22	1:A:269:LEU:HD12	1.68	0.76
1:B:264:LEU:HD22	1:B:269:LEU:HD12	1.67	0.76
1:A:102:ILE:HD11	1:A:175:LEU:HD21	1.68	0.76
1:A:147:LEU:HB3	1:B:321:LEU:HD13	1.67	0.76
1:B:259:VAL:O	1:B:263:ILE:HG13	1.86	0.76
3:F:145:GLN:O	3:F:149:GLN:HG3	1.86	0.76
1:B:139:HIS:O	1:B:140:LEU:CG	2.34	0.75
2:D:12:GLU:O	2:D:12:GLU:HG2	1.85	0.75
2:C:239:ILE:HD13	2:D:239:ILE:HD13	1.68	0.75
1:B:1:MSE:HB3	2:D:108:ASN:HD21	1.51	0.75
1:B:80:LEU:HD21	1:B:236:VAL:HG22	1.67	0.75
1:B:164:ILE:CG2	1:B:175:LEU:HD12	2.05	0.75
1:B:90:LEU:CG	1:B:258:LEU:HD11	2.14	0.75
1:B:163:ALA:O	1:B:166:PHE:HD2	1.70	0.75
1:A:180:MSE:CE	1:A:304:PRO:HG3	2.16	0.74
2:D:87:ALA:H	2:D:125:ASN:ND2	1.84	0.74
2:D:5:MSE:CE	2:D:46:MSE:HE2	2.17	0.74
1:A:259:VAL:O	1:A:263:ILE:HG13	1.88	0.74
1:B:138:ARG:O	1:B:138:ARG:HG2	1.86	0.74
2:D:161:MSE:H	6:D:800:1PE:H262	1.53	0.74
3:F:221:ILE:N	3:F:222:PRO:HD2	2.02	0.74
1:B:271:ASP:OD1	1:B:273:ARG:HG2	1.87	0.74
1:B:14:ARG:HG3	1:B:14:ARG:HH11	1.53	0.74
2:C:19:LEU:HD22	2:C:211:MSE:HB2	1.69	0.74
3:F:168:PHE:HB2	3:F:198:GLN:HE22	1.53	0.73
1:B:95:ASN:O	1:B:99:VAL:HG23	1.89	0.73
1:B:164:ILE:CG2	1:B:175:LEU:HD13	2.14	0.73
1:A:32:SER:HA	1:A:56:ARG:NH1	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLY:C	1:A:255:PHE:HD1	1.90	0.73
1:B:6:ARG:HG3	1:B:7:GLN:N	2.02	0.73
3:F:243:TRP:HE1	3:F:250:ARG:NH2	1.85	0.73
2:C:140:VAL:CG1	2:C:155:LEU:HD11	2.19	0.72
2:C:45:ARG:HD3	2:C:50:THR:HG22	1.70	0.72
1:B:256:ILE:HG23	1:B:260:ILE:HD12	1.71	0.72
2:D:19:LEU:HD22	2:D:211:MSE:HB2	1.70	0.72
1:B:102:ILE:HD12	1:B:160:MSE:HG2	1.70	0.72
1:A:300:ALA:O	3:F:69:MSE:C	2.28	0.71
2:C:17:GLY:HA3	2:C:210:LYS:NZ	2.04	0.71
1:B:172:LEU:O	1:B:176:MSE:HB2	1.90	0.71
1:A:201:LEU:CD2	1:A:242:MSE:HE1	2.20	0.71
1:B:35:GLU:O	1:B:35:GLU:HG2	1.90	0.71
2:C:239:ILE:HG22	2:C:240:GLU:HG3	1.73	0.71
2:D:197:LEU:O	2:D:217:ARG:NH1	2.23	0.71
2:D:239:ILE:HG22	2:D:240:GLU:HG3	1.73	0.71
3:F:214:ILE:HG21	3:F:224:ILE:HG13	1.71	0.71
2:C:87:ALA:N	2:C:125:ASN:HD21	1.89	0.71
1:B:87:GLU:HB3	1:B:258:LEU:HD23	1.72	0.70
1:B:87:GLU:HG2	1:B:89:GLY:N	2.07	0.70
1:B:73:SER:O	1:B:77:MSE:HG3	1.91	0.70
2:C:5:MSE:CE	2:C:46:MSE:HE2	2.17	0.70
1:B:173:ARG:O	1:B:177:TYR:HD1	1.75	0.70
2:C:12:GLU:O	2:C:12:GLU:HG2	1.90	0.70
3:F:149:GLN:O	3:F:153:LYS:HG3	1.92	0.70
2:D:86:PHE:HA	2:D:125:ASN:OD1	1.91	0.69
1:B:87:GLU:HB3	1:B:258:LEU:CD2	2.22	0.69
1:A:262:HIS:HD2	1:A:320:LEU:HD22	1.57	0.69
1:B:291:ASP:OD1	1:B:305:ILE:HD11	1.93	0.69
2:D:140:VAL:CG1	2:D:155:LEU:HD11	2.23	0.69
2:C:82:GLN:NE2	2:C:136:ARG:HH21	1.91	0.68
2:D:75:ARG:HD2	2:D:75:ARG:C	2.13	0.67
1:A:180:MSE:HE2	1:A:304:PRO:CG	2.24	0.67
1:B:101:LEU:HD13	1:B:178:TRP:CZ2	2.29	0.67
1:A:302:GLU:HB3	3:F:68:GLY:HA3	1.75	0.67
1:B:90:LEU:HG	1:B:258:LEU:CD1	2.19	0.67
2:C:75:ARG:C	2:C:75:ARG:HD2	2.14	0.67
3:F:194:VAL:O	3:F:197:PRO:HD3	1.94	0.67
1:B:101:LEU:HD13	1:B:178:TRP:HZ2	1.60	0.67
3:F:109:ALA:HA	3:F:114:GLN:OE1	1.94	0.67
1:B:3:THR:HG22	1:B:7:GLN:HE21	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:GLN:NE2	2:D:136:ARG:HH21	1.93	0.67
1:A:138:ARG:HD2	1:A:140:LEU:HD11	1.76	0.67
2:D:45:ARG:HD3	2:D:50:THR:HG22	1.77	0.67
1:B:113:PRO:O	1:B:117:LEU:HG	1.96	0.66
3:F:192:SER:OG	3:F:197:PRO:HG3	1.94	0.66
1:A:275:LEU:O	1:A:279:CYS:SG	2.53	0.66
1:B:80:LEU:HD21	1:B:236:VAL:HG23	1.77	0.66
1:A:301:ALA:O	3:F:69:MSE:O	2.14	0.66
1:B:1:MSE:HG3	2:D:120:LEU:CD1	2.25	0.66
1:B:314:ALA:HB3	1:B:315:PRO:HD3	1.77	0.66
2:C:161:MSE:H	6:C:800:1PE:H262	1.61	0.66
1:A:302:GLU:CD	3:F:93:GLN:HE22	1.97	0.66
1:B:92:GLY:O	1:B:128:ILE:HD12	1.96	0.66
1:B:168:THR:HG22	1:B:169:SER:N	2.10	0.66
1:A:314:ALA:HB3	1:A:315:PRO:HD3	1.77	0.66
1:B:43:TRP:CD1	1:B:52:VAL:HG21	2.31	0.66
3:F:221:ILE:HD11	3:F:238:PRO:HD3	1.78	0.66
1:B:209:ARG:CB	1:B:210:PRO:HD3	2.27	0.65
1:A:140:LEU:HD22	1:A:144:ARG:HH11	1.60	0.65
1:A:165:TYR:HB2	1:B:180:MSE:HE1	1.76	0.65
1:B:77:MSE:HE1	1:B:129:THR:HG22	1.79	0.65
1:B:298:LEU:CD1	1:B:301:ALA:CB	2.74	0.65
1:A:161:THR:CG2	1:B:180:MSE:HE3	2.26	0.65
1:B:262:HIS:CD2	1:B:320:LEU:HD11	2.28	0.65
1:A:146:LEU:O	1:A:150:VAL:HG23	1.96	0.65
1:A:138:ARG:HB2	1:A:140:LEU:HG	1.79	0.65
2:C:166:VAL:HG23	8:D:904:HOH:O	1.96	0.65
1:B:151:ALA:O	1:B:155:ILE:HG13	1.97	0.64
1:B:114:ASN:HA	1:B:117:LEU:HD12	1.79	0.64
1:B:141:SER:O	1:B:143:SER:N	2.30	0.64
1:A:64:LEU:HD21	1:A:288:LEU:CD1	2.27	0.64
1:B:35:GLU:O	1:B:36:GLN:HG3	1.97	0.64
1:B:87:GLU:CD	1:B:258:LEU:HG	2.18	0.64
2:C:17:GLY:CA	2:C:210:LYS:NZ	2.60	0.64
1:A:276:LEU:HB2	1:A:277:PRO:HD3	1.79	0.64
2:C:197:LEU:O	2:C:217:ARG:NH1	2.30	0.64
