



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:58 AM UTC

PDB ID : 1YAR / pdb_00001yar
Title : Structure of Archeobacterial 20S proteasome mutant D9S- PA26 complex
Authors : Forster, A.; Masters, E.I.; Whitby, F.G.; Robinson, H.; Hill, C.P.
Deposited on : 2004-12-17
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 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

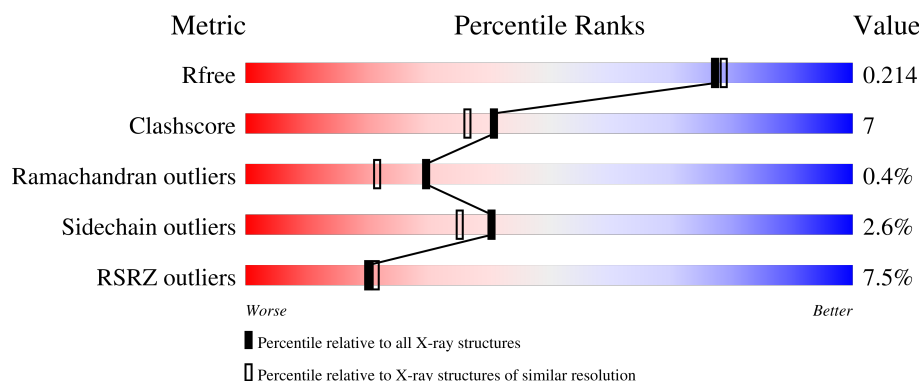
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	233	9% 80% 13% • 5%
1	B	233	12% 85% 9% • 5%
1	C	233	11% 82% 12% 5%
1	D	233	12% 83% 11% 5%
1	E	233	7% 83% 11% • 5%

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Mol	Chain	Length	Quality of chain
1	F	233	
1	G	233	
2	H	217	
2	I	217	
2	J	217	
2	K	217	
2	L	217	
2	M	217	
2	N	217	
3	O	237	
3	P	237	
3	Q	237	
3	R	237	
3	S	237	
3	T	237	
3	U	237	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	G	4007	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 39593 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 Proteasome alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	7	0
			1777	1127	302	345	3			
1	B	221	Total	C	N	O	S	0	7	0
			1777	1127	302	345	3			
1	C	221	Total	C	N	O	S	0	6	0
			1771	1124	301	343	3			
1	D	221	Total	C	N	O	S	0	7	0
			1777	1127	302	345	3			
1	E	221	Total	C	N	O	S	0	6	0
			1771	1124	301	343	3			
1	F	221	Total	C	N	O	S	0	6	0
			1771	1124	301	343	3			
1	G	221	Total	C	N	O	S	0	6	0
			1771	1124	301	343	3			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	SER	ASP	engineered mutation	UNP P25156
B	9	SER	ASP	engineered mutation	UNP P25156
C	9	SER	ASP	engineered mutation	UNP P25156
D	9	SER	ASP	engineered mutation	UNP P25156
E	9	SER	ASP	engineered mutation	UNP P25156
F	9	SER	ASP	engineered mutation	UNP P25156
G	9	SER	ASP	engineered mutation	UNP P25156

- Molecule 2 is a protein called Proteasome beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	203	Total	C	N	O	S	0	7	0
			1613	1019	271	311	12			
2	I	203	Total	C	N	O	S	0	7	0
			1613	1019	271	311	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	203	Total	C	N	O	S	0	7	0
			1613	1019	271	311	12			
2	K	203	Total	C	N	O	S	0	7	0
			1613	1019	271	311	12			
2	L	203	Total	C	N	O	S	0	7	0
			1613	1019	271	311	12			
2	M	203	Total	C	N	O	S	0	7	0
			1613	1019	271	311	12			
2	N	203	Total	C	N	O	S	0	7	0
			1613	1019	271	311	12			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	204	HIS	-	expression tag	UNP P28061
H	205	HIS	-	expression tag	UNP P28061
H	206	HIS	-	expression tag	UNP P28061
H	207	HIS	-	expression tag	UNP P28061
H	208	HIS	-	expression tag	UNP P28061
H	209	HIS	-	expression tag	UNP P28061
I	204	HIS	-	expression tag	UNP P28061
I	205	HIS	-	expression tag	UNP P28061
I	206	HIS	-	expression tag	UNP P28061
I	207	HIS	-	expression tag	UNP P28061
I	208	HIS	-	expression tag	UNP P28061
I	209	HIS	-	expression tag	UNP P28061
J	204	HIS	-	expression tag	UNP P28061
J	205	HIS	-	expression tag	UNP P28061
J	206	HIS	-	expression tag	UNP P28061
J	207	HIS	-	expression tag	UNP P28061
J	208	HIS	-	expression tag	UNP P28061
J	209	HIS	-	expression tag	UNP P28061
K	204	HIS	-	expression tag	UNP P28061
K	205	HIS	-	expression tag	UNP P28061
K	206	HIS	-	expression tag	UNP P28061
K	207	HIS	-	expression tag	UNP P28061
K	208	HIS	-	expression tag	UNP P28061
K	209	HIS	-	expression tag	UNP P28061
L	204	HIS	-	expression tag	UNP P28061
L	205	HIS	-	expression tag	UNP P28061
L	206	HIS	-	expression tag	UNP P28061
L	207	HIS	-	expression tag	UNP P28061
L	208	HIS	-	expression tag	UNP P28061

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Chain	Residue	Modelled	Actual	Comment	Reference
L	209	HIS	-	expression tag	UNP P28061
M	204	HIS	-	expression tag	UNP P28061
M	205	HIS	-	expression tag	UNP P28061
M	206	HIS	-	expression tag	UNP P28061
M	207	HIS	-	expression tag	UNP P28061
M	208	HIS	-	expression tag	UNP P28061
M	209	HIS	-	expression tag	UNP P28061
N	204	HIS	-	expression tag	UNP P28061
N	205	HIS	-	expression tag	UNP P28061
N	206	HIS	-	expression tag	UNP P28061
N	207	HIS	-	expression tag	UNP P28061
N	208	HIS	-	expression tag	UNP P28061
N	209	HIS	-	expression tag	UNP P28061

- Molecule 3 is a protein called proteasome activator protein PA26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	218	Total	C	N	O	S	0	10	0
			1754	1094	309	343	8			
3	P	218	Total	C	N	O	S	0	10	0
			1754	1094	309	343	8			
3	Q	218	Total	C	N	O	S	0	10	0
			1754	1094	309	343	8			
3	R	218	Total	C	N	O	S	0	10	0
			1754	1094	309	343	8			
3	S	218	Total	C	N	O	S	0	10	0
			1754	1094	309	343	8			
3	T	218	Total	C	N	O	S	0	9	0
			1746	1089	308	342	7			
3	U	218	Total	C	N	O	S	0	10	0
			1754	1094	309	343	8			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	MET	-	initiating methionine	GB 5757773
O	-4	HIS	-	expression tag	GB 5757773
O	-3	HIS	-	expression tag	GB 5757773
O	-2	HIS	-	expression tag	GB 5757773
O	-1	HIS	-	expression tag	GB 5757773
O	0	HIS	-	expression tag	GB 5757773
O	1	HIS	-	expression tag	GB 5757773

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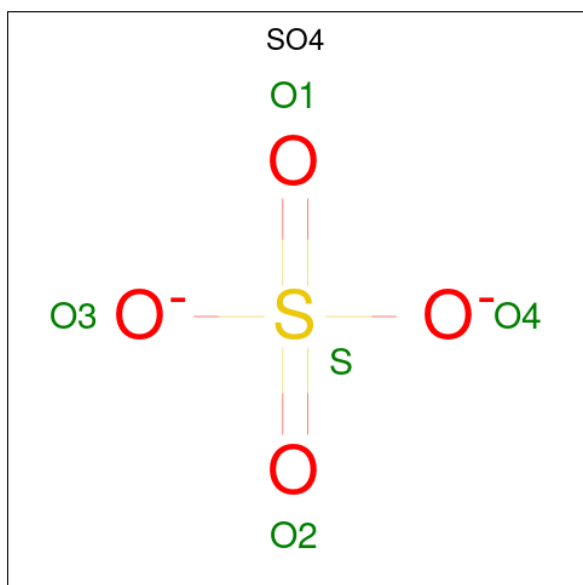
Chain	Residue	Modelled	Actual	Comment	Reference
O	49	VAL	THR	variant	GB 5757773
P	-5	MET	-	initiating methionine	GB 5757773
P	-4	HIS	-	expression tag	GB 5757773
P	-3	HIS	-	expression tag	GB 5757773
P	-2	HIS	-	expression tag	GB 5757773
P	-1	HIS	-	expression tag	GB 5757773
P	0	HIS	-	expression tag	GB 5757773
P	1	HIS	-	expression tag	GB 5757773
P	49	VAL	THR	variant	GB 5757773
Q	-5	MET	-	initiating methionine	GB 5757773
Q	-4	HIS	-	expression tag	GB 5757773
Q	-3	HIS	-	expression tag	GB 5757773
Q	-2	HIS	-	expression tag	GB 5757773
Q	-1	HIS	-	expression tag	GB 5757773
Q	0	HIS	-	expression tag	GB 5757773
Q	1	HIS	-	expression tag	GB 5757773
Q	49	VAL	THR	variant	GB 5757773
R	-5	MET	-	initiating methionine	GB 5757773
R	-4	HIS	-	expression tag	GB 5757773
R	-3	HIS	-	expression tag	GB 5757773
R	-2	HIS	-	expression tag	GB 5757773
R	-1	HIS	-	expression tag	GB 5757773
R	0	HIS	-	expression tag	GB 5757773
R	1	HIS	-	expression tag	GB 5757773
R	49	VAL	THR	variant	GB 5757773
S	-5	MET	-	initiating methionine	GB 5757773
S	-4	HIS	-	expression tag	GB 5757773
S	-3	HIS	-	expression tag	GB 5757773
S	-2	HIS	-	expression tag	GB 5757773
S	-1	HIS	-	expression tag	GB 5757773
S	0	HIS	-	expression tag	GB 5757773
S	1	HIS	-	expression tag	GB 5757773
S	49	VAL	THR	variant	GB 5757773
T	-5	MET	-	initiating methionine	GB 5757773
T	-4	HIS	-	expression tag	GB 5757773
T	-3	HIS	-	expression tag	GB 5757773
T	-2	HIS	-	expression tag	GB 5757773
T	-1	HIS	-	expression tag	GB 5757773
T	0	HIS	-	expression tag	GB 5757773
T	1	HIS	-	expression tag	GB 5757773
T	49	VAL	THR	variant	GB 5757773
U	-5	MET	-	initiating methionine	GB 5757773

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Chain	Residue	Modelled	Actual	Comment	Reference
U	-4	HIS	-	expression tag	GB 5757773
U	-3	HIS	-	expression tag	GB 5757773
U	-2	HIS	-	expression tag	GB 5757773
U	-1	HIS	-	expression tag	GB 5757773
U	0	HIS	-	expression tag	GB 5757773
U	1	HIS	-	expression tag	GB 5757773
U	49	VAL	THR	variant	GB 5757773

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



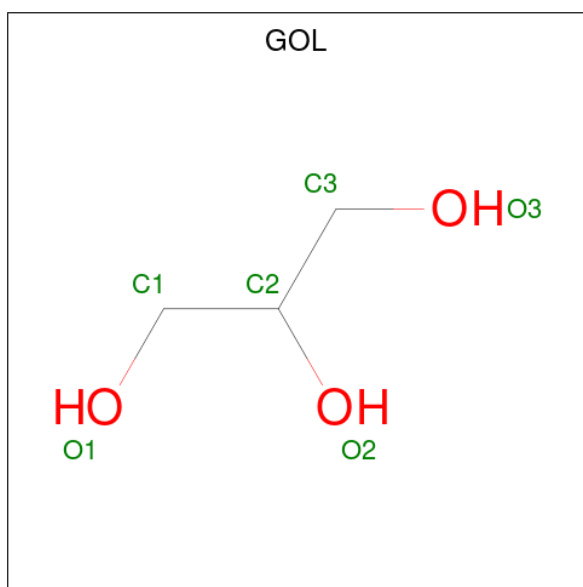
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	N	1	Total	O	S	0	0
			5	4	1		
4	N	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		
5	M	1	Total	C	O	0	0
			6	3	3		
5	N	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	153	Total	O	0	0
			153	153		
6	B	145	Total	O	0	0
			145	145		
6	C	128	Total	O	0	0
			128	128		
6	D	130	Total	O	0	0
			130	130		
6	E	153	Total	O	0	0
			153	153		

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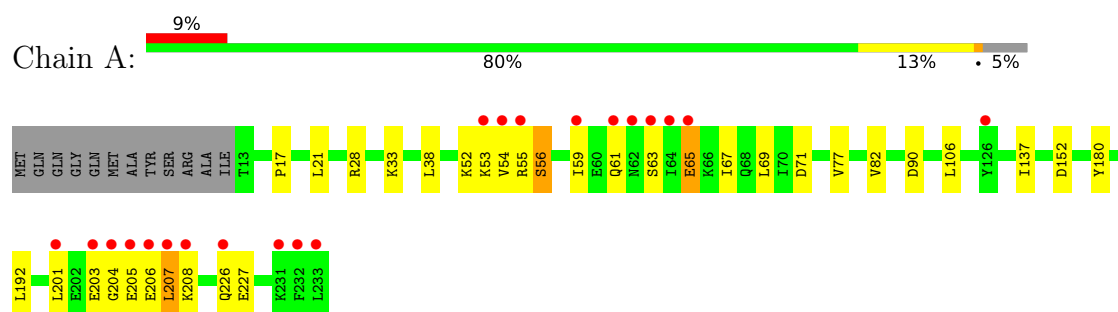
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	122	Total 122	O 122	0	0
6	G	133	Total 133	O 133	0	0
6	H	165	Total 165	O 165	0	0
6	I	165	Total 165	O 165	0	0
6	J	159	Total 159	O 159	0	0
6	K	177	Total 177	O 177	0	0
6	L	153	Total 153	O 153	0	0
6	M	180	Total 180	O 180	0	0
6	N	179	Total 179	O 179	0	0
6	O	178	Total 178	O 178	0	0
6	P	162	Total 162	O 162	0	0
6	Q	161	Total 161	O 161	0	0
6	R	189	Total 189	O 189	0	0
6	S	221	Total 221	O 221	0	0
6	T	207	Total 207	O 207	0	0
6	U	210	Total 210	O 210	0	0

