



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:47 am GMT

PDB ID : 5L52
Title : Yeast 20S proteasome in complex with epoxyketone inhibitor 14
Authors : Groll, M.; Huber, E.M.
Deposited on : 2016-05-27
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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

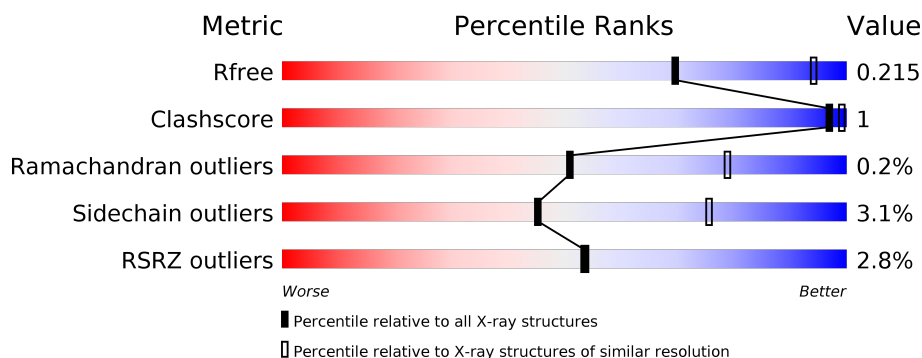
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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 $\leq 5\%$. 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	<div> <div>3%</div> <div>98%</div> <div>•</div> </div>
1	O	250	<div> <div>4%</div> <div>99%</div> <div>•</div> </div>
2	B	258	<div> <div>5%</div> <div>90%</div> <div>• • 5%</div> </div>
2	P	258	<div> <div>5%</div> <div>90%</div> <div>• • 5%</div> </div>
3	C	254	<div> <div>6%</div> <div>90%</div> <div>• • 6%</div> </div>
3	Q	254	<div> <div>10%</div> <div>89%</div> <div>• • 6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MG	X	201	-	-	-	X
15	MG	Z	301	-	-	-	X
17	6N5	N	201	-	-	-	X
17	6N5	b	201	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49836 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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	225	Total	C	N	O	S	0	0	0
			1761	1114	301	339	7			
13	a	225	Total	C	N	O	S	0	0	0
			1761	1114	301	339	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	K	2	Total	Mg	0	0
			2	2		

Continued on next page...

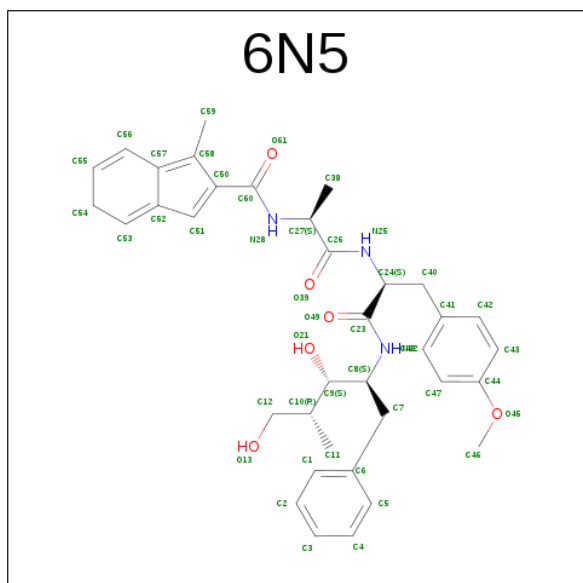
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	I	2	Total	Mg	0	0
			2	2		
15	Z	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		
15	X	1	Total	Mg	0	0
			1	1		
15	Y	1	Total	Mg	0	0
			1	1		
15	L	1	Total	Mg	0	0
			1	1		

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

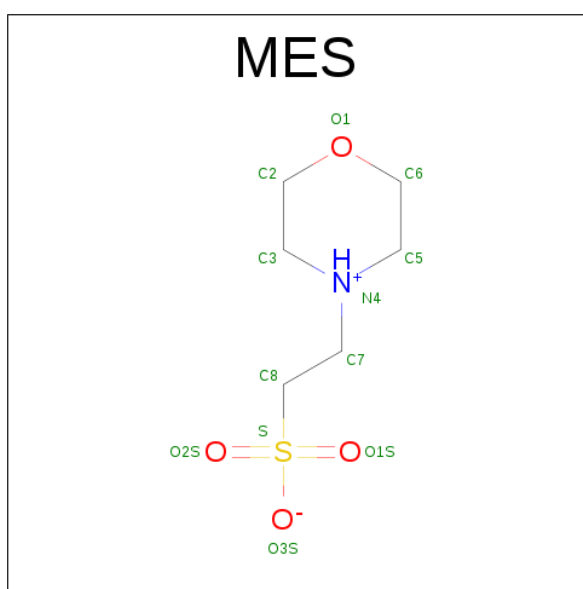
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Cl	0	0
			1	1		
16	U	1	Total	Cl	0	0
			1	1		

- Molecule 17 is {N}-[(2 {S})-1-[(2 {S})-3-(4-methoxyphenyl)-1-[(2 {S},3 {S},4 {R})-4-methyl-3,5-bis(oxidanyl)-1-phenyl-pentan-2-yl]amino]-1-oxidanylidene-propan-2-yl]amino]-1-oxidanylidene-propan-2-yl]-1-methyl-5 {H}-indene-2-carboxamide (three-letter code: 6N5) (formula: C₃₆H₄₃N₃O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	K	1	Total	C	N	O	0	0
			45	36	3	6		
17	N	1	Total	C	N	O	0	0
			45	36	3	6		
17	Y	1	Total	C	N	O	0	0
			45	36	3	6		
17	b	1	Total	C	N	O	0	0
			45	36	3	6		

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	14	Total	O	0	0
			14	14		
19	B	21	Total	O	0	0
			21	21		
19	C	13	Total	O	0	0
			13	13		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	D	9	Total O 9 9	0	0
19	E	6	Total O 6 6	0	0
19	F	11	Total O 11 11	0	0
19	G	21	Total O 21 21	0	0
19	H	20	Total O 20 20	0	0
19	I	18	Total O 18 18	0	0
19	J	26	Total O 26 26	0	0
19	K	28	Total O 28 28	0	0
19	L	21	Total O 21 21	0	0
19	M	16	Total O 16 16	0	0
19	N	16	Total O 16 16	0	0
19	O	8	Total O 8 8	0	0
19	P	14	Total O 14 14	0	0
19	Q	11	Total O 11 11	0	0
19	R	3	Total O 3 3	0	0
19	S	4	Total O 4 4	0	0
19	T	17	Total O 17 17	0	0
19	U	14	Total O 14 14	0	0
19	V	19	Total O 19 19	0	0
19	W	20	Total O 20 20	0	0
19	X	23	Total O 23 23	0	0

Continued on next page...

