



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:08 PM UTC

PDB ID : 4JSQ / pdb_00004jsq
Title : Yeast 20S proteasome in complex with the dimerized linear mimetic of TMC-95A - yCP:4e
Authors : Desvergne, A.; Genin, E.; Marechal, X.; Gallastegui, N.; Dufau, L.; Richy, N.; Groll, M.; Vidal, J.; Reboud-Ravaux, M.
Deposited on : 2013-03-22
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

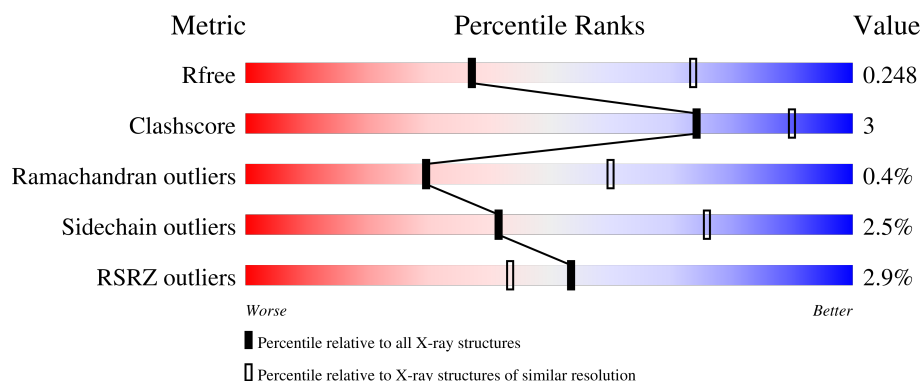
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	250	0% 93% 7%
1	O	250	2% 92% 7%
2	B	258	6% 81% 13% 5%
2	P	258	6% 81% 13% 5%
3	C	254	4% 82% 12% 5%

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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	233	
13	a	233	
14	N	196	
14	b	196	
15	c	8	
15	d	8	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 51011 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	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			
4	R	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
6	T	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	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	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	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			

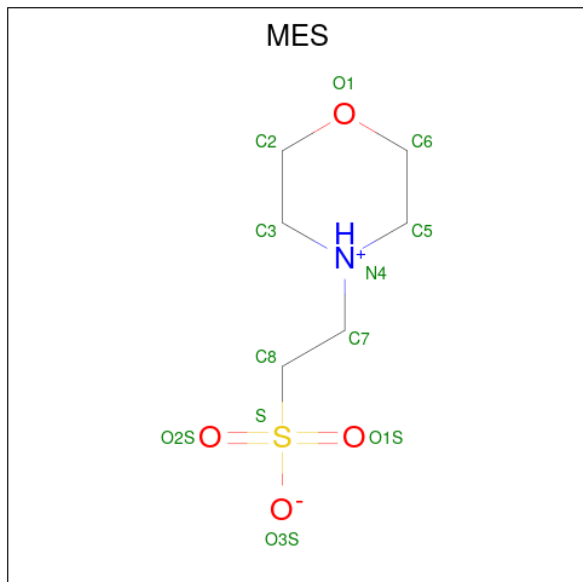
- Molecule 14 is a protein called Proteasome subunit beta type-1.

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 TMC-95A mimic ligand yCP:4e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	5	Total	C	N	O	0	0	0
			56	43	6	7			
15	d	5	Total	C	N	O	0	0	0
			56	43	6	7			

- Molecule 16 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
16	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	59	Total	O	0	0
			59	59		
17	B	39	Total	O	0	0
			39	39		
17	C	43	Total	O	0	0
			43	43		
17	D	36	Total	O	0	0
			36	36		
17	E	21	Total	O	0	0
			21	21		
17	F	47	Total	O	0	0
			47	47		
17	G	60	Total	O	0	0
			60	60		
17	H	52	Total	O	0	0
			52	52		

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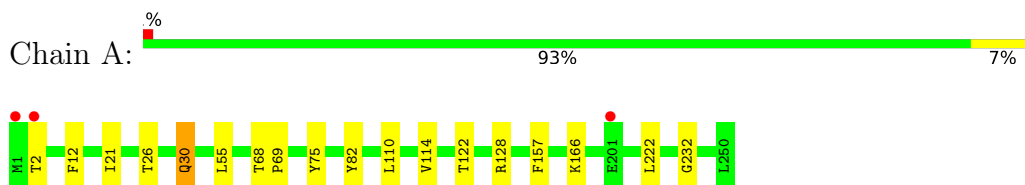
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	I	64	Total 64	O 64	0	0
17	J	53	Total 53	O 53	0	0
17	K	48	Total 48	O 48	0	0
17	L	54	Total 54	O 54	0	0
17	M	81	Total 81	O 81	0	0
17	N	58	Total 58	O 58	0	0
17	O	34	Total 34	O 34	0	0
17	P	30	Total 30	O 30	0	0
17	Q	29	Total 29	O 29	0	0
17	R	27	Total 27	O 27	0	0
17	S	18	Total 18	O 18	0	0
17	T	43	Total 43	O 43	0	0
17	U	55	Total 55	O 55	0	0
17	V	50	Total 50	O 50	0	0
17	W	62	Total 62	O 62	0	0
17	X	41	Total 41	O 41	0	0
17	Y	50	Total 50	O 50	0	0
17	Z	49	Total 49	O 49	0	0
17	a	78	Total 78	O 78	0	0
17	b	56	Total 56	O 56	0	0

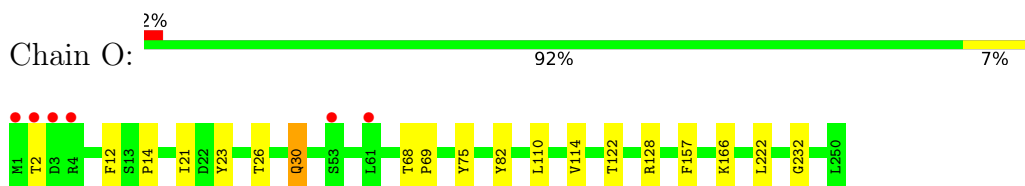
3 Residue-property plots [i](#)

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.

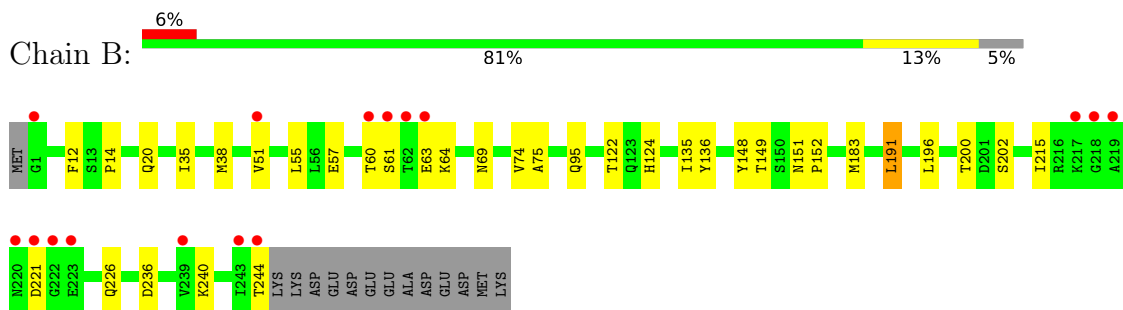
- Molecule 1: Proteasome subunit alpha type-2



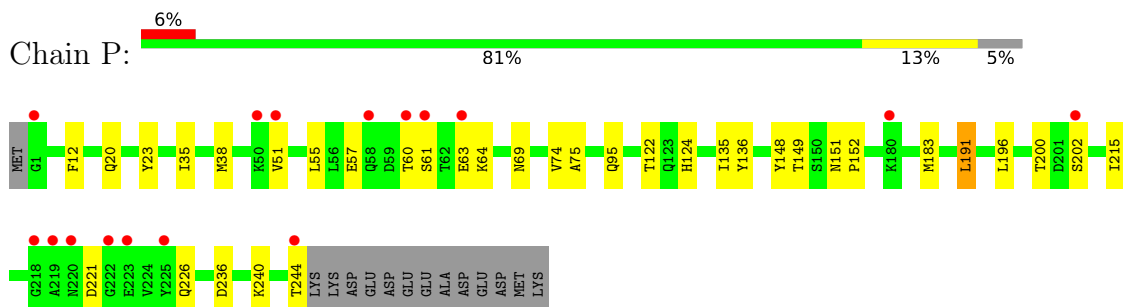
- Molecule 1: Proteasome subunit alpha type-2