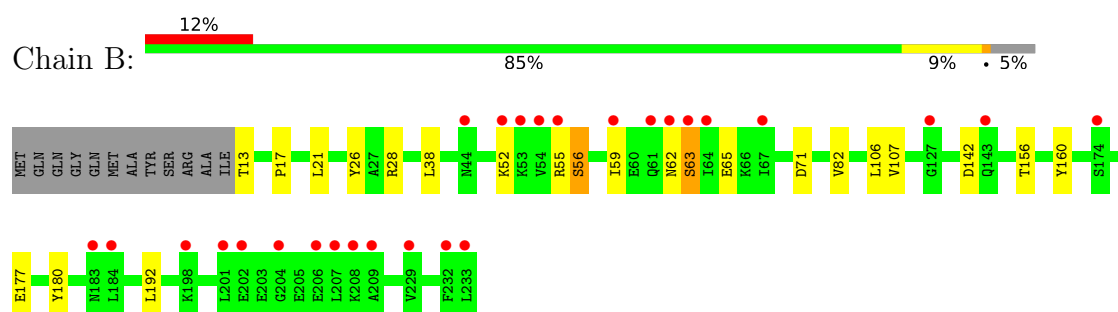
3 Residue-property plots [i](#)

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

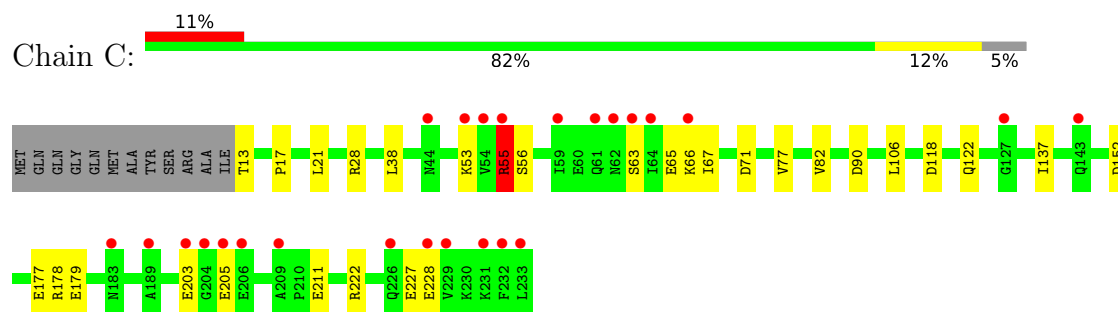
- Molecule 1: Proteasome alpha subunit



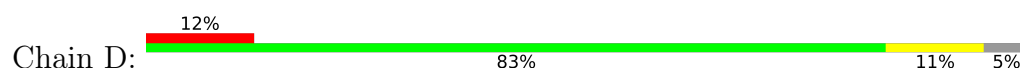
- Molecule 1: Proteasome alpha subunit

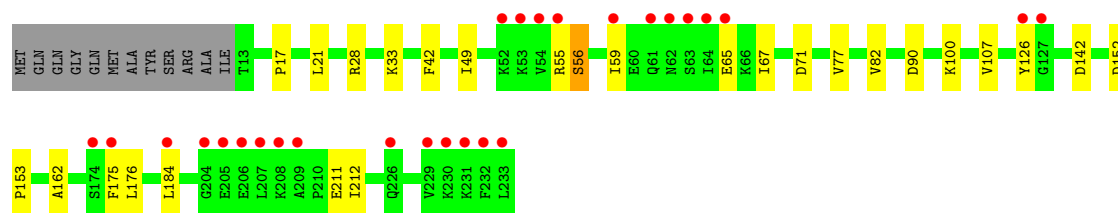


- Molecule 1: Proteasome alpha subunit

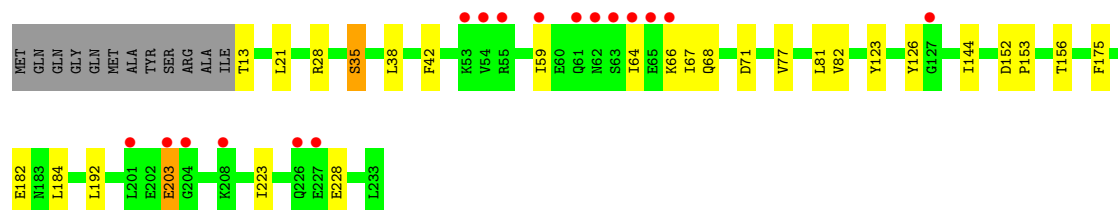
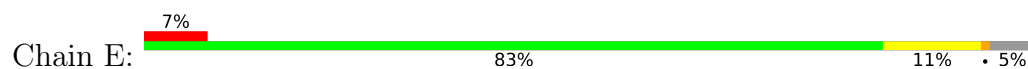


- Molecule 1: Proteasome alpha subunit

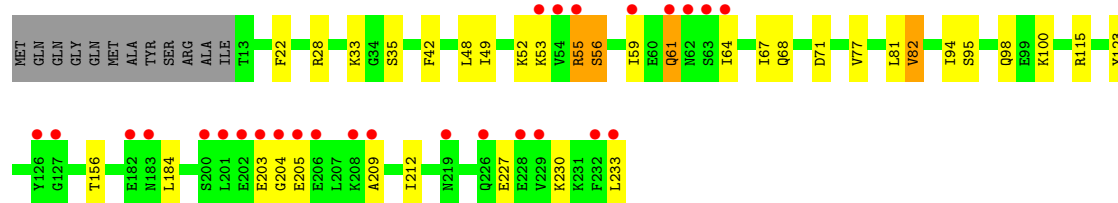
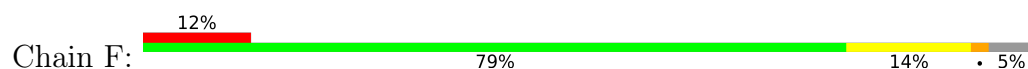




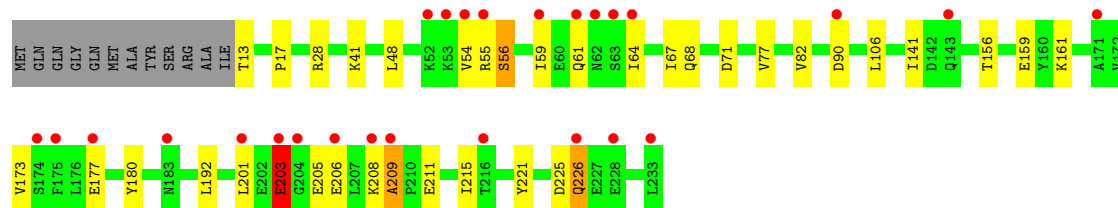
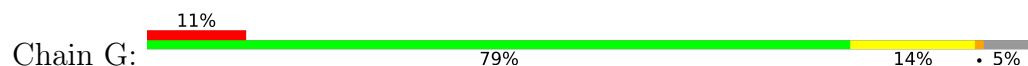
• Molecule 1: Proteasome alpha subunit



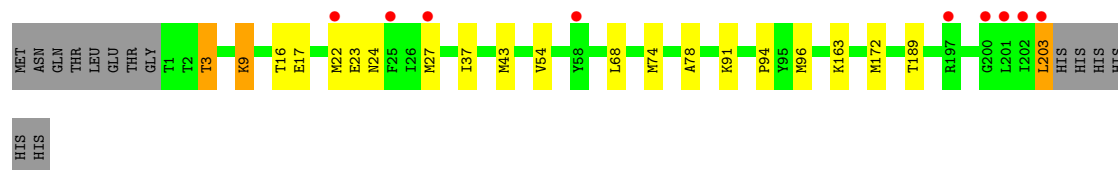
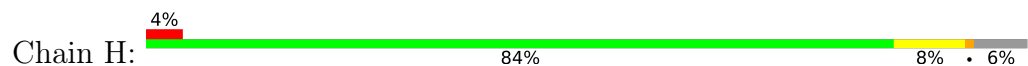
• Molecule 1: Proteasome alpha subunit



