



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2022 – 12:09 PM JST

PDB ID : 5ZIA
Title : Crystal structure of human anti-tau antibody CBTAU-24.1 in complex with its phosphorylated tau peptide
Authors : Zhang, H.; Wilson, I.A.
Deposited on : 2018-03-14
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

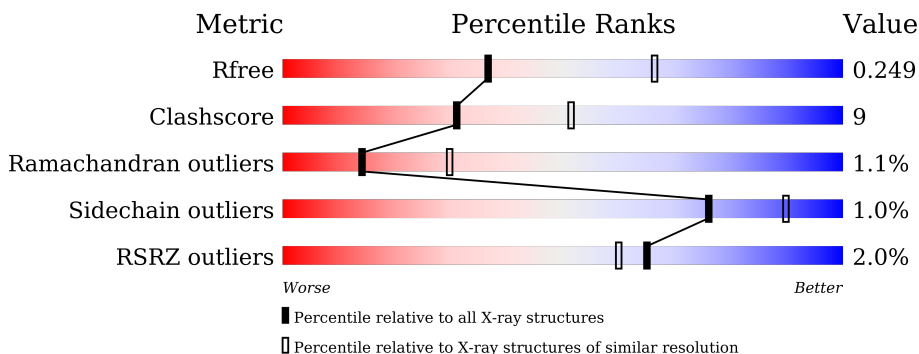
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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X-RAY DIFFRACTION

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












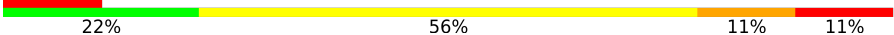


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	226	 <div>2% 86% 12%</div>
1	D	226	 <div>3% 86% 11%</div>
1	G	226	 <div>3% 81% 17%</div>
1	H	226	 <div>3% 85% 12%</div>
1	K	226	 <div>4% 80% 17%</div>
1	O	226	 <div>4% 77% 20%</div>

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Mol	Chain	Length	Quality of chain
2	B	220	 79%19%..
2	E	220	 88%11%.
2	I	220	 2%77%18%..
2	L	220	 %82%14%..
2	M	220	 80%17%..
2	P	220	 %80%18%..
3	C	9	 67%33%
3	F	9	 78%11%11%
3	J	9	 89%11%
3	N	9	 11%22%56%11%11%
3	Q	9	 100%
3	R	9	 78%22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20828 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 Heavy chain of CBTAU-24.1 antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	220	Total	C	N	O	S	0	0	0
			1640	1038	275	320	7			
1	A	220	Total	C	N	O	S	0	0	0
			1640	1038	275	320	7			
1	D	219	Total	C	N	O	S	0	0	0
			1631	1033	273	318	7			
1	H	219	Total	C	N	O	S	0	0	0
			1631	1033	273	318	7			
1	K	220	Total	C	N	O	S	0	0	0
			1640	1038	275	320	7			
1	O	220	Total	C	N	O	S	0	0	0
			1640	1038	275	320	7			

- Molecule 2 is a protein called Light chain (kappa) of CBTAU-24.1 antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	217	Total	C	N	O	S	0	0	0
			1698	1065	283	345	5			
2	B	217	Total	C	N	O	S	0	0	0
			1694	1063	283	343	5			
2	E	218	Total	C	N	O	S	0	0	0
			1702	1067	284	346	5			
2	I	217	Total	C	N	O	S	0	0	0
			1698	1065	283	345	5			
2	M	217	Total	C	N	O	S	0	0	0
			1698	1065	283	345	5			
2	P	217	Total	C	N	O	S	0	0	0
			1698	1065	283	345	5			

- Molecule 3 is a protein called phosphorylated tau peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	9	Total	C	N	O	P	0	0	0
			68	38	13	16	1			
3	C	9	Total	C	N	O	P	0	0	0
			68	38	13	16	1			
3	F	9	Total	C	N	O	P	0	0	0
			68	38	13	16	1			
3	J	9	Total	C	N	O	P	0	0	0
			68	38	13	16	1			
3	N	9	Total	C	N	O	P	0	0	0
			68	38	13	16	1			
3	Q	9	Total	C	N	O	P	0	0	0
			68	38	13	16	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	38	Total	O	0	0
			38	38		
4	L	24	Total	O	0	0
			24	24		
4	R	2	Total	O	0	0
			2	2		
4	A	33	Total	O	0	0
			33	33		
4	B	37	Total	O	0	0
			37	37		
4	D	41	Total	O	0	0
			41	41		
4	E	42	Total	O	0	0
			42	42		
4	F	2	Total	O	0	0
			2	2		
4	H	31	Total	O	0	0
			31	31		
4	I	24	Total	O	0	0
			24	24		
4	J	6	Total	O	0	0
			6	6		
4	K	29	Total	O	0	0
			29	29		
4	M	34	Total	O	0	0
			34	34		
4	N	2	Total	O	0	0
			2	2		

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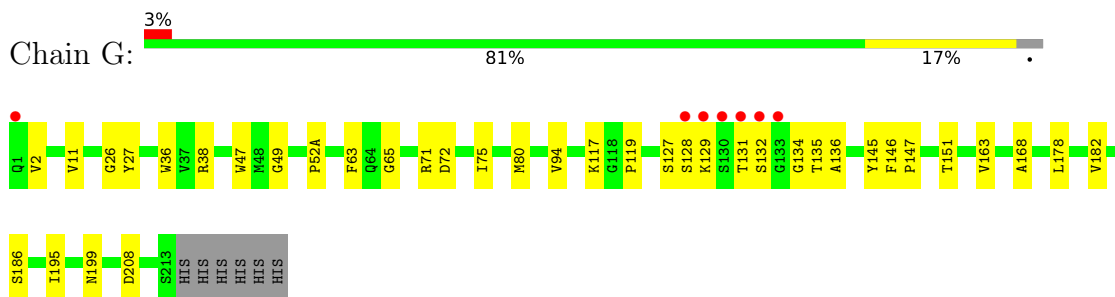
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	24	Total 24	O 24	0	0
4	P	40	Total 40	O 40	0	0
4	Q	1	Total 1	O 1	0	0

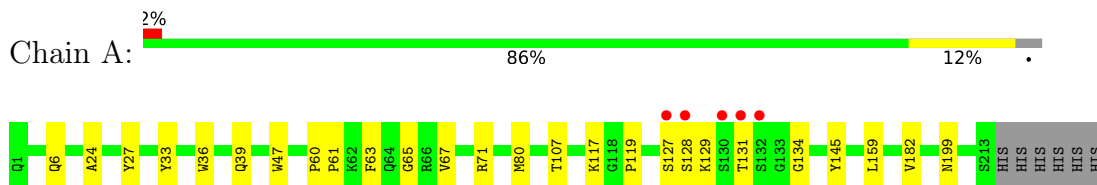
3 Residue-property plots

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.

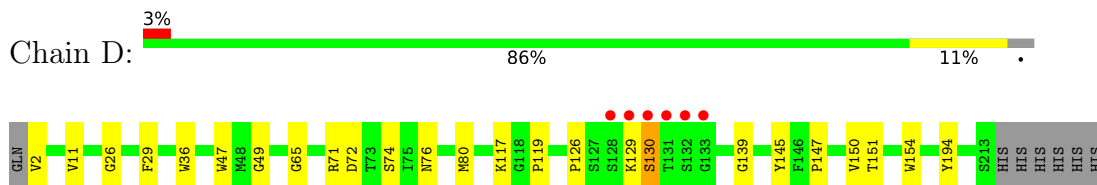
- Molecule 1: Heavy chain of CBTAU-24.1 antibody