1:B:215:ALA:O	2:D:85:PRO:HB3	1.97	0.64
1:B:275:LEU:O	1:B:279:CYS:SG	2.56	0.64
2:C:246:ILE:HD11	2:D:244:MSE:SE	2.48	0.64
1:A:298:LEU:CD1	3:F:67:GLN:NE2	2.61	0.64
1:B:201:LEU:HG	1:B:242:MSE:CE	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLY:C	1:A:255:PHE:CD1	2.71	0.63
2:C:128:SER:OG	2:C:131:GLU:HG3	1.98	0.63
3:F:210:GLN:O	3:F:235:PRO:HD2	1.98	0.63
1:B:164:ILE:CB	1:B:175:LEU:HD13	2.28	0.63
1:B:260:ILE:HD13	1:B:283:GLY:HA2	1.81	0.63
1:B:276:LEU:HB2	1:B:277:PRO:HD3	1.81	0.63
2:D:100:ASP:OD1	2:D:102:THR:HB	1.97	0.63
2:C:17:GLY:HA3	2:C:210:LYS:HZ2	1.63	0.63
1:A:30:SER:HB2	1:A:295:ARG:NH2	2.13	0.63
1:B:87:GLU:CG	1:B:89:GLY:H	2.09	0.63
1:B:167:SER:CB	1:B:171:ASP:HB2	2.21	0.63
1:B:180:MSE:HE2	1:B:304:PRO:HG2	1.79	0.63
3:F:155:LYS:HB3	3:F:186:GLU:HG2	1.81	0.62
1:B:113:PRO:HB2	1:B:115:TRP:CD1	2.33	0.62
2:C:100:ASP:OD1	2:C:102:THR:HB	1.98	0.62
1:B:101:LEU:HG	1:B:121:ALA:HB2	1.80	0.62
3:F:147:LYS:O	3:F:151:ALA:HB2	2.00	0.62
1:A:174:GLN:NE2	3:F:91:GLU:HG3	2.15	0.62
1:B:45:THR:HG22	1:B:47:ARG:H	1.63	0.62
1:A:61:LEU:HB3	1:A:194:MSE:CE	2.30	0.62
1:A:138:ARG:HH12	1:B:322:LEU:CD2	2.09	0.62
1:A:3:THR:O	1:A:6:ARG:HG2	2.00	0.62
1:A:33:ALA:H	1:A:56:ARG:NH1	1.97	0.62
1:A:174:GLN:HE22	3:F:91:GLU:HG3	1.65	0.62
1:A:32:SER:CB	1:A:38:ILE:O	2.48	0.62
2:C:237:LEU:HD11	2:C:246:ILE:HD12	1.82	0.62
2:D:87:ALA:N	2:D:125:ASN:ND2	2.48	0.62
2:C:244:MSE:SE	2:D:246:ILE:HD11	2.50	0.61
1:A:32:SER:HA	1:A:56:ARG:HH11	1.64	0.61
1:A:301:ALA:HB3	3:F:70:ASN:CA	2.27	0.61
1:B:298:LEU:CB	1:B:301:ALA:HB3	2.27	0.61
1:A:151:ALA:O	1:A:155:ILE:HG13	1.99	0.61
1:A:260:ILE:HD13	1:A:283:GLY:HA2	1.83	0.61
1:B:168:THR:HG22	1:B:169:SER:H	1.65	0.61
1:A:61:LEU:HD13	1:A:194:MSE:HE1	1.83	0.61
1:B:83:ASN:ND2	1:B:145:LEU:HD23	2.07	0.61
2:C:11:ALA:HA	2:C:16:LEU:O	2.01	0.61
2:C:232:MSE:HE1	2:D:170:SER:OG	2.01	0.61
2:D:161:MSE:CG	2:D:169:GLN:HG2	2.31	0.60
1:A:35:GLU:HG2	3:F:72:GLU:CG	2.30	0.60
1:A:34:GLY:HA3	1:A:296:LEU:HD22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASN:H	1:A:95:ASN:ND2	2.00	0.60
1:B:33:ALA:HB3	1:B:56:ARG:CZ	2.31	0.60
2:C:236:ARG:NH2	2:C:243:ARG:HD3	2.16	0.60
1:A:92:GLY:HA3	1:A:153:GLY:HA2	1.84	0.60
1:A:255:PHE:CD1	1:A:255:PHE:N	2.69	0.60
3:F:189:PHE:CZ	3:F:199:VAL:HG11	2.37	0.60
1:B:173:ARG:CD	1:B:177:TYR:HE1	2.15	0.60
1:A:45:THR:HG22	1:A:47:ARG:H	1.67	0.60
1:A:176:MSE:HE2	1:A:176:MSE:HA	1.84	0.60
1:B:162:TRP:CD1	1:B:162:TRP:C	2.76	0.59
2:C:106:LEU:CD1	2:C:148:ALA:HB2	2.32	0.59
1:B:270:THR:HG21	2:D:88:THR:HA	1.84	0.59
2:D:86:PHE:C	2:D:125:ASN:HD21	2.05	0.59
1:A:165:TYR:CD1	1:B:177:TYR:HE2	2.19	0.59
1:A:164:ILE:HD13	1:B:176:MSE:HE1	1.84	0.59
1:A:255:PHE:CE2	1:B:155:ILE:HG12	2.38	0.59
2:C:87:ALA:N	2:C:125:ASN:ND2	2.42	0.59
1:B:136:ALA:HA	1:B:140:LEU:HD11	1.83	0.59
2:C:161:MSE:CG	2:C:169:GLN:HG2	2.32	0.59
2:D:237:LEU:HD11	2:D:246:ILE:HD12	1.83	0.59
3:F:165:ASN:HB3	3:F:166:PRO:HD2	1.82	0.59
1:A:72:ILE:HD12	1:A:201:LEU:CD2	2.33	0.59
1:A:172:LEU:O	1:A:176:MSE:HG2	2.02	0.59
2:D:93:TYR:O	2:D:97:HIS:HD2	1.86	0.58
2:D:216:ARG:HB3	2:D:218:GLU:OE2	2.03	0.58
1:B:271:ASP:OD1	1:B:273:ARG:CG	2.50	0.58
1:A:150:VAL:HG11	1:B:146:LEU:HD21	1.84	0.58
3:F:221:ILE:H	3:F:222:PRO:HD2	1.67	0.58
2:D:87:ALA:N	2:D:125:ASN:HD21	2.00	0.58
1:A:207:GLN:HA	1:A:207:GLN:NE2	2.14	0.58
1:B:197:LEU:HG	1:B:245:VAL:CG1	2.33	0.58
3:F:110:THR:O	3:F:110:THR:HG22	2.04	0.58
1:A:12:ASN:OD1	1:A:269:LEU:HD23	2.04	0.58
3:F:86:ARG:HG2	3:F:86:ARG:NH1	2.18	0.58
1:A:219:ILE:HG23	2:C:49:MSE:HE2	1.86	0.57
1:A:259:VAL:HG13	1:A:263:ILE:HD11	1.86	0.57
1:B:209:ARG:HB2	1:B:210:PRO:HD3	1.85	0.57
2:C:106:LEU:HD12	2:C:148:ALA:HB2	1.85	0.57
1:B:197:LEU:HG	1:B:245:VAL:HG11	1.86	0.57
2:D:12:GLU:O	2:D:12:GLU:CG	2.50	0.57
1:B:259:VAL:HG13	1:B:263:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ILE:HG21	1:B:176:MSE:SE	2.54	0.57
1:A:35:GLU:CB	3:F:72:GLU:CG	2.83	0.57
1:B:88:PRO:HA	1:B:93:VAL:HB	1.85	0.56
2:C:17:GLY:CA	2:C:210:LYS:HZ2	2.17	0.56
2:C:216:ARG:HB3	2:C:218:GLU:OE2	2.04	0.56
2:D:236:ARG:NH2	2:D:243:ARG:HD3	2.19	0.56
1:B:173:ARG:HD2	1:B:177:TYR:HE1	1.69	0.56
1:A:27:LEU:HD23	1:A:60:THR:HG21	1.88	0.56
1:A:95:ASN:N	1:A:95:ASN:ND2	2.45	0.56
2:C:159:GLU:HA	6:C:800:1PE:C26	2.34	0.56
2:D:6:GLN:C	2:D:7:LEU:HD23	2.26	0.56
2:D:106:LEU:HD12	2:D:148:ALA:HB2	1.87	0.56
3:F:94:VAL:O	3:F:97:LEU:HB2	2.05	0.56
1:A:121:ALA:HB3	1:A:248:ALA:HB2	1.87	0.56
1:B:172:LEU:CD1	1:B:176:MSE:HG3	2.35	0.56
2:C:93:TYR:O	2:C:97:HIS:HD2	1.88	0.56
2:C:89:PRO:HA	2:C:123:SER:HA	1.87	0.56
2:D:45:ARG:NH2	2:D:52:GLY:C	2.59	0.56
