Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 01:54 pm GMT

PDB ID	:	5LEZ
Title	:	Human 20S proteasome complex with Oprozomib in Mg-Acetate at 2.2 Angstrom
Authors	:	Schrader, J.; Henneberg, F.; Mata, R.; Tittmann, K.; Schneider, T.R.; Stark, H.; Bourenkov, G.; Chari, A.
Deposited on	:	2016-06-30
Resolution	:	2.19 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

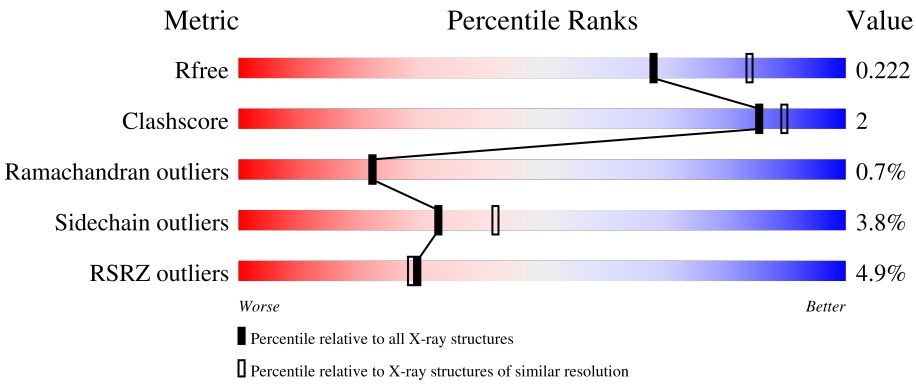
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.19 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	234	2%, 85%, 12%
1	O	234	13%, 87%, 9%
2	B	261	7%, 89%, 6%, 5%
2	P	261	11%, 84%, 10%, 5%
3	C	248	12%, 83%, 9%

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Mol	Chain	Length	Quality of chain
3	Q	248	17% 83% 10% 5%
4	D	241	8% 87% 9%
4	R	241	2% 88% 7%
5	E	263	4% 80% 7% 11%
5	S	263	2% 79% 10% 10%
6	F	255	% 86% 7% 6%
6	T	255	5% 85% 7% 6%
7	G	246	4% 92% 5%
7	U	246	15% 89% 7%
8	H	234	% 87% 7% 6%
8	V	234	3% 86% 7% 6%
9	I	205	92% 7%
9	W	205	2% 95%
10	J	201	% 86% 10%
10	X	201	% 86% 9%
11	K	204	2% 86% 11%
11	Y	204	% 87% 8%
12	L	213	93% 7%
12	Z	213	% 92% 7%
13	M	219	2% 93% 5%
13	a	219	% 94% 5%
14	N	205	% 92% 6%
14	b	205	5% 95%
15	c	4	50% 50%
15	d	4	75% 25%

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Mol	Chain	Length	Quality of chain
15	e	4	50% 50%
15	f	4	50% 50%

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
7	6V1	U	47	X	-	-	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 52158 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 subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	230	1788	1145	301	336	6	0	3	0
1	O	230	1741	1111	293	331	6	0	0	0

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	248	1922	1217	331	363	11	0	2	0
2	P	247	1898	1200	321	366	11	0	2	0

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	237	1798	1121	320	352	5	0	2	0
3	Q	235	1801	1126	316	354	5	0	0	0

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	233	1762	1105	290	356	11	0	1	0
4	R	233	1753	1103	293	346	11	0	1	0

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	234	1822	1144	325	342	11	0	1	0
5	S	238	1875	1175	340	349	11	0	3	0

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	239	1888	1198	325	353	12	0	4	0
6	T	240	1856	1178	315	351	12	0	1	0

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	244	1912	1214	321	364	13	0	2	0
7	U	238	1815	1147	304	350	14	0	1	0

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	220	1664	1047	284	320	13	0	2	0
8	V	220	1622	1023	269	318	12	0	2	0

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	204	1613	1028	270	295	20	0	3	0
9	W	204	1599	1018	267	295	19	0	2	0

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	196	1590	1021	271	288	10	0	3	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	X	196	1576	1012	267	287	10	0	2	0

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	200	1551	977	272	293	9	0	0	0
11	Y	199	1570	991	278	291	10	0	3	0

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	213	1636	1038	277	310	11	0	2	0
12	Z	213	1642	1041	280	310	11	0	1	0

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	216	1692	1067	291	322	12	0	1	0
13	a	216	1688	1064	291	321	12	0	2	0

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	202	1519	953	258	295	13	0	1	0
14	b	203	1524	956	259	296	13	0	1	0

- Molecule 15 is a protein called bound Oprozomib.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	c	4	37	25	4	7	1	0	0	0
15	d	4	37	25	4	7	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	e	4	37	25	4	7	1	0	0	0
			Total	C	N	O	S			
15	f	4	37	25	4	7	1	0	0	0

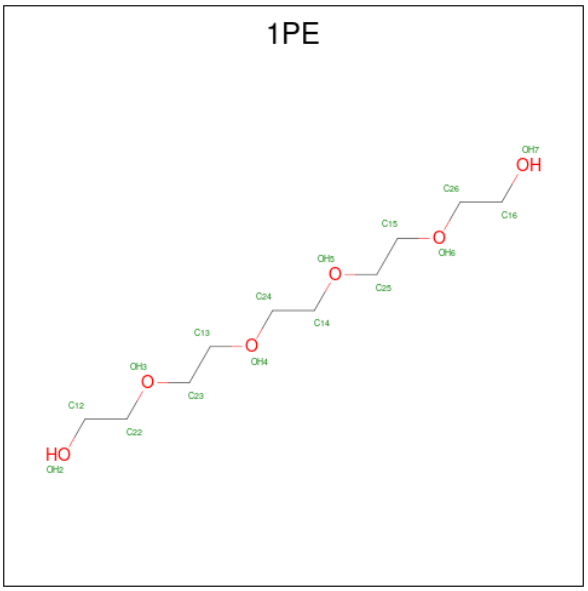
- Molecule 16 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
16	G	1	1	1	0	0
			Total	K		
16	L	1	1	1	0	0
			Total	K		
16	N	1	1	1	0	0
			Total	K		
16	U	1	1	1	0	0
			Total	K		
16	Z	1	1	1	0	0
			Total	K		
16	b	1	1	1	0	0

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

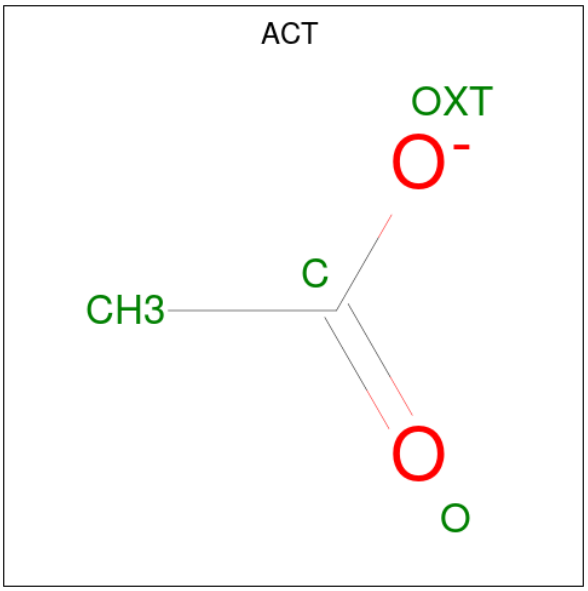
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
17	H	2	2	2	0	0
			Total	Mg		
17	I	2	2	2	0	0
			Total	Mg		
17	J	1	1	1	0	0
			Total	Mg		
17	K	1	1	1	0	0
			Total	Mg		
17	L	1	1	1	0	0
			Total	Mg		
17	V	1	1	1	0	0
			Total	Mg		
17	W	1	1	1	0	0
			Total	Mg		
17	X	1	1	1	0	0

- Molecule 18 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
18	H	1	16	10	6	0	0
			Total	C	O		
18	I	1	16	10	6	0	0
			Total	C	O		
18	K	1	16	10	6	0	0
			Total	C	O		
18	L	1	16	10	6	0	0
			Total	C	O		
18	N	1	16	10	6	0	0
			Total	C	O		
18	U	1	16	10	6	0	0
			Total	C	O		
18	W	1	16	10	6	0	0
			Total	C	O		
18	Y	1	16	10	6	0	0
			Total	C	O		
18	a	1	16	10	6	0	0

- Molecule 19 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	c	1	4	2	2	0	0
19	d	1	4	2	2	0	0
19	e	1	4	2	2	0	0
19	f	1	4	2	2	0	0

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
20	A	120	120	120	0	0
20	B	130	130	130	0	0
20	C	80	80	80	0	0
20	D	99	99	99	0	0
20	E	147	147	147	0	0
20	F	185	185	185	0	0
20	G	196	196	196	0	0
20	H	156	156	156	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	I	161	Total O 161 161	0	0
20	J	136	Total O 136 136	0	0
20	K	106	Total O 106 106	0	0
20	L	127	Total O 127 127	0	0
20	M	155	Total O 155 155	0	0
20	N	160	Total O 160 160	0	0
20	O	94	Total O 94 94	0	0
20	P	127	Total O 127 127	0	0
20	Q	77	Total O 77 77	0	0
20	R	133	Total O 133 133	0	0
20	S	132	Total O 132 132	0	0
20	T	95	Total O 95 95	0	0
20	U	116	Total O 116 116	0	0
20	V	114	Total O 114 114	0	0
20	W	120	Total O 120 120	0	0
20	X	129	Total O 129 129	0	0
20	Y	149	Total O 149 149	0	0
20	Z	168	Total O 168 168	0	0
20	a	179	Total O 179 179	0	0
20	b	118	Total O 118 118	0	0
20	c	2	Total O 2 2	0	0

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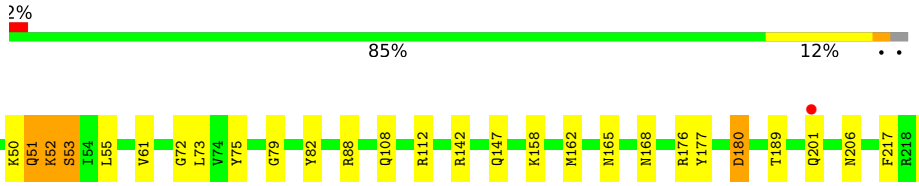
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
20	d	2	2	2	0	0
			Total	O		
20	e	3	3	3	0	0
			Total	O		
20	f	1	1	1	0	0

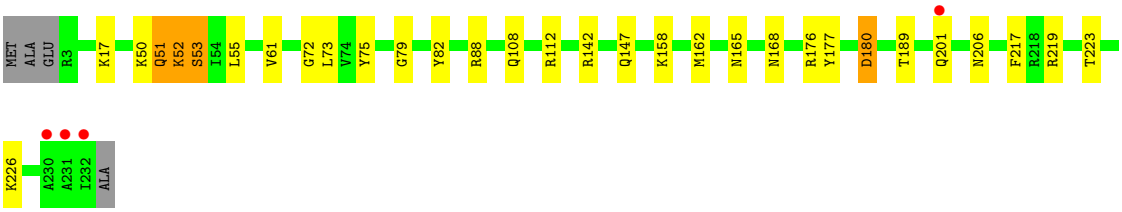
3 Residue-property plots (i)

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 subunit alpha type-2

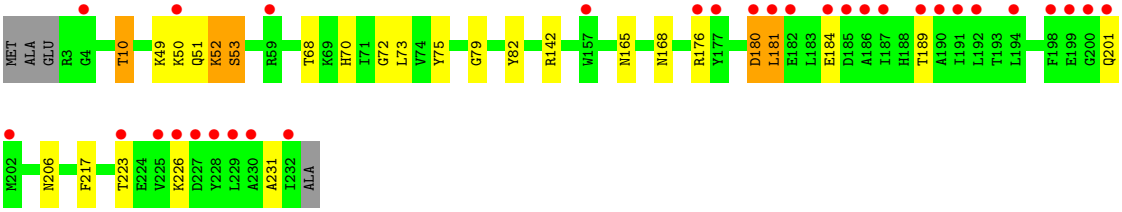
Chain A:





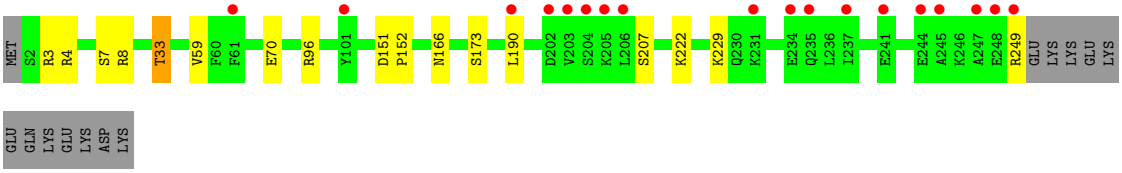
• Molecule 1: Proteasome subunit alpha type-2

Chain O:



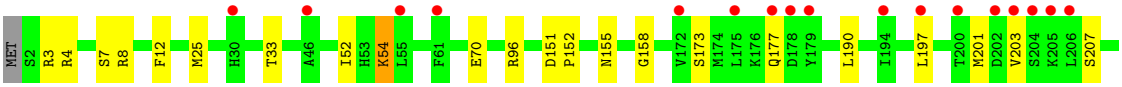
• Molecule 2: Proteasome subunit alpha type-4