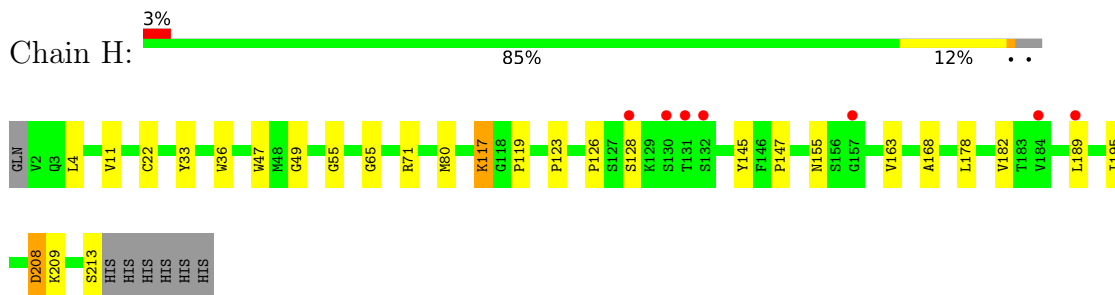
- Molecule 1: Heavy chain of CBTAU-24.1 antibody



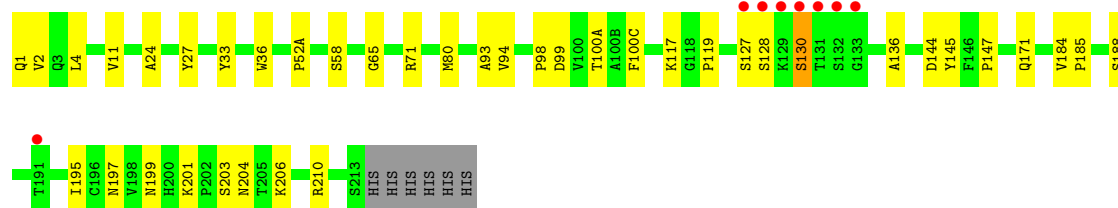
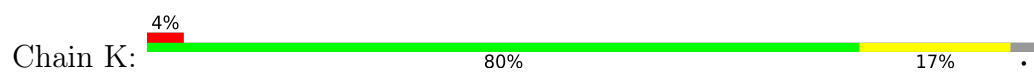
- Molecule 1: Heavy chain of CBTAU-24.1 antibody



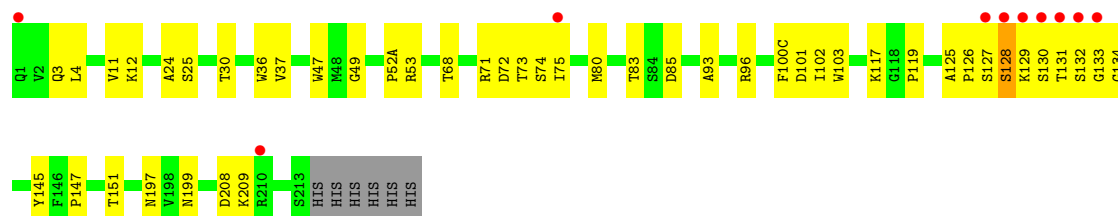
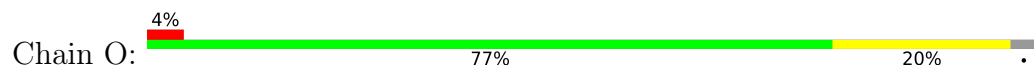
- Molecule 1: Heavy chain of CBTAU-24.1 antibody



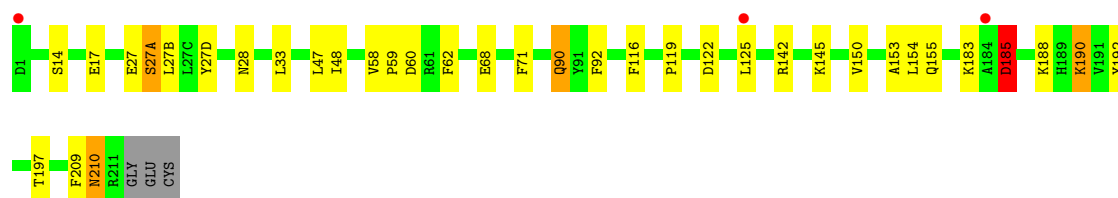
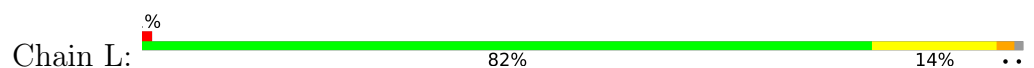
- Molecule 1: Heavy chain of CBTAU-24.1 antibody



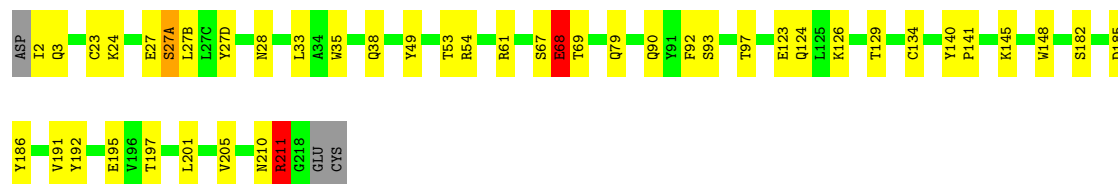
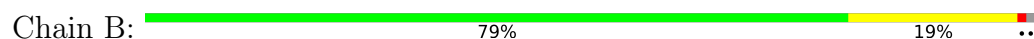
- Molecule 1: Heavy chain of CBTAU-24.1 antibody



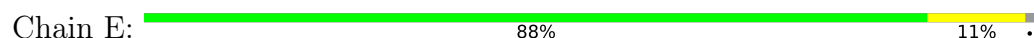
- Molecule 2: Light chain (kappa) of CBTAU-24.1 antibody



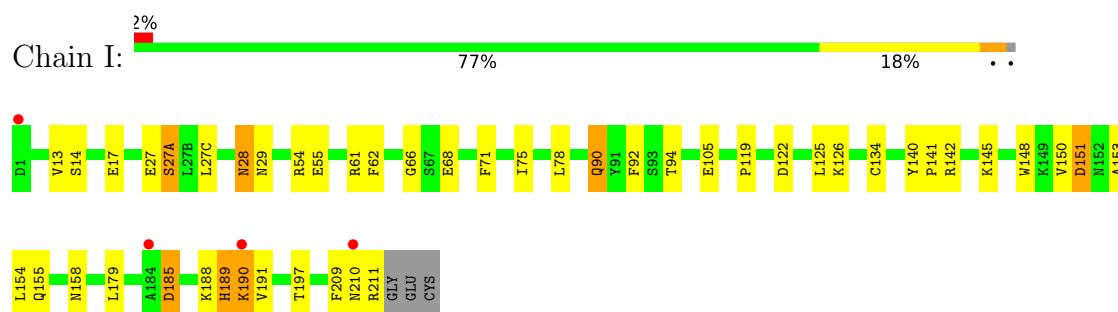
- Molecule 2: Light chain (kappa) of CBTAU-24.1 antibody



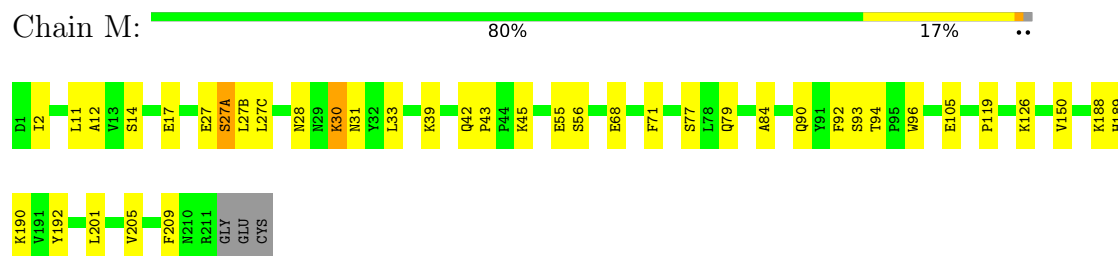
- Molecule 2: Light chain (kappa) of CBTAU-24.1 antibody



