Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:46 PM GMT

PDB ID	:	4Y84
Title	:	Yeast 20S proteasome in complex with N3-A(4,4-F2P)nLL-ep
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2015-02-16
Resolution	:	2.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

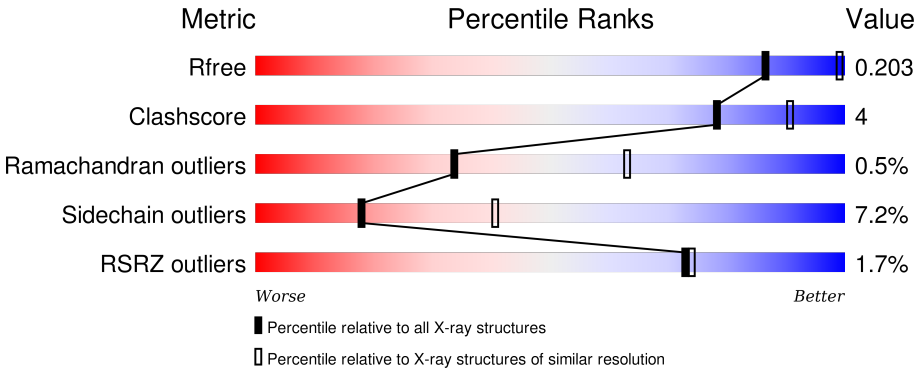
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	2% 92% 6% •
1	O	250	2% 91% 7% •
2	B	258	3% 78% 15% • 5%
2	P	258	4% 80% 14% • 5%
3	C	254	6% 78% 14% • 6%

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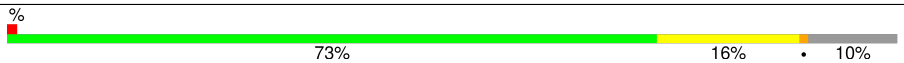
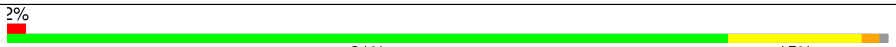
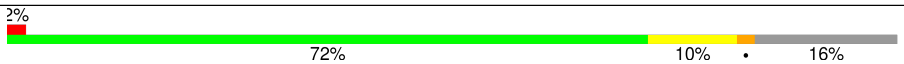
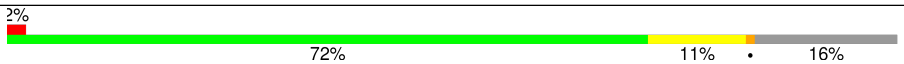
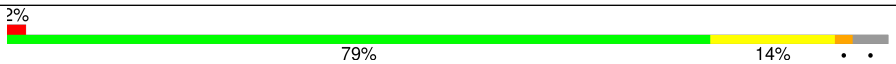
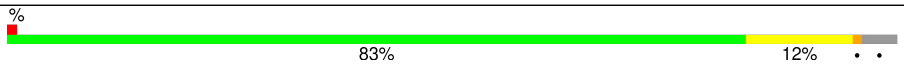
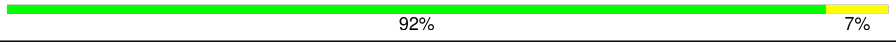
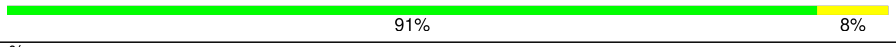
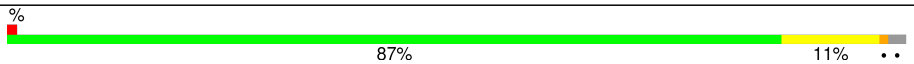
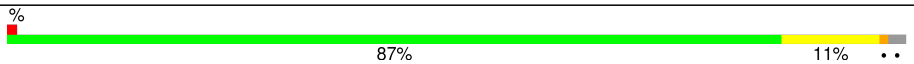
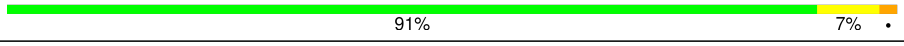
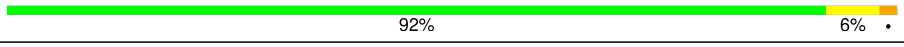
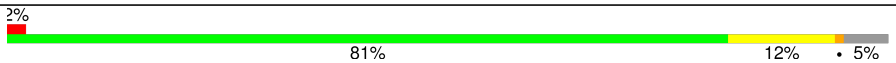
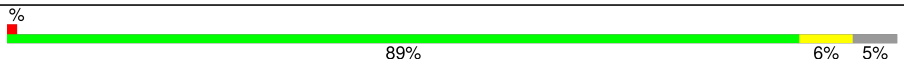
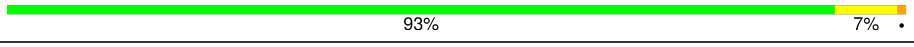
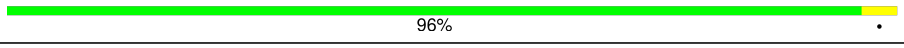
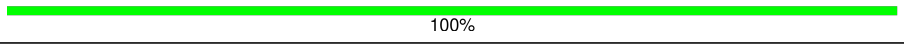
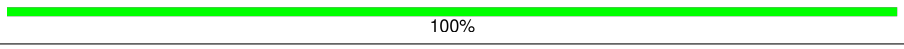
Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	
15	e	6	
15	f	6	

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Mol	Chain	Length	Quality of chain
15	g	6	100%
15	h	6	100%
15	i	6	83% 17%
15	j	6	100%

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
17	MES	K	302	-	-	-	X
17	MES	i	101	-	-	-	X
18	CL	N	202	-	-	-	X
18	CL	b	201	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49927 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	1	0
			1691	1066	295	323	7			
8	V	222	Total	C	N	O	S	0	1	0
			1691	1066	295	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 N3-A(4,4-F2P)nLL-ep.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	e	6	Total	C	F	N	O		0	0	0
			40	25	2	7	6				
15	f	6	Total	C	F	N	O		0	0	0
			40	25	2	7	6				

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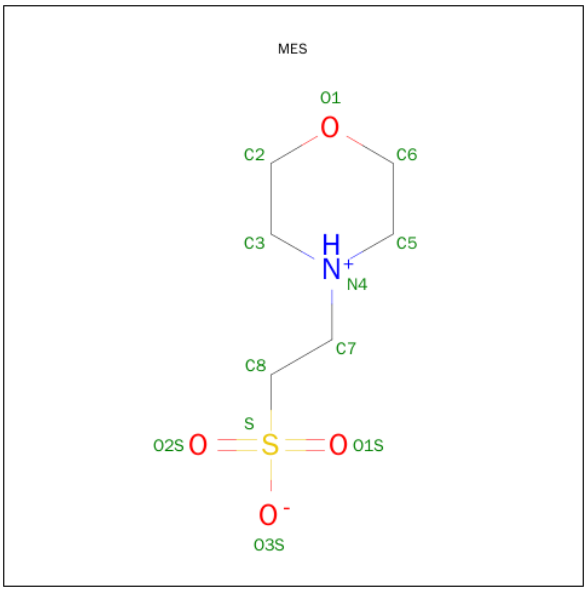
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	g	6	Total	C	F	N	O	0	0	0
			40	25	2	7	6			
15	h	6	Total	C	F	N	O	0	0	0
			40	25	2	7	6			
15	i	6	Total	C	F	N	O	0	0	0
			40	25	2	7	6			
15	j	6	Total	C	F	N	O	0	0	0
			40	25	2	7	6			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Mg	0	0
			1	1		
16	K	1	Total	Mg	0	0
			1	1		
16	I	2	Total	Mg	0	0
			2	2		
16	Z	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		
16	L	1	Total	Mg	0	0
			1	1		

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 18 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	b	1	Total	Cl	0	0
			1	1		
18	N	1	Total	Cl	0	0
			1	1		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	12	Total	O	0	0
			12	12		
19	B	15	Total	O	0	0
			15	15		
19	C	12	Total	O	0	0
			12	12		
19	D	3	Total	O	0	0
			3	3		
19	E	5	Total	O	0	0
			5	5		
19	F	13	Total	O	0	0
			13	13		
19	G	8	Total	O	0	0
			8	8		
19	H	14	Total	O	0	0
			14	14		
19	I	19	Total	O	0	0
			19	19		
19	J	17	Total	O	0	0
			17	17		
19	K	18	Total	O	0	0
			18	18		
19	L	17	Total	O	0	0
			17	17		
19	M	13	Total	O	0	0
			13	13		
19	N	7	Total	O	0	0
			7	7		

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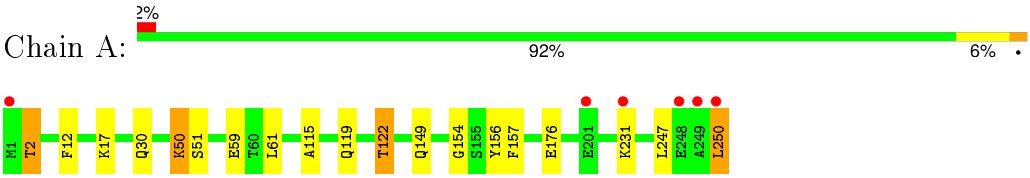
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	O	14	Total O 14 14	0	0
19	P	4	Total O 4 4	0	0
19	Q	8	Total O 8 8	0	0
19	R	4	Total O 4 4	0	0
19	S	6	Total O 6 6	0	0
19	T	13	Total O 13 13	0	0
19	U	12	Total O 12 12	0	0
19	V	12	Total O 12 12	0	0
19	W	5	Total O 5 5	0	0
19	X	13	Total O 13 13	0	0
19	Y	13	Total O 13 13	0	0
19	Z	21	Total O 21 21	0	0
19	a	19	Total O 19 19	0	0
19	b	18	Total O 18 18	0	0
19	e	1	Total O 1 1	0	0
19	f	1	Total O 1 1	0	0
19	g	2	Total O 2 2	0	0
19	h	1	Total O 1 1	0	0
19	i	1	Total O 1 1	0	0
19	j	3	Total O 3 3	0	0

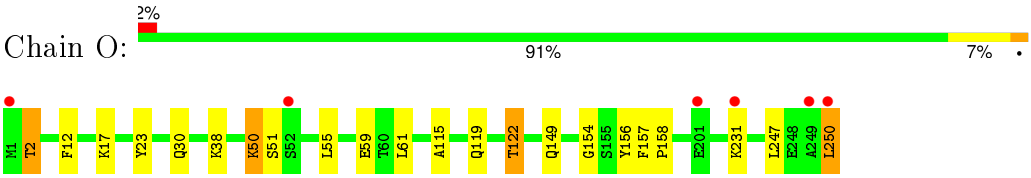
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

