Full wwPDB X-ray Structure Validation Report (i)

Apr 23, 2024 – 10:16 pm BST

PDB ID	:	8RHJ
Title	:	Yeast 20S proteasome in complex with a macrocyclic oxindole epoxyketone (compound 5)
Authors	:	Goetz, M.G.; Godwin, K.; Price, R.; Dorn, R.; Merrill-Steskal, G.; Hansen, H.; Klemmer, W.; Produturi, G.; Rocha, M.; Palmer, M.; Molacek, L.; Strater, Z.; Groll, M.
Deposited on	:	2023-12-15
Resolution	:	3.05 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:

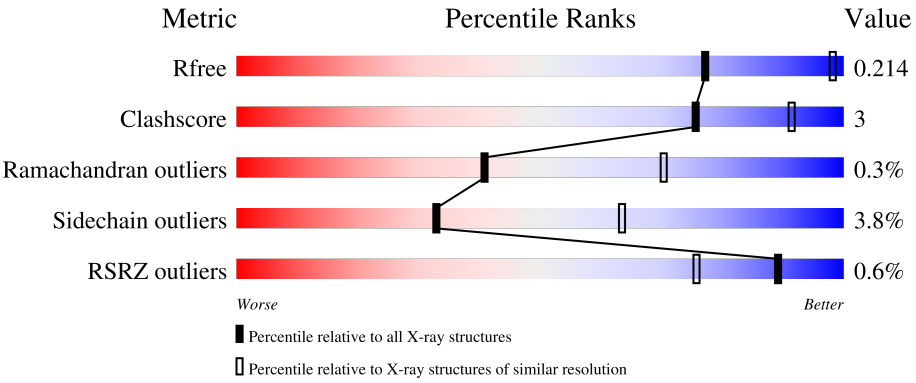
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	250	95% 5%
1	O	250	94% 6%
2	B	258	88% 6% • 5%
2	P	258	88% 5% • 5%

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Mol	Chain	Length	Quality of chain
3	C	254	87% 6% 6%
3	Q	254	4% 87% 6% 6%
4	D	260	84% 6% 10%
4	R	260	84% 6% 10%
5	E	234	93% 6%
5	S	234	% 93% 6%
6	F	288	80% 16%
6	T	288	80% 16%
7	G	252	88% 8%
7	U	252	87% 8%
8	H	232	% 85% 9%
8	V	232	83% 12%
9	I	205	89% 9%
9	W	205	90% 8%
10	J	198	% 87% 9%
10	X	198	% 87% 9%
11	K	212	89% 9%
11	Y	212	90% 9%
12	L	222	89% 10%
12	Z	222	89% 10%
13	M	246	% 87% 7% 5%
13	a	246	% 91% 5%
14	N	196	93% 7%
14	b	196	99%
15	e	5	40% 60%

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Mol	Chain	Length	Quality of chain
15	f	5	40% 60%
15	g	5	40% 60%
15	h	5	40% 40% 20%
15	i	5	40% 40% 20%
15	j	5	40% 40% 20%

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
15	PPN	j	2	-	-	-	X

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 49785 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
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is a protein called Macrocyclic oxindole epoxyketone.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	g	5	Total	C	N	O	0	0	0
			53	37	6	10			
15	e	5	Total	C	N	O	0	0	0
			53	37	6	10			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	i	5	Total C N O 53 37 6 10	0	0	0
15	f	5	Total C N O 53 37 6 10	0	0	0
15	h	5	Total C N O 53 37 6 10	0	0	0
15	j	5	Total C N O 53 37 6 10	0	0	0

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Mg 1 1	0	0
16	I	1	Total Mg 1 1	0	0
16	K	1	Total Mg 1 1	0	0
16	N	1	Total Mg 1 1	0	0
16	V	1	Total Mg 1 1	0	0
16	X	1	Total Mg 1 1	0	0
16	Y	1	Total Mg 1 1	0	0
16	Z	1	Total Mg 1 1	0	0

- Molecule 17 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	G	1	Total Cl 1 1	0	0
17	U	1	Total Cl 1 1	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	B	7	Total O 7 7	0	0
18	C	5	Total O 5 5	0	0
18	D	5	Total O 5 5	0	0
18	E	6	Total O 6 6	0	0
18	F	6	Total O 6 6	0	0
18	G	6	Total O 6 6	0	0
18	H	7	Total O 7 7	0	0
18	I	6	Total O 6 6	0	0
18	J	11	Total O 11 11	0	0
18	K	5	Total O 5 5	0	0
18	L	6	Total O 6 6	0	0
18	M	4	Total O 4 4	0	0
18	N	8	Total O 8 8	0	0
18	O	1	Total O 1 1	0	0
18	P	8	Total O 8 8	0	0
18	Q	7	Total O 7 7	0	0
18	R	4	Total O 4 4	0	0
18	S	2	Total O 2 2	0	0
18	T	3	Total O 3 3	0	0
18	U	5	Total O 5 5	0	0
18	V	5	Total O 5 5	0	0

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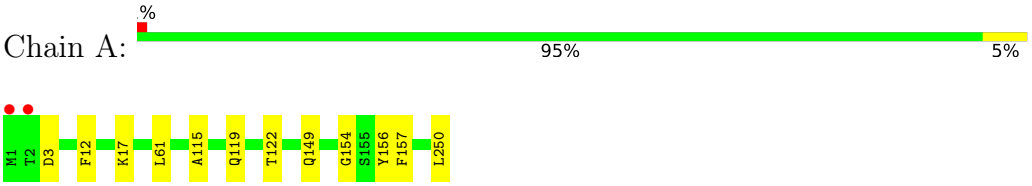
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	W	2	Total O 2 2	0	0
18	X	8	Total O 8 8	0	0
18	Y	5	Total O 5 5	0	0
18	Z	6	Total O 6 6	0	0
18	a	8	Total O 8 8	0	0
18	b	4	Total O 4 4	0	0
18	g	2	Total O 2 2	0	0
18	e	1	Total O 1 1	0	0
18	i	1	Total O 1 1	0	0
18	h	2	Total O 2 2	0	0
18	j	1	Total O 1 1	0	0

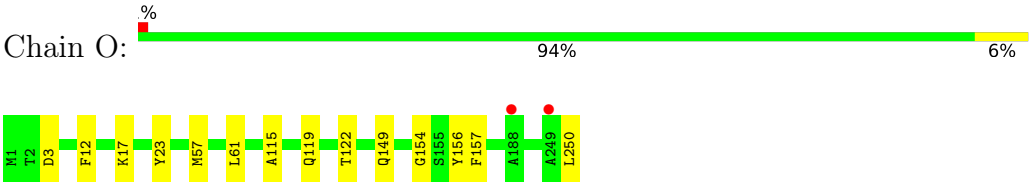
3 Residue-property plots (i)

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.

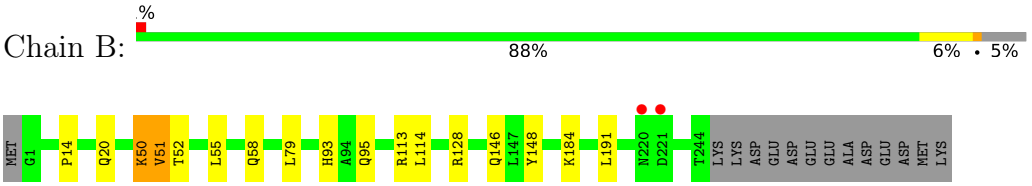
• Molecule 1: Proteasome subunit alpha type-2



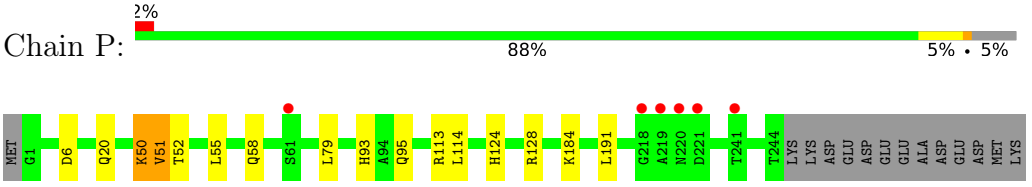
• Molecule 1: Proteasome subunit alpha type-2



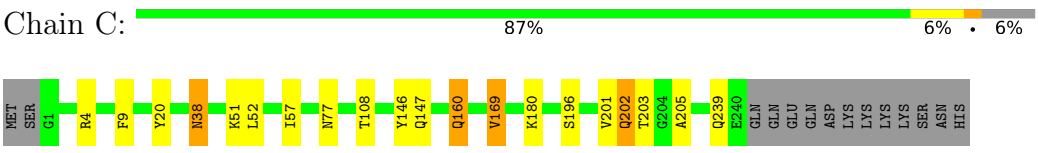
• Molecule 2: Proteasome subunit alpha type-3