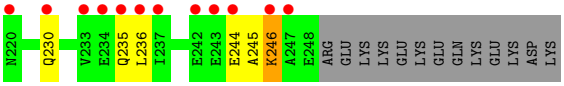
Chain B:



• Molecule 2: Proteasome subunit alpha type-4

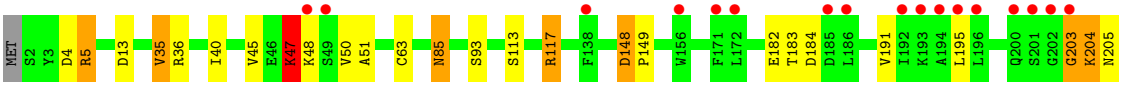
Chain P:

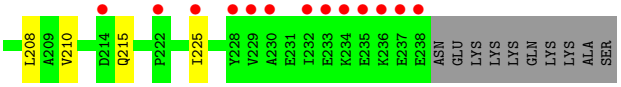




• Molecule 3: Proteasome subunit alpha type-7

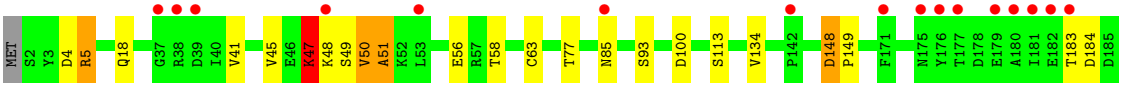
Chain C:

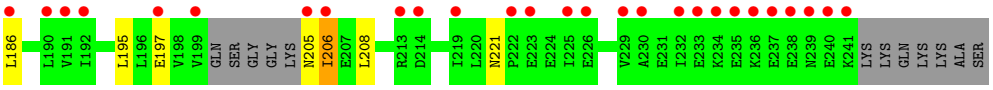




• Molecule 3: Proteasome subunit alpha type-7

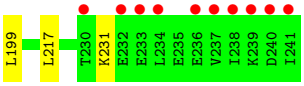
Chain Q:





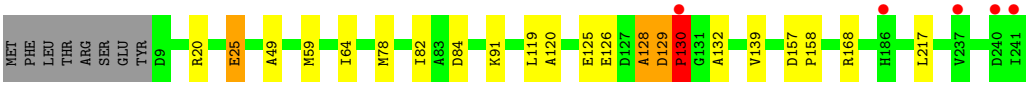
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



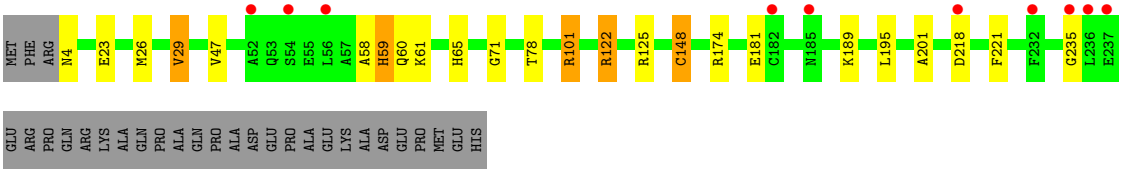
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



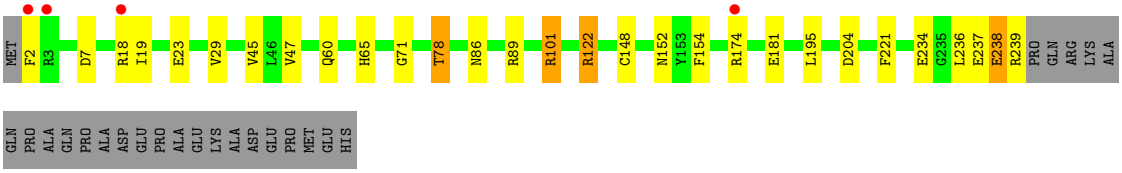
• Molecule 5: Proteasome subunit alpha type-1

Chain E:



- Molecule 5: Proteasome subunit alpha type-1

Chain S:

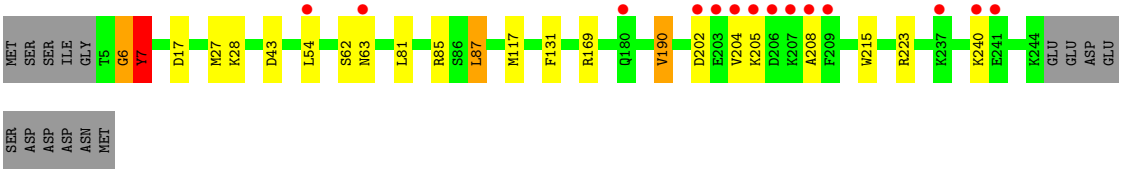


- Molecule 6: Proteasome subunit alpha type-3

Chain F:

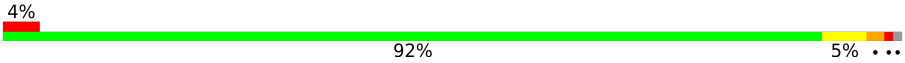
- Molecule 6: Proteasome subunit alpha type-3

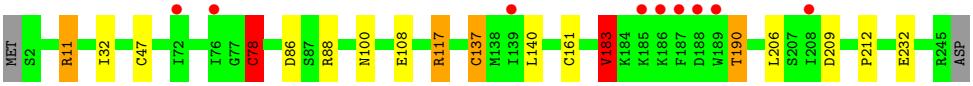
Chain T:



- Molecule 7: Proteasome subunit alpha type-6

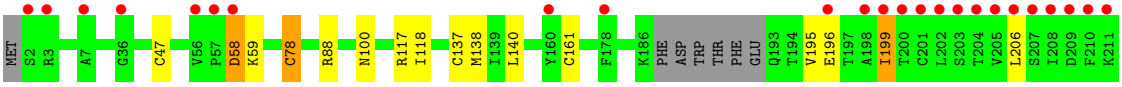
Chain G:

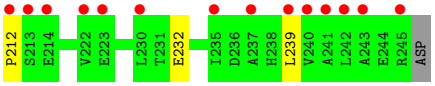




- Molecule 7: Proteasome subunit alpha type-6

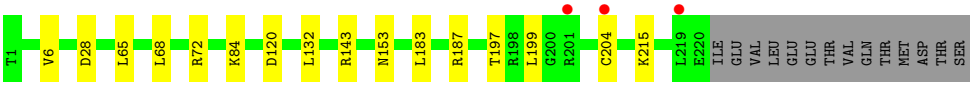
Chain U:





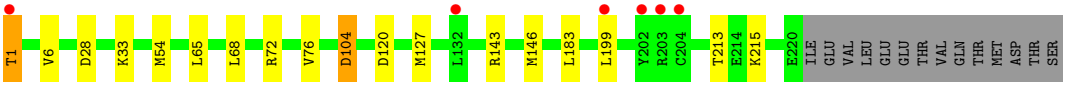
• Molecule 8: Proteasome subunit beta type-7

Chain H:



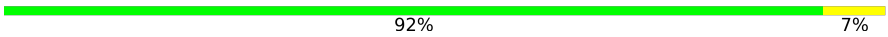
• Molecule 8: Proteasome subunit beta type-7

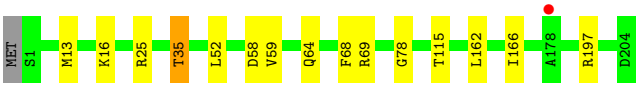
Chain V:



• Molecule 9: Proteasome subunit beta type-3

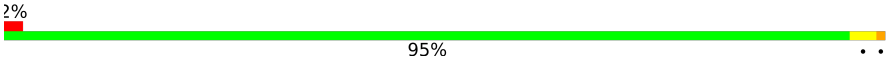
Chain I:





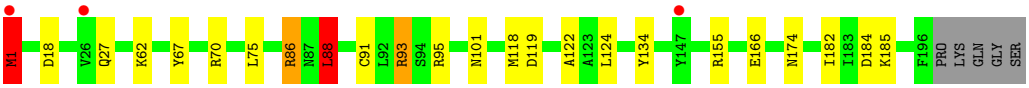
• Molecule 9: Proteasome subunit beta type-3

Chain W:



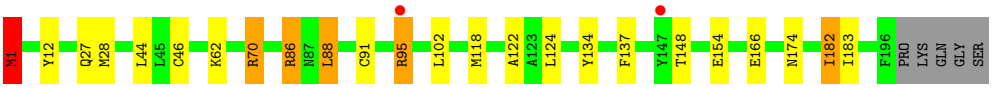
• Molecule 10: Proteasome subunit beta type-2

Chain J:



• Molecule 10: Proteasome subunit beta type-2

Chain X:

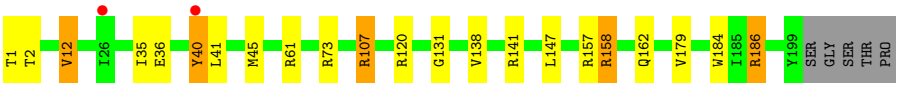


• Molecule 11: Proteasome subunit beta type-5

Chain K:

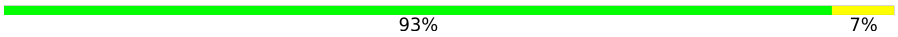
- Molecule 11: Proteasome subunit beta type-5

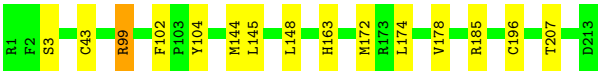
Chain Y:



- Molecule 12: Proteasome subunit beta type-1

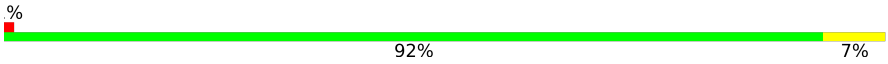
Chain L:

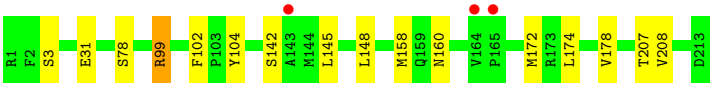




- Molecule 12: Proteasome subunit beta type-1

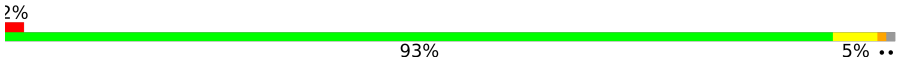
Chain Z:

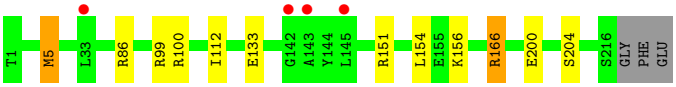




- Molecule 13: Proteasome subunit beta type-4

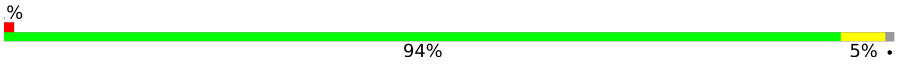
Chain M:

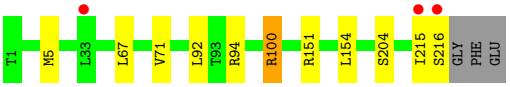




- Molecule 13: Proteasome subunit beta type-4

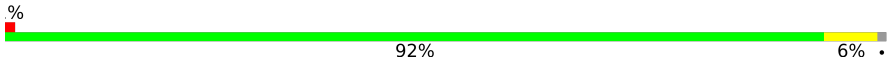
Chain a:

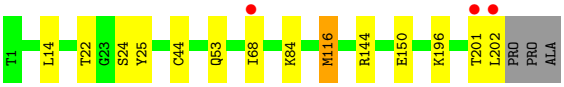




- Molecule 14: Proteasome subunit beta type-6

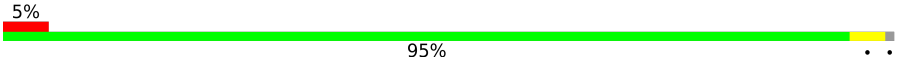
Chain N:





• Molecule 14: Proteasome subunit beta type-6

Chain b:



• Molecule 15: bound Oprozomib

Chain c:

• Molecule 15: bound Oprozomib

Chain d:

• Molecule 15: bound Oprozomib

Chain e:

• Molecule 15: bound Oprozomib

Chain f:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.86Å 203.23Å 315.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.81 – 2.19 49.67 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.4 (170.81-2.19) 99.5 (49.67-2.19)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.181 , 0.222 0.185 , 0.222	Depositor DCC
R_{free} test set	18458 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	49.6	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	52158	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 6V9, 1PE, MG, OAS, 6VA, K, 6V1, YCM, ACT

