Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:23 AM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

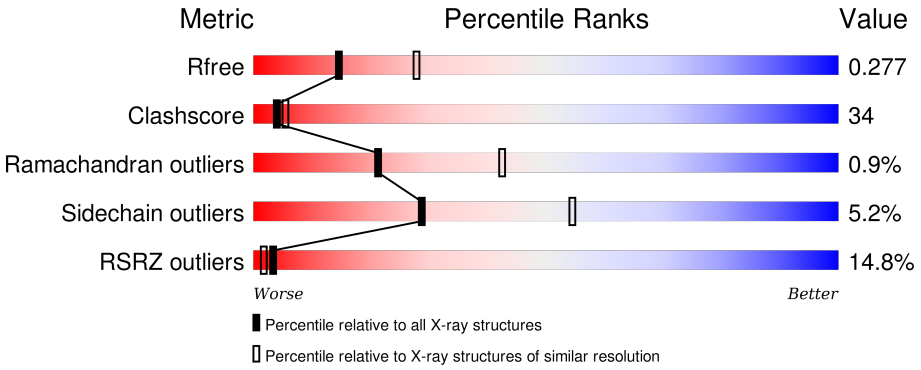
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	326	10% 51% 46%
1	B	326	7% 42% 52% 5%
2	C	249	% 62% 33% 5%
2	D	249	2% 62% 33%
3	F	245	56% 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	C	800	-	-	-	X
6	1PE	D	800	-	-	-	X
7	PEG	D	501	-	-	-	X

2 Entry composition

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
1	A	324	Total	C	N	O	S	Se	0	0	0
			2441	1611	418	400	1	11			
1	B	324	Total	C	N	O	S	Se	0	0	0
			2441	1611	418	400	1	11			

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

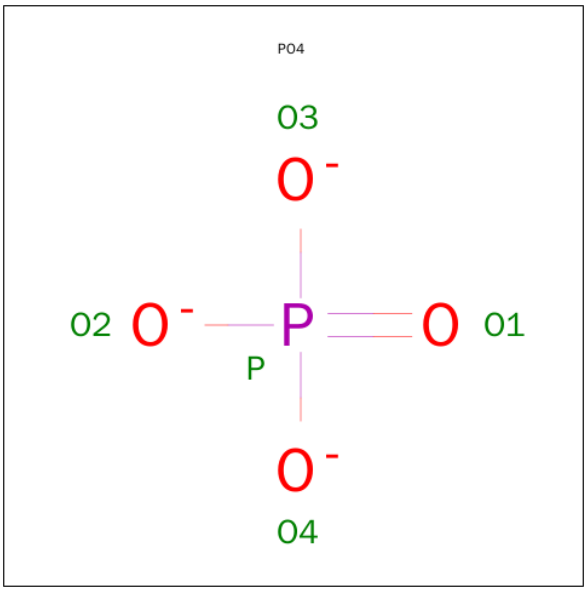
There are 2 discrepancies between the modelled and reference sequences:

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

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

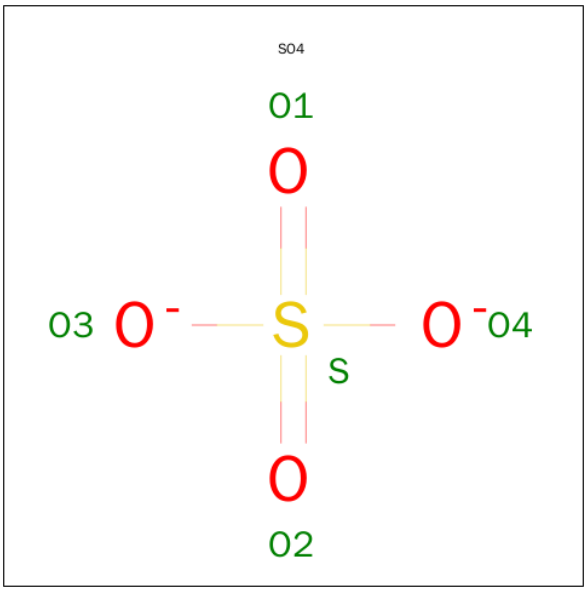
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	245	Total	C	N	O	S	Se	0	0	0
			1908	1216	332	356	2	2			

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



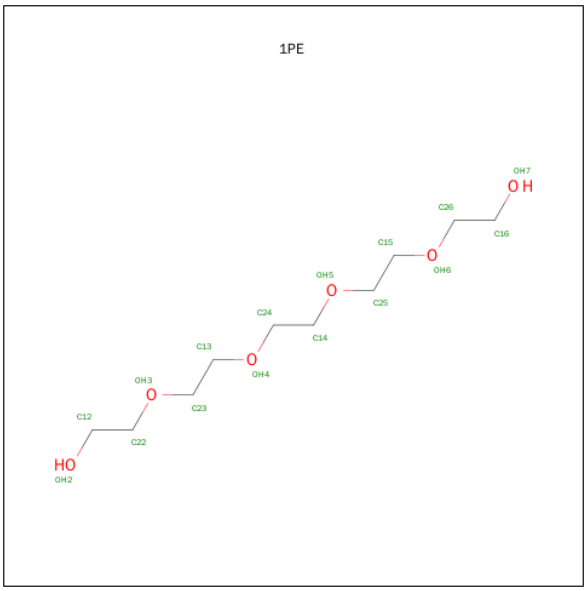
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	O	P		0	0
			5	4	1			
4	D	1	Total	O	P		0	0
			5	4	1			

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



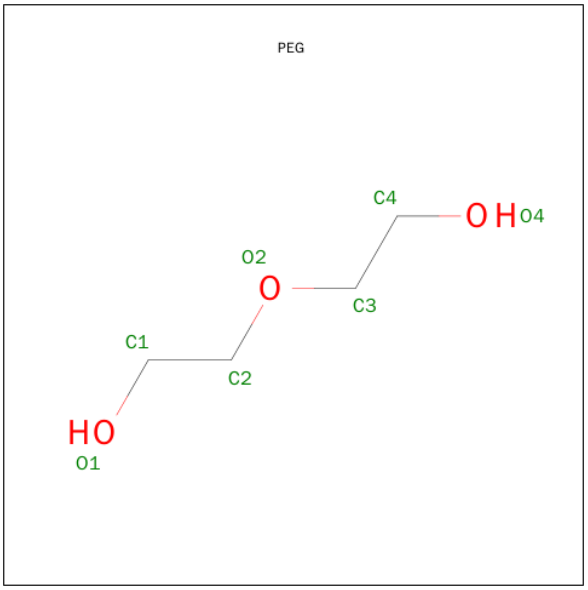
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 16 10 6	0	0
6	D	1	Total C O 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
7	C	1	Total C O 7 4 3	0	0
7	C	1	Total C O 7 4 3	0	0

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

- Molecule 8 is water.