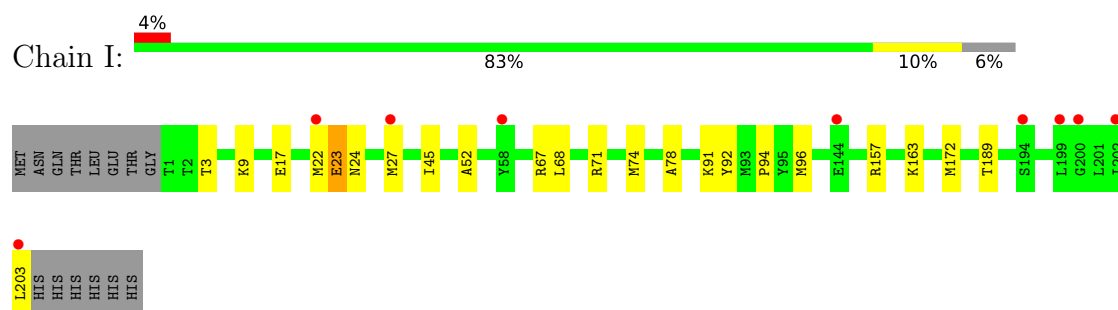
• Molecule 1: Proteasome alpha subunit



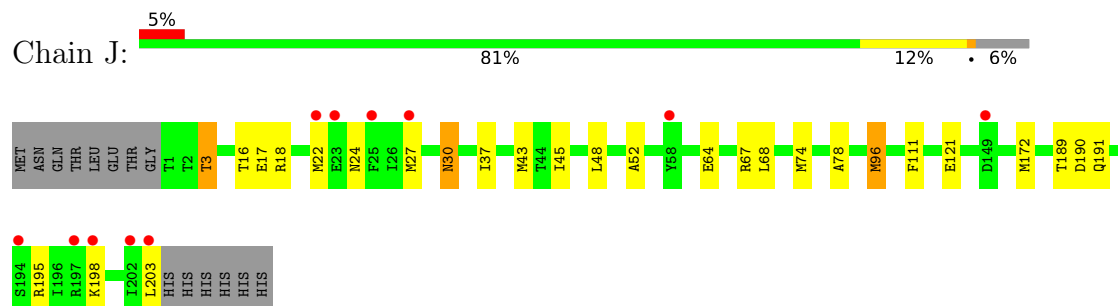
• Molecule 2: Proteasome beta subunit



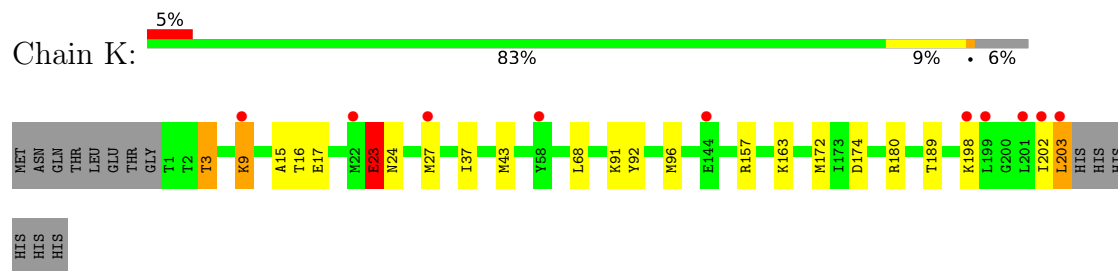
• Molecule 2: Proteasome beta subunit



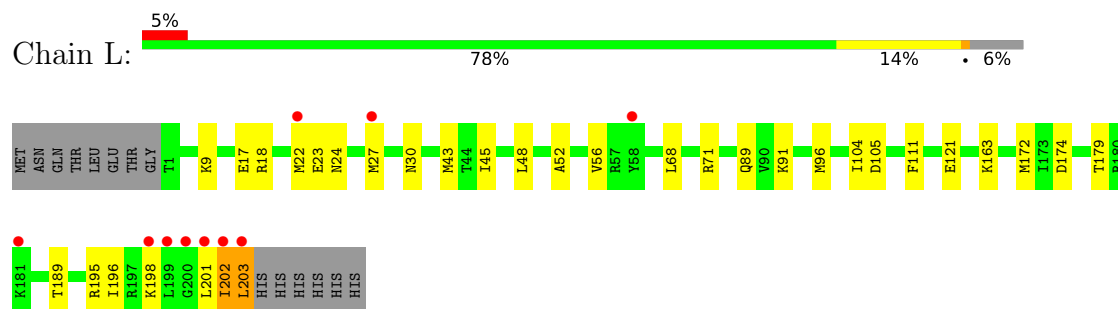
- Molecule 2: Proteasome beta subunit



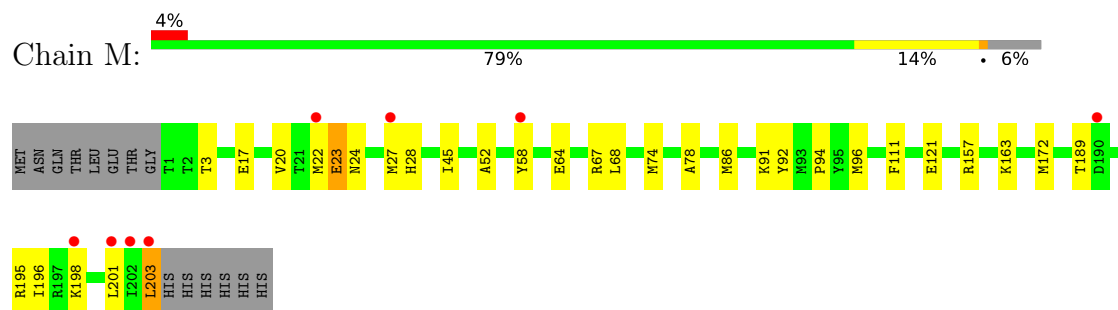
- Molecule 2: Proteasome beta subunit



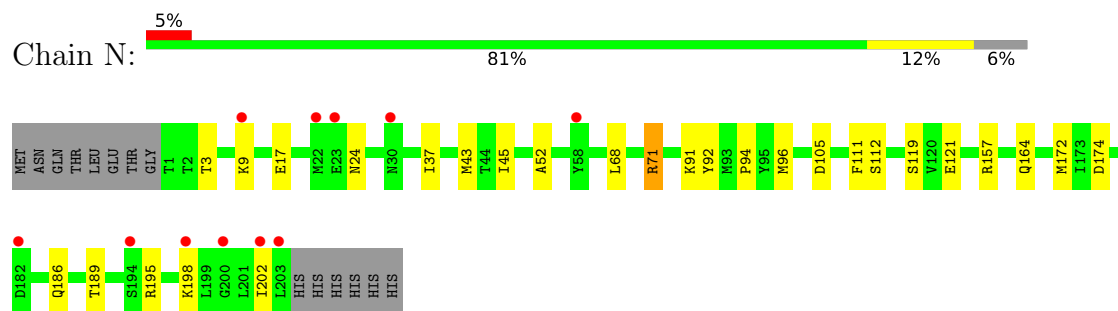
- Molecule 2: Proteasome beta subunit



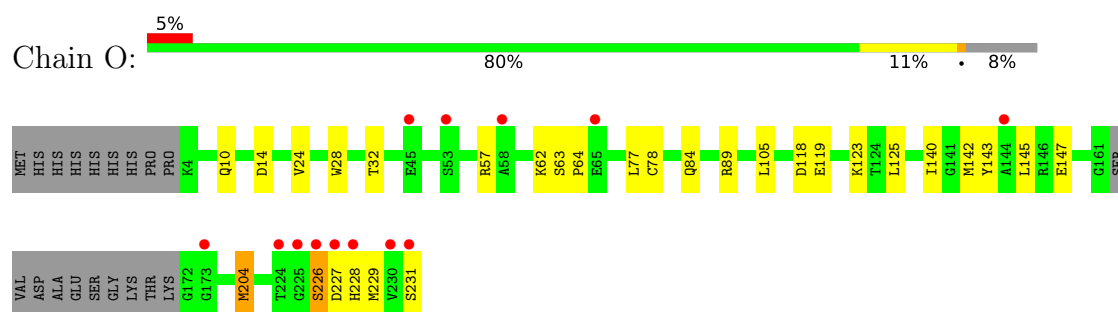
- Molecule 2: Proteasome beta subunit



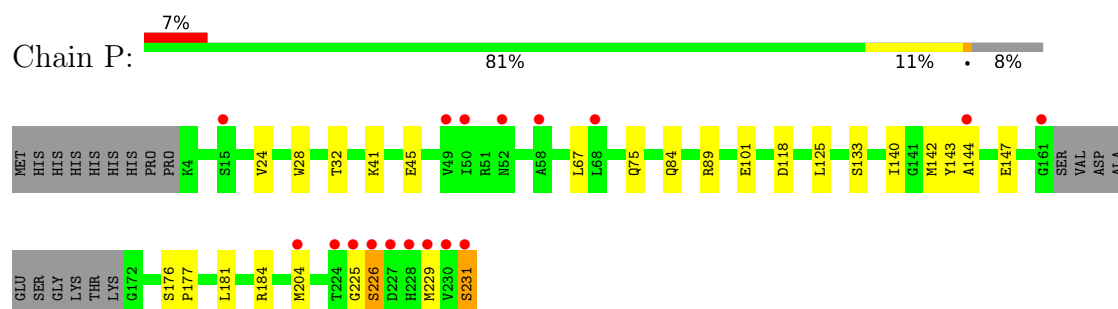
- Molecule 2: Proteasome beta subunit



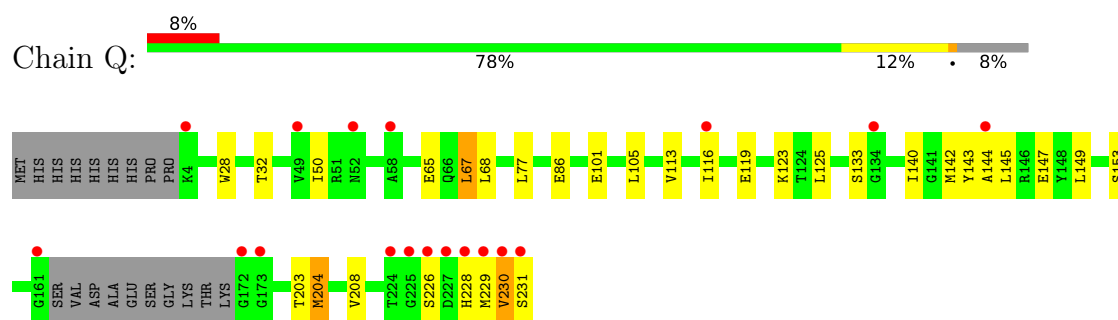
- Molecule 3: proteasome activator protein PA26



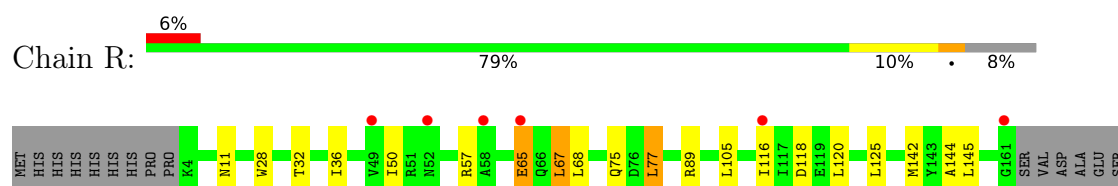
- Molecule 3: proteasome activator protein PA26



- Molecule 3: proteasome activator protein PA26

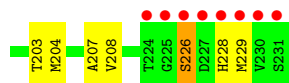
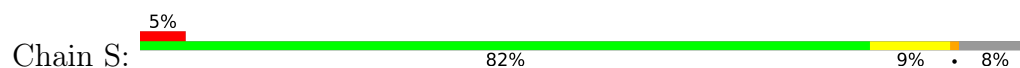


- Molecule 3: proteasome activator protein PA26

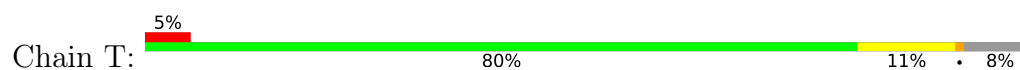




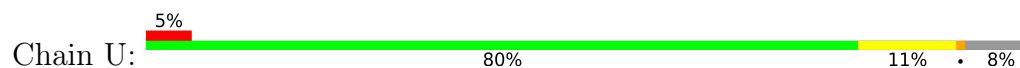
- Molecule 3: proteasome activator protein PA26



- Molecule 3: proteasome activator protein PA26



- Molecule 3: proteasome activator protein PA26



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	254.87Å 127.51Å 181.18Å 90.00° 92.45° 90.00°	Depositor
Resolution (Å)	47.30 – 1.90 47.30 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (47.30-1.90) 97.3 (47.30-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.182 , 0.216 0.182 , 0.214	Depositor DCC
R_{free} test set	1345 reflections (0.30%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.002 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	39593	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, GOL

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	0/1800	0.89	3/2425 (0.1%)
1	B	0.67	0/1800	0.86	0/2425
1	C	0.68	0/1794	0.83	0/2417
1	D	0.67	0/1800	0.85	0/2425
1	E	0.70	0/1794	0.86	0/2417
1	F	0.66	0/1794	0.83	1/2417 (0.0%)
1	G	0.67	0/1794	0.83	0/2417
2	H	0.77	0/1633	0.88	0/2206
2	I	0.75	0/1633	0.90	1/2206 (0.0%)
2	J	0.73	0/1633	0.87	0/2206
2	K	0.73	0/1633	0.89	1/2206 (0.0%)
2	L	0.74	1/1633 (0.1%)	0.88	0/2206
2	M	0.78	0/1633	0.92	0/2206
2	N	0.74	1/1633 (0.1%)	0.88	0/2206
3	O	0.63	0/1777	0.82	0/2398
3	P	0.62	0/1777	0.83	0/2398
3	Q	0.61	0/1777	0.83	0/2398
3	R	0.67	0/1777	0.84	0/2398
3	S	0.73	0/1777	0.85	0/2398
3	T	0.73	0/1769	0.83	0/2388
3	U	0.71	0/1777	0.84	0/2398
All	All	0.70	2/36438 (0.0%)	0.86	6/49161 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	105	ASP	CA-C	5.76	1.55	1.52
2	L	105	ASP	CA-C	5.04	1.54	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	GLU	N-CA-C	-7.53	99.38	110.52
2	K	23	GLU	CB-CA-C	-6.29	109.33	116.63
2	I	23	GLU	CB-CA-C	-5.78	109.93	116.63
1	A	206	GLU	CA-C-N	5.56	131.71	121.70
1	A	206	GLU	C-N-CA	5.56	131.71	121.70
1	F	22	PHE	N-CA-C	5.07	116.81	111.28

There are no chirality outliers.

There are no planarity outliers.

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	1777	0	1809	34	0
1	B	1777	0	1809	22	0
1	C	1771	0	1805	30	0
1	D	1777	0	1809	27	0
1	E	1771	0	1805	29	0
1	F	1771	0	1805	30	0
1	G	1771	0	1805	38	0
2	H	1613	0	1649	17	0
2	I	1613	0	1649	21	0
2	J	1613	0	1649	20	0
2	K	1613	0	1649	23	0
2	L	1613	0	1649	28	0
2	M	1613	0	1649	26	0
2	N	1613	0	1649	17	0
3	O	1754	0	1765	22	0
3	P	1754	0	1765	24	0
3	Q	1754	0	1765	32	0
3	R	1754	0	1765	36	0
3	S	1754	0	1765	38	0
3	T	1746	0	1757	31	0
3	U	1754	0	1765	36	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	5	0	0	0	0
4	F	10	0	0	0	0
4	G	5	0	0	2	0
4	H	10	0	0	1	0
4	I	5	0	0	0	0
4	J	10	0	0	0	0
4	K	10	0	0	0	0
4	L	10	0	0	0	0
4	M	10	0	0	1	0
4	N	10	0	0	0	0
5	H	6	0	8	0	0
5	I	6	0	8	0	0
5	J	6	0	8	0	0
5	K	6	0	8	0	0
5	L	6	0	8	0	0
5	M	6	0	8	0	0
5	N	6	0	8	0	0
6	A	153	0	0	5	0
6	B	145	0	0	4	0
6	C	128	0	0	8	0
6	D	130	0	0	1	0
6	E	153	0	0	6	0
6	F	122	0	0	3	0
6	G	133	0	0	9	0
6	H	165	0	0	5	0
6	I	165	0	0	7	0
6	J	159	0	0	5	0
6	K	177	0	0	4	0
6	L	153	0	0	4	0
6	M	180	0	0	9	0
6	N	179	0	0	6	0
6	O	178	0	0	3	0
6	P	162	0	0	3	0
6	Q	161	0	0	1	0
6	R	189	0	0	6	0
6	S	221	0	0	1	0
6	T	207	0	0	5	0
6	U	210	0	0	3	0
All	All	39593	0	36593	478	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 7.