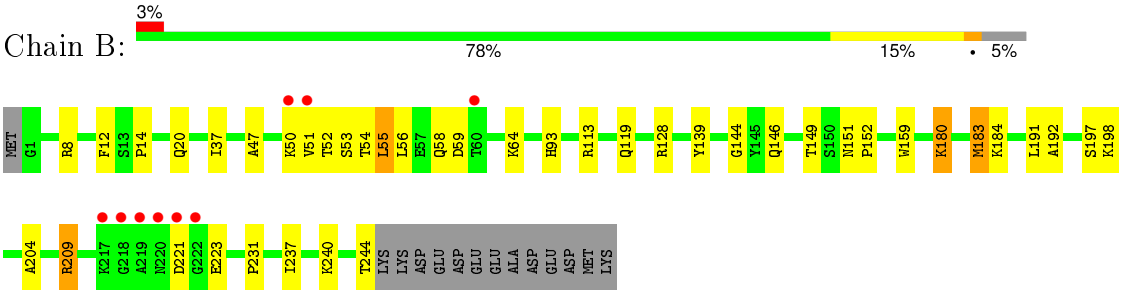
• Molecule 1: Proteasome subunit alpha type-2



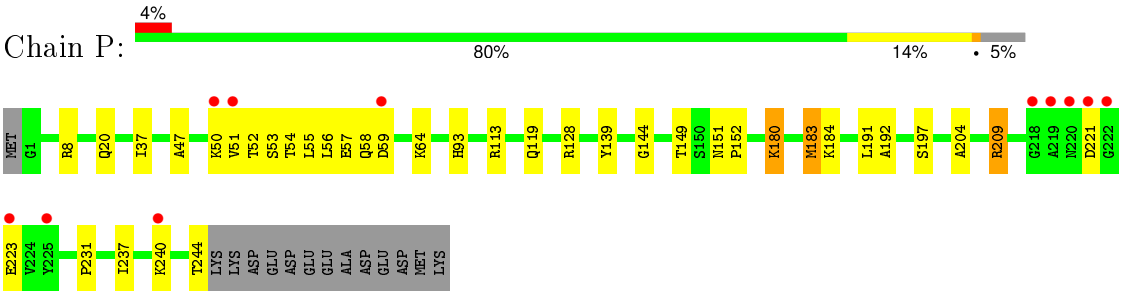
• Molecule 1: Proteasome subunit alpha type-2



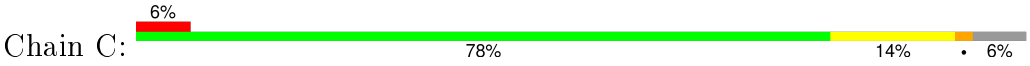
• Molecule 2: Proteasome subunit alpha type-3

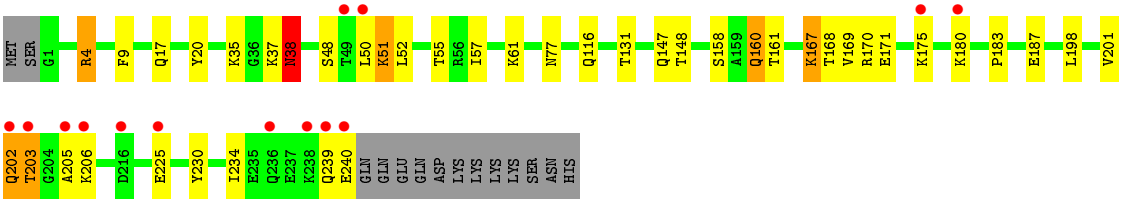


• Molecule 2: Proteasome subunit alpha type-3



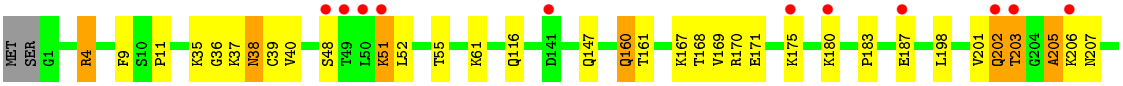
• Molecule 3: Proteasome subunit alpha type-4

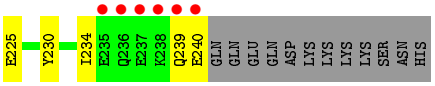




• Molecule 3: Proteasome subunit alpha type-4

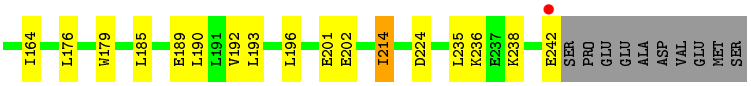
Chain Q:





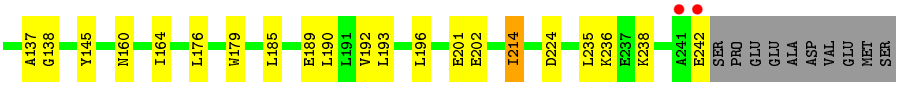
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



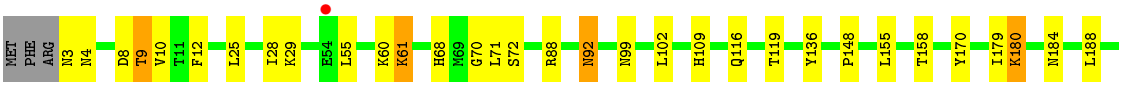
• Molecule 4: Proteasome subunit alpha type-5

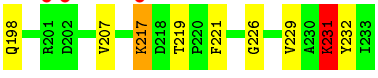
Chain R:



• Molecule 5: Proteasome subunit alpha type-6

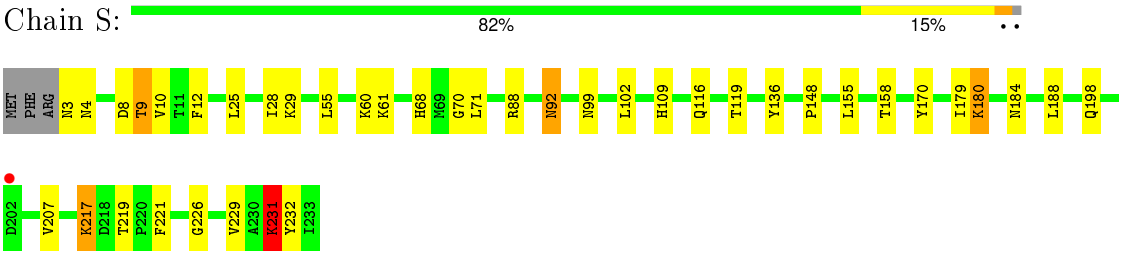
Chain E:





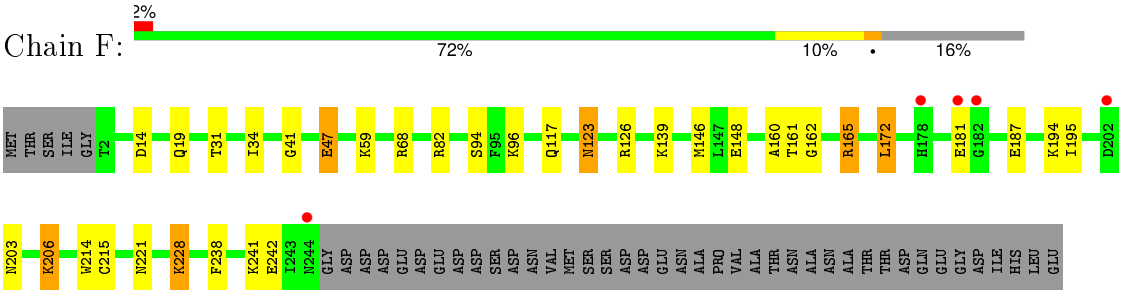
• Molecule 5: Proteasome subunit alpha type-6

Chain S:



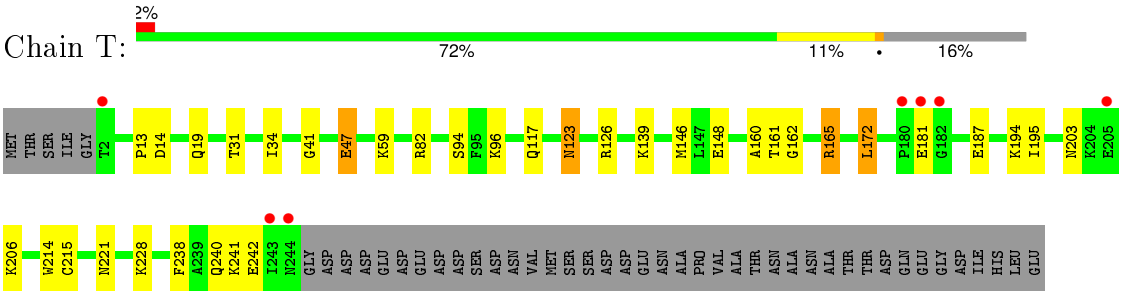
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



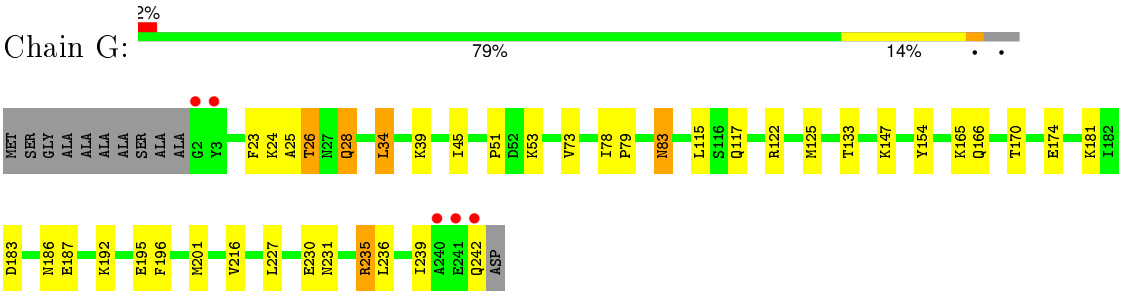
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