3:F:168:PHE:CD1	3:F:169:THR:N	2.74	0.56
1:A:64:LEU:HD21	1:A:288:LEU:HD12	1.87	0.56
2:D:106:LEU:CD1	2:D:148:ALA:HB2	2.35	0.56
1:B:270:THR:CG2	2:D:87:ALA:O	2.51	0.56
2:C:103:ARG:HA	2:C:105:GLU:OE2	2.05	0.56
2:D:59:ALA:HB3	2:D:66:TRP:HZ2	1.71	0.56
1:B:82:GLU:OE2	1:B:217:GLY:HA2	2.06	0.56
1:B:146:LEU:O	1:B:150:VAL:HG23	2.06	0.56
2:C:45:ARG:NH2	2:C:52:GLY:C	2.60	0.56
3:F:32:ALA:HB2	3:F:246:ARG:HB3	1.87	0.55
1:A:203:TRP:HH2	1:A:234:VAL:HG13	1.71	0.55
2:D:213:ALA:HB3	2:D:220:VAL:HG13	1.88	0.55
3:F:159:PHE:HB2	3:F:188:ILE:CD1	2.36	0.55
3:F:189:PHE:CE2	3:F:199:VAL:HG11	2.41	0.55
2:D:30:HIS:HA	2:D:188:MSE:O	2.06	0.55
1:B:189:ARG:HG2	1:B:189:ARG:O	2.06	0.55
2:D:105:GLU:CD	2:D:105:GLU:H	2.08	0.55
3:F:103:LYS:HD3	3:F:125:TRP:CZ2	2.41	0.55
1:A:232:ARG:O	1:A:236:VAL:HG23	2.06	0.55
2:D:50:THR:CG2	2:D:51:SER:N	2.69	0.55
1:A:307:VAL:HG11	1:B:162:TRP:HE3	1.62	0.55
1:B:165:TYR:CE1	3:F:67:GLN:OE1	2.60	0.55
2:C:6:GLN:C	2:C:7:LEU:HD23	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:59:ALA:HB3	2:C:66:TRP:HZ2	1.71	0.55
2:D:128:SER:OG	2:D:131:GLU:HG3	2.07	0.55
1:A:61:LEU:HB3	1:A:194:MSE:HE1	1.89	0.55
2:C:170:SER:OG	2:D:232:MSE:HE1	2.06	0.55
1:A:33:ALA:N	1:A:56:ARG:NH1	2.55	0.55
1:B:192:TRP:HA	1:B:192:TRP:CE3	2.42	0.55
2:D:159:GLU:HA	6:D:800:1PE:C26	2.33	0.55
3:F:29:LEU:HD12	3:F:84:ALA:HB2	1.89	0.55
1:A:138:ARG:NH1	1:B:322:LEU:HD22	2.16	0.54
1:B:64:LEU:HD21	1:B:288:LEU:CD1	2.37	0.54
1:B:173:ARG:HG3	3:F:196:TRP:CE3	2.42	0.54
2:C:50:THR:CG2	2:C:51:SER:N	2.70	0.54
3:F:229:GLY:O	3:F:231:GLN:N	2.40	0.54
1:B:173:ARG:NH1	1:B:177:TYR:OH	2.40	0.54
1:B:177:TYR:CD2	3:F:198:GLN:HG2	2.42	0.54
2:C:86:PHE:HA	2:C:125:ASN:CG	2.28	0.54
2:D:103:ARG:HA	2:D:105:GLU:OE2	2.06	0.54
1:A:87:GLU:HG2	1:A:89:GLY:H	1.72	0.54
1:A:270:THR:HG21	2:C:87:ALA:O	2.07	0.54
1:A:77:MSE:HE2	1:A:77:MSE:HA	1.89	0.54
1:A:307:VAL:HG12	1:B:162:TRP:CE3	2.31	0.54
8:C:904:HOH:O	2:D:166:VAL:HG23	2.06	0.54
1:A:183:PHE:CD1	1:A:305:ILE:HD12	2.43	0.54
2:C:105:GLU:CD	2:C:105:GLU:H	2.09	0.54
2:C:191:HIS:HB2	6:C:800:1PE:H251	1.90	0.54
3:F:165:ASN:CB	3:F:166:PRO:CD	2.82	0.54
3:F:69:MSE:HE1	3:F:94:VAL:HG22	1.88	0.54
3:F:221:ILE:N	3:F:222:PRO:CD	2.68	0.54
1:A:57:LEU:HD23	1:A:188:TRP:HZ2	1.72	0.54
1:A:60:THR:HG23	1:A:288:LEU:HD21	1.89	0.54
3:F:165:ASN:HB3	3:F:166:PRO:HD3	1.88	0.54
1:A:135:PHE:CD1	1:A:148:ALA:HB1	2.43	0.53
1:B:138:ARG:O	1:B:138:ARG:CG	2.56	0.53
2:D:89:PRO:HA	2:D:123:SER:HA	1.89	0.53
1:A:207:GLN:HE21	1:A:207:GLN:CA	2.17	0.53
1:A:307:VAL:CG1	1:B:162:TRP:HB2	2.35	0.53
1:B:254:GLY:O	1:B:255:PHE:HB2	2.08	0.53
1:B:298:LEU:HD12	1:B:301:ALA:HB3	1.90	0.53
3:F:168:PHE:HA	3:F:198:GLN:OE1	2.07	0.53
1:A:72:ILE:O	1:A:76:VAL:HG23	2.08	0.53
1:A:102:ILE:HD11	1:A:175:LEU:CD2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:155:LYS:HD3	3:F:186:GLU:OE2	2.08	0.53
1:A:291:ASP:OD1	1:A:305:ILE:HD11	2.09	0.53
2:D:173:ASP:OD1	2:D:195:HIS:HE1	1.91	0.53
1:A:53:TRP:CE3	1:A:57:LEU:HD22	2.44	0.53
1:A:35:GLU:HB2	3:F:72:GLU:CG	2.38	0.53
3:F:162:PHE:HB2	3:F:168:PHE:CD2	2.43	0.53
3:F:53:TYR:CG	3:F:250:ARG:HD2	2.44	0.53
1:A:201:LEU:HD23	1:A:242:MSE:HE1	1.91	0.53
1:B:232:ARG:O	1:B:236:VAL:HG23	2.08	0.53
2:C:17:GLY:HA3	2:C:210:LYS:CD	2.39	0.53
1:A:102:ILE:CD1	1:A:175:LEU:HD21	2.37	0.53
1:B:87:GLU:HG3	1:B:88:PRO:HD2	1.90	0.53
2:D:85:PRO:O	2:D:124:THR:OG1	2.22	0.53
3:F:28:THR:HG21	3:F:34:THR:HA	1.90	0.53
2:D:7:LEU:HD23	2:D:7:LEU:N	2.24	0.53
3:F:212:ILE:HG13	3:F:234:ILE:CD1	2.38	0.53
2:C:30:HIS:HA	2:C:188:MSE:O	2.10	0.52
2:C:32:VAL:HG22	2:C:190:SER:OG	2.09	0.52
2:C:7:LEU:HD11	2:C:46:MSE:HE3	1.90	0.52
1:A:307:VAL:HG11	1:B:162:TRP:CE3	2.39	0.52
1:B:201:LEU:HG	1:B:242:MSE:HE3	1.91	0.52
2:C:161:MSE:SE	2:C:172:LEU:HD23	2.60	0.52
1:A:136:ALA:HB2	1:A:145:LEU:HD11	1.91	0.52
1:A:143:SER:O	1:A:147:LEU:HG	2.08	0.52
1:B:72:ILE:O	1:B:76:VAL:HG23	2.10	0.52
1:B:173:ARG:HG3	3:F:196:TRP:HE3	1.75	0.52
3:F:71:LEU:HD22	3:F:96:GLN:OE1	2.09	0.52
1:A:168:THR:HG22	1:A:169:SER:N	2.25	0.52
1:B:6:ARG:HG3	1:B:7:GLN:H	1.74	0.52
1:B:274:VAL:C	1:B:277:PRO:HD2	2.30	0.52
3:F:175:ILE:HG12	3:F:251:ILE:HD13	1.91	0.52
1:A:83:ASN:ND2	1:B:147:LEU:HD12	2.25	0.51
1:B:1:MSE:CB	2:D:108:ASN:HD21	2.21	0.51
1:A:183:PHE:HD1	1:A:305:ILE:HD12	1.75	0.51
1:B:35:GLU:OE1	3:F:202:GLU:CG	2.58	0.51
1:B:57:LEU:HD23	1:B:188:TRP:HZ2	1.74	0.51
2:C:7:LEU:HD23	2:C:7:LEU:N	2.26	0.51
1:B:45:THR:HG23	1:B:46:PRO:HD2	1.93	0.51
3:F:221:ILE:HG23	3:F:236:VAL:HG11	1.92	0.51
1:A:164:ILE:CG2	1:B:176:MSE:SE	3.08	0.51
2:C:7:LEU:HD22	2:C:56:ILE:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:HD13	1:A:235:LEU:HD12	1.91	0.51