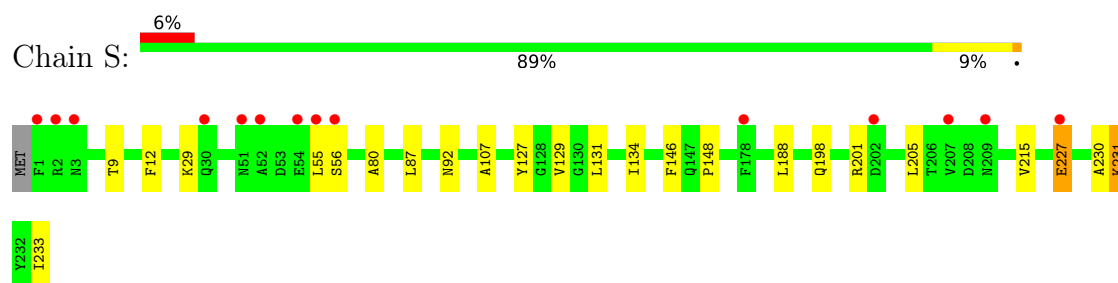
- Molecule 2: Proteasome subunit alpha type-3



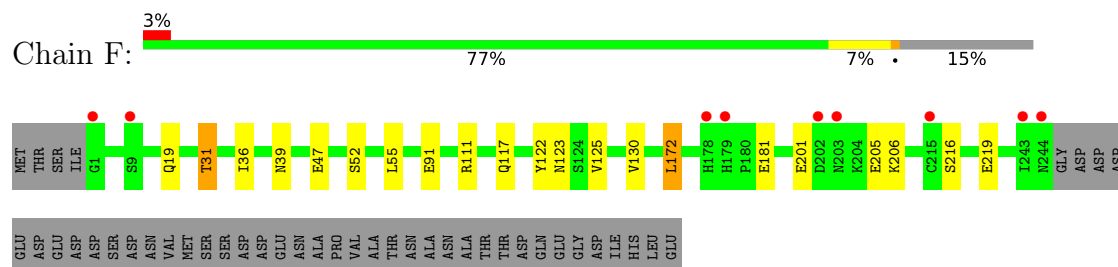
- Molecule 2: Proteasome subunit alpha type-3



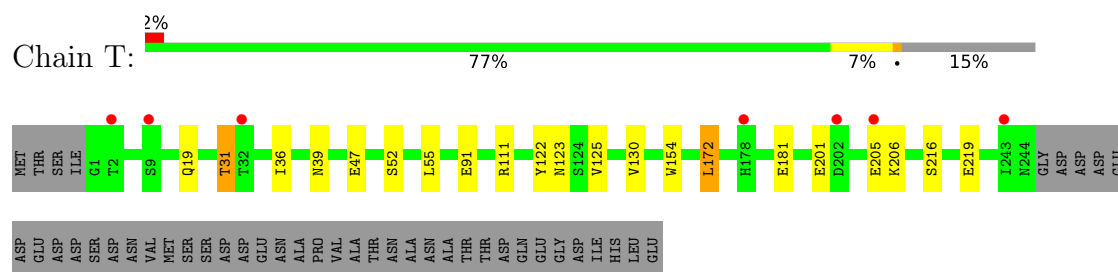
- Molecule 3: Proteasome subunit alpha type-4



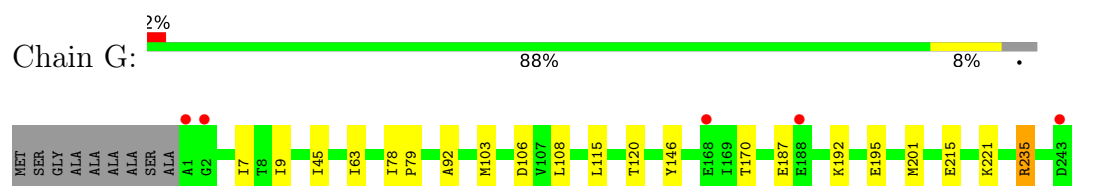
- Molecule 6: Probable proteasome subunit alpha type-7



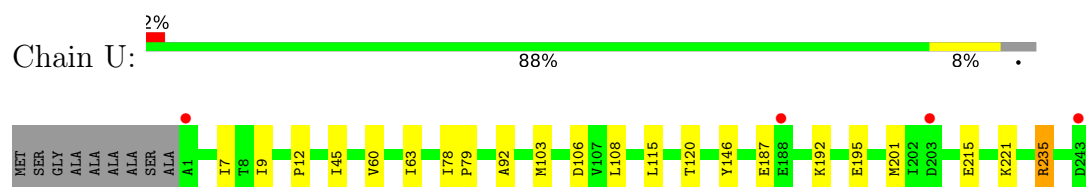
- Molecule 6: Probable proteasome subunit alpha type-7



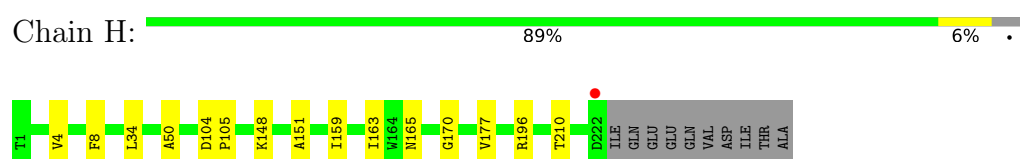
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 7: Proteasome subunit alpha type-1

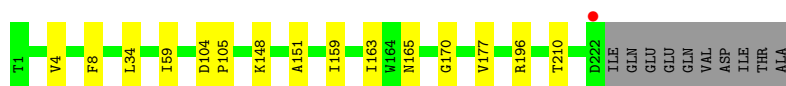


- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2

Chain V:  89% 6%



- Molecule 9: Proteasome subunit beta type-3

Chain I:  88% 11%



- Molecule 9: Proteasome subunit beta type-3

Chain W:  90% 10%



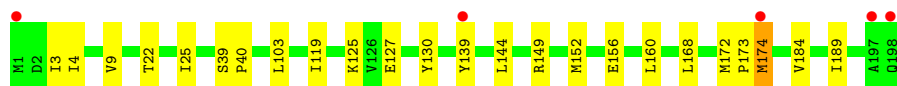
- Molecule 10: Proteasome subunit beta type-4

Chain J:  4% 87% 12%



- Molecule 10: Proteasome subunit beta type-4

Chain X:  3% 88% 12%



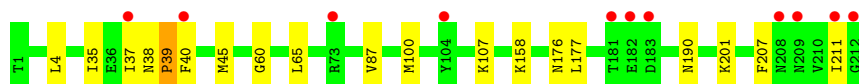
- Molecule 11: Proteasome subunit beta type-5

Chain K:  5% 90% 9%

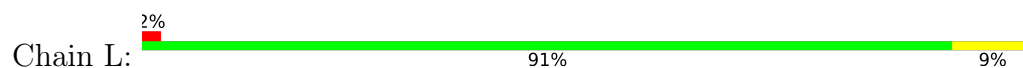


- Molecule 11: Proteasome subunit beta type-5

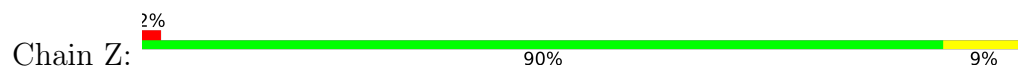
Chain Y:  5% 91% 8%



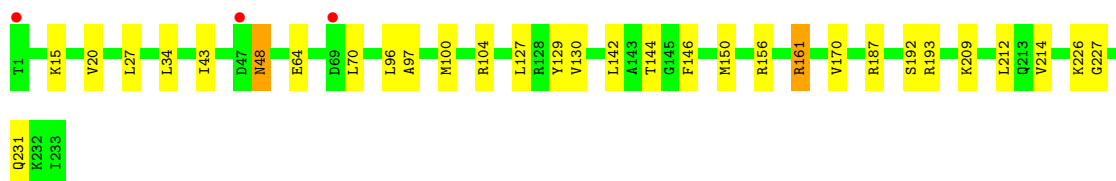
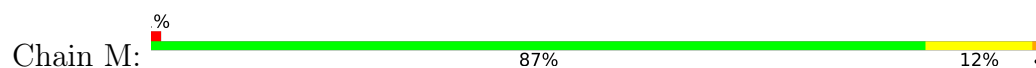
- Molecule 12: Proteasome subunit beta type-6