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	0.70	0/1833	0.80	2/2489 (0.1%)
1	O	0.60	0/1778	0.79	1/2419 (0.0%)
2	B	0.73	0/1958	0.87	4/2645 (0.2%)
2	P	0.67	0/1934	0.86	3/2617 (0.1%)
3	C	0.77	1/1818 (0.1%)	0.94	8/2469 (0.3%)
3	Q	0.71	0/1814	0.88	2/2462 (0.1%)
4	D	0.70	0/1789	0.82	4/2424 (0.2%)
4	R	0.82	2/1780 (0.1%)	0.91	5/2408 (0.2%)
5	E	0.71	1/1842 (0.1%)	0.86	2/2493 (0.1%)
5	S	0.71	0/1901	0.89	5/2571 (0.2%)
6	F	0.78	0/1935	0.89	4/2605 (0.2%)
6	T	0.79	1/1894 (0.1%)	0.93	8/2556 (0.3%)
7	G	0.82	3/1909 (0.2%)	0.88	7/2579 (0.3%)
7	U	0.70	0/1804	0.82	2/2441 (0.1%)
8	H	0.81	1/1697 (0.1%)	0.97	5/2299 (0.2%)
8	V	0.68	2/1655 (0.1%)	0.88	4/2251 (0.2%)
9	I	0.76	0/1648	0.96	8/2219 (0.4%)
9	W	0.62	0/1630	0.89	6/2197 (0.3%)
10	J	0.82	0/1613	0.99	5/2180 (0.2%)
10	X	0.74	1/1599 (0.1%)	0.94	4/2163 (0.2%)
11	K	0.73	0/1582	0.97	9/2138 (0.4%)
11	Y	0.85	1/1610 (0.1%)	1.00	9/2172 (0.4%)
12	L	0.67	0/1672	0.85	3/2257 (0.1%)
12	Z	0.84	4/1675 (0.2%)	0.91	3/2257 (0.1%)
13	M	0.79	0/1728	0.93	5/2339 (0.2%)
13	a	0.83	0/1724	0.93	4/2336 (0.2%)
14	N	0.86	2/1548 (0.1%)	0.90	2/2095 (0.1%)
14	b	0.81	0/1554	0.90	4/2104 (0.2%)
All	All	0.75	19/48924 (0.0%)	0.90	128/66185 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	3
3	Q	0	2
4	D	0	2
4	R	0	1
5	E	0	1
6	F	0	1
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	2
13	a	0	1
All	All	1	17

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	182	GLU	CD-OE2	8.46	1.34	1.25
7	G	108	GLU	CD-OE1	8.18	1.34	1.25
12	Z	3	SER	CB-OG	7.22	1.51	1.42
10	X	154	GLU	C-O	6.91	1.36	1.23
14	N	24	SER	CB-OG	-6.42	1.33	1.42
12	Z	31	GLU	CD-OE2	6.28	1.32	1.25
6	T	7	TYR	N-CA	6.26	1.58	1.46
7	G	108	GLU	CD-OE2	6.26	1.32	1.25
4	R	25	GLU	CG-CD	6.07	1.61	1.51
14	N	150	GLU	CG-CD	5.82	1.60	1.51
7	G	78	CYS	CB-SG	-5.71	1.72	1.81
4	R	25	GLU	CD-OE1	5.64	1.31	1.25
11	Y	40	TYR	CE1-CZ	5.63	1.45	1.38
5	E	4	ASN	N-CA	5.46	1.57	1.46
8	V	104[A]	ASP	CB-CG	-5.43	1.40	1.51
8	V	104[B]	ASP	CB-CG	-5.43	1.40	1.51
12	Z	142	SER	CB-OG	-5.10	1.35	1.42
8	H	120	ASP	CB-CG	5.10	1.62	1.51
12	Z	78	SER	CB-OG	-5.06	1.35	1.42

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	99	ARG	NE-CZ-NH2	-11.67	114.46	120.30
10	J	86	ARG	NE-CZ-NH1	10.77	125.68	120.30
9	I	69	ARG	NE-CZ-NH1	10.36	125.48	120.30
4	R	120[A]	ALA	C-N-CA	9.90	146.45	121.70
4	R	120[B]	ALA	C-N-CA	9.90	146.45	121.70
9	W	69	ARG	NE-CZ-NH1	9.79	125.20	120.30
12	L	99	ARG	NE-CZ-NH2	-9.79	115.41	120.30
10	X	86	ARG	NE-CZ-NH1	9.78	125.19	120.30
12	Z	99	ARG	NE-CZ-NH1	9.35	124.98	120.30
8	H	72	ARG	NE-CZ-NH2	-9.23	115.68	120.30
9	W	16[A]	LYS	C-N-CA	9.19	144.67	121.70
9	W	16[B]	LYS	C-N-CA	9.19	144.67	121.70
10	J	86	ARG	NE-CZ-NH2	-9.03	115.79	120.30
10	X	86	ARG	NE-CZ-NH2	-8.95	115.83	120.30
9	I	69	ARG	NE-CZ-NH2	-8.65	115.97	120.30
9	I	16[A]	LYS	C-N-CA	8.52	143.00	121.70
9	I	16[B]	LYS	C-N-CA	8.52	143.00	121.70
2	B	96	ARG	NE-CZ-NH1	8.29	124.45	120.30
11	Y	120	ARG	NE-CZ-NH1	8.18	124.39	120.30
3	Q	5	ARG	NE-CZ-NH2	-8.11	116.25	120.30
12	L	99	ARG	NE-CZ-NH1	7.97	124.29	120.30
2	P	96	ARG	NE-CZ-NH1	7.82	124.21	120.30
10	J	184	ASP	CB-CG-OD1	7.78	125.31	118.30
11	K	120	ARG	NE-CZ-NH1	7.74	124.17	120.30
11	Y	157	ARG	NE-CZ-NH1	7.64	124.12	120.30
14	b	1	THR	N-CA-CB	7.61	124.75	110.30
11	K	107	ARG	NE-CZ-NH1	7.42	124.01	120.30
9	I	25[A]	ARG	NE-CZ-NH1	7.19	123.89	120.30
9	I	25[B]	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	O	181	LEU	CA-CB-CG	7.15	131.75	115.30
6	T	43	ASP	CB-CG-OD2	7.15	124.73	118.30
9	W	69	ARG	NE-CZ-NH2	-7.06	116.77	120.30
7	U	88	ARG	NE-CZ-NH1	6.94	123.77	120.30
7	G	117	ARG	NE-CZ-NH1	6.84	123.72	120.30
11	K	1	THR	N-CA-CB	6.83	123.27	110.30
7	G	86	ASP	CB-CG-OD1	6.75	124.37	118.30
11	Y	157	ARG	NE-CZ-NH2	-6.74	116.93	120.30
3	C	5	ARG	NE-CZ-NH2	-6.66	116.97	120.30
11	K	157	ARG	NE-CZ-NH1	6.62	123.61	120.30
5	S	122	ARG	NE-CZ-NH2	-6.59	117.00	120.30
6	F	190	VAL	CB-CA-C	-6.56	98.94	111.40
13	M	151	ARG	NE-CZ-NH1	6.55	123.58	120.30
14	N	116	MET	CG-SD-CE	-6.49	89.82	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	120	ARG	NE-CZ-NH2	-6.48	117.06	120.30
11	Y	158	ARG	NE-CZ-NH1	6.47	123.54	120.30
4	R	84	ASP	CB-CG-OD1	6.43	124.08	118.30
7	U	117	ARG	NE-CZ-NH1	6.40	123.50	120.30
6	F	43	ASP	CB-CG-OD1	6.39	124.05	118.30
5	E	122	ARG	NE-CZ-NH2	-6.38	117.11	120.30
8	H	72	ARG	NE-CZ-NH1	6.38	123.49	120.30
10	X	154	GLU	O-C-N	6.37	132.89	122.70
2	B	96	ARG	NE-CZ-NH2	-6.36	117.12	120.30
11	K	154	ASP	CB-CG-OD2	6.35	124.01	118.30
6	F	117	MET	CG-SD-CE	6.34	110.34	100.20
6	T	117	MET	CG-SD-CE	6.26	110.21	100.20
11	Y	107	ARG	NE-CZ-NH1	6.24	123.42	120.30
4	D	175[A]	GLU	N-CA-C	-6.22	94.22	111.00
4	D	175[B]	GLU	N-CA-C	-6.22	94.22	111.00
1	A	219	ARG	NE-CZ-NH1	6.18	123.39	120.30
8	H	28	ASP	CB-CG-OD1	6.13	123.81	118.30
11	Y	1	THR	N-CA-CB	6.11	121.92	110.30
4	D	168	ARG	NE-CZ-NH1	6.11	123.35	120.30
13	M	99	ARG	NE-CZ-NH1	6.08	123.34	120.30
7	G	11	ARG	NE-CZ-NH1	6.04	123.32	120.30
11	K	120	ARG	NE-CZ-NH2	-6.04	117.28	120.30
12	Z	172	MET	CG-SD-CE	-6.03	90.56	100.20
2	B	4	ARG	NE-CZ-NH1	5.99	123.30	120.30
6	T	190	VAL	CB-CA-C	-5.99	100.02	111.40
6	T	6	GLY	C-N-CA	5.99	136.66	121.70
7	G	108	GLU	OE1-CD-OE2	5.97	130.47	123.30
1	A	219	ARG	NE-CZ-NH2	-5.97	117.31	120.30
5	E	174	ARG	NE-CZ-NH1	5.95	123.28	120.30
11	Y	158	ARG	NE-CZ-NH2	-5.90	117.35	120.30
2	P	4	ARG	NE-CZ-NH1	5.89	123.25	120.30
6	T	7	TYR	N-CA-CB	5.89	121.20	110.60
11	K	42	LEU	CA-CB-CG	5.87	128.81	115.30
6	T	27	MET	CG-SD-CE	5.87	109.59	100.20
10	X	70	ARG	NE-CZ-NH2	-5.87	117.37	120.30
3	C	182	GLU	OE1-CD-OE2	-5.81	116.33	123.30
6	F	85	ARG	NE-CZ-NH1	5.77	123.19	120.30
13	a	100	ARG	NE-CZ-NH2	-5.73	117.44	120.30
3	Q	5	ARG	NE-CZ-NH1	5.71	123.16	120.30
9	I	197	ARG	NE-CZ-NH1	5.65	123.13	120.30
13	M	166	ARG	NE-CZ-NH1	5.64	123.12	120.30
8	V	72	ARG	NE-CZ-NH1	5.62	123.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	89	ARG	NE-CZ-NH2	-5.61	117.50	120.30
14	b	116	MET	CG-SD-CE	-5.55	91.33	100.20
4	R	168	ARG	NE-CZ-NH1	5.54	123.07	120.30
10	J	88	LEU	CB-CG-CD2	5.52	120.38	111.00
3	C	5	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	P	3	ARG	NE-CZ-NH2	-5.49	117.55	120.30
3	C	117	ARG	CG-CD-NE	5.43	123.22	111.80
8	V	120	ASP	CB-CG-OD1	5.43	123.19	118.30
14	b	45	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	B	3	ARG	NE-CZ-NH2	-5.39	117.60	120.30
13	a	5	MET	CG-SD-CE	5.39	108.82	100.20
5	S	174	ARG	NE-CZ-NH1	5.36	122.98	120.30
6	T	169	ARG	NE-CZ-NH1	5.35	122.98	120.30
13	a	151	ARG	NE-CZ-NH1	5.35	122.98	120.30
3	C	85[A]	ASN	CB-CA-C	5.34	121.08	110.40
3	C	85[B]	ASN	CB-CA-C	5.34	121.08	110.40
8	H	187[A]	ARG	NE-CZ-NH2	-5.34	117.63	120.30
8	H	187[B]	ARG	NE-CZ-NH2	-5.34	117.63	120.30
7	G	183	VAL	CB-CA-C	-5.33	101.28	111.40
5	S	122	ARG	NE-CZ-NH1	5.32	122.96	120.30
13	M	166	ARG	NE-CZ-NH2	-5.30	117.65	120.30
9	W	25[A]	ARG	NE-CZ-NH1	5.28	122.94	120.30
9	W	25[B]	ARG	NE-CZ-NH1	5.28	122.94	120.30
11	K	157	ARG	NE-CZ-NH2	-5.26	117.67	120.30
3	C	47	LYS	N-CA-C	5.24	125.15	111.00
13	M	5	MET	CG-SD-CE	5.24	108.58	100.20
14	N	144	ARG	NE-CZ-NH1	5.21	122.91	120.30
4	D	84	ASP	CB-CG-OD1	5.19	122.97	118.30
7	G	11	ARG	CG-CD-NE	5.18	122.68	111.80
7	G	117	ARG	NE-CZ-NH2	-5.13	117.73	120.30
9	I	58	ASP	CB-CG-OD2	5.12	122.91	118.30
8	V	28	ASP	CB-CG-OD1	5.12	122.91	118.30
11	K	154	ASP	CB-CG-OD1	-5.12	113.69	118.30
4	R	128	ALA	N-CA-C	5.11	124.80	111.00
14	b	29	ARG	CB-CA-C	-5.10	100.20	110.40
8	V	72	ARG	NE-CZ-NH2	-5.09	117.76	120.30
12	L	172	MET	CG-SD-CE	-5.08	92.07	100.20
11	Y	61	ARG	NE-CZ-NH1	5.06	122.83	120.30
13	a	67	LEU	CA-CB-CG	5.05	126.91	115.30
3	C	36	ARG	NE-CZ-NH1	5.03	122.81	120.30
6	T	85	ARG	NE-CZ-NH1	5.03	122.81	120.30
10	J	93	ARG	NE-CZ-NH1	5.03	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	7	ASP	CB-CG-OD1	-5.01	113.79	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Peptide
5	E	235	GLY	Peptide
6	F	206	ASP	Peptide
9	I	78	GLY	Peptide
10	J	1[A]	MET	Peptide
10	J	1[B]	MET	Peptide
2	P	244	GLU	Peptide
2	P	245	ALA	Peptide
2	P	54	LYS	Peptide
3	Q	47	LYS	Peptide
3	Q	49	SER	Peptide
4	R	130	PRO	Peptide
9	W	78	GLY	Peptide
10	X	1	MET	Peptide
10	X	148	THR	Mainchain
13	a	215	ILE	Peptide