1:B:139:HIS:O	1:B:140:LEU:CD2	2.59	0.51
2:C:213:ALA:HB3	2:C:220:VAL:HG13	1.91	0.51
1:A:165:TYR:CE1	1:B:177:TYR:HE2	2.29	0.51
1:B:140:LEU:HD13	1:B:145:LEU:HD13	1.93	0.51
1:B:49:GLU:HA	1:B:53:TRP:HD1	1.76	0.51
1:B:88:PRO:CA	1:B:93:VAL:HB	2.41	0.51
3:F:175:ILE:O	3:F:179:VAL:HG23	2.11	0.51
1:A:136:ALA:HB2	1:A:145:LEU:HD21	1.93	0.51
1:A:193:LEU:HB3	1:A:249:LEU:HD22	1.90	0.51
1:A:198:ILE:N	1:A:199:PRO:HD2	2.25	0.51
1:A:167:SER:O	3:F:195:PRO:CG	2.59	0.50
1:A:209:ARG:HB2	1:A:210:PRO:HD3	1.93	0.50
1:A:249:LEU:O	3:F:92:ARG:NH1	2.45	0.50
1:B:200:VAL:HG21	1:B:241:TRP:CD1	2.46	0.50
1:A:201:LEU:HD21	1:A:242:MSE:HE1	1.94	0.50
3:F:85:TRP:O	3:F:89:ASN:HB2	2.11	0.50
1:A:80:LEU:HD11	1:A:232:ARG:HA	1.93	0.50
1:A:81:PHE:CD2	1:A:146:LEU:HD13	2.46	0.50
1:A:209:ARG:CB	1:A:210:PRO:HD3	2.42	0.50
1:B:35:GLU:O	1:B:36:GLN:CG	2.59	0.50
1:A:32:SER:HB3	1:A:38:ILE:O	2.11	0.50
1:A:263:ILE:HD11	1:A:316:VAL:HG11	1.93	0.50
1:B:141:SER:O	1:B:142:THR:C	2.49	0.50
3:F:214:ILE:HD12	3:F:220:GLN:O	2.12	0.50
1:A:117:LEU:O	1:A:120:SER:HB2	2.10	0.50
1:A:270:THR:CG2	2:C:87:ALA:O	2.60	0.50
1:A:274:VAL:C	1:A:277:PRO:HD2	2.31	0.50
1:A:302:GLU:HG2	3:F:68:GLY:CA	2.29	0.50
1:B:113:PRO:HB2	1:B:115:TRP:NE1	2.27	0.50
1:B:123:ALA:O	1:B:127:ILE:HG12	2.12	0.50
1:B:35:GLU:O	1:B:35:GLU:CG	2.58	0.50
1:B:77:MSE:HE1	1:B:129:THR:CG2	2.40	0.50
1:B:84:PRO:HD3	2:D:86:PHE:CD2	2.46	0.50
1:A:50:LEU:HD23	1:A:54:GLN:OE1	2.11	0.50
1:A:140:LEU:HB3	1:A:144:ARG:HD2	1.93	0.50
1:B:112:LEU:HD23	1:B:113:PRO:HD2	1.94	0.50
1:B:136:ALA:HA	1:B:140:LEU:CD1	2.42	0.50
1:B:216:LEU:HD21	2:D:96:LEU:HD12	1.94	0.50
3:F:195:PRO:O	3:F:196:TRP:HD1	1.94	0.50
3:F:248:SER:HB2	3:F:249:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLU:HB3	3:F:72:GLU:HB3	1.73	0.50
1:A:57:LEU:N	1:A:58:PRO:HD2	2.27	0.50
2:C:140:VAL:HG13	2:C:155:LEU:HD11	1.92	0.50
1:B:139:HIS:O	1:B:140:LEU:HD23	2.11	0.49
2:C:97:HIS:CG	2:C:139:ALA:HB1	2.47	0.49
2:D:5:MSE:HE3	2:D:23:VAL:HG21	1.94	0.49
3:F:221:ILE:HD11	3:F:238:PRO:HG3	1.92	0.49
1:A:203:TRP:HH2	1:A:234:VAL:CG1	2.24	0.49
1:B:294:ALA:HB1	1:B:303:LEU:O	2.12	0.49
1:B:88:PRO:HA	1:B:93:VAL:CG2	2.43	0.49
3:F:219:ASP:O	3:F:222:PRO:HD2	2.12	0.49
2:C:123:SER:OG	2:C:126:GLN:HG3	2.12	0.49
1:B:299:ALA:O	1:B:300:ALA:HB3	2.12	0.49
1:B:77:MSE:HE1	1:B:93:VAL:HG21	1.94	0.49
3:F:150:TYR:HA	3:F:153:LYS:HB2	1.95	0.49
3:F:69:MSE:HE3	3:F:93:GLN:HB3	1.94	0.49
3:F:221:ILE:HD11	3:F:238:PRO:CD	2.41	0.49
2:D:123:SER:OG	2:D:126:GLN:HG3	2.13	0.49
3:F:161:GLN:OE1	3:F:224:ILE:HG23	2.12	0.49
1:A:270:THR:HG21	2:C:88:THR:HA	1.95	0.49
1:B:57:LEU:N	1:B:58:PRO:HD2	2.27	0.49
2:D:161:MSE:SE	2:D:172:LEU:HD23	2.62	0.49
1:A:59:ARG:HA	1:A:186:VAL:HG11	1.94	0.49
1:B:30:SER:HB2	1:B:295:ARG:NH2	2.21	0.49
1:A:35:GLU:CB	3:F:72:GLU:HG3	2.43	0.48
1:A:150:VAL:HG11	1:B:146:LEU:CD2	2.43	0.48
2:D:97:HIS:CG	2:D:139:ALA:HB1	2.48	0.48
1:A:154:ILE:HG21	1:B:255:PHE:HZ	1.78	0.48
1:B:81:PHE:CE2	1:B:133:LEU:HD23	2.48	0.48
1:B:119:LEU:HD23	1:B:122:ILE:HD12	1.93	0.48
1:B:86:ALA:HA	1:B:91:LEU:HD11	1.96	0.48
3:F:229:GLY:C	3:F:231:GLN:H	2.15	0.48
1:A:174:GLN:HE22	3:F:91:GLU:CG	2.26	0.48
1:A:275:LEU:HG	1:A:279:CYS:SG	2.54	0.48
2:C:162:ASN:O	2:C:163:SER:HB2	2.14	0.48
3:F:159:PHE:HB2	3:F:188:ILE:HD13	1.95	0.48
1:A:123:ALA:O	1:A:127:ILE:HG12	2.13	0.48
1:B:62:ALA:HA	1:B:194:MSE:HE3	1.94	0.48
1:B:78:GLN:HE22	1:B:261:PRO:HG2	1.79	0.48
1:B:231:TRP:O	1:B:235:LEU:HG	2.14	0.48
2:C:249:ILE:HG22	2:C:249:ILE:OXT	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:249:ILE:HG22	2:D:249:ILE:OXT	2.14	0.48
3:F:69:MSE:HE1	3:F:94:VAL:CG2	2.44	0.48
1:B:275:LEU:HG	1:B:279:CYS:SG	2.54	0.48
2:C:232:MSE:HE1	2:D:170:SER:CB	2.43	0.48
1:B:101:LEU:HD23	1:B:117:LEU:O	2.14	0.48
1:B:163:ALA:O	1:B:166:PHE:CE2	2.65	0.48
1:B:167:SER:CB	1:B:171:ASP:CB	2.85	0.48
2:D:191:HIS:HB2	6:D:800:1PE:H251	1.95	0.48
1:A:95:ASN:O	1:A:99:VAL:HG23	2.13	0.47
1:A:136:ALA:CA	1:A:145:LEU:HD21	2.44	0.47
1:A:32:SER:HB2	1:A:38:ILE:O	2.15	0.47
1:A:316:VAL:O	1:A:320:LEU:HG	2.13	0.47
2:C:86:PHE:HA	2:C:125:ASN:OD1	2.14	0.47
2:D:7:LEU:HD22	2:D:56:ILE:HG23	1.95	0.47
3:F:221:ILE:HD11	3:F:238:PRO:CG	2.44	0.47
1:A:58:PRO:HB3	1:A:188:TRP:CD2	2.49	0.47
1:A:231:TRP:O	1:A:235:LEU:HG	2.14	0.47
1:B:122:ILE:HD13	1:B:241:TRP:CE3	2.49	0.47
2:D:7:LEU:HD11	2:D:46:MSE:HE3	1.94	0.47
2:D:235:ARG:HE	2:D:237:LEU:HD21	1.79	0.47
3:F:179:VAL:O	3:F:182:VAL:HG12	2.15	0.47
1:B:55:ILE:HG22	1:B:56:ARG:N	2.29	0.47
1:B:194:MSE:O	1:B:198:ILE:HG13	2.14	0.47
1:B:45:THR:CG2	1:B:46:PRO:HD2	2.45	0.47