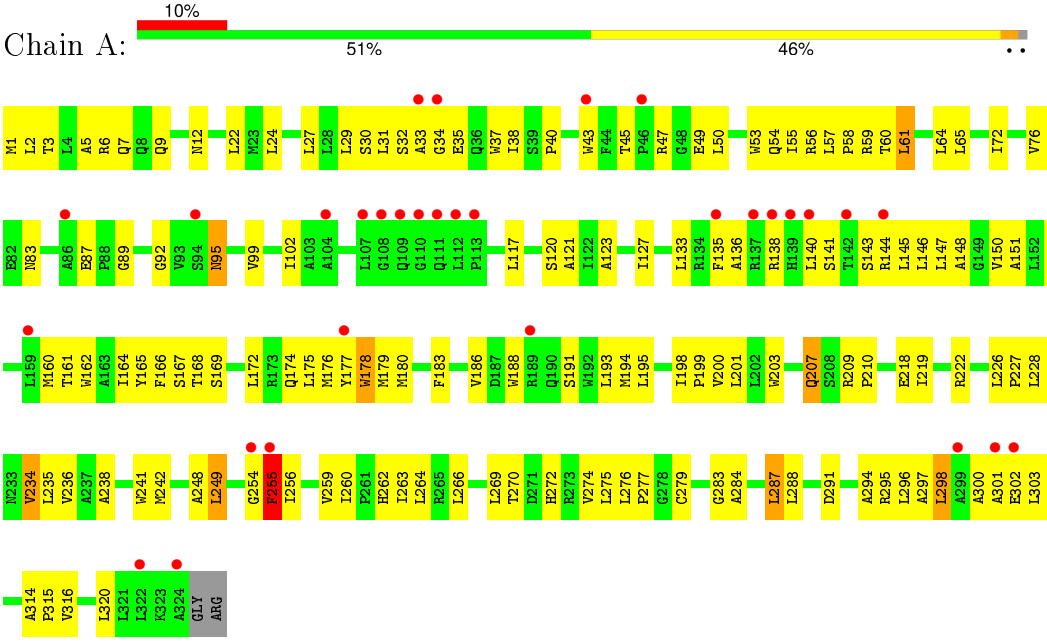
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	8	Total O 8 8	0	0
8	D	8	Total O 8 8	0	0

3 Residue-property plots (i)

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

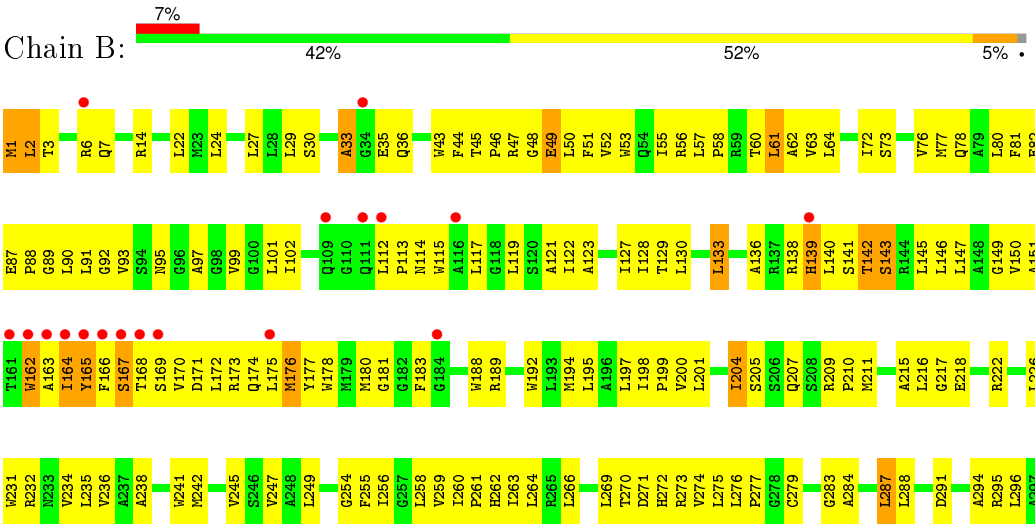
- Molecule 1: Vitamin B12 import system permease protein btuC

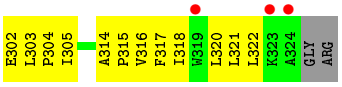
Chain A:



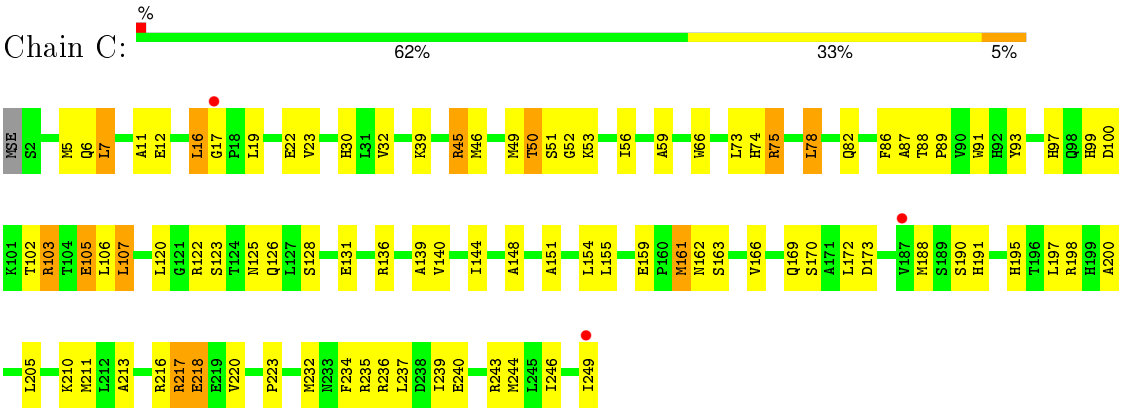
- Molecule 1: Vitamin B12 import system permease protein btuC

Chain B:

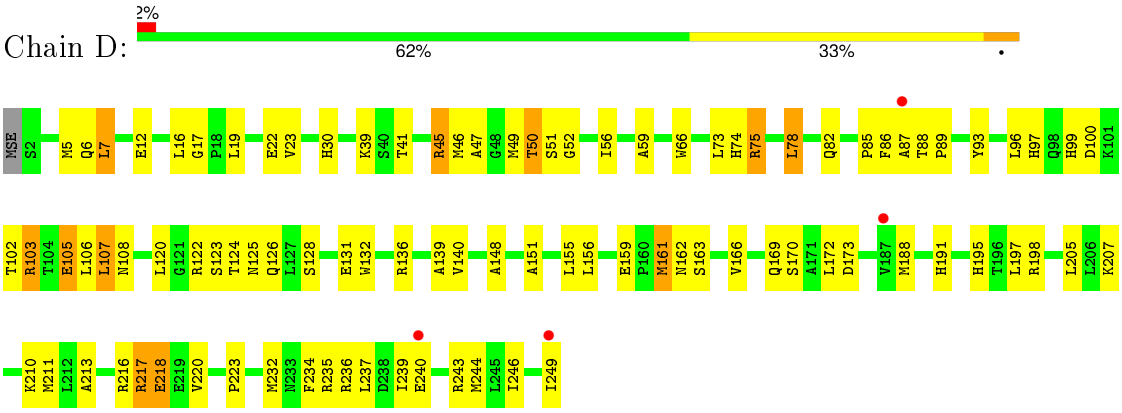




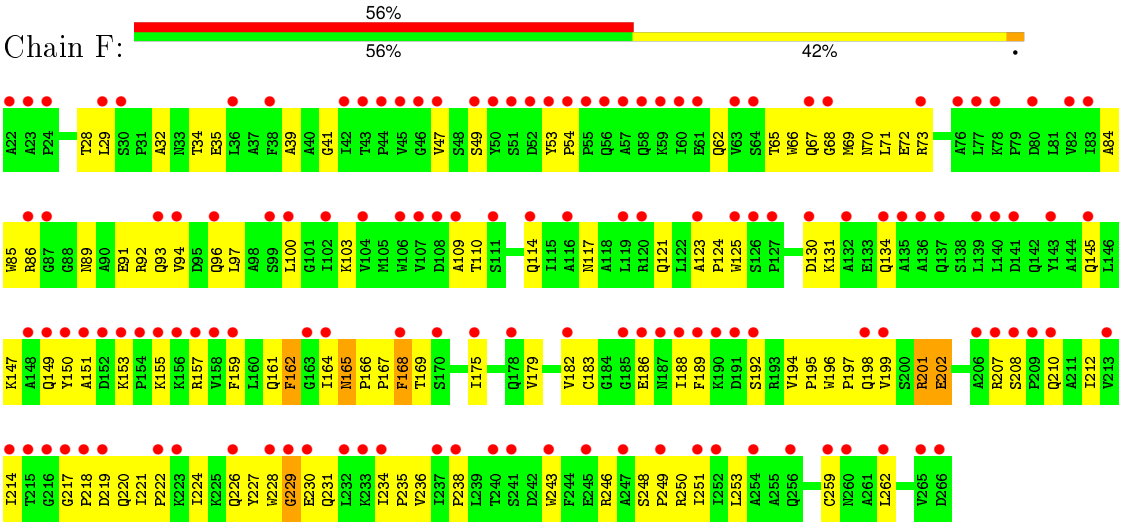
• Molecule 2: Vitamin B12 import ATP-binding protein btuD