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	1788	0	1761	12	0
1	O	1741	0	1683	9	0
2	B	1922	0	1913	4	0
2	P	1898	0	1861	11	0
3	C	1798	0	1718	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	1801	0	1735	14	0
4	D	1762	0	1709	10	0
4	R	1753	0	1726	10	0
5	E	1822	0	1779	11	0
5	S	1875	0	1818	15	0
6	F	1888	0	1882	4	0
6	T	1856	0	1816	4	0
7	G	1912	0	1882	7	0
7	U	1815	0	1748	6	0
8	H	1664	0	1681	6	0
8	V	1622	0	1595	8	0
9	I	1613	0	1646	5	0
9	W	1599	0	1621	4	0
10	J	1590	0	1581	14	0
10	X	1576	0	1561	16	0
11	K	1551	0	1506	9	0
11	Y	1570	0	1547	11	0
12	L	1636	0	1625	7	0
12	Z	1642	0	1635	6	0
13	M	1692	0	1670	4	0
13	a	1688	0	1658	0	0
14	N	1519	0	1493	6	0
14	b	1524	0	1493	0	0
15	c	37	0	6	0	0
15	d	37	0	6	0	0
15	e	37	0	6	0	0
15	f	37	0	6	0	0
16	G	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	Z	1	0	0	0	0
16	b	1	0	0	0	0
17	H	2	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	K	1	0	0	0	0
17	L	1	0	0	0	0
17	V	1	0	0	0	0
17	W	1	0	0	0	0
17	X	1	0	0	0	0
18	H	16	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	I	16	0	22	0	0
18	K	16	0	22	0	0
18	L	16	0	22	0	0
18	N	16	0	22	0	0
18	U	16	0	22	0	0
18	W	16	0	22	0	0
18	Y	16	0	22	0	0
18	a	16	0	22	0	0
19	c	4	0	3	0	0
19	d	4	0	3	0	0
19	e	4	0	3	0	0
19	f	4	0	3	0	0
20	A	120	0	0	2	0
20	B	130	0	0	1	0
20	C	80	0	0	1	0
20	D	99	0	0	1	0
20	E	147	0	0	3	0
20	F	185	0	0	1	1
20	G	196	0	0	2	1
20	H	156	0	0	1	0
20	I	161	0	0	1	0
20	J	136	0	0	2	0
20	K	106	0	0	1	0
20	L	127	0	0	0	0
20	M	155	0	0	0	0
20	N	160	0	0	0	0
20	O	94	0	0	1	0
20	P	127	0	0	2	0
20	Q	77	0	0	0	0
20	R	133	0	0	1	0
20	S	132	0	0	5	0
20	T	95	0	0	0	0
20	U	116	0	0	0	0
20	V	114	0	0	1	0
20	W	120	0	0	2	0
20	X	129	0	0	0	0
20	Y	149	0	0	1	0
20	Z	168	0	0	0	0
20	a	179	0	0	0	0
20	b	118	0	0	0	0
20	c	2	0	0	0	0
20	d	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	e	3	0	0	0	0
20	f	1	0	0	0	0
All	All	52158	0	47577	199	1

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 2.

All (199) 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)
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.64	0.80
6:F:227:VAL:O	6:F:232[B]:ARG:NH1	2.14	0.80
5:S:18[B]:ARG:HG2	5:S:23:GLU:OE2	1.84	0.78
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.65	0.77
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.51	0.74
2:P:12:PHE:H	3:Q:18:GLN:HE22	1.35	0.74
5:S:65[A]:HIS:CE1	20:S:304:HOH:O	2.39	0.74
5:S:152[B]:ASN:ND2	20:S:301:HOH:O	2.22	0.73
6:T:202:ASP:O	6:T:205:LYS:O	2.05	0.73
11:Y:35:ILE:HD11	11:Y:45:MET:SD	2.29	0.72
12:L:144:MET:HE1	12:L:185:ARG:HB2	1.72	0.72
11:K:35:ILE:HD11	11:K:45:MET:SD	2.29	0.72
8:V:1:THR:HB	8:V:33:LYS:HZ3	1.55	0.70
9:I:64:GLN:OE1	10:J:86:ARG:NH2	2.26	0.69
3:C:47:LYS:CB	3:C:48:LYS:O	2.41	0.68
5:E:58:ALA:O	5:E:59:HIS:CB	2.43	0.66
6:F:169[A]:ARG:NH1	20:F:302:HOH:O	2.30	0.65
10:X:1:MET:HE1	10:X:134:TYR:H	1.60	0.65
20:H:542:HOH:O	12:Z:160:ASN:CB	2.44	0.64
7:U:199:ILE:HD11	7:U:239:LEU:HD23	1.81	0.63
9:I:35:THR:HG21	20:I:437:HOH:O	1.98	0.63
10:J:1[A]:MET:HE1	10:J:134:TYR:N	2.14	0.63
5:S:86:ASN:ND2	20:S:302:HOH:O	2.33	0.62
5:S:101:ARG:NH1	20:S:303:HOH:O	2.34	0.60
8:V:54:MET:HE1	20:W:448:HOH:O	2.01	0.60
4:R:129:ASP:CB	4:R:130:PRO:CD	2.80	0.59
4:D:96:THR:OG1	20:D:301:HOH:O	2.17	0.59
12:L:144:MET:CE	12:L:185:ARG:HB2	2.32	0.59
11:K:141:ARG:NH1	10:X:166:GLU:OE2	2.35	0.59
9:W:13:MET:HE1	9:W:166:ILE:N	2.18	0.59
8:V:1:THR:HB	8:V:33:LYS:NZ	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:195:VAL:O	7:U:199:ILE:HG23	2.05	0.57
3:Q:41:VAL:HG11	3:Q:134:VAL:HB	1.87	0.57
4:R:49:ALA:HB2	4:R:217:LEU:HD12	1.87	0.57
4:R:78:MET:HG3	4:R:82:ILE:HD12	1.87	0.56
4:R:20:ARG:HD2	4:R:25:GLU:CD	2.26	0.56
5:S:238:GLU:CB	5:S:239:ARG:C	2.74	0.56
13:M:5:MET:HE3	14:N:116:MET:HB2	1.88	0.56
10:X:1:MET:HE1	10:X:134:TYR:N	2.21	0.56
4:D:20:ARG:HD2	4:D:25:GLU:CD	2.27	0.55
10:J:101:ASN:HD22	10:J:119:ASP:HA	1.71	0.55
10:J:166:GLU:OE2	11:Y:141[A]:ARG:NH1	2.40	0.55
9:W:64:GLN:OE1	10:X:86:ARG:NH2	2.40	0.55
4:D:49:ALA:HB2	4:D:217:LEU:HD12	1.88	0.54
11:Y:40:TYR:CD2	11:Y:73:ARG:CZ	2.90	0.54
3:C:203:GLY:CA	3:C:204:LYS:CB	2.87	0.53
7:G:11:ARG:HH11	7:G:11:ARG:HG2	1.74	0.53
9:I:13[A]:MET:HE1	9:I:166:ILE:N	2.23	0.53
1:O:10:THR:HG23	20:O:301:HOH:O	2.09	0.53
7:U:78:CYS:HB2	7:U:140:LEU:HD23	1.90	0.53
4:D:78:MET:HG3	4:D:82:ILE:HD12	1.91	0.52
5:E:23:GLU:HA	5:E:26:MET:HE2	1.90	0.52
8:H:204:CYS:SG	12:Z:158:MET:CE	2.97	0.52
6:F:51:LYS:NZ	6:F:62:SER:O	2.28	0.52
10:X:118:MET:HE2	10:X:124:LEU:HD13	1.91	0.52
1:A:108:GLN:HE21	1:A:112:ARG:HH12	1.57	0.52
12:L:148:LEU:HD23	12:L:178:VAL:CG1	2.39	0.52
3:Q:4:ASP:O	4:R:125:GLU:HB2	2.10	0.52
7:G:78:CYS:HB2	7:G:140:LEU:HD23	1.90	0.52
11:Y:158:ARG:HE	11:Y:162:GLN:HE21	1.56	0.51
3:C:4:ASP:O	4:D:125:GLU:HB2	2.11	0.51
10:X:28:MET:HE3	20:Y:487:HOH:O	2.10	0.51
11:Y:35:ILE:CD1	11:Y:45:MET:SD	2.98	0.51
8:H:132:LEU:HD22	14:N:25:TYR:CE2	2.46	0.51
6:T:87:LEU:HD13	6:T:131:PHE:CE1	2.46	0.51
6:T:6:GLY:HA3	6:T:7:TYR:CD2	2.47	0.50
5:E:23:GLU:HA	5:E:26:MET:CE	2.41	0.50
11:K:35:ILE:CD1	11:K:45:MET:SD	2.99	0.50
12:Z:148:LEU:HD23	12:Z:178:VAL:CG1	2.41	0.50
2:P:155:ASN:OD1	3:Q:77:THR:OG1	2.25	0.50
12:L:43[B]:CYS:HG	12:L:196:CYS:HG	1.57	0.50
10:X:1:MET:HE3	10:X:1:MET:C	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASP:OD1	1:A:180:ASP:N	2.44	0.49
10:X:88:LEU:HB3	10:X:122:ALA:HB2	1.94	0.49
11:K:40:TYR:CD2	11:K:73:ARG:CZ	2.95	0.49
2:P:8:ARG:NH2	3:Q:5:ARG:HD2	2.27	0.49
3:C:35:VAL:HG13	3:C:191:VAL:CG2	2.42	0.49
10:X:46[B]:CYS:SG	10:X:102:LEU:HD22	2.52	0.49
5:S:60:GLN:HE22	5:S:78:THR:HG21	1.78	0.49
11:K:36:GLU:HG2	11:K:184:TRP:CZ2	2.48	0.49
12:Z:145:LEU:HD22	12:Z:178:VAL:HB	1.94	0.48
3:C:183:THR:OG1	3:C:184:ASP:N	2.45	0.48
5:E:101[A]:ARG:NH1	20:E:304:HOH:O	2.46	0.48
7:G:32:ILE:HD13	7:G:137:YCM:HD2	1.95	0.48
7:G:190:THR:HG23	20:G:421:HOH:O	2.12	0.48
3:C:203:GLY:HA2	3:C:204:LYS:CB	2.44	0.48
5:E:71:GLY:HA3	5:E:221:PHE:CZ	2.48	0.48
2:P:155:ASN:ND2	20:P:301:HOH:O	2.43	0.48
1:O:180:ASP:N	1:O:180:ASP:OD1	2.46	0.47
3:C:47:LYS:CB	3:C:48:LYS:C	2.82	0.47
4:D:59:MET:SD	4:D:64:ILE:HD11	2.54	0.47
2:P:246:LYS:N	2:P:246:LYS:HE3	2.29	0.47
1:A:52:LYS:CB	20:A:402:HOH:O	2.62	0.47
4:R:132:ALA:HB1	20:R:306:HOH:O	2.14	0.47
8:H:204:CYS:SG	12:Z:158:MET:HE2	2.55	0.47
12:L:145:LEU:HD22	12:L:178:VAL:HB	1.96	0.47
2:P:25[B]:MET:HA	2:P:25[B]:MET:CE	2.45	0.47
8:V:76:VAL:HG23	8:V:104[A]:ASP:OD2	2.15	0.47
8:H:132:LEU:HD22	14:N:25:TYR:CZ	2.49	0.47
10:J:67:TYR:CD1	10:J:75:LEU:HG	2.50	0.47
8:V:213:THR:HB	9:W:198:THR:OG1	2.14	0.47
10:X:95:ARG:HB2	10:X:95:ARG:HH11	1.79	0.47
1:A:79:GLY:O	1:A:82:TYR:HB3	2.15	0.46
5:E:60:GLN:NE2	5:E:78:THR:HG21	2.30	0.46
10:J:88:LEU:HB3	10:J:122:ALA:HB2	1.97	0.46
4:R:59:MET:SD	4:R:64:ILE:HD11	2.55	0.46
9:I:13[A]:MET:HE3	9:I:162:LEU:HD12	1.98	0.46
8:V:127[B]:MET:HE2	8:V:127[B]:MET:HB3	1.79	0.46
12:Z:99:ARG:HG3	12:Z:104:TYR:CE2	2.50	0.46
1:O:79:GLY:O	1:O:82:TYR:HB3	2.16	0.46
13:M:86:ARG:NH1	13:M:133:GLU:OE2	2.49	0.46
11:Y:36:GLU:HG2	11:Y:184:TRP:CZ2	2.51	0.46
2:B:8:ARG:NH2	3:C:5:ARG:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:27[B]:GLN:NE2	10:J:174:ASN:O	2.49	0.46
10:J:118:MET:HE2	10:J:124:LEU:HD13	1.97	0.46
3:Q:50:VAL:O	3:Q:51:ALA:HB3	2.15	0.46
3:C:215:GLN:CB	20:C:375:HOH:O	2.64	0.46
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.56	0.45
5:E:29:VAL:HG22	5:E:148:6V1:C3	2.47	0.45
7:G:212:PRO:HB2	7:G:232:GLU:HG3	1.99	0.45
10:J:185:LYS:NZ	20:J:405:HOH:O	2.50	0.45
4:R:129:ASP:CB	4:R:130:PRO:HD2	2.46	0.45
11:Y:2:THR:OG1	11:Y:131:GLY:HA3	2.17	0.45
1:A:88[B]:ARG:NH2	20:A:302:HOH:O	2.50	0.45
1:A:158:LYS:HB3	1:A:177:TYR:CE1	2.51	0.45
10:X:44:LEU:HG	10:X:46[B]:CYS:SG	2.57	0.45
3:C:85[B]:ASN:OD1	10:J:70:ARG:NH1	2.50	0.45
3:Q:183:THR:CG2	3:Q:186:LEU:HD13	2.47	0.45
5:S:65[A]:HIS:ND1	20:S:304:HOH:O	2.36	0.45
1:O:72:GLY:HA3	1:O:217:PHE:CE1	2.52	0.45
3:Q:183:THR:OG1	3:Q:184:ASP:N	2.50	0.45
5:S:154:PHE:HD2	6:T:63:ASN:HD21	1.65	0.45
1:A:55:LEU:HD23	7:G:183:VAL:HG21	1.99	0.44
1:O:75:TYR:HB3	1:O:82:TYR:CD2	2.52	0.44
1:A:72:GLY:HA3	1:A:217:PHE:CE1	2.52	0.44
11:K:133:VAL:HG21	10:X:137:PHE:HB3	1.99	0.44
13:M:112:ILE:HD12	13:M:112:ILE:N	2.32	0.44
2:P:151:ASP:HB2	2:P:152:PRO:CD	2.48	0.44
3:C:85[B]:ASN:OD1	10:J:70:ARG:CZ	2.65	0.44
5:E:65:HIS:HB2	20:E:376:HOH:O	2.18	0.44
9:I:52:LEU:HB2	9:I:59:VAL:HG13	2.00	0.44
3:C:40:ILE:HD11	3:C:210:VAL:HG13	1.99	0.44
8:H:84:LYS:NZ	14:N:53:GLN:OE1	2.46	0.43
11:K:2:THR:OG1	11:K:131:GLY:HA3	2.18	0.43
5:E:201:ALA:O	20:E:301:HOH:O	2.21	0.43
7:G:117:ARG:NH2	20:G:403:HOH:O	2.47	0.43
3:Q:47:LYS:HA	3:Q:205:ASN:HA	1.99	0.43
11:K:73:ARG:HG3	20:K:489:HOH:O	2.19	0.43
3:Q:148:ASP:HB2	3:Q:149:PRO:CD	2.48	0.43
3:C:148:ASP:HB2	3:C:149:PRO:CD	2.48	0.43
1:O:165:ASN:OD1	1:O:168:ASN:HB2	2.18	0.43
5:S:237:GLU:O	5:S:238:GLU:CB	2.66	0.43
10:J:93:ARG:HD2	20:J:508:HOH:O	2.17	0.43
7:U:118:ILE:HG21	7:U:138:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:182:ILE:HG13	10:X:183:ILE:N	2.34	0.43
2:P:197:LEU:HB3	2:P:201:MET:HE3	2.01	0.43
7:U:58:ASP:O	7:U:59:LYS:CB	2.66	0.42
1:A:165:ASN:OD1	1:A:168:ASN:HB2	2.19	0.42
1:A:147:GLN:HG3	1:A:162:MET:HE1	2.01	0.42
2:B:151:ASP:HB2	2:B:152:PRO:CD	2.49	0.42
12:L:99:ARG:HG3	12:L:104:TYR:CE2	2.54	0.42
11:Y:12:VAL:HG13	11:Y:179:VAL:HB	2.01	0.42
11:K:12:VAL:HG13	11:K:179:VAL:HB	2.01	0.42
7:U:212:PRO:HB2	7:U:232:GLU:HG3	2.02	0.42
4:R:157:ASP:HB2	4:R:158:PRO:CD	2.50	0.42
5:S:71:GLY:HA3	5:S:221:PHE:CZ	2.54	0.42
4:D:91:LYS:HG2	4:D:119:LEU:HD11	2.00	0.42
3:Q:100:ASP:OD1	11:Y:107:ARG:NH2	2.52	0.42
4:R:91:LYS:HG2	4:R:119:LEU:HD11	2.00	0.42
1:O:49:LYS:O	1:O:51:GLN:N	2.53	0.42
2:P:25[B]:MET:HE2	20:P:304:HOH:O	2.18	0.42
11:Y:186[A]:ARG:HE	11:Y:186[A]:ARG:HB2	1.69	0.41
2:B:33:THR:HB	2:B:166:ASN:O	2.20	0.41
4:D:157:ASP:HB2	4:D:158:PRO:CD	2.50	0.41
1:O:51:GLN:C	1:O:52:LYS:O	2.59	0.41
1:A:51:GLN:C	1:A:52:LYS:O	2.58	0.41
9:W:35:THR:HG21	20:W:417:HOH:O	2.20	0.41
3:C:5:ARG:HD3	4:D:125:GLU:OE2	2.20	0.41
2:P:158:GLY:HA3	3:Q:58:THR:HG21	2.03	0.41
3:Q:85:ASN:OD1	10:X:70:ARG:CZ	2.69	0.41
8:V:143:ARG:HE	8:V:143:ARG:HB2	1.67	0.41
11:Y:40:TYR:CD2	11:Y:73:ARG:NH1	2.89	0.41
6:F:87:LEU:HD13	6:F:131:PHE:CE2	2.55	0.41
1:A:75:TYR:HB3	1:A:82:TYR:CD2	2.56	0.41
8:H:143:ARG:HE	8:H:143:ARG:HB2	1.67	0.41
12:L:144:MET:HB3	12:L:144:MET:HE2	1.84	0.41
13:M:166:ARG:NH2	13:M:200:GLU:OE2	2.53	0.41
8:V:146:MET:HE2	20:V:450:HOH:O	2.21	0.41
1:O:68:THR:HG1	1:O:70:HIS:CE1	2.39	0.41
4:D:127:ASP:HB3	5:E:125:ARG:HD3	2.03	0.40
2:P:25[B]:MET:HA	2:P:25[B]:MET:HE3	2.02	0.40
3:Q:85:ASN:OD1	10:X:70:ARG:NH1	2.55	0.40
10:X:12:TYR:HB2	10:X:182:ILE:HD11	2.03	0.40
14:N:201:THR:HG22	14:N:202:LEU:N	2.37	0.40
5:S:18[B]:ARG:HG3	5:S:19:ILE:N	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:LYS:NZ	20:B:303:HOH:O	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:F:465:HOH:O	20:G:566:HOH:O[4_475]	2.06	0.14