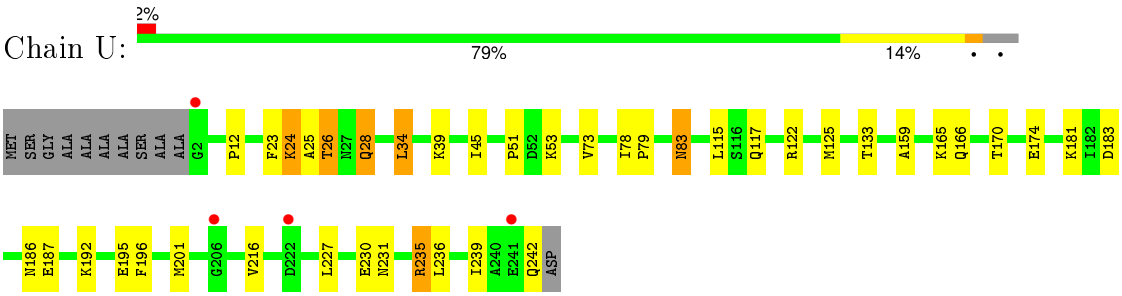
• Molecule 7: Proteasome subunit alpha type-1

Chain G:



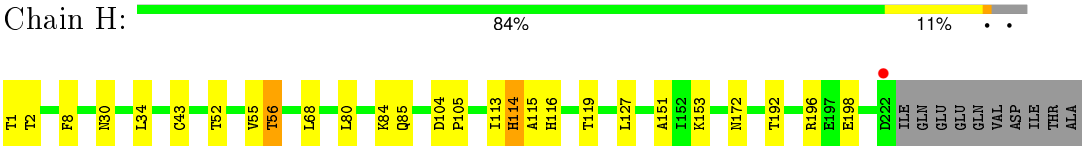
• Molecule 7: Proteasome subunit alpha type-1

Chain U:



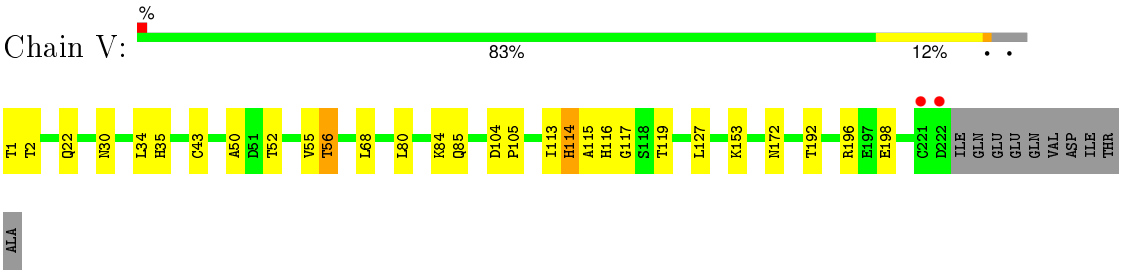
• Molecule 8: Proteasome subunit beta type-2

Chain H:



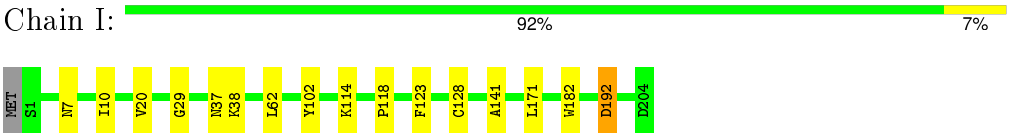
• Molecule 8: Proteasome subunit beta type-2

Chain V:



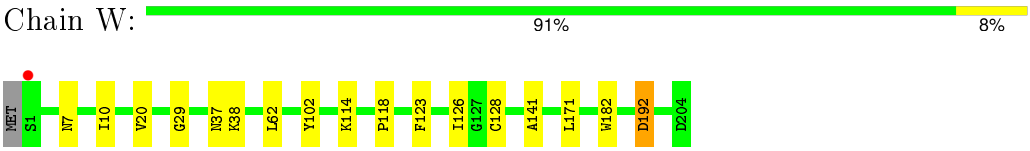
• Molecule 9: Proteasome subunit beta type-3

Chain I:



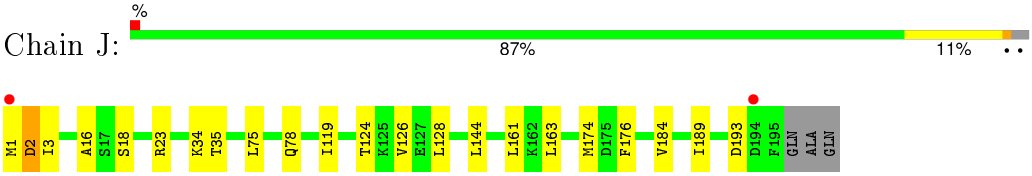
• Molecule 9: Proteasome subunit beta type-3

Chain W:



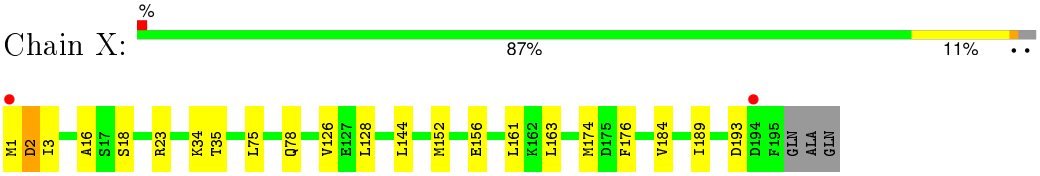
• Molecule 10: Proteasome subunit beta type-4

Chain J:



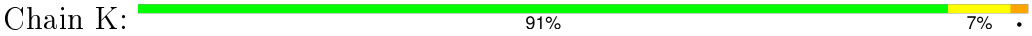
• Molecule 10: Proteasome subunit beta type-4

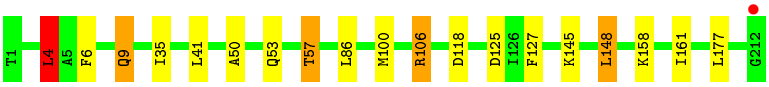
Chain X:



• Molecule 11: Proteasome subunit beta type-5

Chain K:



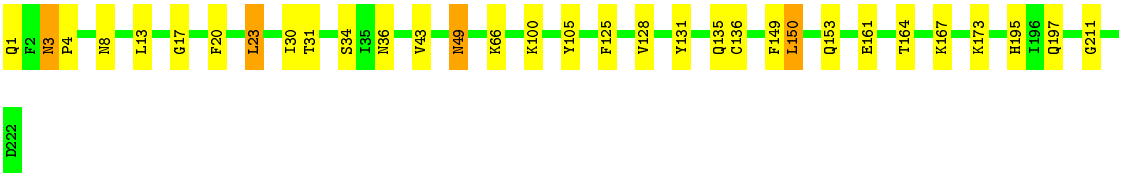


• Molecule 11: Proteasome subunit beta type-5

Chain Y:

• Molecule 12: Proteasome subunit beta type-6

Chain L:

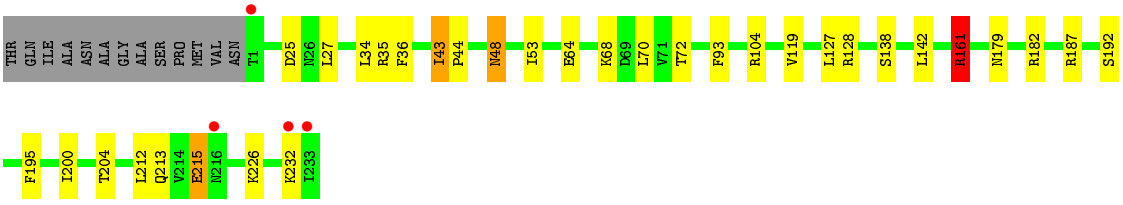


• Molecule 12: Proteasome subunit beta type-6

Chain Z:

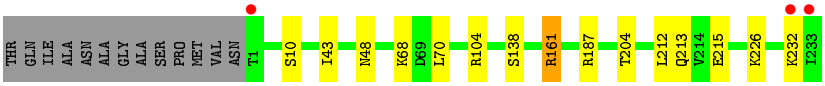
• Molecule 13: Proteasome subunit beta type-7

Chain M:



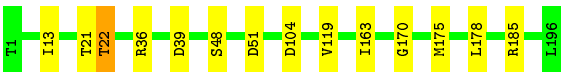
• Molecule 13: Proteasome subunit beta type-7

Chain a:



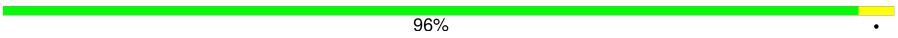
• Molecule 14: Proteasome subunit beta type-1

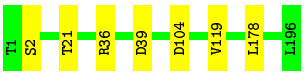
Chain N:



• Molecule 14: Proteasome subunit beta type-1

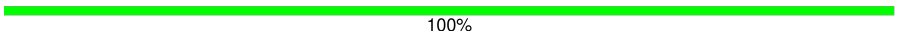
Chain b:





• Molecule 15: N3-A(4,4-F2P)nLL-ep

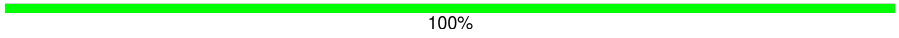
Chain e:



There are no outlier residues recorded for this chain.

• Molecule 15: N3-A(4,4-F2P)nLL-ep

Chain f:



There are no outlier residues recorded for this chain.

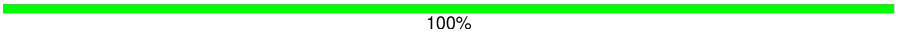
• Molecule 15: N3-A(4,4-F2P)nLL-ep

Chain g:

There are no outlier residues recorded for this chain.

• Molecule 15: N3-A(4,4-F2P)nLL-ep

Chain h:



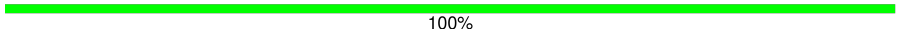
There are no outlier residues recorded for this chain.