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



• Molecule 3: Vitamin B12-binding protein btuF



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	CNS	Depositor
R, R_{free}	0.262 , 0.280 0.260 , 0.277	Depositor DCC
R_{free} test set	3727 reflections (5.05%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 74100 reflections (0.003%)	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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:35:GLU:CD	3:F:72:GLU:CG	2.39	0.90
1:A:30:SER:HB2	1:A:295:ARG:HH22	1.35	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:HD22	1:A:95:ASN:N	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:B:164:ILE:HG23	1:B:175:LEU:HD11	1.59	0.84
1:A:35:GLU:CG	3:F:72:GLU:CG	2.55	0.84
1:A:161:THR:HG22	1:B:180:MSE:HE3	1.59	0.84
1:A:147:LEU:HD13	1:B:321:LEU:HD22	1.60	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:HB2	3:F:72:GLU:CB	2.09	0.83
1:A:35:GLU:HG2	3:F:72:GLU:CB	2.07	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: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:12:ASN:HB3	1:A:274:VAL:HG11	1.60	0.81
1:A:302:GLU:CD	3:F:93:GLN:NE2	2.34	0.81
1:A:207:GLN:HE21	1:A:207:GLN:HA	1.46	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:307:VAL:HG13	1:B:162:TRP:HB2	1.65	0.78
1:A:95:ASN:HD22	1:A:95:ASN:H	1.31	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
3:F:86:ARG:HH11	3:F:86:ARG:HG2	1.49	0.77
1:A:256:ILE:HG23	1:A:260:ILE:HD12	1.65	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: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
1:A:102:ILE:HD11	1:A:175:LEU:HD21	1.68	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:HG2	2:D:12:GLU:O	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:163:ALA:O	1:B:166:PHE:HD2	1.70	0.75
1:B:90:LEU:CG	1:B:258:LEU:HD11	2.14	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
2:D:161:MSE:H	6:D:800:1PE:H262	1.53	0.74
1:B:138:ARG:HG2	1:B:138:ARG:O	1.86	0.74
3:F:221:ILE:N	3:F:222:PRO:HD2	2.02	0.74
1:A:259:VAL:O	1:A:263:ILE:HG13	1.88	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)
3:F:243:TRP:HE1	3:F:250:ARG:NH2	1.85	0.73
1:B:6:ARG:HG3	1:B:7:GLN:N	2.02	0.73
1:A:254:GLY:C	1:A:255:PHE:HD1	1.90	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
2:C:239:ILE:HG22	2:C:240:GLU:HG3	1.73	0.71
2:D:239:ILE:HG22	2:D:240:GLU:HG3	1.73	0.71
1:B:35:GLU:HG2	1:B:35:GLU:O	1.90	0.71
2:D:197:LEU:O	2:D:217:ARG:NH1	2.23	0.71
1:A:201:LEU:CD2	1:A:242:MSE:HE1	2.20	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
2:D:140:VAL:CG1	2:D:155:LEU:HD11	2.23	0.69
1:B:291:ASP:OD1	1:B:305:ILE:HD11	1.93	0.69
2:C:82:GLN:NE2	2:C:136:ARG:HH21	1.91	0.68
2:D:75:ARG:C	2:D:75:ARG:HD2	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:B:80:LEU:HD21	1:B:236:VAL:HG23	1.77	0.66
1:A:275:LEU:O	1:A:279:CYS:SG	2.53	0.66
1:A:301:ALA:O	3:F:69:MSE:O	2.14	0.66
2:C:161:MSE:H	6:C:800:1PE:H262	1.61	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
1:A:302:GLU:CD	3:F:93:GLN:HE22	1.97	0.66
1:B:168:THR:HG22	1:B:169:SER:N	2.10	0.66
1:B:92:GLY:O	1:B:128:ILE:HD12	1.96	0.66
1:A:314:ALA:HB3	1:A:315:PRO:HD3	1.77	0.66
3:F:221:ILE:HD11	3:F:238:PRO:HD3	1.78	0.66
1:B:43:TRP:CD1	1:B:52:VAL:HG21	2.31	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:141:SER:O	1:B:143:SER:N	2.30	0.64
1:B:114:ASN:HA	1:B:117:LEU:HD12	1.79	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:B:35:GLU:O	1:B:36:GLN:HG3	1.97	0.64
1:A:64:LEU:HD21	1:A:288:LEU:CD1	2.27	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:275:LEU:O	1:B:279:CYS:SG	2.56	0.64
1:B:215:ALA:O	2:D:85:PRO:HB3	1.97	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:B:87:GLU:CG	1:B:89:GLY:H	2.09	0.63
1:A:30:SER:HB2	1:A:295:ARG:NH2	2.13	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:B:45:THR:HG22	1:B:47:ARG:H	1.63	0.62
1:A:174:GLN:NE2	3:F:91:GLU:HG3	2.15	0.62
1:A:138:ARG:HH12	1:B:322:LEU:CD2	2.09	0.62
1:A:61:LEU:HB3	1:A:194:MSE:CE	2.30	0.62
1:A:33:ALA:H	1:A:56:ARG:NH1	1.97	0.62
1:A:3:THR:O	1:A:6:ARG:HG2	2.00	0.62
1:A:174:GLN:HE22	3:F:91:GLU:HG3	1.65	0.62
2:D:87:ALA:N	2:D:125:ASN:ND2	2.48	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: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:260:ILE:HD13	1:A:283:GLY:HA2	1.83	0.61
1:A:151:ALA:O	1:A:155:ILE:HG13	1.99	0.61
1:B:168:THR:HG22	1:B:169:SER:H	1.65	0.61
1:B:83:ASN:ND2	1:B:145:LEU:HD23	2.07	0.61
1:A:61:LEU:HD13	1:A:194:MSE:HE1	1.83	0.61
2:C:232:MSE:HE1	2:D:170:SER:OG	2.01	0.61
2:C:11:ALA:HA	2:C:16:LEU:O	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:ND2	1:A:95:ASN:H	2.00	0.60
2:C:236:ARG:NH2	2:C:243:ARG:HD3	2.16	0.60
1:B:33:ALA:HB3	1:B:56:ARG:CZ	2.31	0.60
1:A:255:PHE:N	1:A:255:PHE:CD1	2.69	0.60
1:A:92:GLY:HA3	1:A:153:GLY:HA2	1.84	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:176:MSE:HE2	1:A:176:MSE:HA	1.84	0.60
1:A:45:THR:HG22	1:A:47:ARG:H	1.67	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
2:D:86:PHE:C	2:D:125:ASN:HD21	2.05	0.59
1:B:270:THR:HG21	2:D:88:THR:HA	1.84	0.59
1:A:165:TYR:CD1	1:B:177:TYR:HE2	2.19	0.59
2:C:87:ALA:N	2:C:125:ASN:ND2	2.42	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
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
3:F:165:ASN:HB3	3:F:166:PRO:HD2	1.82	0.59
2:D:237:LEU:HD11	2:D:246:ILE:HD12	1.83	0.59
1:A:172:LEU:O	1:A:176:MSE:HG2	2.02	0.59
1:A:72:ILE:HD12	1:A:201:LEU:CD2	2.33	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:NH1	3:F:86:ARG:HG2	2.18	0.58
1:A:259:VAL:HG13	1:A:263:ILE:HD11	1.86	0.57
1:A:219:ILE:HG23	2:C:49:MSE:HE2	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
2:D:12:GLU:CG	2:D:12:GLU:O	2.50	0.57
1:B:197:LEU:HG	1:B:245:VAL:HG11	1.86	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:D:236:ARG:NH2	2:D:243:ARG:HD3	2.19	0.56
2:C:216:ARG:HB3	2:C:218:GLU:OE2	2.04	0.56
1:B:173:ARG:HD2	1:B:177:TYR:HE1	1.69	0.56
2:D:6:GLN:C	2:D:7:LEU:HD23	2.26	0.56
3:F:94:VAL:O	3:F:97:LEU:HB2	2.05	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
1:A:27:LEU:HD23	1:A:60:THR:HG21	1.88	0.56
2:D:106:LEU:HD12	2:D:148:ALA:HB2	1.87	0.56
1:B:172:LEU:CD1	1:B:176:MSE:HG3	2.35	0.56
1:A:121:ALA:HB3	1:A:248:ALA:HB2	1.87	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
3:F:168:PHE:CD1	3:F:169:THR:N	2.74	0.56
2:D:45:ARG:NH2	2:D:52:GLY:C	2.59	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: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
1:B:82:GLU:OE2	1:B:217:GLY:HA2	2.06	0.56