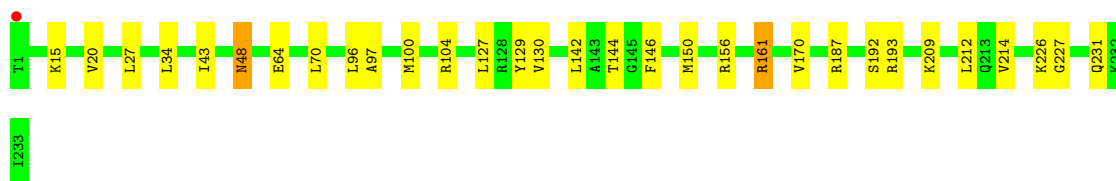
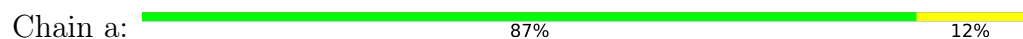
- Molecule 12: Proteasome subunit beta type-6



- Molecule 13: Proteasome subunit beta type-7



- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1

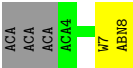


- Molecule 14: Proteasome subunit beta type-1

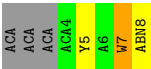




● Molecule 15: TMC-95A mimic ligand yCP:4e



● Molecule 15: TMC-95A mimic ligand yCP:4e



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.77Å 300.22Å 144.26Å 90.00° 112.86° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (15.00-2.80) 98.6 (15.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.235 , 0.241 0.241 , 0.248	Depositor DCC
R_{free} test set	12835 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	51011	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RE0, MES, ABN, ACA, TY5

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	0.49	0/1952	0.77	0/2642
1	O	0.49	0/1952	0.77	0/2642
2	B	0.46	0/1934	0.74	0/2618
2	P	0.46	0/1934	0.74	0/2618
3	C	0.47	0/1919	0.77	0/2598
3	Q	0.47	0/1919	0.77	0/2598
4	D	0.53	0/1886	0.75	0/2541
4	R	0.53	0/1886	0.75	0/2541
5	E	0.48	0/1823	0.74	0/2463
5	S	0.48	0/1823	0.74	0/2463
6	F	0.58	0/1936	0.78	0/2614
6	T	0.58	0/1936	0.78	0/2614
7	G	0.49	0/1959	0.75	0/2652
7	U	0.48	0/1959	0.75	0/2652
8	H	0.61	0/1715	0.75	0/2326
8	V	0.62	0/1715	0.75	0/2326
9	I	0.45	0/1611	0.73	0/2174
9	W	0.45	0/1611	0.73	0/2174
10	J	0.48	0/1613	0.74	0/2173
10	X	0.48	0/1613	0.74	0/2173
11	K	0.58	0/1681	0.74	0/2274
11	Y	0.58	0/1681	0.74	0/2274
12	L	0.51	0/1795	0.72	0/2420
12	Z	0.51	0/1795	0.72	0/2420
13	M	0.47	0/1855	0.73	0/2514
13	a	0.47	0/1855	0.73	0/2514
14	N	0.52	0/1541	0.74	0/2087
14	b	0.52	0/1541	0.74	0/2087
15	c	0.61	0/4	0.76	0/4
15	d	0.61	0/4	0.75	0/4
All	All	0.51	0/50448	0.75	0/68200