3:F:198:GLN:OE1	3:F:198:GLN:HA	2.13	0.47
1:A:95:ASN:HB3	1:A:156:SER:HB3	1.97	0.47
1:B:173:ARG:O	1:B:177:TYR:CD1	2.62	0.47
1:B:298:LEU:CD1	1:B:301:ALA:HB1	2.36	0.47
2:D:140:VAL:HG13	2:D:155:LEU:HD11	1.97	0.47
3:F:53:TYR:CE2	3:F:250:ARG:HD2	2.50	0.47
1:A:136:ALA:CB	1:A:145:LEU:HD11	2.44	0.47
1:B:162:TRP:CD1	1:B:163:ALA:N	2.83	0.47
2:C:122:ARG:NH2	2:C:131:GLU:OE2	2.46	0.47
1:B:99:VAL:HG22	1:B:160:MSE:HG3	1.96	0.47
1:B:160:MSE:O	1:B:164:ILE:CG1	2.59	0.47
2:D:162:ASN:O	2:D:163:SER:HB2	2.15	0.47
1:A:55:ILE:HG22	1:A:56:ARG:N	2.29	0.47
1:B:27:LEU:HD23	1:B:60:THR:HG21	1.96	0.47
1:B:168:THR:CG2	1:B:169:SER:H	2.28	0.46
2:C:39:LYS:HG3	4:C:701:PO4:O1	2.14	0.46
3:F:65:THR:OG1	3:F:67:GLN:HG2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:168:PHE:HB2	3:F:198:GLN:NE2	2.26	0.46
3:F:229:GLY:C	3:F:231:GLN:N	2.69	0.46
1:B:165:TYR:HE1	3:F:67:GLN:OE1	1.98	0.46
1:B:302:GLU:OE1	1:B:302:GLU:HA	2.14	0.46
2:D:17:GLY:HA3	2:D:210:LYS:HD3	1.97	0.46
1:B:168:THR:CG2	1:B:169:SER:N	2.78	0.46
2:C:235:ARG:HE	2:C:237:LEU:HD21	1.80	0.46
2:C:236:ARG:HH21	2:C:243:ARG:HD3	1.78	0.46
2:D:223:PRO:HB3	2:D:234:PHE:O	2.15	0.46
1:B:270:THR:HG21	2:D:89:PRO:HD2	1.97	0.46
1:B:102:ILE:HD11	1:B:160:MSE:HE2	1.96	0.46
1:B:170:VAL:O	1:B:174:GLN:HG3	2.14	0.46
3:F:227:TYR:C	3:F:229:GLY:H	2.17	0.46
1:B:64:LEU:HD21	1:B:288:LEU:HD12	1.97	0.46
2:C:246:ILE:HG23	2:D:198:ARG:NH1	2.30	0.46
1:A:53:TRP:HE3	1:A:57:LEU:HD22	1.78	0.46
1:A:177:TYR:HD2	1:A:178:TRP:CE3	2.33	0.46
1:A:33:ALA:H	1:A:56:ARG:CZ	2.29	0.46
1:B:172:LEU:HD11	1:B:176:MSE:HG3	1.97	0.46
1:B:195:LEU:O	1:B:199:PRO:HD2	2.15	0.46
2:C:17:GLY:HA3	2:C:210:LYS:HD3	1.97	0.46
3:F:157:ARG:HH12	3:F:207:ARG:HD3	1.80	0.46
3:F:188:ILE:HG13	3:F:189:PHE:CD1	2.51	0.46
1:B:14:ARG:HH11	1:B:14:ARG:CG	2.24	0.46
2:C:17:GLY:CA	2:C:210:LYS:HZ3	2.28	0.46
1:A:193:LEU:HD13	1:A:249:LEU:HD22	1.98	0.45
1:B:35:GLU:OE1	3:F:202:GLU:HG3	2.16	0.45
1:B:204:ILE:HG22	1:B:205:SER:N	2.31	0.45
3:F:222:PRO:O	3:F:226:GLN:HG3	2.17	0.45
1:A:6:ARG:HG3	1:A:7:GLN:N	2.32	0.45
2:C:5:MSE:HE3	2:C:23:VAL:HG21	1.96	0.45
2:D:207:LYS:NZ	7:D:500:PEG:H31	2.31	0.45
3:F:212:ILE:HG13	3:F:234:ILE:HD12	1.98	0.45
3:F:248:SER:HB2	3:F:249:PRO:CD	2.46	0.45
1:A:162:TRP:O	1:A:166:PHE:HD1	1.99	0.45
1:B:275:LEU:HG	1:B:279:CYS:HG	1.81	0.45
2:D:75:ARG:C	2:D:75:ARG:CD	2.84	0.45
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.52	0.45
1:A:61:LEU:HB3	1:A:194:MSE:HE3	1.96	0.45
1:A:191:SER:O	1:A:195:LEU:HG	2.16	0.45
1:B:35:GLU:OE1	3:F:202:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:144:ILE:CD1	2:C:154:LEU:O	2.65	0.45
3:F:47:VAL:O	3:F:62:GLN:HA	2.16	0.45
1:A:40:PRO:HA	1:A:43:TRP:CD2	2.52	0.45
1:B:22:LEU:HD23	1:B:22:LEU:O	2.16	0.45
1:B:183:PHE:CE1	1:B:305:ILE:HD12	2.52	0.45
2:C:75:ARG:C	2:C:75:ARG:CD	2.84	0.45
2:C:170:SER:CB	2:D:232:MSE:HE1	2.47	0.45
2:C:173:ASP:OD1	2:C:195:HIS:HE1	1.99	0.45
2:C:198:ARG:NH1	2:D:246:ILE:HG23	2.32	0.45
1:A:22:LEU:O	1:A:22:LEU:HD23	2.17	0.45
1:B:44:PHE:CD1	1:B:44:PHE:N	2.84	0.45
1:B:97:ALA:HB3	1:B:247:VAL:HG21	1.97	0.45
1:B:272:HIS:HA	1:B:275:LEU:HB3	1.99	0.45
2:D:97:HIS:CD2	2:D:139:ALA:HB1	2.52	0.45
3:F:167:PRO:HG2	3:F:227:TYR:CZ	2.52	0.45
1:A:167:SER:O	3:F:195:PRO:HG3	2.17	0.45
1:B:192:TRP:HA	1:B:192:TRP:HE3	1.81	0.45
2:C:239:ILE:HG21	2:D:239:ILE:HD13	1.98	0.45
3:F:207:ARG:O	3:F:208:SER:C	2.56	0.45
3:F:243:TRP:CE3	3:F:253:LEU:HB3	2.51	0.45
1:A:133:LEU:HD21	1:A:236:VAL:HG11	1.98	0.45
1:B:14:ARG:HG3	1:B:14:ARG:NH1	2.28	0.45
1:B:162:TRP:HD1	1:B:163:ALA:N	2.15	0.45
3:F:35:GLU:OE1	3:F:250:ARG:HG3	2.17	0.45
3:F:159:PHE:HB2	3:F:188:ILE:HD11	1.99	0.45
1:A:59:ARG:HA	1:A:186:VAL:CG1	2.47	0.45
1:A:201:LEU:HG	1:A:242:MSE:HE3	1.98	0.45
1:B:77:MSE:CE	1:B:129:THR:HG22	2.46	0.44
1:B:270:THR:HG21	2:D:89:PRO:CD	2.48	0.44
1:B:80:LEU:CD2	1:B:236:VAL:HG22	2.43	0.44
1:B:143:SER:O	1:B:147:LEU:HG	2.17	0.44
1:B:226:LEU:HA	1:B:227:PRO:HD3	1.80	0.44
2:D:74:HIS:CE1	2:D:151:ALA:HB1	2.52	0.44
1:A:1:MSE:SE	1:A:9:GLN:HE22	2.51	0.44
1:A:307:VAL:HG13	1:B:162:TRP:HE3	1.69	0.44
1:B:183:PHE:CD1	1:B:305:ILE:HD12	2.53	0.44
1:B:259:VAL:CG1	1:B:263:ILE:HD11	2.48	0.44
1:B:318:ILE:C	1:B:320:LEU:H	2.21	0.44
2:C:5:MSE:CE	2:C:23:VAL:HG21	2.48	0.44
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.86	0.44
1:B:1:MSE:O	1:B:3:THR:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:GLU:HG3	1:B:88:PRO:CD	2.47	0.44
2:C:45:ARG:NH2	2:C:53:LYS:O	2.43	0.44
1:B:1:MSE:HB2	2:D:108:ASN:OD1	2.16	0.44
3:F:162:PHE:N	3:F:162:PHE:CD1	2.85	0.44
1:A:259:VAL:CG1	1:A:263:ILE:HD11	2.48	0.44
