Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 10:20 am GMT

PDB ID	:	5L54
Title	:	Yeast 20S proteasome in complex with epoxyketone inhibitor 16
Authors	:	Groll, M.; Huber, E.M.
Deposited on	:	2016-05-27
Resolution	:	2.80 Å(reported)

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

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

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

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

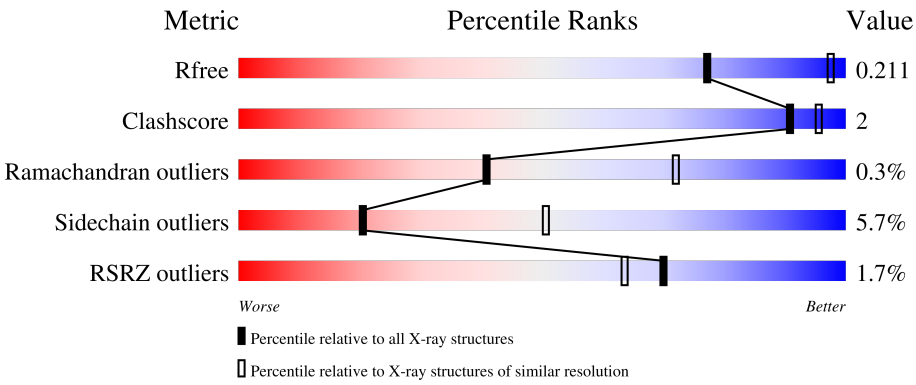
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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%, 96%, •
1	O	250	2%, 96%, •
2	B	258	3%, 83%, 11%, • 5%
2	P	258	4%, 84%, 10%, 5%
3	C	254	4%, 85%, 7%, • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	5% 84% 8% 6%
4	D	260	% 82% 8% 10%
4	R	260	% 81% 9% 10%
5	E	234	2% 87% 11%
5	S	234	% 87% 11%
6	F	288	% 79% 16%
6	T	288	2% 78% 5% 16%
7	G	252	2% 87% 9%
7	U	252	2% 87% 8%
8	H	232	% 90% 5%
8	V	232	% 90%
9	I	205	% 93% 7%
9	W	205	2% 93% 6%
10	J	198	% 90% 8%
10	X	198	2% 90% 8%
11	K	212	93% 5%
11	Y	212	% 91% 8%
12	L	222	88% 11%
12	Z	222	89% 10%
13	M	246	2% 87% 7% 5%
13	a	246	90% 5% 5%
14	N	196	% 95% 5%
14	b	196	97%

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 49779 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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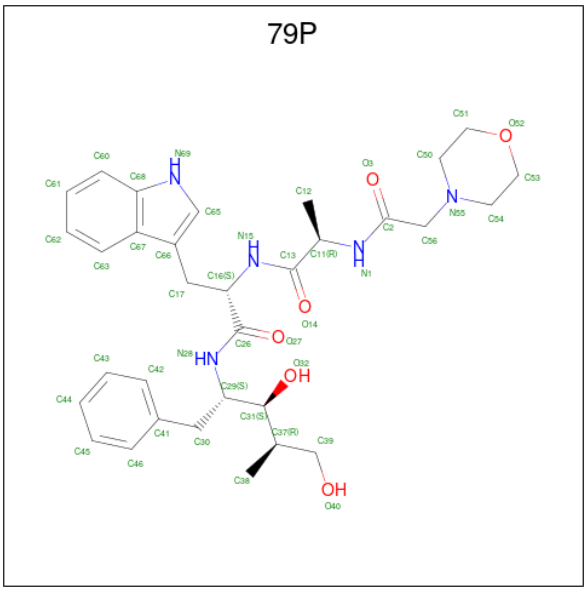
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