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	10	0
1	O	1915	0	1929	10	0
2	B	1904	0	1904	17	0
2	P	1904	0	1904	17	0
3	C	1890	0	1903	19	0
3	Q	1890	0	1903	14	0
4	D	1861	0	1839	18	0
4	R	1861	0	1839	13	0
5	E	1795	0	1800	17	0
5	S	1795	0	1800	15	0
6	F	1896	0	1889	11	0
6	T	1896	0	1889	11	0
7	G	1921	0	1913	10	0
7	U	1921	0	1913	11	0
8	H	1684	0	1688	8	0
8	V	1684	0	1688	7	0
9	I	1581	0	1574	13	0
9	W	1581	0	1574	10	0
10	J	1585	0	1590	17	0
10	X	1585	0	1590	15	0
11	K	1644	0	1595	11	0
11	Y	1644	0	1595	8	0
12	L	1757	0	1711	13	0
12	Z	1757	0	1711	14	0
13	M	1824	0	1832	18	0
13	a	1824	0	1832	18	0
14	N	1512	0	1481	3	0
14	b	1512	0	1481	3	0
15	c	56	0	42	2	0
15	d	56	0	42	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	K	12	0	13	0	0
16	Y	12	0	13	0	0
17	A	59	0	0	0	0
17	B	39	0	0	0	0
17	C	43	0	0	0	0
17	D	36	0	0	0	0
17	E	21	0	0	0	0
17	F	47	0	0	0	0
17	G	60	0	0	0	0
17	H	52	0	0	0	0
17	I	64	0	0	0	0
17	J	53	0	0	2	0
17	K	48	0	0	0	0
17	L	54	0	0	0	0
17	M	81	0	0	0	0
17	N	58	0	0	0	0
17	O	34	0	0	0	0
17	P	30	0	0	0	0
17	Q	29	0	0	0	0
17	R	27	0	0	0	0
17	S	18	0	0	0	0
17	T	43	0	0	0	0
17	U	55	0	0	0	0
17	V	50	0	0	0	0
17	W	62	0	0	0	0
17	X	41	0	0	0	0
17	Y	50	0	0	0	0
17	Z	49	0	0	0	0
17	a	78	0	0	0	0
17	b	56	0	0	0	0
All	All	51011	0	49406	302	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 (302) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:PHE:H	4:D:15:GLN:HE22	1.33	0.77
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.67	0.76
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.51	0.75
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.67	0.74
12:Z:109:THR:HG23	12:Z:125:PHE:HB2	1.72	0.72
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.40	0.70
12:L:109:THR:HG23	12:L:125:PHE:HB2	1.71	0.70
13:a:161:ARG:HG3	13:a:161:ARG:HH11	1.56	0.69
4:R:161:ALA:HB3	5:S:55:LEU:HD23	1.75	0.69
5:S:12:PHE:H	6:T:19:GLN:HE22	1.41	0.69
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.57	0.69
1:O:12:PHE:H	2:P:20:GLN:HE22	1.42	0.67
5:E:12:PHE:H	6:F:19:GLN:HE22	1.44	0.65
13:a:48:ASN:H	13:a:48:ASN:HD22	1.45	0.64
11:Y:45:MET:HB3	15:d:8:ABN:H3	1.79	0.64
10:J:174:MET:HE3	10:X:174:MET:HE3	1.79	0.64
13:M:48:ASN:H	13:M:48:ASN:HD22	1.45	0.64
10:X:4:ILE:HG22	10:X:103:LEU:HD12	1.80	0.62
10:J:4:ILE:HG22	10:J:103:LEU:HD12	1.80	0.62
2:B:12:PHE:H	3:C:17:GLN:HE22	1.47	0.61
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.82	0.61
1:A:12:PHE:H	2:B:20:GLN:HE22	1.49	0.61
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.48	0.61
14:b:175:MET:HB2	14:b:186:LEU:HB2	1.82	0.61
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.84	0.60
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.82	0.60
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.82	0.60
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.68	0.59
7:U:92:ALA:HA	7:U:103:MET:HE2	1.84	0.59
2:P:200:THR:HG22	2:P:202:SER:H	1.67	0.59
2:B:200:THR:HG22	2:B:202:SER:H	1.67	0.59
11:K:107:LYS:H	11:K:107:LYS:HD2	1.68	0.59
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.68	0.58
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.51	0.58
11:Y:107:LYS:H	11:Y:107:LYS:HD2	1.68	0.58
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.86	0.58
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.86	0.58
7:G:92:ALA:HA	7:G:103:MET:HE2	1.84	0.58
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.86	0.57
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.86	0.57
10:X:168:LEU:O	10:X:172:MET:HB2	2.05	0.57
4:D:44:LYS:HE3	4:D:210:GLN:HB2	1.86	0.57
2:P:215:ILE:HG12	2:P:226:GLN:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.86	0.57
10:J:168:LEU:O	10:J:172:MET:HB2	2.04	0.57
4:D:73:LEU:HD12	4:D:131:GLY:HA3	1.87	0.56
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.87	0.56
3:C:161:THR:HG21	3:C:169:VAL:HG13	1.86	0.56
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.87	0.56
4:R:44:LYS:HE3	4:R:210:GLN:HB2	1.86	0.56
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.54	0.56
4:R:73:LEU:HD12	4:R:131:GLY:HA3	1.88	0.56
9:I:28:LEU:HB3	9:I:36:SER:HB3	1.88	0.56
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.87	0.56
2:B:215:ILE:HG12	2:B:226:GLN:HG2	1.86	0.56
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.87	0.55
8:H:165:ASN:HD22	13:a:156:ARG:HH11	1.54	0.55
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.87	0.55
4:D:77:ALA:O	4:D:81:ILE:HG12	2.07	0.55
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.87	0.55
4:R:77:ALA:O	4:R:81:ILE:HG12	2.06	0.55
3:C:214:LYS:HB2	3:C:218:ASP:HB3	1.88	0.55
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.53	0.55
9:W:28:LEU:HB3	9:W:36:SER:HB3	1.88	0.55
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.89	0.54
12:L:195:HIS:HD2	12:L:197:GLN:H	1.56	0.54
2:P:63:GLU:HG3	2:P:64:LYS:HG3	1.90	0.54
2:P:75:ALA:HB3	2:P:135:ILE:HB	1.89	0.54
3:Q:214:LYS:HB2	3:Q:218:ASP:HB3	1.89	0.54
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.55	0.54
2:B:75:ALA:HB3	2:B:135:ILE:HB	1.89	0.54
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.89	0.54
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.54	0.54
13:M:43:ILE:HG12	13:M:64:GLU:HG2	1.91	0.53
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.90	0.53
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.91	0.53
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.89	0.53
6:T:91:GLU:HG3	6:T:111:ARG:HH11	1.74	0.53
2:B:63:GLU:HG3	2:B:64:LYS:HG3	1.90	0.53
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.90	0.53
13:a:43:ILE:HG12	13:a:64:GLU:HG2	1.91	0.53
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.89	0.53
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.43	0.53
4:D:119:ALA:HA	5:E:124:GLY:HA2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:35:ILE:HD12	2:P:196:LEU:HG	1.90	0.52
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.90	0.52
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.07	0.52
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.91	0.52
6:F:91:GLU:HG3	6:F:111:ARG:HH11	1.73	0.52
2:B:35:ILE:HD12	2:B:196:LEU:HG	1.90	0.52
2:P:183:MET:HE1	2:P:191:LEU:HD12	1.92	0.51
2:B:183:MET:HE1	2:B:191:LEU:HD12	1.92	0.51
5:E:231:LYS:H	5:E:231:LYS:HD2	1.76	0.51
11:K:45:MET:HB3	15:c:8:ABN:H3	1.92	0.51
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.07	0.51
5:E:227:GLU:CD	5:E:227:GLU:H	2.18	0.51
10:J:139:TYR:OH	10:X:25:ILE:HG12	2.10	0.51
5:S:227:GLU:CD	5:S:227:GLU:H	2.18	0.51
5:S:231:LYS:H	5:S:231:LYS:HD2	1.76	0.51
1:A:110:LEU:O	1:A:114:VAL:HG23	2.11	0.51
1:O:110:LEU:O	1:O:114:VAL:HG23	2.11	0.51
10:J:39:SER:HB2	10:J:40:PRO:HD2	1.93	0.51
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.93	0.51
5:S:80:ALA:HB2	5:S:129:VAL:HG21	1.93	0.51
10:X:39:SER:HB2	10:X:40:PRO:HD2	1.93	0.51
7:G:63:ILE:HD12	7:G:215:GLU:HG2	1.93	0.51
6:T:31:THR:HG21	6:T:47:GLU:O	2.11	0.51
6:F:31:THR:HG21	6:F:47:GLU:O	2.11	0.50
9:I:35:VAL:HG13	17:J:241:HOH:O	2.10	0.50
10:J:3:ILE:HD13	10:J:168:LEU:HD13	1.94	0.50
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.46	0.50
13:a:127:LEU:HG	13:a:142:LEU:HD12	1.93	0.50
3:C:186:VAL:HG21	3:C:214:LYS:HE2	1.94	0.50
5:E:80:ALA:HB2	5:E:129:VAL:HG21	1.93	0.50
8:V:148:LYS:HE3	8:V:177:VAL:HG11	1.93	0.50
6:T:31:THR:HG23	6:T:47:GLU:HB3	1.93	0.50
12:Z:126:ASP:HB2	12:Z:130:SER:HB3	1.94	0.50
7:G:78:ILE:N	7:G:79:PRO:HD2	2.27	0.50
9:W:94:LEU:HD11	9:W:106:PRO:HG2	1.93	0.50
8:H:148:LYS:HE3	8:H:177:VAL:HG11	1.94	0.50
1:O:26:THR:O	1:O:30:GLN:HG2	2.12	0.50
10:X:3:ILE:HD13	10:X:168:LEU:HD13	1.94	0.50
3:Q:186:VAL:HG21	3:Q:214:LYS:HE2	1.94	0.49
10:J:139:TYR:HD1	17:J:227:HOH:O	1.95	0.49
6:F:31:THR:HG23	6:F:47:GLU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:195:GLU:HG3	7:G:235:ARG:HG3	1.94	0.49
13:M:27:LEU:HB2	13:M:192:SER:HB2	1.95	0.49
7:U:63:ILE:HD12	7:U:215:GLU:HG2	1.93	0.49
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.94	0.49
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.94	0.49
15:d:5:TY5:H47	15:d:7:RE0:H18	1.95	0.49
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.93	0.49
10:J:119:ILE:HG12	10:J:125:LYS:HG3	1.94	0.49
12:L:126:ASP:HB2	12:L:130:SER:HB3	1.94	0.49
3:Q:157:TRP:CE2	4:R:51:LEU:HD23	2.48	0.49
7:U:78:ILE:N	7:U:79:PRO:HD2	2.27	0.49
2:B:122:THR:HG22	3:C:125:ARG:HH21	1.78	0.49
3:Q:70:VAL:HG13	3:Q:219:ILE:HD13	1.95	0.49
1:A:21:ILE:HD11	1:A:122:THR:HG21	1.95	0.49
10:J:25:ILE:HG12	10:X:139:TYR:OH	2.12	0.49
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.76	0.48
10:X:119:ILE:HG12	10:X:125:LYS:HG3	1.94	0.48
1:A:26:THR:O	1:A:30:GLN:HG2	2.12	0.48
12:Z:17:GLY:HA2	12:Z:174:TYR:HE1	1.78	0.48
3:C:70:VAL:HG13	3:C:219:ILE:HD13	1.95	0.48
13:M:150:MET:HE1	13:M:187:ARG:HG3	1.96	0.48
1:O:21:ILE:HD11	1:O:122:THR:HG21	1.95	0.48
10:X:149:ARG:HB2	10:X:152:MET:HG3	1.96	0.48
13:a:27:LEU:HB2	13:a:192:SER:HB2	1.95	0.48
12:L:17:GLY:HA2	12:L:174:TYR:HE1	1.78	0.48
8:V:210:THR:HG21	9:W:167:SER:HB3	1.96	0.47