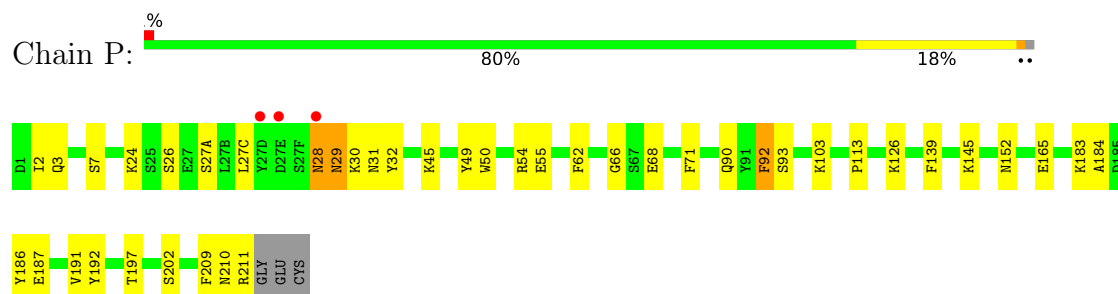
- Molecule 2: Light chain (kappa) of CBTAU-24.1 antibody



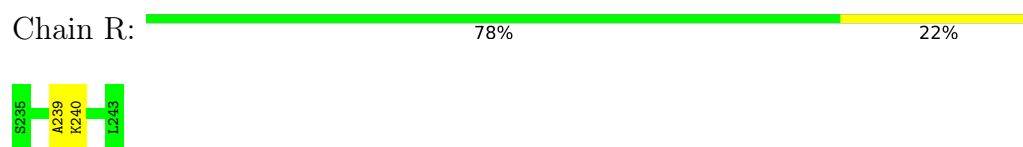
- Molecule 2: Light chain (kappa) of CBTAU-24.1 antibody



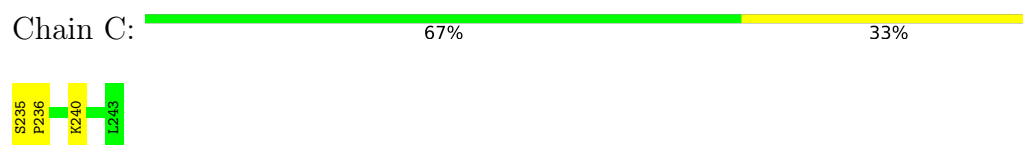
- Molecule 2: Light chain (kappa) of CBTAU-24.1 antibody



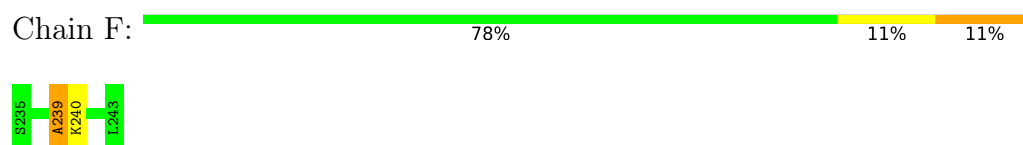
- Molecule 3: phosphorylated tau peptide




- Molecule 3: phosphorylated tau peptide



- Molecule 3: phosphorylated tau peptide



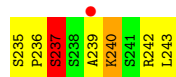
- Molecule 3: phosphorylated tau peptide

Chain J:  89% 11%



- Molecule 3: phosphorylated tau peptide

Chain N:  11% 22% 56% 11% 11%



- Molecule 3: phosphorylated tau peptide

Chain Q:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	86.35Å 107.81Å 107.93Å 62.16° 71.02° 90.77°	Depositor
Resolution (Å)	46.86 – 2.60 46.87 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.7 (46.86-2.60) 90.7 (46.87-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.200 , 0.249 0.203 , 0.249	Depositor DCC
R_{free} test set	4623 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,k,k-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20828	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: SEP

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	0.50	0/1685	0.62	0/2307
1	D	0.47	0/1676	0.61	0/2295
1	G	0.43	0/1685	0.61	0/2307
1	H	0.43	0/1676	0.61	0/2295
1	K	0.46	0/1685	0.59	0/2307
1	O	0.52	0/1685	0.63	0/2307
2	B	0.60	0/1733	0.60	0/2355
2	E	0.53	0/1741	0.61	0/2366
2	I	0.56	0/1737	0.65	0/2361
2	L	0.54	0/1737	0.65	0/2361
2	M	0.53	0/1737	0.60	0/2361
2	P	0.62	0/1737	0.64	0/2361
3	C	0.80	0/57	0.63	0/73
3	F	0.62	0/57	0.56	0/73
3	J	0.32	0/57	0.54	0/73
3	N	0.39	0/57	0.63	0/73
3	Q	0.78	0/57	0.84	0/73
3	R	0.60	0/57	1.05	0/73
All	All	0.52	0/20856	0.62	0/28421

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1640	0	1602	16	0
1	D	1631	0	1591	18	0
1	G	1640	0	1602	23	0
1	H	1631	0	1591	15	0
1	K	1640	0	1602	35	0
1	O	1640	0	1602	41	0
2	B	1694	0	1632	36	0
2	E	1702	0	1639	20	0
2	I	1698	0	1636	47	0
2	L	1698	0	1636	44	0
2	M	1698	0	1636	42	0
2	P	1698	0	1636	38	0
3	C	68	0	67	3	0
3	F	68	0	67	1	0
3	J	68	0	67	1	0
3	N	68	0	66	11	0
3	Q	68	0	67	0	0
3	R	68	0	67	1	0
4	A	33	0	0	0	0
4	B	37	0	0	3	0
4	D	41	0	0	4	0
4	E	42	0	0	1	0
4	F	2	0	0	0	0
4	G	38	0	0	0	0
4	H	31	0	0	0	0
4	I	24	0	0	0	0
4	J	6	0	0	0	0
4	K	29	0	0	3	0
4	L	24	0	0	1	0
4	M	34	0	0	0	0
4	N	2	0	0	0	0
4	O	24	0	0	0	0
4	P	40	0	0	2	0
4	Q	1	0	0	0	0
4	R	2	0	0	0	0
All	All	20828	0	19806	366	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 9.