• Molecule 2: Proteasome subunit alpha type-3

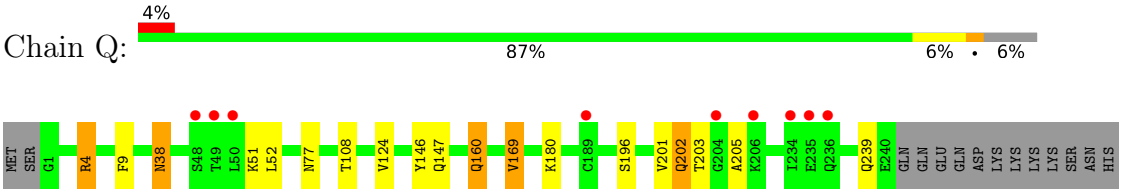


• Molecule 3: Proteasome subunit alpha type-4



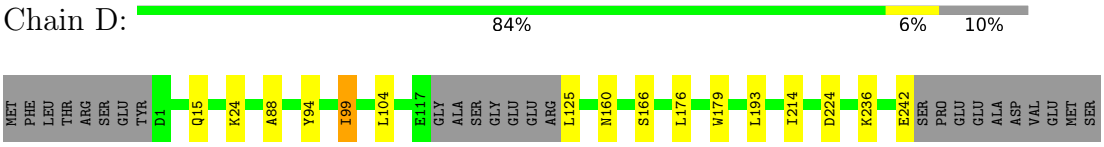
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



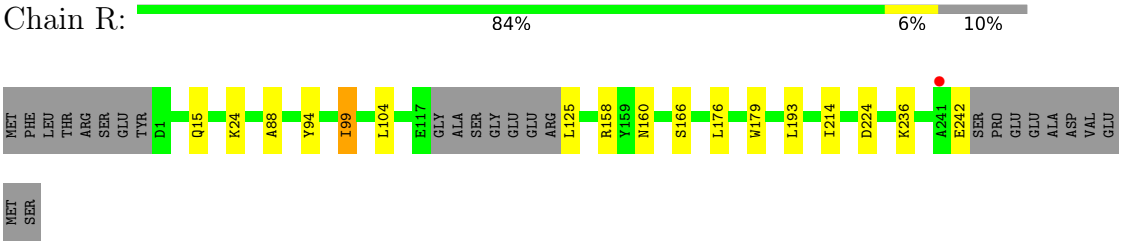
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



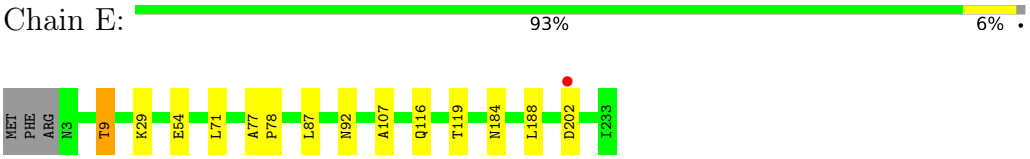
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



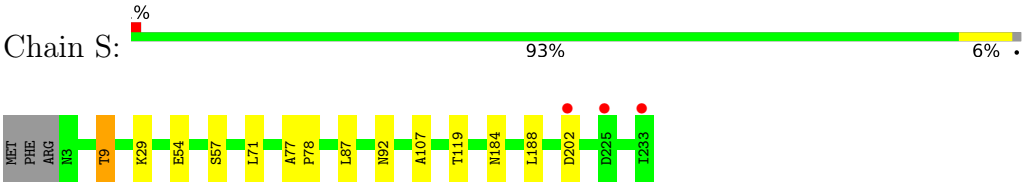
• Molecule 5: Proteasome subunit alpha type-6

Chain E:



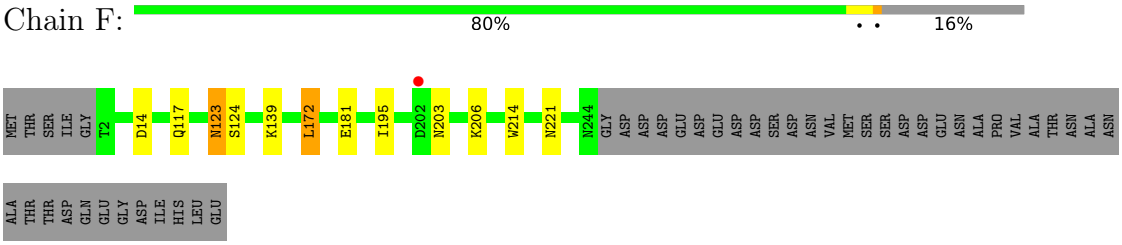
• Molecule 5: Proteasome subunit alpha type-6

Chain S:



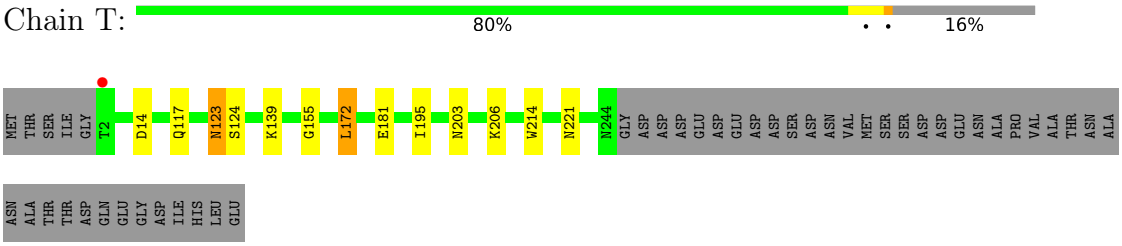
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



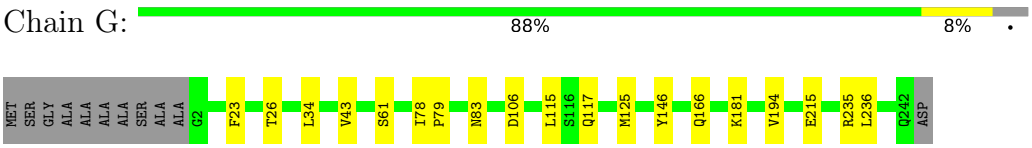
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



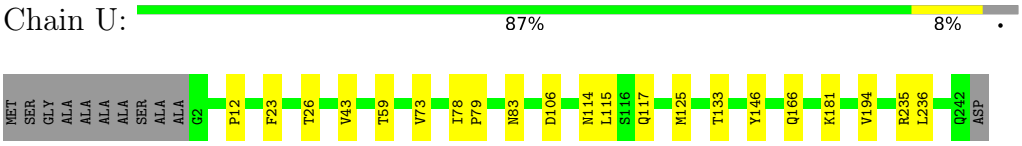
• Molecule 7: Proteasome subunit alpha type-1

Chain G:



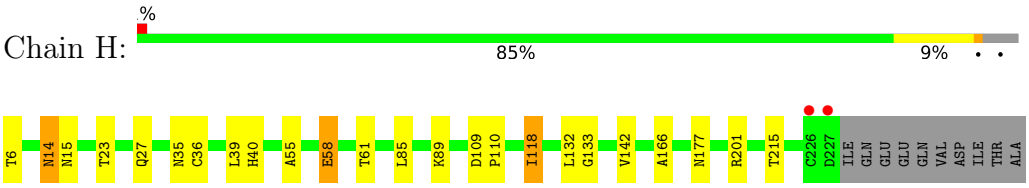
• Molecule 7: Proteasome subunit alpha type-1

Chain U:



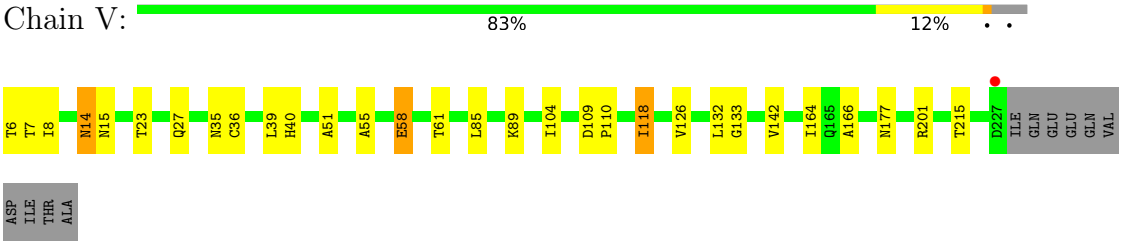
• Molecule 8: Proteasome subunit beta type-2