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	231/234 (99%)	222 (96%)	4 (2%)	5 (2%)	6 4
1	O	228/234 (97%)	218 (96%)	4 (2%)	6 (3%)	5 3
2	B	248/261 (95%)	240 (97%)	8 (3%)	0	100 100
2	P	247/261 (95%)	233 (94%)	11 (4%)	3 (1%)	13 10
3	C	236/248 (95%)	217 (92%)	14 (6%)	5 (2%)	7 4
3	Q	230/248 (93%)	216 (94%)	8 (4%)	6 (3%)	5 3
4	D	232/241 (96%)	224 (97%)	5 (2%)	3 (1%)	12 9
4	R	232/241 (96%)	224 (97%)	4 (2%)	4 (2%)	9 6
5	E	232/263 (88%)	226 (97%)	5 (2%)	1 (0%)	34 37
5	S	238/263 (90%)	232 (98%)	4 (2%)	2 (1%)	19 19
6	F	241/255 (94%)	235 (98%)	5 (2%)	1 (0%)	34 37
6	T	239/255 (94%)	229 (96%)	6 (2%)	4 (2%)	9 6
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100 100
7	U	232/246 (94%)	227 (98%)	4 (2%)	1 (0%)	34 37
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	V	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
9	I	205/205 (100%)	202 (98%)	3 (2%)	0	100	100
9	W	204/205 (100%)	200 (98%)	2 (1%)	2 (1%)	15	14
10	J	195/201 (97%)	192 (98%)	3 (2%)	0	100	100
10	X	195/201 (97%)	191 (98%)	4 (2%)	0	100	100
11	K	198/204 (97%)	196 (99%)	2 (1%)	0	100	100
11	Y	200/204 (98%)	197 (98%)	3 (2%)	0	100	100
12	L	213/213 (100%)	211 (99%)	2 (1%)	0	100	100
12	Z	212/213 (100%)	210 (99%)	2 (1%)	0	100	100
13	M	215/219 (98%)	207 (96%)	8 (4%)	0	100	100
13	a	216/219 (99%)	206 (95%)	10 (5%)	0	100	100
14	N	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
14	b	202/205 (98%)	199 (98%)	3 (2%)	0	100	100
All	All	6203/6458 (96%)	6023 (97%)	137 (2%)	43 (1%)	22	22

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	53	SER
3	C	47	LYS
3	C	204	LYS
4	D	176	GLY
6	F	62	SER
1	O	50	LYS
1	O	52	LYS
1	O	53	SER
2	P	54	LYS
3	Q	47	LYS
3	Q	206	ILE
4	R	128	ALA
4	R	129	ASP
4	R	130	PRO
5	S	238	GLU
6	T	7	TYR
6	T	62	SER
6	T	208	ALA

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Mol	Chain	Res	Type
1	A	52	LYS
4	D	175[A]	GLU
4	D	175[B]	GLU
5	E	59	HIS
1	O	231	ALA
2	P	52	ILE
3	Q	48	LYS
3	Q	221	ASN
1	A	176	ARG
1	O	176	ARG
7	U	58	ASP
3	C	50	VAL
3	Q	50	VAL
9	W	16[A]	LYS
9	W	16[B]	LYS
3	C	51	ALA
1	O	201	GLN
3	Q	51	ALA
4	R	126	GLU
5	S	236	LEU
1	A	201	GLN
2	P	203	VAL
3	C	203	GLY
6	T	204	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/191 (97%)	174 (94%)	11 (6%)	19	23
1	O	176/191 (92%)	165 (94%)	11 (6%)	18	20
2	B	199/221 (90%)	190 (96%)	9 (4%)	27	34
2	P	196/221 (89%)	184 (94%)	12 (6%)	18	21
3	C	179/210 (85%)	168 (94%)	11 (6%)	18	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	183/210 (87%)	174 (95%)	9 (5%)	25	31
4	D	189/203 (93%)	185 (98%)	4 (2%)	53	67
4	R	187/203 (92%)	186 (100%)	1 (0%)	88	94
5	E	192/223 (86%)	184 (96%)	8 (4%)	30	38
5	S	197/223 (88%)	188 (95%)	9 (5%)	27	34
6	F	199/212 (94%)	189 (95%)	10 (5%)	24	30
6	T	192/212 (91%)	183 (95%)	9 (5%)	26	33
7	G	202/207 (98%)	195 (96%)	7 (4%)	36	46
7	U	186/207 (90%)	181 (97%)	5 (3%)	44	57
8	H	181/195 (93%)	173 (96%)	8 (4%)	28	35
8	V	172/195 (88%)	165 (96%)	7 (4%)	30	39
9	I	176/174 (101%)	173 (98%)	3 (2%)	60	74
9	W	173/174 (99%)	172 (99%)	1 (1%)	86	93
10	J	166/170 (98%)	158 (95%)	8 (5%)	25	32
10	X	165/170 (97%)	158 (96%)	7 (4%)	30	38
11	K	155/159 (98%)	146 (94%)	9 (6%)	20	23
11	Y	158/159 (99%)	152 (96%)	6 (4%)	33	42
12	L	175/178 (98%)	169 (97%)	6 (3%)	37	47
12	Z	175/178 (98%)	171 (98%)	4 (2%)	50	63
13	M	180/181 (99%)	176 (98%)	4 (2%)	52	65
13	a	178/181 (98%)	171 (96%)	7 (4%)	32	41
14	N	158/159 (99%)	154 (98%)	4 (2%)	47	60
14	b	158/159 (99%)	152 (96%)	6 (4%)	33	42
All	All	5032/5366 (94%)	4836 (96%)	196 (4%)	33	41

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	51	GLN
1	A	53	SER
1	A	61	VAL
1	A	73	LEU
1	A	142	ARG