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

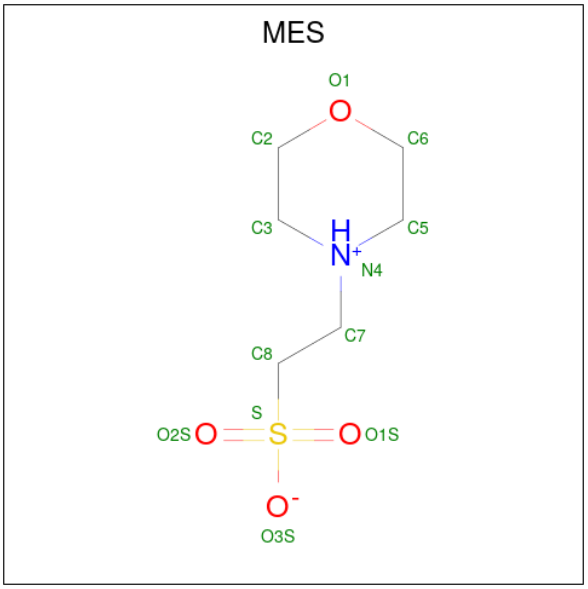
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is (2 {S})-3-(1 {H}-indol-3-yl)- {N}-[(2 {S},3 {S},4 {R})-4-methyl-3,5-bis(oxidanyl)-1-phenyl-pentan-2-yl]-2-[[(2 {R})-2-(2-morpholin-4-ylethanoylamino)propanoyl]amino]propanamide (three-letter code: 79P) (formula: $C_{32}H_{43}N_5O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	K	1	Total C N O 43 32 5 6	0	0
17	Y	1	Total C N O 43 32 5 6	0	0

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
19	A	14	14	14	0	0
			Total	O		
19	B	17	17	17	0	0
			Total	O		
19	C	11	11	11	0	0
			Total	O		
19	D	4	4	4	0	0
			Total	O		
19	E	8	8	8	0	0
			Total	O		
19	F	9	9	9	0	0
			Total	O		
19	G	18	18	18	0	0
			Total	O		
19	H	12	12	12	0	0

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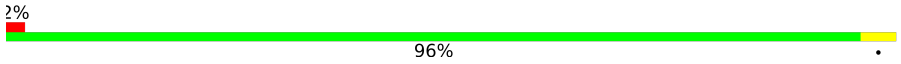
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
19	I	14	14	14	0	0
			Total	O		
19	J	15	15	15	0	0
			Total	O		
19	K	24	24	24	0	0
			Total	O		
19	L	16	16	16	0	0
			Total	O		
19	M	14	14	14	0	0
			Total	O		
19	N	12	12	12	0	0
			Total	O		
19	O	11	11	11	0	0
			Total	O		
19	P	12	12	12	0	0
			Total	O		
19	Q	5	5	5	0	0
			Total	O		
19	R	10	10	10	0	0
			Total	O		
19	S	4	4	4	0	0
			Total	O		
19	T	11	11	11	0	0
			Total	O		
19	U	15	15	15	0	0
			Total	O		
19	V	8	8	8	0	0
			Total	O		
19	W	9	9	9	0	0
			Total	O		
19	X	24	24	24	0	0
			Total	O		
19	Y	17	17	17	0	0
			Total	O		
19	Z	21	21	21	0	0
			Total	O		
19	a	15	15	15	0	0
			Total	O		
19	b	14	14	14	0	0

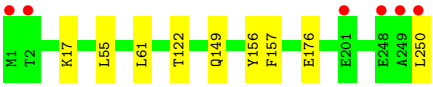
3 Residue-property plots (i)

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

• Molecule 1: Proteasome subunit alpha type-2

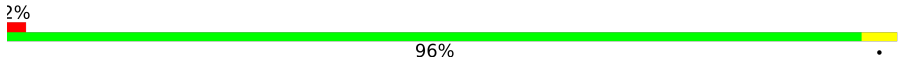
Chain A:





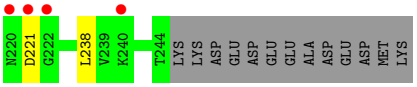
• Molecule 1: Proteasome subunit alpha type-2

Chain O:



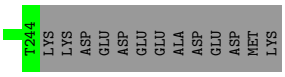
• Molecule 2: Proteasome subunit alpha type-3

Chain B:



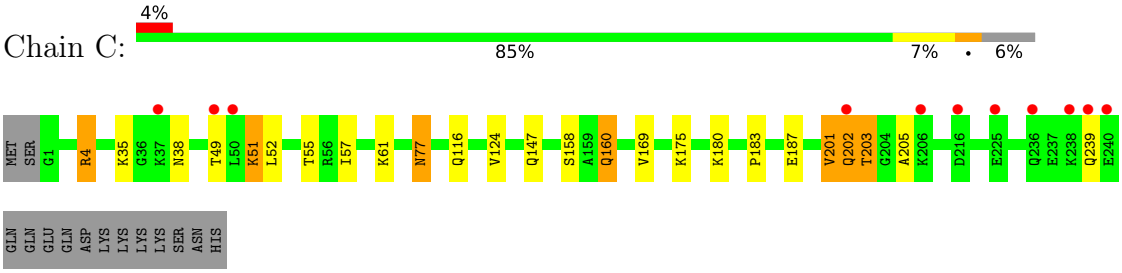
• Molecule 2: Proteasome subunit alpha type-3

Chain P:



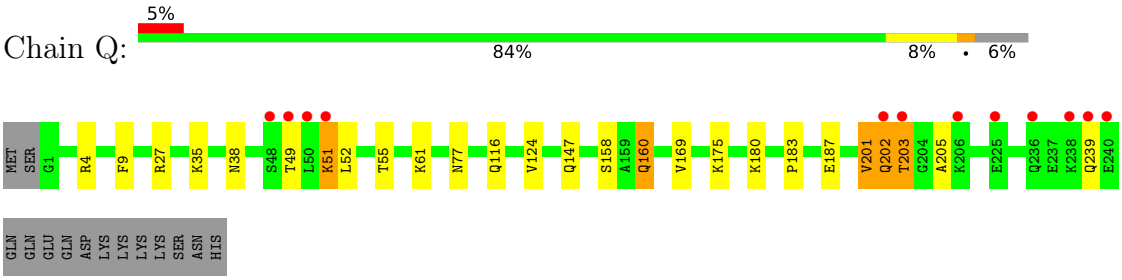
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



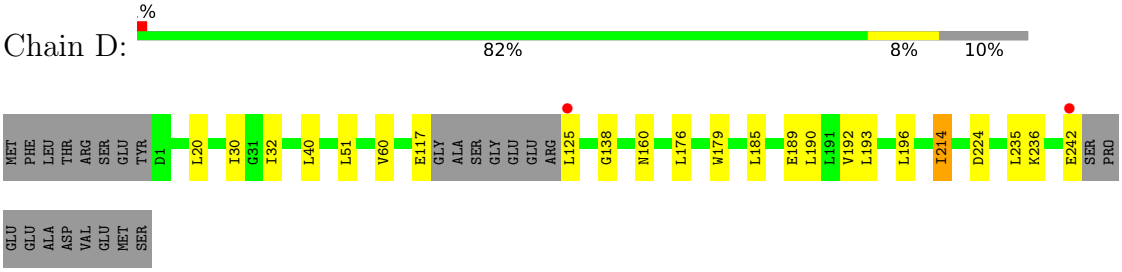
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