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.12	0.47
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.94	0.47
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.49	0.47
1:A:68:THR:HB	1:A:69:PRO:HD2	1.96	0.47
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.49	0.47
12:Z:124:SER:HB3	12:Z:137:ARG:HG2	1.96	0.47
10:J:149:ARG:HB2	10:J:152:MET:HG3	1.96	0.47
13:M:209:LYS:HB3	13:M:212:LEU:HD11	1.96	0.47
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.45	0.47
12:Z:135:GLN:HG3	12:Z:174:TYR:OH	2.15	0.47
4:D:113:LEU:HD12	5:E:78:PRO:HB2	1.96	0.47
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.80	0.47
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.63	0.47
2:B:236:ASP:O	2:B:240:LYS:HG2	2.15	0.47
11:Y:158:LYS:HB2	11:Y:177:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:150:MET:HE1	13:a:187:ARG:HG3	1.96	0.47
1:A:55:LEU:HD12	7:G:170:THR:HG23	1.97	0.46
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.13	0.46
11:K:38:ASN:HB2	11:K:39:PRO:HD2	1.96	0.46
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	1.96	0.46
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.98	0.46
2:P:236:ASP:O	2:P:240:LYS:HG2	2.15	0.46
11:Y:38:ASN:C	11:Y:40:PHE:H	2.24	0.46
12:L:135:GLN:HG3	12:L:174:TYR:OH	2.15	0.46
13:a:209:LYS:HB3	13:a:212:LEU:HD11	1.95	0.46
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.45	0.46
4:D:5:SER:HB2	5:E:125:ARG:HD3	1.97	0.46
11:K:38:ASN:C	11:K:40:PHE:H	2.24	0.46
12:L:124:SER:HB3	12:L:137:ARG:HG2	1.96	0.46
1:O:68:THR:HB	1:O:69:PRO:HD2	1.96	0.46
13:a:48:ASN:HD22	13:a:48:ASN:N	2.08	0.46
6:F:122:TYR:HB2	6:F:125:VAL:HG22	1.98	0.46
13:M:96:LEU:O	13:M:100:MET:HG2	2.16	0.46
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.98	0.46
11:K:158:LYS:HB2	11:K:177:LEU:HD11	1.97	0.46
4:D:176:LEU:HD22	5:E:55:LEU:HD13	1.99	0.45
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.99	0.45
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.97	0.45
13:a:15:LYS:HB3	13:a:20:VAL:HG12	1.98	0.45
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.80	0.45
6:T:122:TYR:HB2	6:T:125:VAL:HG22	1.99	0.45
13:a:96:LEU:O	13:a:100:MET:HG2	2.16	0.45
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.97	0.45
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.80	0.45
13:a:129:TYR:HE1	13:a:144:THR:HG22	1.81	0.45
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.98	0.45
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.98	0.45
5:S:131:LEU:HB2	5:S:146:PHE:HB3	1.98	0.45
2:B:136:TYR:HB2	2:B:148:TYR:HB2	1.99	0.45
10:J:184:VAL:HG22	10:J:189:ILE:HG12	1.99	0.45
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.52	0.45
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.97	0.45
11:Y:201:LYS:HG3	11:Y:207:PHE:HB2	1.98	0.45
9:I:52:ILE:HB	9:I:59:VAL:HG13	1.99	0.45
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.99	0.45
11:K:201:LYS:HG3	11:K:207:PHE:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:129:TYR:HE1	13:M:144:THR:HG22	1.81	0.44
13:M:15:LYS:HB3	13:M:20:VAL:HG12	1.98	0.44
3:C:155:SER:HB2	4:D:51:LEU:HD21	1.99	0.44
3:C:108:THR:HG21	3:C:146:TYR:HB3	1.99	0.44
4:D:229:ALA:HA	4:D:232:ILE:HD12	1.99	0.44
12:Z:111:ILE:HG12	12:Z:125:PHE:HE1	1.83	0.44
13:M:161:ARG:HG3	13:M:161:ARG:NH1	2.28	0.44
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.98	0.44
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.99	0.44
13:a:227:GLY:HA3	13:a:231:GLN:HB3	2.00	0.44
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.52	0.44
13:M:48:ASN:HD22	13:M:48:ASN:N	2.07	0.44
2:P:136:TYR:HB2	2:P:148:TYR:HB2	1.98	0.44
12:L:111:ILE:HG12	12:L:125:PHE:HE1	1.82	0.44
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.00	0.43
3:C:204:GLY:HA3	3:C:207:ASN:HB2	2.00	0.43
5:E:131:LEU:HB2	5:E:146:PHE:HB3	1.98	0.43
10:J:22:THR:HG21	10:X:173:PRO:HB3	2.01	0.43
10:J:173:PRO:HB3	10:X:22:THR:HG21	2.00	0.43
10:X:184:VAL:HG22	10:X:189:ILE:HG12	1.99	0.43
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	1.99	0.43
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.00	0.43
10:J:152:MET:HE1	10:J:160:LEU:HD22	1.99	0.43
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.99	0.43
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.54	0.43
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.99	0.43
10:J:152:MET:HE2	10:J:156:GLU:HB3	2.00	0.43
11:K:31:VAL:HG11	15:c:8:ABN:C5	2.48	0.43
4:R:229:ALA:HA	4:R:232:ILE:HD12	1.99	0.43
13:a:161:ARG:HG3	13:a:161:ARG:NH1	2.28	0.43
5:S:134:ILE:HD12	5:S:215:VAL:HG12	2.01	0.43
8:V:4:VAL:HG22	8:V:159:ILE:HD11	2.01	0.43
9:W:106:PRO:HD2	9:W:123:PHE:HB2	2.01	0.43
13:M:227:GLY:HA3	13:M:231:GLN:HB3	2.00	0.43
6:T:52:SER:H	6:T:55:LEU:HD13	1.83	0.43
7:G:7:ILE:HG13	7:G:9:ILE:HG12	2.01	0.43
5:S:230:ALA:HA	5:S:233:ILE:HD12	2.01	0.43
7:U:7:ILE:HG13	7:U:9:ILE:HG12	2.01	0.43
11:K:100:MET:HE2	11:K:100:MET:HB2	1.88	0.43
2:P:57:GLU:O	2:P:61:SER:HB2	2.19	0.42
3:Q:204:GLY:HA3	3:Q:207:ASN:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:152:MET:HE1	10:X:160:LEU:HD22	1.99	0.42
2:P:122:THR:HG22	3:Q:125:ARG:HH21	1.84	0.42
4:D:161:ALA:HB1	4:D:175:LEU:HD22	2.00	0.42
5:E:230:ALA:HA	5:E:233:ILE:HD12	2.01	0.42
5:S:127:TYR:O	5:S:148:PRO:HB3	2.18	0.42
3:C:46:ARG:HB2	3:C:207:ASN:HA	2.01	0.42
3:Q:46:ARG:HB2	3:Q:207:ASN:HA	2.01	0.42
4:D:186:LYS:O	4:D:190:LEU:HD22	2.20	0.42
9:I:106:PRO:HD2	9:I:123:PHE:HB2	2.01	0.42
5:E:134:ILE:HD12	5:E:215:VAL:HG12	2.01	0.42
6:T:205:GLU:HG3	6:T:206:LYS:HG3	2.02	0.42
4:D:43:GLU:HG3	4:D:200:MET:HE3	2.02	0.42
5:E:127:TYR:O	5:E:148:PRO:HB3	2.19	0.42
7:G:103:MET:HE3	7:G:108:LEU:HD13	2.02	0.42
13:a:27:LEU:HD11	13:a:34:LEU:HB3	2.02	0.42
2:B:57:GLU:O	2:B:61:SER:HB2	2.19	0.42
4:R:161:ALA:HB1	4:R:175:LEU:HD22	2.01	0.42
10:X:152:MET:HE2	10:X:156:GLU:HB3	2.00	0.42
6:F:205:GLU:HG3	6:F:206:LYS:HG3	2.01	0.42
9:I:23:ALA:HB1	9:I:170:LEU:HD22	2.01	0.42
13:M:27:LEU:HD11	13:M:34:LEU:HB3	2.01	0.42
13:M:193:ARG:HG3	13:M:214:VAL:HB	2.02	0.42
6:T:36:ILE:HG12	6:T:172:LEU:HD11	2.02	0.42
6:F:52:SER:H	6:F:55:LEU:HD13	1.83	0.41
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.02	0.41
1:A:30:GLN:HE21	1:A:30:GLN:HA	1.85	0.41
6:F:36:ILE:HG12	6:F:172:LEU:HD11	2.02	0.41
8:H:4:VAL:HG22	8:H:159:ILE:HD11	2.01	0.41
4:R:186:LYS:O	4:R:190:LEU:HD22	2.20	0.41
3:C:29:THR:HB	3:C:45:GLU:HG3	2.02	0.41
10:X:130:TYR:HB2	10:X:144:LEU:HD13	2.02	0.41
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.56	0.41
7:U:103:MET:HE3	7:U:108:LEU:HD13	2.02	0.41
13:a:193:ARG:HG3	13:a:214:VAL:HB	2.02	0.41
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.03	0.41
3:C:159:ALA:HB3	4:D:50:LEU:HD22	2.03	0.41
5:E:205:LEU:HD23	5:E:205:LEU:H	1.86	0.41
11:K:176:ASN:HD21	11:K:190:ASN:HD22	1.69	0.41
4:R:43:GLU:HG3	4:R:200:MET:HE3	2.03	0.41
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.56	0.41
9:W:23:ALA:HB1	9:W:170:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:210:THR:HG21	9:I:167:SER:HB3	2.03	0.41
9:I:15:THR:HG22	9:I:20:VAL:HG12	2.04	0.40
4:D:28:THR:HG21	4:D:199:VAL:HG21	2.04	0.40
11:Y:176:ASN:HD21	11:Y:190:ASN:HD22	1.69	0.40
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.03	0.40
8:H:50:ALA:HB2	9:I:128:CYS:HB2	2.04	0.40
5:S:205:LEU:HD23	5:S:205:LEU:H	1.86	0.40
12:Z:17:GLY:HA2	12:Z:174:TYR:CE1	2.57	0.40
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.04	0.40
6:F:117:GLN:HE21	6:F:117:GLN:HB3	1.69	0.40
10:J:130:TYR:HB2	10:J:144:LEU:HD13	2.02	0.40
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	240 (97%)	6 (2%)	2 (1%)	16	44
1	O	248/250 (99%)	240 (97%)	6 (2%)	2 (1%)	16	44
2	B	242/258 (94%)	235 (97%)	5 (2%)	2 (1%)	16	44
2	P	242/258 (94%)	235 (97%)	5 (2%)	2 (1%)	16	44
3	C	239/254 (94%)	233 (98%)	3 (1%)	3 (1%)	9	31
3	Q	239/254 (94%)	233 (98%)	3 (1%)	3 (1%)	9	31
4	D	240/260 (92%)	235 (98%)	2 (1%)	3 (1%)	9	31
4	R	240/260 (92%)	235 (98%)	2 (1%)	3 (1%)	9	31
5	E	231/234 (99%)	224 (97%)	6 (3%)	1 (0%)	30	60
5	S	231/234 (99%)	224 (97%)	6 (3%)	1 (0%)	30	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	242/288 (84%)	233 (96%)	9 (4%)	0	100	100
6	T	242/288 (84%)	233 (96%)	9 (4%)	0	100	100
7	G	241/252 (96%)	236 (98%)	5 (2%)	0	100	100
7	U	241/252 (96%)	236 (98%)	5 (2%)	0	100	100
8	H	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
8	V	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	194 (96%)	7 (4%)	1 (0%)	24	55
9	W	202/205 (98%)	194 (96%)	7 (4%)	1 (0%)	24	55
10	J	196/198 (99%)	189 (96%)	6 (3%)	1 (0%)	24	55
10	X	196/198 (99%)	189 (96%)	6 (3%)	1 (0%)	24	55
11	K	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	24	55
11	Y	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	24	55
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	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
13	a	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
15	c	1/8 (12%)	1 (100%)	0	0	100	100
15	d	1/8 (12%)	1 (100%)	0	0	100	100
All	All	6314/6604 (96%)	6120 (97%)	166 (3%)	28 (0%)	30	60