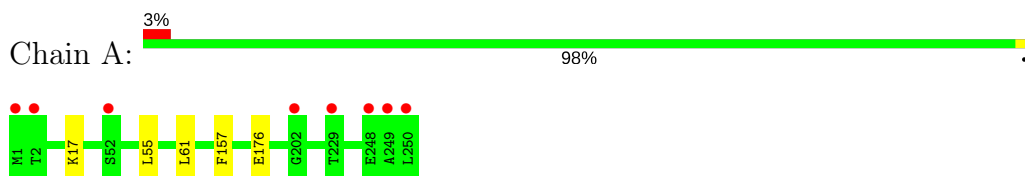
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	Y	14	Total 14	O 14	0	0
19	Z	26	Total 26	O 26	0	0
19	a	22	Total 22	O 22	0	0
19	b	15	Total 15	O 15	0	0

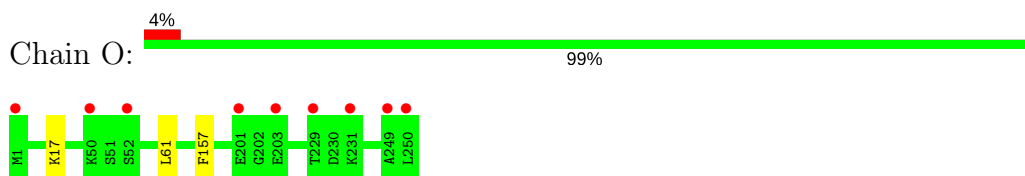
3 Residue-property plots [i](#)

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

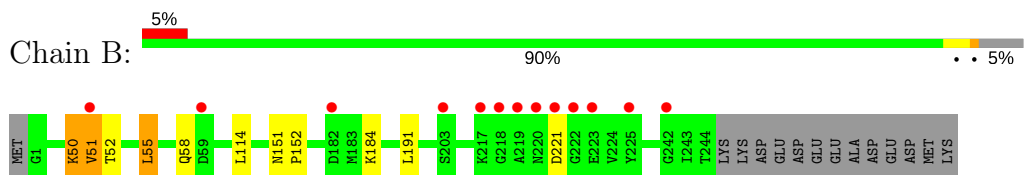
- Molecule 1: Proteasome subunit alpha type-2



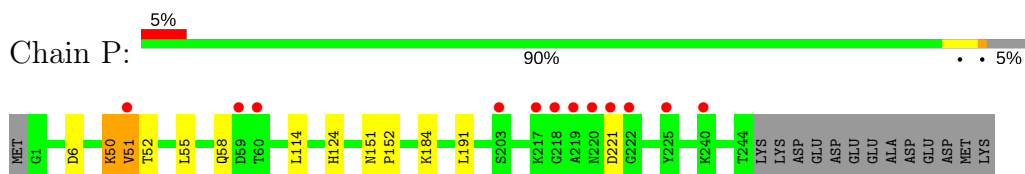
- Molecule 1: Proteasome subunit alpha type-2



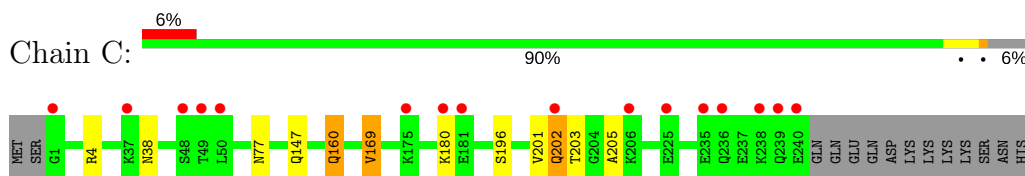
- Molecule 2: Proteasome subunit alpha type-3



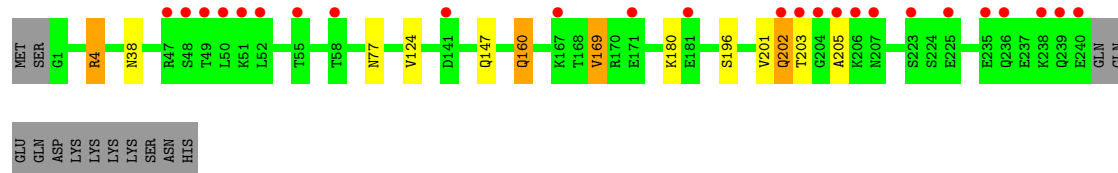
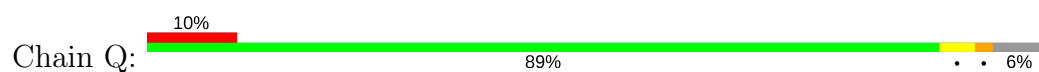
- Molecule 2: Proteasome subunit alpha type-3



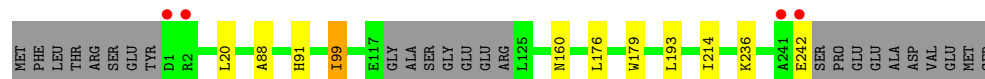
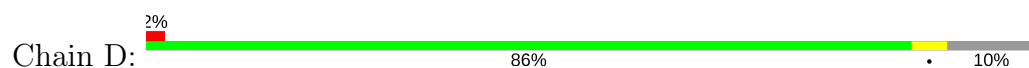
- Molecule 3: Proteasome subunit alpha type-4



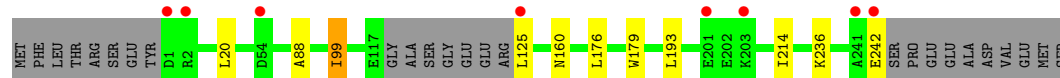
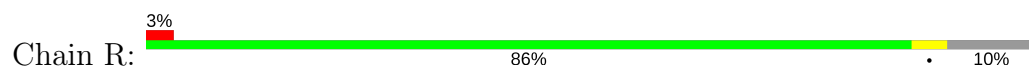
- Molecule 3: Proteasome subunit alpha type-4



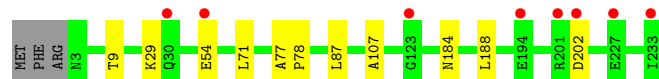
• Molecule 4: Proteasome subunit alpha type-5