All (478) 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:D:28[B]:ARG:HH22	3:U:229:MET:CG	1.49	1.23
2:K:96[B]:MET:HE3	2:L:91:LYS:NZ	1.58	1.19
3:S:116[B]:ILE:HD11	3:S:204[B]:MET:HE1	1.22	1.14
1:E:28[B]:ARG:HH22	3:O:229:MET:HG3	0.98	1.09
1:F:28[B]:ARG:HH22	3:P:229:MET:HG2	1.10	1.09
2:L:202:ILE:HG22	2:L:203:LEU:H	1.05	1.08
1:C:28[A]:ARG:HH22	3:T:229:MET:CG	1.66	1.08
3:R:89[A]:ARG:HD3	3:S:203:THR:HG21	1.11	1.08
1:D:28[B]:ARG:HH22	3:U:229:MET:HG3	1.14	1.07
3:P:89[A]:ARG:HD3	3:Q:203:THR:HG21	1.10	1.05
1:E:28[B]:ARG:NH2	3:O:229:MET:HG3	1.72	1.05
3:S:89[A]:ARG:HD3	3:T:203:THR:HG21	1.07	1.04
1:A:65:GLU:HB3	4:G:4007:SO4:O1	1.57	1.04
3:P:89[A]:ARG:HD3	3:Q:203:THR:CG2	1.88	1.03
1:B:28[B]:ARG:HH22	3:S:229:MET:CG	1.71	1.03
1:G:28[B]:ARG:HH22	3:Q:229:MET:HG2	1.19	1.02
1:C:28[A]:ARG:HH22	3:T:229:MET:HG3	1.23	1.00
2:K:96[B]:MET:HE3	2:L:91:LYS:HZ2	1.19	0.98
1:F:28[B]:ARG:NH2	3:P:229:MET:HG2	1.79	0.97
1:E:28[B]:ARG:HH22	3:O:229:MET:CG	1.76	0.97
3:S:116[B]:ILE:CD1	3:S:204[B]:MET:HE1	1.94	0.97
2:L:202:ILE:HG22	2:L:203:LEU:N	1.77	0.97
3:P:89[A]:ARG:CD	3:Q:203:THR:HG21	1.95	0.96
3:Q:101:GLU:HG3	3:R:105:LEU:HD22	1.47	0.95
1:G:90:ASP:HB3	6:M:5136:HOH:O	1.66	0.95
3:T:89[A]:ARG:NH1	3:T:118:ASP:OD1	2.01	0.94
1:D:28[B]:ARG:NH2	3:U:229:MET:HG3	1.82	0.94
3:S:89[A]:ARG:HD3	3:T:203:THR:CG2	1.99	0.93
3:S:89[A]:ARG:CD	3:T:203:THR:HG21	1.97	0.93
3:U:37[A]:GLU:OE1	6:U:344:HOH:O	1.86	0.93
1:F:68[B]:GLN:NE2	6:F:4108:HOH:O	2.02	0.92
3:S:116[B]:ILE:HD11	3:S:204[B]:MET:CE	1.99	0.92
1:D:28[B]:ARG:HH22	3:U:229:MET:HG2	1.33	0.91
3:T:89[A]:ARG:HD3	3:U:203:THR:HG21	1.52	0.91
3:T:11:ASN:OD1	6:T:310:HOH:O	1.87	0.91
1:D:28[B]:ARG:NH2	3:U:229:MET:CG	2.34	0.91
2:I:67:ARG:NH1	6:I:5168:HOH:O	2.02	0.91
1:F:28[B]:ARG:HH22	3:P:229:MET:CG	1.82	0.90
6:K:5105:HOH:O	2:L:91:LYS:HE2	1.72	0.89
3:R:89[A]:ARG:HD3	3:S:203:THR:CG2	2.00	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:89[A]:ARG:NH1	3:U:118:ASP:OD1	2.05	0.89
6:H:5089:HOH:O	2:I:91:LYS:HE2	1.70	0.89
1:A:28[B]:ARG:HH22	3:R:229:MET:HG2	1.36	0.88
3:R:89[A]:ARG:CD	3:S:203:THR:HG21	2.02	0.88
3:S:204[B]:MET:HE2	3:S:208:VAL:HG23	1.56	0.86
1:G:28[B]:ARG:NH2	3:Q:229:MET:HG2	1.93	0.83
1:B:28[B]:ARG:HH22	3:S:229:MET:HG2	1.44	0.83
2:K:96[B]:MET:HE3	2:L:91:LYS:HZ1	1.41	0.82
3:T:144:ALA:HA	3:T:147:GLU:HG3	1.61	0.82
2:N:172:MET:HE2	2:N:189:THR:HG23	1.59	0.82
6:A:4015:HOH:O	3:Q:230:VAL:HG13	1.79	0.81
2:M:91:LYS:HE3	2:M:92:TYR:CE1	2.15	0.81
1:C:66:LYS:HB2	6:C:4131:HOH:O	1.78	0.81
3:R:75:GLN:OE1	6:R:419:HOH:O	1.99	0.81
2:I:172:MET:HE2	2:I:189:THR:HG23	1.60	0.80
1:C:28[A]:ARG:NH2	3:T:229:MET:HG3	1.97	0.78
1:G:68[B]:GLN:OE1	6:G:4058:HOH:O	2.01	0.78
1:A:65:GLU:CB	4:G:4007:SO4:O1	2.32	0.78
1:B:28[B]:ARG:HH22	3:S:229:MET:HG3	1.47	0.76
2:I:22:MET:HB2	2:I:27:MET:SD	2.25	0.76
1:C:28[A]:ARG:NH2	3:T:229:MET:CG	2.48	0.76
1:C:106:LEU:HD21	6:C:4072:HOH:O	1.86	0.75
2:H:9:LYS:HG2	6:H:5060:HOH:O	1.85	0.75
1:G:67:ILE:HD12	1:G:211:GLU:HG2	1.67	0.74
3:R:11:ASN:OD1	6:R:276:HOH:O	2.04	0.74
1:A:28[B]:ARG:NH2	6:A:4056:HOH:O	2.18	0.74
1:B:21:LEU:HD12	3:S:229:MET:HE1	1.70	0.74
3:S:89[A]:ARG:NH1	3:S:118:ASP:OD1	2.21	0.74
1:G:82[A]:VAL:HG11	3:P:231:SER:HB3	1.68	0.73
2:L:202:ILE:CG2	2:L:203:LEU:N	2.46	0.73
3:S:49:VAL:HG21	6:S:412:HOH:O	1.87	0.73
2:I:67:ARG:NE	6:I:5152:HOH:O	2.22	0.73
2:J:48:LEU:HD22	2:J:96[B]:MET:HE3	1.71	0.72
2:H:172:MET:HE2	2:H:189:THR:HG23	1.72	0.72
3:Q:101:GLU:HG3	3:R:105:LEU:CD2	2.20	0.72
3:U:125:LEU:O	3:U:142[A]:MET:HG3	1.89	0.71
1:E:68[B]:GLN:NE2	6:E:371:HOH:O	2.23	0.71
1:F:67:ILE:HG12	1:F:77[B]:VAL:HG12	1.72	0.71
2:J:22:MET:HB2	2:J:27:MET:SD	2.29	0.71
1:A:65:GLU:HG3	1:A:67:ILE:O	1.90	0.71
2:J:67:ARG:HD2	6:J:5151:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:ILE:HG12	1:D:77[A]:VAL:CG1	2.21	0.71
1:A:28[A]:ARG:NH2	3:R:228:HIS:CD2	2.59	0.70
1:G:67:ILE:HG12	1:G:77[A]:VAL:CG1	2.22	0.70
1:A:28[B]:ARG:HH22	3:R:229:MET:CG	2.03	0.69
2:I:9:LYS:HG3	6:I:5017:HOH:O	1.92	0.69
2:M:96[B]:MET:HE2	2:M:96[B]:MET:HA	1.75	0.69
6:O:261:HOH:O	3:U:129:GLU:HG2	1.93	0.69
3:O:125:LEU:O	3:O:142[A]:MET:HG3	1.92	0.69
3:S:116[B]:ILE:CG1	3:S:204[B]:MET:HE1	2.22	0.69
2:K:157:ARG:HD2	6:K:5018:HOH:O	1.93	0.68
2:M:172:MET:HE2	2:M:189:THR:HG23	1.75	0.68
1:A:54:VAL:HG21	1:A:61:GLN:HE22	1.57	0.67
3:T:144:ALA:HA	3:T:147:GLU:CG	2.25	0.67
1:C:21:LEU:HD12	3:T:229:MET:HE1	1.76	0.67
1:D:21:LEU:HD12	3:U:229:MET:HE1	1.76	0.67
2:N:91:LYS:HE3	2:N:92:TYR:CE1	2.29	0.67
1:A:90:ASP:HB3	6:N:5079:HOH:O	1.93	0.67
1:G:82[A]:VAL:CG1	3:P:231:SER:HB3	2.23	0.67
2:L:18:ARG:NH1	2:L:30:ASN:OD1	2.26	0.67
2:M:27:MET:HB3	6:N:5104:HOH:O	1.95	0.66
3:O:119:GLU:HG3	3:O:123:LYS:HD2	1.77	0.66
3:P:125:LEU:O	3:P:142[A]:MET:HG3	1.96	0.66
2:J:18:ARG:HH11	2:J:30:ASN:HD21	1.44	0.66
3:Q:101:GLU:CG	3:R:105:LEU:HD22	2.25	0.65
3:S:204[B]:MET:HE2	3:S:208:VAL:CG2	2.26	0.65
1:D:90:ASP:HB3	6:J:5096:HOH:O	1.97	0.65
1:B:28[B]:ARG:NH2	3:S:229:MET:CG	2.53	0.64
1:D:28[B]:ARG:NH2	3:U:229:MET:HG2	2.09	0.64
2:H:94:PRO:CG	2:H:96[A]:MET:HE3	2.28	0.64
1:F:68[B]:GLN:OE1	6:F:4082:HOH:O	2.15	0.64
3:U:89[A]:ARG:CZ	3:U:118:ASP:OD1	2.45	0.64
2:L:96[B]:MET:HE2	6:M:5041:HOH:O	1.96	0.64
1:F:67:ILE:HG12	1:F:77[B]:VAL:CG1	2.28	0.63
3:R:144:ALA:N	6:R:419:HOH:O	2.31	0.63
1:B:28[B]:ARG:NH2	3:S:229:MET:HG3	2.12	0.63
2:N:157:ARG:HD2	6:N:5014:HOH:O	1.98	0.63
1:E:228:GLU:OE1	6:E:386:HOH:O	2.16	0.63
1:G:173:VAL:O	1:G:177:GLU:HG3	1.99	0.63
2:K:24:ASN:HD22	2:K:24:ASN:H	1.47	0.63
3:O:140:ILE:HA	3:U:129:GLU:OE2	1.98	0.62
3:R:125:LEU:O	3:R:142[A]:MET:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ILE:HG12	1:C:77[A]:VAL:CG1	2.30	0.61
3:S:204[B]:MET:HE3	3:S:207:ALA:HB3	1.80	0.61
1:E:28[B]:ARG:NH2	6:E:288:HOH:O	2.21	0.61
2:L:96[B]:MET:CE	6:M:5041:HOH:O	2.48	0.61
1:F:156:THR:HG23	1:G:82[B]:VAL:HG11	1.81	0.61
1:A:21:LEU:HD12	3:R:229:MET:HE1	1.81	0.61
1:G:141:ILE:HD12	1:G:215:ILE:HG12	1.81	0.61
1:G:67:ILE:HG12	1:G:77[A]:VAL:HG12	1.83	0.60
3:S:113:VAL:O	3:S:116[B]:ILE:HG22	2.01	0.60
3:Q:144:ALA:HB3	6:Q:340:HOH:O	2.00	0.60
1:C:28[A]:ARG:NH2	6:C:4118:HOH:O	2.29	0.60
2:K:27:MET:HB3	6:L:5075:HOH:O	2.02	0.60
1:A:55:ARG:O	1:A:56:SER:CB	2.49	0.60
3:R:226:SER:HB2	3:R:228:HIS:NE2	2.16	0.60
1:G:106:LEU:HD21	6:G:4020:HOH:O	2.01	0.60
3:S:78:CYS:HB3	3:S:142[A]:MET:HG2	1.84	0.60
3:T:89[A]:ARG:CD	3:U:203:THR:HG21	2.30	0.59
3:Q:125:LEU:O	3:Q:142[A]:MET:HG3	2.03	0.59
1:C:28[A]:ARG:HH22	3:T:229:MET:HG2	1.61	0.59
2:K:172:MET:HE2	2:K:189:THR:HG23	1.85	0.58
3:R:224:THR:HG23	6:R:315:HOH:O	2.02	0.58
2:L:24:ASN:H	2:L:24:ASN:HD22	1.52	0.58
3:Q:140:ILE:CD1	3:Q:144:ALA:HB1	2.32	0.58
1:F:71:ASP:HA	2:L:68:LEU:HD11	1.86	0.58
2:J:96[B]:MET:HE2	2:K:91:LYS:HZ2	1.69	0.58
1:F:100:LYS:NZ	6:L:5117:HOH:O	2.35	0.58
2:H:22:MET:HB2	2:H:27:MET:SD	2.44	0.57
3:R:116[B]:ILE:HG13	3:R:204[B]:MET:HE1	1.85	0.57
3:Q:140:ILE:HD11	3:Q:144:ALA:HB1	1.86	0.57
1:E:35:SER:HB2	3:U:231:SER:OXT	2.04	0.57
3:P:89[A]:ARG:NH1	3:P:118:ASP:OD1	2.37	0.57
1:E:64:ILE:HG22	1:E:64:ILE:O	2.05	0.57
2:H:94:PRO:HG2	2:H:96[A]:MET:HE3	1.86	0.57
2:J:18:ARG:HH11	2:J:30:ASN:ND2	2.02	0.57
3:S:226:SER:HB2	3:S:228:HIS:CD2	2.40	0.57
3:Q:116[A]:ILE:HD12	3:Q:208:VAL:HG22	1.85	0.57
2:H:96[A]:MET:HE2	2:H:96[A]:MET:HA	1.87	0.56
2:M:163:LYS:HZ1	2:M:203:LEU:HB3	1.69	0.56
1:F:48:LEU:HD13	1:F:77[B]:VAL:HG13	1.86	0.56
4:H:4015:SO4:O4	6:H:5044:HOH:O	2.18	0.56
3:R:89[A]:ARG:NH1	3:R:118:ASP:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:THR:N	6:C:4077:HOH:O	2.37	0.56
1:A:55:ARG:O	1:A:55:ARG:HG3	2.05	0.56
2:M:94:PRO:HG2	2:M:96[B]:MET:HE3	1.88	0.56
1:D:67:ILE:HG12	1:D:77[A]:VAL:HG12	1.86	0.56
1:E:67:ILE:HG12	1:E:77[A]:VAL:CG1	2.35	0.56
2:M:157:ARG:HD2	6:M:5024:HOH:O	2.05	0.56
1:B:63:SER:HB3	6:B:4160:HOH:O	2.06	0.56
3:S:125:LEU:O	3:S:142[A]:MET:HG3	2.05	0.56
1:F:49:ILE:HG12	1:F:212:ILE:HG12	1.88	0.55
2:M:91:LYS:HE2	6:M:5038:HOH:O	2.05	0.55
1:D:28[B]:ARG:NH2	6:D:4062:HOH:O	2.37	0.55
1:G:48:LEU:HD13	1:G:77[A]:VAL:HG13	1.89	0.55
2:N:9:LYS:HG3	6:N:5013:HOH:O	2.06	0.55
1:E:21:LEU:HD12	3:O:229:MET:HE1	1.89	0.55
2:N:195:ARG:HA	2:N:198:LYS:HG2	1.88	0.55
6:P:295:HOH:O	3:Q:204[A]:MET:HE3	2.07	0.55
1:E:13:THR:N	6:E:350:HOH:O	2.39	0.55
1:B:177:GLU:OE1	1:C:56:SER:HB2	2.06	0.55
2:H:9:LYS:HE2	6:H:5060:HOH:O	2.06	0.55
2:I:163:LYS:NZ	2:I:203:LEU:HB3	2.21	0.54
2:N:174[B]:ASP:OD1	2:N:186:GLN:NE2	2.32	0.54
1:C:53:LYS:NZ	6:C:4091:HOH:O	2.41	0.54
1:E:82[B]:VAL:HG12	3:U:229:MET:O	2.08	0.54
2:I:27:MET:HB3	6:J:5084:HOH:O	2.08	0.54
1:A:28[B]:ARG:NH2	3:R:229:MET:HG2	2.16	0.54
2:L:174[B]:ASP:OD2	6:L:5076:HOH:O	2.18	0.54
1:D:71:ASP:HB2	2:J:64:GLU:OE2	2.08	0.54
2:N:96[B]:MET:HA	2:N:96[B]:MET:HE2	1.90	0.54
1:E:126:TYR:HH	1:F:123:TYR:HH	1.53	0.54
1:D:126:TYR:HH	1:E:123:TYR:HH	1.53	0.54
6:T:330:HOH:O	3:U:200:HIS:CE1	2.61	0.54
2:M:195:ARG:HA	2:M:198:LYS:HG2	1.90	0.53
3:P:143:TYR:O	3:P:147:GLU:HG3	2.08	0.53
3:R:226:SER:O	3:R:228:HIS:CD2	2.60	0.53
1:A:82[B]:VAL:HG11	1:G:156:THR:HG23	1.89	0.53
1:B:17:PRO:HB3	3:T:105:LEU:HD11	1.90	0.53
3:Q:119:GLU:HG3	3:Q:123:LYS:HD2	1.89	0.53
3:S:116[B]:ILE:CG1	3:S:204[B]:MET:CE	2.86	0.53
3:S:129:GLU:HG3	3:T:138:THR:O	2.09	0.53
1:G:55:ARG:O	1:G:56:SER:HB2	2.09	0.53
1:G:211:GLU:HG3	6:G:4030:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLU:CG	1:A:67:ILE:O	2.56	0.53
3:T:160:LEU:O	3:T:161:GLY:C	2.50	0.53
1:B:28[B]:ARG:NH2	3:S:229:MET:HG2	2.17	0.52
3:S:28:TRP:HA	3:S:32:THR:HB	1.91	0.52
1:C:178:ARG:HD2	1:C:179:GLU:OE2	2.09	0.52
1:D:55:ARG:O	1:D:56:SER:CB	2.57	0.52
3:O:28:TRP:HA	3:O:32:THR:HB	1.91	0.52
1:B:71:ASP:HA	2:H:68:LEU:HD11	1.92	0.52
3:Q:65:GLU:HA	3:Q:68:LEU:HD12	1.92	0.52
1:D:55:ARG:O	1:D:56:SER:HB3	2.09	0.52
1:A:38:LEU:HD12	1:A:38:LEU:C	2.34	0.52
1:B:82[B]:VAL:HG12	3:R:229:MET:O	2.09	0.52
1:F:156:THR:HG23	1:G:82[B]:VAL:CG1	2.39	0.52
1:D:49:ILE:HG23	1:D:212:ILE:HD13	1.91	0.51
3:O:89[A]:ARG:NH1	3:O:118:ASP:OD1	2.44	0.51
1:C:66:LYS:O	6:C:4130:HOH:O	2.19	0.51
2:K:96[B]:MET:CE	2:L:91:LYS:HZ1	2.18	0.51
1:G:68[B]:GLN:NE2	6:G:4063:HOH:O	2.35	0.51
2:N:37:ILE:HG21	2:N:43:MET:HE2	1.93	0.51
1:F:28[B]:ARG:NH2	6:F:4059:HOH:O	2.43	0.51
3:T:143:TYR:O	3:T:147:GLU:HG2	2.10	0.51
6:R:317:HOH:O	3:S:204[A]:MET:HG2	2.10	0.51
3:R:120:LEU:HD13	3:R:204[B]:MET:HG3	1.93	0.51
3:P:225:GLY:O	3:P:226:SER:HB3	2.09	0.51
1:A:90:ASP:OD1	6:A:4070:HOH:O	2.20	0.50
2:K:24:ASN:H	2:K:24:ASN:ND2	2.09	0.50
2:H:3:THR:HB	2:H:16:THR:HG22	1.93	0.50
2:I:27:MET:HG2	6:J:5154:HOH:O	2.11	0.50
1:G:82[A]:VAL:HG22	3:P:229:MET:O	2.11	0.50
3:S:116[B]:ILE:CD1	3:S:204[B]:MET:CE	2.72	0.50
2:I:24:ASN:H	2:I:24:ASN:HD22	1.58	0.50
3:O:204[A]:MET:HE3	3:O:204[A]:MET:HA	1.92	0.50
3:U:64:PRO:HB2	3:U:67:LEU:HG	1.94	0.50
1:G:71:ASP:HA	2:M:68:LEU:HD11	1.93	0.50
2:H:91:LYS:HD3	6:H:5075:HOH:O	2.11	0.50
3:Q:226:SER:HB2	3:Q:228:HIS:NE2	2.26	0.49
3:Q:230:VAL:O	3:Q:231:SER:HB3	2.12	0.49
2:J:111:PHE:CE2	2:J:121:GLU:HB2	2.48	0.49
1:E:81:LEU:HD22	3:U:229:MET:HE2	1.94	0.49
1:G:28[B]:ARG:NH2	6:G:4066:HOH:O	2.37	0.49
2:H:24:ASN:HD22	2:H:24:ASN:H	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:9:LYS:HE2	6:K:5172:HOH:O	2.12	0.49
3:U:78:CYS:HB3	3:U:142[A]:MET:HG2	1.94	0.49
1:C:222:ARG:HH12	1:C:228:GLU:CD	2.20	0.49