3:F:32:ALA:HB2	3:F:246:ARG:HB3	1.87	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:213:ALA:HB3	2:D:220:VAL:HG13	1.88	0.55
1:A:203:TRP:HH2	1:A:234:VAL:HG13	1.71	0.55
2:D:30:HIS:HA	2:D:188:MSE:O	2.06	0.55
1:B:189:ARG:O	1:B:189:ARG:HG2	2.06	0.55
2:D:105:GLU:H	2:D:105:GLU:CD	2.08	0.55
3:F:103:LYS:HD3	3:F:125:TRP:CZ2	2.41	0.55
2:D:50:THR:CG2	2:D:51:SER:N	2.69	0.55
1:A:232:ARG:O	1:A:236:VAL:HG23	2.06	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:D:128:SER:OG	2:D:131:GLU:HG3	2.07	0.55
2:C:59:ALA:HB3	2:C:66:TRP:HZ2	1.71	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
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:B:192:TRP:HA	1:B:192:TRP:CE3	2.42	0.55
1:A:138:ARG:NH1	1:B:322:LEU:HD22	2.16	0.54
1:B:173:ARG:HG3	3:F:196:TRP:CE3	2.42	0.54
3:F:229:GLY:O	3:F:231:GLN:N	2.40	0.54
2:C:50:THR:CG2	2:C:51:SER:N	2.70	0.54
1:B:64:LEU:HD21	1:B:288:LEU:CD1	2.37	0.54
2:C:86:PHE:HA	2:C:125:ASN:CG	2.28	0.54
1:B:177:TYR:CD2	3:F:198:GLN:HG2	2.42	0.54
1:B:173:ARG:NH1	1:B:177:TYR:OH	2.40	0.54
2:D:103:ARG:HA	2:D:105:GLU:OE2	2.06	0.54
1:A:270:THR:HG21	2:C:87:ALA:O	2.07	0.54
1:A:87:GLU:HG2	1:A:89:GLY:H	1.72	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:77:MSE:HE2	1:A:77:MSE:HA	1.89	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
2:C:105:GLU:CD	2:C:105:GLU:H	2.09	0.54
1:A:183:PHE:CD1	1:A:305:ILE:HD12	2.43	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
3:F:165:ASN:HB3	3:F:166:PRO:HD3	1.88	0.54
1:A:60:THR:HG23	1:A:288:LEU:HD21	1.89	0.54
1:A:57:LEU:HD23	1:A:188:TRP:HZ2	1.72	0.54
2:D:89:PRO:HA	2:D:123:SER:HA	1.89	0.53
1:B:138:ARG:O	1:B:138:ARG:CG	2.56	0.53
1:A:135:PHE:CD1	1:A:148:ALA:HB1	2.43	0.53
1:A:307:VAL:CG1	1:B:162:TRP:HB2	2.35	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:207:GLN:HE21	1:A:207:GLN:CA	2.17	0.53
1:B:254:GLY:O	1:B:255:PHE:HB2	2.08	0.53
1:A:102:ILE:HD11	1:A:175:LEU:CD2	2.37	0.53
1:A:72:ILE:O	1:A:76:VAL:HG23	2.08	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: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:201:LEU:HD23	1:A:242:MSE:HE1	1.91	0.53
1:B:87:GLU:HG3	1:B:88:PRO:HD2	1.90	0.53
1:A:102:ILE:CD1	1:A:175:LEU:HD21	2.37	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:N	2:D:7:LEU:HD23	2.24	0.53
3:F:212:ILE:HG13	3:F:234:ILE:CD1	2.38	0.53
2:C:32:VAL:HG22	2:C:190:SER:OG	2.09	0.52
2:C:30:HIS:HA	2:C:188:MSE:O	2.10	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
2:C:161:MSE:SE	2:C:172:LEU:HD23	2.60	0.52
1:B:201:LEU:HG	1:B:242:MSE:HE3	1.91	0.52
1:A:143:SER:O	1:A:147:LEU:HG	2.08	0.52
1:A:136:ALA:HB2	1:A:145:LEU:HD11	1.91	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: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
1:A:168:THR:HG22	1:A:169:SER:N	2.25	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:B:35:GLU:OE1	3:F:202:GLU:CG	2.58	0.51
1:A:183:PHE:HD1	1:A:305:ILE:HD12	1.75	0.51
1:B:57:LEU:HD23	1:B:188:TRP:HZ2	1.74	0.51
2:C:7:LEU:N	2:C:7:LEU:HD23	2.26	0.51
3:F:221:ILE:HG23	3:F:236:VAL:HG11	1.92	0.51
1:B:45:THR:HG23	1:B:46:PRO:HD2	1.93	0.51
2:C:7:LEU:HD22	2:C:56:ILE:HG23	1.93	0.51
1:A:164:ILE:CG2	1:B:176:MSE:SE	3.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:HIS:O	1:B:140:LEU:CD2	2.59	0.51
1:A:80:LEU:HD13	1:A:235:LEU:HD12	1.91	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: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:B:49:GLU:HA	1:B:53:TRP:HD1	1.76	0.51
1:A:193:LEU:HB3	1:A:249:LEU:HD22	1.90	0.51
1:A:136:ALA:HB2	1:A:145:LEU:HD21	1.93	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: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:209:ARG:HB2	1:A:210:PRO:HD3	1.93	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:81:PHE:CD2	1:A:146:LEU:HD13	2.46	0.50
1:B:35:GLU:O	1:B:36:GLN:CG	2.59	0.50
1:A:80:LEU:HD11	1:A:232:ARG:HA	1.93	0.50
1:A:209:ARG:CB	1:A:210:PRO:HD3	2.42	0.50
1:B:141:SER:O	1:B:142:THR:C	2.49	0.50
1:A:32:SER:HB3	1:A:38:ILE:O	2.11	0.50
3:F:214:ILE:HD12	3:F:220:GLN:O	2.12	0.50
1:A:263:ILE:HD11	1:A:316:VAL:HG11	1.93	0.50
1:A:270:THR:CG2	2:C:87:ALA:O	2.60	0.50
1:A:302:GLU:HG2	3:F:68:GLY:CA	2.29	0.50
1:A:274:VAL:C	1:A:277:PRO:HD2	2.31	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:A:117:LEU:O	1:A:120:SER:HB2	2.10	0.50
1:B:84:PRO:HD3	2:D:86:PHE:CD2	2.46	0.50
1:B:77:MSE:HE1	1:B:129:THR:CG2	2.40	0.50
1:B:35:GLU:CG	1:B:35:GLU:O	2.58	0.50
1:B:136:ALA:HA	1:B:140:LEU:CD1	2.42	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:216:LEU:HD21	2:D:96:LEU:HD12	1.94	0.50
1:A:50:LEU:HD23	1:A:54:GLN:OE1	2.11	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
2:C:140:VAL:HG13	2:C:155:LEU:HD11	1.92	0.50
1:A:57:LEU:N	1:A:58:PRO:HD2	2.27	0.50
1:B:139:HIS:O	1:B:140:LEU:HD23	2.11	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
2:C:97:HIS:CG	2:C:139:ALA:HB1	2.47	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
2:D:161:MSE:SE	2:D:172:LEU:HD23	2.62	0.49
1:B:57:LEU:N	1:B:58:PRO:HD2	2.27	0.49
1:B:30:SER:HB2	1:B:295:ARG:NH2	2.21	0.49
1:A:59:ARG:HA	1:A:186:VAL:HG11	1.94	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:119:LEU:HD23	1:B:122:ILE:HD12	1.93	0.48
1:B:81:PHE:CE2	1:B:133:LEU:HD23	2.48	0.48
3:F:229:GLY:C	3:F:231:GLN:H	2.15	0.48
1:B:86:ALA:HA	1:B:91:LEU:HD11	1.96	0.48
1:A:275:LEU:HG	1:A:279:CYS:SG	2.54	0.48
3:F:159:PHE:HB2	3:F:188:ILE:HD13	1.95	0.48
1:A:174:GLN:HE22	3:F:91:GLU:CG	2.26	0.48
2:C:162:ASN:O	2:C:163:SER:HB2	2.14	0.48
1:B:62:ALA:HA	1:B:194:MSE:HE3	1.94	0.48
3:F:69:MSE:HE1	3:F:94:VAL:CG2	2.44	0.48
1:B:78:GLN:HE22	1:B:261:PRO:HG2	1.79	0.48
2:C:249:ILE:OXT	2:C:249:ILE:HG22	2.14	0.48
2:D:249:ILE:HG22	2:D:249:ILE:OXT	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:TRP:O	1:B:235:LEU:HG	2.14	0.48
1:A:123:ALA:O	1:A:127:ILE:HG12	2.13	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:163:ALA:O	1:B:166:PHE:CE2	2.65	0.48
1:B:101:LEU:HD23	1:B:117:LEU:O	2.14	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
2:D:7:LEU:HD22	2:D:56:ILE:HG23	1.95	0.47
2:C:86:PHE:HA	2:C:125:ASN:OD1	2.14	0.47
1:A:32:SER:HB2	1:A:38:ILE:O	2.15	0.47
3:F:221:ILE:HD11	3:F:238:PRO:CG	2.44	0.47
1:A:316:VAL:O	1:A:320:LEU:HG	2.13	0.47
2:D:7:LEU:HD11	2:D:46:MSE:HE3	1.94	0.47
1:A:231:TRP:O	1:A:235:LEU:HG	2.14	0.47
1:A:58:PRO:HB3	1:A:188:TRP:CD2	2.49	0.47
1:B:122:ILE:HD13	1:B:241:TRP:CE3	2.49	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:194:MSE:O	1:B:198:ILE:HG13	2.14	0.47
1:B:55:ILE:HG22	1:B:56:ARG:N	2.29	0.47
3:F:198:GLN:OE1	3:F:198:GLN:HA	2.13	0.47