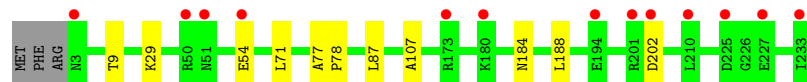
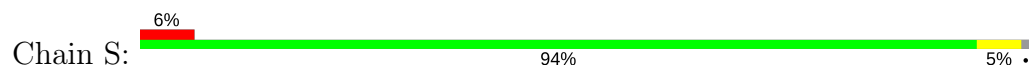
• Molecule 4: Proteasome subunit alpha type-5



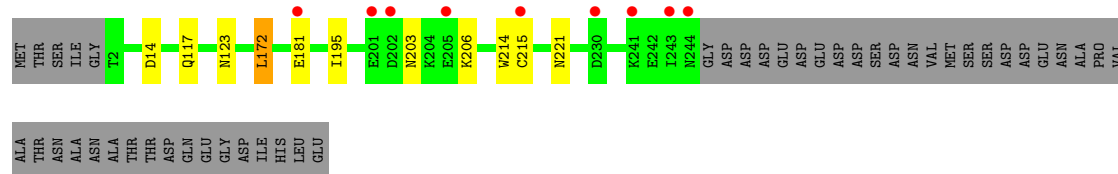
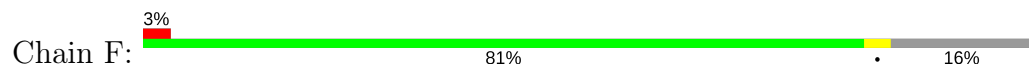
• Molecule 5: Proteasome subunit alpha type-6



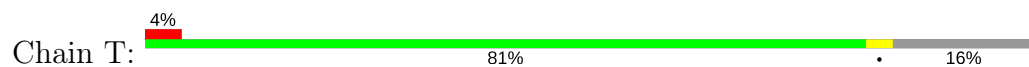
• Molecule 5: Proteasome subunit alpha type-6

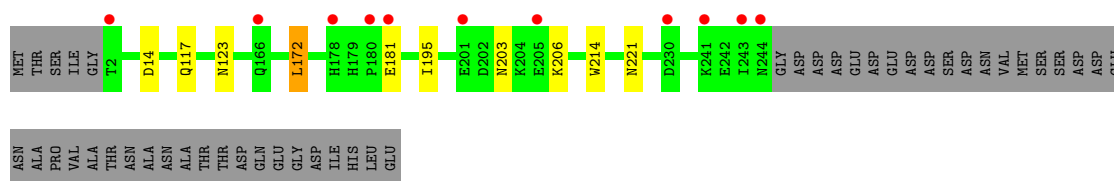


• Molecule 6: Probable proteasome subunit alpha type-7

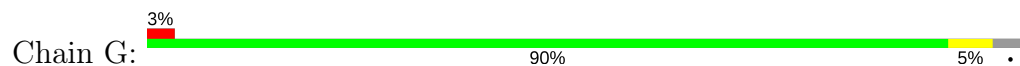


• Molecule 6: Probable proteasome subunit alpha type-7

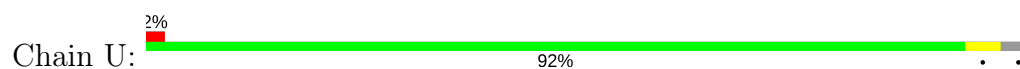




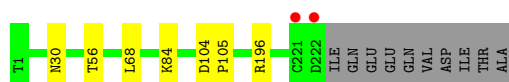
- Molecule 7: Proteasome subunit alpha type-1



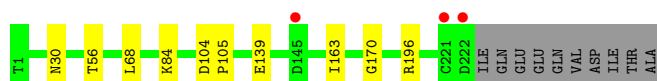
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2



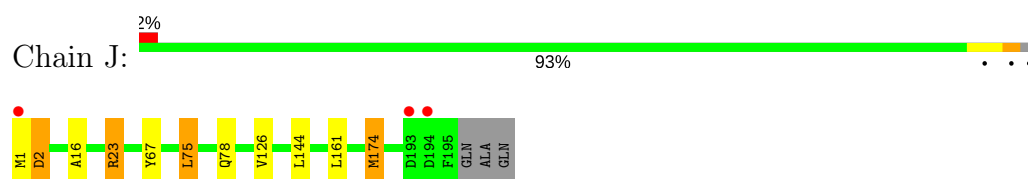
- Molecule 9: Proteasome subunit beta type-3



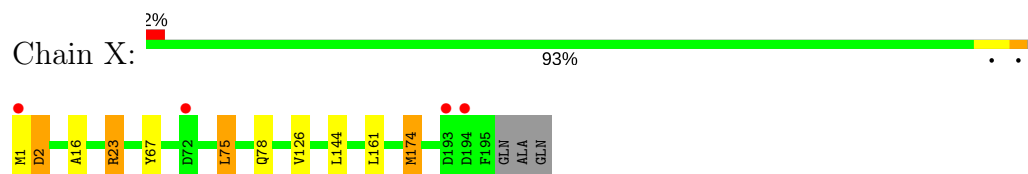
- Molecule 9: Proteasome subunit beta type-3



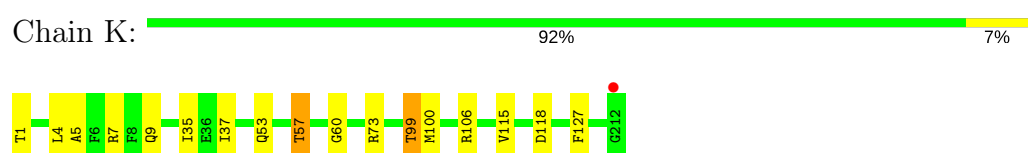
- Molecule 10: Proteasome subunit beta type-4



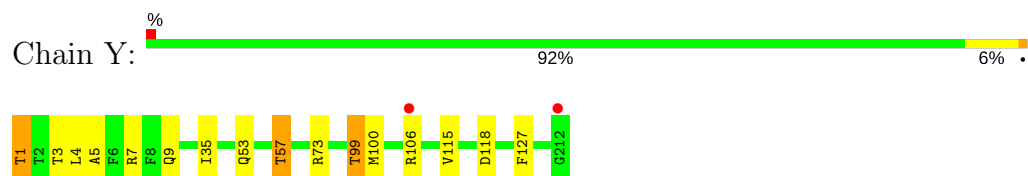
- Molecule 10: Proteasome subunit beta type-4



