



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:24 PM UTC

PDB ID : 2QI9 / pdb_00002qi9
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.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

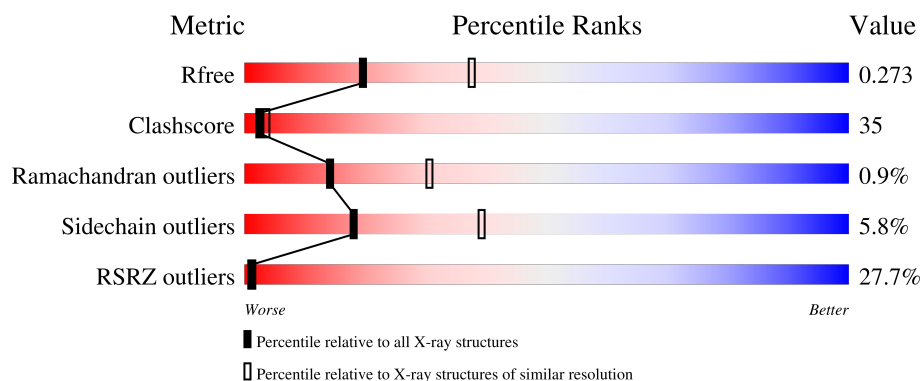
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	326	23% 48% 46% ..
1	B	326	21% 41% 50% 8% ..
2	C	249	8% 62% 32% 6%
2	D	249	8% 61% 33% 6%
3	F	245	78% 54% 42% ..

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 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
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				

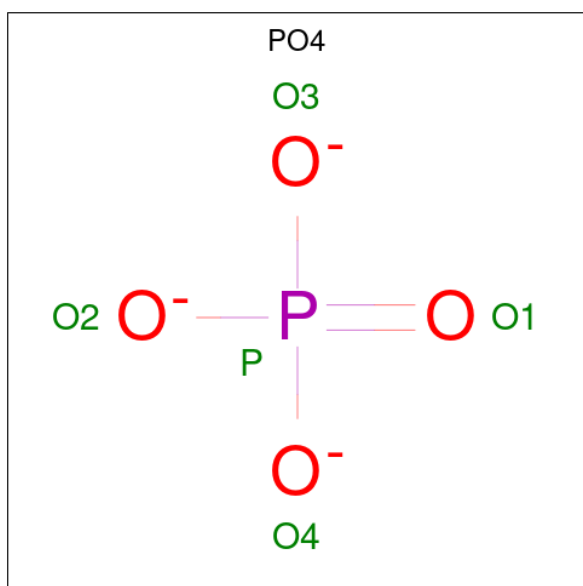
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	180	SER	CYS	engineered 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
3	F	245	Total	C	N	O	S	Se	0	0	0
			1908	1216	332	356	2	2			

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



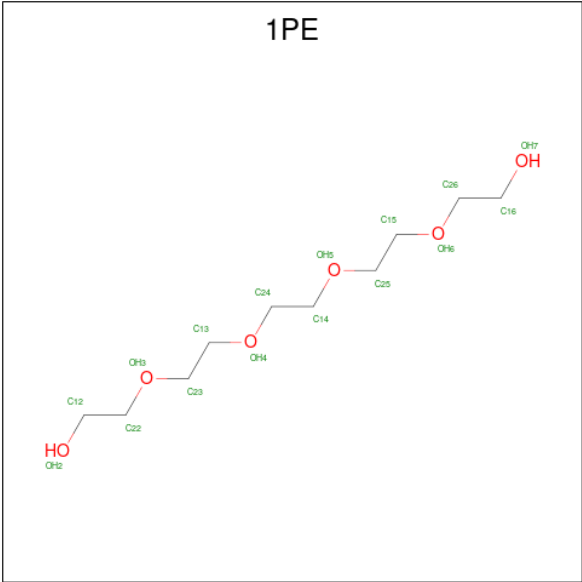
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



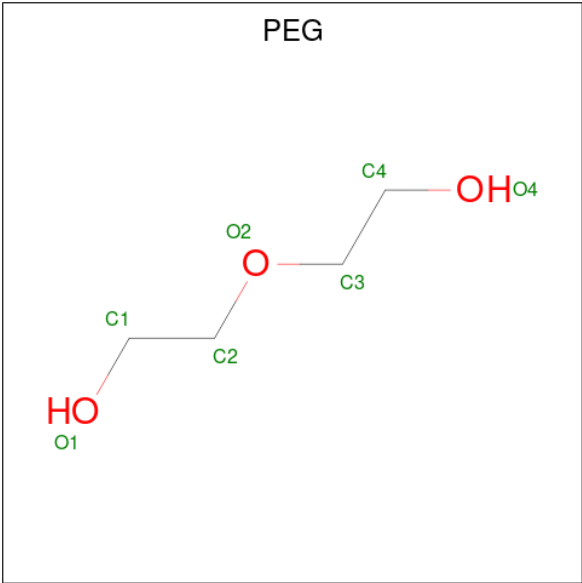
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