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	52	LEU
3	Q	52	LEU
1	A	2	THR
1	A	166	LYS
4	D	122	GLU
11	K	39	PRO
1	O	166	LYS
4	R	122	GLU
11	Y	39	PRO
2	B	51	VAL

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Mol	Chain	Res	Type
2	B	221	ASP
3	C	183	PRO
3	C	203	THR
4	D	121	GLY
5	E	201	ARG
1	O	2	THR
2	P	51	VAL
2	P	221	ASP
3	Q	183	PRO
3	Q	203	THR
4	R	121	GLY
5	S	201	ARG
4	D	118	GLY
4	R	118	GLY
9	I	100	GLY
9	W	100	GLY
10	J	9	VAL
10	X	9	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	207 (99%)	2 (1%)	68	88
1	O	209/209 (100%)	207 (99%)	2 (1%)	68	88
2	B	203/216 (94%)	195 (96%)	8 (4%)	28	64
2	P	203/216 (94%)	195 (96%)	8 (4%)	28	64
3	C	213/226 (94%)	207 (97%)	6 (3%)	38	73
3	Q	213/226 (94%)	207 (97%)	6 (3%)	38	73
4	D	198/215 (92%)	190 (96%)	8 (4%)	28	63
4	R	198/215 (92%)	190 (96%)	8 (4%)	28	63
5	E	192/193 (100%)	186 (97%)	6 (3%)	35	70
5	S	192/193 (100%)	186 (97%)	6 (3%)	35	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	201/239 (84%)	194 (96%)	7 (4%)	32	67
6	T	201/239 (84%)	194 (96%)	7 (4%)	32	67
7	G	207/210 (99%)	202 (98%)	5 (2%)	43	77
7	U	207/210 (99%)	202 (98%)	5 (2%)	43	77
8	H	181/190 (95%)	179 (99%)	2 (1%)	65	87
8	V	181/190 (95%)	178 (98%)	3 (2%)	53	83
9	I	172/173 (99%)	170 (99%)	2 (1%)	63	87
9	W	172/173 (99%)	170 (99%)	2 (1%)	63	87
10	J	175/175 (100%)	173 (99%)	2 (1%)	65	87
10	X	175/175 (100%)	173 (99%)	2 (1%)	65	87
11	K	169/169 (100%)	163 (96%)	6 (4%)	31	66
11	Y	169/169 (100%)	163 (96%)	6 (4%)	31	66
12	L	185/185 (100%)	182 (98%)	3 (2%)	55	83
12	Z	185/185 (100%)	181 (98%)	4 (2%)	45	78
13	M	199/199 (100%)	192 (96%)	7 (4%)	32	67
13	a	199/199 (100%)	192 (96%)	7 (4%)	32	67
14	N	162/162 (100%)	161 (99%)	1 (1%)	78	92
14	b	162/162 (100%)	161 (99%)	1 (1%)	78	92
All	All	5332/5522 (97%)	5200 (98%)	132 (2%)	42	76

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	157	PHE
2	B	38	MET
2	B	55	LEU
2	B	60	THR
2	B	69	ASN
2	B	74	VAL
2	B	149	THR
2	B	191	LEU
2	B	244	THR
3	C	19	GLU
3	C	107	LEU
3	C	147	GLN

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Mol	Chain	Res	Type
3	C	160	GLN
3	C	169	VAL
3	C	171	GLU
4	D	40	LEU
4	D	44	LYS
4	D	102	GLU
4	D	124	ARG
4	D	176	LEU
4	D	190	LEU
4	D	214	ILE
4	D	235	LEU
5	E	9	THR
5	E	29	LYS
5	E	188	LEU
5	E	198	GLN
5	E	227	GLU
5	E	231	LYS
6	F	31	THR
6	F	39	ASN
6	F	123	ASN
6	F	130	VAL
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
7	G	45	ILE
7	G	115	LEU
7	G	201	MET
7	G	221	LYS
7	G	235	ARG
8	H	34	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	127	GLU
10	J	174	MET
11	K	4	LEU
11	K	35	ILE
11	K	65	LEU
11	K	87	VAL
11	K	100	MET
11	K	211	ILE
12	L	23	LEU

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Mol	Chain	Res	Type
12	L	49	ASN
12	L	109	THR
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	146	PHE
13	M	161	ARG
13	M	170	VAL
13	M	226	LYS
14	N	119	VAL
1	O	30	GLN
1	O	157	PHE
2	P	38	MET
2	P	55	LEU
2	P	60	THR
2	P	69	ASN
2	P	74	VAL
2	P	149	THR
2	P	191	LEU
2	P	244	THR
3	Q	19	GLU
3	Q	107	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	171	GLU
4	R	40	LEU
4	R	44	LYS
4	R	102	GLU
4	R	124	ARG
4	R	176	LEU
4	R	190	LEU
4	R	214	ILE
4	R	235	LEU
5	S	9	THR
5	S	29	LYS
5	S	188	LEU
5	S	198	GLN
5	S	227	GLU
5	S	231	LYS
6	T	31	THR
6	T	39	ASN

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Mol	Chain	Res	Type
6	T	123	ASN
6	T	130	VAL
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
7	U	45	ILE
7	U	115	LEU
7	U	201	MET
7	U	221	LYS
7	U	235	ARG
8	V	34	LEU
8	V	59	ILE
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	127	GLU
10	X	174	MET
11	Y	4	LEU
11	Y	35	ILE
11	Y	65	LEU
11	Y	87	VAL
11	Y	100	MET
11	Y	211	ILE
12	Z	23	LEU
12	Z	49	ASN
12	Z	109	THR
12	Z	128	VAL
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	146	PHE
13	a	161	ARG
13	a	170	VAL
13	a	226	LYS
14	b	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (180) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	143	ASN
2	B	20	GLN