Chain H:



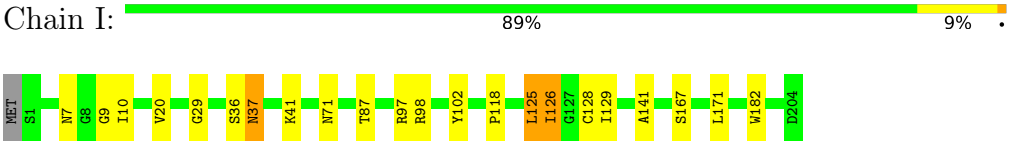
• Molecule 8: Proteasome subunit beta type-2

Chain V:



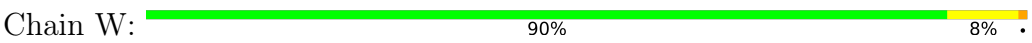
• Molecule 9: Proteasome subunit beta type-3

Chain I:



• Molecule 9: Proteasome subunit beta type-3

Chain W:

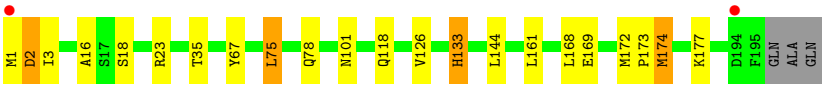


• Molecule 10: Proteasome subunit beta type-4

Chain J:

• Molecule 10: Proteasome subunit beta type-4

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-6

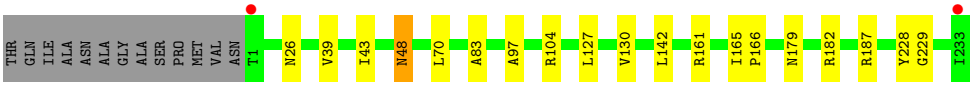
Chain L:

• Molecule 12: Proteasome subunit beta type-6

Chain Z:

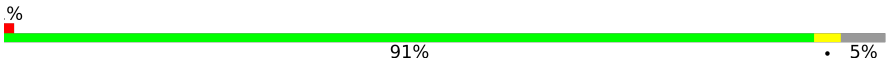
• Molecule 13: Proteasome subunit beta type-7

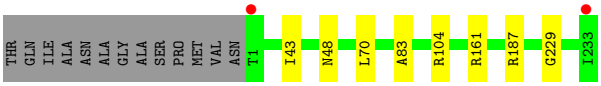
Chain M:



• Molecule 13: Proteasome subunit beta type-7

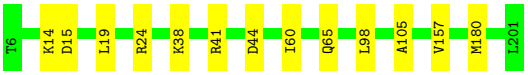
Chain a:





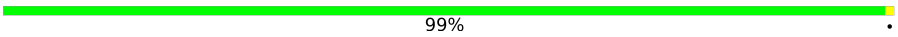
• Molecule 14: Proteasome subunit beta type-1

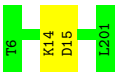
Chain N:



• Molecule 14: Proteasome subunit beta type-1

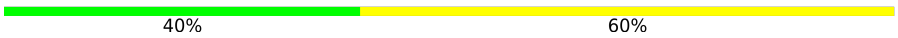
Chain b:





• Molecule 15: Macrocyclic oxindole epoxyketone

Chain g:



• Molecule 15: Macrocyclic oxindole epoxyketone

Chain e:

• Molecule 15: Macrocyclic oxindole epoxyketone

Chain i:

• Molecule 15: Macrocyclic oxindole epoxyketone

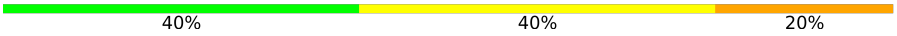
Chain f:

• Molecule 15: Macrocyclic oxindole epoxyketone

Chain h:

• Molecule 15: Macrocyclic oxindole epoxyketone

Chain j:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.69Å 302.01Å 144.24Å 90.00° 113.18° 90.00°	Depositor
Resolution (Å)	30.00 – 3.05 48.79 – 3.05	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.00-3.05) 96.4 (48.79-3.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.176 , 0.212 0.173 , 0.214	Depositor DCC
R_{free} test set	9741 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	67.9	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 40.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	49785	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: MG, CL, ACE, PPN, 6VO, A1H45

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	0.65	0/1952	0.70	0/2642
1	O	0.66	0/1952	0.70	0/2642
2	B	0.65	0/1934	0.71	0/2618
2	P	0.66	0/1934	0.71	0/2618
3	C	0.66	0/1910	0.72	0/2586
3	Q	0.66	0/1910	0.72	0/2586
4	D	0.66	0/1837	0.71	0/2475
4	R	0.66	0/1837	0.71	0/2475
5	E	0.66	0/1800	0.71	0/2433
5	S	0.66	0/1800	0.71	0/2433
6	F	0.65	0/1932	0.71	0/2609
6	T	0.65	0/1932	0.70	0/2609
7	G	0.64	0/1945	0.70	0/2634
7	U	0.64	0/1945	0.70	0/2634
8	H	0.65	0/1715	0.73	0/2326
8	V	0.64	0/1715	0.73	0/2326
9	I	0.65	0/1611	0.72	0/2174
9	W	0.65	0/1611	0.73	0/2174
10	J	0.64	0/1589	0.70	0/2142
10	X	0.64	0/1589	0.70	0/2142
11	K	0.65	0/1681	0.73	0/2274
11	Y	0.65	0/1681	0.72	0/2274
12	L	0.64	0/1795	0.71	0/2420
12	Z	0.64	0/1795	0.71	0/2420
13	M	0.64	0/1855	0.72	0/2514
13	a	0.65	0/1855	0.72	0/2514
14	N	0.64	0/1541	0.70	0/2087
14	b	0.64	0/1541	0.70	0/2087
15	e	2.08	1/7 (14.3%)	1.08	0/8
15	f	2.03	1/7 (14.3%)	1.04	0/8
15	g	2.09	1/7 (14.3%)	1.09	0/8
15	h	2.05	1/7 (14.3%)	1.00	0/8

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
15	i	2.04	1/7 (14.3%)	1.04	0/8
15	j	2.04	1/7 (14.3%)	1.08	0/8
All	All	0.65	6/50236 (0.0%)	0.71	0/67916

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	g	3	LEU	CA-C	-5.42	1.38	1.52
15	e	3	LEU	CA-C	-5.40	1.39	1.52
15	h	3	LEU	CA-C	-5.30	1.39	1.52
15	i	3	LEU	CA-C	-5.28	1.39	1.52
15	f	3	LEU	CA-C	-5.26	1.39	1.52
15	j	3	LEU	CA-C	-5.25	1.39	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	5	0
1	O	1915	0	1929	7	0
2	B	1904	0	1904	8	0
2	P	1904	0	1904	7	0
3	C	1881	0	1895	13	0
3	Q	1881	0	1895	12	0
4	D	1813	0	1797	9	0
4	R	1813	0	1797	10	0
5	E	1773	0	1775	6	0
5	S	1773	0	1775	7	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1684	0	1684	13	0
8	V	1684	0	1684	20	0
9	I	1581	0	1574	14	0
9	W	1581	0	1574	13	0
10	J	1561	0	1569	17	0
10	X	1561	0	1569	16	0
11	K	1644	0	1591	19	0
11	Y	1644	0	1591	17	0
12	L	1757	0	1711	20	0
12	Z	1757	0	1711	18	0
13	M	1824	0	1832	8	0
13	a	1824	0	1832	0	0
14	N	1512	0	1477	6	0
14	b	1512	0	1477	0	0
15	e	53	0	20	0	0
15	f	53	0	20	0	0
15	g	53	0	20	0	0
15	h	53	0	20	0	0
15	i	53	0	20	0	0
15	j	53	0	20	0	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	K	1	0	0	0	0
16	N	1	0	0	0	0
16	V	1	0	0	0	0
16	X	1	0	0	0	0
16	Y	1	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	U	1	0	0	0	0
18	A	4	0	0	0	0
18	B	7	0	0	0	0
18	C	5	0	0	0	0
18	D	5	0	0	0	0
18	E	6	0	0	0	0
18	F	6	0	0	0	0
18	G	6	0	0	0	0
18	H	7	0	0	0	0
18	I	6	0	0	0	0
18	J	11	0	0	0	0
18	K	5	0	0	0	0
18	L	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	M	4	0	0	0	0
18	N	8	0	0	0	0
18	O	1	0	0	0	0
18	P	8	0	0	0	0
18	Q	7	0	0	1	0
18	R	4	0	0	0	0
18	S	2	0	0	0	0
18	T	3	0	0	0	0
18	U	5	0	0	1	0
18	V	5	0	0	0	0
18	W	2	0	0	0	0
18	X	8	0	0	0	0
18	Y	5	0	0	0	0
18	Z	6	0	0	0	0
18	a	8	0	0	0	0
18	b	4	0	0	0	0
18	e	1	0	0	0	0
18	g	2	0	0	0	0
18	h	2	0	0	0	0
18	i	1	0	0	0	0
18	j	1	0	0	0	0
All	All	49785	0	49164	232	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 3.