• Molecule 15: N3-A(4,4-F2P)nLL-ep

Chain i:

• Molecule 15: N3-A(4,4-F2P)nLL-ep

Chain j:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.95Å 299.90Å 145.79Å 90.00° 113.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.4 (15.00-2.70) 97.4 (15.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.185 , 0.203 0.185 , 0.203	Depositor DCC
R_{free} test set	14297 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	60.5	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 285933 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	49927	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: AZI, MG, ACE, CL, NLE, MES, PDF, 05W

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	0.30	0/1952	0.58	0/2642
1	O	0.30	0/1952	0.58	0/2642
2	B	0.30	0/1934	0.62	0/2618
2	P	0.30	0/1934	0.62	0/2618
3	C	0.31	0/1910	0.64	1/2586 (0.0%)
3	Q	0.33	0/1910	0.64	1/2586 (0.0%)
4	D	0.30	0/1837	0.61	1/2475 (0.0%)
4	R	0.30	0/1837	0.61	1/2475 (0.0%)
5	E	0.30	0/1800	0.61	1/2433 (0.0%)
5	S	0.30	0/1800	0.61	1/2433 (0.0%)
6	F	0.31	0/1932	0.55	0/2609
6	T	0.31	0/1932	0.55	0/2609
7	G	0.30	0/1945	0.57	0/2634
7	U	0.30	0/1945	0.57	0/2634
8	H	0.43	2/1726 (0.1%)	0.66	4/2341 (0.2%)
8	V	0.44	2/1726 (0.1%)	0.65	2/2341 (0.1%)
9	I	0.30	0/1611	0.58	0/2174
9	W	0.30	0/1611	0.58	0/2174
10	J	0.29	0/1589	0.58	0/2142
10	X	0.29	0/1589	0.58	0/2142
11	K	0.32	0/1681	0.60	1/2274 (0.0%)
11	Y	0.31	0/1681	0.59	1/2274 (0.0%)
12	L	0.29	0/1795	0.55	0/2420
12	Z	0.32	0/1795	0.55	0/2420
13	M	0.31	0/1855	0.62	1/2514 (0.0%)
13	a	0.34	0/1855	0.63	1/2514 (0.0%)
14	N	0.32	0/1541	0.56	0/2087
14	b	0.33	0/1541	0.55	0/2087
15	e	0.83	0/5	0.86	0/6
15	f	0.54	0/5	1.44	0/6
15	g	0.38	0/5	0.82	0/6
15	h	1.03	0/5	1.28	0/6

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
15	i	0.66	0/5	1.73	0/6
15	j	1.25	0/5	1.40	0/6
All	All	0.32	4/50246 (0.0%)	0.60	16/67934 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	1
9	W	0	1
12	L	0	1
12	Z	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	114[A]	HIS	CA-C	8.12	1.74	1.52
8	H	114[B]	HIS	CA-C	8.12	1.74	1.52
8	V	114[A]	HIS	CA-C	7.47	1.72	1.52
8	V	114[B]	HIS	CA-C	7.47	1.72	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	114[A]	HIS	CA-C-O	8.01	136.92	120.10
8	H	114[B]	HIS	CA-C-O	8.01	136.92	120.10
3	C	167	LYS	CD-CE-NZ	7.73	129.47	111.70
3	Q	167	LYS	CD-CE-NZ	7.49	128.92	111.70
8	V	114[A]	HIS	CA-C-O	7.20	135.21	120.10
8	V	114[B]	HIS	CA-C-O	7.20	135.21	120.10
5	S	180	LYS	CD-CE-NZ	6.99	127.78	111.70
5	E	180	LYS	CD-CE-NZ	6.47	126.58	111.70
13	a	161	ARG	NE-CZ-NH1	5.42	123.01	120.30
13	M	161	ARG	NE-CZ-NH1	5.34	122.97	120.30
4	D	51	LEU	CA-CB-CG	5.27	127.42	115.30
4	R	51	LEU	CA-CB-CG	5.26	127.39	115.30
11	K	4	LEU	CA-CB-CG	5.19	127.23	115.30
11	Y	4	LEU	CA-CB-CG	5.17	127.18	115.30
8	H	114[A]	HIS	CA-C-N	-5.07	106.04	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	114[B]	HIS	CA-C-N	-5.07	106.04	117.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	192	ASP	Peptide
12	L	135	GLN	Peptide
9	W	192	ASP	Peptide
12	Z	135	GLN	Peptide

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	9	0
1	O	1915	0	1929	12	0
2	B	1904	0	1904	22	0
2	P	1904	0	1904	17	0
3	C	1881	0	1895	23	0
3	Q	1881	0	1895	23	0
4	D	1813	0	1797	15	0
4	R	1813	0	1797	18	0
5	E	1773	0	1775	13	0
5	S	1773	0	1775	12	0
6	F	1892	0	1883	15	0
6	T	1892	0	1883	15	0
7	G	1907	0	1901	17	0
7	U	1907	0	1901	19	0
8	H	1691	0	1692	10	0
8	V	1691	0	1692	13	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	10	0
11	K	1644	0	1592	11	0
11	Y	1644	0	1592	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	1757	0	1711	15	0
12	Z	1757	0	1711	14	0
13	M	1824	0	1832	15	0
13	a	1824	0	1832	0	0
14	N	1512	0	1479	5	0
14	b	1512	0	1478	0	0
15	e	40	0	40	0	0
15	f	40	0	39	0	0
15	g	40	0	40	0	0
15	h	40	0	39	0	0
15	i	40	0	39	0	0
15	j	40	0	39	0	0
16	G	1	0	0	0	0
16	I	2	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	Z	1	0	0	0	0
17	K	12	0	13	0	0
17	i	12	0	13	0	0
18	N	1	0	0	0	0
18	b	1	0	0	0	0
19	A	12	0	0	0	0
19	B	15	0	0	0	0
19	C	12	0	0	0	0
19	D	3	0	0	0	0
19	E	5	0	0	0	0
19	F	13	0	0	0	0
19	G	8	0	0	0	0
19	H	14	0	0	0	0
19	I	19	0	0	0	0
19	J	17	0	0	0	0
19	K	18	0	0	0	0
19	L	17	0	0	0	0
19	M	13	0	0	0	0
19	N	7	0	0	1	0
19	O	14	0	0	0	0
19	P	4	0	0	0	0
19	Q	8	0	0	0	0
19	R	4	0	0	0	0
19	S	6	0	0	0	0
19	T	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	U	12	0	0	0	0
19	V	12	0	0	0	0
19	W	5	0	0	0	0
19	X	13	0	0	0	0
19	Y	13	0	0	0	0
19	Z	21	0	0	0	0
19	a	19	0	0	0	0
19	b	18	0	0	0	0
19	e	1	0	0	0	0
19	f	1	0	0	0	0
19	g	2	0	0	0	0
19	h	1	0	0	0	0
19	i	1	0	0	0	0
19	j	3	0	0	0	0
All	All	49927	0	49327	323	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 4.