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



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

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

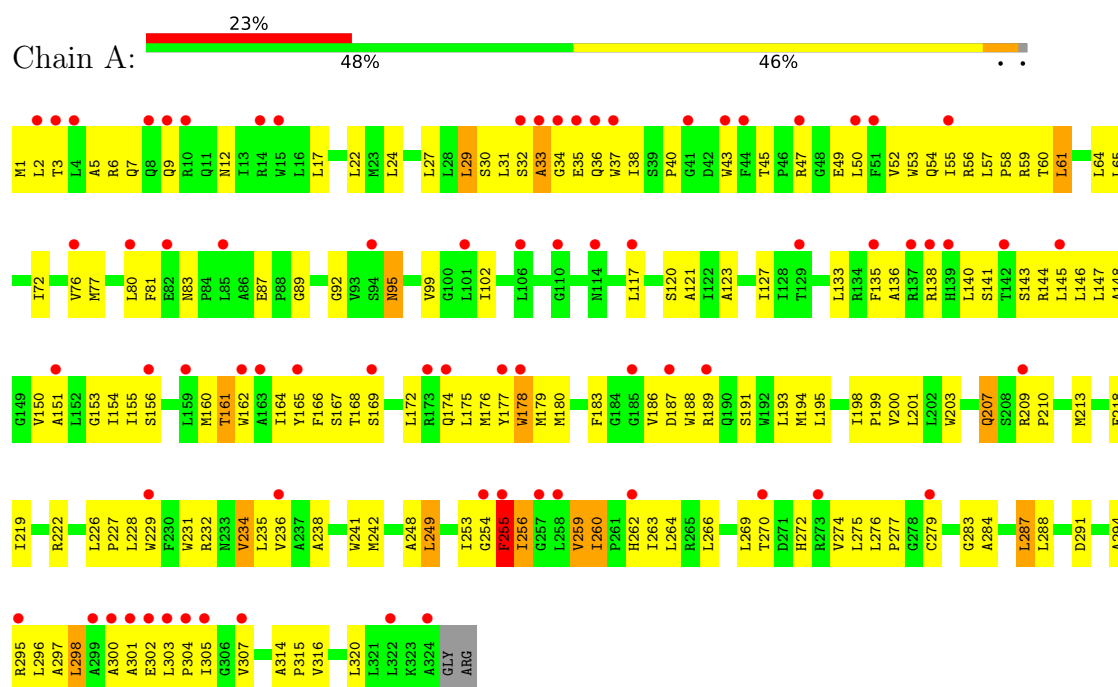
- Molecule 8 is water.

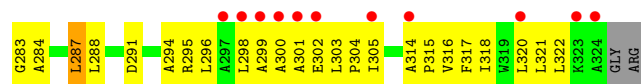
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	8	Total	O	0	0
			8	8		
8	D	8	Total	O	0	0
			8	8		

3 Residue-property plots

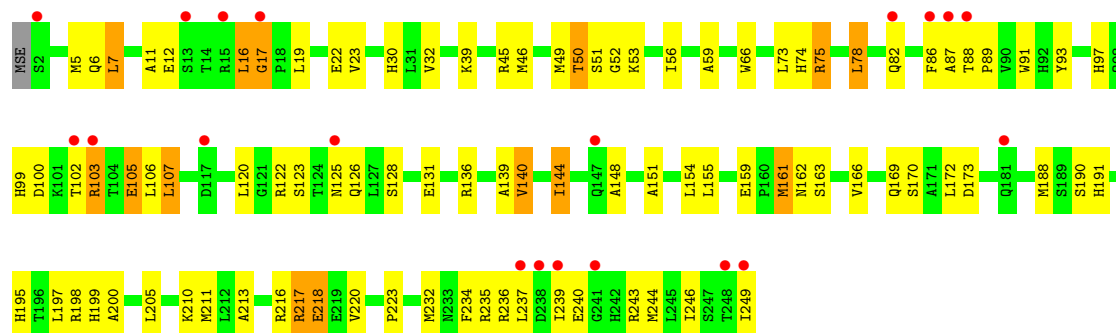
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