2:L:43:MET:HE3	2:L:56:VAL:HG22	1.95	0.49
2:M:58[B]:TYR:CE2	2:M:86:MET:HE1	2.48	0.49
1:G:17:PRO:HB3	3:R:105:LEU:HD11	1.95	0.49
2:N:24:ASN:HB3	6:N:5109:HOH:O	2.12	0.49
3:U:113:VAL:O	3:U:116[B]:ILE:HG22	2.12	0.49
1:A:54:VAL:O	1:A:208:LYS:NZ	2.46	0.49
1:E:66:LYS:HB2	6:E:318:HOH:O	2.12	0.49
1:G:55:ARG:O	1:G:56:SER:CB	2.61	0.49
4:M:4020:SO4:O1	6:M:5097:HOH:O	2.20	0.49
2:N:24:ASN:H	2:N:24:ASN:HD22	1.61	0.49
2:I:157:ARG:CZ	6:I:5068:HOH:O	2.61	0.48
2:M:22:MET:HE1	6:N:5180:HOH:O	2.13	0.48
2:M:157:ARG:HD3	6:M:5116:HOH:O	2.13	0.48
1:D:71:ASP:HA	2:J:68:LEU:HD11	1.95	0.48
1:G:206:GLU:HG2	6:G:4120:HOH:O	2.12	0.48
3:T:28:TRP:HA	3:T:32:THR:HB	1.94	0.48
2:I:94:PRO:CG	2:I:96[B]:MET:HE3	2.44	0.48
2:L:48:LEU:HD22	2:L:96[B]:MET:HE3	1.94	0.48
2:K:163:LYS:NZ	2:K:203:LEU:HB3	2.28	0.48
2:J:96[A]:MET:HE2	2:J:96[A]:MET:HA	1.96	0.48
2:M:111:PHE:CE2	2:M:121:GLU:HB2	2.49	0.48
2:N:111:PHE:CE2	2:N:121:GLU:HB2	2.49	0.48
3:R:28:TRP:HA	3:R:32:THR:HB	1.96	0.48
3:P:24:VAL:HG13	3:P:84:GLN:HB3	1.96	0.48
2:I:74:MET:HG2	2:I:78:ALA:HB3	1.96	0.47
2:L:195:ARG:HA	2:L:198:LYS:HG2	1.95	0.47
3:Q:28:TRP:HA	3:Q:32:THR:HB	1.96	0.47
3:U:28:TRP:HA	3:U:32:THR:HB	1.94	0.47
2:L:172:MET:HE2	2:L:189:THR:HG23	1.96	0.47
1:F:82[A]:VAL:HG22	3:O:229:MET:O	2.14	0.47
1:G:13:THR:N	6:G:4083:HOH:O	2.47	0.47
2:K:37:ILE:HG21	2:K:43:MET:HE2	1.95	0.47
2:L:111:PHE:CE2	2:L:121:GLU:HB2	2.50	0.47
1:A:33:LYS:O	1:A:53:LYS:NZ	2.47	0.47
1:A:180:TYR:HA	1:A:192:LEU:HD21	1.96	0.47
1:E:42:PHE:HB2	1:E:184:LEU:O	2.14	0.47
2:J:45:ILE:HB	2:J:52:ALA:HB1	1.96	0.47
2:M:196:ILE:HG23	2:M:201:LEU:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:94:PRO:CG	2:N:96[B]:MET:HE3	2.45	0.47
3:T:112:ALA:O	3:T:116[A]:ILE:HG23	2.14	0.47
2:K:202:ILE:HG22	2:K:203:LEU:N	2.30	0.47
3:P:41:LYS:O	3:P:45:GLU:HG2	2.15	0.47
1:A:106:LEU:HD21	6:A:4023:HOH:O	2.15	0.47
1:C:65:GLU:HG3	6:I:5134:HOH:O	2.15	0.47
1:G:201:LEU:HB3	1:G:205:GLU:HB3	1.97	0.47
1:C:28[A]:ARG:NH2	3:T:229:MET:HG2	2.25	0.46
1:E:67:ILE:HG12	1:E:77[A]:VAL:HG12	1.97	0.46
1:F:64:ILE:HG22	1:F:64:ILE:O	2.15	0.46
2:J:172:MET:HE2	2:J:189:THR:HG23	1.97	0.46
2:N:45:ILE:HB	2:N:52:ALA:HB1	1.97	0.46
1:G:208:LYS:O	1:G:209:ALA:HB2	2.16	0.46
1:A:28[A]:ARG:NH1	1:A:152:ASP:OD2	2.49	0.46
1:A:54:VAL:HG21	1:A:61:GLN:NE2	2.28	0.46
2:L:104:ILE:HD12	2:L:179:THR:HA	1.98	0.46
3:T:39:ILE:HG12	3:T:73:ARG:HG2	1.97	0.46
3:T:113:VAL:O	3:T:116[B]:ILE:HG22	2.16	0.46
1:C:228:GLU:OE1	6:C:4129:HOH:O	2.20	0.46
1:E:144:ILE:N	1:E:144:ILE:HD12	2.31	0.46
2:I:91:LYS:HE3	2:I:92:TYR:CE1	2.50	0.46
2:M:74:MET:HG2	2:M:78:ALA:HB3	1.98	0.46
3:U:123:LYS:HD2	6:U:385:HOH:O	2.14	0.46
2:L:196:ILE:HG23	2:L:201:LEU:HB2	1.97	0.46
1:A:77[A]:VAL:HG12	1:A:137:ILE:HB	1.96	0.46
2:I:96[B]:MET:HA	2:I:96[B]:MET:HE2	1.98	0.46
2:K:3:THR:HB	2:K:16:THR:HG22	1.98	0.46
2:M:24:ASN:HD22	2:M:24:ASN:H	1.63	0.46
2:M:94:PRO:CG	2:M:96[B]:MET:HE3	2.45	0.46
3:P:101:GLU:CG	3:Q:105:LEU:HD22	2.46	0.46
3:U:226:SER:HB2	3:U:228:HIS:CD2	2.51	0.46
1:F:95:SER:HG	1:F:115:ARG:HE	1.63	0.46
6:O:307:HOH:O	3:P:204[A]:MET:HG2	2.15	0.46
1:D:67:ILE:HD12	1:D:211:GLU:HB3	1.96	0.46
2:H:163:LYS:NZ	2:H:203:LEU:HB3	2.31	0.46
1:F:33:LYS:O	1:F:53:LYS:NZ	2.39	0.45
2:K:91:LYS:HE3	2:K:92:TYR:CE1	2.51	0.45
1:A:201:LEU:HD11	1:A:207:LEU:HB2	1.97	0.45
2:M:58[A]:TYR:CE2	6:M:5099:HOH:O	2.68	0.45
3:P:133:SER:N	3:Q:133:SER:O	2.50	0.45
3:Q:113:VAL:O	3:Q:116[B]:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:37[B]:GLU:OE2	3:S:41:LYS:HE2	2.16	0.45
1:D:28[B]:ARG:CZ	3:U:229:MET:HG3	2.43	0.45
1:E:71:ASP:HA	2:K:68:LEU:HD11	1.98	0.45
1:F:42:PHE:HB2	1:F:184:LEU:O	2.16	0.45
3:U:77:LEU:O	3:U:77:LEU:HG	2.16	0.45
3:U:89[A]:ARG:NH2	3:U:118:ASP:OD1	2.50	0.45
2:I:91:LYS:HE3	2:I:92:TYR:CZ	2.52	0.45
3:P:75:GLN:NE2	6:P:297:HOH:O	2.47	0.45
1:D:33:LYS:HB2	3:T:230:VAL:HG11	1.98	0.45
3:T:89[A]:ARG:NH2	6:T:402:HOH:O	2.49	0.45
3:Q:143:TYR:O	3:Q:147:GLU:HG3	2.17	0.45
3:R:50:ILE:HD11	3:R:67:LEU:HD21	1.99	0.45
1:C:90:ASP:OD1	6:C:4116:HOH:O	2.21	0.44
2:L:45:ILE:HB	2:L:52:ALA:HB1	1.99	0.44
3:Q:153[B]:SER:OG	3:R:179:LEU:HB2	2.18	0.44
3:R:75:GLN:HE21	3:S:192:LEU:CD2	2.31	0.44
1:C:67:ILE:HD12	1:C:211:GLU:HB3	1.99	0.44
2:J:74:MET:HG2	2:J:78:ALA:HB3	1.99	0.44
3:U:90:THR:O	3:U:94:ILE:HG12	2.17	0.44
3:O:143:TYR:O	3:O:147:GLU:HG3	2.18	0.44
2:I:94:PRO:HG2	2:I:96[B]:MET:HE3	1.99	0.44
2:M:96[B]:MET:HA	2:M:96[B]:MET:CE	2.46	0.44
3:O:24:VAL:HG13	3:O:84:GLN:HB3	1.99	0.44
1:F:61:GLN:HE21	1:F:61:GLN:HB3	1.66	0.44
2:K:15:ALA:HA	2:K:174[B]:ASP:O	2.18	0.44
1:D:107:VAL:O	1:D:142:ASP:HB2	2.18	0.44
1:B:107:VAL:O	1:B:142:ASP:HB2	2.18	0.44
1:C:82[A]:VAL:HG22	3:S:229:MET:O	2.18	0.44
1:C:38:LEU:HD12	1:C:38:LEU:C	2.43	0.43
1:B:13:THR:HA	6:B:4090:HOH:O	2.17	0.43
1:G:41:LYS:HD3	1:G:161:LYS:HA	2.01	0.43
1:G:208:LYS:O	1:G:209:ALA:CB	2.66	0.43
2:M:24:ASN:H	2:M:24:ASN:ND2	2.15	0.43
2:J:37:ILE:HG21	2:J:43:MET:HE2	2.00	0.43
3:P:144:ALA:N	6:P:314:HOH:O	2.51	0.43
3:R:65:GLU:HA	3:R:68:LEU:HD12	1.99	0.43
1:C:71:ASP:HA	2:I:68:LEU:HD11	2.00	0.43
1:F:55:ARG:O	1:F:56:SER:HB2	2.18	0.43
1:G:64:ILE:HG22	1:G:64:ILE:O	2.19	0.43
1:G:226:GLN:H	1:G:226:GLN:HG3	1.66	0.43
2:H:37:ILE:HG21	2:H:43:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:89:GLN:HG3	6:L:5064:HOH:O	2.18	0.43
3:R:77:LEU:O	3:R:77:LEU:HG	2.15	0.43
1:B:106:LEU:HD21	6:B:4063:HOH:O	2.19	0.43
3:R:75:GLN:HE21	3:S:192:LEU:HD22	1.82	0.43
1:A:82[A]:VAL:HG22	3:Q:229:MET:O	2.19	0.43
1:C:17:PRO:HB3	3:U:105:LEU:HD11	2.00	0.43
3:Q:68:LEU:HD21	3:Q:149:LEU:HD21	2.00	0.43
3:Q:140:ILE:HG12	3:Q:144:ALA:HB2	2.01	0.43
1:B:160:TYR:OH	1:C:55:ARG:NH1	2.51	0.43
1:E:223:ILE:N	1:E:223:ILE:HD12	2.34	0.43
3:S:116[B]:ILE:HG12	3:S:204[B]:MET:CE	2.48	0.43
1:A:17:PRO:HA	1:B:26:TYR:CD2	2.54	0.43
3:P:28:TRP:HA	3:P:32:THR:HB	2.01	0.43
3:Q:142[A]:MET:HE1	3:R:196:LEU:HD11	2.00	0.43
1:B:28[B]:ARG:NH2	6:B:4091:HOH:O	2.43	0.43
3:Q:86:GLU:HG3	3:R:199[A]:THR:HG22	2.01	0.43
1:C:77[B]:VAL:HG12	1:C:137:ILE:HB	2.00	0.43
2:I:45:ILE:HB	2:I:52:ALA:HB1	1.99	0.43
3:O:226:SER:O	3:O:228:HIS:N	2.50	0.43
1:E:28[A]:ARG:NH1	1:E:152:ASP:OD2	2.52	0.42
3:P:176:SER:HA	3:P:177:PRO:HD2	1.93	0.42
3:S:142[A]:MET:HE1	3:T:196:LEU:HD11	2.01	0.42
1:B:156:THR:HG23	1:C:82[B]:VAL:HG11	1.99	0.42
1:E:175:PHE:HE1	1:E:192:LEU:HD12	1.84	0.42
1:G:180:TYR:HA	1:G:192:LEU:HD21	2.00	0.42
2:L:24:ASN:H	2:L:24:ASN:ND2	2.17	0.42
1:A:65:GLU:OE2	2:N:71:ARG:NH1	2.53	0.42
2:J:190[B]:ASP:OD1	2:J:191:GLN:N	2.51	0.42
3:O:77:LEU:HD13	3:O:77:LEU:C	2.45	0.42
3:Q:50:ILE:HD11	3:Q:67:LEU:HD21	2.00	0.42
6:T:330:HOH:O	3:U:204[A]:MET:HG2	2.19	0.42
1:B:38:LEU:C	1:B:38:LEU:HD12	2.44	0.42
2:M:23:GLU:HB3	2:M:24:ASN:H	1.58	0.42
2:N:112[B]:SER:O	2:N:119:SER:HA	2.19	0.42
2:N:164:GLN:HE22	2:N:202:ILE:HD11	1.83	0.42
3:R:11:ASN:HB2	6:R:316:HOH:O	2.18	0.42
3:R:36:ILE:HG21	3:R:202[B]:SER:OG	2.19	0.42
3:T:144:ALA:CA	3:T:147:GLU:HG3	2.39	0.42
3:R:225:GLY:O	3:R:226:SER:HB3	2.19	0.42
1:A:55:ARG:O	1:A:56:SER:HB3	2.20	0.42
2:J:24:ASN:HD22	2:J:24:ASN:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:63:SER:HA	3:O:64:PRO:HD3	1.85	0.42
1:A:77[A]:VAL:HG22	6:A:4142:HOH:O	2.19	0.42
1:B:55:ARG:O	1:B:56:SER:CB	2.68	0.42
1:E:156:THR:HG23	1:F:82[B]:VAL:HG11	2.02	0.42
1:F:82[A]:VAL:HG11	3:O:231:SER:HB3	2.02	0.42
2:H:9:LYS:HG2	2:H:9:LYS:H	1.68	0.42
3:R:204[A]:MET:HA	3:R:204[A]:MET:HE2	2.01	0.42
1:F:203:GLU:O	1:F:205:GLU:N	2.53	0.42
1:F:209:ALA:HA	1:F:233:LEU:HD11	2.00	0.42
1:G:56:SER:HB3	1:G:59:ILE:HG12	2.01	0.42
3:P:181:LEU:HD22	3:P:184:ARG:HH12	1.85	0.42
2:K:202:ILE:CG2	2:K:203:LEU:N	2.82	0.41
3:Q:204[A]:MET:HE2	3:Q:204[A]:MET:HA	2.01	0.41
1:G:13:THR:CA	6:G:4083:HOH:O	2.67	0.41
2:H:24:ASN:H	2:H:24:ASN:ND2	2.18	0.41
1:D:152:ASP:HB2	1:D:153:PRO:CD	2.50	0.41
1:E:156:THR:HG23	1:F:82[B]:VAL:CG1	2.51	0.41
1:F:81:LEU:HD22	3:O:229:MET:HE2	2.02	0.41
2:L:22:MET:HB2	2:L:27:MET:SD	2.60	0.41
1:D:42:PHE:HB2	1:D:184:LEU:O	2.21	0.41
1:G:13:THR:HA	6:G:4083:HOH:O	2.20	0.41
2:L:163:LYS:HB3	2:L:203:LEU:HD13	2.01	0.41
2:M:20:VAL:HB	2:M:28:HIS:HB2	2.02	0.41
3:U:217:LYS:HD2	6:U:375:HOH:O	2.19	0.41
1:D:175:PHE:CD2	1:D:175:PHE:C	2.98	0.41
2:H:54:VAL:HG23	6:I:5043:HOH:O	2.18	0.41
2:K:163:LYS:HZ1	2:K:203:LEU:HB3	1.86	0.41
3:S:50:ILE:HD11	3:S:67:LEU:HD21	2.01	0.41
2:K:180:ARG:HD3	6:K:5101:HOH:O	2.20	0.41
2:K:23:GLU:HB3	2:K:24:ASN:HD22	1.85	0.41
2:M:91:LYS:HD2	6:M:5041:HOH:O	2.20	0.41
3:T:75:GLN:HE21	3:U:192:LEU:CD2	2.34	0.41
1:C:118:ASP:O	1:C:122:GLN:HG3	2.21	0.41
3:P:229:MET:HE2	3:P:229:MET:HB3	1.92	0.41
1:A:207:LEU:HD12	1:A:207:LEU:HA	1.95	0.41
1:D:100:LYS:NZ	6:J:5095:HOH:O	2.54	0.41
1:E:38:LEU:HD12	1:E:38:LEU:C	2.45	0.41
1:E:203:GLU:H	1:E:203:GLU:HG3	1.57	0.41
2:J:3:THR:HB	2:J:16:THR:HG22	2.02	0.41
3:U:78:CYS:CB	3:U:142[B]:MET:HB2	2.51	0.41
2:L:22:MET:SD	2:L:27:MET:HE1	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:64:GLU:HG3	2:M:67:ARG:HH21	1.86	0.41
1:B:180:TYR:HA	1:B:192:LEU:HD21	2.03	0.40
1:C:28[B]:ARG:NH1	1:C:152:ASP:OD2	2.54	0.40
1:E:152:ASP:HB2	1:E:153:PRO:CD	2.51	0.40
2:J:195:ARG:HA	2:J:198:LYS:HG2	2.02	0.40
3:O:10:GLN:NE2	3:O:14:ASP:OD1	2.49	0.40
6:O:261:HOH:O	3:U:129:GLU:CG	2.60	0.40
3:T:221:GLN:NE2	6:T:304:HOH:O	2.54	0.40
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.91	0.40
1:A:71:ASP:HA	2:N:68:LEU:HD11	2.03	0.40
1:F:55:ARG:O	1:F:56:SER:CB	2.70	0.40
2:M:45:ILE:HB	2:M:52:ALA:HB1	2.02	0.40
3:U:119:GLU:CD	3:U:204[B]:MET:HE1	2.46	0.40
1:A:63:SER:HB2	1:G:159:GLU:OE1	2.21	0.40
1:D:17:PRO:HB3	3:O:105:LEU:HD11	2.03	0.40
1:D:162:ALA:HB1	1:D:176:LEU:HD13	2.02	0.40
1:E:182:GLU:HG2	6:E:341:HOH:O	2.19	0.40
1:F:94:ILE:O	1:F:98:GLN:HG3	2.21	0.40
2:H:74:MET:HG2	2:H:78:ALA:HB3	2.01	0.40
2:J:96[B]:MET:HE2	2:K:91:LYS:NZ	2.36	0.40
3:O:204[A]:MET:HA	3:O:204[A]:MET:CE	2.52	0.40
1:G:203:GLU:H	1:G:203:GLU:HG3	1.58	0.40
2:I:163:LYS:HZ3	2:I:203:LEU:HB3	1.86	0.40
2:J:18:ARG:NH1	2:J:30:ASN:HD21	2.15	0.40
3:O:78:CYS:HB3	3:O:142[A]:MET:HG2	2.04	0.40
2:I:71:ARG:NE	6:I:5169:HOH:O	2.54	0.40
2:L:23:GLU:HB3	2:L:24:ASN:H	1.72	0.40
3:T:89[B]:ARG:HG3	3:T:117:ILE:HG21	2.03	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	226/233 (97%)	219 (97%)	5 (2%)	2 (1%)	14	6
1	B	226/233 (97%)	218 (96%)	7 (3%)	1 (0%)	30	22
1	C	225/233 (97%)	220 (98%)	4 (2%)	1 (0%)	30	22
1	D	226/233 (97%)	219 (97%)	6 (3%)	1 (0%)	30	22
1	E	225/233 (97%)	220 (98%)	5 (2%)	0	100	100
1	F	225/233 (97%)	216 (96%)	7 (3%)	2 (1%)	14	6
1	G	225/233 (97%)	217 (96%)	5 (2%)	3 (1%)	9	3
2	H	208/217 (96%)	204 (98%)	4 (2%)	0	100	100
2	I	208/217 (96%)	202 (97%)	6 (3%)	0	100	100
2	J	208/217 (96%)	204 (98%)	4 (2%)	0	100	100
2	K	208/217 (96%)	204 (98%)	4 (2%)	0	100	100
2	L	208/217 (96%)	201 (97%)	6 (3%)	1 (0%)	24	16
2	M	208/217 (96%)	204 (98%)	4 (2%)	0	100	100
2	N	208/217 (96%)	204 (98%)	4 (2%)	0	100	100
3	O	224/237 (94%)	220 (98%)	2 (1%)	2 (1%)	14	6
3	P	224/237 (94%)	218 (97%)	5 (2%)	1 (0%)	30	22
3	Q	224/237 (94%)	221 (99%)	3 (1%)	0	100	100
3	R	224/237 (94%)	220 (98%)	3 (1%)	1 (0%)	30	22
3	S	224/237 (94%)	217 (97%)	6 (3%)	1 (0%)	30	22
3	T	223/237 (94%)	219 (98%)	3 (1%)	1 (0%)	30	22
3	U	224/237 (94%)	219 (98%)	4 (2%)	1 (0%)	30	22
All	All	4601/4809 (96%)	4486 (98%)	97 (2%)	18 (0%)	30	22