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Mol	Chain	Res	Type
2	B	69	ASN
2	B	93	HIS
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	155	ASN
2	B	176	GLN
2	B	220	ASN
2	B	232	GLN
3	C	17	GLN
3	C	77	ASN
3	C	115	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	241	GLN
4	D	15	GLN
4	D	100	ASN
4	D	146	GLN
4	D	160	ASN
4	D	210	GLN
4	D	225	ASN
5	E	30	GLN
5	E	68	HIS
5	E	99	ASN
5	E	109	HIS
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
5	E	165	GLN
5	E	184	ASN
5	E	198	GLN
5	E	209	ASN
6	F	19	GLN
6	F	39	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	143	HIS
6	F	224	HIS

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Mol	Chain	Res	Type
7	G	30	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
7	G	186	ASN
7	G	212	ASN
7	G	231	ASN
8	H	30	ASN
8	H	141	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	63	ASN
9	I	88	GLN
10	J	37	GLN
10	J	55	GLN
10	J	63	ASN
10	J	118	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	158	ASN
12	L	165	ASN
12	L	197	GLN
13	M	2	GLN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	171	GLN
13	M	179	ASN
13	M	213	GLN
14	N	69	GLN
14	N	141	ASN
14	N	145	ASN

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Mol	Chain	Res	Type
14	N	161	GLN
1	O	30	GLN
1	O	143	ASN
2	P	20	GLN
2	P	69	ASN
2	P	93	HIS
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
2	P	220	ASN
2	P	232	GLN
3	Q	17	GLN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	241	GLN
4	R	15	GLN
4	R	100	ASN
4	R	146	GLN
4	R	160	ASN
4	R	210	GLN
4	R	225	ASN
5	S	30	GLN
5	S	68	HIS
5	S	99	ASN
5	S	109	HIS
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	165	GLN
5	S	184	ASN
5	S	198	GLN
5	S	209	ASN
6	T	19	GLN
6	T	39	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN

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Mol	Chain	Res	Type
6	T	143	HIS
6	T	224	HIS
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
7	U	212	ASN
7	U	231	ASN
8	V	30	ASN
8	V	141	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	63	ASN
9	W	88	GLN
10	X	37	GLN
10	X	55	GLN
10	X	63	ASN
10	X	86	GLN
10	X	118	GLN
10	X	198	GLN
11	Y	62	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	92	ASN
12	Z	158	ASN
12	Z	165	ASN
12	Z	197	GLN
13	a	2	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN

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Mol	Chain	Res	Type
13	a	108	ASN
13	a	171	GLN
13	a	179	ASN
13	a	213	GLN
14	b	69	GLN
14	b	106	ASN
14	b	141	ASN
14	b	145	ASN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	ACA	d	4	15	6,7,8	0.73	0	5,6,8	0.51	0
15	TY5	c	5	15	19,20,21	1.08	0	20,25,27	0.55	0
15	RE0	d	7	15	15,17,18	1.29	1 (6%)	19,25,27	1.99	5 (26%)
15	RE0	c	7	15	15,17,18	1.35	1 (6%)	19,25,27	2.00	5 (26%)
15	TY5	d	5	15	19,20,21	1.08	0	20,25,27	0.43	0
15	ACA	c	4	15	6,7,8	0.75	0	5,6,8	0.47	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
15	ACA	d	4	15	-	4/5/5/6	-
15	TY5	c	5	15	-	4/10/11/13	0/2/2/2
15	RE0	d	7	15	-	0/6/23/25	0/2/2/2
15	RE0	c	7	15	-	0/6/23/25	0/2/2/2
15	TY5	d	5	15	-	5/10/11/13	0/2/2/2
15	ACA	c	4	15	-	3/5/5/6	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	7	RE0	CG-CD2	3.61	1.54	1.51
15	d	7	RE0	CG-CD2	3.36	1.54	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	c	7	RE0	CG-CD2-CE2	-4.29	107.11	108.86
15	d	7	RE0	CG-CD2-CE2	-4.16	107.16	108.86
15	c	7	RE0	CD2-CE2-NE1	3.42	111.89	109.60
15	d	7	RE0	CD2-CE2-NE1	3.42	111.89	109.60
15	c	7	RE0	CG-CD1-NE1	3.35	110.43	108.43
15	d	7	RE0	CG-CD1-NE1	3.25	110.37	108.43
15	d	7	RE0	CE2-NE1-CD1	-3.24	109.70	111.85
15	c	7	RE0	CE2-NE1-CD1	-3.17	109.75	111.85
15	c	7	RE0	CZ2-CE2-NE1	-2.80	125.16	130.83
15	d	7	RE0	CZ2-CE2-NE1	-2.77	125.23	130.83

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	c	4	ACA	C-C2-C3-C4
15	d	4	ACA	O-C-C2-C3
15	c	5	TY5	CE2-CZ-OH-C49
15	d	5	TY5	CE1-CZ-OH-C49
15	d	5	TY5	CE2-CZ-OH-C49
15	c	5	TY5	CE1-CZ-OH-C49
15	c	4	ACA	C2-C3-C4-C5
15	d	4	ACA	C2-C3-C4-C5
15	c	4	ACA	C3-C4-C5-C6
15	d	5	TY5	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
15	d	4	ACA	C-C2-C3-C4
15	c	5	TY5	CA-CB-CG-CD1
15	c	5	TY5	CA-CB-CG-CD2
15	d	5	TY5	CA-CB-CG-CD2
15	d	5	TY5	CA-CB-CG-CD1
15	d	4	ACA	C4-C5-C6-N

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	d	7	RE0	1	0
15	d	5	TY5	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	MES	K	301	-	12,12,12	1.31	2 (16%)	15,16,16	1.43	2 (13%)
16	MES	Y	301	-	12,12,12	1.39	2 (16%)	15,16,16	1.78	5 (33%)

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
16	MES	K	301	-	-	5/6/14/14	0/1/1/1
16	MES	Y	301	-	-	4/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	301	MES	C8-S	2.98	1.81	1.77
16	K	301	MES	C8-S	2.87	1.81	1.77
16	K	301	MES	O2S-S	2.04	1.50	1.45
16	Y	301	MES	O2S-S	2.03	1.50	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	301	MES	O2S-S-C8	-3.06	102.10	106.73
16	K	301	MES	O3S-S-O1S	2.88	118.62	111.40
16	Y	301	MES	O3S-S-O1S	2.88	118.60	111.40
16	K	301	MES	O2S-S-C8	-2.73	102.60	106.73
16	Y	301	MES	C6-C5-N4	2.53	113.96	110.12
16	Y	301	MES	C5-N4-C3	2.48	114.18	108.84
16	Y	301	MES	C2-C3-N4	2.35	113.69	110.12

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Y	301	MES	C7-C8-S-O2S
16	Y	301	MES	C7-C8-S-O3S
16	Y	301	MES	N4-C7-C8-S
16	K	301	MES	C8-C7-N4-C3
16	K	301	MES	C8-C7-N4-C5
16	K	301	MES	C7-C8-S-O3S
16	K	301	MES	C7-C8-S-O1S
16	K	301	MES	C7-C8-S-O2S
16	Y	301	MES	C8-C7-N4-C5