All (232) 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)
10:X:101:ASN:HB3	10:X:133:HIS:CD2	1.85	1.12
10:J:101:ASN:HB3	10:J:133:HIS:CD2	1.84	1.11
4:R:94:TYR:HD1	12:Z:95:HIS:HD1	1.22	0.85
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.45	0.80
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.45	0.80
10:J:101:ASN:HB3	10:J:133:HIS:HD2	1.44	0.80
11:K:40:ILE:HD12	11:K:50:MET:CE	2.13	0.79
8:V:6:THR:HG21	8:V:51:ALA:HB2	1.65	0.77
10:X:101:ASN:HB3	10:X:133:HIS:HD2	1.44	0.77
4:R:94:TYR:HD1	12:Z:95:HIS:ND1	1.84	0.76
10:J:101:ASN:CB	10:J:133:HIS:CD2	2.67	0.75
11:Y:40:ILE:HD12	11:Y:50:MET:CE	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:101:ASN:CB	10:X:133:HIS:CD2	2.68	0.75
10:J:101:ASN:CB	10:J:133:HIS:HD2	2.02	0.72
14:N:157:VAL:HA	14:N:180:MET:HE1	1.73	0.70
11:Y:6:THR:HG22	11:Y:7:THR:N	2.08	0.69
8:V:6:THR:HG21	8:V:51:ALA:CB	2.22	0.68
10:X:101:ASN:CB	10:X:133:HIS:HD2	2.03	0.68
11:K:12:ARG:NH2	11:K:115:PRO:O	2.23	0.68
11:K:40:ILE:HD12	11:K:50:MET:HE2	1.76	0.68
7:U:23:PHE:O	7:U:26:THR:HB	1.94	0.67
11:K:6:THR:HG22	11:K:7:THR:N	2.07	0.67
4:D:94:TYR:HD1	12:L:95:HIS:ND1	1.92	0.67
7:G:23:PHE:O	7:G:26:THR:HB	1.96	0.66
8:V:58:GLU:OE2	8:V:58:GLU:HA	1.98	0.64
6:F:123:ASN:C	6:F:123:ASN:HD22	2.02	0.62
11:Y:40:ILE:HD12	11:Y:50:MET:HE2	1.80	0.62
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.81	0.62
8:H:55:ALA:CB	9:I:126:ILE:HG22	2.30	0.62
8:H:23:THR:HG21	8:H:177:ASN:HB2	1.83	0.61
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.64	0.61
8:V:85:LEU:HD12	8:V:118:ILE:HD11	1.83	0.61
10:J:174:MET:HA	10:X:174:MET:HA	1.81	0.60
8:V:23:THR:HG21	8:V:177:ASN:HB2	1.83	0.60
6:T:123:ASN:C	6:T:123:ASN:HD22	2.05	0.60
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.81	0.60
8:H:85:LEU:HD12	8:H:118:ILE:HD11	1.83	0.60
11:K:6:THR:CG2	11:K:7:THR:N	2.65	0.60
8:V:6:THR:CG2	8:V:51:ALA:HB2	2.32	0.59
9:W:87:THR:HG22	9:W:129:ILE:HD13	1.83	0.59
11:K:78:ARG:HG2	11:K:78:ARG:HH11	1.66	0.59
8:H:58:GLU:OE2	8:H:58:GLU:HA	2.01	0.59
3:Q:51:LYS:NZ	18:Q:301:HOH:O	2.26	0.59
4:D:94:TYR:HD1	12:L:95:HIS:HD1	1.47	0.59
11:Y:78:ARG:HG2	11:Y:78:ARG:HH11	1.68	0.59
9:I:87:THR:HG22	9:I:129:ILE:HD13	1.84	0.58
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.02	0.58
11:Y:6:THR:CG2	11:Y:7:THR:N	2.67	0.57
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.71	0.56
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.72	0.55
6:F:123:ASN:HD22	6:F:124:SER:N	2.05	0.55
9:W:98:ARG:HD2	9:W:126:ILE:HG13	1.89	0.55
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:98:ARG:HD2	9:I:126:ILE:HG13	1.88	0.54
8:V:55:ALA:CB	9:W:126:ILE:HG22	2.38	0.54
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.42	0.54
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.43	0.53
6:T:123:ASN:HD22	6:T:124:SER:N	2.06	0.53
3:C:38:ASN:C	3:C:38:ASN:HD22	2.12	0.53
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.06	0.53
11:K:59:PHE:HE1	12:L:95:HIS:HD2	1.57	0.53
8:V:40:HIS:HB3	8:V:61:THR:HG21	1.90	0.52
3:Q:38:ASN:C	3:Q:38:ASN:HD22	2.11	0.52
8:V:215:THR:HG21	9:W:167:SER:HB3	1.91	0.52
8:H:40:HIS:HB3	8:H:61:THR:HG21	1.90	0.52
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.92	0.51
11:Y:6:THR:HG23	11:Y:38:LYS:NZ	2.25	0.51
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.46	0.51
10:X:101:ASN:HB3	10:X:133:HIS:NE2	2.22	0.51
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.45	0.51
4:R:94:TYR:CD1	12:Z:95:HIS:ND1	2.66	0.51
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.93	0.50
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.93	0.50
10:J:101:ASN:HB3	10:J:133:HIS:NE2	2.22	0.50
1:O:12:PHE:H	2:P:20:GLN:HE22	1.59	0.50
8:V:8:ILE:HG13	8:V:104:ILE:HD12	1.92	0.50
1:O:119:GLN:O	1:O:122:THR:HB	2.11	0.50
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.93	0.50
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.11	0.50
12:L:8:ASN:HA	12:L:30:ILE:O	2.12	0.49
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.94	0.49
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.94	0.49
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.58	0.49
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.28	0.49
1:A:119:GLN:O	1:A:122:THR:HB	2.12	0.49
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.95	0.49
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.95	0.49
7:U:78:ILE:N	7:U:79:PRO:CD	2.75	0.49
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.95	0.49
7:G:78:ILE:N	7:G:79:PRO:CD	2.76	0.49
4:R:94:TYR:HD1	12:Z:95:HIS:CE1	2.31	0.49
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.62	0.48
11:Y:9:LEU:HD22	11:Y:9:LEU:O	2.12	0.48
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:147:MET:N	12:L:148:PRO:HD2	2.28	0.48
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.43	0.48
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.95	0.48
11:K:9:LEU:HD22	11:K:9:LEU:O	2.14	0.48
10:J:1:MET:O	10:J:2:ASP:HB2	2.14	0.48
1:O:57:MET:HE1	18:U:403:HOH:O	2.14	0.48
8:V:7:THR:O	8:V:164:ILE:HD12	2.14	0.48
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.95	0.47
8:H:215:THR:HG21	9:I:167:SER:HB3	1.95	0.47
7:G:61:SER:OG	7:G:215:GLU:OE2	2.22	0.47
14:N:60:ILE:HD11	14:N:98:LEU:HD13	1.97	0.47
9:W:102:TYR:O	9:W:125:LEU:HD12	2.14	0.47
3:C:108:THR:HG21	3:C:146:TYR:HB3	1.97	0.47
4:D:94:TYR:CD1	12:L:95:HIS:ND1	2.78	0.47
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.96	0.47
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.13	0.47
1:A:12:PHE:H	2:B:20:GLN:HE22	1.63	0.47
8:H:109:ASP:HB2	8:H:110:PRO:HD2	1.97	0.47
11:Y:9:LEU:HD22	11:Y:9:LEU:C	2.35	0.47
8:V:55:ALA:HB2	9:W:128:CYS:HB2	1.97	0.47
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.43	0.47
8:V:40:HIS:CB	8:V:61:THR:HG21	2.45	0.47
8:H:40:HIS:CB	8:H:61:THR:HG21	2.46	0.46
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.97	0.46
10:J:177:LYS:NZ	10:X:169:GLU:O	2.48	0.46
8:H:55:ALA:HB2	9:I:128:CYS:HB2	1.98	0.46
11:K:9:LEU:HD22	11:K:9:LEU:C	2.36	0.46
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.96	0.46
1:O:149:GLN:O	1:O:156:TYR:HA	2.15	0.46
10:X:168:LEU:O	10:X:172:MET:HB2	2.16	0.46
3:C:201:VAL:HG13	3:C:202:GLN:N	2.30	0.46
4:D:94:TYR:HD1	12:L:95:HIS:CE1	2.33	0.46
1:A:149:GLN:O	1:A:156:TYR:HA	2.16	0.45
3:C:160:GLN:HA	3:C:160:GLN:NE2	2.23	0.45
5:S:77:ALA:N	5:S:78:PRO:CD	2.79	0.45