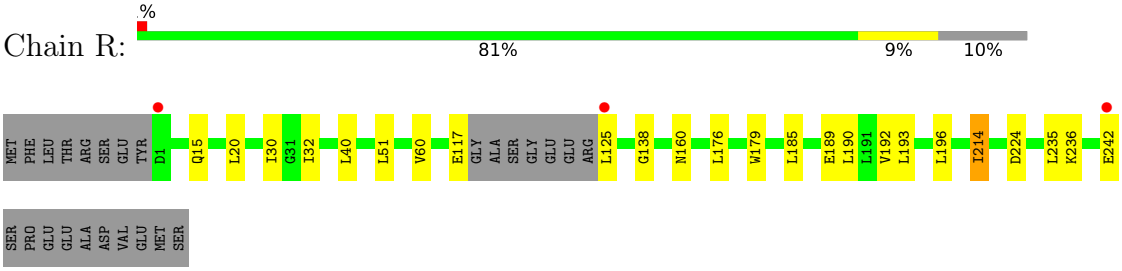
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



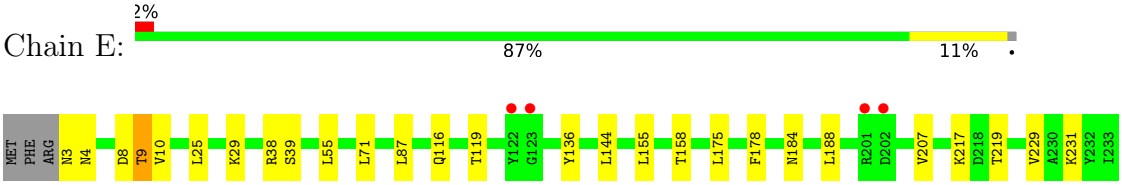
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



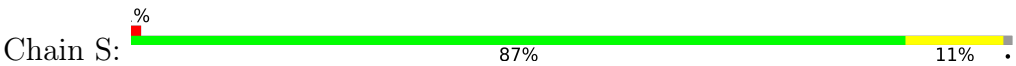
• Molecule 5: Proteasome subunit alpha type-6

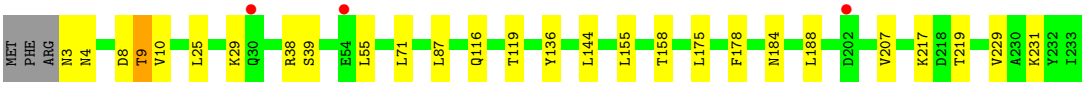
Chain E:



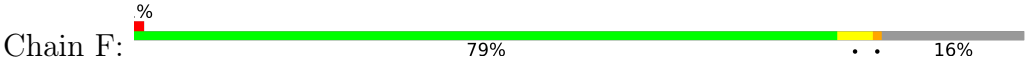
• Molecule 5: Proteasome subunit alpha type-6

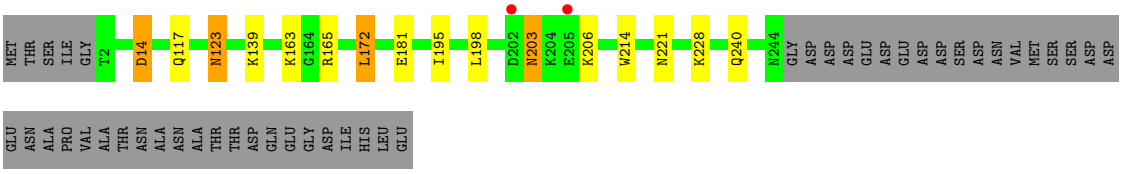
Chain S:



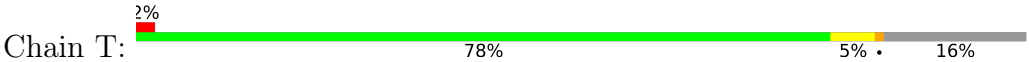


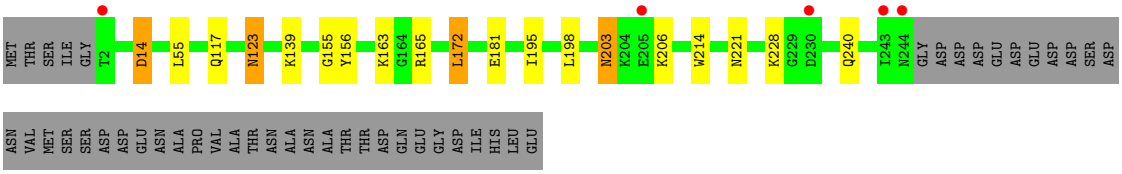
• Molecule 6: Probable proteasome subunit alpha type-7