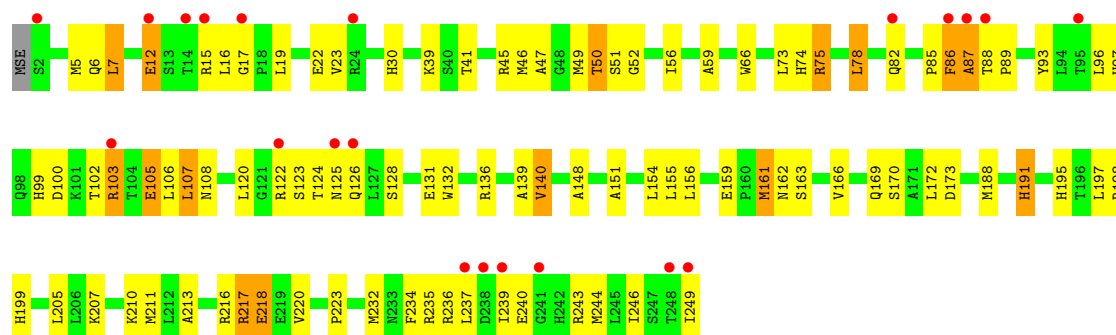




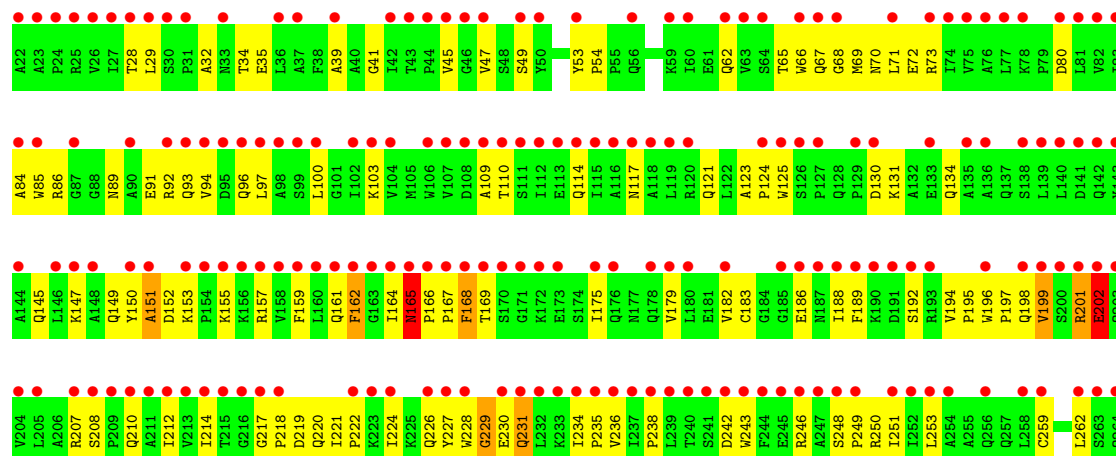
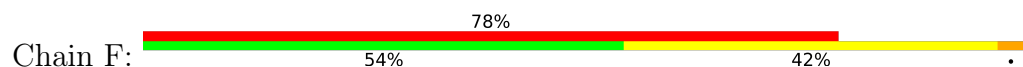
• Molecule 2: Vitamin B12 import ATP-binding protein btuD



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



• Molecule 3: Vitamin B12-binding protein btuF





4 Data and refinement statistics

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 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.81-2.60) 99.7 (29.81-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.02%)	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 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PO4, PEG, 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	0.67	1/2485 (0.0%)	1.09	15/3378 (0.4%)
1	B	0.72	5/2485 (0.2%)	1.21	27/3378 (0.8%)
2	C	0.52	0/1919	0.89	4/2587 (0.2%)
2	D	0.53	2/1919 (0.1%)	0.92	5/2587 (0.2%)
3	F	0.39	0/1950	0.98	10/2655 (0.4%)
All	All	0.59	8/10758 (0.1%)	1.04	61/14585 (0.4%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	PHE	C-N	-22.83	1.11	1.33
1	B	167	SER	C-N	12.14	1.49	1.33
1	B	164	ILE	C-N	10.85	1.48	1.33
1	B	296	LEU	C-N	-9.17	1.20	1.33
1	B	160	MSE	C-N	-8.93	1.21	1.33
1	B	139	HIS	C-N	-5.84	1.25	1.33
2	D	87	ALA	C-N	5.49	1.37	1.33
2	D	15	ARG	N-CA	5.05	1.52	1.46

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	296	LEU	O-C-N	-14.95	98.91	121.63
1	B	160	MSE	O-C-N	-13.52	107.79	122.12
1	B	296	LEU	CA-C-N	12.00	144.06	122.46
1	B	296	LEU	C-N-CA	12.00	144.06	122.46
1	A	253	ILE	CA-C-N	11.60	131.56	121.58
1	A	253	ILE	C-N-CA	11.60	131.56	121.58
1	B	259	VAL	N-CA-C	10.87	120.86	110.42
1	A	255	PHE	CA-C-N	10.56	134.81	122.35
1	A	255	PHE	C-N-CA	10.56	134.81	122.35
1	A	259	VAL	N-CA-C	10.56	120.54	110.30
1	A	255	PHE	O-C-N	-10.07	108.92	122.41
1	B	36	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	A	36	GLN	OE1-CD-NE2	-9.77	112.83	122.60
2	D	15	ARG	N-CA-C	8.10	122.43	112.23
1	B	167	SER	CA-C-N	8.05	136.19	121.06
1	B	167	SER	C-N-CA	8.05	136.19	121.06
1	B	83	ASN	CA-C-N	7.09	126.77	119.82
1	B	83	ASN	C-N-CA	7.09	126.77	119.82
3	F	202	GLU	N-CA-C	-6.92	105.77	114.56
3	F	151	ALA	N-CA-C	-6.81	103.65	112.23
1	A	33	ALA	N-CA-C	6.70	118.65	110.41
1	A	36	GLN	CG-CD-NE2	6.65	126.37	116.40
1	B	36	GLN	CG-CD-NE2	6.63	126.35	116.40
3	F	242	ASP	N-CA-C	6.58	119.01	111.11
3	F	165	ASN	CA-C-N	-6.44	113.75	120.38
3	F	165	ASN	C-N-CA	-6.44	113.75	120.38
2	D	191	HIS	N-CA-C	-6.14	105.59	114.12
2	D	199	HIS	N-CA-C	6.12	120.74	113.28
1	A	52	VAL	N-CA-C	6.08	116.26	110.42
1	B	260	ILE	N-CA-C	6.04	119.60	112.35
1	B	52	VAL	N-CA-C	6.03	116.21	110.42
2	C	199	HIS	N-CA-C	5.98	120.57	113.16
1	A	33	ALA	CA-C-N	5.94	131.37	120.79
1	A	33	ALA	C-N-CA	5.94	131.37	120.79
1	A	260	ILE	N-CA-C	5.92	119.45	112.35
1	B	160	MSE	CA-C-N	5.66	128.32	120.29
1	B	160	MSE	C-N-CA	5.66	128.32	120.29
1	B	209	ARG	CA-C-N	5.65	125.32	119.05
1	B	209	ARG	C-N-CA	5.65	125.32	119.05
1	B	139	HIS	CA-C-N	-5.58	110.88	121.54
1	B	139	HIS	C-N-CA	-5.58	110.88	121.54
1	B	29	LEU	N-CA-C	5.50	116.96	111.07
1	A	29	LEU	N-CA-C	5.43	116.88	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	TRP	CA-C-N	-5.43	112.20	121.97
1	B	37	TRP	C-N-CA	-5.43	112.20	121.97
2	C	17	GLY	CA-C-N	5.36	126.55	119.84
2	C	17	GLY	C-N-CA	5.36	126.55	119.84
3	F	152	ASP	N-CA-C	-5.36	106.51	113.16
1	B	164	ILE	O-C-N	5.34	127.30	121.90
1	B	198	ILE	N-CA-C	5.32	119.32	112.67
3	F	199	VAL	N-CA-C	5.32	117.54	108.86
1	B	117	LEU	N-CA-C	-5.32	105.93	112.90
3	F	45	VAL	N-CA-C	-5.30	106.70	112.80
1	A	161	THR	N-CA-C	-5.23	105.18	112.45
3	F	231	GLN	N-CA-C	-5.19	106.21	112.54
1	B	167	SER	O-C-N	-5.14	117.18	122.94
1	B	17	LEU	N-CA-C	-5.12	105.39	110.97
2	D	86	PHE	CA-CB-CG	5.08	118.88	113.80
2	C	144	ILE	N-CA-C	5.04	119.83	109.34
3	F	80	ASP	N-CA-C	-5.03	106.99	113.23
2	D	154	LEU	N-CA-C	5.02	117.24	108.76