1:B:45:THR:CG2	1:B:46:PRO:HD2	2.45	0.47
1:B:298:LEU:CD1	1:B:301:ALA:HB1	2.36	0.47
1:A:95:ASN:HB3	1:A:156:SER:HB3	1.97	0.47
3:F:53:TYR:CE2	3:F:250:ARG:HD2	2.50	0.47
1:B:173:ARG:O	1:B:177:TYR:CD1	2.62	0.47
2:D:140:VAL:HG13	2:D:155:LEU:HD11	1.97	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:A:136:ALA:CB	1:A:145:LEU:HD11	2.44	0.47
1:B:160:MSE:O	1:B:164:ILE:CG1	2.59	0.47
1:B:99:VAL:HG22	1:B:160:MSE:HG3	1.96	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
3:F:65:THR:OG1	3:F:67:GLN:HG2	2.14	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:165:TYR:HE1	3:F:67:GLN:OE1	1.98	0.46
2:D:17:GLY:HA3	2:D:210:LYS:HD3	1.97	0.46
1:B:302:GLU:HA	1:B:302:GLU:OE1	2.14	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
3:F:227:TYR:C	3:F:229:GLY:H	2.17	0.46
1:B:170:VAL:O	1:B:174:GLN:HG3	2.14	0.46
2:C:246:ILE:HG23	2:D:198:ARG:NH1	2.30	0.46
1:B:64:LEU:HD21	1:B:288:LEU:HD12	1.97	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
3:F:188:ILE:HG13	3:F:189:PHE:CD1	2.51	0.46
2:C:17:GLY:HA3	2:C:210:LYS:HD3	1.97	0.46
1:B:195:LEU:O	1:B:199:PRO:HD2	2.15	0.46
3:F:157:ARG:HH12	3:F:207:ARG:HD3	1.80	0.46
1:B:14:ARG:CG	1:B:14:ARG:HH11	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
3:F:222:PRO:O	3:F:226:GLN:HG3	2.17	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
2:C:5:MSE:HE3	2:C:23:VAL:HG21	1.96	0.45
1:A:6:ARG:HG3	1:A:7:GLN:N	2.32	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
2:D:207:LYS:NZ	7:D:500:PEG:H31	2.31	0.45
1:A:162:TRP:O	1:A:166:PHE:HD1	1.99	0.45
2:D:75:ARG:C	2:D:75:ARG:CD	2.84	0.45
1:B:275:LEU:HG	1:B:279:CYS:HG	1.81	0.45
1:B:35:GLU:OE1	3:F:202:GLU:HG2	2.17	0.45
1:A:61:LEU:HB3	1:A:194:MSE:HE3	1.96	0.45
2:C:144:ILE:CD1	2:C:154:LEU:O	2.65	0.45
1:A:191:SER:O	1:A:195:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:47:VAL:O	3:F:62:GLN:HA	2.16	0.45
1:A:31:LEU:HA	1:A:31:LEU:HD23	1.52	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:198:ARG:NH1	2:D:246:ILE:HG23	2.32	0.45
2:C:170:SER:CB	2:D:232:MSE:HE1	2.47	0.45
1:A:40:PRO:HA	1:A:43:TRP:CD2	2.52	0.45
2:C:173:ASP:OD1	2:C:195:HIS:HE1	1.99	0.45
1:B:22:LEU:O	1:B:22:LEU:HD23	2.16	0.45
3:F:167:PRO:HG2	3:F:227:TYR:CZ	2.52	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
1:A:22:LEU:HD23	1:A:22:LEU:O	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
3:F:243:TRP:CE3	3:F:253:LEU:HB3	2.51	0.45
1:A:167:SER:O	3:F:195:PRO:HG3	2.17	0.45
2:C:239:ILE:HG21	2:D:239:ILE:HD13	1.98	0.45
1:B:192:TRP:HA	1:B:192:TRP:HE3	1.81	0.45
3:F:207:ARG:O	3:F:208:SER:C	2.56	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:B:14:ARG:HG3	1:B:14:ARG:NH1	2.28	0.45
1:A:133:LEU:HD21	1:A:236:VAL:HG11	1.98	0.45
1:A:201:LEU:HG	1:A:242:MSE:HE3	1.98	0.45
1:A:59:ARG:HA	1:A:186:VAL:CG1	2.47	0.45
1:B:270:THR:HG21	2:D:89:PRO:CD	2.48	0.44
1:B:77:MSE:CE	1:B:129:THR:HG22	2.46	0.44
1:B:143:SER:O	1:B:147:LEU:HG	2.17	0.44
1:B:80:LEU:CD2	1:B:236:VAL:HG22	2.43	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:307:VAL:HG13	1:B:162:TRP:HE3	1.69	0.44
1:A:1:MSE:SE	1:A:9:GLN:HE22	2.51	0.44
2:C:5:MSE:CE	2:C:23:VAL:HG21	2.48	0.44
1:B:318:ILE:C	1:B:320:LEU:H	2.21	0.44
1:B:259:VAL:CG1	1:B:263:ILE:HD11	2.48	0.44
1:B:183:PHE:CD1	1:B:305:ILE:HD12	2.53	0.44
1:B:87:GLU:HG3	1:B:88:PRO:CD	2.47	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)
2:C:45:ARG:NH2	2:C:53:LYS:O	2.43	0.44
1:A:287:LEU:HA	1:A:287:LEU:HD23	1.86	0.44
3:F:162:PHE:CD1	3:F:162:PHE:N	2.85	0.44
1:B:1:MSE:HB2	2:D:108:ASN:OD1	2.16	0.44
3:F:49:SER:HB3	3:F:65:THR:HG22	1.99	0.44
1:A:272:HIS:HA	1:A:275:LEU:HB3	2.00	0.44
1:A:259:VAL:CG1	1:A:263:ILE:HD11	2.48	0.44
1:A:167:SER:OG	1:A:172:LEU:HD13	2.17	0.44
3:F:150:TYR:HA	3:F:153:LYS:HG3	1.99	0.44
1:A:255:PHE:CZ	1:B:155:ILE:HG12	2.52	0.44
1:A:64:LEU:HD22	1:A:284:ALA:HB1	2.00	0.44
3:F:73:ARG:HD2	3:F:73:ARG:HA	1.77	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: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
1:A:226:LEU:HA	1:A:227:PRO:HD3	1.79	0.43
3:F:183:CYS:O	3:F:262:LEU:HD23	2.18	0.43
3:F:150:TYR:CD2	3:F:153:LYS:HD2	2.53	0.43
1:B:33:ALA:HB3	1:B:56:ARG:NH2	2.33	0.43
1:A:154:ILE:HG21	1:B:255:PHE:CZ	2.53	0.43
3:F:248:SER:O	3:F:251:ILE:HG22	2.18	0.43
2:D:66:TRP:HZ3	2:D:74:HIS:CD2	2.36	0.43
2:D:17:GLY:HA3	2:D:210:LYS:CD	2.48	0.43
2:D:86:PHE:CB	2:D:125:ASN:HD21	2.29	0.43
1:A:168:THR:CG2	1:A:169:SER:N	2.82	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:55:ILE:HD13	3:F:201:ARG:O	2.19	0.43
1:A:1:MSE:HE3	1:A:5:ALA:CB	2.49	0.43
1:B:83:ASN:OD1	1:B:84:PRO:HD2	2.19	0.43
3:F:218:PRO:HA	3:F:238:PRO:HG3	2.00	0.43
2:C:200:ALA:O	2:C:217:ARG:HD2	2.18	0.43
2:D:236:ARG:HH21	2:D:243:ARG:HD3	1.83	0.43
2:D:39:LYS:HG3	4:D:701:PO4:O4	2.19	0.43
1:B:222:ARG:HB2	2:D:49:MSE:HE1	2.00	0.43
1:B:317:PHE:O	1:B:320:LEU:HB3	2.19	0.42
1:B:48:GLY:O	1:B:49:GLU:C	2.58	0.42
3:F:183:CYS:HB3	3:F:259:CYS:HA	2.01	0.42
1:B:207:GLN:O	1:B:211:MSE:HE3	2.19	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)
2:C:106:LEU:O	2:C:107:LEU:C	2.58	0.42
1:B:64:LEU:HD22	1:B:284:ALA:HB1	2.01	0.42
1:B:87:GLU:OE2	1:B:258:LEU:HG	2.19	0.42
2:D:5:MSE:CE	2:D:23:VAL:HG21	2.48	0.42
3:F:168:PHE:C	3:F:168:PHE:CD1	2.93	0.42
1:A:269:LEU:HD22	1:A:274:VAL:CG1	2.49	0.42
2:C:106:LEU:HA	2:C:106:LEU:HD23	1.89	0.42
3:F:103:LYS:HD3	3:F:125:TRP:CH2	2.54	0.42
3:F:39:ALA:CB	3:F:249:PRO:HG2	2.49	0.42
1:A:160:MSE:SE	1:A:179:MSE:HE3	2.68	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
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:218:GLU:HG2	1:B:228:LEU:HD21	2.02	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
2:C:45:ARG:CD	2:C:50:THR:HG22	2.46	0.42
2:C:75:ARG:O	2:C:75:ARG:HD2	2.20	0.42
1:A:65:LEU:HD13	1:A:194:MSE:O	2.20	0.42
2:D:106:LEU:O	2:D:107:LEU:C	2.58	0.42
1:B:165:TYR:CD1	1:B:165:TYR:O	2.73	0.42
3:F:159:PHE:CD1	3:F:188:ILE:HD11	2.54	0.42
2:D:50:THR:HG23	2:D:51:SER:N	2.35	0.42
1:B:209:ARG:CB	1:B:210:PRO:CD	2.97	0.42
1:B:201:LEU:CD2	1:B:242:MSE:HE1	2.50	0.42
3:F:130:ASP:O	3:F:134:GLN:HG3	2.20	0.42
1:A:228:LEU:HB3	1:A:229:TRP:CE3	2.55	0.42
1:A:298:LEU:HD21	1:A:303:LEU:HD13	2.02	0.42
2:C:50:THR:HG23	2:C:51:SER:N	2.34	0.42
1:B:91:LEU:HA	1:B:149:GLY:HA3	2.01	0.42
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: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:B:130:LEU:HA	1:B:130:LEU:HD23	1.89	0.41
3:F:164:ILE:O	3:F:165:ASN:C	2.57	0.41
1:A:2:LEU:HG	1:A:3:THR:N	2.35	0.41
3:F:103:LYS:NZ	3:F:125:TRP:HZ2	2.18	0.41
1:A:168:THR:O	1:A:169:SER:C	2.59	0.41