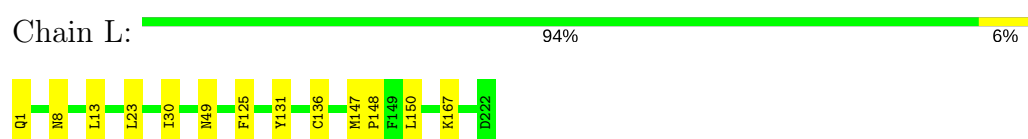
- Molecule 11: Proteasome subunit beta type-5



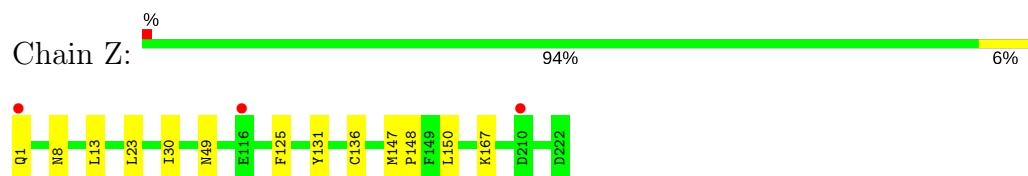
- Molecule 11: Proteasome subunit beta type-5



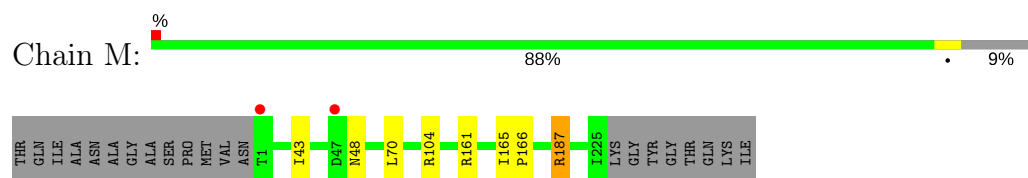
- Molecule 12: Proteasome subunit beta type-6



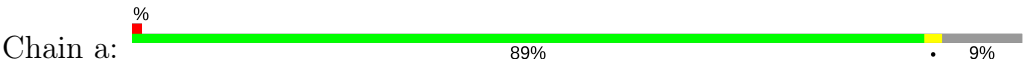
- Molecule 12: Proteasome subunit beta type-6



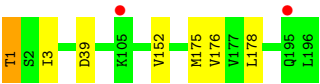
- Molecule 13: Proteasome subunit beta type-7



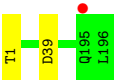
- Molecule 13: Proteasome subunit beta type-7



• Molecule 14: Proteasome subunit beta type-1



• Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.44Å 300.22Å 144.34Å 90.00° 112.98° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.8 (15.00-2.70) 96.8 (15.00-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.186 , 0.210 0.192 , 0.215	Depositor DCC
R_{free} test set	13930 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.0	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	0.95	EDS
Total number of atoms	49836	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 6N5, MES, CL

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	0.27	0/1952	0.47	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.48	0/2618
2	P	0.27	0/1934	0.48	0/2618
3	C	0.27	0/1910	0.50	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.27	0/1837	0.47	0/2475
4	R	0.27	0/1837	0.47	0/2475
5	E	0.27	0/1800	0.46	0/2433
5	S	0.26	0/1800	0.46	0/2433
6	F	0.27	0/1932	0.44	0/2609
6	T	0.26	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.27	0/1945	0.47	0/2634
8	H	0.25	0/1715	0.48	0/2326
8	V	0.25	0/1715	0.48	0/2326
9	I	0.31	1/1611 (0.1%)	0.70	2/2174 (0.1%)
9	W	0.33	1/1611 (0.1%)	0.70	3/2174 (0.1%)
10	J	0.26	0/1589	0.49	0/2142
10	X	0.26	0/1589	0.49	0/2142
11	K	0.28	0/1681	0.52	1/2274 (0.0%)
11	Y	0.27	0/1681	0.52	1/2274 (0.0%)
12	L	0.27	0/1795	0.47	0/2420
12	Z	0.29	0/1795	0.48	0/2420
13	M	0.27	0/1791	0.52	0/2431
13	a	0.26	0/1791	0.52	0/2431
14	N	0.25	0/1541	0.50	1/2087 (0.0%)
14	b	0.25	0/1541	0.50	1/2087 (0.0%)
All	All	0.27	2/50066 (0.0%)	0.50	9/67702 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	126	ILE	CB-CG2	-6.91	1.31	1.52
9	I	126	ILE	CB-CG2	-5.52	1.35	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	126	ILE	CG1-CB-CG2	-20.20	66.95	111.40
9	W	126	ILE	CG1-CB-CG2	-17.71	72.43	111.40
9	W	126	ILE	CA-CB-CG1	11.58	133.01	111.00
9	I	126	ILE	CA-CB-CG1	9.60	129.23	111.00
14	N	1	THR	N-CA-C	5.42	125.64	111.00
9	W	126	ILE	CB-CA-C	-5.42	100.76	111.60
14	b	1	THR	N-CA-C	5.38	125.52	111.00
11	Y	1	THR	N-CA-C	5.05	124.65	111.00
11	K	1	THR	N-CA-C	5.03	124.57	111.00

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	2	0
1	O	1915	0	1929	0	0
2	B	1904	0	1904	4	0
2	P	1904	0	1904	5	0
3	C	1881	0	1895	4	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	2	0
5	E	1773	0	1775	2	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	2	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	2	0
8	H	1684	0	1688	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	V	1684	0	1688	3	0
9	I	1581	0	1574	10	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	6	0
10	X	1561	0	1569	6	0
11	K	1644	0	1592	8	0
11	Y	1644	0	1592	8	0
12	L	1757	0	1711	4	0
12	Z	1757	0	1711	4	0
13	M	1761	0	1765	2	0
13	a	1761	0	1765	0	0
14	N	1512	0	1478	3	0
14	b	1512	0	1478	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	K	2	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	X	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	K	45	0	0	1	0
17	N	45	0	0	0	0
17	Y	45	0	0	0	0
17	b	45	0	0	0	0
18	K	12	0	13	1	0
18	Y	12	0	13	1	0
19	A	14	0	0	0	0
19	B	21	0	0	0	0
19	C	13	0	0	0	0
19	D	9	0	0	0	0
19	E	6	0	0	0	0
19	F	11	0	0	1	0
19	G	21	0	0	0	0
19	H	20	0	0	0	0
19	I	18	0	0	0	0
19	J	26	0	0	0	0
19	K	28	0	0	0	0
19	L	21	0	0	0	0
19	M	16	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	N	16	0	0	0	0
19	O	8	0	0	0	0
19	P	14	0	0	0	0
19	Q	11	0	0	0	0
19	R	3	0	0	0	0
19	S	4	0	0	0	0
19	T	17	0	0	0	0
19	U	14	0	0	0	0
19	V	19	0	0	0	0
19	W	20	0	0	0	0
19	X	23	0	0	0	0
19	Y	14	0	0	0	0
19	Z	26	0	0	0	0
19	a	22	0	0	0	0
19	b	15	0	0	0	0
All	All	49836	0	48948	93	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 1.