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

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	229	0
1	B	2441	0	2605	276	0
2	C	1893	0	1925	103	0
2	D	1893	0	1925	108	0
3	F	1908	0	1924	156	0
4	C	5	0	0	1	0
4	D	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	11068	758	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 35.

All (758) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLU:CD	3:F:72:GLU:HG3	1.47	1.38
1:B:164:ILE:HG23	1:B:175:LEU:CD1	1.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:35:GLU:CD	3:F:72:GLU:CG	2.39	0.94
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: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
2:D:86:PHE:HA	2:D:125:ASN:CG	1.98	0.88
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
1:A:302:GLU:CD	3:F:93:GLN:NE2	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:A:254:GLY:C	1:A:255:PHE:HD1	1.90	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:300:ALA:O	3:F:69:MSE:C	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:D:75:ARG:HD2	2:D:75:ARG:C	2.13	0.72
1:B:256:ILE:HG23	1:B:260:ILE:HD12	1.71	0.72
2:C:75:ARG:C	2:C:75:ARG:HD2	2.14	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
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
1:A:302:GLU:CD	3:F:93:GLN:HE22	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:87:GLU:CD	1:B:258:LEU:HG	2.18	0.69
1:A:262:HIS:HD2	1:A:320:LEU:HD22	1.57	0.69
1:A:254:GLY:C	1:A:255:PHE:CD1	2.71	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
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
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
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: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
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:168:THR:HG22	1:B:169:SER:N	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:162:TRP:CD1	1:B:162:TRP:C	2.76	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
2:C:17:GLY:CA	2:C:210:LYS:NZ	2.60	0.64
2:D:86:PHE:C	2:D:125:ASN:HD21	2.05	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:6:GLN:C	2:D:7:LEU:HD23	2.26	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:45:ARG:NH2	2:D:52:GLY:C	2.59	0.60
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
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:45:ARG:NH2	2:C:52:GLY:C	2.60	0.60
2:C:236:ARG:NH2	2:C:243:ARG:HD3	2.16	0.60
2:D:105:GLU:CD	2:D:105:GLU:H	2.08	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
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
1:A:165:TYR:CD1	1:B:177:TYR:HE2	2.19	0.59
2:C:6:GLN:C	2:C:7:LEU:HD23	2.26	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
2:C:17:GLY:HA3	2:C:210:LYS:HZ2	1.67	0.59
2:C:86:PHE:HA	2:C:125:ASN:CG	2.28	0.59
1:B:136:ALA:HA	1:B:140:LEU:HD11	1.83	0.59
2:C:105:GLU:CD	2:C:105:GLU:H	2.09	0.59
2:C:161:MSE:CG	2:C:169:GLN:HG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:274:VAL:C	1:B:277:PRO:HD2	2.30	0.56
2:C:159:GLU:HA	6:C:800:1PE:C26	2.34	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
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
1:B:275:LEU:HG	1:B:279:CYS:HG	1.70	0.56
2:D:106:LEU:CD1	2:D:148:ALA:HB2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:141:SER:O	1:B:142:THR:C	2.49	0.55
1:B:165:TYR:CE1	3:F:67:GLN:OE1	2.60	0.55
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
1:A:274:VAL:C	1:A:277:PRO:HD2	2.31	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:17:GLY:CA	2:C:210:LYS:HZ2	2.21	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
3:F:229:GLY:C	3:F:231:GLN:H	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:F:227:TYR:C	3:F:229:GLY:H	2.17	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
2:D:75:ARG:C	2:D:75:ARG:CD	2.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:75:ARG:C	2:C:75:ARG:CD	2.84	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: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
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:17:GLY:CA	2:C:210:LYS:HZ3	2.24	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
3:F:207:ARG:O	3:F:208:SER:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:229:GLY:C	3:F:231:GLN:N	2.69	0.48
1:B:86:ALA:HA	1:B:91:LEU:HD11	1.96	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
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
1:B:318:ILE:C	1:B:320:LEU:H	2.21	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:48:GLY:O	1:B:49:GLU:C	2.58	0.47
1:B:122:ILE:HD13	1:B:241:TRP:CE3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:106:LEU:O	2:C:107:LEU:C	2.58	0.47
1:B:45:THR:CG2	1:B:46:PRO:HD2	2.45	0.47
3:F:168:PHE:CD1	3:F:168:PHE:C	2.93	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
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
2:D:106:LEU:O	2:D:107:LEU:C	2.58	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
3:F:168:PHE:HB2	3:F:198:GLN:NE2	2.26	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:A:303:LEU:O	1:A:304:PRO:C	2.57	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
3:F:164:ILE:O	3:F:165:ASN:C	2.57	0.46
1:A:168:THR:O	1:A:169:SER:C	2.59	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
1:B:64:LEU:HD21	1:B:288:LEU:HD12	1.97	0.46
1:B:272:HIS:C	1:B:274:VAL:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:272:HIS:C	1:A:274:VAL:H	2.23	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
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: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
3:F:217:GLY:C	3:F:219:ASP:H	2.24	0.45
3:F:53:TYR:HA	3:F:54:PRO:C	2.40	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:C:86:PHE:C	2:C:125:ASN:HD21	2.24	0.45
2:D:97:HIS:CD2	2:D:139:ALA:HB1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:162:ASN:O	2:D:163:SER:HB2	2.15	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:82:GLN:CD	2:D:136:ARG:HH21	2.24	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
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
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:A:207:GLN:C	1:A:210:PRO:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1:MSE:C	1:B:3:THR:N	2.75	0.43
1:B:33:ALA:HB3	1:B:56:ARG:NH2	2.33	0.43
1:B:318:ILE:C	1:B:320:LEU:N	2.76	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
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: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
2:C:82:GLN:CD	2:C:136:ARG:HH21	2.26	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
1:B:64:LEU:HD22	1:B:284:ALA:HB1	2.01	0.42
1:A:160:MSE:SE	1:A:179:MSE:HE3	2.68	0.42
1:A:168:THR:CG2	1:A:169:SER:N	2.82	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:D:100:ASP:C	2:D:102:THR:H	2.28	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: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
3:F:103:LYS:NZ	3:F:125:TRP:HZ2	2.18	0.41
1:A:2:LEU:O	1:A:3:THR:C	2.62	0.41
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
1:B:272:HIS:C	1:B:274:VAL:N	2.79	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
2:C:100:ASP:C	2:C:102:THR:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:SER:O	1:B:33:ALA:C	2.63	0.41
1:A:95:ASN:N	1:A:95:ASN:ND2	2.45	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:187:ASP:C	1:A:189:ARG:N	2.77	0.41
1:A:200:VAL:HG21	1:A:241:TRP:CD1	2.56	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:A:272:HIS:C	1:A:274:VAL:N	2.79	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:1:MSE:C	1:B:3:THR:H	2.29	0.40
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
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
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
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
1:B:165:TYR:CD1	1:B:165:TYR:C	2.97	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%)	21	42
1	B	322/326 (99%)	285 (88%)	32 (10%)	5 (2%)	7	16
2	C	246/249 (99%)	232 (94%)	13 (5%)	1 (0%)	30	51
2	D	246/249 (99%)	237 (96%)	8 (3%)	1 (0%)	30	51
3	F	243/245 (99%)	225 (93%)	15 (6%)	3 (1%)	10	23
All	All	1379/1395 (99%)	1270 (92%)	97 (7%)	12 (1%)	14	30