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:ALA:HB2	2:D:156:LEU:CD1	2.51	0.40
2:C:91:TRP:HD1	2:C:120:LEU:O	2.05	0.40
3:F:41:GLY:CA	3:F:131:LYS:HD3	2.51	0.40
3:F:168:PHE:CA	3:F:198:GLN:OE1	2.70	0.40
2:C:239:ILE:HD13	2:D:239:ILE:HG21	2.02	0.40
1:B:48:GLY:O	1:B:51:PHE:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	322/326 (99%)	291 (90%)	29 (9%)	2 (1%)	30	56
1	B	322/326 (99%)	285 (88%)	32 (10%)	5 (2%)	12	24
2	C	246/249 (99%)	232 (94%)	13 (5%)	1 (0%)	39	65
2	D	246/249 (99%)	237 (96%)	8 (3%)	1 (0%)	39	65
3	F	243/245 (99%)	225 (93%)	15 (6%)	3 (1%)	16	33
All	All	1379/1395 (99%)	1270 (92%)	97 (7%)	12 (1%)	21	42

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

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%)	31	58
1	B	249/239 (104%)	236 (95%)	13 (5%)	29	54
2	C	200/192 (104%)	187 (94%)	13 (6%)	21	42
2	D	200/192 (104%)	187 (94%)	13 (6%)	21	42
3	F	205/203 (101%)	199 (97%)	6 (3%)	50	77
All	All	1103/1065 (104%)	1046 (95%)	57 (5%)	29	54

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

Some 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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (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	$\#\|Z\| > 2$
7	PEG	C	500	-	6,6,6	0.64	0	5,5,5	0.68	0
7	PEG	C	501	-	6,6,6	0.50	0	5,5,5	0.69	0
5	SO4	C	601	-	4,4,4	1.43	0	6,6,6	1.03	0
5	SO4	C	602	-	4,4,4	1.54	0	6,6,6	0.90	0
5	SO4	C	603	-	4,4,4	1.50	0	6,6,6	0.95	0
4	PO4	C	701	-	4,4,4	1.87	1 (25%)	6,6,6	0.28	0
6	1PE	C	800	-	15,15,15	0.62	0	14,14,14	0.64	0
7	PEG	D	500	-	6,6,6	0.49	0	5,5,5	0.75	0
7	PEG	D	501	-	6,6,6	0.50	0	5,5,5	0.70	0
5	SO4	D	601	-	4,4,4	1.50	0	6,6,6	1.01	0
5	SO4	D	602	-	4,4,4	1.54	0	6,6,6	0.89	0
5	SO4	D	603	-	4,4,4	1.45	0	6,6,6	0.97	0
4	PO4	D	701	-	4,4,4	1.70	0	6,6,6	0.28	0
6	1PE	D	800	-	15,15,15	0.60	0	14,14,14	0.73	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	-	-	0/4/4/4	0/0/0/0
7	PEG	C	501	-	-	0/4/4/4	0/0/0/0
5	SO4	C	601	-	-	0/0/0/0	0/0/0/0
5	SO4	C	602	-	-	0/0/0/0	0/0/0/0
5	SO4	C	603	-	-	0/0/0/0	0/0/0/0
4	PO4	C	701	-	-	0/0/0/0	0/0/0/0
6	1PE	C	800	-	-	0/13/13/13	0/0/0/0
7	PEG	D	500	-	-	0/4/4/4	0/0/0/0
7	PEG	D	501	-	-	0/4/4/4	0/0/0/0
5	SO4	D	601	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	D	602	-	-	0/0/0/0	0/0/0/0
5	SO4	D	603	-	-	0/0/0/0	0/0/0/0
4	PO4	D	701	-	-	0/0/0/0	0/0/0/0
6	1PE	D	800	-	-	0/13/13/13	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	701	PO4	P-O2	2.19	1.61	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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
6	C	800	1PE	6	0
7	D	500	PEG	1	0
4	D	701	PO4	1	0
6	D	800	1PE	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	313/326 (96%)	0.50	32 (10%) 9 5	41, 74, 147, 197	0
1	B	313/326 (96%)	0.35	23 (7%) 18 12	37, 71, 140, 184	0
2	C	240/249 (96%)	-0.10	3 (1%) 79 75	23, 46, 89, 176	0
2	D	240/249 (96%)	-0.07	4 (1%) 73 68	25, 45, 91, 180	0
3	F	243/245 (99%)	2.60	137 (56%) 0 0	73, 156, 195, 200	0
All	All	1349/1395 (96%)	0.64	199 (14%) 3 2	23, 69, 172, 200	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	GLY	12.4
3	F	154	PRO	9.0
3	F	56	GLN	8.1
1	A	139	HIS	8.1
3	F	153	LYS	8.1
3	F	207	ARG	7.6
1	B	164	ILE	7.3
3	F	230	GLU	7.2
3	F	152	ASP	7.0
1	A	137	ARG	7.0
3	F	182	VAL	7.0
3	F	143	TYR	6.9
3	F	163	GLY	6.9
3	F	126	SER	6.4
3	F	148	ALA	6.4
3	F	53	TYR	6.3
3	F	145	GLN	6.3
3	F	150	TYR	6.2
3	F	234	ILE	6.1
1	B	34	GLY	6.1