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	B	56	SER
1	D	56	SER
1	F	56	SER
1	G	56	SER
1	G	209	ALA
3	P	226	SER
3	R	226	SER
3	T	226	SER
1	F	204	GLY

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Mol	Chain	Res	Type
3	O	226	SER
1	C	55	ARG
1	G	203	GLU
3	S	226	SER
3	U	226	SER
2	L	202	ILE
3	O	227	ASP
1	A	204	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/193 (99%)	183 (96%)	8 (4%)	26	19
1	B	191/193 (99%)	186 (97%)	5 (3%)	40	35
1	C	190/193 (98%)	184 (97%)	6 (3%)	34	27
1	D	191/193 (99%)	187 (98%)	4 (2%)	47	44
1	E	190/193 (98%)	187 (98%)	3 (2%)	55	54
1	F	190/193 (98%)	181 (95%)	9 (5%)	23	15
1	G	190/193 (98%)	184 (97%)	6 (3%)	34	27
2	H	177/183 (97%)	172 (97%)	5 (3%)	38	32
2	I	177/183 (97%)	174 (98%)	3 (2%)	53	52
2	J	177/183 (97%)	171 (97%)	6 (3%)	32	25
2	K	177/183 (97%)	171 (97%)	6 (3%)	32	25
2	L	177/183 (97%)	173 (98%)	4 (2%)	44	40
2	M	177/183 (97%)	173 (98%)	4 (2%)	44	40
2	N	177/183 (97%)	174 (98%)	3 (2%)	53	52
3	O	189/196 (96%)	184 (97%)	5 (3%)	40	35
3	P	189/196 (96%)	186 (98%)	3 (2%)	55	54
3	Q	189/196 (96%)	183 (97%)	6 (3%)	34	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	R	189/196 (96%)	181 (96%)	8 (4%)	26	19
3	S	189/196 (96%)	187 (99%)	2 (1%)	65	67
3	T	188/196 (96%)	181 (96%)	7 (4%)	30	22
3	U	189/196 (96%)	187 (99%)	2 (1%)	65	67
All	All	3894/4004 (97%)	3789 (97%)	105 (3%)	40	34