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Mol	Chain	Res	Type
1	A	180	ASP
1	A	189	THR
1	A	206	ASN
1	A	223	THR
1	A	226	LYS
2	B	7	SER
2	B	33	THR
2	B	59	VAL
2	B	70	GLU
2	B	173	SER
2	B	190	LEU
2	B	207	SER
2	B	229	LYS
2	B	249	ARG
3	C	13	ASP
3	C	35	VAL
3	C	45	VAL
3	C	93	SER
3	C	113	SER
3	C	117	ARG
3	C	148	ASP
3	C	195	LEU
3	C	205	ASN
3	C	208	LEU
3	C	225	ILE
4	D	126	GLU
4	D	139	VAL
4	D	199	LEU
4	D	231	LYS
5	E	29	VAL
5	E	61	LYS
5	E	101[A]	ARG
5	E	101[B]	ARG
5	E	122	ARG
5	E	181	GLU
5	E	189	LYS
5	E	218	ASP
6	F	17	ASP
6	F	28	LYS
6	F	53	VAL
6	F	81	LEU
6	F	87	LEU

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Mol	Chain	Res	Type
6	F	187	ARG
6	F	190	VAL
6	F	215	TRP
6	F	240	LYS
6	F	244	LYS
7	G	78	CYS
7	G	88	ARG
7	G	100	ASN
7	G	183	VAL
7	G	190	THR
7	G	206	LEU
7	G	209	ASP
8	H	6	VAL
8	H	65	LEU
8	H	68	LEU
8	H	153	ASN
8	H	183	LEU
8	H	197	THR
8	H	199	LEU
8	H	215	LYS
9	I	35	THR
9	I	68	PHE
9	I	115	THR
10	J	1[A]	MET
10	J	1[B]	MET
10	J	18	ASP
10	J	62	LYS
10	J	88	LEU
10	J	95	ARG
10	J	155	ARG
10	J	182	ILE
11	K	8	PHE
11	K	12	VAL
11	K	42	LEU
11	K	72	GLU
11	K	138	VAL
11	K	147	LEU
11	K	158	ARG
11	K	174	VAL
11	K	187	VAL
12	L	3[A]	SER
12	L	3[B]	SER

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Mol	Chain	Res	Type
12	L	102	PHE
12	L	163	HIS
12	L	174	LEU
12	L	207	THR
13	M	100	ARG
13	M	154	LEU
13	M	156	LYS
13	M	204	SER
14	N	22	THR
14	N	68	ILE
14	N	84	LYS
14	N	196	LYS
1	O	10	THR
1	O	53	SER
1	O	73	LEU
1	O	142	ARG
1	O	180	ASP
1	O	181	LEU
1	O	184	GLU
1	O	189	THR
1	O	206	ASN
1	O	223	THR
1	O	226	LYS
2	P	7[A]	SER
2	P	7[B]	SER
2	P	33	THR
2	P	70	GLU
2	P	173	SER
2	P	177	GLN
2	P	190	LEU
2	P	207	SER
2	P	230	GLN
2	P	235	GLN
2	P	236	LEU
2	P	246	LYS
3	Q	45	VAL
3	Q	56	GLU
3	Q	93	SER
3	Q	113	SER
3	Q	148	ASP
3	Q	195	LEU
3	Q	197	GLU

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Mol	Chain	Res	Type
3	Q	206	ILE
3	Q	208	LEU
4	R	139	VAL
5	S	2	PHE
5	S	29	VAL
5	S	45	VAL
5	S	78	THR
5	S	101	ARG
5	S	122	ARG
5	S	181	GLU
5	S	204	ASP
5	S	234	GLU
6	T	17	ASP
6	T	28	LYS
6	T	54	LEU
6	T	81	LEU
6	T	87	LEU
6	T	190	VAL
6	T	215	TRP
6	T	223	ARG
6	T	240	LYS
7	U	78	CYS
7	U	100	ASN
7	U	196	GLU
7	U	199	ILE
7	U	206	LEU
8	V	1	THR
8	V	6	VAL
8	V	65	LEU
8	V	68	LEU
8	V	183	LEU
8	V	199	LEU
8	V	215	LYS
9	W	35	THR
10	X	1	MET
10	X	27	GLN
10	X	62	LYS
10	X	88	LEU
10	X	95	ARG
10	X	174	ASN
10	X	182	ILE
11	Y	12	VAL

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Mol	Chain	Res	Type
11	Y	41	LEU
11	Y	138	VAL
11	Y	147	LEU
11	Y	186[A]	ARG
11	Y	186[B]	ARG
12	Z	102	PHE
12	Z	174	LEU
12	Z	207	THR
12	Z	208	VAL
13	a	71	VAL
13	a	92	LEU
13	a	94	ARG
13	a	100	ARG
13	a	154	LEU
13	a	204	SER
13	a	216	SER
14	b	22	THR
14	b	29	ARG
14	b	35	THR
14	b	84	LYS
14	b	92	GLU
14	b	196	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	206	ASN
2	B	40	ASN
5	E	60	GLN
5	E	65	HIS
5	E	185	ASN
6	F	63	ASN
6	F	143	ASN
9	I	161	HIS
10	J	87	ASN
10	J	101	ASN
10	J	132	HIS
11	K	10	HIS
11	K	162	GLN
12	L	77	HIS
12	L	131	GLN

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Mol	Chain	Res	Type
12	L	157	ASN
13	M	47	ASN
1	O	118	GLN
1	O	206	ASN
2	P	40	ASN
2	P	146	GLN
3	Q	18	GLN
4	R	186	HIS
5	S	60	GLN
5	S	86	ASN
6	T	68	ASN
9	W	172	ASN
10	X	24	ASN
10	X	82	ASN
10	X	174	ASN
11	Y	162	GLN
12	Z	157	ASN
13	a	47	ASN
13	a	89	HIS
13	a	162	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

24 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	$\#\|Z\| > 2$
7	6V1	U	161	7	12,15,16	2.30	3 (25%)	9,20,22	3.02	4 (44%)
15	6V9	d	1	15	6,8,9	1.34	2 (33%)	3,10,12	5.66	2 (66%)
15	OAS	e	3	15	5,6,9	0.50	0	2,6,11	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	6V1	X	91	10	12,15,16	1.63	5 (41%)	9,20,22	4.02	5 (55%)
15	OAS	e	2	15	5,6,9	1.03	1 (20%)	2,6,11	1.90	1 (50%)
7	YCM	G	137	7	7,9,10	1.67	2 (28%)	4,10,12	2.71	2 (50%)
3	YCM	Q	63	3	7,9,10	1.29	1 (14%)	4,10,12	2.80	2 (50%)
5	6V1	E	148	5	12,15,16	1.65	4 (33%)	9,20,22	2.49	3 (33%)
5	6V1	S	148	5	12,15,16	1.68	4 (33%)	9,20,22	2.58	4 (44%)
15	OAS	c	3	15	5,6,9	0.60	0	2,6,11	0.69	0
15	6V9	c	1	15	6,8,9	0.87	0	3,10,12	3.22	2 (66%)
15	OAS	f	2	15	5,6,9	0.55	0	2,6,11	1.56	1 (50%)
15	OAS	d	3	15	5,6,9	0.90	0	2,6,11	0.87	0
3	YCM	C	63	3	7,9,10	1.02	1 (14%)	4,10,12	1.27	1 (25%)
15	6V9	f	1	15	6,8,9	1.40	0	3,10,12	5.63	2 (66%)
15	OAS	d	2	15	5,6,9	0.55	0	2,6,11	1.64	0
7	6V1	G	47	7	12,15,16	1.77	3 (25%)	9,20,22	1.98	2 (22%)
10	6V1	J	91	10	12,15,16	1.71	4 (33%)	9,20,22	4.21	5 (55%)
7	6V1	G	161	7	12,15,16	1.57	4 (33%)	9,20,22	2.02	3 (33%)
15	OAS	f	3	15	5,6,9	0.99	0	2,6,11	1.13	0
7	YCM	U	137	7	7,9,10	1.00	0	4,10,12	3.22	1 (25%)
7	6V1	U	47	7	12,15,16	1.64	3 (25%)	9,20,22	2.02	2 (22%)
15	OAS	c	2	15	5,6,9	0.67	0	2,6,11	2.41	2 (100%)
15	6V9	e	1	15	6,8,9	0.78	0	3,10,12	2.95	2 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	6V1	U	161	7	-	1/6/25/27	0/1/1/1
15	6V9	d	1	15	-	0/0/2/4	0/1/1/1
15	OAS	e	3	15	-	1/3/5/9	-
10	6V1	X	91	10	-	2/6/25/27	0/1/1/1
15	OAS	e	2	15	-	3/3/5/9	-
7	YCM	G	137	7	-	2/6/8/10	-
3	YCM	Q	63	3	-	3/6/8/10	-
5	6V1	E	148	5	-	2/6/25/27	0/1/1/1
5	6V1	S	148	5	-	0/6/25/27	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	OAS	c	3	15	-	1/3/5/9	-
15	6V9	c	1	15	-	0/0/2/4	0/1/1/1
15	OAS	f	2	15	-	0/3/5/9	-
15	OAS	d	3	15	-	0/3/5/9	-
3	YCM	C	63	3	-	0/6/8/10	-
15	6V9	f	1	15	-	0/0/2/4	0/1/1/1
15	OAS	d	2	15	-	0/3/5/9	-
7	6V1	G	47	7	-	0/6/25/27	0/1/1/1
10	6V1	J	91	10	-	2/6/25/27	0/1/1/1
7	6V1	G	161	7	-	0/6/25/27	0/1/1/1
15	OAS	f	3	15	-	1/3/5/9	-
7	YCM	U	137	7	-	1/6/8/10	-
7	6V1	U	47	7	1/1/5/6	1/6/25/27	0/1/1/1
15	OAS	c	2	15	-	3/3/5/9	-
15	6V9	e	1	15	-	0/0/2/4	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	161	6V1	C1-SG	-5.11	1.77	1.83
7	U	161	6V1	CB-SG	-4.69	1.77	1.82
7	G	47	6V1	CB-SG	-4.38	1.77	1.82
7	U	47	6V1	CB-SG	-4.04	1.77	1.82
10	J	91	6V1	C4-N3	-3.70	1.32	1.38
5	E	148	6V1	CB-SG	-3.63	1.78	1.82
10	J	91	6V1	C1-SG	-3.02	1.79	1.83
3	Q	63	YCM	CD-SG	-3.02	1.73	1.81
5	S	148	6V1	CB-SG	-3.00	1.78	1.82
7	G	161	6V1	C1-SG	-2.98	1.80	1.83
10	X	91	6V1	C4-N3	-2.97	1.33	1.38
5	S	148	6V1	C2-N3	-2.93	1.34	1.38
7	U	161	6V1	C2-N3	-2.71	1.34	1.38
7	G	47	6V1	C2-N3	-2.63	1.35	1.38
7	G	137	YCM	CD-SG	2.57	1.88	1.81
7	G	137	YCM	CE-NZ2	2.56	1.41	1.32
7	U	47	6V1	C4-N3	-2.56	1.34	1.38
5	S	148	6V1	C5-C4	2.56	1.54	1.50
10	X	91	6V1	C1-SG	-2.50	1.80	1.83
5	E	148	6V1	C2-N3	-2.49	1.35	1.38
7	G	161	6V1	CB-SG	-2.36	1.79	1.82
10	X	91	6V1	O7-C2	2.26	1.26	1.22
7	G	161	6V1	C2-N3	-2.22	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	161	6V1	C4-N3	-2.20	1.35	1.38
3	C	63	YCM	CD-SG	-2.20	1.75	1.81
5	E	148	6V1	C4-N3	-2.20	1.35	1.38
10	X	91	6V1	CB-SG	-2.19	1.79	1.82
5	E	148	6V1	C5-C4	2.18	1.54	1.50
15	d	1	6V9	C2-C1	2.15	1.53	1.49
10	J	91	6V1	O7-C2	2.11	1.26	1.22
10	X	91	6V1	C5-C4	2.08	1.53	1.50
15	e	2	OAS	CA-N	-2.08	1.41	1.48
7	U	47	6V1	C2-N3	-2.07	1.35	1.38
10	J	91	6V1	CB-SG	-2.06	1.79	1.82
7	G	47	6V1	C5-C4	2.06	1.53	1.50
15	d	1	6V9	C21-N	2.02	1.39	1.36
5	S	148	6V1	C1-SG	-2.02	1.81	1.83