All (366) 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)
3:N:239:ALA:O	3:N:240:LYS:HG2	1.09	1.24
2:B:68:GLU:CG	2:B:69:THR:H	1.43	1.22
2:B:68:GLU:HG3	2:B:69:THR:N	1.43	1.14
3:N:239:ALA:O	3:N:240:LYS:CG	1.95	1.13
2:L:125:LEU:HD11	2:L:183:LYS:HE3	1.31	1.09
2:I:158:ASN:ND2	2:I:179:LEU:HD11	1.67	1.08
2:I:158:ASN:ND2	2:I:179:LEU:CD1	2.21	1.04
2:L:125:LEU:HD11	2:L:183:LYS:CE	1.90	1.02
2:L:59:PRO:HG2	2:L:62:PHE:HD2	1.26	1.00
1:O:71:ARG:HH11	1:O:73:THR:HG23	1.25	0.99
2:P:145:LYS:HB3	2:P:197:THR:HG22	1.46	0.98
2:L:125:LEU:CD1	2:L:183:LYS:HE3	1.93	0.98
2:L:59:PRO:HG2	2:L:62:PHE:CD2	2.01	0.94
1:K:1:GLN:HG3	1:K:2:VAL:N	1.84	0.92
2:M:2:ILE:HG12	2:M:27:GLU:HG3	1.54	0.89
1:K:65:GLY:CA	1:O:117:LYS:HE3	2.05	0.87
1:O:71:ARG:NH1	1:O:73:THR:HG23	1.88	0.86
2:P:2:ILE:HG21	2:P:90:GLN:HG3	1.57	0.86
2:I:158:ASN:HD21	2:I:179:LEU:HD11	1.37	0.86
1:A:39:GLN:HE22	2:B:38:GLN:HE22	1.19	0.86
1:K:65:GLY:C	1:O:117:LYS:HE3	1.97	0.85
1:G:151:THR:OG1	1:G:199:ASN:HB3	1.77	0.84
2:M:31:ASN:HD21	2:M:68:GLU:H	1.26	0.84
2:P:27(C):LEU:HB2	2:P:31:ASN:ND2	1.93	0.83
1:O:71:ARG:HH11	1:O:73:THR:CG2	1.91	0.83
2:B:27(B):LEU:HD12	2:B:33:LEU:HD23	1.60	0.82
2:L:125:LEU:CD1	2:L:183:LYS:CE	2.55	0.81
1:K:98:PRO:O	1:K:99:ASP:HB2	1.79	0.81
1:O:71:ARG:NH1	1:O:73:THR:CG2	2.44	0.81
2:I:150:VAL:HB	2:I:155:GLN:NE2	1.96	0.80
1:K:65:GLY:HA2	1:O:117:LYS:HE3	1.65	0.79
2:L:125:LEU:HD11	2:L:183:LYS:NZ	1.98	0.79
2:L:145:LYS:HB3	2:L:197:THR:HB	1.65	0.78
1:K:1:GLN:HG3	1:K:2:VAL:H	1.48	0.78
2:M:27(C):LEU:HD13	2:M:31:ASN:OD1	1.85	0.77
1:O:30:THR:O	1:O:53:ARG:HD2	1.84	0.76
2:M:68:GLU:O	2:M:71:PHE:CE2	2.39	0.76
2:M:90:GLN:HE21	2:M:93:SER:H	1.34	0.76
2:L:59:PRO:CG	2:L:62:PHE:CD2	2.69	0.75
2:B:27(B):LEU:CD1	2:B:33:LEU:HD23	2.16	0.75
2:M:190:LYS:N	2:M:190:LYS:HD2	2.02	0.74
2:M:31:ASN:ND2	2:M:68:GLU:H	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:201:LEU:HD13	2:M:205:VAL:HG23	1.71	0.73
2:P:145:LYS:HB3	2:P:197:THR:CG2	2.18	0.73
2:E:90:GLN:HE21	2:E:93:SER:H	1.34	0.73
2:I:68:GLU:O	2:I:71:PHE:CE1	2.42	0.73
2:M:14:SER:HB2	2:M:17:GLU:HG3	1.71	0.73
2:E:184:ALA:O	2:E:188:LYS:HE3	1.89	0.72
2:M:68:GLU:O	2:M:71:PHE:CZ	2.42	0.72
1:K:127:SER:O	1:K:128:SER:OG	2.07	0.72
2:M:188:LYS:HB2	2:M:189:HIS:HD2	1.55	0.72
2:M:11:LEU:HD12	2:M:12:ALA:N	2.06	0.71
2:L:185:ASP:HA	2:L:188:LYS:HD3	1.73	0.70
2:B:68:GLU:HG3	2:B:69:THR:H	0.58	0.70
2:L:154:LEU:HD22	2:P:3:GLN:OE1	1.90	0.70
2:L:58:VAL:HG13	2:L:59:PRO:HD2	1.73	0.70
2:M:77:SER:O	2:M:79:GLN:NE2	2.24	0.69
2:L:59:PRO:CG	2:L:62:PHE:HD2	2.02	0.69
2:M:55:GLU:HG3	2:M:56:SER:N	2.07	0.69
2:P:152:ASN:ND2	4:P:302:HOH:O	2.25	0.69
2:P:145:LYS:HE2	2:P:197:THR:HG21	1.75	0.68
2:L:60:ASP:OD1	2:L:60:ASP:O	2.11	0.68
2:E:27(D):TYR:HB3	2:E:28:ASN:OD1	1.93	0.68
2:M:11:LEU:HD12	2:M:12:ALA:H	1.59	0.68
2:L:122:ASP:O	2:L:125:LEU:N	2.23	0.67
2:P:90:GLN:NE2	2:P:93:SER:H	1.92	0.67
1:O:30:THR:HB	1:O:53:ARG:HG2	1.75	0.66
2:P:28:ASN:O	2:P:30:LYS:N	2.28	0.66
1:D:71:ARG:NH1	4:D:301:HOH:O	2.26	0.66
2:M:28:ASN:ND2	2:M:30:LYS:HG3	2.11	0.66
2:L:150:VAL:HG22	2:L:155:GLN:NE2	2.11	0.66
1:K:136:ALA:N	1:K:184:VAL:O	2.25	0.66
1:G:163:VAL:HG22	1:G:182:VAL:HB	1.77	0.65
2:B:90:GLN:NE2	2:B:93:SER:H	1.94	0.65
2:M:188:LYS:HB2	2:M:189:HIS:CD2	2.30	0.65
1:K:203:SER:O	1:K:204:ASN:OD1	2.14	0.65
2:P:191:VAL:HG22	2:P:210:ASN:OD1	1.97	0.64
1:G:132:SER:HB3	2:L:116:PHE:HE2	1.62	0.64
1:A:117:LYS:HE2	1:D:65:GLY:HA2	1.79	0.64
1:K:71:ARG:NH2	4:K:302:HOH:O	2.31	0.64
2:E:90:GLN:NE2	2:E:93:SER:H	1.94	0.64
2:I:158:ASN:HD21	2:I:179:LEU:CD1	2.01	0.64
1:K:36:TRP:CE2	1:K:80:MET:HB2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:VAL:HG21	1:D:147:PRO:HG3	1.80	0.63
1:G:36:TRP:CE2	1:G:80:MET:HB2	2.34	0.63
3:N:239:ALA:O	3:N:240:LYS:CB	2.46	0.63
1:K:195:ILE:HG12	1:K:210:ARG:HG2	1.81	0.63
2:B:210:ASN:O	2:B:211:ARG:HB2	1.99	0.62
1:A:36:TRP:CE2	1:A:80:MET:HB2	2.35	0.62
2:M:94:THR:HG21	2:P:126:LYS:HE3	1.80	0.62
1:O:127:SER:O	1:O:128:SER:CB	2.48	0.62
1:K:65:GLY:C	1:O:117:LYS:CE	2.68	0.62
2:I:158:ASN:ND2	2:I:179:LEU:HD12	2.14	0.61
1:K:199:ASN:ND2	1:K:206:LYS:HG2	2.14	0.61
3:F:239:ALA:O	3:F:240:LYS:HD3	2.01	0.61
2:B:145:LYS:HB2	2:B:197:THR:HB	1.82	0.60
2:L:122:ASP:O	2:L:125:LEU:HB3	2.01	0.60
2:I:148:TRP:CE3	2:I:179:LEU:HD22	2.36	0.60
1:G:132:SER:HB3	2:L:116:PHE:CE2	2.35	0.60
2:L:125:LEU:CD1	2:L:183:LYS:NZ	2.65	0.60
2:B:61:ARG:CZ	2:B:79:GLN:HG3	2.31	0.60
1:D:36:TRP:CE2	1:D:80:MET:HB2	2.37	0.60
2:P:27(C):LEU:HB2	2:P:31:ASN:HD21	1.65	0.60
2:P:31:ASN:ND2	2:P:68:GLU:H	2.00	0.60
1:O:36:TRP:CE2	1:O:80:MET:HB2	2.37	0.60
2:I:188:LYS:HG2	2:I:189:HIS:N	2.17	0.59
2:I:191:VAL:HG12	2:I:210:ASN:HA	1.82	0.59
1:D:194:TYR:HD2	4:D:340:HOH:O	1.85	0.59
1:K:144:ASP:OD1	1:K:171:GLN:NE2	2.20	0.59
2:M:190:LYS:N	2:M:190:LYS:CD	2.64	0.59
2:I:90:GLN:HG2	2:I:92:PHE:H	1.68	0.59
1:D:119:PRO:HB3	1:D:145:TYR:HB3	1.84	0.59
1:K:1:GLN:CG	1:K:2:VAL:N	2.56	0.59
2:L:125:LEU:HD11	2:L:183:LYS:HZ1	1.67	0.59
1:G:119:PRO:HB3	1:G:145:TYR:HB3	1.85	0.58
1:H:195:ILE:HD11	1:H:208:ASP:HB3	1.84	0.58
2:I:151:ASP:OD1	2:I:189:HIS:HB3	2.03	0.58
1:K:185:PRO:HG2	1:K:188:SER:OG	2.03	0.58
2:B:90:GLN:OE1	2:B:97:THR:OG1	2.21	0.58
2:P:29:ASN:O	2:P:29:ASN:CG	2.42	0.58
1:K:119:PRO:HB3	1:K:145:TYR:HB3	1.86	0.57
1:G:52(A):PRO:HA	1:G:71:ARG:HD2	1.86	0.57
1:O:37:VAL:HG11	1:O:103:TRP:CZ3	2.39	0.57
2:P:103:LYS:NZ	2:P:165:GLU:OE2	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:32:TYR:CD2	2:P:50:TRP:HZ3	2.22	0.57
1:H:117:LYS:HE2	1:O:68:THR:OG1	2.04	0.57
2:L:58:VAL:CG1	2:L:59:PRO:HD2	2.33	0.57
2:M:39:LYS:HG2	2:M:84:ALA:HB2	1.86	0.57