All (93) 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)
11:Y:53:GLN:O	11:Y:57:THR:OG1	2.09	0.71
10:J:1:MET:O	10:J:2:ASP:HB2	1.92	0.69
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.75	0.69
11:K:53:GLN:O	11:K:57:THR:OG1	2.11	0.68
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.75	0.67
10:X:1:MET:O	10:X:2:ASP:HB2	1.92	0.67
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.80	0.64
9:I:98:ARG:HD2	9:I:126:ILE:HD11	1.79	0.63
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.81	0.63
14:N:152:VAL:HA	14:N:175:MET:HE1	1.81	0.62
9:W:98:ARG:HD2	9:W:126:ILE:HD12	1.83	0.60
11:K:99:THR:HG22	11:K:115:VAL:HB	1.84	0.59
11:Y:99:THR:HG22	11:Y:115:VAL:HB	1.85	0.59
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.40	0.56
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.41	0.55
11:Y:73:ARG:HH11	11:Y:73:ARG:HG2	1.72	0.55
10:J:23:ARG:NH2	18:K:304:MES:O1	2.40	0.54
11:K:73:ARG:HG2	11:K:73:ARG:HH11	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:98:ARG:HD2	9:I:126:ILE:CD1	2.39	0.53
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.90	0.53
10:J:174:MET:HA	10:X:174:MET:HA	1.90	0.53
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.92	0.51
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.51
7:U:23:PHE:O	7:U:26:THR:HB	2.11	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.50
9:I:98:ARG:NH2	9:I:126:ILE:HD11	2.26	0.50
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.94	0.50
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.94	0.49
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.93	0.49
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.93	0.49
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.93	0.49
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.93	0.49
6:F:215:CYS:HB3	19:F:301:HOH:O	2.12	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.46
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.98	0.45
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.98	0.45
9:I:98:ARG:CD	9:I:126:ILE:HD11	2.46	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.45
9:I:98:ARG:CZ	9:I:126:ILE:HD11	2.46	0.45
12:L:8:ASN:HA	12:L:30:ILE:O	2.17	0.45
14:N:1:THR:CG2	14:N:3:ILE:HG23	2.46	0.44
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.48	0.44
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.99	0.44
11:K:5:ALA:HB3	11:K:100:MET:CE	2.47	0.44
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.99	0.44
11:K:100:MET:CE	11:K:127:PHE:HB2	2.48	0.44
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.17	0.44
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.00	0.43
1:A:176:GLU:HG2	2:B:55:LEU:HD13	2.00	0.43
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.48	0.43
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.01	0.43
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.43
3:C:201:VAL:HG13	3:C:202:GLN:N	2.33	0.43
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.01	0.43
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.48	0.43
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.33	0.43
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.00	0.43
2:P:50:LYS:O	2:P:51:VAL:C	2.57	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.54	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.50	0.43
10:X:23:ARG:NH2	18:Y:303:MES:O1	2.51	0.43
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.01	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.43
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.42
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.48	0.42
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.55	0.42
5:S:77:ALA:N	5:S:78:PRO:CD	2.83	0.42
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.85	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.42
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.35	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.55	0.41
2:B:50:LYS:O	2:B:51:VAL:C	2.58	0.41
8:V:163:ILE:HG23	8:V:170:GLY:HA2	2.02	0.41
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.01	0.41
1:A:55:LEU:HD12	7:G:170:THR:HG23	2.03	0.41
12:L:147:MET:N	12:L:148:PRO:HD2	2.35	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.03	0.41
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.85	0.41
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.02	0.41
11:Y:1:THR:CG2	11:Y:3:THR:HG23	2.51	0.41
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.02	0.41
17:K:301:6N5:C48	17:K:301:6N5:N25	2.84	0.41
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.04	0.41
2:P:6:ASP:OD2	3:Q:4:ARG:HG3	2.20	0.41
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.03	0.40
11:K:37:ILE:HG23	11:K:60:GLY:HA2	2.03	0.40
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.03	0.40
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.52	0.40
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.51	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%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
2	B	242/258 (94%)	235 (97%)	5 (2%)	2 (1%)	22	49
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	22	49
3	C	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	22	49
3	Q	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	22	49
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
8	V	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	32	60
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	32	60
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
12	Z	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
13	M	223/246 (91%)	216 (97%)	7 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	223/246 (91%)	216 (97%)	7 (3%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
All	All	6260/6614 (95%)	6098 (97%)	152 (2%)	10 (0%)	51	79

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
10	J	2	ASP
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
3	C	205	ALA
3	Q	205	ALA
2	B	221	ASP
2	P	221	ASP

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%)	206 (99%)	3 (1%)	71	90
1	O	209/209 (100%)	206 (99%)	3 (1%)	71	90
2	B	203/216 (94%)	196 (97%)	7 (3%)	42	73
2	P	203/216 (94%)	196 (97%)	7 (3%)	42	73
3	C	212/226 (94%)	204 (96%)	8 (4%)	38	68
3	Q	212/226 (94%)	204 (96%)	8 (4%)	38	68
4	D	194/215 (90%)	187 (96%)	7 (4%)	40	70
4	R	194/215 (90%)	186 (96%)	8 (4%)	35	66
5	E	190/193 (98%)	183 (96%)	7 (4%)	39	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	190/193 (98%)	183 (96%)	7 (4%)	39	70
6	F	201/239 (84%)	192 (96%)	9 (4%)	32	62
6	T	201/239 (84%)	192 (96%)	9 (4%)	32	62
7	G	206/210 (98%)	200 (97%)	6 (3%)	48	77
7	U	206/210 (98%)	200 (97%)	6 (3%)	48	77
8	H	181/190 (95%)	176 (97%)	5 (3%)	49	79
8	V	181/190 (95%)	176 (97%)	5 (3%)	49	79
9	I	172/173 (99%)	168 (98%)	4 (2%)	56	84
9	W	172/173 (99%)	168 (98%)	4 (2%)	56	84
10	J	173/175 (99%)	168 (97%)	5 (3%)	48	77
10	X	173/175 (99%)	168 (97%)	5 (3%)	48	77
11	K	169/169 (100%)	161 (95%)	8 (5%)	30	60
11	Y	169/169 (100%)	161 (95%)	8 (5%)	30	60
12	L	185/185 (100%)	180 (97%)	5 (3%)	50	80
12	Z	185/185 (100%)	180 (97%)	5 (3%)	50	80
13	M	193/208 (93%)	187 (97%)	6 (3%)	45	75
13	a	193/208 (93%)	187 (97%)	6 (3%)	45	75
14	N	162/162 (100%)	161 (99%)	1 (1%)	89	97
14	b	162/162 (100%)	161 (99%)	1 (1%)	89	97
All	All	5300/5540 (96%)	5137 (97%)	163 (3%)	45	75