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	59	ILE
1	A	65	GLU
1	A	203	GLU
1	A	205	GLU
1	A	207	LEU
1	A	226	GLN
1	A	227	GLU
1	B	52	LYS
1	B	59	ILE
1	B	62	ASN
1	B	63	SER
1	B	65	GLU
1	C	55	ARG
1	C	63	SER
1	C	177	GLU
1	C	203	GLU
1	C	205	GLU
1	C	227	GLU
1	D	59	ILE
1	D	65	GLU
1	D	82[A]	VAL
1	D	82[B]	VAL
1	E	35	SER
1	E	59	ILE
1	E	203	GLU
1	F	35	SER
1	F	52	LYS
1	F	55	ARG
1	F	59	ILE
1	F	61	GLN
1	F	82[A]	VAL

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Mol	Chain	Res	Type
1	F	82[B]	VAL
1	F	227	GLU
1	F	230	LYS
1	G	54	VAL
1	G	61	GLN
1	G	203	GLU
1	G	221	TYR
1	G	225	ASP
1	G	226	GLN
2	H	3	THR
2	H	9	LYS
2	H	17	GLU
2	H	23	GLU
2	H	203	LEU
2	I	3	THR
2	I	17	GLU
2	I	23	GLU
2	J	3	THR
2	J	17	GLU
2	J	30	ASN
2	J	96[A]	MET
2	J	96[B]	MET
2	J	203	LEU
2	K	3	THR
2	K	9	LYS
2	K	17	GLU
2	K	23	GLU
2	K	198	LYS
2	K	203	LEU
2	L	9	LYS
2	L	17	GLU
2	L	71	ARG
2	L	203	LEU
2	M	3	THR
2	M	17	GLU
2	M	23	GLU
2	M	203	LEU
2	N	3	THR
2	N	17	GLU
2	N	71	ARG
3	O	57	ARG
3	O	62	LYS

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Mol	Chain	Res	Type
3	O	145	LEU
3	O	204[A]	MET
3	O	204[B]	MET
3	P	67	LEU
3	P	140	ILE
3	P	231	SER
3	Q	67	LEU
3	Q	77	LEU
3	Q	145	LEU
3	Q	204[A]	MET
3	Q	204[B]	MET
3	Q	230	VAL
3	R	57	ARG
3	R	65	GLU
3	R	67	LEU
3	R	77	LEU
3	R	145	LEU
3	R	204[A]	MET
3	R	204[B]	MET
3	R	224	THR
3	S	67	LEU
3	S	77	LEU
3	T	116[A]	ILE
3	T	116[B]	ILE
3	T	140	ILE
3	T	142[A]	MET
3	T	142[B]	MET
3	T	147	GLU
3	T	157	ASP
3	U	67	LEU
3	U	77	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	219	ASN
1	A	226	GLN
1	B	143	GLN
1	B	219	ASN
1	C	183	ASN
1	C	219	ASN

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Mol	Chain	Res	Type
1	D	61	GLN
1	D	111	ASN
1	D	226	GLN
1	E	61	GLN
1	E	158	ASN
1	E	219	ASN
1	E	226	GLN
1	F	61	GLN
1	F	143	GLN
1	F	158	ASN
1	F	219	ASN
1	G	61	GLN
1	G	97	GLN
1	G	219	ASN
1	G	226	GLN
2	H	24	ASN
2	H	191	GLN
2	I	24	ASN
2	J	24	ASN
2	J	30	ASN
2	J	89	GLN
2	J	141	GLN
2	J	191	GLN
2	K	24	ASN
2	L	24	ASN
2	M	24	ASN
2	M	73	ASN
2	N	24	ASN
2	N	164	GLN
3	O	99	HIS
3	P	75	GLN
3	P	79	HIS
3	P	185	GLN
3	P	228	HIS
3	Q	185	GLN
3	R	75	GLN
3	R	99	HIS
3	R	228	HIS
3	S	79	HIS
3	S	99	HIS
3	S	175	GLN
3	S	185	GLN

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Mol	Chain	Res	Type
3	T	79	HIS
3	T	175	GLN
3	T	221	GLN
3	U	79	HIS
3	U	185	GLN
3	U	228	HIS

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 ⓘ

28 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	SO4	N	4021	-	4,4,4	0.25	0	6,6,6	0.16	0
4	SO4	K	4018	-	4,4,4	0.26	0	6,6,6	0.47	0
4	SO4	H	4015	-	4,4,4	0.30	0	6,6,6	0.28	0
4	SO4	K	4013	-	4,4,4	0.20	0	6,6,6	0.66	0
4	SO4	J	4012	-	4,4,4	0.14	0	6,6,6	0.36	0
5	GOL	L	5001	-	5,5,5	0.35	0	5,5,5	0.49	0
4	SO4	B	4016	-	4,4,4	0.23	0	6,6,6	0.42	0
4	SO4	C	4003	-	4,4,4	0.24	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	F	4006	-	4,4,4	0.30	0	6,6,6	0.12	0
5	GOL	M	5002	-	5,5,5	0.27	0	5,5,5	0.47	0
4	SO4	A	4001	-	4,4,4	0.24	0	6,6,6	0.10	0
5	GOL	J	5006	-	5,5,5	0.54	0	5,5,5	0.64	0
4	SO4	L	4014	-	4,4,4	0.28	0	6,6,6	0.48	0
4	SO4	G	4007	-	4,4,4	0.21	0	6,6,6	0.30	0
4	SO4	F	4005	-	4,4,4	0.25	0	6,6,6	0.10	0
4	SO4	H	4008	-	4,4,4	0.35	0	6,6,6	0.42	0
4	SO4	D	4004	-	4,4,4	0.26	0	6,6,6	0.12	0
4	SO4	N	4009	-	4,4,4	0.29	0	6,6,6	0.26	0
5	GOL	H	5004	-	5,5,5	0.46	0	5,5,5	1.48	1 (20%)
4	SO4	M	4020	-	4,4,4	0.15	0	6,6,6	0.13	0
4	SO4	J	4017	-	4,4,4	0.22	0	6,6,6	0.08	0
4	SO4	I	4011	-	4,4,4	0.19	0	6,6,6	0.34	0
4	SO4	L	4019	-	4,4,4	0.20	0	6,6,6	0.16	0
5	GOL	K	5007	-	5,5,5	0.39	0	5,5,5	0.86	0
4	SO4	B	4002	-	4,4,4	0.28	0	6,6,6	0.22	0
4	SO4	M	4010	-	4,4,4	0.35	0	6,6,6	0.39	0
5	GOL	N	5003	-	5,5,5	0.34	0	5,5,5	0.73	0
5	GOL	I	5005	-	5,5,5	0.37	0	5,5,5	0.57	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
5	GOL	K	5007	-	-	0/4/4/4	-
5	GOL	N	5003	-	-	0/4/4/4	-
5	GOL	M	5002	-	-	3/4/4/4	-
5	GOL	H	5004	-	-	4/4/4/4	-
5	GOL	J	5006	-	-	1/4/4/4	-
5	GOL	L	5001	-	-	2/4/4/4	-
5	GOL	I	5005	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	5004	GOL	O2-C2-C1	2.39	119.06	109.18

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	5004	GOL	C1-C2-C3-O3
5	M	5002	GOL	O1-C1-C2-C3
5	H	5004	GOL	O1-C1-C2-C3
5	L	5001	GOL	O1-C1-C2-C3
5	H	5004	GOL	O1-C1-C2-O2
5	H	5004	GOL	O2-C2-C3-O3
5	L	5001	GOL	O1-C1-C2-O2
5	M	5002	GOL	O1-C1-C2-O2
5	M	5002	GOL	C1-C2-C3-O3
5	J	5006	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	4015	SO4	1	0
4	G	4007	SO4	2	0
4	M	4020	SO4	1	0

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	221/233 (94%)	0.44	21 (9%) 14 14	10, 28, 61, 71	7 (3%)
1	B	221/233 (94%)	0.54	27 (12%) 8 9	9, 29, 60, 71	7 (3%)
1	C	221/233 (94%)	0.43	25 (11%) 10 10	9, 28, 63, 70	6 (2%)
1	D	221/233 (94%)	0.62	27 (12%) 8 9	10, 31, 62, 73	7 (3%)
1	E	221/233 (94%)	0.37	17 (7%) 19 21	10, 27, 55, 65	6 (2%)
1	F	221/233 (94%)	0.57	27 (12%) 8 9	10, 30, 63, 75	6 (2%)
1	G	221/233 (94%)	0.52	26 (11%) 9 9	10, 30, 58, 70	6 (2%)
2	H	203/217 (93%)	0.01	9 (4%) 39 41	10, 23, 38, 65	7 (3%)
2	I	203/217 (93%)	0.05	9 (4%) 39 41	10, 24, 40, 61	7 (3%)
2	J	203/217 (93%)	0.14	11 (5%) 31 33	11, 25, 41, 65	7 (3%)
2	K	203/217 (93%)	0.13	10 (4%) 35 37	10, 25, 40, 62	7 (3%)
2	L	203/217 (93%)	0.15	10 (4%) 35 37	11, 24, 40, 65	7 (3%)
2	M	203/217 (93%)	0.05	8 (3%) 43 46	9, 22, 37, 60	7 (3%)
2	N	203/217 (93%)	0.06	11 (5%) 31 33	10, 24, 39, 65	7 (3%)
3	O	218/237 (91%)	0.40	13 (5%) 27 29	11, 30, 47, 61	10 (4%)
3	P	218/237 (91%)	0.56	17 (7%) 19 20	13, 32, 50, 67	10 (4%)
3	Q	218/237 (91%)	0.58	18 (8%) 17 18	13, 32, 51, 79	10 (4%)
3	R	218/237 (91%)	0.39	14 (6%) 25 27	12, 28, 49, 63	10 (4%)
3	S	218/237 (91%)	0.19	13 (5%) 27 29	9, 25, 42, 66	10 (4%)
3	T	218/237 (91%)	0.20	11 (5%) 34 36	9, 25, 44, 61	9 (4%)
3	U	218/237 (91%)	0.17	12 (5%) 30 32	9, 26, 41, 64	10 (4%)
All	All	4494/4809 (93%)	0.32	336 (7%) 20 21	9, 27, 54, 79	163 (3%)