2:B:67:SER:O	2:B:68:GLU:HG2	2.05	0.57
2:E:59:PRO:CG	2:E:61:ARG:NH1	2.67	0.57
2:I:119:PRO:HB3	2:I:209:PHE:CE1	2.39	0.57
1:D:151:THR:HG22	4:D:326:HOH:O	2.04	0.56
2:E:90:GLN:HG2	2:E:92:PHE:H	1.70	0.56
2:I:188:LYS:HG2	2:I:189:HIS:H	1.70	0.56
2:L:150:VAL:HG22	2:L:155:GLN:HE22	1.70	0.56
1:K:100(A):THR:OG1	3:N:239:ALA:HA	2.05	0.56
1:G:195:ILE:HD11	1:G:208:ASP:HB3	1.86	0.56
2:P:68:GLU:O	2:P:71:PHE:CE1	2.58	0.56
2:I:158:ASN:HD22	2:I:179:LEU:HD11	1.65	0.56
2:E:68:GLU:O	2:E:71:PHE:CE2	2.59	0.56
2:E:210:ASN:O	2:E:211:ARG:HB2	2.06	0.56
1:K:4:LEU:HD11	1:K:94:VAL:HG23	1.88	0.55
2:P:183:LYS:O	2:P:187:GLU:HG3	2.05	0.55
2:I:150:VAL:O	2:I:150:VAL:HG13	2.06	0.55
2:I:148:TRP:CD2	2:I:179:LEU:HD22	2.41	0.55
2:L:122:ASP:O	2:L:125:LEU:CB	2.55	0.55
2:I:189:HIS:O	2:I:190:LYS:O	2.24	0.55
1:O:71:ARG:NH1	1:O:73:THR:HG21	2.20	0.55
2:P:31:ASN:HD21	2:P:68:GLU:H	1.54	0.55
2:B:90:GLN:HE21	2:B:93:SER:H	1.53	0.55
1:A:131:THR:HG22	1:A:134:GLY:H	1.73	0.54
1:D:29:PHE:HB3	1:D:76:ASN:HD22	1.73	0.54
1:O:11:VAL:HG21	1:O:147:PRO:HG3	1.89	0.54
2:L:59:PRO:CG	2:L:62:PHE:CE2	2.90	0.54
1:O:52(A):PRO:O	1:O:71:ARG:HD2	2.08	0.54
2:B:2:ILE:O	2:B:97:THR:HG21	2.07	0.54
2:M:190:LYS:HD2	2:M:190:LYS:H	1.73	0.54
2:I:14:SER:HB2	2:I:17:GLU:HG3	1.90	0.54
1:G:132:SER:HB2	1:G:135:THR:O	2.08	0.54
2:I:68:GLU:O	2:I:71:PHE:CZ	2.61	0.54
2:E:59:PRO:HG3	2:E:61:ARG:NH1	2.22	0.54
1:O:119:PRO:HB3	1:O:145:TYR:HB3	1.89	0.54
1:H:65:GLY:HA2	1:K:117:LYS:HE2	1.91	0.53
3:N:236:PRO:O	3:N:237:SER:O	2.27	0.53
2:P:90:GLN:HE21	2:P:92:PHE:N	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:30:THR:O	1:O:53:ARG:CD	2.55	0.53
2:B:90:GLN:HG2	2:B:92:PHE:H	1.74	0.53
2:I:122:ASP:HA	2:I:125:LEU:CD1	2.39	0.53
2:M:90:GLN:HG2	2:M:92:PHE:H	1.73	0.53
1:H:36:TRP:CE2	1:H:80:MET:HB2	2.43	0.53
1:O:72:ASP:OD1	1:O:74:SER:OG	2.27	0.53
1:D:29:PHE:CB	1:D:76:ASN:HD22	2.21	0.52
1:D:117:LYS:NZ	4:D:304:HOH:O	2.37	0.52
2:L:125:LEU:HD12	2:L:183:LYS:CE	2.39	0.52
1:A:117:LYS:HE2	1:D:65:GLY:CA	2.40	0.52
1:D:145:TYR:CE2	1:D:150:VAL:HG23	2.44	0.52
2:P:49:TYR:HE1	2:P:55:GLU:OE1	1.92	0.52
1:O:125:ALA:O	1:O:127:SER:N	2.43	0.52
1:G:65:GLY:HA2	1:D:117:LYS:HE2	1.92	0.52
2:M:28:ASN:HD21	2:M:30:LYS:NZ	2.07	0.52
2:M:27:GLU:O	2:M:27(A):SER:CB	2.58	0.52
2:I:150:VAL:HB	2:I:155:GLN:HE21	1.74	0.51
2:P:90:GLN:HE21	2:P:92:PHE:H	1.58	0.51
1:K:11:VAL:HG21	1:K:147:PRO:HG3	1.91	0.51
1:K:98:PRO:O	1:K:99:ASP:CB	2.51	0.51
1:K:195:ILE:CD1	1:K:210:ARG:HG2	2.40	0.51
2:I:145:LYS:HB3	2:I:197:THR:HB	1.92	0.51
1:O:83:THR:HG22	1:O:85:ASP:H	1.76	0.51
2:M:27(B):LEU:HD12	2:M:33:LEU:HB2	1.92	0.51
2:P:145:LYS:HE2	2:P:197:THR:CG2	2.41	0.51
2:E:188:LYS:HE2	2:P:184:ALA:HB1	1.94	0.50
1:G:2:VAL:HG22	1:G:26:GLY:O	2.11	0.50
2:L:183:LYS:C	2:L:185:ASP:H	2.15	0.50
1:A:33:TYR:CZ	3:C:240:LYS:HD2	2.45	0.50
2:E:37:GLN:HB2	2:E:86:TYR:CE1	2.47	0.50
1:A:159:LEU:HD21	1:A:182:VAL:HG21	1.93	0.50
1:O:93:ALA:HB1	1:O:100(C):PHE:HB3	1.94	0.50
2:B:182:SER:OG	2:B:185:ASP:OD1	2.30	0.50
1:H:155:ASN:OD1	1:H:195:ILE:HG22	2.10	0.50
2:I:94:THR:HG21	2:M:126:LYS:HE3	1.93	0.50
2:I:105:GLU:OE1	2:I:142:ARG:NH2	2.44	0.50
2:M:190:LYS:CD	2:M:190:LYS:H	2.24	0.50
2:L:27(B):LEU:HD22	2:L:90:GLN:HG3	1.94	0.49
2:L:190:LYS:O	2:L:210:ASN:HA	2.12	0.49
2:P:32:TYR:CD2	2:P:50:TRP:CZ3	2.99	0.49
1:O:96:ARG:NH2	1:O:101:ASP:OD2	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:GLN:HE21	2:B:92:PHE:N	2.10	0.49
2:L:59:PRO:HG3	2:L:62:PHE:CE2	2.48	0.49
2:B:201:LEU:HD13	2:B:205:VAL:HG23	1.95	0.49
2:B:191:VAL:HG22	2:B:210:ASN:OD1	2.13	0.49
2:L:150:VAL:HG12	2:L:192:TYR:CD2	2.48	0.48
1:O:131:THR:C	1:O:133:GLY:H	2.16	0.48
2:L:190:LYS:HG3	2:L:210:ASN:HB3	1.95	0.48
1:O:37:VAL:HG11	1:O:103:TRP:HZ3	1.77	0.48
2:I:134:CYS:HB2	2:I:148:TRP:CZ2	2.48	0.48
1:O:47:TRP:CZ2	1:O:49:GLY:HA2	2.49	0.48
1:G:38:ARG:NH2	1:G:63:PHE:HZ	2.12	0.48
1:H:126:PRO:HG2	1:H:213:SER:OG	2.14	0.48
2:M:150:VAL:HG12	2:M:189:HIS:ND1	2.27	0.48
1:O:52(A):PRO:HA	1:O:71:ARG:HD3	1.95	0.48
1:D:47:TRP:CZ2	1:D:49:GLY:HA2	2.48	0.48
1:G:132:SER:HB2	1:G:136:ALA:HA	1.95	0.47
2:I:27:GLU:O	2:I:27(A):SER:HB3	2.14	0.47
1:K:184:VAL:HB	1:K:185:PRO:HD2	1.96	0.47
1:O:11:VAL:C	1:O:12:LYS:HG2	2.34	0.47
1:K:52(A):PRO:HD2	3:N:243:LEU:HD11	1.95	0.47
2:M:27:GLU:O	2:M:27(A):SER:HB3	2.15	0.47
2:M:90:GLN:NE2	2:M:93:SER:H	2.08	0.47
1:H:55:GLY:HA2	1:H:71:ARG:HD2	1.96	0.47
2:I:13:VAL:HB	2:I:78:LEU:HD22	1.97	0.47
1:G:47:TRP:CZ2	1:G:49:GLY:HA2	2.50	0.47
1:K:52(A):PRO:HA	1:K:71:ARG:HD2	1.95	0.47
1:O:127:SER:O	1:O:128:SER:HB3	2.13	0.47
1:O:197:ASN:ND2	1:O:208:ASP:OD1	2.35	0.47
2:B:195:GLU:OE2	4:B:301:HOH:O	2.20	0.46
2:I:188:LYS:O	2:I:189:HIS:HB2	2.15	0.46
1:A:127:SER:O	1:A:129:LYS:N	2.48	0.46
2:M:2:ILE:HG12	2:M:27:GLU:CG	2.35	0.46
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.97	0.46
1:O:30:THR:HB	1:O:53:ARG:CG	2.44	0.46
2:P:7:SER:CB	2:P:24:LYS:HZ1	2.28	0.46
2:I:140:TYR:CG	2:I:141:PRO:HA	2.51	0.46
2:L:119:PRO:HB3	2:L:209:PHE:CE2	2.50	0.46
1:A:47:TRP:CE3	1:A:60:PRO:HG3	2.50	0.46
1:D:139:GLY:HA2	1:D:154:TRP:CH2	2.51	0.46
2:B:23:CYS:HB2	2:B:35:TRP:CH2	2.51	0.46
1:K:24:ALA:HB1	1:K:27:TYR:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:188:LYS:CG	2:I:189:HIS:H	2.29	0.45
2:I:68:GLU:O	2:I:71:PHE:HE1	1.97	0.45
2:L:68:GLU:O	2:L:71:PHE:CE2	2.70	0.45
2:P:30:LYS:HD2	2:P:50:TRP:CH2	2.52	0.45
2:B:124:GLN:HG2	2:B:129:THR:O	2.16	0.45
2:I:54:ARG:NE	2:I:62:PHE:O	2.44	0.45
2:I:188:LYS:CG	2:I:189:HIS:N	2.78	0.45
2:M:42:GLN:HB3	2:M:43:PRO:HD2	1.98	0.45
2:M:45:LYS:HB2	2:M:45:LYS:HE2	1.61	0.45
2:I:90:GLN:HE21	2:I:90:GLN:HB3	1.58	0.45