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
2	B	50	LYS
2	B	52	THR
2	B	55	LEU
2	B	58	GLN
2	B	114	LEU
2	B	184	LYS
2	B	191	LEU
3	C	4	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	203	THR
4	D	20	LEU
4	D	99	ILE
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP
6	F	117	GLN
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	115	LEU
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	56	THR
8	H	68	LEU
8	H	84	LYS
8	H	196	ARG
9	I	37	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	126	ILE
9	I	171	LEU
9	I	182	TRP
10	J	23	ARG
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	7	ARG
11	K	9	GLN
11	K	35	ILE
11	K	57	THR
11	K	99	THR
11	K	106	ARG
11	K	118	ASP
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	136	CYS
12	L	167	LYS
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	39	ASP
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	52	THR
2	P	55	LEU
2	P	58	GLN
2	P	114	LEU
2	P	184	LYS
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	203	THR
4	R	20	LEU
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	14	ASP
6	T	117	GLN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	115	LEU
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	56	THR
8	V	68	LEU
8	V	84	LYS
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	W	182	TRP
10	X	23	ARG
10	X	75	LEU
10	X	78	GLN
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	7	ARG
11	Y	9	GLN
11	Y	35	ILE
11	Y	57	THR
11	Y	99	THR
11	Y	106	ARG
11	Y	118	ASP
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	136	CYS
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	39	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	38	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	91	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	70	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	38	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	S	184	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
10	X	55	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	70	ASN
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	6N5	K	301	11	48,48,48	1.75	8 (16%)	55,66,66	1.27	8 (14%)
18	MES	K	304	-	12,12,12	2.27	1 (8%)	14,16,16	1.63	2 (14%)
17	6N5	N	201	14	48,48,48	1.79	9 (18%)	55,66,66	1.45	10 (18%)
17	6N5	Y	301	11	48,48,48	1.77	9 (18%)	55,66,66	1.29	9 (16%)
18	MES	Y	303	-	12,12,12	2.22	1 (8%)	14,16,16	1.81	2 (14%)
17	6N5	b	201	14	48,48,48	1.76	9 (18%)	55,66,66	1.46	10 (18%)

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	6N5	K	301	11	-	0/44/67/67	0/4/4/4
18	MES	K	304	-	-	0/6/14/14	0/1/1/1
17	6N5	N	201	14	-	0/44/67/67	0/4/4/4
17	6N5	Y	301	11	-	0/44/67/67	0/4/4/4
18	MES	Y	303	-	-	0/6/14/14	0/1/1/1
17	6N5	b	201	14	-	0/44/67/67	0/4/4/4