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
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%)	234 (94%)	15 (6%)	17	37
1	B	249/239 (104%)	233 (94%)	16 (6%)	16	35
2	C	200/192 (104%)	187 (94%)	13 (6%)	15	35
2	D	200/192 (104%)	186 (93%)	14 (7%)	14	31
3	F	205/203 (101%)	199 (97%)	6 (3%)	37	65
All	All	1103/1065 (104%)	1039 (94%)	64 (6%)	18	39

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
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	213	MSE
1	A	234	VAL
1	A	249	LEU
1	A	255	PHE
1	A	256	ILE
1	A	287	LEU
1	A	298	LEU
1	B	1	MSE
1	B	17	LEU
1	B	24	LEU
1	B	29	LEU
1	B	61	LEU
1	B	133	LEU
1	B	139	HIS
1	B	162	TRP
1	B	176	MSE
1	B	201	LEU
1	B	204	ILE
1	B	213	MSE
1	B	234	VAL
1	B	249	LEU
1	B	273	ARG
1	B	287	LEU

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Mol	Chain	Res	Type
2	C	7	LEU
2	C	16	LEU
2	C	22	GLU
2	C	50	THR
2	C	75	ARG
2	C	78	LEU
2	C	105	GLU
2	C	107	LEU
2	C	140	VAL
2	C	161	MSE
2	C	205	LEU
2	C	217	ARG
2	C	218	GLU
2	D	7	LEU
2	D	12	GLU
2	D	16	LEU
2	D	22	GLU
2	D	50	THR
2	D	75	ARG
2	D	78	LEU
2	D	105	GLU
2	D	107	LEU
2	D	140	VAL
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 (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	9	GLN
1	A	36	GLN
1	A	95	ASN
1	A	207	GLN

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Mol	Chain	Res	Type
1	A	262	HIS
1	B	7	GLN
1	B	36	GLN
1	B	114	ASN
1	B	174	GLN
1	B	262	HIS
2	C	61	GLN
2	C	80	GLN
2	C	82	GLN
2	C	92	HIS
2	C	97	HIS
2	C	99	HIS
2	C	125	ASN
2	C	147	GLN
2	C	195	HIS
2	D	61	GLN
2	D	80	GLN
2	D	82	GLN
2	D	97	HIS
2	D	99	HIS
2	D	108	ASN
2	D	125	ASN
2	D	147	GLN
2	D	195	HIS
3	F	62	GLN
3	F	93	GLN
3	F	145	GLN
3	F	149	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 oligosaccharides in this entry.