2:M:189:HIS:CD2	2:M:189:HIS:N	2.83	0.45
1:H:168:ALA:HA	1:H:178:LEU:HB3	1.99	0.45
2:L:59:PRO:HG3	2:L:62:PHE:HE2	1.82	0.45
1:K:33:TYR:CE2	3:N:243:LEU:HD23	2.51	0.45
1:G:127:SER:O	1:G:129:LYS:N	2.49	0.45
2:P:30:LYS:HD2	2:P:50:TRP:CZ3	2.52	0.45
1:O:30:THR:O	1:O:53:ARG:CG	2.65	0.44
2:P:186:TYR:HA	2:P:192:TYR:OH	2.16	0.44
1:H:47:TRP:CZ2	1:H:49:GLY:HA2	2.52	0.44
1:O:75:ILE:HG22	1:O:75:ILE:O	2.18	0.44
2:E:55:GLU:HG3	2:E:56:SER:N	2.33	0.44
2:I:126:LYS:HB2	2:I:126:LYS:HE3	1.67	0.44
1:G:38:ARG:NH2	1:G:63:PHE:CZ	2.85	0.44
2:M:28:ASN:CG	2:M:30:LYS:HG3	2.37	0.44
2:M:94:THR:HG22	3:N:237:SER:OG	2.18	0.44
1:O:131:THR:HG22	1:O:134:GLY:H	1.83	0.44
2:L:90:GLN:HG2	2:L:92:PHE:H	1.82	0.44
1:A:119:PRO:HB3	1:A:145:TYR:HB3	2.00	0.44
2:P:202:SER:N	4:P:310:HOH:O	2.44	0.44
1:O:4:LEU:HD23	1:O:24:ALA:HA	2.00	0.44
2:B:54:ARG:NH1	4:B:307:HOH:O	2.50	0.43
2:E:27(D):TYR:O	2:E:28:ASN:OD1	2.36	0.43
2:I:150:VAL:HG12	2:I:153:ALA:O	2.18	0.43
3:N:239:ALA:C	3:N:240:LYS:CG	2.80	0.43
2:B:186:TYR:HA	2:B:192:TYR:OH	2.18	0.43
2:I:122:ASP:HA	2:I:125:LEU:HD13	2.00	0.43
1:G:117:LYS:HE2	1:A:65:GLY:HA2	2.00	0.43
2:B:126:LYS:HD3	2:E:94:THR:HG21	1.99	0.43
2:B:134:CYS:HB2	2:B:148:TRP:CH2	2.53	0.43
2:E:28:ASN:ND2	2:E:30:LYS:HB2	2.33	0.43
2:E:60:ASP:OD1	2:E:61:ARG:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:195:ILE:CG1	1:K:210:ARG:HG2	2.46	0.43
2:P:3:GLN:HB3	2:P:26:SER:HB2	1.99	0.43
2:I:210:ASN:O	2:I:211:ARG:CB	2.67	0.43
2:M:119:PRO:HB3	2:M:209:PHE:CE1	2.53	0.43
1:O:151:THR:OG1	1:O:199:ASN:HB3	2.19	0.43
2:I:66:GLY:HA3	2:I:71:PHE:HA	2.01	0.43
1:K:58:SER:OG	4:K:301:HOH:O	2.20	0.43
2:L:47:LEU:O	2:L:48:ILE:HG13	2.19	0.43
2:P:209:PHE:HD1	2:P:210:ASN:O	2.02	0.43
1:A:47:TRP:CZ3	1:A:60:PRO:HG3	2.54	0.42
2:E:199:GLN:N	4:E:306:HOH:O	2.46	0.42
2:I:188:LYS:C	2:I:189:HIS:ND1	2.73	0.42
2:P:113:PRO:HB3	2:P:139:PHE:HB3	2.01	0.42
2:L:27(B):LEU:HD12	2:L:33:LEU:HB2	2.01	0.42
2:L:27(D):TYR:HB3	2:L:28:ASN:OD1	2.19	0.42
2:L:153:ALA:O	2:L:155:GLN:NE2	2.50	0.42
1:A:60:PRO:CB	1:A:61:PRO:HD2	2.50	0.42
1:G:146:PHE:HA	1:G:147:PRO:HA	1.80	0.42
1:A:63:PHE:O	1:A:67:VAL:HG12	2.19	0.42
2:B:68:GLU:CG	2:B:69:THR:N	2.23	0.42
2:I:27:GLU:O	2:I:27(A):SER:CB	2.67	0.42
2:M:12:ALA:HA	2:M:105:GLU:O	2.19	0.42
1:G:72:ASP:OD2	1:G:75:ILE:HG12	2.19	0.42
2:L:27:GLU:O	2:L:27(A):SER:CB	2.67	0.42
2:I:151:ASP:OD1	2:I:151:ASP:N	2.52	0.42
2:I:210:ASN:OD1	2:I:210:ASN:C	2.57	0.42
1:O:3:GLN:HG3	1:O:25:SER:HB3	2.01	0.42
1:D:72:ASP:OD1	1:D:74:SER:OG	2.32	0.42
2:I:27(C):LEU:HD11	2:I:29:ASN:HD22	1.84	0.42
2:B:49:TYR:O	2:B:53:THR:HB	2.20	0.42
3:C:235:SER:HA	3:C:236:PRO:HD3	1.94	0.42
1:O:129:LYS:HE2	1:O:129:LYS:HB3	1.69	0.42
2:B:92:PHE:CE2	3:C:236:PRO:HG3	2.55	0.42
1:H:11:VAL:HG21	1:H:147:PRO:HG3	2.02	0.42
1:A:6:GLN:NE2	1:A:107:THR:OG1	2.53	0.42
2:E:68:GLU:O	2:E:71:PHE:CZ	2.73	0.42
1:O:96:ARG:CZ	1:O:102:ILE:HD11	2.50	0.42
1:K:201:LYS:HA	1:K:201:LYS:HD2	1.91	0.42
2:M:31:ASN:ND2	2:M:68:GLU:N	2.62	0.42
2:P:210:ASN:O	2:P:211:ARG:HB2	2.20	0.41
1:O:52(A):PRO:O	1:O:71:ARG:CD	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:54:ARG:HD3	2:P:62:PHE:O	2.19	0.41
2:B:24:LYS:HB3	2:B:24:LYS:HE2	1.82	0.41
1:H:4:LEU:HB3	1:H:22:CYS:SG	2.60	0.41
1:G:168:ALA:HA	1:G:178:LEU:HB3	2.02	0.41
1:D:129:LYS:O	1:D:130:SER:HB3	2.21	0.41
2:M:150:VAL:HG13	2:M:192:TYR:CE2	2.55	0.41
2:P:27(C):LEU:HD11	2:P:29:ASN:HA	2.02	0.41
1:G:11:VAL:HG21	1:G:147:PRO:HG3	2.02	0.41
1:H:33:TYR:CE2	3:J:243:LEU:HD23	2.56	0.41
3:N:235:SER:HA	3:N:236:PRO:HD3	1.91	0.41
1:G:134:GLY:O	1:G:186:SER:OG	2.36	0.41
2:B:90:GLN:HE21	2:B:92:PHE:H	1.69	0.41
2:B:123:GLU:OE1	2:B:123:GLU:N	2.51	0.41
3:R:239:ALA:O	3:R:240:LYS:HD3	2.21	0.41
1:H:163:VAL:HG22	1:H:182:VAL:HB	2.03	0.41
1:K:93:ALA:HB1	1:K:100(C):PHE:HB3	2.03	0.41
1:G:27:TYR:OH	1:G:94:VAL:HG21	2.20	0.41
2:L:14:SER:HB2	2:L:17:GLU:HG3	2.03	0.41
2:L:125:LEU:HD12	2:L:183:LYS:HD2	2.02	0.41
2:B:27:GLU:O	2:B:27(A):SER:HB3	2.21	0.41
2:I:55:GLU:HA	2:I:55:GLU:OE2	2.20	0.41
1:K:201:LYS:NZ	4:K:306:HOH:O	2.50	0.41
3:N:242:ARG:HE	3:N:242:ARG:HB3	1.63	0.41
2:B:27(D):TYR:HB3	2:B:28:ASN:OD1	2.21	0.41
2:E:90:GLN:NE2	2:E:93:SER:O	2.53	0.41
2:P:66:GLY:HA3	2:P:71:PHE:HA	2.03	0.41
2:B:140:TYR:CG	2:B:141:PRO:HA	2.57	0.40
2:E:107:LYS:HA	2:E:140:TYR:OH	2.21	0.40
2:I:61:ARG:O	2:I:75:ILE:HA	2.20	0.40
1:A:24:ALA:HB1	1:A:27:TYR:CE1	2.56	0.40
2:B:2:ILE:N	4:B:310:HOH:O	2.53	0.40
1:D:2:VAL:HG22	1:D:26:GLY:O	2.22	0.40
1:H:123:PRO:HD3	1:H:209:LYS:HE2	2.03	0.40
2:P:92:PHE:C	2:P:92:PHE:CD1	2.94	0.40
1:K:100(A):THR:HG21	2:M:96:TRP:CE2	2.57	0.40
2:L:27:GLU:O	4:L:301:HOH:O	2.21	0.40
2:M:33:LEU:HD22	2:M:71:PHE:CG	2.56	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	218/226 (96%)	207 (95%)	10 (5%)	1 (0%)	29	52
1	D	217/226 (96%)	208 (96%)	7 (3%)	2 (1%)	17	35
1	G	218/226 (96%)	207 (95%)	9 (4%)	2 (1%)	17	35
1	H	217/226 (96%)	204 (94%)	11 (5%)	2 (1%)	17	35
1	K	218/226 (96%)	206 (94%)	11 (5%)	1 (0%)	29	52
1	O	218/226 (96%)	206 (94%)	8 (4%)	4 (2%)	8	16
2	B	215/220 (98%)	206 (96%)	6 (3%)	3 (1%)	11	22
2	E	216/220 (98%)	207 (96%)	8 (4%)	1 (0%)	29	52
2	I	215/220 (98%)	202 (94%)	8 (4%)	5 (2%)	6	11
2	L	215/220 (98%)	205 (95%)	8 (4%)	2 (1%)	17	35
2	M	215/220 (98%)	209 (97%)	5 (2%)	1 (0%)	29	52
2	P	215/220 (98%)	204 (95%)	8 (4%)	3 (1%)	11	22
3	C	6/9 (67%)	4 (67%)	2 (33%)	0	100	100
3	F	6/9 (67%)	3 (50%)	2 (33%)	1 (17%)	0	0
3	J	6/9 (67%)	4 (67%)	2 (33%)	0	100	100
3	N	6/9 (67%)	2 (33%)	2 (33%)	2 (33%)	0	0
3	Q	6/9 (67%)	4 (67%)	2 (33%)	0	100	100
3	R	6/9 (67%)	5 (83%)	1 (17%)	0	100	100
All	All	2633/2730 (96%)	2493 (95%)	110 (4%)	30 (1%)	14	30