1:A:272:HIS:HA	1:A:275:LEU:HB3	2.00	0.44
3:F:49:SER:HB3	3:F:65:THR:HG22	1.99	0.44
1:A:64:LEU:HD22	1:A:284:ALA:HB1	2.00	0.44
1:A:167:SER:OG	1:A:172:LEU:HD13	2.17	0.44
1:A:255:PHE:CZ	1:B:155:ILE:HG12	2.52	0.44
3:F:73:ARG:HD2	3:F:73:ARG:HA	1.77	0.44
3:F:150:TYR:HA	3:F:153:LYS:HG3	1.99	0.44
2:C:19:LEU:CD2	2:C:211:MSE:HB2	2.44	0.43
2:C:223:PRO:HB3	2:C:234:PHE:O	2.18	0.43
1:A:226:LEU:HA	1:A:227:PRO:HD3	1.79	0.43
1:B:92:GLY:O	1:B:128:ILE:CD1	2.65	0.43
2:D:122:ARG:NH2	2:D:131:GLU:OE2	2.51	0.43
3:F:183:CYS:O	3:F:262:LEU:HD23	2.18	0.43
1:A:154:ILE:HG21	1:B:255:PHE:CZ	2.53	0.43
1:B:33:ALA:HB3	1:B:56:ARG:NH2	2.33	0.43
3:F:150:TYR:CD2	3:F:153:LYS:HD2	2.53	0.43
3:F:248:SER:O	3:F:251:ILE:HG22	2.18	0.43
2:D:17:GLY:HA3	2:D:210:LYS:CD	2.48	0.43
2:D:66:TRP:HZ3	2:D:74:HIS:CD2	2.36	0.43
1:A:168:THR:CG2	1:A:169:SER:N	2.82	0.43
2:D:86:PHE:CB	2:D:125:ASN:HD21	2.29	0.43
1:A:1:MSE:HE3	1:A:5:ALA:CB	2.49	0.43
1:B:55:ILE:HD13	3:F:201:ARG:O	2.19	0.43
1:B:262:HIS:O	1:B:266:LEU:HG	2.19	0.43
2:C:78:LEU:CD2	2:C:136:ARG:NH2	2.82	0.43
1:B:83:ASN:OD1	1:B:84:PRO:HD2	2.19	0.43
1:B:222:ARG:HB2	2:D:49:MSE:HE1	2.00	0.43
2:C:200:ALA:O	2:C:217:ARG:HD2	2.18	0.43
2:D:39:LYS:HG3	4:D:701:PO4:O4	2.19	0.43
2:D:236:ARG:HH21	2:D:243:ARG:HD3	1.83	0.43
3:F:218:PRO:HA	3:F:238:PRO:HG3	2.00	0.43
1:B:48:GLY:O	1:B:49:GLU:C	2.58	0.42
1:B:207:GLN:O	1:B:211:MSE:HE3	2.19	0.42
1:B:317:PHE:O	1:B:320:LEU:HB3	2.19	0.42
3:F:183:CYS:HB3	3:F:259:CYS:HA	2.01	0.42
1:A:262:HIS:O	1:A:266:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LEU:HD22	1:B:284:ALA:HB1	2.01	0.42
2:C:106:LEU:O	2:C:107:LEU:C	2.58	0.42
1:A:160:MSE:SE	1:A:179:MSE:HE3	2.68	0.42
1:A:269:LEU:HD22	1:A:274:VAL:CG1	2.49	0.42
1:B:87:GLU:OE2	1:B:258:LEU:HG	2.19	0.42
2:C:106:LEU:HD23	2:C:106:LEU:HA	1.89	0.42
2:D:5:MSE:CE	2:D:23:VAL:HG21	2.48	0.42
3:F:39:ALA:CB	3:F:249:PRO:HG2	2.49	0.42
3:F:103:LYS:HD3	3:F:125:TRP:CH2	2.54	0.42
3:F:168:PHE:CD1	3:F:168:PHE:C	2.93	0.42
1:A:297:ALA:CB	1:A:303:LEU:HD22	2.49	0.42
1:B:61:LEU:CB	1:B:194:MSE:HE1	2.28	0.42
1:B:218:GLU:HG2	1:B:228:LEU:HD21	2.02	0.42
2:D:19:LEU:CD2	2:D:211:MSE:HB2	2.46	0.42
2:D:75:ARG:HD2	2:D:75:ARG:O	2.18	0.42
1:B:1:MSE:HE2	1:B:2:LEU:CA	2.42	0.42
1:B:201:LEU:HD23	1:B:242:MSE:HE1	2.01	0.42
2:C:73:LEU:HD23	2:C:99:HIS:CE1	2.54	0.42
1:A:65:LEU:HD13	1:A:194:MSE:O	2.20	0.42
2:C:45:ARG:CD	2:C:50:THR:HG22	2.46	0.42
2:C:75:ARG:HD2	2:C:75:ARG:O	2.20	0.42
2:D:106:LEU:O	2:D:107:LEU:C	2.58	0.42
1:A:228:LEU:HB3	1:A:229:TRP:CE3	2.55	0.42
1:B:165:TYR:O	1:B:165:TYR:CD1	2.73	0.42
1:B:201:LEU:CD2	1:B:242:MSE:HE1	2.50	0.42
1:B:209:ARG:CB	1:B:210:PRO:CD	2.97	0.42
2:D:50:THR:HG23	2:D:51:SER:N	2.35	0.42
3:F:130:ASP:O	3:F:134:GLN:HG3	2.20	0.42
3:F:159:PHE:CD1	3:F:188:ILE:HD11	2.54	0.42
1:A:298:LEU:HD21	1:A:303:LEU:HD13	2.02	0.42
1:B:91:LEU:HA	1:B:149:GLY:HA3	2.01	0.42
2:C:50:THR:HG23	2:C:51:SER:N	2.34	0.42
1:A:165:TYR:HD2	1:A:166:PHE:CE1	2.38	0.41
1:A:176:MSE:SE	1:B:176:MSE:HE3	2.70	0.41
1:A:303:LEU:O	1:A:304:PRO:C	2.57	0.41
1:B:61:LEU:HD22	1:B:194:MSE:CE	2.50	0.41
1:B:130:LEU:HD23	1:B:130:LEU:HA	1.89	0.41
1:A:2:LEU:HG	1:A:3:THR:N	2.35	0.41
1:A:168:THR:O	1:A:169:SER:C	2.59	0.41
3:F:103:LYS:NZ	3:F:125:TRP:HZ2	2.18	0.41
3:F:164:ILE:O	3:F:165:ASN:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ALA:O	1:A:242:MSE:HG3	2.20	0.41
1:B:48:GLY:O	1:B:50:LEU:N	2.53	0.41
1:B:218:GLU:O	1:B:222:ARG:HG3	2.20	0.41
1:B:228:LEU:HB3	1:B:229:TRP:CE3	2.55	0.41
2:D:87:ALA:H	2:D:125:ASN:HD22	1.65	0.41
3:F:147:LYS:O	3:F:151:ALA:CB	2.67	0.41
1:B:2:LEU:HA	1:B:2:LEU:HD12	1.92	0.41
1:B:272:HIS:C	1:B:274:VAL:H	2.23	0.41
2:D:132:TRP:O	2:D:136:ARG:HG3	2.20	0.41
3:F:202:GLU:HG3	3:F:202:GLU:O	2.21	0.41
1:A:5:ALA:HB1	1:A:9:GLN:HE21	1.85	0.41
1:A:218:GLU:O	1:A:222:ARG:HG3	2.21	0.41
1:A:294:ALA:HB1	1:A:303:LEU:O	2.20	0.41
1:B:173:ARG:HD3	1:B:177:TYR:HE1	1.82	0.41
1:B:287:LEU:HD21	1:B:305:ILE:HG21	2.02	0.41
1:A:275:LEU:HG	1:A:279:CYS:HG	1.86	0.41
1:A:302:GLU:HB3	3:F:68:GLY:CA	2.48	0.41
2:D:73:LEU:HD23	2:D:99:HIS:CE1	2.56	0.41
3:F:117:ASN:O	3:F:121:GLN:HG2	2.21	0.41
1:A:200:VAL:HG21	1:A:241:TRP:CD1	2.56	0.41
1:A:272:HIS:C	1:A:274:VAL:H	2.23	0.41
1:B:49:GLU:HA	1:B:53:TRP:CD1	2.54	0.41
1:B:63:VAL:HG11	1:B:288:LEU:HA	2.01	0.41
1:B:316:VAL:O	1:B:320:LEU:HB2	2.21	0.41
2:D:12:GLU:OE1	2:D:41:THR:HG23	2.21	0.41
2:D:78:LEU:CD2	2:D:136:ARG:NH2	2.84	0.41
1:A:5:ALA:HB1	1:A:9:GLN:NE2	2.36	0.41
1:A:174:GLN:OE1	1:A:174:GLN:HA	2.21	0.41
1:A:218:GLU:HG2	1:A:228:LEU:HD21	2.02	0.41
1:B:14:ARG:CG	1:B:14:ARG:NH1	2.84	0.41