5.6 Ligand geometry

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
4	PO4	D	701	-	4,4,4	2.58	1 (25%)	6,6,6	0.66	0
4	PO4	C	701	-	4,4,4	2.75	3 (75%)	6,6,6	0.62	0
6	1PE	C	800	-	15,15,15	0.62	0	14,14,14	0.62	0
5	SO4	D	603	-	4,4,4	1.04	0	6,6,6	0.59	0
5	SO4	C	601	-	4,4,4	1.02	0	6,6,6	0.61	0
7	PEG	C	501	-	6,6,6	0.52	0	5,5,5	0.67	0
5	SO4	D	601	-	4,4,4	1.06	0	6,6,6	0.58	0
5	SO4	C	602	-	4,4,4	1.09	0	6,6,6	0.56	0
5	SO4	C	603	-	4,4,4	1.06	0	6,6,6	0.58	0
7	PEG	C	500	-	6,6,6	0.65	0	5,5,5	0.66	0
5	SO4	D	602	-	4,4,4	1.08	0	6,6,6	0.55	0
7	PEG	D	501	-	6,6,6	0.51	0	5,5,5	0.67	0
6	1PE	D	800	-	15,15,15	0.60	0	14,14,14	0.71	0
7	PEG	D	500	-	6,6,6	0.50	0	5,5,5	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
6	1PE	C	800	-	-	4/13/13/13	-
7	PEG	C	501	-	-	1/4/4/4	-
7	PEG	C	500	-	-	1/4/4/4	-
7	PEG	D	501	-	-	1/4/4/4	-
6	1PE	D	800	-	-	4/13/13/13	-
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	3.94	1.59	1.50
4	C	701	PO4	P-O1	3.82	1.59	1.50
4	C	701	PO4	P-O4	-2.69	1.46	1.54
4	C	701	PO4	P-O2	2.28	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	D	701	PO4	1	0
4	C	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	313/326 (96%)	1.38	74 (23%) 2 1	41, 74, 147, 197	0
1	B	313/326 (96%)	1.29	69 (22%) 2 2	37, 71, 140, 184	0
2	C	240/249 (96%)	0.34	20 (8%) 17 13	23, 46, 89, 176	0
2	D	240/249 (96%)	0.43	21 (8%) 15 12	25, 45, 91, 180	0
3	F	243/245 (99%)	3.10	190 (78%) 0 0	73, 156, 195, 200	0
All	All	1349/1395 (96%)	1.32	374 (27%) 1 1	23, 69, 172, 200	0

All (374) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	249	ILE	10.1
2	D	87	ALA	9.3
1	A	177	TYR	9.0
3	F	247	ALA	8.9
1	A	178	TRP	8.8
2	C	249	ILE	8.3
3	F	251	ILE	8.0
1	B	164	ILE	7.5
1	B	324	ALA	7.0
3	F	168	PHE	6.4
3	F	139	LEU	6.4
3	F	109	ALA	6.3
3	F	107	VAL	6.3
3	F	182	VAL	6.3
3	F	99	SER	6.3
1	A	2	LEU	6.2
1	A	301	ALA	6.1
3	F	164	ILE	6.1
1	A	302	GLU	6.0
3	F	106	TRP	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	255	PHE	5.8
3	F	63	VAL	5.7
1	B	161	THR	5.7
3	F	100	LEU	5.7
3	F	175	ILE	5.6
3	F	67	GLN	5.6
3	F	75	VAL	5.6
1	A	34	GLY	5.5
1	B	165	TYR	5.5
1	B	170	VAL	5.5
1	B	166	PHE	5.4
1	B	258	LEU	5.4
3	F	189	PHE	5.4
3	F	252	ILE	5.4
3	F	163	GLY	5.3
3	F	115	ILE	5.3
3	F	214	ILE	5.3
3	F	30	SER	5.3
1	A	324	ALA	5.2
3	F	143	TYR	5.2
3	F	170	SER	5.1
3	F	199	VAL	5.1
3	F	93	GLN	5.1
3	F	119	LEU	5.1
1	A	305	ILE	5.0
1	B	305	ILE	5.0
3	F	82	VAL	5.0
3	F	104	VAL	5.0
3	F	233	LYS	5.0
3	F	198	GLN	4.9
1	B	167	SER	4.9
1	B	300	ALA	4.9
3	F	213	VAL	4.9
3	F	234	ILE	4.8
3	F	228	TRP	4.8
3	F	241	SER	4.8
3	F	29	LEU	4.8
1	B	163	ALA	4.7
3	F	245	GLU	4.7
3	F	243	TRP	4.7
1	A	229	TRP	4.7
3	F	237	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
3	F	43	THR	4.6
1	A	50	LEU	4.6
3	F	249	PRO	4.6
3	F	159	PHE	4.5
3	F	112	ILE	4.4
3	F	205	LEU	4.4
3	F	94	VAL	4.3
3	F	83	ILE	4.3
1	A	101	LEU	4.2
3	F	92	ARG	4.2
3	F	157	ARG	4.2
1	B	169	SER	4.2
3	F	215	THR	4.2
3	F	85	TRP	4.2
3	F	87	GLY	4.2
3	F	186	GLU	4.2
3	F	36	LEU	4.1
3	F	96	GLN	4.1
3	F	240	THR	4.1
1	A	36	GLN	4.1
1	A	139	HIS	4.1
3	F	200	SER	4.1
3	F	166	PRO	4.0
3	F	210	GLN	4.0
3	F	231	GLN	4.0
3	F	90	ALA	4.0
3	F	160	LEU	4.0
3	F	161	GLN	4.0
2	C	17	GLY	4.0
2	D	17	GLY	4.0
1	B	185	GLY	4.0
2	C	125	ASN	4.0
3	F	173	GLU	4.0
3	F	146	LEU	4.0
1	B	177	TYR	4.0
1	B	162	TRP	3.9
1	A	209	ARG	3.9
2	D	103	ARG	3.9
1	B	34	GLY	3.9
1	B	229	TRP	3.9
1	B	168	THR	3.9
3	F	110	THR	3.9