10:X:1:MET:O	10:X:2:ASP:HB2	2.16	0.45
12:Z:108:HIS:HD2	12:Z:139:GLY:HA3	1.80	0.45
11:Y:9:LEU:HD11	11:Y:166:ILE:HG12	1.98	0.45
8:V:109:ASP:HB2	8:V:110:PRO:HD2	1.99	0.45
11:Y:59:PHE:CE1	12:Z:95:HIS:CD2	3.04	0.45
5:E:77:ALA:N	5:E:78:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:3:ILE:HB	10:J:18:SER:HB3	1.99	0.45
13:M:228:TYR:HA	8:V:126:VAL:HG23	1.98	0.45
14:N:19:LEU:HD11	14:N:105:ALA:HB3	1.99	0.45
8:V:14:ASN:HD22	8:V:15:ASN:N	2.15	0.45
12:L:108:HIS:HD2	12:L:139:GLY:HA3	1.82	0.45
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.31	0.45
11:K:59:PHE:CE1	12:L:95:HIS:CD2	3.05	0.44
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.64	0.44
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.52	0.44
10:J:168:LEU:O	10:J:172:MET:HB2	2.16	0.44
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	1.98	0.44
10:X:3:ILE:HB	10:X:18:SER:HB3	1.99	0.44
5:E:9:THR:HG21	5:E:119:THR:HA	1.99	0.44
11:K:55:ALA:CB	12:L:128:VAL:HG23	2.47	0.44
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.66	0.44
11:Y:59:PHE:HE1	12:Z:95:HIS:CD2	2.36	0.44
8:H:55:ALA:HB1	9:I:126:ILE:HG22	1.98	0.44
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.47	0.44
14:N:41:ARG:HH21	14:N:65:GLN:HE21	1.65	0.44
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.64	0.44
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.99	0.44
11:Y:181:ASN:ND2	11:Y:195:ASN:HD22	2.15	0.44
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.82	0.44
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.47	0.44
11:K:9:LEU:HD11	11:K:166:ILE:HG12	2.00	0.44
13:M:228:TYR:HA	8:V:126:VAL:CG2	2.48	0.44
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.52	0.44
8:H:14:ASN:HD22	8:H:15:ASN:N	2.16	0.43
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.00	0.43
3:C:201:VAL:O	3:C:202:GLN:CB	2.66	0.43
10:J:169:GLU:O	10:X:177:LYS:NZ	2.51	0.43
5:S:9:THR:HG21	5:S:119:THR:HA	2.00	0.43
14:N:41:ARG:NH1	14:N:44:ASP:OD2	2.51	0.43
2:P:6:ASP:OD2	3:Q:4:ARG:HG3	2.17	0.43
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.84	0.43
2:B:148:TYR:OH	3:C:57:ILE:HB	2.19	0.43
3:C:9:PHE:H	4:D:15:GLN:HE22	1.66	0.43
10:J:118:GLN:HG2	10:J:133:HIS:HE1	1.84	0.43
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.99	0.43
4:D:99:ILE:HD11	4:D:104:LEU:HB2	2.00	0.43
9:I:102:TYR:O	9:I:125:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:6:THR:O	8:V:133:GLY:HA3	2.19	0.43
8:H:6:THR:O	8:H:133:GLY:HA3	2.19	0.43
14:N:24:ARG:O	14:N:38:LYS:NZ	2.48	0.43
4:R:24:LYS:O	4:R:166:SER:HA	2.19	0.43
8:V:55:ALA:HB1	9:W:126:ILE:HG22	2.01	0.43
8:H:142:VAL:HG21	8:H:166:ALA:HB2	2.00	0.42
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.83	0.42
10:X:118:GLN:HG2	10:X:133:HIS:HE1	1.84	0.42
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.54	0.42
3:Q:160:GLN:HA	3:Q:160:GLN:NE2	2.24	0.42
11:Y:55:ALA:CB	12:Z:128:VAL:HG23	2.49	0.42
4:D:24:LYS:O	4:D:166:SER:HA	2.19	0.42
11:K:42:ILE:HG23	11:K:65:GLY:HA2	2.01	0.42
11:Y:78:ARG:HH11	11:Y:78:ARG:CG	2.31	0.42
9:I:37:ASN:ND2	11:Y:214:ASN:O	2.52	0.42
11:K:181:ASN:ND2	11:K:195:ASN:HD22	2.17	0.42
13:M:179:ASN:HD22	13:M:182:ARG:NH1	2.17	0.42
4:R:158:ARG:O	5:S:57:SER:N	2.45	0.42
1:A:115:ALA:HB1	1:A:154:GLY:O	2.19	0.42
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.00	0.42
7:G:43:VAL:HG11	7:G:194:VAL:HA	2.02	0.42
8:V:142:VAL:HG21	8:V:166:ALA:HB2	2.01	0.42
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.55	0.42
11:K:78:ARG:HH11	11:K:78:ARG:CG	2.30	0.42
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.00	0.42
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.66	0.41
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.55	0.41
11:K:59:PHE:CE1	12:L:95:HIS:HD2	2.35	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.41
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.18	0.41
11:K:6:THR:HG23	11:K:38:LYS:NZ	2.35	0.41
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.55	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.02	0.41
6:T:155:GLY:HA3	7:U:59:THR:HG21	2.02	0.41
11:Y:42:ILE:HG23	11:Y:65:GLY:HA2	2.02	0.41
11:Y:60:TRP:HB2	11:Y:102:MET:CE	2.50	0.41
11:K:46:LEU:HD23	11:K:46:LEU:HA	1.87	0.41
7:G:34:LEU:C	7:G:34:LEU:HD23	2.41	0.41
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.20	0.41
9:I:7:ASN:HA	9:I:29:GLY:O	2.20	0.41
13:M:26:ASN:HA	13:M:39:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.03	0.41
7:U:43:VAL:HG11	7:U:194:VAL:HA	2.01	0.41
2:B:50:LYS:O	2:B:51:VAL:C	2.59	0.41
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.86	0.41
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.20	0.40
11:K:214:ASN:O	9:W:37:ASN:ND2	2.54	0.40
1:O:115:ALA:HB1	1:O:154:GLY:O	2.20	0.40
7:U:78:ILE:HG22	7:U:79:PRO:HD3	2.04	0.40
3:C:51:LYS:O	3:C:52:LEU:HB2	2.20	0.40
7:U:73:VAL:HG12	7:U:133:THR:HB	2.02	0.40
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.56	0.40
10:J:118:GLN:CG	10:J:133:HIS:CE1	3.04	0.40
13:M:48:ASN:H	13:M:48:ASN:HD22	1.67	0.40
7:U:114:ASN:HD22	7:U:114:ASN:HA	1.70	0.40
10:J:22:THR:HG21	10:X:173:PRO:HB3	2.04	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	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34	64
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34	64
2	B	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	34	64
2	P	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	34	64
3	C	238/254 (94%)	228 (96%)	7 (3%)	3 (1%)	12	38
3	Q	238/254 (94%)	228 (96%)	7 (3%)	3 (1%)	12	38
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
6	T	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
7	G	239/252 (95%)	232 (97%)	7 (3%)	0	100	100
7	U	239/252 (95%)	232 (97%)	7 (3%)	0	100	100
8	H	220/232 (95%)	217 (99%)	3 (1%)	0	100	100
8	V	220/232 (95%)	217 (99%)	3 (1%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	60
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	60
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	222 (96%)	7 (3%)	2 (1%)	17	47
13	a	231/246 (94%)	223 (96%)	6 (3%)	2 (1%)	17	47
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
15	e	1/5 (20%)	1 (100%)	0	0	100	100
15	f	1/5 (20%)	1 (100%)	0	0	100	100
15	g	1/5 (20%)	1 (100%)	0	0	100	100
15	h	1/5 (20%)	1 (100%)	0	0	100	100
15	i	1/5 (20%)	1 (100%)	0	0	100	100
15	j	1/5 (20%)	1 (100%)	0	0	100	100
All	All	6282/6644 (95%)	6109 (97%)	157 (2%)	16 (0%)	41	70