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	f	1	6V9	O-C-C3	-8.97	115.72	124.22
15	d	1	6V9	O-C-C3	-8.68	116.00	124.22
10	J	91	6V1	C6-N3-C2	6.60	131.74	123.36
10	X	91	6V1	C6-N3-C2	6.46	131.56	123.36
7	U	161	6V1	C5-C4-N3	6.35	111.87	108.13
10	J	91	6V1	O7-C2-N3	6.21	131.74	124.14
7	U	137	YCM	CE-CD-SG	5.98	131.20	113.59
5	E	148	6V1	C2-N3-C4	-5.94	109.52	113.04
10	X	91	6V1	O7-C2-N3	5.90	131.36	124.14
10	J	91	6V1	C5-C4-N3	5.85	111.58	108.13
10	X	91	6V1	C5-C4-N3	4.95	111.05	108.13
10	X	91	6V1	C2-N3-C4	-4.92	110.12	113.04
3	Q	63	YCM	CE-CD-SG	-4.86	99.30	113.59
10	J	91	6V1	C2-N3-C4	-4.81	110.18	113.04
7	G	137	YCM	CE-CD-SG	4.61	127.17	113.59
7	U	47	6V1	C2-N3-C4	-4.53	110.35	113.04
7	U	161	6V1	C2-N3-C4	-4.34	110.47	113.04
15	c	1	6V9	O-C-C3	-4.31	120.14	124.22
15	e	1	6V9	O-C-C3	-4.16	120.28	124.22
15	d	1	6V9	C2-C1-N	4.14	132.77	121.87
7	G	47	6V1	C2-N3-C4	-4.09	110.61	113.04
5	S	148	6V1	C2-N3-C4	-4.08	110.62	113.04
5	S	148	6V1	C5-C4-N3	3.92	110.44	108.13
10	X	91	6V1	C6-N3-C4	-3.91	117.50	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	91	6V1	C6-N3-C4	-3.88	117.53	122.59
7	U	161	6V1	O8-C4-C5	-3.70	121.85	127.24
7	G	161	6V1	O8-C4-N3	3.69	128.01	123.92
15	f	1	6V9	C2-C1-N	3.64	131.44	121.87
5	S	148	6V1	C6-N3-C4	3.57	127.24	122.59
5	E	148	6V1	C5-C4-N3	3.52	110.21	108.13
7	G	47	6V1	C5-C4-N3	3.44	110.16	108.13
15	c	1	6V9	C2-C1-N	3.39	130.78	121.87
5	S	148	6V1	O7-C2-N3	-3.25	120.16	124.14
7	G	161	6V1	O8-C4-C5	-3.15	122.65	127.24
15	c	2	OAS	OG-CB-CA	2.63	116.78	109.39
15	e	2	OAS	OG-CB-CA	2.56	116.60	109.39
3	C	63	YCM	CE-CD-SG	-2.38	106.59	113.59
7	U	47	6V1	C5-C4-N3	2.35	109.52	108.13
15	e	1	6V9	C2-C1-N	2.31	127.93	121.87
3	Q	63	YCM	CA-CB-SG	-2.26	105.48	113.74
15	c	2	OAS	C1A-OG-CB	2.17	121.53	112.42
15	f	2	OAS	OG-CB-CA	-2.16	103.33	109.39
7	U	161	6V1	O8-C4-N3	2.13	126.28	123.92
5	E	148	6V1	C6-N3-C4	2.10	125.34	122.59
7	G	161	6V1	C5-C4-N3	2.04	109.33	108.13
7	G	137	YCM	OZ1-CE-NZ2	-2.00	117.04	122.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	148	6V1	C3-C6-N3-C4
7	G	137	YCM	CE-CD-SG-CB
7	G	137	YCM	SG-CD-CE-NZ2
10	J	91	6V1	C3-C6-N3-C2
10	J	91	6V1	C3-C6-N3-C4
3	Q	63	YCM	SG-CD-CE-OZ1
3	Q	63	YCM	SG-CD-CE-NZ2
10	X	91	6V1	C3-C6-N3-C2
10	X	91	6V1	C3-C6-N3-C4
15	c	2	OAS	N-CA-CB-OG
15	c	2	OAS	C-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
15	e	2	OAS	N-CA-CB-OG
15	e	2	OAS	C-CA-CB-OG
5	E	148	6V1	C3-C6-N3-C2
15	c	2	OAS	CA-CB-OG-C1A
15	f	3	OAS	CA-CB-OG-C1A
7	U	137	YCM	CE-CD-SG-CB
7	U	47	6V1	C3-C6-N3-C4
15	e	3	OAS	CA-CB-OG-C1A
3	Q	63	YCM	CE-CD-SG-CB
7	U	161	6V1	N-CA-CB-SG
15	e	2	OAS	CA-CB-OG-C1A
15	c	3	OAS	CA-CB-OG-C1A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	137	YCM	1	0
5	E	148	6V1	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 16 are monoatomic - leaving 13 for Mogul analysis.

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	$\#\|Z\| > 2$
18	1PE	W	302	-	15,15,15	0.68	0	14,14,14	0.33	0
18	1PE	N	301	-	15,15,15	0.56	0	14,14,14	0.51	0
18	1PE	Y	301	-	15,15,15	0.63	0	14,14,14	0.62	0
18	1PE	K	302	-	15,15,15	0.70	0	14,14,14	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	ACT	c	101	-	3,3,3	0.75	0	3,3,3	0.98	0
18	1PE	I	302	-	15,15,15	0.73	0	14,14,14	0.84	0
18	1PE	U	301	-	15,15,15	0.65	0	14,14,14	0.68	0
18	1PE	a	301	-	15,15,15	0.59	0	14,14,14	0.39	0
19	ACT	f	101	-	3,3,3	0.96	0	3,3,3	0.70	0
19	ACT	e	101	-	3,3,3	0.83	0	3,3,3	0.41	0
19	ACT	d	101	-	3,3,3	0.68	0	3,3,3	0.87	0
18	1PE	L	301	-	15,15,15	0.59	0	14,14,14	0.46	0
18	1PE	H	303	-	15,15,15	0.64	0	14,14,14	0.76	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
18	1PE	W	302	-	-	5/13/13/13	-
18	1PE	N	301	-	-	5/13/13/13	-
18	1PE	Y	301	-	-	7/13/13/13	-
18	1PE	K	302	-	-	7/13/13/13	-
18	1PE	I	302	-	-	9/13/13/13	-
18	1PE	U	301	-	-	6/13/13/13	-
18	1PE	a	301	-	-	6/13/13/13	-
18	1PE	L	301	-	-	5/13/13/13	-
18	1PE	H	303	-	-	7/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	I	302	1PE	C15-C25-OH5-C14
18	H	303	1PE	C24-C14-OH5-C25
18	K	302	1PE	C16-C26-OH6-C15
18	Y	301	1PE	C16-C26-OH6-C15
18	H	303	1PE	OH4-C13-C23-OH3
18	K	302	1PE	OH5-C14-C24-OH4
18	L	301	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
18	Y	301	1PE	OH6-C15-C25-OH5
18	U	301	1PE	OH4-C13-C23-OH3
18	W	302	1PE	OH6-C15-C25-OH5
18	K	302	1PE	OH6-C15-C25-OH5
18	H	303	1PE	OH5-C14-C24-OH4
18	U	301	1PE	OH6-C15-C25-OH5
18	a	301	1PE	OH4-C13-C23-OH3
18	a	301	1PE	OH5-C14-C24-OH4
18	H	303	1PE	OH7-C16-C26-OH6
18	U	301	1PE	C24-C14-OH5-C25
18	L	301	1PE	OH5-C14-C24-OH4
18	N	301	1PE	OH4-C13-C23-OH3
18	I	302	1PE	OH2-C12-C22-OH3
18	K	302	1PE	OH2-C12-C22-OH3
18	N	301	1PE	OH2-C12-C22-OH3
18	W	302	1PE	OH2-C12-C22-OH3
18	a	301	1PE	OH7-C16-C26-OH6
18	L	301	1PE	OH6-C15-C25-OH5
18	L	301	1PE	OH2-C12-C22-OH3
18	N	301	1PE	OH7-C16-C26-OH6
18	I	302	1PE	OH6-C15-C25-OH5
18	K	302	1PE	C25-C15-OH6-C26
18	a	301	1PE	OH6-C15-C25-OH5
18	L	301	1PE	C14-C24-OH4-C13
18	Y	301	1PE	C15-C25-OH5-C14
18	I	302	1PE	C24-C14-OH5-C25
18	a	301	1PE	C25-C15-OH6-C26
18	Y	301	1PE	C23-C13-OH4-C24
18	W	302	1PE	C14-C24-OH4-C13
18	a	301	1PE	C14-C24-OH4-C13
18	Y	301	1PE	OH2-C12-C22-OH3
18	U	301	1PE	OH7-C16-C26-OH6
18	U	301	1PE	C13-C23-OH3-C22
18	I	302	1PE	C14-C24-OH4-C13
18	Y	301	1PE	C12-C22-OH3-C23
18	H	303	1PE	C16-C26-OH6-C15
18	K	302	1PE	C13-C23-OH3-C22
18	H	303	1PE	C15-C25-OH5-C14
18	Y	301	1PE	OH7-C16-C26-OH6
18	K	302	1PE	C12-C22-OH3-C23
18	N	301	1PE	C13-C23-OH3-C22
18	I	302	1PE	OH7-C16-C26-OH6

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Mol	Chain	Res	Type	Atoms
18	W	302	1PE	C24-C14-OH5-C25
18	U	301	1PE	OH5-C14-C24-OH4
18	I	302	1PE	OH4-C13-C23-OH3
18	H	303	1PE	OH6-C15-C25-OH5
18	I	302	1PE	C13-C23-OH3-C22
18	W	302	1PE	C23-C13-OH4-C24
18	N	301	1PE	C16-C26-OH6-C15
18	I	302	1PE	OH5-C14-C24-OH4

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	230/234 (98%)	-0.06	4 (1%)	70	68	42, 62, 99, 120	0
1	O	230/234 (98%)	0.61	31 (13%)	3	2	55, 82, 127, 151	0
2	B	248/261 (95%)	0.30	18 (7%)	15	14	47, 67, 118, 170	0
2	P	247/261 (94%)	0.55	29 (11%)	4	4	53, 80, 137, 171	0
3	C	236/248 (95%)	0.68	30 (12%)	3	3	48, 78, 130, 180	0
3	Q	234/248 (94%)	0.95	43 (18%)	1	1	44, 81, 152, 204	0
4	D	233/241 (96%)	0.28	19 (8%)	11	10	51, 76, 109, 141	0
4	R	233/241 (96%)	-0.03	5 (2%)	63	61	39, 55, 84, 118	0
5	E	233/263 (88%)	0.09	10 (4%)	35	33	40, 56, 99, 130	0
5	S	237/263 (90%)	-0.19	4 (1%)	70	68	41, 58, 94, 125	0
6	F	239/255 (93%)	-0.09	2 (0%)	86	85	39, 51, 77, 98	0
6	T	240/255 (94%)	0.17	14 (5%)	23	22	43, 63, 105, 134	0
7	G	241/246 (97%)	0.25	9 (3%)	41	39	38, 54, 99, 148	0
7	U	235/246 (95%)	0.68	38 (16%)	1	1	53, 74, 111, 148	0
8	H	220/234 (94%)	-0.15	3 (1%)	75	73	34, 48, 82, 112	0
8	V	220/234 (94%)	0.12	6 (2%)	54	52	45, 62, 106, 126	0
9	I	204/205 (99%)	0.04	1 (0%)	91	90	37, 49, 77, 96	0
9	W	204/205 (99%)	0.03	4 (1%)	65	63	48, 66, 98, 109	0
10	J	195/201 (97%)	-0.09	3 (1%)	73	72	38, 53, 74, 91	0
10	X	195/201 (97%)	-0.04	2 (1%)	82	81	44, 56, 77, 95	0
11	K	200/204 (98%)	0.16	5 (2%)	57	55	46, 60, 90, 109	0
11	Y	199/204 (97%)	0.08	2 (1%)	82	81	35, 47, 72, 83	0
12	L	213/213 (100%)	-0.07	0	100	100	43, 65, 91, 114	0
12	Z	213/213 (100%)	-0.03	3 (1%)	75	73	33, 48, 78, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	216/219 (98%)	0.11	4 (1%) 66 65	35, 51, 77, 115	0
13	a	216/219 (98%)	0.03	3 (1%) 75 73	33, 47, 73, 107	0
14	N	202/205 (98%)	0.03	3 (1%) 73 72	35, 44, 70, 117	0
14	b	203/205 (99%)	0.23	10 (4%) 29 28	39, 50, 81, 131	0
15	c	0/4	-	-	-	-
15	d	0/4	-	-	-	-
15	e	0/4	-	-	-	-
15	f	0/4	-	-	-	-
All	All	6216/6474 (96%)	0.17	305 (4%) 29 28	33, 59, 107, 204	0