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	27(A)	SER
2	B	27(A)	SER
2	E	27(A)	SER
1	H	128	SER

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Mol	Chain	Res	Type
1	H	189	LEU
2	I	27(A)	SER
2	I	185	ASP
2	I	190	LYS
1	K	130	SER
2	M	27(A)	SER
3	N	237	SER
3	N	240	LYS
1	O	128	SER
1	O	130	SER
2	P	27(A)	SER
2	P	28	ASN
1	G	128	SER
1	G	131	THR
2	L	185	ASP
1	A	128	SER
2	B	211	ARG
1	D	130	SER
1	O	132	SER
2	B	68	GLU
3	F	239	ALA
2	I	28	ASN
2	I	189	HIS
1	O	126	PRO
2	P	29	ASN
1	D	126	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/190 (97%)	182 (99%)	2 (1%)	73	88
1	D	183/190 (96%)	183 (100%)	0	100	100
1	G	184/190 (97%)	184 (100%)	0	100	100
1	H	183/190 (96%)	181 (99%)	2 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	184/190 (97%)	182 (99%)	2 (1%)	73	88
1	O	184/190 (97%)	183 (100%)	1 (0%)	88	96
2	B	193/196 (98%)	190 (98%)	3 (2%)	62	82
2	E	194/196 (99%)	194 (100%)	0	100	100
2	I	194/196 (99%)	189 (97%)	5 (3%)	46	72
2	L	194/196 (99%)	189 (97%)	5 (3%)	46	72
2	M	194/196 (99%)	193 (100%)	1 (0%)	88	96
2	P	194/196 (99%)	192 (99%)	2 (1%)	76	90
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	7 (100%)	0	100	100
3	J	7/7 (100%)	7 (100%)	0	100	100
3	N	7/7 (100%)	6 (86%)	1 (14%)	3	5
3	Q	7/7 (100%)	7 (100%)	0	100	100
3	R	7/7 (100%)	7 (100%)	0	100	100
All	All	2307/2358 (98%)	2283 (99%)	24 (1%)	76	90