All (323) 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)
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.31	0.94
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.32	0.93
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.78	0.84
3:Q:38:ASN:HD22	3:Q:38:ASN:H	1.24	0.83
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.09	0.83
11:K:100:MET:CE	11:K:127:PHE:HB2	2.09	0.82
11:K:53:GLN:O	11:K:57:THR:HG23	1.80	0.80
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.63	0.79
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.62	0.79
3:C:201:VAL:O	3:C:202:GLN:HB2	1.85	0.76
3:C:202:GLN:HG3	3:C:203:THR:H	1.50	0.76
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.50	0.76
3:Q:201:VAL:O	3:Q:202:GLN:HB2	1.85	0.76
3:C:51:LYS:O	3:C:52:LEU:HB2	1.86	0.75
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.34	0.75
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.35	0.74
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.87	0.74
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.53	0.74
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.70	0.73
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.54	0.72
7:U:23:PHE:O	7:U:26:THR:HB	1.90	0.71
7:G:23:PHE:O	7:G:26:THR:HB	1.90	0.71
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.72	0.71
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.73	0.70
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.73	0.69
3:Q:35:LYS:HB2	3:Q:40:VAL:HG22	1.74	0.69
11:K:106:ARG:HB3	11:K:106:ARG:HH11	1.59	0.68
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.09	0.67
5:E:12:PHE:H	6:F:19:GLN:HE22	1.41	0.67
11:Y:106:ARG:HH11	11:Y:106:ARG:HB3	1.59	0.67
5:S:12:PHE:H	6:T:19:GLN:HE22	1.45	0.65
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.44	0.65
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.79	0.65
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.78	0.65
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.79	0.64
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.79	0.64
3:C:201:VAL:O	3:C:202:GLN:CB	2.44	0.64
8:H:52:THR:O	8:H:56:THR:HB	1.98	0.64
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.79	0.64
8:V:52:THR:O	8:V:56:THR:HB	1.98	0.63
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.64	0.62
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.82	0.62
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.81	0.61
13:M:161:ARG:HH11	13:M:161:ARG:HG3	1.64	0.61
11:K:100:MET:HE3	11:K:127:PHE:CB	2.30	0.61
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.65	0.61
1:O:12:PHE:H	2:P:20:GLN:HE22	1.49	0.61
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.82	0.60
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.81	0.60
11:Y:100:MET:HE3	11:Y:127:PHE:CB	2.29	0.60
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.84	0.60
3:C:198:LEU:HA	3:C:201:VAL:HG12	1.84	0.59
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.84	0.59
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.84	0.59
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.85	0.59
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.84	0.59
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.15	0.59
12:L:17:GLY:HA3	12:L:20:PHE:CE1	2.39	0.58
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:17:GLY:HA3	12:Z:20:PHE:CE1	2.38	0.58
6:F:31:THR:HB	6:F:47:GLU:HG2	1.86	0.58
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.84	0.58
6:T:31:THR:HB	6:T:47:GLU:HG2	1.85	0.58
3:C:230:TYR:O	3:C:234:ILE:HG13	2.04	0.58
3:Q:38:ASN:N	3:Q:38:ASN:HD22	1.91	0.58
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.52	0.58
3:Q:230:TYR:O	3:Q:234:ILE:HG13	2.04	0.58
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.17	0.57
8:V:50:ALA:HB3	9:W:126:ILE:HD12	1.85	0.56
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.87	0.56
1:O:247:LEU:O	1:O:250:LEU:HB2	2.06	0.56
1:A:247:LEU:O	1:A:250:LEU:HB2	2.06	0.55
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.71	0.55
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.36	0.55
6:T:34:ILE:HG22	6:T:160:ALA:HB2	1.89	0.55
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.89	0.54
6:F:123:ASN:C	6:F:123:ASN:HD22	2.11	0.54
6:F:34:ILE:HG22	6:F:160:ALA:HB2	1.89	0.54
1:A:12:PHE:H	2:B:20:GLN:HE22	1.55	0.54
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.90	0.53
3:C:160:GLN:HE21	3:C:161:THR:H	1.57	0.53
3:Q:168:THR:O	3:Q:171:GLU:HB3	2.09	0.53
6:T:123:ASN:HD22	6:T:123:ASN:C	2.11	0.53
3:Q:160:GLN:HE21	3:Q:161:THR:H	1.57	0.53
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.89	0.53
4:D:99:ILE:CD1	4:D:104:LEU:HB2	2.39	0.53
7:G:45:ILE:HG22	7:G:216:VAL:HG13	1.91	0.53
2:P:8:ARG:HD2	3:Q:4:ARG:NH2	2.24	0.52
4:R:99:ILE:CD1	4:R:104:LEU:HB2	2.39	0.52
8:V:172:ASN:HD22	8:V:192:THR:HA	1.74	0.52
4:R:185:LEU:O	4:R:189:GLU:HG3	2.10	0.52
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.09	0.52
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.36	0.52
7:U:45:ILE:HG22	7:U:216:VAL:HG13	1.91	0.52
3:C:168:THR:O	3:C:171:GLU:HB3	2.10	0.52
2:B:204:ALA:O	2:B:209:ARG:NH2	2.43	0.52
12:L:8:ASN:HA	12:L:30:ILE:O	2.09	0.52
7:U:242:GLN:OE1	7:U:242:GLN:HA	2.11	0.51
5:E:9:THR:HG21	5:E:119:THR:HA	1.93	0.51
2:B:59:ASP:HB3	2:B:231:PRO:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:172:ASN:HD22	8:H:192:THR:HA	1.75	0.51
2:P:59:ASP:HB3	2:P:231:PRO:HG2	1.92	0.51
2:P:204:ALA:O	2:P:209:ARG:NH2	2.44	0.51
14:N:185:ARG:NH1	19:N:303:HOH:O	2.42	0.51
10:X:1:MET:HA	10:X:34:LYS:CE	2.41	0.51
7:G:34:LEU:HD23	7:G:34:LEU:C	2.31	0.51
7:G:242:GLN:HA	7:G:242:GLN:OE1	2.10	0.51
2:P:180:LYS:O	2:P:183:MET:HB2	2.11	0.51
10:J:1:MET:HA	10:J:34:LYS:HE3	1.93	0.51
2:B:8:ARG:HD2	3:C:4:ARG:HH21	1.76	0.50
10:J:1:MET:HA	10:J:34:LYS:CE	2.41	0.50
2:B:12:PHE:H	3:C:17:GLN:HE22	1.59	0.50
4:D:185:LEU:O	4:D:189:GLU:HG3	2.11	0.50
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.94	0.50
12:L:195:HIS:HD2	12:L:197:GLN:H	1.60	0.50
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.94	0.50
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.47	0.50
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.47	0.50
5:S:9:THR:HG21	5:S:119:THR:HA	1.93	0.50
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.47	0.50
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.93	0.50
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.93	0.50
7:G:83:ASN:C	7:G:83:ASN:HD22	2.16	0.50
2:B:93:HIS:CG	2:B:113:ARG:HE	2.30	0.49
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.60	0.49
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.94	0.49
14:N:22:THR:O	14:N:22:THR:HG23	2.12	0.49
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.94	0.49
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.94	0.49
7:U:34:LEU:C	7:U:34:LEU:HD23	2.32	0.49
2:B:180:LYS:O	2:B:183:MET:HB2	2.12	0.49
5:E:68:HIS:HE1	5:E:102:LEU:O	1.96	0.49
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.60	0.49
7:U:83:ASN:C	7:U:83:ASN:HD22	2.16	0.49
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.94	0.49
5:E:70:GLY:HA3	5:E:221:PHE:CE2	2.47	0.48
2:P:237:ILE:HD12	2:P:240:LYS:HE3	1.94	0.48
3:C:38:ASN:N	3:C:38:ASN:HD22	2.10	0.48
4:D:60:VAL:HG11	4:D:81:ILE:HD12	1.95	0.48
10:X:1:MET:HA	10:X:34:LYS:HE3	1.93	0.48
7:U:73:VAL:HG12	7:U:133:THR:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.44	0.48
11:Y:50:ALA:CB	12:Z:128:VAL:HG23	2.43	0.48
2:B:237:ILE:HD12	2:B:240:LYS:HE3	1.94	0.48
2:P:93:HIS:CG	2:P:113:ARG:HE	2.31	0.48
5:S:68:HIS:HE1	5:S:102:LEU:O	1.96	0.48
7:G:73:VAL:HG12	7:G:133:THR:HB	1.95	0.48
7:U:170:THR:O	7:U:174:GLU:HG3	2.14	0.48
3:Q:35:LYS:CB	3:Q:40:VAL:HG22	2.41	0.47
11:K:100:MET:HE2	11:K:127:PHE:HB2	1.92	0.47
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.43	0.47
7:G:170:THR:O	7:G:174:GLU:HG3	2.14	0.47
4:R:60:VAL:HG11	4:R:81:ILE:HD12	1.95	0.47
5:S:109:HIS:HB3	6:T:82:ARG:NH2	2.29	0.47
3:Q:38:ASN:ND2	3:Q:38:ASN:H	2.02	0.47
1:O:149:GLN:O	1:O:156:TYR:HA	2.15	0.47
10:J:3:ILE:HB	10:J:18:SER:HB3	1.96	0.47
1:O:158:PRO:HB2	2:P:57:GLU:HB3	1.96	0.47
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.79	0.47
11:K:50:ALA:CB	12:L:128:VAL:HG23	2.45	0.47
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.96	0.47
7:G:195:GLU:HG3	7:G:235:ARG:HG3	1.96	0.47
13:M:119:VAL:HG23	13:M:200:ILE:HG22	1.97	0.47
3:C:9:PHE:H	4:D:15:GLN:HE22	1.63	0.47
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.96	0.46
1:A:149:GLN:O	1:A:156:TYR:HA	2.14	0.46
1:O:119:GLN:O	1:O:122:THR:HB	2.16	0.46
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.97	0.46
2:P:37:ILE:HD12	2:P:192:ALA:HB2	1.97	0.46
5:E:109:HIS:HB3	6:F:82:ARG:NH2	2.30	0.46
4:D:71:SER:HB3	4:D:164:ILE:HD12	1.97	0.46