All (305) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	187	PHE	12.9
3	Q	232	ILE	11.9
1	O	232	ILE	9.3
14	b	203	PRO	9.2
2	P	204	SER	8.6
7	G	188	ASP	8.3
7	U	242	LEU	8.3
13	a	216	SER	8.3
3	Q	238	GLU	7.9
3	Q	239	ASN	7.1
3	Q	234	LYS	6.8
3	Q	225	ILE	6.7
7	G	189	TRP	6.7
4	D	241	ILE	6.5
3	Q	229	VAL	6.4
5	E	237	GLU	6.2
7	U	235	ILE	6.1
4	R	130	PRO	6.1
5	S	2	PHE	6.0
3	C	225	ILE	5.9
2	B	204	SER	5.9
2	B	205	LYS	5.9
3	Q	181	ILE	5.8
14	b	201	THR	5.8
1	O	229	LEU	5.8
3	Q	237	GLU	5.8
3	Q	233	GLU	5.6
3	Q	240	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	230	ALA	5.6
3	C	232	ILE	5.6
3	C	229	VAL	5.5
2	P	246	LYS	5.5
7	U	202	LEU	5.4
3	C	230	ALA	5.4
2	P	234	GLU	5.4
3	Q	236	LYS	5.3
4	D	237	VAL	5.3
1	O	223	THR	5.1
3	C	203	GLY	5.0
8	V	203	ARG	5.0
3	Q	186	LEU	5.0
3	C	234	LYS	5.0
3	C	201	SER	5.0
3	C	200	GLN	5.0
1	O	50	LYS	4.9
7	U	204	THR	4.8
4	R	241	ILE	4.7
11	K	40	TYR	4.7
7	U	208	ILE	4.6
1	O	177	TYR	4.6
3	C	236	LYS	4.6
2	P	61	PHE	4.6
3	Q	230	ALA	4.6
3	Q	171	PHE	4.5
1	O	192	LEU	4.5
5	E	235	GLY	4.5
6	T	203	GLU	4.4
2	B	248	GLU	4.4
2	B	247	ALA	4.4
6	T	208	ALA	4.4
7	U	198	ALA	4.4
2	P	203	VAL	4.4
3	Q	223	GLU	4.4
4	D	188	SER	4.4
14	b	202	LEU	4.4
3	Q	48	LYS	4.4
11	K	145	TYR	4.3
2	B	203	VAL	4.3
1	O	200	GLY	4.3
1	O	176	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
7	U	212	PRO	4.2
3	Q	192	ILE	4.2
3	Q	37	GLY	4.2
7	U	200	THR	4.1
4	D	234	LEU	4.1
1	A	231	ALA	4.1
7	U	206	LEU	4.1
7	U	199	ILE	4.1
1	O	199	GLU	4.0
2	P	233	VAL	4.0
14	N	202	LEU	4.0
3	Q	179	GLU	4.0
3	Q	177	THR	4.0
1	O	225	VAL	3.9
2	P	197	LEU	3.9
10	J	1[A]	MET	3.9
1	A	232	ILE	3.9
2	B	61	PHE	3.9
7	U	243	ALA	3.8
3	Q	182	GLU	3.7
2	P	237	ILE	3.7
3	Q	190	LEU	3.7
7	U	213	SER	3.7
11	Y	40	TYR	3.6
7	U	210	PHE	3.6
2	P	244	GLU	3.6
14	b	199	VAL	3.6
2	P	202	ASP	3.6
2	P	177	GLN	3.5
14	b	200	ALA	3.5
1	O	191	ILE	3.5
7	U	239	LEU	3.5
14	b	26	ILE	3.5
3	Q	222	PRO	3.5
2	P	236	LEU	3.5
7	G	185	LYS	3.5
5	E	236	LEU	3.5
3	C	228	TYR	3.5
7	U	2	SER	3.5
3	C	185	ASP	3.4
1	O	227	ASP	3.4
1	O	228	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
2	P	247	ALA	3.4
6	T	241	GLU	3.4
2	B	249	ARG	3.4
8	V	132	LEU	3.3
3	C	237	GLU	3.3
5	E	232	PHE	3.3
2	B	206	LEU	3.2
1	O	189	THR	3.2
1	O	4	GLY	3.2
1	O	198	PHE	3.2
3	C	192	ILE	3.2
1	O	201	GLN	3.2
7	U	3	ARG	3.2
3	C	233	GLU	3.2
6	T	204	VAL	3.2
7	U	57	PRO	3.2
7	U	36	GLY	3.2
2	P	242	GLU	3.2
7	U	58	ASP	3.2
2	P	220	ASN	3.1
5	S	3	ARG	3.1
1	O	226	LYS	3.1
1	O	202	MET	3.1
3	C	156	TRP	3.1
7	U	211	LYS	3.1
2	P	205	LYS	3.1
5	E	52	ALA	3.1
4	D	230	THR	3.1
4	D	232	GLU	3.1
4	D	236	GLU	3.0
8	H	201	ARG	3.0
3	C	238	GLU	3.0
6	T	209	PHE	3.0
7	U	240	VAL	3.0
4	D	183	GLU	3.0
6	F	243	LEU	3.0
7	U	237	ALA	3.0
13	M	33	LEU	2.9
3	Q	191	VAL	2.9
1	O	194	LEU	2.9
7	G	72	ILE	2.9
8	H	204	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	235	GLU	2.9
7	U	178	PHE	2.9
1	O	185	ASP	2.9
4	D	191	LEU	2.9
4	D	131	GLY	2.8
1	O	190	ALA	2.8
4	D	130	PRO	2.8
1	O	181	LEU	2.8
2	B	245	ALA	2.8
3	C	194	ALA	2.8
14	b	198	ALA	2.8
7	U	207	SER	2.8
7	U	56	VAL	2.8
7	U	7	ALA	2.8
9	W	113	PRO	2.8
10	X	95	ARG	2.8
3	Q	241	LYS	2.8
8	V	1	THR	2.7
8	V	202	TYR	2.7
3	Q	38	ARG	2.7
3	C	138	PHE	2.7
7	U	203	SER	2.7
3	Q	205	ASN	2.7
6	T	207	LYS	2.7
1	O	186	ALA	2.7
3	Q	180	ALA	2.7
1	A	201	GLN	2.7
4	D	195	ILE	2.6
5	E	218	ASP	2.6
4	D	194	ALA	2.6
2	P	206	LEU	2.6
8	V	204	CYS	2.6
4	D	238	ILE	2.6
1	O	184	GLU	2.6
8	H	219	LEU	2.6
2	P	243	GLU	2.6
12	Z	164	VAL	2.6
2	B	237	ILE	2.6
2	P	178	ASP	2.6
3	C	48	LYS	2.6
1	O	180	ASP	2.6
2	P	194	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
3	Q	226	GLU	2.6
6	T	237	LYS	2.6
7	G	186	LYS	2.6
5	E	54	SER	2.6
3	C	186	LEU	2.6
3	Q	39	ASP	2.5
6	T	202	ASP	2.5
7	U	245	ARG	2.5
1	O	230	ALA	2.5
2	B	202	ASP	2.5
5	E	56	LEU	2.5
6	T	54	LEU	2.5
4	D	184	VAL	2.5
1	O	59	ARG	2.5
13	M	145	LEU	2.5
6	T	205	LYS	2.5
1	O	157	TRP	2.5
7	U	209	ASP	2.5
7	U	222	VAL	2.5
3	Q	206	ILE	2.5
3	Q	175	ASN	2.5
7	U	230	LEU	2.4
3	Q	142	PRO	2.4
3	C	195	LEU	2.4
1	O	182	GLU	2.4
2	B	101	TYR	2.4
2	P	230	GLN	2.4
11	Y	26	ILE	2.4
4	D	240	ASP	2.4
6	T	206	ASP	2.4
4	R	237	VAL	2.4
3	Q	183	THR	2.4
3	C	196	LEU	2.4
4	D	239	LYS	2.4
11	K	163	ALA	2.4
1	O	187	ILE	2.4
7	G	76	ILE	2.4
3	C	202	GLY	2.4
3	Q	213	ARG	2.4
13	M	142	GLY	2.4
3	C	214	ASP	2.4
6	F	203	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	172	LEU	2.3
8	V	199	LEU	2.3
2	B	244	GLU	2.3
2	P	179	TYR	2.3
14	b	25	TYR	2.3
3	C	171	PHE	2.3
13	a	33	LEU	2.3
5	E	182	CYS	2.3
2	P	235	GLN	2.3
7	U	214	GLU	2.3
2	P	46	ALA	2.3
14	N	201	THR	2.3
7	U	223	GLU	2.3
3	C	49	SER	2.3
3	Q	235	GLU	2.3
4	D	233	GLU	2.3
7	U	196	GLU	2.3
7	G	208	ILE	2.3
14	b	150	GLU	2.3
2	P	175	LEU	2.2
3	C	193	LYS	2.2
3	Q	197	GLU	2.2
4	R	186	HIS	2.2
10	J	147	TYR	2.2
2	B	235	GLN	2.2
2	B	231	LYS	2.2
2	P	30	HIS	2.2
5	S	18[A]	ARG	2.2
7	U	241	ALA	2.2
3	Q	85	ASN	2.2
12	Z	165	PRO	2.2
2	P	172	VAL	2.2
5	S	174	ARG	2.2
14	b	27	ALA	2.2
7	G	139	ILE	2.2
13	a	215	ILE	2.2
2	B	190	LEU	2.2
6	T	240	LYS	2.2
6	T	180	GLN	2.2
7	U	201	CYS	2.2
10	J	26	VAL	2.2
9	I	178	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
7	U	160	TYR	2.1
4	R	240	ASP	2.1
9	W	192	ASP	2.1
3	Q	199	VAL	2.1
3	Q	176	TYR	2.1
10	X	147	TYR	2.1
2	P	200	THR	2.1
7	U	205	VAL	2.1
6	T	63	ASN	2.1
2	B	234	GLU	2.1
9	W	189	ILE	2.1
3	Q	53	LEU	2.1
9	W	31	ALA	2.1
13	M	143	ALA	2.1
11	K	9	ARG	2.1
11	K	11	GLY	2.1
3	Q	219	ILE	2.1
14	N	68	ILE	2.0
3	Q	214	ASP	2.0
3	C	222	PRO	2.0
4	D	190	THR	2.0
5	E	185	ASN	2.0
2	B	241	GLU	2.0
2	P	55	LEU	2.0
12	Z	143	ALA	2.0

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
7	YCM	U	137	10/11	0.84	0.18	60,70,87,87	0
7	6V1	U	47	15/16	0.87	0.33	94,131,141,141	0
5	6V1	S	148	15/16	0.88	0.16	44,74,82,83	0
5	6V1	E	148	15/16	0.89	0.17	47,68,74,76	0
7	6V1	U	161	15/16	0.91	0.12	70,89,97,99	0
15	OAS	f	2	7/10	0.91	0.11	53,56,58,60	0
7	6V1	G	161	15/16	0.92	0.17	46,69,77,78	0
7	6V1	G	47	15/16	0.92	0.16	53,79,84,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	6V1	X	91	15/16	0.92	0.17	48,69,76,76	0
15	6V9	f	1	8/9	0.92	0.13	61,63,68,68	0
7	YCM	G	137	10/11	0.92	0.15	46,53,68,69	0
3	YCM	Q	63	10/11	0.93	0.15	67,72,78,79	0
10	6V1	J	91	15/16	0.93	0.17	43,64,69,69	0
3	YCM	C	63	10/11	0.94	0.12	63,69,85,89	0
15	OAS	c	2	7/10	0.95	0.14	49,50,52,54	0
15	OAS	d	2	7/10	0.95	0.10	45,46,47,49	0
15	6V9	d	1	8/9	0.95	0.12	52,55,61,63	0
15	OAS	f	3	7/10	0.97	0.09	52,53,58,60	0
15	6V9	c	1	8/9	0.98	0.09	51,52,53,53	0
15	OAS	c	3	7/10	0.98	0.14	47,48,48,48	0
15	OAS	d	3	7/10	0.98	0.10	42,45,51,52	0
15	OAS	e	3	7/10	0.98	0.13	35,35,38,39	0
15	OAS	e	2	7/10	0.98	0.14	34,37,43,48	0
15	6V9	e	1	8/9	0.99	0.10	41,42,44,45	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	1PE	I	302	16/16	0.70	0.29	76,88,94,95	0
18	1PE	W	302	16/16	0.71	0.37	75,93,100,103	0
18	1PE	K	302	16/16	0.75	0.19	78,86,93,94	0
18	1PE	Y	301	16/16	0.77	0.18	64,80,88,91	0
17	MG	H	301	1/1	0.78	0.17	59,59,59,59	0
18	1PE	L	301	16/16	0.80	0.33	80,89,117,117	0
18	1PE	H	303	16/16	0.83	0.27	71,82,101,107	0
18	1PE	N	301	16/16	0.83	0.13	51,64,78,79	0
18	1PE	a	301	16/16	0.86	0.23	77,82,114,116	0
18	1PE	U	301	16/16	0.88	0.17	57,66,87,89	0
17	MG	K	301	1/1	0.89	0.07	50,50,50,50	0
17	MG	V	301	1/1	0.91	0.16	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	K	L	302	1/1	0.91	0.09	77,77,77,77	0
19	ACT	f	101	4/4	0.92	0.18	59,60,63,67	0
16	K	Z	301	1/1	0.93	0.04	67,67,67,67	0
17	MG	L	303	1/1	0.94	0.05	49,49,49,49	0
17	MG	I	303	1/1	0.95	0.09	40,40,40,40	0
17	MG	H	302	1/1	0.96	0.07	45,45,45,45	0
17	MG	X	301	1/1	0.96	0.07	65,65,65,65	0
17	MG	J	301	1/1	0.96	0.11	61,61,61,61	0
16	K	G	301	1/1	0.97	0.12	59,59,59,59	0
16	K	N	302	1/1	0.97	0.06	56,56,56,56	0
16	K	U	302	1/1	0.97	0.21	62,62,62,62	0
19	ACT	c	101	4/4	0.97	0.12	63,65,65,66	0
19	ACT	d	101	4/4	0.97	0.15	54,60,61,65	0
19	ACT	e	101	4/4	0.97	0.13	47,48,49,49	0
17	MG	I	301	1/1	0.97	0.09	43,43,43,43	0
16	K	b	301	1/1	0.98	0.05	60,60,60,60	0
17	MG	W	301	1/1	0.99	0.03	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.