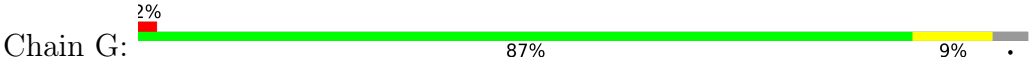


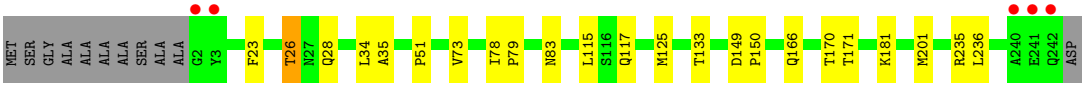
• Molecule 6: Probable proteasome subunit alpha type-7



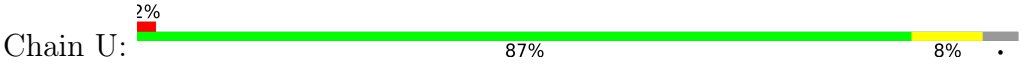


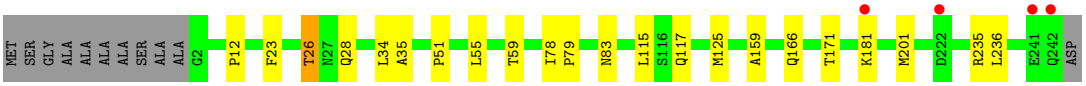
• Molecule 7: Proteasome subunit alpha type-1



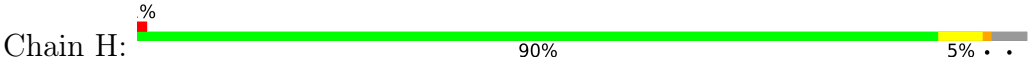


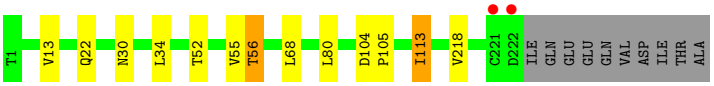
• Molecule 7: Proteasome subunit alpha type-1



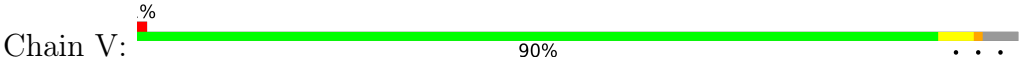


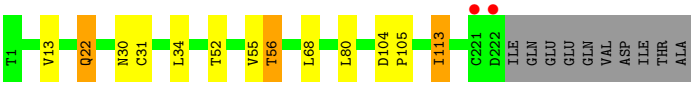
• Molecule 8: Proteasome subunit beta type-2





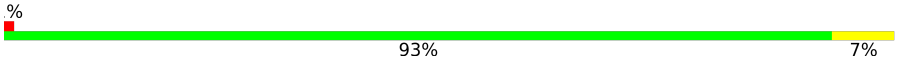
• Molecule 8: Proteasome subunit beta type-2

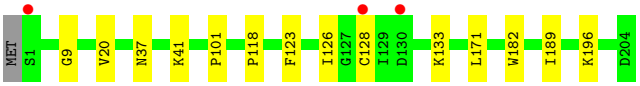




• Molecule 9: Proteasome subunit beta type-3

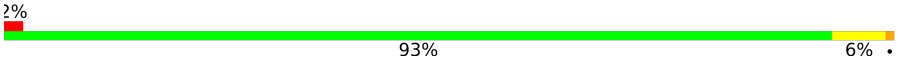
Chain I:

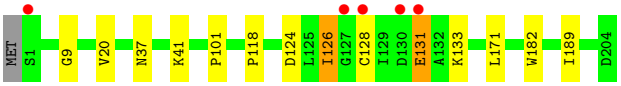




• Molecule 9: Proteasome subunit beta type-3

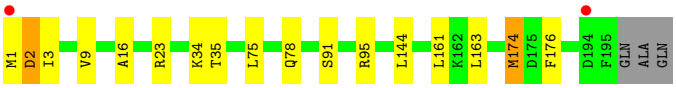
Chain W:





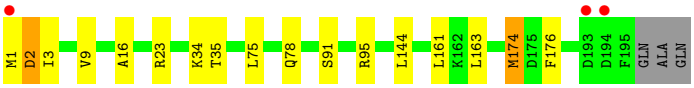
• Molecule 10: Proteasome subunit beta type-4

Chain J:



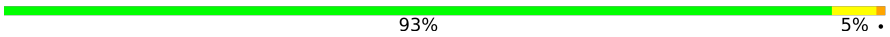
• Molecule 10: Proteasome subunit beta type-4

Chain X:



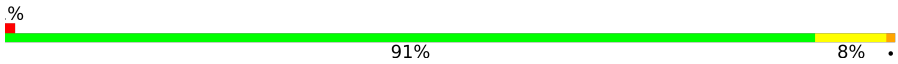
• Molecule 11: Proteasome subunit beta type-5

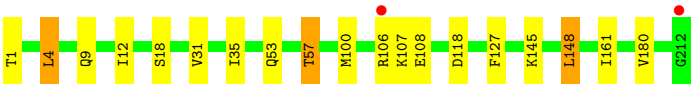
Chain K:



• Molecule 11: Proteasome subunit beta type-5

Chain Y:



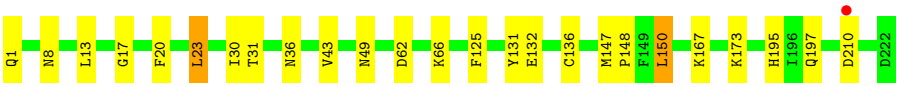


• Molecule 12: Proteasome subunit beta type-6

Chain L:

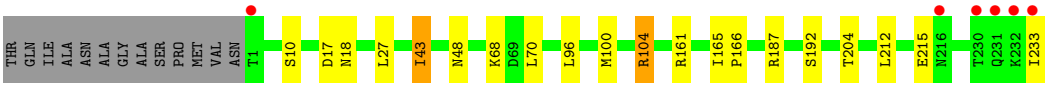
• Molecule 12: Proteasome subunit beta type-6

Chain Z:



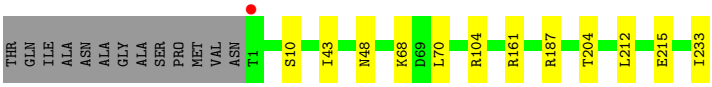
• Molecule 13: Proteasome subunit beta type-7

Chain M:



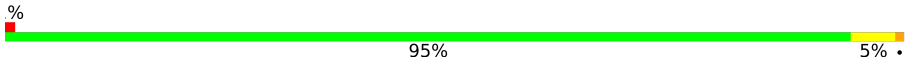
• Molecule 13: Proteasome subunit beta type-7

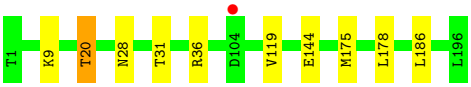
Chain a:



• Molecule 14: Proteasome subunit beta type-1

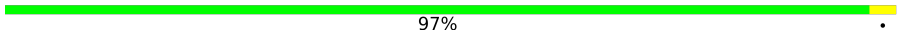
Chain N:





• Molecule 14: Proteasome subunit beta type-1

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.44Å 299.14Å 145.47Å 90.00° 112.87° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (15.00-2.80) 97.0 (15.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.90 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.186 , 0.206 0.190 , 0.211	Depositor DCC
R_{free} test set	12666 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	61.3	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	49779	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 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 79P, MG, MES

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	0.28	0/1952	0.50	0/2642
1	O	0.28	0/1952	0.50	0/2642
2	B	0.28	0/1934	0.53	0/2618
2	P	0.28	0/1934	0.53	0/2618
3	C	0.28	0/1910	0.55	0/2586
3	Q	0.28	0/1910	0.55	0/2586
4	D	0.27	0/1837	0.52	0/2475
4	R	0.27	0/1837	0.52	0/2475
5	E	0.28	0/1800	0.51	0/2433
5	S	0.28	0/1800	0.51	0/2433
6	F	0.28	0/1932	0.49	0/2609
6	T	0.28	0/1932	0.49	0/2609
7	G	0.28	0/1945	0.51	0/2634
7	U	0.28	0/1945	0.50	0/2634
8	H	0.25	0/1715	0.52	0/2326
8	V	0.25	0/1715	0.52	0/2326
9	I	0.29	0/1611	0.55	0/2174
9	W	0.30	0/1611	0.55	0/2174
10	J	0.27	0/1589	0.51	0/2142
10	X	0.27	0/1589	0.51	0/2142
11	K	0.28	0/1681	0.56	0/2274
11	Y	0.29	0/1681	0.56	1/2274 (0.0%)
12	L	0.28	0/1795	0.52	0/2420
12	Z	0.30	0/1795	0.53	0/2420
13	M	0.26	0/1855	0.55	0/2514
13	a	0.26	0/1855	0.55	0/2514
14	N	0.25	0/1541	0.50	0/2087
14	b	0.25	0/1541	0.50	0/2087
All	All	0.28	0/50194	0.52	1/67868 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Y	1	THR	N-CA-C	5.22	125.10	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	3	0
1	O	1915	0	1929	4	0
2	B	1904	0	1904	10	0
2	P	1904	0	1904	6	0
3	C	1881	0	1895	10	0
3	Q	1881	0	1895	9	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	6	0
5	E	1773	0	1775	5	0
5	S	1773	0	1775	6	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	6	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	7	0
8	H	1684	0	1688	4	0
8	V	1684	0	1688	5	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	6	0
10	X	1561	0	1569	6	0
11	K	1644	0	1592	6	0
11	Y	1644	0	1592	8	0
12	L	1757	0	1711	12	0
12	Z	1757	0	1711	10	0
13	M	1824	0	1832	6	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	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	43	0	0	1	0
17	Y	43	0	0	0	0
18	K	12	0	13	0	0
18	Y	12	0	13	0	0
19	A	14	0	0	0	0
19	B	17	0	0	0	0
19	C	11	0	0	0	0
19	D	4	0	0	0	0
19	E	8	0	0	0	0
19	F	9	0	0	0	0
19	G	18	0	0	0	0
19	H	12	0	0	0	0
19	I	14	0	0	0	0
19	J	15	0	0	0	0
19	K	24	0	0	0	0
19	L	16	0	0	0	0
19	M	14	0	0	0	0
19	N	12	0	0	0	0
19	O	11	0	0	0	0
19	P	12	0	0	0	0
19	Q	5	0	0	0	0
19	R	10	0	0	0	0
19	S	4	0	0	0	0
19	T	11	0	0	0	0
19	U	15	0	0	0	0
19	V	8	0	0	1	0
19	W	9	0	0	1	0
19	X	24	0	0	0	0
19	Y	17	0	0	0	0
19	Z	21	0	0	0	0
19	a	15	0	0	0	0
19	b	14	0	0	0	0
All	All	49779	0	49088	153	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 2.