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.98	0.46
8:H:84:LYS:HG3	8:H:85:GLN:N	2.29	0.46
10:X:3:ILE:HB	10:X:18:SER:HB3	1.96	0.46
4:R:71:SER:HB3	4:R:164:ILE:HD12	1.97	0.46
8:V:84:LYS:HG3	8:V:85:GLN:N	2.30	0.46
3:C:35:LYS:HG2	3:C:158:SER:O	2.16	0.46
13:M:93:PHE:CE2	13:M:128:ARG:HD3	2.50	0.46
7:G:83:ASN:ND2	7:G:83:ASN:C	2.69	0.46
6:T:238:PHE:O	6:T:242:GLU:HG2	2.16	0.46
6:F:238:PHE:O	6:F:242:GLU:HG2	2.16	0.46
2:B:37:ILE:HD12	2:B:192:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:48:ASN:H	13:M:48:ASN:HD22	1.64	0.45
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.97	0.45
6:T:34:ILE:HG22	6:T:160:ALA:CB	2.47	0.45
10:X:3:ILE:HD12	10:X:176:PHE:CD2	2.52	0.45
8:V:1:THR:HG22	8:V:2:THR:N	2.30	0.45
9:W:123:PHE:HA	9:W:128:CYS:O	2.17	0.45
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.51	0.45
7:U:83:ASN:C	7:U:83:ASN:ND2	2.70	0.45
4:R:51:LEU:C	4:R:51:LEU:HD12	2.37	0.45
5:E:155:LEU:HD13	5:E:158:THR:HB	1.99	0.45
1:A:119:GLN:O	1:A:122:THR:HB	2.16	0.45
1:O:50:LYS:HG3	1:O:50:LYS:O	2.16	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.99	0.45
7:G:25:ALA:O	7:G:28:GLN:HB2	2.17	0.45
5:E:226:GLY:O	5:E:229:VAL:HG22	2.17	0.45
11:Y:100:MET:HE2	11:Y:127:PHE:HB2	1.93	0.45
5:S:155:LEU:HD13	5:S:158:THR:HB	1.99	0.45
10:J:3:ILE:HD12	10:J:176:PHE:CD2	2.52	0.44
14:N:13:ILE:HG21	14:N:175:MET:CE	2.47	0.44
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.99	0.44
1:O:115:ALA:HB1	1:O:154:GLY:O	2.18	0.44
3:Q:202:GLN:CG	3:Q:203:THR:H	2.24	0.44
6:F:34:ILE:HG22	6:F:160:ALA:CB	2.46	0.44
6:T:194:LYS:HD3	6:T:242:GLU:HG3	2.00	0.44
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.44
7:U:25:ALA:O	7:U:28:GLN:HB2	2.17	0.44
5:S:226:GLY:O	5:S:229:VAL:HG22	2.17	0.44
13:M:182:ARG:NH2	13:M:215:GLU:O	2.51	0.44
6:T:13:PRO:O	7:U:24:LYS:HD2	2.18	0.44
4:D:51:LEU:C	4:D:51:LEU:HD12	2.37	0.44
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.53	0.44
9:I:123:PHE:HA	9:I:128:CYS:O	2.17	0.44
6:F:194:LYS:HD3	6:F:242:GLU:HG3	2.00	0.44
8:V:35:HIS:CG	8:V:56:THR:HG21	2.53	0.44
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.53	0.44
11:K:6:PHE:HA	11:K:125:ASP:O	2.18	0.44
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.18	0.44
1:A:50:LYS:O	1:A:50:LYS:HG3	2.17	0.44
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.00	0.44
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:193:ASP:N	10:X:193:ASP:OD1	2.51	0.43
5:S:231:LYS:HD2	5:S:232:TYR:CE2	2.53	0.43
3:C:202:GLN:HG3	3:C:203:THR:N	2.27	0.43
8:H:114[A]:HIS:CD2	8:H:116:HIS:H	2.37	0.43
14:N:48:SER:HB3	14:N:51:ASP:HB2	2.00	0.43
5:E:231:LYS:HD2	5:E:232:TYR:CE2	2.54	0.43
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.84	0.43
10:J:184:VAL:HG22	10:J:189:ILE:HG12	2.01	0.43
1:A:115:ALA:HB1	1:A:154:GLY:O	2.19	0.43
3:C:51:LYS:HA	3:C:51:LYS:HD2	1.58	0.43
10:X:184:VAL:HG22	10:X:189:ILE:HG12	2.01	0.43
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.53	0.43
8:V:114[A]:HIS:CD2	8:V:116:HIS:H	2.37	0.43
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.48	0.43
5:S:28:ILE:HD11	5:S:148:PRO:CD	2.48	0.43
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.84	0.43
11:Y:86:LEU:HD13	11:Y:86:LEU:C	2.39	0.43
7:G:196:PHE:C	7:G:196:PHE:CD1	2.92	0.42
9:I:7:ASN:HA	9:I:29:GLY:O	2.19	0.42
4:R:99:ILE:HD13	4:R:104:LEU:HB2	2.01	0.42
5:S:136:TYR:CE1	5:S:217:LYS:HA	2.53	0.42
11:K:86:LEU:HD13	11:K:86:LEU:C	2.40	0.42
13:M:43:ILE:HG21	13:M:64:GLU:HG2	2.01	0.42
13:M:43:ILE:HD11	13:M:53:ILE:CD1	2.49	0.42
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.54	0.42
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.54	0.42
4:D:99:ILE:HD13	4:D:104:LEU:HB2	2.01	0.42
5:E:136:TYR:CE1	5:E:217:LYS:HA	2.53	0.42
7:G:227:LEU:HB3	7:G:231:ASN:HB2	2.00	0.42
6:F:228:LYS:HB2	6:F:228:LYS:HE3	1.88	0.42
9:W:7:ASN:HA	9:W:29:GLY:O	2.19	0.42
13:M:25:ASP:HA	13:M:195:PHE:CB	2.49	0.42
7:U:39:LYS:HD2	7:U:186:ASN:ND2	2.35	0.42
6:T:41:GLY:HA3	6:T:215:CYS:O	2.20	0.42
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.85	0.42
3:Q:202:GLN:HG3	3:Q:203:THR:N	2.27	0.42
7:U:227:LEU:HB3	7:U:231:ASN:HB2	2.01	0.42
7:G:39:LYS:HD2	7:G:186:ASN:ND2	2.35	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
1:O:38:LYS:NZ	2:P:57:GLU:OE2	2.34	0.41
7:U:196:PHE:C	7:U:196:PHE:CD1	2.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:146:MET:CE	6:T:161:THR:HB	2.50	0.41
13:M:27:LEU:HB2	13:M:192:SER:HB3	2.03	0.41
1:O:55:LEU:HB3	7:U:159:ALA:O	2.20	0.41
8:H:84:LYS:HE2	8:H:119:THR:HG23	2.02	0.41
6:T:165:ARG:HE	6:T:165:ARG:HB3	1.76	0.41
8:H:1:THR:HG22	8:H:2:THR:N	2.35	0.41
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.84	0.41
3:C:160:GLN:NE2	3:C:161:THR:H	2.16	0.41
6:F:41:GLY:HA3	6:F:215:CYS:O	2.20	0.41
4:R:77:ALA:O	4:R:81:ILE:HG12	2.21	0.41
2:P:139:TYR:CE2	2:P:144:GLY:HA2	2.56	0.41
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.56	0.41
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.56	0.41
4:D:4:VAL:HG13	4:D:15:GLN:HG3	2.02	0.41
2:B:139:TYR:CE2	2:B:144:GLY:HA2	2.56	0.41
4:R:4:VAL:HG13	4:R:15:GLN:HG3	2.03	0.41
13:M:43:ILE:HA	13:M:44:PRO:HD3	1.85	0.41
6:F:146:MET:CE	6:F:161:THR:HB	2.51	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
6:F:206:LYS:HA	6:F:206:LYS:HE3	2.03	0.41
6:T:162:GLY:O	6:T:165:ARG:HB3	2.21	0.41
5:S:170:TYR:HB2	5:S:198:GLN:HG3	2.02	0.41
13:M:35:ARG:HG3	13:M:36:PHE:CZ	2.56	0.41
9:I:62:LEU:HD21	9:I:102:TYR:CD2	2.56	0.41
7:G:147:LYS:O	7:G:154:TYR:HA	2.21	0.41
5:E:170:TYR:HB2	5:E:198:GLN:HG3	2.02	0.41
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.02	0.40
12:Z:161:GLU:HB3	12:Z:164:THR:CG2	2.51	0.40
4:R:38:VAL:HG11	4:R:137:ALA:HB1	2.03	0.40
6:T:240:GLN:HA	6:T:240:GLN:NE2	2.36	0.40
8:V:22:GLN:HG3	8:V:22:GLN:O	2.21	0.40
12:L:161:GLU:HB3	12:L:164:THR:HG21	2.03	0.40
3:Q:36:GLY:N	3:Q:39:CYS:O	2.51	0.40
3:Q:160:GLN:NE2	3:Q:161:THR:H	2.17	0.40
12:L:161:GLU:HB3	12:L:164:THR:CG2	2.51	0.40
5:S:88:ARG:O	5:S:92:ASN:HB2	2.21	0.40
5:E:88:ARG:O	5:E:92:ASN:HB2	2.21	0.40
10:J:193:ASP:OD1	10:J:193:ASP:N	2.51	0.40
12:Z:100:LYS:HD3	12:Z:105:TYR:CZ	2.57	0.40
12:L:149:PHE:CE1	12:L:153:GLN:HG3	2.57	0.40
14:N:163:ILE:HG23	14:N:170:GLY:HA2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:205:ALA:C	3:Q:207:ASN:H	2.25	0.40
5:E:61:LYS:O	5:E:72:SER:HA	2.21	0.40
3:C:131:THR:OG1	3:C:148:THR:OG1	2.35	0.40
11:K:4:LEU:HD13	11:K:161:ILE:HD11	2.03	0.40
10:X:152:MET:HE3	10:X:156:GLU:HB3	2.03	0.40
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.56	0.40
2:B:159:TRP:HH2	3:C:50:LEU:HD22	1.86	0.40
10:J:119:ILE:HA	10:J:124:THR:O	2.22	0.40
6:F:162:GLY:O	6:F:165:ARG:HB3	2.22	0.40
7:U:239:ILE:O	7:U:242:GLN:HB3	2.22	0.40
7:G:239:ILE:O	7:G:242:GLN:HB3	2.21	0.40
9:W:62:LEU:HD21	9:W:102:TYR:CD2	2.57	0.40
6:F:68:ARG:NH1	13:M:72:THR:OG1	2.55	0.40
2:B:198:LYS:HE2	2:B:198:LYS:HB3	1.86	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%)	238 (96%)	9 (4%)	1 (0%)	39 69
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	39 69
2	B	242/258 (94%)	228 (94%)	11 (4%)	3 (1%)	16 39
2	P	242/258 (94%)	228 (94%)	11 (4%)	3 (1%)	16 39
3	C	238/254 (94%)	224 (94%)	9 (4%)	5 (2%)	9 23
3	Q	238/254 (94%)	225 (94%)	9 (4%)	4 (2%)	11 29
4	D	231/260 (89%)	224 (97%)	5 (2%)	2 (1%)	21 49
4	R	231/260 (89%)	224 (97%)	5 (2%)	2 (1%)	21 49
5	E	229/234 (98%)	215 (94%)	12 (5%)	2 (1%)	21 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	S	229/234 (98%)	215 (94%)	12 (5%)	2 (1%)	21 49
6	F	241/288 (84%)	234 (97%)	7 (3%)	0	100 100
6	T	241/288 (84%)	234 (97%)	7 (3%)	0	100 100
7	G	239/252 (95%)	231 (97%)	7 (3%)	1 (0%)	39 69
7	U	239/252 (95%)	230 (96%)	8 (3%)	1 (0%)	39 69
8	H	221/232 (95%)	214 (97%)	7 (3%)	0	100 100
8	V	221/232 (95%)	215 (97%)	6 (3%)	0	100 100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100 100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100 100
10	J	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	34 63
10	X	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	34 63
11	K	210/212 (99%)	205 (98%)	4 (2%)	1 (0%)	34 63
11	Y	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	34 63
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100 100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100 100
13	M	231/246 (94%)	224 (97%)	7 (3%)	0	100 100
13	a	231/246 (94%)	224 (97%)	7 (3%)	0	100 100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100 100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100 100
15	e	1/6 (17%)	1 (100%)	0	0	100 100
15	f	1/6 (17%)	1 (100%)	0	0	100 100
15	g	1/6 (17%)	1 (100%)	0	0	100 100
15	h	1/6 (17%)	1 (100%)	0	0	100 100
15	i	1/6 (17%)	0	0	1 (100%)	0 0
15	j	1/6 (17%)	1 (100%)	0	0	100 100
All	All	6284/6650 (94%)	6053 (96%)	199 (3%)	32 (0%)	34 63