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Mol	Chain	Res	Type	RSRZ
3	F	127	PRO	3.9
3	F	178	GLN	3.9
3	F	223	LYS	3.9
2	D	125	ASN	3.8
1	A	35	GLU	3.8
3	F	77	LEU	3.8
3	F	153	LYS	3.8
3	F	208	SER	3.8
3	F	136	ALA	3.8
2	D	2	SER	3.7
3	F	196	TRP	3.7
3	F	84	ALA	3.7
3	F	209	PRO	3.7
1	B	262	HIS	3.7
1	B	178	TRP	3.7
1	A	174	GLN	3.7
1	B	35	GLU	3.7
3	F	97	LEU	3.6
3	F	154	PRO	3.6
3	F	212	ILE	3.6
1	A	165	TYR	3.6
1	A	299	ALA	3.5
1	B	33	ALA	3.5
2	D	241	GLY	3.5
3	F	64	SER	3.5
3	F	254	ALA	3.5
3	F	44	PRO	3.5
1	A	156	SER	3.4
1	B	90	LEU	3.4
3	F	147	LYS	3.4
3	F	248	SER	3.4
1	B	301	ALA	3.4
3	F	116	ALA	3.4
3	F	236	VAL	3.4
3	F	66	TRP	3.4
2	D	88	THR	3.4
3	F	169	THR	3.4
3	F	218	PRO	3.4
3	F	50	TYR	3.3
3	F	45	VAL	3.3
1	B	55	ILE	3.3
3	F	111	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	33	ALA	3.3
1	A	51	PHE	3.3
3	F	165	ASN	3.3
3	F	191	ASP	3.3
3	F	102	ILE	3.3
1	B	11	GLN	3.3
3	F	135	ALA	3.3
1	A	307	VAL	3.3
1	B	171	ASP	3.3
3	F	190	LYS	3.3
3	F	224	ILE	3.3
3	F	265	VAL	3.3
3	F	266	ASP	3.3
3	F	53	TYR	3.2
1	B	299	ALA	3.2
3	F	24	PRO	3.2
2	D	14	THR	3.2
1	A	169	SER	3.2
3	F	158	VAL	3.2
1	A	145	LEU	3.2
1	A	270	THR	3.2
1	A	254	GLY	3.2
3	F	187	ASN	3.2
2	D	15	ARG	3.2
3	F	120	ARG	3.2
1	B	140	LEU	3.2
3	F	201	ARG	3.1
3	F	204	VAL	3.1
1	A	85	LEU	3.1
2	C	82	GLN	3.1
3	F	176	GLN	3.1
1	A	43	TRP	3.1
1	B	252	ALA	3.1
3	F	155	LYS	3.1
1	A	159	LEU	3.1
1	B	101	LEU	3.1
1	B	147	LEU	3.1
2	C	87	ALA	3.1
1	B	175	LEU	3.1
3	F	180	LEU	3.1
1	B	302	GLU	3.1
3	F	80	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
3	F	31	PRO	3.1
3	F	23	ALA	3.1
1	A	80	LEU	3.0
1	A	262	HIS	3.0
3	F	144	ALA	3.0
3	F	141	ASP	3.0
3	F	256	GLN	3.0
1	A	173	ARG	3.0
3	F	226	GLN	3.0
1	A	189	ARG	3.0
1	A	142	THR	3.0
1	B	297	ALA	3.0
3	F	39	ALA	3.0
3	F	26	VAL	3.0
3	F	244	PHE	3.0
1	A	236	VAL	3.0
1	B	41	GLY	2.9
1	A	37	TRP	2.9
1	A	94	SER	2.9
3	F	126	SER	2.9
1	A	322	LEU	2.9
3	F	232	LEU	2.9
3	F	150	TYR	2.9
3	F	230	GLU	2.8
1	A	8	GLN	2.8
2	C	13	SER	2.8
3	F	188	ILE	2.8
3	F	148	ALA	2.8
1	A	137	ARG	2.8
3	F	207	ARG	2.8
3	F	140	LEU	2.8
3	F	98	ALA	2.8
2	D	86	PHE	2.8
2	D	82	GLN	2.8
3	F	114	GLN	2.8
1	A	187	ASP	2.8
1	A	300	ALA	2.8
1	A	10	ARG	2.8
2	C	103	ARG	2.8
3	F	42	ILE	2.8
3	F	125	TRP	2.8
3	F	71	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
3	F	216	GLY	2.8
3	F	217	GLY	2.8
3	F	130	ASP	2.8
3	F	76	ALA	2.8
3	F	113	GLU	2.8
1	A	47	ARG	2.8
1	B	146	LEU	2.7
2	C	2	SER	2.7
1	A	82	GLU	2.7
3	F	78	LYS	2.7
2	C	239	ILE	2.7
1	A	185	GLY	2.7
3	F	192	SER	2.7
1	B	174	GLN	2.7
3	F	103	LYS	2.7
1	B	249	LEU	2.7
1	B	141	SER	2.7
2	C	15	ARG	2.7
3	F	179	VAL	2.7
3	F	235	PRO	2.7
1	B	139	HIS	2.7
3	F	46	GLY	2.7
2	C	237	LEU	2.6
1	B	40	PRO	2.6
2	D	239	ILE	2.6
3	F	27	ILE	2.6
3	F	185	GLY	2.6
2	C	86	PHE	2.6
3	F	22	ALA	2.6