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	304	MES	C8-S	-7.59	1.66	1.77
18	Y	303	MES	C8-S	-7.39	1.66	1.77
17	K	301	6N5	C40-C41	-4.30	1.41	1.51
17	Y	301	6N5	C40-C41	-4.26	1.41	1.51
17	b	201	6N5	C40-C41	-4.21	1.41	1.51
17	N	201	6N5	C40-C41	-4.18	1.41	1.51
17	Y	301	6N5	C50-C60	-4.09	1.35	1.50
17	K	301	6N5	C50-C60	-4.04	1.35	1.50
17	Y	301	6N5	C57-C52	-3.71	1.34	1.46
17	N	201	6N5	C50-C60	-3.67	1.37	1.50
17	b	201	6N5	C50-C60	-3.67	1.37	1.50
17	K	301	6N5	C57-C52	-3.66	1.34	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	201	6N5	C7-C6	-3.66	1.42	1.51
17	N	201	6N5	C7-C6	-3.66	1.42	1.51
17	b	201	6N5	C57-C52	-3.63	1.34	1.46
17	N	201	6N5	C57-C52	-3.63	1.34	1.46
17	Y	301	6N5	C7-C6	-3.61	1.42	1.51
17	K	301	6N5	C7-C6	-3.61	1.42	1.51
17	N	201	6N5	C54-C53	-2.97	1.39	1.49
17	b	201	6N5	C54-C53	-2.97	1.39	1.49
17	Y	301	6N5	C54-C53	-2.96	1.39	1.49
17	K	301	6N5	C54-C53	-2.93	1.39	1.49
17	K	301	6N5	C56-C57	-2.41	1.34	1.40
17	Y	301	6N5	C56-C57	-2.40	1.34	1.40
17	N	201	6N5	C56-C57	-2.16	1.35	1.40
17	b	201	6N5	C56-C57	-2.15	1.35	1.40
17	Y	301	6N5	C57-C58	-2.03	1.33	1.37
17	N	201	6N5	C27-N28	2.05	1.50	1.46
17	b	201	6N5	C27-N28	2.16	1.50	1.46
17	Y	301	6N5	C56-C55	2.17	1.39	1.33
17	K	301	6N5	C56-C55	2.19	1.39	1.33
17	b	201	6N5	C56-C55	2.42	1.40	1.33
17	N	201	6N5	C56-C55	2.43	1.40	1.33
17	b	201	6N5	C10-C9	5.77	1.64	1.53
17	K	301	6N5	C10-C9	5.98	1.64	1.53
17	Y	301	6N5	C10-C9	6.21	1.64	1.53
17	N	201	6N5	C10-C9	6.23	1.64	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	201	6N5	C11-C10-C12	-4.94	103.64	109.87
17	b	201	6N5	C11-C10-C12	-4.89	103.70	109.87
17	b	201	6N5	C26-C27-N28	-3.20	103.71	111.65
17	N	201	6N5	C26-C27-N28	-3.19	103.73	111.65
17	Y	301	6N5	C41-C40-C24	-3.16	104.55	113.41
17	K	301	6N5	C41-C40-C24	-3.16	104.58	113.41
17	Y	301	6N5	O13-C12-C10	-3.09	105.20	111.51
17	K	301	6N5	O13-C12-C10	-2.99	105.40	111.51
17	N	201	6N5	C59-C58-C57	-2.58	121.93	128.47
17	b	201	6N5	C59-C58-C57	-2.56	121.98	128.47
17	b	201	6N5	O13-C12-C10	-2.50	106.40	111.51
17	Y	301	6N5	C59-C58-C57	-2.50	122.14	128.47
17	K	301	6N5	C59-C58-C57	-2.48	122.19	128.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	201	6N5	C7-C6-C1	-2.38	116.10	120.91
17	N	201	6N5	C7-C6-C1	-2.35	116.16	120.91
17	K	301	6N5	C7-C6-C1	-2.24	116.38	120.91
17	N	201	6N5	O13-C12-C10	-2.19	107.05	111.51
17	Y	301	6N5	C7-C6-C1	-2.16	116.55	120.91
17	Y	301	6N5	C7-C8-N22	-2.14	107.66	110.17
17	N	201	6N5	C40-C24-N25	-2.14	106.28	110.80
17	b	201	6N5	C40-C24-N25	-2.07	106.41	110.80
17	Y	301	6N5	C46-O45-C44	-2.04	113.05	117.50
17	K	301	6N5	C7-C8-N22	-2.02	107.80	110.17
17	N	201	6N5	C53-C54-C55	2.01	118.06	113.83
17	b	201	6N5	C53-C54-C55	2.02	118.07	113.83
17	Y	301	6N5	C53-C54-C55	2.23	118.52	113.83
17	K	301	6N5	C53-C54-C55	2.25	118.55	113.83
17	N	201	6N5	C38-C27-N28	2.26	114.61	110.34
17	b	201	6N5	C38-C27-N28	2.27	114.63	110.34
17	K	301	6N5	C7-C6-C5	2.53	126.02	120.91
17	Y	301	6N5	C7-C6-C5	2.55	126.05	120.91
17	N	201	6N5	C7-C6-C5	2.59	126.14	120.91
17	b	201	6N5	C7-C6-C5	2.67	126.29	120.91
17	K	301	6N5	C50-C60-N28	2.88	118.94	116.00
17	Y	301	6N5	C50-C60-N28	3.09	119.15	116.00
18	K	304	MES	O2S-S-C8	3.24	109.58	106.79
18	K	304	MES	O3S-S-C8	3.93	110.89	106.06
18	Y	303	MES	O2S-S-C8	4.19	110.39	106.79
18	Y	303	MES	O3S-S-C8	4.26	111.30	106.06
17	b	201	6N5	C27-N28-C60	4.74	128.59	121.33
17	N	201	6N5	C27-N28-C60	4.86	128.78	121.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	301	6N5	1	0
18	K	304	MES	1	0
18	Y	303	MES	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	250/250 (100%)	-0.26	8 (3%)	48	48	42, 55, 98, 147	0
1	O	250/250 (100%)	-0.24	9 (3%)	43	42	45, 64, 105, 151	0
2	B	244/258 (94%)	-0.07	13 (5%)	27	25	40, 61, 111, 169	0
2	P	244/258 (94%)	-0.09	12 (4%)	30	29	42, 65, 110, 159	0
3	C	240/254 (94%)	-0.04	16 (6%)	19	16	39, 65, 126, 153	0
3	Q	240/254 (94%)	0.26	25 (10%)	7	5	46, 80, 167, 208	0
4	D	235/260 (90%)	-0.25	4 (1%)	70	72	40, 64, 96, 143	0
4	R	235/260 (90%)	-0.19	8 (3%)	46	45	46, 70, 113, 164	0
5	E	231/234 (98%)	-0.17	8 (3%)	44	44	44, 69, 105, 149	0
5	S	231/234 (98%)	0.02	13 (5%)	25	23	49, 80, 133, 171	0
6	F	243/288 (84%)	-0.30	9 (3%)	42	41	38, 63, 113, 148	0
6	T	243/288 (84%)	-0.14	11 (4%)	34	32	43, 73, 132, 167	0
7	G	241/252 (95%)	-0.31	7 (2%)	52	52	37, 58, 100, 145	0
7	U	241/252 (95%)	-0.31	4 (1%)	70	72	43, 60, 96, 132	0
8	H	222/232 (95%)	-0.20	2 (0%)	84	85	42, 58, 89, 125	0
8	V	222/232 (95%)	-0.17	3 (1%)	75	76	45, 61, 89, 128	0
9	I	204/205 (99%)	-0.61	1 (0%)	90	92	35, 50, 80, 104	0
9	W	204/205 (99%)	-0.54	2 (0%)	82	82	36, 53, 82, 108	0
10	J	195/198 (98%)	-0.46	3 (1%)	74	75	35, 51, 80, 120	0
10	X	195/198 (98%)	-0.46	4 (2%)	64	65	37, 53, 84, 132	0
11	K	212/212 (100%)	-0.54	1 (0%)	90	92	30, 51, 76, 99	0
11	Y	212/212 (100%)	-0.48	2 (0%)	84	85	25, 53, 81, 109	0
12	L	222/222 (100%)	-0.52	0	100	100	33, 53, 83, 102	0
12	Z	222/222 (100%)	-0.44	3 (1%)	75	76	34, 56, 85, 105	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	M	225/246 (91%)	-0.51	2 (0%)	84	85	31, 55, 82, 108	0
13	a	225/246 (91%)	-0.44	3 (1%)	77	78	33, 56, 83, 118	0
14	N	196/196 (100%)	-0.47	2 (1%)	82	82	30, 52, 82, 107	0
14	b	196/196 (100%)	-0.49	1 (0%)	90	92	30, 53, 85, 109	0
All	All	6320/6614 (95%)	-0.29	176 (2%)	53	54	25, 60, 109, 208	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	219	ALA	10.6
2	P	219	ALA	10.4
8	V	222	ASP	10.2
2	B	220	ASN	9.6
8	H	222	ASP	8.6
2	B	221	ASP	8.1
2	P	220	ASN	7.9
3	Q	50	LEU	7.1
1	O	1	MET	6.4
2	P	218	GLY	6.3
3	Q	206	LYS	6.1
2	P	222	GLY	5.9
1	A	1	MET	5.9
10	X	1	MET	5.8
8	H	221	CYS	5.7
3	Q	49	THR	5.7
1	O	249	ALA	5.6
3	Q	48	SER	5.4
8	V	221	CYS	5.4
10	J	1	MET	5.4
2	B	51	VAL	5.3
5	E	202	ASP	5.3
3	Q	239	GLN	5.2
2	P	221	ASP	5.2
4	D	242	GLU	5.2
5	S	202	ASP	5.1
4	R	241	ALA	4.9
2	P	51	VAL	4.9
6	T	2	THR	4.6
3	Q	205	ALA	4.5
3	Q	223	SER	4.5
3	Q	238	LYS	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Q	51	LYS	4.3
5	S	54	GLU	4.2
3	C	206	LYS	4.1
11	Y	212	GLY	4.1
3	Q	236	GLN	4.0
5	E	123	GLY	4.0
10	X	194	ASP	3.9
9	W	1	SER	3.9
3	C	202	GLN	3.9
3	C	238	LYS	3.8
2	B	222	GLY	3.8
3	Q	240	GLU	3.7
3	Q	202	GLN	3.7
3	C	49	THR	3.6
10	J	194	ASP	3.5
7	G	222	ASP	3.5
5	S	51	ASN	3.5
13	M	1	THR	3.4
6	F	202	ASP	3.4
7	U	222	ASP	3.4
3	Q	55	THR	3.3
2	B	242	GLY	3.3
5	S	233	ILE	3.2
7	U	242	GLN	3.2
6	T	243	ILE	3.2
6	T	181	GLU	3.2
7	G	242	GLN	3.2
3	C	239	GLN	3.1
5	S	225	ASP	3.1
5	S	3	ASN	3.1
1	A	250	LEU	3.1
6	T	244	ASN	3.1
6	F	181	GLU	3.0
3	C	225	GLU	3.0
13	a	1	THR	3.0
5	E	201	ARG	2.9
4	R	242	GLU	2.9
2	P	225	TYR	2.9
7	G	241	GLU	2.9
3	C	236	GLN	2.8
3	Q	204	GLY	2.8
6	T	230	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	F	243	ILE	2.8
11	Y	106	ARG	2.8
9	W	133	LYS	2.8
6	F	244	ASN	2.8
5	E	233	ILE	2.8
7	U	2	GLY	2.8
7	U	241	GLU	2.7
1	O	52	SER	2.7
4	D	2	ARG	2.7
4	D	241	ALA	2.7
6	T	180	PRO	2.7
10	X	193	ASP	2.7
3	C	235	GLU	2.7
3	C	50	LEU	2.7
6	T	241	LYS	2.7
13	a	225	ILE	2.7
1	O	229	THR	2.7
3	C	37	LYS	2.7
3	C	180	LYS	2.7
2	B	218	GLY	2.7
6	T	178	HIS	2.7
1	A	249	ALA	2.6
5	S	173	ARG	2.6
7	G	240	ALA	2.6
6	T	166	GLN	2.6
1	A	2	THR	2.6
10	J	193	ASP	2.6
2	B	225	TYR	2.6
1	O	201	GLU	2.6
4	R	201	GLU	2.6
11	K	212	GLY	2.5
4	R	1	ASP	2.5
6	F	201	GLU	2.5
6	T	205	GLU	2.5
3	Q	207	ASN	2.5
5	S	201	ARG	2.5
3	Q	225	GLU	2.5
14	N	105	LYS	2.5
13	a	224	ASP	2.5
3	Q	58	THR	2.4
4	R	125	LEU	2.4
1	A	248	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	1	SER	2.4
14	N	195	GLN	2.4
3	C	48	SER	2.4
2	B	223	GLU	2.4
3	Q	52	LEU	2.4
1	O	203	GLU	2.4
2	P	59	ASP	2.4
3	Q	167	LYS	2.4
13	M	47	ASP	2.4
1	A	229	THR	2.3
2	B	203	SER	2.3
4	R	54	ASP	2.3
5	S	180	LYS	2.3
7	G	3	TYR	2.3
3	Q	181	GLU	2.3
12	Z	210	ASP	2.3
4	D	1	ASP	2.3
6	F	230	ASP	2.3
12	Z	1	GLN	2.3
6	F	205	GLU	2.3
2	B	182	ASP	2.3
3	C	181	GLU	2.3
3	C	175	LYS	2.3
5	E	54	GLU	2.3
8	V	145	ASP	2.3
1	A	52	SER	2.2
5	E	30	GLN	2.2
1	O	250	LEU	2.2
6	F	215	CYS	2.2
2	P	203	SER	2.2
2	B	217	LYS	2.2
7	G	68	ARG	2.2
3	Q	235	GLU	2.2
3	Q	141	ASP	2.2
2	B	59	ASP	2.2
3	Q	171	GLU	2.2
6	F	241	LYS	2.2
2	P	217	LYS	2.2
3	C	1	GLY	2.2
4	R	203	LYS	2.1
3	C	240	GLU	2.1
5	S	194	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	Z	116	GLU	2.1
3	Q	47	ARG	2.1
7	G	188	GLU	2.1
6	T	201	GLU	2.1
10	X	72	ASP	2.1
5	E	194	GLU	2.1
2	P	60	THR	2.1
5	S	50	ARG	2.1
4	R	2	ARG	2.1
3	Q	203	THR	2.1
5	E	227	GLU	2.1
1	O	50	LYS	2.0
1	O	231	LYS	2.0
2	P	240	LYS	2.0
5	S	227	GLU	2.0
5	S	210	LEU	2.0
1	A	202	GLY	2.0
14	b	195	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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, 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	LLDF	B-factors(Å ²)	Q<0.9
15	MG	X	201	1/1	0.98	0.34	9.53	34,34,34,34	0
15	MG	Z	301	1/1	0.95	0.39	8.29	66,66,66,66	0
17	6N5	N	201	45/45	0.82	0.26	7.10	27,41,53,56	45