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	52	THR
3	C	202	GLN

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Mol	Chain	Res	Type
3	C	205	ALA
1	O	2	THR
2	P	52	THR
3	Q	202	GLN
3	Q	205	ALA
15	i	3	ALA
2	B	51	VAL
3	C	38	ASN
10	J	2	ASP
11	K	9	GLN
2	P	51	VAL
10	X	2	ASP
11	Y	9	GLN
3	C	183	PRO
3	C	206	LYS
5	E	231	LYS
7	G	51	PRO
3	Q	183	PRO
3	Q	206	LYS
5	S	231	LYS
7	U	51	PRO
2	B	221	ASP
4	D	2	ARG
4	D	201	GLU
5	E	217	LYS
2	P	221	ASP
4	R	2	ARG
5	S	217	LYS
4	R	201	GLU

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%)	198 (95%)	11 (5%)	28 57
1	O	209/209 (100%)	198 (95%)	11 (5%)	28 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	203/216 (94%)	187 (92%)	16 (8%)	15 34
2	P	203/216 (94%)	187 (92%)	16 (8%)	15 34
3	C	212/226 (94%)	192 (91%)	20 (9%)	11 25
3	Q	212/226 (94%)	194 (92%)	18 (8%)	13 30
4	D	194/215 (90%)	173 (89%)	21 (11%)	8 18
4	R	194/215 (90%)	172 (89%)	22 (11%)	7 16
5	E	190/193 (98%)	169 (89%)	21 (11%)	8 17
5	S	190/193 (98%)	169 (89%)	21 (11%)	8 17
6	F	201/239 (84%)	181 (90%)	20 (10%)	9 22
6	T	201/239 (84%)	181 (90%)	20 (10%)	9 22
7	G	206/210 (98%)	188 (91%)	18 (9%)	13 29
7	U	206/210 (98%)	188 (91%)	18 (9%)	13 29
8	H	182/190 (96%)	172 (94%)	10 (6%)	27 55
8	V	182/190 (96%)	172 (94%)	10 (6%)	27 55
9	I	172/173 (99%)	166 (96%)	6 (4%)	43 74
9	W	172/173 (99%)	166 (96%)	6 (4%)	43 74
10	J	173/175 (99%)	165 (95%)	8 (5%)	33 64
10	X	173/175 (99%)	165 (95%)	8 (5%)	33 64
11	K	169/169 (100%)	159 (94%)	10 (6%)	24 51
11	Y	169/169 (100%)	159 (94%)	10 (6%)	24 51
12	L	185/185 (100%)	175 (95%)	10 (5%)	27 56
12	Z	185/185 (100%)	175 (95%)	10 (5%)	27 56
13	M	199/208 (96%)	185 (93%)	14 (7%)	19 42
13	a	199/208 (96%)	184 (92%)	15 (8%)	17 38
14	N	162/162 (100%)	155 (96%)	7 (4%)	35 66
14	b	162/162 (100%)	155 (96%)	7 (4%)	35 66
All	All	5314/5540 (96%)	4930 (93%)	384 (7%)	18 41

All (384) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	17	LYS

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Mol	Chain	Res	Type
1	A	30	GLN
1	A	50	LYS
1	A	51	SER
1	A	59	GLU
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	231	LYS
1	A	250	LEU
2	B	50	LYS
2	B	53	SER
2	B	54	THR
2	B	55	LEU
2	B	56	LEU
2	B	58	GLN
2	B	119	GLN
2	B	149	THR
2	B	180	LYS
2	B	183	MET
2	B	184	LYS
2	B	191	LEU
2	B	197	SER
2	B	209	ARG
2	B	223	GLU
2	B	244	THR
3	C	4	ARG
3	C	37	LYS
3	C	38	ASN
3	C	48	SER
3	C	51	LYS
3	C	55	THR
3	C	61	LYS
3	C	77	ASN
3	C	116	GLN
3	C	147	GLN
3	C	160	GLN
3	C	167	LYS
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	187	GLU
3	C	203	THR

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Mol	Chain	Res	Type
3	C	225	GLU
3	C	239	GLN
3	C	240	GLU
4	D	1	ASP
4	D	12	ARG
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	54	ASP
4	D	60	VAL
4	D	78	ARG
4	D	99	ILE
4	D	117	GLU
4	D	125	LEU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	202	GLU
4	D	214	ILE
4	D	224	ASP
4	D	235	LEU
4	D	236	LYS
4	D	238	LYS
4	D	242	GLU
5	E	3	ASN
5	E	4	ASN
5	E	8	ASP
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	55	LEU
5	E	60	LYS
5	E	61	LYS
5	E	71	LEU
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	179	ILE
5	E	180	LYS
5	E	184	ASN
5	E	188	LEU

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Mol	Chain	Res	Type
5	E	207	VAL
5	E	219	THR
5	E	231	LYS
6	F	14	ASP
6	F	47	GLU
6	F	59	LYS
6	F	94	SER
6	F	96	LYS
6	F	117	GLN
6	F	123	ASN
6	F	126	ARG
6	F	139	LYS
6	F	148	GLU
6	F	165	ARG
6	F	172	LEU
6	F	181	GLU
6	F	187	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
6	F	228	LYS
6	F	241	LYS
7	G	24	LYS
7	G	26	THR
7	G	28	GLN
7	G	34	LEU
7	G	53	LYS
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	165	LYS
7	G	166	GLN
7	G	181	LYS
7	G	183	ASP
7	G	201	MET
7	G	230	GLU
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN

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Mol	Chain	Res	Type
8	H	34	LEU
8	H	43	CYS
8	H	55	VAL
8	H	56	THR
8	H	68	LEU
8	H	127	LEU
8	H	153	LYS
8	H	196	ARG
8	H	198	GLU
9	I	37	ASN
9	I	38	LYS
9	I	114	LYS
9	I	171	LEU
9	I	182	TRP
9	I	192	ASP
10	J	2	ASP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	163	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	41	LEU
11	K	57	THR
11	K	106	ARG
11	K	118	ASP
11	K	148	LEU
11	K	158	LYS
11	K	177	LEU
12	L	1	GLN
12	L	3	ASN
12	L	23	LEU
12	L	34	SER
12	L	49	ASN
12	L	66	LYS
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS

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Mol	Chain	Res	Type
12	L	173	LYS
13	M	43	ILE
13	M	48	ASN
13	M	68	LYS
13	M	70	LEU
13	M	104	ARG
13	M	138	SER
13	M	161	ARG
13	M	187	ARG
13	M	204	THR
13	M	212	LEU
13	M	213	GLN
13	M	215	GLU
13	M	226	LYS
13	M	232	LYS
14	N	21	THR
14	N	22	THR
14	N	36	ARG
14	N	39	ASP
14	N	104	ASP
14	N	119	VAL
14	N	178	LEU
1	O	2	THR
1	O	17	LYS
1	O	30	GLN
1	O	50	LYS
1	O	51	SER
1	O	59	GLU
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
1	O	231	LYS
1	O	250	LEU
2	P	50	LYS
2	P	53	SER
2	P	54	THR
2	P	55	LEU
2	P	56	LEU
2	P	58	GLN
2	P	119	GLN
2	P	149	THR
2	P	180	LYS

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Mol	Chain	Res	Type
2	P	183	MET
2	P	184	LYS
2	P	191	LEU
2	P	197	SER
2	P	209	ARG
2	P	223	GLU
2	P	244	THR
3	Q	4	ARG
3	Q	37	LYS
3	Q	38	ASN
3	Q	48	SER
3	Q	51	LYS
3	Q	55	THR
3	Q	61	LYS
3	Q	116	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	187	GLU
3	Q	203	THR
3	Q	225	GLU
3	Q	239	GLN
3	Q	240	GLU
4	R	1	ASP
4	R	12	ARG
4	R	20	LEU
4	R	40	LEU
4	R	48	SER
4	R	51	LEU
4	R	54	ASP
4	R	60	VAL
4	R	78	ARG
4	R	99	ILE
4	R	117	GLU
4	R	125	LEU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	202	GLU
4	R	214	ILE

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Mol	Chain	Res	Type
4	R	224	ASP
4	R	235	LEU
4	R	236	LYS
4	R	238	LYS
4	R	242	GLU
5	S	3	ASN
5	S	4	ASN
5	S	8	ASP
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	55	LEU
5	S	60	LYS
5	S	61	LYS
5	S	71	LEU
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	179	ILE
5	S	180	LYS
5	S	184	ASN
5	S	188	LEU
5	S	207	VAL
5	S	219	THR
5	S	231	LYS
6	T	14	ASP
6	T	47	GLU
6	T	59	LYS
6	T	94	SER
6	T	96	LYS
6	T	117	GLN
6	T	123	ASN
6	T	126	ARG
6	T	139	LYS
6	T	148	GLU
6	T	165	ARG
6	T	172	LEU
6	T	181	GLU
6	T	187	GLU
6	T	203	ASN
6	T	206	LYS

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Mol	Chain	Res	Type
6	T	214	TRP
6	T	221	ASN
6	T	228	LYS
6	T	241	LYS
7	U	24	LYS
7	U	26	THR
7	U	28	GLN
7	U	34	LEU
7	U	53	LYS
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	165	LYS
7	U	166	GLN
7	U	181	LYS
7	U	183	ASP
7	U	201	MET
7	U	230	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	34	LEU
8	V	43	CYS
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	127	LEU
8	V	153	LYS
8	V	196	ARG
8	V	198	GLU
9	W	37	ASN
9	W	38	LYS
9	W	114	LYS
9	W	171	LEU
9	W	182	TRP
9	W	192	ASP
10	X	2	ASP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU

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Mol	Chain	Res	Type
10	X	78	GLN
10	X	144	LEU
10	X	163	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	41	LEU
11	Y	57	THR
11	Y	106	ARG
11	Y	118	ASP
11	Y	148	LEU
11	Y	158	LYS
11	Y	177	LEU
12	Z	1	GLN
12	Z	3	ASN
12	Z	23	LEU
12	Z	34	SER
12	Z	49	ASN
12	Z	66	LYS
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
12	Z	173	LYS
13	a	10	SER
13	a	43	ILE
13	a	48	ASN
13	a	68	LYS
13	a	70	LEU
13	a	104	ARG
13	a	138	SER
13	a	161	ARG
13	a	187	ARG
13	a	204	THR
13	a	212	LEU
13	a	213	GLN
13	a	215	GLU
13	a	226	LYS
13	a	232	LYS
14	b	2	SER
14	b	21	THR
14	b	36	ARG

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Mol	Chain	Res	Type
14	b	39	ASP
14	b	104	ASP
14	b	119	VAL
14	b	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (143) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	102	ASN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	233	GLN
4	D	15	GLN
4	D	100	ASN
4	D	106	GLN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN

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Mol	Chain	Res	Type
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	167	GLN
7	G	175	ASN
7	G	186	ASN
8	H	30	ASN
8	H	57	GLN
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
9	I	88	GLN
10	J	55	GLN
10	J	118	GLN
10	J	191	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	158	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	38	HIS
14	N	69	GLN
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN

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Mol	Chain	Res	Type
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	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	233	GLN
4	R	15	GLN
4	R	100	ASN
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	165	GLN
5	S	184	ASN
6	T	19	GLN
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
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
8	V	30	ASN
8	V	57	GLN
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN

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Mol	Chain	Res	Type
8	V	172	ASN
8	V	189	ASN
9	W	37	ASN
9	W	88	GLN
10	X	55	GLN
10	X	86	GLN
10	X	191	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	158	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	38	HIS
14	b	69	GLN
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	NLE	e	5	15	5,7,8	0.65	0	5,7,9	1.72	1 (20%)
15	NLE	f	5	15	5,7,8	1.42	1 (20%)	5,7,9	1.47	1 (20%)
15	NLE	g	5	15	5,7,8	0.65	0	5,7,9	1.37	1 (20%)
15	NLE	h	5	15	5,7,8	1.01	1 (20%)	5,7,9	1.29	1 (20%)
15	NLE	i	5	15	5,7,8	1.25	1 (20%)	5,7,9	1.30	0
15	NLE	j	5	15	5,7,8	0.90	0	5,7,9	1.35	1 (20%)