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN

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Mol	Chain	Res	Type
10	J	2	ASP
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
3	C	205	ALA
3	C	239	GLN
3	Q	205	ALA
3	Q	239	GLN
1	A	3	ASP
13	M	83	ALA
1	O	3	ASP
13	a	83	ALA
13	M	229	GLY
13	a	229	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	205 (98%)	4 (2%)	57	79
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	79
2	B	203/216 (94%)	195 (96%)	8 (4%)	32	63
2	P	203/216 (94%)	195 (96%)	8 (4%)	32	63
3	C	212/226 (94%)	204 (96%)	8 (4%)	33	63
3	Q	212/226 (94%)	204 (96%)	8 (4%)	33	63
4	D	194/215 (90%)	186 (96%)	8 (4%)	30	61
4	R	194/215 (90%)	186 (96%)	8 (4%)	30	61
5	E	190/193 (98%)	182 (96%)	8 (4%)	30	60
5	S	190/193 (98%)	183 (96%)	7 (4%)	34	64
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	54
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	54
7	G	206/210 (98%)	198 (96%)	8 (4%)	32	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	U	206/210 (98%)	198 (96%)	8 (4%)	32 63
8	H	181/190 (95%)	171 (94%)	10 (6%)	21 50
8	V	181/190 (95%)	171 (94%)	10 (6%)	21 50
9	I	172/173 (99%)	166 (96%)	6 (4%)	36 66
9	W	172/173 (99%)	166 (96%)	6 (4%)	36 66
10	J	173/175 (99%)	166 (96%)	7 (4%)	31 62
10	X	173/175 (99%)	166 (96%)	7 (4%)	31 62
11	K	169/169 (100%)	161 (95%)	8 (5%)	26 56
11	Y	169/169 (100%)	162 (96%)	7 (4%)	30 61
12	L	185/185 (100%)	179 (97%)	6 (3%)	39 68
12	Z	185/185 (100%)	177 (96%)	8 (4%)	29 59
13	M	199/208 (96%)	193 (97%)	6 (3%)	41 69
13	a	199/208 (96%)	193 (97%)	6 (3%)	41 69
14	N	162/162 (100%)	160 (99%)	2 (1%)	71 87
14	b	162/162 (100%)	160 (99%)	2 (1%)	71 87
15	e	1/1 (100%)	1 (100%)	0	100 100
15	f	1/1 (100%)	1 (100%)	0	100 100
15	g	1/1 (100%)	1 (100%)	0	100 100
15	h	1/1 (100%)	0	1 (100%)	0 0
15	i	1/1 (100%)	0	1 (100%)	0 0
15	j	1/1 (100%)	0	1 (100%)	0 0
All	All	5318/5546 (96%)	5117 (96%)	201 (4%)	33 63

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	52	THR
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU

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Mol	Chain	Res	Type
2	B	114	LEU
2	B	184	LYS
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	203	THR
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	224	ASP
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	125	MET
7	G	166	GLN

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Mol	Chain	Res	Type
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	14	ASN
8	H	27	GLN
8	H	35	ASN
8	H	36	CYS
8	H	39	LEU
8	H	58	GLU
8	H	89	LYS
8	H	118	ILE
8	H	132	LEU
8	H	201	ARG
9	I	37	ASN
9	I	97	ARG
9	I	125	LEU
9	I	126	ILE
9	I	171	LEU
9	I	182	TRP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	78	GLN
10	J	133	HIS
10	J	144	LEU
10	J	174	MET
11	K	9	LEU
11	K	12	ARG
11	K	14	GLN
11	K	40	ILE
11	K	104	THR
11	K	105	MET
11	K	111	ARG
11	K	123	ASP
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	126	ASP
12	L	136	CYS
12	L	167	LYS
13	M	43	ILE
13	M	48	ASN

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Mol	Chain	Res	Type
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	14	LYS
14	N	15	ASP
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	52	THR
2	P	55	LEU
2	P	58	GLN
2	P	79	LEU
2	P	114	LEU
2	P	184	LYS
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	203	THR
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	224	ASP
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	14	ASP

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Mol	Chain	Res	Type
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	14	ASN
8	V	27	GLN
8	V	35	ASN
8	V	36	CYS
8	V	39	LEU
8	V	58	GLU
8	V	89	LYS
8	V	118	ILE
8	V	132	LEU
8	V	201	ARG
9	W	37	ASN
9	W	97	ARG
9	W	125	LEU
9	W	126	ILE
9	W	171	LEU
9	W	182	TRP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	78	GLN
10	X	133	HIS
10	X	144	LEU
10	X	174	MET
11	Y	9	LEU
11	Y	14	GLN

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Mol	Chain	Res	Type
11	Y	40	ILE
11	Y	104	THR
11	Y	105	MET
11	Y	111	ARG
11	Y	123	ASP
12	Z	1	GLN
12	Z	23	LEU
12	Z	34	SER
12	Z	49	ASN
12	Z	126	ASP
12	Z	130	SER
12	Z	136	CYS
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	14	LYS
14	b	15	ASP
15	i	3	LEU
15	h	3	LEU
15	j	3	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	146	GLN

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Mol	Chain	Res	Type
4	D	160	ASN
4	D	198	GLN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	147	GLN
5	E	184	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	6	HIS
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
8	H	14	ASN
8	H	119	HIS
8	H	177	ASN
9	I	88	GLN
10	J	55	GLN
10	J	118	GLN
10	J	133	HIS
10	J	146	HIS
10	J	191	GLN
11	K	14	GLN
11	K	90	ASN
11	K	148	ASN
11	K	181	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	80	ASN
12	L	152	ASN
12	L	153	GLN

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Mol	Chain	Res	Type
12	L	158	ASN
12	L	159	GLN
12	L	165	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	65	GLN
14	N	166	GLN
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	146	GLN
4	R	160	ASN
4	R	198	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	147	GLN
5	S	151	ASN
5	S	184	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	114	ASN

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Mol	Chain	Res	Type
7	U	117	GLN
7	U	121	GLN
7	U	175	ASN
8	V	14	ASN
8	V	121	HIS
8	V	177	ASN
9	W	88	GLN
10	X	55	GLN
10	X	118	GLN
10	X	133	HIS
10	X	146	HIS
10	X	191	GLN
11	Y	14	GLN
11	Y	90	ASN
11	Y	148	ASN
11	Y	181	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	158	ASN
12	Z	165	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	65	GLN
14	b	166	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)

12 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	$\#\|Z\| > 2$
15	PPN	j	2	15	12,14,15	3.95	3 (25%)	13,18,20	1.40	3 (23%)
15	A1H45	j	4	15	14,17,18	3.27	6 (42%)	16,24,26	2.62	6 (37%)
15	A1H45	g	4	15	14,17,18	3.37	7 (50%)	16,24,26	2.68	6 (37%)
15	A1H45	e	4	15	14,17,18	3.29	6 (42%)	16,24,26	2.58	4 (25%)
15	A1H45	i	4	15	14,17,18	3.31	7 (50%)	16,24,26	2.62	5 (31%)
15	PPN	f	2	15	12,14,15	3.83	3 (25%)	13,18,20	1.34	2 (15%)
15	A1H45	h	4	15	14,17,18	3.38	7 (50%)	16,24,26	2.70	6 (37%)
15	PPN	g	2	15	12,14,15	3.63	3 (25%)	13,18,20	1.39	3 (23%)
15	PPN	h	2	15	12,14,15	3.71	3 (25%)	13,18,20	1.37	2 (15%)
15	A1H45	f	4	15	14,17,18	3.29	6 (42%)	16,24,26	2.57	4 (25%)
15	PPN	i	2	15	12,14,15	3.84	3 (25%)	13,18,20	1.49	3 (23%)
15	PPN	e	2	15	12,14,15	3.71	3 (25%)	13,18,20	1.30	2 (15%)