3	F	211	ALA	2.6
1	A	110	GLY	2.6
3	F	259	CYS	2.6
3	F	25	ARG	2.6
3	F	59	LYS	2.6
3	F	124	PRO	2.6
1	B	86	ALA	2.5
1	B	279	CYS	2.5
2	C	88	THR	2.5
1	B	172	LEU	2.5
1	B	320	LEU	2.5
1	A	44	PHE	2.5
1	A	163	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	147	GLN	2.5
3	F	37	ALA	2.5
2	C	248	THR	2.5
1	B	159	LEU	2.5
3	F	81	LEU	2.5
1	A	76	VAL	2.5
3	F	56	GLN	2.5
1	A	138	ARG	2.5
1	B	50	LEU	2.5
1	B	298	LEU	2.5
3	F	49	SER	2.5
3	F	262	LEU	2.5
2	D	24	ARG	2.4
1	A	304	PRO	2.4
3	F	151	ALA	2.4
3	F	263	SER	2.4
3	F	171	GLY	2.4
3	F	172	LYS	2.4
1	A	4	LEU	2.4
1	B	239	THR	2.4
1	A	135	PHE	2.4
1	A	273	ARG	2.4
1	B	137	ARG	2.4
3	F	73	ARG	2.4
1	A	55	ILE	2.4
3	F	33	ASN	2.4
2	D	12	GLU	2.4
2	D	238	ASP	2.4
1	B	2	LEU	2.3
1	B	270	THR	2.3
3	F	156	LYS	2.3
1	A	279	CYS	2.3
1	B	47	ARG	2.3
1	B	143	SER	2.3
3	F	108	ASP	2.3
1	B	192	TRP	2.3
2	D	237	LEU	2.3
1	B	127	ILE	2.3
1	B	138	ARG	2.3
1	B	189	ARG	2.3
3	F	167	PRO	2.3
1	A	9	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	74	ILE	2.3
1	B	323	LYS	2.3
2	C	102	THR	2.3
1	A	32	SER	2.3
1	B	10	ARG	2.3
1	B	144	ARG	2.3
3	F	242	ASP	2.3
1	A	106	LEU	2.3
1	B	142	THR	2.2
2	C	117	ASP	2.2
1	A	303	LEU	2.2
1	B	145	LEU	2.2
1	B	314	ALA	2.2
3	F	202	GLU	2.2
1	A	41	GLY	2.2
1	A	257	GLY	2.2
1	A	15	TRP	2.2
3	F	47	VAL	2.2
1	A	3	THR	2.2
2	D	95	THR	2.2
3	F	129	PRO	2.2
3	F	142	GLN	2.2
2	C	241	GLY	2.2
3	F	253	LEU	2.2
1	A	295	ARG	2.2
2	C	181	GLN	2.2
3	F	62	GLN	2.2
3	F	68	GLY	2.2
3	F	258	LEU	2.2
3	F	95	ASP	2.2
1	A	14	ARG	2.1
2	D	126	GLN	2.1
3	F	227	TYR	2.1
1	A	258	LEU	2.1
2	C	238	ASP	2.1
1	A	162	TRP	2.1
1	B	82	GLU	2.1
3	F	193	ARG	2.1
3	F	246	ARG	2.1
1	A	129	THR	2.1
3	F	203	GLN	2.1
3	F	264	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	114	ASN	2.1
3	F	162	PHE	2.1
3	F	118	ALA	2.1
2	D	248	THR	2.1
3	F	28	THR	2.1
3	F	222	PRO	2.1
1	B	109	GLN	2.1
3	F	60	ILE	2.1
1	A	151	ALA	2.0
3	F	133	GLU	2.0
1	B	266	LEU	2.0
3	F	117	ASN	2.0
1	B	14	ARG	2.0
2	D	122	ARG	2.0
3	F	138	SER	2.0
3	F	238	PRO	2.0
1	A	117	LEU	2.0
3	F	239	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	D	602	5/5	0.67	0.20	106,106,106,106	0
7	PEG	C	500	7/7	0.68	0.21	67,67,67,67	0
6	1PE	D	800	16/16	0.75	0.26	69,69,69,69	0
5	SO4	C	602	5/5	0.75	0.12	113,113,113,113	0
7	PEG	D	500	7/7	0.77	0.35	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	1PE	C	800	16/16	0.78	0.25	69,69,69,69	0
5	SO4	C	603	5/5	0.80	0.19	141,141,141,141	0
5	SO4	D	603	5/5	0.82	0.15	119,119,119,119	0
7	PEG	D	501	7/7	0.83	0.17	71,71,71,71	0
5	SO4	D	601	5/5	0.86	0.12	85,85,85,85	0
5	SO4	C	601	5/5	0.86	0.10	78,78,78,78	0
7	PEG	C	501	7/7	0.93	0.11	71,71,71,71	0
4	PO4	C	701	5/5	0.98	0.06	28,28,28,28	0
4	PO4	D	701	5/5	0.98	0.06	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.