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	90	GLN
2	L	142	ARG
2	L	185	ASP
2	L	190	LYS
2	L	210	ASN
1	A	71	ARG
1	A	199	ASN
2	B	3	GLN
2	B	68	GLU
2	B	211	ARG
1	H	117	LYS
1	H	208	ASP
2	I	28	ASN
2	I	90	GLN
2	I	151	ASP
2	I	154	LEU
2	I	185	ASP
1	K	130	SER

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Mol	Chain	Res	Type
1	K	197	ASN
2	M	30	LYS
3	N	237	SER
1	O	209	LYS
2	P	45	LYS
2	P	92	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	42	GLN
2	L	199	GLN
2	L	210	ASN
1	A	199	ASN
2	B	38	GLN
1	D	43	GLN
1	D	76	ASN
2	E	42	GLN
2	E	90	GLN
2	E	210	ASN
2	I	29	ASN
2	I	42	GLN
2	I	90	GLN
2	I	158	ASN
1	K	39	GLN
1	K	164	HIS
1	K	199	ASN
2	M	28	ASN
2	M	31	ASN
2	M	42	GLN
2	M	90	GLN
2	M	189	HIS
2	M	199	GLN
2	P	31	ASN
2	P	90	GLN
2	P	199	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
3	SEP	R	238	3	8,9,10	0.76	0	8,12,14	1.15	0
3	SEP	N	238	3	8,9,10	0.78	0	8,12,14	1.15	0
3	SEP	Q	238	3	8,9,10	0.76	0	8,12,14	1.14	0
3	SEP	C	238	3	8,9,10	0.80	0	8,12,14	1.14	0
3	SEP	J	238	3	8,9,10	0.77	0	8,12,14	1.14	0
3	SEP	F	238	3	8,9,10	0.77	0	8,12,14	1.14	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
3	SEP	R	238	3	-	4/5/8/10	-
3	SEP	N	238	3	-	3/5/8/10	-
3	SEP	Q	238	3	-	4/5/8/10	-
3	SEP	C	238	3	-	4/5/8/10	-
3	SEP	J	238	3	-	4/5/8/10	-
3	SEP	F	238	3	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	238	SEP	N-CA-CB-OG
3	R	238	SEP	CB-OG-P-O1P
3	R	238	SEP	CB-OG-P-O2P

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Mol	Chain	Res	Type	Atoms
3	R	238	SEP	CB-OG-P-O3P
3	C	238	SEP	N-CA-CB-OG
3	C	238	SEP	CB-OG-P-O1P
3	C	238	SEP	CB-OG-P-O2P
3	C	238	SEP	CB-OG-P-O3P
3	J	238	SEP	N-CA-CB-OG
3	J	238	SEP	CB-OG-P-O1P
3	J	238	SEP	CB-OG-P-O2P
3	J	238	SEP	CB-OG-P-O3P
3	N	238	SEP	N-CA-CB-OG
3	Q	238	SEP	N-CA-CB-OG
3	Q	238	SEP	CB-OG-P-O2P
3	Q	238	SEP	CB-OG-P-O3P
3	N	238	SEP	CB-OG-P-O1P
3	Q	238	SEP	CB-OG-P-O1P
3	F	238	SEP	N-CA-CB-OG
3	N	238	SEP	CB-OG-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 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	220/226 (97%)	-0.44	5 (2%) 60 54	16, 29, 56, 98	0
1	D	219/226 (96%)	-0.44	6 (2%) 54 48	14, 26, 52, 100	0
1	G	220/226 (97%)	-0.42	7 (3%) 47 40	17, 31, 61, 92	0
1	H	219/226 (96%)	-0.25	7 (3%) 47 40	16, 32, 83, 95	0
1	K	220/226 (97%)	-0.38	8 (3%) 42 35	20, 30, 60, 107	0
1	O	220/226 (97%)	-0.25	10 (4%) 33 26	20, 34, 61, 103	0
2	B	217/220 (98%)	-0.43	0 100 100	21, 33, 48, 61	0
2	E	218/220 (99%)	-0.51	0 100 100	17, 29, 46, 59	0
2	I	217/220 (98%)	-0.28	4 (1%) 68 64	16, 36, 82, 99	0
2	L	217/220 (98%)	-0.41	3 (1%) 75 71	17, 32, 61, 74	0
2	M	217/220 (98%)	-0.32	0 100 100	21, 35, 52, 77	0
2	P	217/220 (98%)	-0.37	3 (1%) 75 71	21, 33, 60, 81	0
3	C	8/9 (88%)	-0.42	0 100 100	30, 38, 43, 50	0
3	F	8/9 (88%)	-0.24	0 100 100	17, 24, 29, 34	0
3	J	8/9 (88%)	-0.34	0 100 100	22, 24, 31, 41	0
3	N	8/9 (88%)	0.38	1 (12%) 3 2	31, 38, 49, 52	0
3	Q	8/9 (88%)	0.18	0 100 100	44, 51, 62, 66	0
3	R	8/9 (88%)	-0.56	0 100 100	22, 24, 29, 42	0
All	All	2669/2730 (97%)	-0.37	54 (2%) 65 60	14, 32, 61, 107	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	THR	8.1
1	K	128	SER	7.3
1	D	130	SER	7.2

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Mol	Chain	Res	Type	RSRZ
1	D	131	THR	6.6
1	H	131	THR	6.6
1	G	131	THR	6.5
1	G	130	SER	6.3
1	H	130	SER	6.2
1	O	131	THR	5.9
1	O	129	LYS	5.7
1	A	130	SER	5.5
2	I	210	ASN	5.3
1	D	132	SER	5.3
1	K	133	GLY	5.1
3	N	239	ALA	5.1
1	A	128	SER	4.8
2	I	190	LYS	4.6
1	O	133	GLY	4.5
1	D	128	SER	4.5
1	D	133	GLY	4.0
1	O	130	SER	4.0
1	K	132	SER	3.9
1	K	191	THR	3.6
1	O	127	SER	3.6
1	K	131	THR	3.5
1	O	132	SER	3.3
1	K	129	LYS	3.3
1	G	128	SER	3.2
1	O	1	GLN	3.2
1	G	132	SER	3.2
2	L	184	ALA	3.2
1	H	184	VAL	3.1
1	A	127	SER	3.1
1	K	127	SER	3.0
2	P	27(D)	TYR	2.9
1	H	189	LEU	2.9
1	D	129	LYS	2.8
1	H	157	GLY	2.8
1	G	129	LYS	2.7
1	O	128	SER	2.7
1	K	130	SER	2.7
1	H	132	SER	2.5
2	L	1	ASP	2.5
2	I	184	ALA	2.5
2	I	1	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	P	27(E)	ASP	2.4
1	O	210	ARG	2.4
2	P	28	ASN	2.4
1	O	75	ILE	2.3
1	H	128	SER	2.3
1	G	1	GLN	2.3
1	G	133	GLY	2.2
1	A	132	SER	2.1
2	L	125	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
3	SEP	F	238	10/11	0.84	0.19	23,29,59,72	0
3	SEP	C	238	10/11	0.86	0.20	39,46,66,72	0
3	SEP	N	238	10/11	0.86	0.17	44,55,85,86	0
3	SEP	Q	238	10/11	0.88	0.13	48,59,76,92	0
3	SEP	R	238	10/11	0.90	0.13	26,33,50,66	0
3	SEP	J	238	10/11	0.93	0.12	26,31,50,65	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.