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
15	PPN	j	2	15	-	0/7/10/12	0/1/1/1
15	A1H45	j	4	15	-	3/5/18/20	0/2/2/2
15	A1H45	g	4	15	-	1/5/18/20	0/2/2/2
15	A1H45	e	4	15	-	3/5/18/20	0/2/2/2
15	A1H45	i	4	15	-	3/5/18/20	0/2/2/2
15	PPN	f	2	15	-	5/7/10/12	0/1/1/1
15	A1H45	h	4	15	-	2/5/18/20	0/2/2/2
15	PPN	g	2	15	-	2/7/10/12	0/1/1/1
15	PPN	h	2	15	-	2/7/10/12	0/1/1/1
15	A1H45	f	4	15	-	3/5/18/20	0/2/2/2
15	PPN	i	2	15	-	4/7/10/12	0/1/1/1
15	PPN	e	2	15	-	4/7/10/12	0/1/1/1

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	j	2	PPN	O1-N1	11.65	1.42	1.22
15	f	2	PPN	O1-N1	11.30	1.42	1.22
15	i	2	PPN	O1-N1	11.24	1.41	1.22
15	e	2	PPN	O1-N1	10.81	1.41	1.22
15	h	2	PPN	O1-N1	10.65	1.40	1.22
15	g	2	PPN	O1-N1	10.35	1.40	1.22
15	h	4	A1H45	CE2-CD2	-7.46	1.33	1.39
15	g	4	A1H45	CE2-CD2	-7.36	1.33	1.39
15	i	4	A1H45	CE2-CD2	-7.31	1.33	1.39
15	e	4	A1H45	CE2-CD2	-7.30	1.33	1.39
15	f	4	A1H45	CE2-CD2	-7.23	1.33	1.39
15	g	4	A1H45	CD2-CG	-7.23	1.38	1.51
15	j	4	A1H45	CE2-CD2	-7.22	1.33	1.39
15	h	4	A1H45	CD2-CG	-7.18	1.38	1.51
15	j	4	A1H45	CD2-CG	-7.06	1.39	1.51
15	i	4	A1H45	CD2-CG	-7.04	1.39	1.51
15	e	4	A1H45	CD2-CG	-7.03	1.39	1.51
15	f	4	A1H45	CD2-CG	-7.00	1.39	1.51
15	h	2	PPN	CB-CG	-5.12	1.39	1.51
15	j	2	PPN	CB-CG	-5.09	1.39	1.51
15	i	2	PPN	CB-CG	-5.09	1.39	1.51
15	g	2	PPN	CB-CG	-5.08	1.39	1.51
15	h	2	PPN	CZ-N1	-4.91	1.33	1.45
15	f	2	PPN	CB-CG	-4.89	1.39	1.51
15	g	2	PPN	CZ-N1	-4.88	1.33	1.45
15	j	2	PPN	CZ-N1	-4.86	1.33	1.45
15	e	2	PPN	CB-CG	-4.86	1.39	1.51
15	i	2	PPN	CZ-N1	-4.85	1.33	1.45
15	e	2	PPN	CZ-N1	-4.82	1.33	1.45
15	f	2	PPN	CZ-N1	-4.78	1.33	1.45
15	g	4	A1H45	CE3-CD2	-3.91	1.33	1.39
15	h	4	A1H45	CE3-CD2	-3.89	1.33	1.39
15	i	4	A1H45	CE3-CD2	-3.87	1.33	1.39
15	j	4	A1H45	CE3-CD2	-3.81	1.33	1.39
15	f	4	A1H45	CE3-CD2	-3.79	1.33	1.39
15	e	4	A1H45	CE3-CD2	-3.76	1.33	1.39
15	f	4	A1H45	CZ2-CE2	-3.75	1.33	1.39
15	e	4	A1H45	CZ2-CE2	-3.71	1.33	1.39
15	g	4	A1H45	CZ2-CE2	-3.68	1.33	1.39
15	h	4	A1H45	CZ2-CE2	-3.65	1.33	1.39
15	i	4	A1H45	CZ2-CE2	-3.63	1.33	1.39
15	j	4	A1H45	CZ2-CE2	-3.63	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	f	4	A1H45	CD1-NE1	-3.02	1.33	1.35
15	h	4	A1H45	CD1-NE1	-3.00	1.33	1.35
15	e	4	A1H45	CD1-NE1	-2.99	1.33	1.35
15	g	4	A1H45	CD1-NE1	-2.97	1.33	1.35
15	g	4	A1H45	CE2-NE1	-2.91	1.33	1.38
15	h	4	A1H45	CE2-NE1	-2.88	1.33	1.38
15	f	4	A1H45	CE2-NE1	-2.87	1.33	1.38
15	e	4	A1H45	CE2-NE1	-2.85	1.33	1.38
15	j	4	A1H45	CE2-NE1	-2.85	1.33	1.38
15	i	4	A1H45	CD1-NE1	-2.83	1.33	1.35
15	i	4	A1H45	CE2-NE1	-2.83	1.33	1.38
15	j	4	A1H45	CD1-NE1	-2.81	1.33	1.35
15	h	4	A1H45	CB-CG	-2.40	1.51	1.54
15	g	4	A1H45	CB-CG	-2.24	1.51	1.54
15	i	4	A1H45	CB-CG	-2.16	1.51	1.54

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	g	4	A1H45	CE2-NE1-CD1	-7.49	107.77	111.85
15	h	4	A1H45	CE2-NE1-CD1	-7.48	107.77	111.85
15	e	4	A1H45	CE2-NE1-CD1	-7.32	107.86	111.85
15	j	4	A1H45	CE2-NE1-CD1	-7.30	107.87	111.85
15	i	4	A1H45	CE2-NE1-CD1	-7.25	107.90	111.85
15	f	4	A1H45	CE2-NE1-CD1	-7.15	107.95	111.85
15	i	4	A1H45	CE3-CD2-CE2	4.95	123.97	120.33
15	h	4	A1H45	CE3-CD2-CE2	4.90	123.93	120.33
15	g	4	A1H45	CE3-CD2-CE2	4.87	123.91	120.33
15	e	4	A1H45	CE3-CD2-CE2	4.85	123.89	120.33
15	f	4	A1H45	CE3-CD2-CE2	4.82	123.87	120.33
15	j	4	A1H45	CE3-CD2-CE2	4.65	123.75	120.33
15	i	2	PPN	CE2-CZ-N1	3.33	121.88	119.38
15	f	2	PPN	CE2-CZ-N1	3.30	121.86	119.38
15	j	2	PPN	CE2-CZ-N1	3.16	121.75	119.38
15	h	4	A1H45	CD2-CE2-NE1	-3.13	107.86	109.31
15	e	2	PPN	CE2-CZ-N1	3.12	121.72	119.38
15	j	4	A1H45	CD2-CE2-NE1	-3.11	107.87	109.31
15	g	2	PPN	CE2-CZ-N1	3.10	121.71	119.38
15	g	4	A1H45	CD2-CE2-NE1	-3.09	107.88	109.31
15	h	2	PPN	CE2-CZ-N1	3.08	121.70	119.38
15	i	4	A1H45	CD2-CE2-NE1	-3.02	107.91	109.31
15	f	4	A1H45	CD2-CE2-NE1	-2.94	107.94	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	e	4	A1H45	CD2-CE2-NE1	-2.82	108.00	109.31
15	g	4	A1H45	CB-CG-CD2	-2.57	109.22	114.53
15	i	4	A1H45	CB-CG-CD2	-2.50	109.37	114.53
15	h	4	A1H45	CB-CG-CD2	-2.46	109.45	114.53
15	i	2	PPN	CG-CB-CA	-2.45	109.14	114.10
15	h	2	PPN	CE1-CZ-N1	-2.45	117.53	119.38
15	j	4	A1H45	CB-CG-CD2	-2.40	109.57	114.53
15	i	2	PPN	CE1-CZ-N1	-2.39	117.58	119.38
15	g	2	PPN	CE1-CZ-N1	-2.38	117.58	119.38
15	h	4	A1H45	CD2-CG-CD1	-2.37	101.61	102.40
15	j	2	PPN	CE1-CZ-N1	-2.37	117.60	119.38
15	j	2	PPN	CG-CB-CA	-2.26	109.53	114.10
15	f	2	PPN	CE1-CZ-N1	-2.22	117.70	119.38
15	f	4	A1H45	CB-CG-CD2	-2.22	109.94	114.53
15	j	4	A1H45	CD2-CG-CD1	-2.17	101.67	102.40
15	h	4	A1H45	CB-CG-CD1	-2.17	108.55	113.69
15	g	4	A1H45	CB-CG-CD1	-2.17	108.55	113.69
15	g	4	A1H45	CD2-CG-CD1	-2.16	101.68	102.40
15	e	2	PPN	CE1-CZ-N1	-2.14	117.77	119.38
15	g	2	PPN	CG-CB-CA	-2.12	109.80	114.10
15	j	4	A1H45	CB-CG-CD1	-2.10	108.72	113.69
15	e	4	A1H45	CB-CG-CD2	-2.08	110.23	114.53
15	i	4	A1H45	CZ2-CE2-CD2	-2.00	119.90	121.54