3:F:221:ILE:HG23	3:F:236:VAL:CG1	2.50	0.41
1:B:62:ALA:CA	1:B:194:MSE:HE3	2.51	0.40
1:B:88:PRO:HA	1:B:93:VAL:CB	2.51	0.40
2:C:74:HIS:CE1	2:C:151:ALA:HB1	2.56	0.40
3:F:217:GLY:C	3:F:219:ASP:H	2.24	0.40
1:A:262:HIS:CD2	1:A:320:LEU:HD22	2.47	0.40
2:C:161:MSE:HB2	6:C:800:1PE:OH7	2.21	0.40
3:F:53:TYR:HA	3:F:54:PRO:C	2.40	0.40
1:B:77:MSE:CE	1:B:129:THR:CG2	2.98	0.40
1:B:204:ILE:HA	1:B:204:ILE:HD13	1.90	0.40
1:B:238:ALA:O	1:B:242:MSE:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:TRP:HD1	2:C:120:LEU:O	2.05	0.40
2:D:47:ALA:HB2	2:D:156:LEU:CD1	2.51	0.40
3:F:41:GLY:CA	3:F:131:LYS:HD3	2.51	0.40
1:B:48:GLY:O	1:B:51:PHE:N	2.55	0.40
2:C:239:ILE:HD13	2:D:239:ILE:HG21	2.02	0.40
3:F:168:PHE:CA	3:F:198:GLN:OE1	2.70	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	322/326 (99%)	291 (90%)	29 (9%)	2 (1%)	25 47
1	B	322/326 (99%)	285 (88%)	32 (10%)	5 (2%)	9 19
2	C	246/249 (99%)	232 (94%)	13 (5%)	1 (0%)	34 57
2	D	246/249 (99%)	237 (96%)	8 (3%)	1 (0%)	34 57
3	F	243/245 (99%)	225 (93%)	15 (6%)	3 (1%)	13 27
All	All	1379/1395 (99%)	1270 (92%)	97 (7%)	12 (1%)	17 35

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	103	ARG
3	F	165	ASN
3	F	230	GLU
1	B	33	ALA
2	D	103	ARG
1	A	49	GLU
1	A	141	SER
1	B	2	LEU

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Mol	Chain	Res	Type
1	B	49	GLU
1	B	142	THR
1	B	181	GLY
3	F	229	GLY

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	249/239 (104%)	237 (95%)	12 (5%)	25	49
1	B	249/239 (104%)	236 (95%)	13 (5%)	23	46
2	C	200/192 (104%)	187 (94%)	13 (6%)	17	34
2	D	200/192 (104%)	187 (94%)	13 (6%)	17	34
3	F	205/203 (101%)	199 (97%)	6 (3%)	42	68
All	All	1103/1065 (104%)	1046 (95%)	57 (5%)	23	46

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	29	LEU
1	A	37	TRP
1	A	61	LEU
1	A	95	ASN
1	A	178	TRP
1	A	207	GLN
1	A	234	VAL
1	A	249	LEU
1	A	255	PHE
1	A	287	LEU
1	A	298	LEU
1	B	1	MSE
1	B	24	LEU
1	B	29	LEU

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Mol	Chain	Res	Type
1	B	61	LEU
1	B	133	LEU
1	B	139	HIS
1	B	162	TRP
1	B	165	TYR
1	B	176	MSE
1	B	204	ILE
1	B	234	VAL
1	B	249	LEU
1	B	287	LEU
2	C	7	LEU
2	C	16	LEU
2	C	22	GLU
2	C	45	ARG
2	C	50	THR
2	C	75	ARG
2	C	78	LEU
2	C	105	GLU
2	C	107	LEU
2	C	161	MSE
2	C	205	LEU
2	C	217	ARG
2	C	218	GLU
2	D	7	LEU
2	D	16	LEU
2	D	22	GLU
2	D	45	ARG
2	D	50	THR
2	D	75	ARG
2	D	78	LEU
2	D	105	GLU
2	D	107	LEU
2	D	161	MSE
2	D	205	LEU
2	D	217	ARG
2	D	218	GLU
3	F	66	TRP
3	F	162	PHE
3	F	168	PHE
3	F	201	ARG
3	F	202	GLU
3	F	228	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	9	GLN
1	A	95	ASN
1	A	207	GLN
1	A	262	HIS
1	B	7	GLN
1	B	174	GLN
1	B	262	HIS
2	C	8	GLN
2	C	82	GLN
2	C	97	HIS
2	C	99	HIS
2	C	125	ASN
2	C	195	HIS
2	D	8	GLN
2	D	82	GLN
2	D	97	HIS
2	D	99	HIS
2	D	125	ASN
2	D	195	HIS
3	F	62	GLN
3	F	67	GLN
3	F	93	GLN
3	F	145	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	D	602	-	4,4,4	1.03	0	6,6,6	0.63	0
4	PO4	C	701	-	4,4,4	2.66	3 (75%)	6,6,6	0.59	0
4	PO4	D	701	-	4,4,4	2.49	1 (25%)	6,6,6	0.63	0
7	PEG	C	500	-	6,6,6	0.65	0	5,5,5	0.67	0
5	SO4	D	603	-	4,4,4	0.98	0	6,6,6	0.67	0
6	1PE	C	800	-	15,15,15	0.62	0	14,14,14	0.63	0
7	PEG	C	501	-	6,6,6	0.51	0	5,5,5	0.67	0
5	SO4	C	603	-	4,4,4	1.01	0	6,6,6	0.66	0
6	1PE	D	800	-	15,15,15	0.60	0	14,14,14	0.72	0
7	PEG	D	501	-	6,6,6	0.50	0	5,5,5	0.68	0
5	SO4	C	601	-	4,4,4	0.96	0	6,6,6	0.69	0
7	PEG	D	500	-	6,6,6	0.50	0	5,5,5	0.74	0
5	SO4	D	601	-	4,4,4	1.00	0	6,6,6	0.66	0
5	SO4	C	602	-	4,4,4	1.03	0	6,6,6	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PEG	C	500	-	-	1/4/4/4	-
6	1PE	C	800	-	-	4/13/13/13	-
7	PEG	C	501	-	-	1/4/4/4	-
6	1PE	D	800	-	-	4/13/13/13	-
7	PEG	D	501	-	-	1/4/4/4	-
7	PEG	D	500	-	-	1/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	701	PO4	P-O1	3.79	1.59	1.50
4	C	701	PO4	P-O1	3.68	1.59	1.50
4	C	701	PO4	P-O4	-2.59	1.46	1.54
4	C	701	PO4	P-O2	2.22	1.61	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	500	PEG	O2-C3-C4-O4
7	D	500	PEG	O2-C3-C4-O4
6	D	800	1PE	OH5-C14-C24-OH4
6	C	800	1PE	OH5-C14-C24-OH4
7	C	501	PEG	O2-C3-C4-O4
6	C	800	1PE	OH2-C12-C22-OH3
7	D	501	PEG	O2-C3-C4-O4
6	D	800	1PE	OH2-C12-C22-OH3
6	D	800	1PE	OH4-C13-C23-OH3
6	C	800	1PE	OH4-C13-C23-OH3
6	C	800	1PE	OH6-C15-C25-OH5
6	D	800	1PE	OH6-C15-C25-OH5

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	701	PO4	1	0
4	D	701	PO4	1	0
6	C	800	1PE	6	0
6	D	800	1PE	5	0
7	D	500	PEG	1	0

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
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	255:PHE	C	256:ILE	N	1.11