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
17	6N5	b	201	45/45	0.86	0.23	6.32	27,41,55,60	0
15	MG	N	202	1/1	0.93	0.16	1.26	60,60,60,60	0
15	MG	I	301	1/1	0.97	0.17	1.13	60,60,60,60	0
18	MES	K	304	12/12	0.97	0.15	1.05	34,35,41,50	12
17	6N5	Y	301	45/45	0.94	0.14	0.59	24,36,49,56	0
17	6N5	K	301	45/45	0.93	0.15	0.46	28,39,50,57	0
15	MG	G	301	1/1	0.89	0.15	0.22	61,61,61,61	0
18	MES	Y	303	12/12	0.97	0.12	0.02	32,35,36,39	12
15	MG	L	301	1/1	0.96	0.15	0.01	72,72,72,72	0
15	MG	K	302	1/1	0.98	0.06	-1.76	56,56,56,56	0
15	MG	I	302	1/1	0.98	0.07	-1.86	55,55,55,55	0
15	MG	K	303	1/1	0.94	0.18	-	46,46,46,46	0
16	CL	G	302	1/1	1.00	0.11	-	44,44,44,44	0
16	CL	U	301	1/1	0.99	0.10	-	46,46,46,46	0
15	MG	Y	302	1/1	0.98	0.08	-	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.