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	NLE	e	5	15	-	0/4/6/8	0/0/0/0
15	NLE	f	5	15	-	0/4/6/8	0/0/0/0
15	NLE	g	5	15	-	0/4/6/8	0/0/0/0
15	NLE	h	5	15	-	0/4/6/8	0/0/0/0
15	NLE	i	5	15	-	0/4/6/8	0/0/0/0
15	NLE	j	5	15	-	0/4/6/8	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	f	5	NLE	CB-CA	-3.11	1.49	1.53
15	i	5	NLE	CB-CA	-2.69	1.49	1.53
15	h	5	NLE	CB-CA	-2.15	1.50	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	e	5	NLE	CG-CB-CA	-3.01	101.43	114.00
15	j	5	NLE	O-C-CA	-2.59	118.78	125.72
15	f	5	NLE	O-C-CA	-2.36	119.39	125.72
15	h	5	NLE	O-C-CA	-2.19	119.85	125.72
15	g	5	NLE	CB-CA-N	2.06	116.34	110.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	MES	K	302	-	12,12,12	2.08	1 (8%)	15,16,16	1.77	3 (20%)
17	MES	i	101	-	12,12,12	2.12	1 (8%)	15,16,16	1.77	3 (20%)

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
17	MES	K	302	-	-	0/6/14/14	0/1/1/1
17	MES	i	101	-	-	0/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	i	101	MES	C8-S	-7.02	1.67	1.77
17	K	302	MES	C8-S	-6.84	1.67	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	i	101	MES	O3S-S-C8	2.23	109.62	104.99
17	K	302	MES	O3S-S-C8	2.42	110.01	104.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	i	101	MES	O1S-S-C8	2.65	108.74	106.87
17	K	302	MES	O2S-S-C8	3.72	109.49	106.87
17	K	302	MES	O1S-S-C8	4.08	109.75	106.87
17	i	101	MES	O2S-S-C8	4.72	110.20	106.87

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 (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, 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	6 (2%)	62	62	40, 56, 86, 130	0
1	O	250/250 (100%)	-0.46	6 (2%)	62	62	42, 63, 102, 134	0
2	B	244/258 (94%)	-0.37	9 (3%)	45	45	42, 61, 107, 153	0
2	P	244/258 (94%)	-0.33	11 (4%)	37	36	45, 64, 110, 156	0
3	C	240/254 (94%)	-0.22	14 (5%)	26	25	43, 64, 125, 148	0
3	Q	240/254 (94%)	-0.06	17 (7%)	19	17	48, 74, 144, 154	0
4	D	235/260 (90%)	-0.49	1 (0%)	93	94	42, 64, 93, 138	0
4	R	235/260 (90%)	-0.43	3 (1%)	79	79	45, 67, 102, 140	0
5	E	231/234 (98%)	-0.39	4 (1%)	73	74	48, 69, 99, 131	0
5	S	231/234 (98%)	-0.34	1 (0%)	93	94	49, 69, 102, 139	0
6	F	243/288 (84%)	-0.44	5 (2%)	67	68	43, 62, 107, 136	0
6	T	243/288 (84%)	-0.42	7 (2%)	55	55	41, 62, 102, 136	0
7	G	241/252 (95%)	-0.46	5 (2%)	67	68	39, 58, 92, 138	0
7	U	241/252 (95%)	-0.50	4 (1%)	73	74	39, 58, 91, 116	0
8	H	222/232 (95%)	-0.61	1 (0%)	91	93	40, 56, 79, 126	0
8	V	222/232 (95%)	-0.57	2 (0%)	85	86	42, 58, 81, 141	0
9	I	204/205 (99%)	-0.74	0	100	100	41, 53, 80, 102	0
9	W	204/205 (99%)	-0.72	1 (0%)	91	93	37, 54, 82, 114	0
10	J	195/198 (98%)	-0.62	2 (1%)	84	85	37, 55, 81, 140	0
10	X	195/198 (98%)	-0.61	2 (1%)	84	85	41, 57, 83, 147	0
11	K	212/212 (100%)	-0.68	1 (0%)	91	93	39, 53, 80, 106	0
11	Y	212/212 (100%)	-0.69	0	100	100	43, 56, 83, 105	0
12	L	222/222 (100%)	-0.67	0	100	100	42, 57, 82, 99	0
12	Z	222/222 (100%)	-0.67	0	100	100	40, 55, 80, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.61	4 (1%) 73 74	40, 56, 79, 121	0
13	a	233/246 (94%)	-0.60	3 (1%) 79 79	38, 53, 77, 129	0
14	N	196/196 (100%)	-0.70	0 100 100	39, 52, 79, 107	0
14	b	196/196 (100%)	-0.69	0 100 100	39, 52, 77, 104	0
15	e	1/6 (16%)	1.32	0 100 100	74, 74, 74, 74	0
15	f	1/6 (16%)	0.06	0 100 100	69, 69, 69, 69	0
15	g	1/6 (16%)	0.09	0 100 100	62, 62, 62, 62	0
15	h	1/6 (16%)	-0.41	0 100 100	71, 71, 71, 71	0
15	i	1/6 (16%)	0.29	0 100 100	73, 73, 73, 73	0
15	j	1/6 (16%)	-0.65	0 100 100	61, 61, 61, 61	0
All	All	6342/6650 (95%)	-0.51	109 (1%) 73 74	37, 59, 98, 156	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	a	233	ILE	7.6
3	C	206	LYS	7.4
8	V	222	ASP	6.6
2	B	220	ASN	6.1
2	P	219	ALA	6.1
3	Q	50	LEU	6.0
2	B	219	ALA	5.7
3	Q	49	THR	5.6
10	X	194	ASP	4.8
2	P	221	ASP	4.8
10	J	1	MET	4.7
3	C	49	THR	4.6
8	H	222	ASP	4.5
2	P	218	GLY	4.3
2	B	222	GLY	4.1
3	Q	206	LYS	4.0
2	P	59	ASP	3.9
2	P	51	VAL	3.9
3	C	239	GLN	3.9
2	B	221	ASP	3.8
10	J	194	ASP	3.8
3	C	238	LYS	3.7
3	Q	239	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
13	M	233	ILE	3.7
2	P	222	GLY	3.6
3	Q	238	LYS	3.6
8	V	221	CYS	3.6
3	Q	236	GLN	3.6
3	Q	203	THR	3.5
5	E	202	ASP	3.5
6	T	2	THR	3.4
2	P	220	ASN	3.3
6	T	243	ILE	3.3
4	D	242	GLU	3.2
9	W	1	SER	3.2
3	C	236	GLN	3.2
5	S	202	ASP	3.2
7	G	2	GLY	3.2
2	B	51	VAL	3.2
7	G	240	ALA	3.1
2	B	218	GLY	3.1
6	T	205	GLU	3.1
3	C	225	GLU	3.1
1	A	1	MET	3.1
3	Q	240	GLU	3.0
1	O	231	LYS	3.0
13	a	1	THR	2.9
3	C	50	LEU	2.9
6	T	244	ASN	2.9
2	P	223	GLU	2.9
13	a	232	LYS	2.9
3	Q	48	SER	2.8
3	Q	175	LYS	2.8
1	A	231	LYS	2.8
4	R	242	GLU	2.7
3	Q	51	LYS	2.7
10	X	1	MET	2.7
1	O	201	GLU	2.7
6	F	202	ASP	2.7
1	O	1	MET	2.6
6	F	181	GLU	2.6
13	M	1	THR	2.6
13	M	216	ASN	2.6
3	Q	202	GLN	2.5
3	C	205	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	Q	187	GLU	2.5
13	M	232	LYS	2.5
2	B	50	LYS	2.5
4	R	241	ALA	2.5
7	G	3	TYR	2.5
1	O	52	SER	2.4
7	G	242	GLN	2.4
7	G	241	GLU	2.4
7	U	206	GLY	2.4
1	A	249	ALA	2.4
4	R	125	LEU	2.4
3	C	202	GLN	2.4
3	C	240	GLU	2.4
1	A	250	LEU	2.4
1	O	250	LEU	2.4
3	Q	237	GLU	2.3
2	P	225	TYR	2.3
6	T	181	GLU	2.3
2	P	240	LYS	2.3
7	U	2	GLY	2.3
3	Q	180	LYS	2.3
2	P	50	LYS	2.2
7	U	241	GLU	2.2
6	T	180	PRO	2.2
5	E	54	GLU	2.2
1	A	201	GLU	2.2
3	C	180	LYS	2.2
3	Q	235	GLU	2.2
2	B	217	LYS	2.1
1	A	248	GLU	2.1
3	C	216	ASP	2.1
2	B	60	THR	2.1
3	C	203	THR	2.1
3	C	175	LYS	2.1
7	U	222	ASP	2.1
11	K	212	GLY	2.1
1	O	249	ALA	2.1
6	F	178	HIS	2.1
5	E	201	ARG	2.1
6	F	244	ASN	2.1
6	T	182	GLY	2.0
5	E	217	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	Q	141	ASP	2.0
6	F	182	GLY	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
15	NLE	j	5	8/9	0.95	0.15	-	52,53,59,59	0
15	NLE	e	5	8/9	0.93	0.17	-	59,62,75,85	0
15	NLE	g	5	8/9	0.92	0.22	-	44,45,52,52	0
15	NLE	i	5	8/9	0.95	0.16	-	47,49,54,55	0
15	NLE	f	5	8/9	0.95	0.15	-	50,50,60,60	0
15	NLE	h	5	8/9	0.94	0.19	-	62,69,72,77	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
18	CL	b	201	1/1	0.97	0.33	14.51	30,30,30,30	0
18	CL	N	202	1/1	0.95	0.30	11.29	30,30,30,30	0
17	MES	i	101	12/12	0.91	0.25	6.51	69,80,94,95	0
17	MES	K	302	12/12	0.92	0.23	5.45	74,86,98,98	0
16	MG	G	301	1/1	0.93	0.18	1.03	64,64,64,64	0
16	MG	I	301	1/1	0.98	0.14	0.51	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
16	MG	I	302	1/1	0.99	0.13	0.34	65,65,65,65	0
16	MG	Z	301	1/1	0.96	0.13	-0.10	60,60,60,60	0
16	MG	N	201	1/1	0.95	0.11	-0.30	61,61,61,61	0
16	MG	K	301	1/1	0.97	0.08	-1.33	63,63,63,63	0
16	MG	L	301	1/1	0.98	0.08	-1.44	81,81,81,81	0

6.5 Other polymers

There are no such residues in this entry.