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	g	2	PPN	CE1-CZ-N1-O1
15	g	2	PPN	CE2-CZ-N1-O1
15	e	2	PPN	N-CA-CB-CG
15	e	2	PPN	C-CA-CB-CG
15	e	2	PPN	CE1-CZ-N1-O1
15	e	2	PPN	CE2-CZ-N1-O1
15	i	2	PPN	N-CA-CB-CG
15	i	2	PPN	C-CA-CB-CG
15	i	2	PPN	CE1-CZ-N1-O1
15	i	2	PPN	CE2-CZ-N1-O1
15	f	2	PPN	O-C-CA-CB
15	f	2	PPN	N-CA-CB-CG
15	f	2	PPN	C-CA-CB-CG
15	f	2	PPN	CE1-CZ-N1-O1

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Mol	Chain	Res	Type	Atoms
15	f	2	PPN	CE2-CZ-N1-O1
15	h	2	PPN	CE1-CZ-N1-O1
15	h	2	PPN	CE2-CZ-N1-O1
15	g	4	A1H45	N-CA-CB-CG
15	e	4	A1H45	N-CA-CB-CG
15	e	4	A1H45	C-CA-CB-CG
15	e	4	A1H45	CA-CB-CG-CD1
15	i	4	A1H45	N-CA-CB-CG
15	i	4	A1H45	CA-CB-CG-CD2
15	f	4	A1H45	N-CA-CB-CG
15	f	4	A1H45	C-CA-CB-CG
15	h	4	A1H45	N-CA-CB-CG
15	j	4	A1H45	N-CA-CB-CG
15	j	4	A1H45	C-CA-CB-CG
15	j	4	A1H45	CA-CB-CG-CD2
15	i	4	A1H45	C-CA-CB-CG
15	h	4	A1H45	CA-CB-CG-CD2
15	f	4	A1H45	CA-CB-CG-CD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.50	2 (0%) 86 70	57, 74, 108, 167	0
1	O	250/250 (100%)	-0.39	2 (0%) 86 70	62, 84, 123, 165	0
2	B	244/258 (94%)	-0.34	2 (0%) 86 70	58, 81, 135, 187	0
2	P	244/258 (94%)	-0.24	6 (2%) 57 32	64, 84, 145, 171	0
3	C	240/254 (94%)	-0.30	0 100 100	58, 84, 135, 156	0
3	Q	240/254 (94%)	-0.08	9 (3%) 40 20	68, 102, 158, 182	0
4	D	235/260 (90%)	-0.50	0 100 100	57, 82, 112, 149	0
4	R	235/260 (90%)	-0.35	1 (0%) 92 82	60, 91, 126, 160	0
5	E	231/234 (98%)	-0.39	1 (0%) 92 82	60, 83, 114, 138	0
5	S	231/234 (98%)	-0.17	3 (1%) 77 56	63, 94, 135, 155	0
6	F	243/288 (84%)	-0.44	1 (0%) 92 82	54, 77, 117, 141	0
6	T	243/288 (84%)	-0.37	1 (0%) 92 82	60, 88, 128, 148	0
7	G	241/252 (95%)	-0.52	0 100 100	55, 71, 105, 136	0
7	U	241/252 (95%)	-0.53	0 100 100	58, 78, 107, 143	0
8	H	222/232 (95%)	-0.47	2 (0%) 84 66	54, 70, 97, 144	0
8	V	222/232 (95%)	-0.48	1 (0%) 91 79	61, 74, 99, 151	0
9	I	204/205 (99%)	-0.53	0 100 100	53, 70, 94, 115	0
9	W	204/205 (99%)	-0.55	0 100 100	51, 69, 95, 126	0
10	J	195/198 (98%)	-0.57	1 (0%) 91 79	54, 71, 95, 126	0
10	X	195/198 (98%)	-0.52	2 (1%) 82 63	55, 74, 96, 147	0
11	K	212/212 (100%)	-0.51	0 100 100	54, 70, 94, 120	0
11	Y	212/212 (100%)	-0.55	0 100 100	57, 73, 99, 119	0
12	L	222/222 (100%)	-0.50	0 100 100	48, 71, 97, 120	0
12	Z	222/222 (100%)	-0.44	0 100 100	55, 74, 106, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.55	2 (0%) 84 66	53, 69, 91, 124	0
13	a	233/246 (94%)	-0.57	2 (0%) 84 66	50, 68, 91, 120	0
14	N	196/196 (100%)	-0.58	0 100 100	51, 65, 91, 122	0
14	b	196/196 (100%)	-0.55	0 100 100	55, 67, 91, 115	0
15	e	1/5 (20%)	-0.66	0 100 100	81, 81, 81, 81	0
15	f	1/5 (20%)	-0.61	0 100 100	86, 86, 86, 86	0
15	g	1/5 (20%)	-0.47	0 100 100	65, 65, 65, 65	0
15	h	1/5 (20%)	-0.90	0 100 100	78, 78, 78, 78	0
15	i	1/5 (20%)	-0.23	0 100 100	92, 92, 92, 92	0
15	j	1/5 (20%)	0.19	0 100 100	103, 103, 103, 103	0
All	All	6342/6644 (95%)	-0.44	38 (0%) 89 76	48, 76, 122, 187	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	227	ASP	5.3
8	H	227	ASP	5.2
3	Q	234	ILE	4.2
5	S	202	ASP	3.8
3	Q	204	GLY	3.7
2	P	218	GLY	3.6
3	Q	50	LEU	3.5
5	S	233	ILE	3.5
3	Q	48	SER	3.3
4	R	241	ALA	3.3
8	H	226	CYS	3.3
2	P	220	ASN	3.2
10	J	1	MET	3.2
1	A	1	MET	3.2
3	Q	189	CYS	3.0
13	a	233	ILE	3.0
2	B	220	ASN	3.0
2	P	61	SER	2.8
13	M	1	THR	2.7
6	T	2	THR	2.7
10	X	1	MET	2.7
2	P	241	THR	2.7
1	O	249	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	221	ASP	2.5
3	Q	235	GLU	2.5
3	Q	49	THR	2.5
3	Q	206	LYS	2.5
5	E	202	ASP	2.4
13	a	1	THR	2.4
2	P	221	ASP	2.4
10	X	194	ASP	2.3
2	P	219	ALA	2.1
1	A	2	THR	2.1
5	S	225	ASP	2.1
1	O	188	ALA	2.0
13	M	233	ILE	2.0
6	F	202	ASP	2.0
3	Q	236	GLN	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	PPN	j	2	14/15	0.69	0.59	118,121,125,132	0
15	PPN	f	2	14/15	0.73	0.30	85,101,113,115	0
15	A1H45	j	4	16/17	0.78	0.33	92,109,112,114	0
15	PPN	i	2	14/15	0.82	0.39	101,113,121,123	0
15	PPN	e	2	14/15	0.82	0.36	87,99,106,114	0
15	A1H45	e	4	16/17	0.86	0.23	86,105,112,112	0
15	A1H45	f	4	16/17	0.88	0.32	88,104,113,116	0
15	A1H45	i	4	16/17	0.89	0.33	84,108,117,118	0
15	PPN	g	2	14/15	0.91	0.20	66,77,87,96	0
15	PPN	h	2	14/15	0.93	0.23	74,77,90,91	0
15	A1H45	h	4	16/17	0.95	0.14	64,74,80,84	0
15	A1H45	g	4	16/17	0.95	0.13	62,71,74,78	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	MG	Z	301	1/1	0.88	0.36	95,95,95,95	0
16	MG	G	301	1/1	0.90	0.21	68,68,68,68	0
17	CL	G	302	1/1	0.94	0.11	59,59,59,59	0
17	CL	U	301	1/1	0.96	0.07	74,74,74,74	0
16	MG	X	201	1/1	0.97	0.21	52,52,52,52	0
16	MG	K	301	1/1	0.97	0.14	76,76,76,76	0
16	MG	Y	301	1/1	0.98	0.25	89,89,89,89	0
16	MG	I	301	1/1	0.98	0.29	98,98,98,98	0
16	MG	V	301	1/1	0.99	0.08	99,99,99,99	0
16	MG	N	301	1/1	0.99	0.12	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.