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	0.11	3 (1%) 76 68	58, 71, 92, 109	0
1	O	250/250 (100%)	0.14	6 (2%) 59 49	61, 77, 101, 118	0
2	B	244/258 (94%)	0.36	16 (6%) 24 18	58, 75, 111, 120	0
2	P	244/258 (94%)	0.44	16 (6%) 24 18	64, 79, 109, 124	0
3	C	241/254 (94%)	0.23	9 (3%) 45 36	56, 75, 112, 143	0
3	Q	241/254 (94%)	0.53	15 (6%) 26 20	69, 92, 139, 169	0
4	D	242/260 (93%)	0.29	9 (3%) 45 36	61, 76, 103, 120	0
4	R	242/260 (93%)	0.39	9 (3%) 45 36	65, 84, 114, 129	0
5	E	233/234 (99%)	0.21	5 (2%) 63 54	64, 79, 99, 112	0
5	S	233/234 (99%)	0.41	14 (6%) 27 21	65, 86, 112, 124	0
6	F	244/288 (84%)	0.24	9 (3%) 45 36	59, 74, 102, 125	0
6	T	244/288 (84%)	0.25	7 (2%) 53 43	61, 78, 112, 134	0
7	G	243/252 (96%)	0.20	5 (2%) 63 54	56, 73, 96, 130	0
7	U	243/252 (96%)	0.16	4 (1%) 70 61	60, 72, 91, 116	0
8	H	222/232 (95%)	0.02	1 (0%) 87 82	56, 67, 81, 98	0
8	V	222/232 (95%)	-0.00	1 (0%) 87 82	55, 66, 81, 105	0
9	I	204/205 (99%)	-0.12	1 (0%) 87 82	53, 63, 79, 83	0
9	W	204/205 (99%)	0.01	1 (0%) 87 82	59, 66, 82, 91	0
10	J	198/198 (100%)	0.13	8 (4%) 42 33	54, 66, 83, 116	0
10	X	198/198 (100%)	0.08	5 (2%) 58 48	59, 68, 83, 116	0
11	K	212/212 (100%)	0.25	11 (5%) 33 25	52, 66, 85, 91	0
11	Y	212/212 (100%)	0.24	11 (5%) 33 25	58, 68, 88, 96	0
12	L	222/222 (100%)	0.12	4 (1%) 67 58	55, 65, 89, 96	0
12	Z	222/222 (100%)	0.09	5 (2%) 61 51	56, 66, 88, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/233 (100%)	-0.09	3 (1%) 75 66	53, 64, 77, 80	0
13	a	233/233 (100%)	-0.12	1 (0%) 88 84	53, 65, 76, 80	0
14	N	196/196 (100%)	-0.07	0 100 100	55, 62, 78, 86	0
14	b	196/196 (100%)	-0.10	3 (1%) 72 63	54, 62, 77, 85	0
15	c	1/8 (12%)	0.69	0 100 100	58, 58, 58, 58	0
15	d	1/8 (12%)	0.66	0 100 100	56, 56, 56, 56	0
All	All	6370/6604 (96%)	0.16	182 (2%) 53 43	52, 71, 104, 169	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	119	ALA	8.0
4	D	119	ALA	7.7
3	Q	50	LEU	7.2
11	Y	104	TYR	7.1
4	D	120	SER	6.9
4	D	118	GLY	6.8
11	K	104	TYR	6.7
12	L	174	TYR	6.7
12	Z	174	TYR	6.6
4	R	120	SER	5.8
11	Y	209	ASN	5.8
7	U	243	ASP	5.4
2	P	219	ALA	5.4
11	Y	182	GLU	5.2
5	S	1	PHE	5.2
2	B	219	ALA	5.2
10	X	139	TYR	5.2
11	K	208	ASN	5.0
6	F	202	ASP	5.0
2	B	218	GLY	4.9
4	R	118	GLY	4.9
11	K	182	GLU	4.9
13	M	1	THR	4.9
5	E	1	PHE	4.9
11	K	209	ASN	4.7
4	R	121	GLY	4.5
1	A	2	THR	4.5
2	P	218	GLY	4.5
3	Q	52	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	4.5
2	P	61	SER	4.3
6	T	178	HIS	4.3
2	B	220	ASN	4.2
10	X	198	GLN	4.2
3	C	50	LEU	4.2
10	J	139	TYR	4.1
11	K	40	PHE	4.1
1	O	2	THR	4.0
12	Z	173	LYS	4.0
7	U	1	ALA	4.0
10	J	197	ALA	4.0
2	B	1	GLY	3.8
2	P	1	GLY	3.8
10	J	198	GLN	3.7
3	Q	203	THR	3.7
10	J	1	MET	3.6
4	R	124	ARG	3.6
11	Y	183	ASP	3.6
3	Q	53	GLN	3.6
13	a	1	THR	3.6
5	S	52	ALA	3.5
6	T	9	SER	3.5
5	S	202	ASP	3.5
3	C	49	THR	3.5
11	Y	208	ASN	3.5
2	B	222	GLY	3.4
2	B	63	GLU	3.4
7	G	1	ALA	3.4
1	O	1	MET	3.4
4	D	125	LEU	3.3
11	Y	40	PHE	3.3
2	B	61	SER	3.3
4	D	124	ARG	3.2
6	F	1	GLY	3.2
5	S	209	ASN	3.2
2	B	60	THR	3.2
10	J	174	MET	3.2
11	K	183	ASP	3.2
4	D	121	GLY	3.1
10	X	1	MET	3.1
4	R	157	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
9	W	1	SER	3.1
13	M	47	ASP	3.1
6	F	179	HIS	3.0
3	Q	49	THR	3.0
1	O	53	SER	3.0
2	P	244	THR	3.0
13	M	69	ASP	2.9
6	F	9	SER	2.9
10	X	174	MET	2.9
2	P	222	GLY	2.9
6	F	244	ASN	2.9
2	P	220	ASN	2.8
11	Y	181	THR	2.8
1	A	201	GLU	2.8
5	S	2	ARG	2.8
4	R	125	LEU	2.8
2	B	239	VAL	2.8
4	D	241	ALA	2.8
6	F	243	ILE	2.7
2	B	244	THR	2.7
10	J	196	GLN	2.7
11	K	73	ARG	2.7
5	E	41	THR	2.7
11	Y	73	ARG	2.7
5	S	178	PHE	2.7
6	F	203	ASN	2.7
3	Q	205	ALA	2.6
7	G	2	GLY	2.6
8	H	222	ASP	2.6
10	X	197	ALA	2.6
5	S	3	ASN	2.6
2	P	225	TYR	2.6
11	K	181	THR	2.6
1	O	3	ASP	2.6
2	B	223	GLU	2.5
6	T	32	THR	2.5
6	F	215	CYS	2.5
4	D	240	ALA	2.5
14	b	116	GLY	2.5
12	L	126	ASP	2.5
3	C	48	SER	2.5
3	Q	48	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	P	51	VAL	2.5
6	T	2	THR	2.5
12	L	173	LYS	2.5
5	S	56	SER	2.5
3	Q	171	GLU	2.5
1	O	4	ARG	2.5
2	P	58	GLN	2.5
3	Q	51	LYS	2.5
8	V	222	ASP	2.4
3	C	203	THR	2.4
11	Y	212	GLY	2.4
7	U	203	ASP	2.4
3	C	206	LYS	2.4
12	L	165	ASN	2.4
5	E	202	ASP	2.4
11	K	147	ASP	2.3
3	C	205	ALA	2.3
5	S	54	GLU	2.3
10	J	172	MET	2.3
2	B	62	THR	2.3
5	E	2	ARG	2.3
2	P	223	GLU	2.3
6	T	205	GLU	2.3
12	Z	132	GLU	2.3
14	b	149	GLU	2.3
5	S	55	LEU	2.3
2	B	217	LYS	2.3
10	J	142	SER	2.3
11	Y	211	ILE	2.3
2	B	51	VAL	2.3
5	S	51	ASN	2.3
7	G	188	GLU	2.3
4	R	1	ASP	2.3
11	Y	37	ILE	2.2
4	R	228	THR	2.2
12	Z	172	LEU	2.2
2	B	243	ILE	2.2
2	P	63	GLU	2.2
3	C	58	THR	2.2
3	C	53	GLN	2.2
3	C	241	GLN	2.2
5	S	30	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
3	Q	238	LYS	2.2
1	O	61	LEU	2.2
11	K	211	ILE	2.1
3	Q	241	GLN	2.1
2	B	221	ASP	2.1
7	G	243	ASP	2.1
3	Q	26	LYS	2.1
3	Q	55	THR	2.1
14	b	107	LYS	2.1
9	I	1	SER	2.1
6	T	243	ILE	2.1
6	F	178	HIS	2.1
11	K	39	PRO	2.1
12	Z	168	VAL	2.1
3	Q	234	ILE	2.1
2	P	202	SER	2.1
4	D	27	SER	2.1
5	E	209	ASN	2.1
2	P	50	LYS	2.0
2	P	60	THR	2.0
6	T	202	ASP	2.0
7	G	168	GLU	2.0
3	Q	58	THR	2.0
2	P	180	LYS	2.0
5	S	227	GLU	2.0
7	U	188	GLU	2.0
5	S	207	VAL	2.0

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

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
15	ACA	d	4	8/9	0.49	0.21	61,63,64,64	0
15	ACA	c	4	8/9	0.59	0.17	63,64,65,65	0
15	TY5	d	5	19/20	0.81	0.12	58,60,61,61	0
15	RE0	d	7	16/17	0.84	0.10	56,57,57,58	0
15	TY5	c	5	19/20	0.85	0.11	60,62,63,63	0
15	RE0	c	7	16/17	0.86	0.10	56,57,58,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	MES	Y	301	12/12	0.86	0.19	60,64,66,66	0
16	MES	K	301	12/12	0.93	0.14	61,62,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.