All (336) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	203	LEU	11.0
2	I	203	LEU	10.7
2	K	203	LEU	9.6
2	H	203	LEU	8.6
2	L	203	LEU	8.5
1	B	64	ILE	8.1
2	M	203	LEU	7.9
2	J	203	LEU	7.9
2	N	202	ILE	7.6
2	H	202	ILE	7.6
3	U	226	SER	7.2
3	S	226	SER	7.0
3	R	226	SER	6.9
3	Q	230	VAL	6.6
3	T	225	GLY	6.5
3	O	225	GLY	6.5
2	J	202	ILE	6.0
2	L	202	ILE	6.0
1	E	64	ILE	5.9
1	D	54	VAL	5.9
2	K	202	ILE	5.9
3	Q	227	ASP	5.8
3	Q	231	SER	5.8
3	U	228	HIS	5.7
3	P	230	VAL	5.7
3	S	225	GLY	5.7
3	Q	226	SER	5.7
1	D	64	ILE	5.5
3	T	226	SER	5.4
3	S	230	VAL	5.2
1	F	64	ILE	5.2
3	R	225	GLY	5.2
2	I	202	ILE	5.2
1	G	54	VAL	5.2
2	M	202	ILE	5.0
1	G	55	ARG	5.0
2	I	58[A]	TYR	4.9
3	O	226	SER	4.9
1	A	53	LYS	4.9
1	C	64	ILE	4.8
3	Q	228	HIS	4.8
3	P	227	ASP	4.8
1	F	61	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
3	R	231	SER	4.7
3	T	161	GLY	4.6
2	L	58[A]	TYR	4.6
3	S	227	ASP	4.6
1	G	64	ILE	4.5
3	P	226	SER	4.5
1	B	54	VAL	4.5
1	D	206	GLU	4.5
3	U	225	GLY	4.5
3	U	231	SER	4.5
3	R	230	VAL	4.4
1	D	63	SER	4.4
3	S	224	THR	4.3
3	Q	229	MET	4.3
3	Q	225	GLY	4.3
3	P	144	ALA	4.2
3	T	227	ASP	4.2
2	M	58[A]	TYR	4.2
1	E	61	GLN	4.2
1	C	55	ARG	4.1
1	B	204	GLY	4.1
2	N	58[A]	TYR	4.1
3	R	228	HIS	4.1
1	A	204	GLY	4.1
3	S	228	HIS	4.1
1	E	53	LYS	4.1
1	G	208	LYS	4.0
1	D	61	GLN	4.0
2	M	22	MET	4.0
3	T	228	HIS	3.9
1	A	207	LEU	3.9
1	B	55	ARG	3.9
1	B	61	GLN	3.8
2	K	58[A]	TYR	3.8
3	P	231	SER	3.8
2	H	58[A]	TYR	3.8
1	G	209	ALA	3.8
3	O	227	ASP	3.8
3	R	227	ASP	3.8
1	E	203	GLU	3.8
1	G	53	LYS	3.8
1	D	55	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	204	GLY	3.7
3	T	172	GLY	3.7
2	J	58[A]	TYR	3.6
1	C	59	ILE	3.6
3	O	228	HIS	3.6
3	S	231	SER	3.5
1	A	64	ILE	3.5
3	Q	52	ASN	3.5
3	S	52	ASN	3.5
1	C	127	GLY	3.5
3	P	228	HIS	3.5
1	A	62	ASN	3.5
1	C	61	GLN	3.5
1	F	201	LEU	3.5
3	S	229	MET	3.4
3	U	230	VAL	3.4
1	D	209	ALA	3.4
1	F	63	SER	3.4
3	Q	161	GLY	3.4
1	D	230	LYS	3.3
1	C	54	VAL	3.3
1	F	209	ALA	3.3
2	L	27	MET	3.3
1	E	65	GLU	3.3
1	A	54	VAL	3.3
1	E	127	GLY	3.3
1	F	202	GLU	3.2
1	F	203	GLU	3.2
2	J	198	LYS	3.2
3	Q	58	ALA	3.2
1	F	55	ARG	3.2
3	U	161	GLY	3.2
2	H	22	MET	3.2
1	A	55	ARG	3.2
1	E	54	VAL	3.2
1	F	54	VAL	3.2
1	C	233	LEU	3.2
2	J	27	MET	3.2
2	L	201	LEU	3.1
1	A	65	GLU	3.1
1	F	62	ASN	3.1
3	O	65	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	55	ARG	3.1
1	B	63	SER	3.1
3	P	225	GLY	3.1
3	R	49	VAL	3.1
3	T	230	VAL	3.1
1	D	208	LYS	3.1
1	D	204	GLY	3.1
3	O	144	ALA	3.1
3	O	230	VAL	3.0
1	A	205	GLU	3.0
2	K	9	LYS	3.0
2	N	22	MET	3.0
3	Q	49	VAL	3.0
1	A	63	SER	3.0
3	P	224	THR	3.0
2	L	22	MET	3.0
3	R	52	ASN	3.0
3	P	68	LEU	2.9
1	F	229	VAL	2.9
3	Q	172	GLY	2.9
1	G	59	ILE	2.9
3	U	227	ASP	2.9
2	J	22	MET	2.9
1	G	62	ASN	2.9
1	B	209	ALA	2.9
2	K	198	LYS	2.9
1	A	206	GLU	2.9
2	H	27	MET	2.9
2	K	27	MET	2.9
1	G	204	GLY	2.9
1	G	143	GLN	2.9
1	D	53	LYS	2.9
2	I	22	MET	2.9
2	K	22	MET	2.9
3	R	161	GLY	2.9
1	D	231	LYS	2.8
3	S	4	LYS	2.8
3	T	231	SER	2.8
3	Q	173	GLY	2.8
1	B	208	LYS	2.8
1	C	53	LYS	2.8
1	F	228	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	209	ALA	2.8
1	G	63	SER	2.8
3	Q	116[A]	ILE	2.8
1	F	206	GLU	2.8
1	B	229	VAL	2.8
2	L	200	GLY	2.8
3	U	224	THR	2.8
1	C	203	GLU	2.7
3	S	161	GLY	2.7
3	U	172	GLY	2.7
2	M	201	LEU	2.7
1	E	59	ILE	2.7
1	C	62	ASN	2.7
1	E	204	GLY	2.7
3	R	224	THR	2.7
1	A	231	LYS	2.7
3	O	58	ALA	2.7
1	B	127	GLY	2.7
3	Q	224	THR	2.7
1	C	63	SER	2.7
1	E	201	LEU	2.7
1	G	174	SER	2.7
1	E	62	ASN	2.7
1	D	229	VAL	2.7
3	R	58	ALA	2.6
3	T	224	THR	2.6
1	C	231	LYS	2.6
3	O	231	SER	2.6
1	B	183	ASN	2.6
1	F	127	GLY	2.6
1	C	226	GLN	2.6
3	U	52	ASN	2.6
1	G	201	LEU	2.6
1	F	59	ILE	2.6
1	B	143	GLN	2.6
3	O	173	GLY	2.6
1	D	205	GLU	2.6
1	F	205	GLU	2.6
1	G	177	GLU	2.6
1	F	208	LYS	2.6
1	D	233	LEU	2.6
2	M	27	MET	2.6

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Mol	Chain	Res	Type	RSRZ
2	I	200	GLY	2.6
1	C	229	VAL	2.6
2	H	197	ARG	2.5
1	B	233	LEU	2.5
1	A	59	ILE	2.5
3	P	161	GLY	2.5
3	R	116[A]	ILE	2.5
1	C	232	PHE	2.5
2	L	198	LYS	2.5
1	G	233	LEU	2.5
1	C	204	GLY	2.5
1	A	201	LEU	2.5
1	B	232	PHE	2.5
1	C	44	ASN	2.5
1	B	174	SER	2.5
1	B	206	GLU	2.5
1	D	52	LYS	2.5
2	L	199	LEU	2.4
1	C	206	GLU	2.4
1	G	61	GLN	2.4
1	G	228	GLU	2.4
3	U	35	GLU	2.4
1	D	174	SER	2.4
2	N	194	SER	2.4
2	M	198	LYS	2.4
2	J	149	ASP	2.4
1	G	226	GLN	2.4
1	D	59	ILE	2.4
1	G	171	ALA	2.4
1	D	65	GLU	2.4
2	N	23	GLU	2.4
1	D	126	TYR	2.4
1	A	232	PHE	2.4
1	D	232	PHE	2.4
1	G	175	PHE	2.4
2	H	25	PHE	2.4
2	M	190[A]	ASP	2.4
2	I	144	GLU	2.4
1	C	183	ASN	2.4
3	P	52	ASN	2.4
2	I	27	MET	2.4
1	E	63	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	52	LYS	2.4
2	N	198	LYS	2.4
1	A	233	LEU	2.3
2	H	201	LEU	2.3
1	G	203	GLU	2.3
3	R	65	GLU	2.3
1	F	226	GLN	2.3
1	B	44	ASN	2.3
1	B	62	ASN	2.3
2	N	30	ASN	2.3
3	P	229	MET	2.3
1	F	53	LYS	2.3
2	K	144	GLU	2.3
1	B	201	LEU	2.3
1	F	232	PHE	2.3
1	G	52	LYS	2.3
1	A	226	GLN	2.3
1	D	62	ASN	2.3
1	D	175	PHE	2.3
2	N	200	GLY	2.3
3	S	57	ARG	2.3
1	B	53	LYS	2.3
1	B	207	LEU	2.3
1	C	66	LYS	2.3
1	D	207	LEU	2.3
1	A	126	TYR	2.2
1	B	202	GLU	2.2
3	P	58	ALA	2.2
1	A	61	GLN	2.2
1	F	200	SER	2.2
3	Q	4	LYS	2.2
1	E	227	GLU	2.2
1	D	127	GLY	2.2
3	O	53	SER	2.2
3	Q	134	GLY	2.2
3	R	172	GLY	2.2
3	T	6	ALA	2.2
1	F	183	ASN	2.2
1	D	184	LEU	2.2
1	E	66	LYS	2.2
1	A	203	GLU	2.1
2	J	25	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	67	ILE	2.1
1	F	233	LEU	2.1
2	K	201	LEU	2.1
1	A	208	LYS	2.1
2	L	181	LYS	2.1
3	Q	144	ALA	2.1
3	S	58	ALA	2.1
1	G	216	THR	2.1
2	J	194	SER	2.1
3	P	49	VAL	2.1
1	B	184	LEU	2.1
1	G	183	ASN	2.1
2	I	199	LEU	2.1
3	T	52	ASN	2.1
1	C	189	ALA	2.1
1	F	126	TYR	2.1
3	P	50	ILE	2.1
2	I	194	SER	2.1
1	C	205	GLU	2.1
2	J	23	GLU	2.1
2	N	9	LYS	2.1
1	F	219	ASN	2.1
1	E	226	GLN	2.1
3	U	30	ALA	2.1
1	G	90	ASP	2.1
2	J	197	ARG	2.1
1	B	59	ILE	2.0
1	B	198	LYS	2.0
1	E	208	LYS	2.0
1	F	182	GLU	2.0
3	O	45	GLU	2.0
3	P	15[A]	SER	2.0
3	O	224	THR	2.0
2	H	200	GLY	2.0
2	K	199	LEU	2.0
2	N	182	ASP	2.0
1	C	228	GLU	2.0
1	G	206	GLU	2.0
3	P	204[A]	MET	2.0
1	C	143	GLN	2.0
1	D	226	GLN	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($\text{\AA}^2$)	Q<0.9
4	SO4	A	4001	5/5	0.70	0.18	105,106,106,106	0
4	SO4	D	4004	5/5	0.70	0.16	86,86,87,87	0
4	SO4	F	4005	5/5	0.72	0.16	106,106,106,106	0
4	SO4	C	4003	5/5	0.82	0.15	97,98,98,98	0
4	SO4	F	4006	5/5	0.82	0.13	68,69,69,70	0
4	SO4	B	4002	5/5	0.84	0.14	68,69,69,69	0
4	SO4	G	4007	5/5	0.85	0.10	70,71,72,72	0
4	SO4	B	4016	5/5	0.89	0.11	54,55,55,56	0
5	GOL	H	5004	6/6	0.90	0.11	33,37,38,38	0
5	GOL	J	5006	6/6	0.90	0.12	35,37,39,43	0
4	SO4	K	4018	5/5	0.91	0.09	46,49,51,51	0
4	SO4	L	4019	5/5	0.92	0.09	51,54,54,55	0
5	GOL	I	5005	6/6	0.92	0.10	31,34,35,40	0
4	SO4	M	4010	5/5	0.92	0.10	43,46,47,49	0
5	GOL	M	5002	6/6	0.92	0.10	35,36,37,38	0
4	SO4	J	4017	5/5	0.93	0.09	50,51,52,52	0
4	SO4	H	4015	5/5	0.93	0.09	45,47,48,49	0
4	SO4	M	4020	5/5	0.93	0.09	51,52,53,53	0
4	SO4	N	4021	5/5	0.93	0.08	52,53,54,54	0
5	GOL	N	5003	6/6	0.93	0.10	30,33,36,38	0
5	GOL	K	5007	6/6	0.94	0.08	32,36,37,38	0
5	GOL	L	5001	6/6	0.94	0.08	35,36,37,39	0
4	SO4	I	4011	5/5	0.94	0.17	35,40,41,43	0
4	SO4	H	4008	5/5	0.94	0.14	38,40,42,42	0
4	SO4	K	4013	5/5	0.95	0.16	36,39,41,42	0
4	SO4	N	4009	5/5	0.95	0.15	38,39,42,42	0
4	SO4	J	4012	5/5	0.96	0.15	34,38,39,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	L	4014	5/5	0.96	0.12	36,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.