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	313/326 (96%)	0.47	31 (9%)	7	5	41, 74, 147, 197	0
1	B	313/326 (96%)	0.32	21 (6%)	17	13	37, 71, 140, 184	0
2	C	240/249 (96%)	-0.13	2 (0%)	86	84	23, 46, 89, 176	0
2	D	240/249 (96%)	-0.11	4 (1%)	70	66	25, 45, 91, 180	0
3	F	243/245 (99%)	2.53	134 (55%)	0	0	73, 156, 195, 200	0
All	All	1349/1395 (96%)	0.60	192 (14%)	2	1	23, 69, 172, 200	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	GLY	12.2
3	F	154	PRO	8.8
3	F	153	LYS	8.0
1	A	139	HIS	8.0
3	F	56	GLN	7.9
3	F	207	ARG	7.5
1	B	164	ILE	7.2
3	F	230	GLU	7.0
3	F	182	VAL	7.0
1	A	137	ARG	6.9
3	F	152	ASP	6.9
3	F	143	TYR	6.8
3	F	163	GLY	6.6
3	F	126	SER	6.4
3	F	148	ALA	6.3
3	F	53	TYR	6.2
3	F	145	GLN	6.1
3	F	234	ILE	6.1
1	B	34	GLY	6.1
3	F	150	TYR	6.0

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Mol	Chain	Res	Type	RSRZ
3	F	266	ASP	5.9
3	F	251	ILE	5.8
3	F	130	ASP	5.7
3	F	245	GLU	5.6
1	A	301	ALA	5.5
3	F	240	THR	5.4
3	F	233	LYS	5.4
3	F	57	ALA	5.3
1	B	167	SER	5.2
1	B	324	ALA	5.2
3	F	52	ASP	5.2
3	F	186	GLU	5.1
3	F	106	TRP	5.0
1	B	168	THR	5.0
1	B	163	ALA	5.0
3	F	256	GLN	5.0
2	D	249	ILE	4.9
3	F	226	GLN	4.8
2	D	87	ALA	4.7
1	B	166	PHE	4.7
3	F	190	LYS	4.7
3	F	141	ASP	4.7
3	F	216	GLY	4.7
3	F	58	GLN	4.6
3	F	214	ILE	4.6
2	C	249	ILE	4.5
1	B	111	GLN	4.5
3	F	24	PRO	4.4
3	F	218	PRO	4.3
3	F	252	ILE	4.3
3	F	136	ALA	4.3
3	F	156	LYS	4.2
3	F	50	TYR	4.2
3	F	137	GLN	4.2
3	F	30	SER	4.2
1	A	111	GLN	4.2
3	F	104	VAL	4.2
1	A	138	ARG	4.1
3	F	219	ASP	4.1
3	F	59	LYS	4.0
1	B	165	TYR	4.0
3	F	149	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
3	F	247	ALA	4.0
3	F	170	SER	3.9
3	F	60	ILE	3.9
3	F	168	PHE	3.9
3	F	157	ARG	3.9
3	F	80	ASP	3.9
1	A	108	GLY	3.9
3	F	120	ARG	3.9
3	F	99	SER	3.8
3	F	109	ALA	3.8
3	F	155	LYS	3.8
3	F	67	GLN	3.7
3	F	77	LEU	3.7
3	F	45	VAL	3.7
3	F	210	GLN	3.6
3	F	63	VAL	3.6
1	A	109	GLN	3.6
3	F	139	LEU	3.6
3	F	189	PHE	3.6
3	F	151	ALA	3.6
3	F	125	TRP	3.6
1	A	255	PHE	3.5
3	F	132	ALA	3.5
1	A	144	ARG	3.5
3	F	208	SER	3.5
3	F	262	LEU	3.5
3	F	49	SER	3.5
3	F	185	GLY	3.5
3	F	93	GLN	3.5
3	F	159	PHE	3.4
3	F	55	PRO	3.4
3	F	51	SER	3.3
3	F	73	ARG	3.2
1	B	323	LYS	3.2
3	F	46	GLY	3.2
3	F	100	LEU	3.2
3	F	241	SER	3.2
3	F	215	THR	3.1
3	F	119	LEU	3.1
3	F	265	VAL	3.1
1	B	112	LEU	3.1
1	A	112	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
3	F	213	VAL	3.1
3	F	175	ILE	3.1
1	A	177	TYR	3.1
3	F	229	GLY	3.1
3	F	127	PRO	3.0
3	F	260	ASN	3.0
3	F	23	ALA	3.0
3	F	96	GLN	3.0
3	F	206	ALA	3.0
3	F	87	GLY	2.9
3	F	199	VAL	2.9
1	A	104	ALA	2.9
1	B	162	TRP	2.8
1	A	110	GLY	2.8
3	F	22	ALA	2.8
3	F	64	SER	2.8
3	F	243	TRP	2.8
3	F	82	VAL	2.8
3	F	54	PRO	2.7
1	A	189	ARG	2.7
3	F	164	ILE	2.7
1	B	175	LEU	2.7
3	F	238	PRO	2.7
3	F	76	ALA	2.7
1	A	324	ALA	2.7
3	F	94	VAL	2.7
3	F	188	ILE	2.7
3	F	259	CYS	2.6
3	F	135	ALA	2.6
1	A	322	LEU	2.6
3	F	237	ILE	2.6
1	A	33	ALA	2.6
1	B	301	ALA	2.6
1	A	107	LEU	2.5
1	A	254	GLY	2.5
3	F	217	GLY	2.5
1	A	86	ALA	2.5
3	F	43	THR	2.5
1	B	319	TRP	2.5
3	F	47	VAL	2.5
3	F	111	SER	2.5
3	F	192	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	107	VAL	2.5
1	B	300	ALA	2.5
3	F	232	LEU	2.5
1	A	302	GLU	2.4
1	A	159	LEU	2.4
1	B	109	GLN	2.4
3	F	102	ILE	2.4
1	A	46	PRO	2.4
1	A	113	PRO	2.4
3	F	108	ASP	2.4
3	F	86	ARG	2.3
3	F	187	ASN	2.3
3	F	134	GLN	2.3
3	F	29	LEU	2.3
3	F	44	PRO	2.3
2	D	240	GLU	2.3
1	B	169	SER	2.2
3	F	178	GLN	2.2
3	F	61	GLU	2.2
3	F	123	ALA	2.2
1	A	135	PHE	2.2
3	F	158	VAL	2.2
1	A	142	THR	2.2
3	F	140	LEU	2.2
3	F	249	PRO	2.2
2	C	187	VAL	2.1
1	A	299	ALA	2.1
3	F	254	ALA	2.1
1	A	305	ILE	2.1
3	F	36	LEU	2.1
3	F	209	PRO	2.1
3	F	222	PRO	2.1
3	F	198	GLN	2.1
3	F	68	GLY	2.1
3	F	191	ASP	2.1
3	F	78	LYS	2.1
3	F	83	ILE	2.1
1	A	43	TRP	2.1
2	D	187	VAL	2.1
3	F	116	ALA	2.1
1	A	94	SER	2.1
3	F	223	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	F	42	ILE	2.0
1	B	184	GLY	2.0
1	B	139	HIS	2.0
1	B	6	ARG	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PEG	C	500	7/7	0.64	0.23	67,67,67,67	0
7	PEG	D	500	7/7	0.73	0.41	81,81,81,81	0
6	1PE	D	800	16/16	0.74	0.51	69,69,69,69	0
6	1PE	C	800	16/16	0.77	0.39	69,69,69,69	0
7	PEG	D	501	7/7	0.78	0.26	71,71,71,71	0
5	SO4	D	602	5/5	0.82	0.28	106,106,106,106	0
5	SO4	C	603	5/5	0.82	0.25	141,141,141,141	0
5	SO4	C	602	5/5	0.86	0.19	113,113,113,113	0
5	SO4	D	603	5/5	0.88	0.23	119,119,119,119	0
5	SO4	D	601	5/5	0.92	0.16	85,85,85,85	0
7	PEG	C	501	7/7	0.92	0.15	71,71,71,71	0
5	SO4	C	601	5/5	0.93	0.15	78,78,78,78	0
4	PO4	D	701	5/5	0.98	0.14	30,30,30,30	0
4	PO4	C	701	5/5	0.99	0.12	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.