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Mol	Chain	Res	Type	RSRZ
3	F	266	ASP	6.1
3	F	130	ASP	6.0
3	F	251	ILE	5.8
3	F	245	GLU	5.7
1	A	301	ALA	5.6
3	F	240	THR	5.5
3	F	52	ASP	5.5
3	F	233	LYS	5.4
3	F	57	ALA	5.4
1	B	167	SER	5.3
3	F	186	GLU	5.2
1	B	324	ALA	5.2
1	B	168	THR	5.2
1	B	163	ALA	5.2
3	F	256	GLN	5.1
3	F	106	TRP	5.1
2	D	249	ILE	5.0
3	F	226	GLN	4.9
1	B	166	PHE	4.9
2	D	87	ALA	4.9
3	F	141	ASP	4.9
3	F	190	LYS	4.9
3	F	58	GLN	4.7
3	F	216	GLY	4.7
3	F	214	ILE	4.7
1	B	111	GLN	4.6
2	C	249	ILE	4.5
3	F	24	PRO	4.4
3	F	136	ALA	4.4
3	F	137	GLN	4.4
3	F	252	ILE	4.4
3	F	218	PRO	4.4
3	F	50	TYR	4.4
1	A	111	GLN	4.3
3	F	219	ASP	4.3
3	F	156	LYS	4.3
3	F	30	SER	4.2
1	A	138	ARG	4.2
3	F	59	LYS	4.2
3	F	104	VAL	4.2
1	B	165	TYR	4.1
3	F	149	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
3	F	80	ASP	4.1
3	F	60	ILE	4.1
3	F	247	ALA	4.0
3	F	170	SER	4.0
1	A	108	GLY	4.0
3	F	168	PHE	4.0
3	F	157	ARG	4.0
3	F	120	ARG	3.9
3	F	155	LYS	3.9
3	F	109	ALA	3.9
3	F	99	SER	3.9
3	F	45	VAL	3.8
3	F	77	LEU	3.8
3	F	210	GLN	3.7
3	F	151	ALA	3.7
3	F	67	GLN	3.7
3	F	63	VAL	3.7
1	A	109	GLN	3.7
3	F	189	PHE	3.7
1	A	144	ARG	3.6
3	F	93	GLN	3.6
3	F	185	GLY	3.6
3	F	125	TRP	3.6
3	F	139	LEU	3.6
1	A	255	PHE	3.6
3	F	208	SER	3.6
3	F	262	LEU	3.6
3	F	49	SER	3.5
3	F	132	ALA	3.5
3	F	159	PHE	3.5
3	F	46	GLY	3.4
3	F	55	PRO	3.4
3	F	51	SER	3.4
1	B	323	LYS	3.3
3	F	100	LEU	3.2
3	F	241	SER	3.2
3	F	73	ARG	3.2
1	A	177	TYR	3.2
3	F	119	LEU	3.2
3	F	215	THR	3.2
3	F	213	VAL	3.2
3	F	175	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	112	LEU	3.1
3	F	260	ASN	3.1
3	F	265	VAL	3.1
3	F	127	PRO	3.1
1	B	112	LEU	3.1
3	F	96	GLN	3.1
3	F	229	GLY	3.0
3	F	23	ALA	3.0
3	F	87	GLY	3.0
3	F	206	ALA	3.0
3	F	199	VAL	2.9
1	B	162	TRP	2.9
1	A	104	ALA	2.9
1	A	110	GLY	2.9
3	F	22	ALA	2.9
3	F	64	SER	2.8
3	F	243	TRP	2.8
3	F	82	VAL	2.8
1	A	189	ARG	2.8
3	F	54	PRO	2.8
3	F	135	ALA	2.8
3	F	164	ILE	2.8
3	F	76	ALA	2.8
3	F	238	PRO	2.8
1	B	175	LEU	2.7
3	F	94	VAL	2.7
3	F	259	CYS	2.7
3	F	188	ILE	2.7
1	A	33	ALA	2.7
1	A	322	LEU	2.6
1	A	86	ALA	2.6
1	A	324	ALA	2.6
1	B	301	ALA	2.6
3	F	237	ILE	2.6
3	F	217	GLY	2.6
1	A	254	GLY	2.6
1	B	319	TRP	2.6
3	F	43	THR	2.6
3	F	47	VAL	2.6
1	B	300	ALA	2.5
1	A	107	LEU	2.5
1	A	302	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	107	VAL	2.5
3	F	232	LEU	2.5
3	F	111	SER	2.5
3	F	192	SER	2.5
1	A	159	LEU	2.5
3	F	108	ASP	2.5
1	A	46	PRO	2.5
3	F	102	ILE	2.4
1	A	113	PRO	2.4
3	F	187	ASN	2.4
1	B	109	GLN	2.4
2	D	240	GLU	2.4
3	F	86	ARG	2.4
3	F	178	GLN	2.3
3	F	44	PRO	2.3
1	B	169	SER	2.3
3	F	134	GLN	2.3
3	F	123	ALA	2.3
1	A	135	PHE	2.3
3	F	158	VAL	2.3
3	F	61	GLU	2.3
3	F	29	LEU	2.3
1	A	142	THR	2.3
3	F	78	LYS	2.3
3	F	254	ALA	2.2
2	C	187	VAL	2.2
3	F	36	LEU	2.2
3	F	222	PRO	2.2
3	F	249	PRO	2.2
3	F	191	ASP	2.2
1	A	299	ALA	2.2
3	F	140	LEU	2.2
1	B	139	HIS	2.2
1	A	305	ILE	2.2
3	F	83	ILE	2.2
3	F	198	GLN	2.2
1	A	43	TRP	2.1
2	D	187	VAL	2.1
3	F	209	PRO	2.1
3	F	223	LYS	2.1
3	F	68	GLY	2.1
3	F	42	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	94	SER	2.1
1	B	184	GLY	2.1
3	F	116	ALA	2.1
3	F	228	TRP	2.1
3	F	114	GLN	2.0
1	B	6	ARG	2.0
2	C	17	GLY	2.0
1	A	140	LEU	2.0
1	B	161	THR	2.0
1	B	116	ALA	2.0
3	F	38	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	1PE	D	800	16/16	0.74	0.51	9.61	69,69,69,69	0
6	1PE	C	800	16/16	0.76	0.39	9.25	69,69,69,69	0
7	PEG	D	501	7/7	0.78	0.26	3.75	71,71,71,71	0
4	PO4	D	701	5/5	0.98	0.14	0.94	30,30,30,30	0
4	PO4	C	701	5/5	0.99	0.12	0.10	28,28,28,28	0
7	PEG	C	501	7/7	0.92	0.15	-0.46	71,71,71,71	0
5	SO4	D	602	5/5	0.83	0.28	-	106,106,106,106	0
7	PEG	C	500	7/7	0.63	0.23	-	67,67,67,67	0
5	SO4	D	603	5/5	0.88	0.23	-	119,119,119,119	0
5	SO4	C	602	5/5	0.86	0.20	-	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	SO4	D	601	5/5	0.92	0.16	-	85,85,85,85	0
5	SO4	C	601	5/5	0.93	0.15	-	78,78,78,78	0
7	PEG	D	500	7/7	0.72	0.41	-	81,81,81,81	0
5	SO4	C	603	5/5	0.82	0.24	-	141,141,141,141	0

6.5 Other polymers (i)

There are no such residues in this entry.