All (153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:1:MET:HA	10:X:34:LYS:HE3	1.73	0.71
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.92	0.70
10:J:1:MET:HA	10:J:34:LYS:HE3	1.73	0.69
17:K:301:79P:O40	17:K:301:79P:N28	2.26	0.69
11:K:53:GLN:O	11:K:57:THR:HG23	1.92	0.68
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.62	0.65
8:V:22:GLN:NE2	19:V:401:HOH:O	2.30	0.65
3:C:202:GLN:HG3	3:C:203:THR:H	1.61	0.64
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.64	0.63
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.82	0.62
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.65	0.61
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.84	0.60
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.82	0.59
9:I:123:PHE:HA	9:I:128:CYS:O	2.02	0.59
9:W:124:ASP:OD1	9:W:128:CYS:N	2.20	0.58
14:N:20:THR:HG22	14:N:31:THR:OG1	2.03	0.58
3:C:51:LYS:O	3:C:52:LEU:HB2	2.05	0.57
7:U:23:PHE:O	7:U:26:THR:HB	2.04	0.57
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.05	0.57
9:W:131:GLU:O	9:W:131:GLU:HG2	2.04	0.56
7:G:23:PHE:O	7:G:26:THR:HB	2.04	0.56
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.71	0.56
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.71	0.56
1:A:55:LEU:HD12	7:G:170:THR:HG23	1.88	0.55
10:J:1:MET:HA	10:J:34:LYS:CE	2.37	0.54
10:X:1:MET:HA	10:X:34:LYS:CE	2.37	0.54
10:J:174:MET:HA	10:X:174:MET:HA	1.90	0.54
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.38	0.53
5:E:9:THR:HG21	5:E:119:THR:HA	1.91	0.53
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.91	0.52
2:P:149:THR:HG1	2:P:159:TRP:HE1	1.56	0.52
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.39	0.52
2:P:15:GLU:O	3:Q:27:ARG:NH1	2.42	0.52
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.91	0.52
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.10	0.52
3:C:201:VAL:O	3:C:202:GLN:HB2	2.10	0.51
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:THR:HG1	2:B:159:TRP:HE1	1.56	0.51
3:C:201:VAL:HG13	3:C:202:GLN:N	2.25	0.51
5:S:9:THR:HG21	5:S:119:THR:HA	1.91	0.51
13:M:43:ILE:O	13:M:43:ILE:HG12	2.12	0.50
6:F:14:ASP:OD2	6:F:14:ASP:N	2.41	0.50
12:L:8:ASN:HA	12:L:30:ILE:O	2.12	0.50
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.93	0.50
9:I:101:PRO:HB3	9:I:126:ILE:CD1	2.42	0.49
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.95	0.49
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.12	0.49
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.78	0.48
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.95	0.48
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.95	0.48
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.96	0.48
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.96	0.48
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.95	0.48
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.95	0.48
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.95	0.48
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.96	0.48
5:S:155:LEU:HD13	5:S:158:THR:HB	1.96	0.48
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.79	0.47
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.29	0.47
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.96	0.47
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.95	0.47
12:L:17:GLY:HA3	12:L:20:PHE:CE1	2.49	0.47
5:E:155:LEU:HD13	5:E:158:THR:HB	1.96	0.47
12:Z:17:GLY:HA3	12:Z:20:PHE:CE1	2.49	0.47
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.95	0.47
13:M:27:LEU:HB2	13:M:192:SER:HB3	1.97	0.47
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.97	0.46
9:W:126:ILE:HD12	9:W:126:ILE:HA	1.69	0.46
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.51	0.46
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.50	0.46
11:K:100:MET:CE	11:K:127:PHE:HB2	2.45	0.46
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.45	0.46
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.98	0.46
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.45	0.46
5:S:155:LEU:HD23	6:T:55:LEU:HD23	1.98	0.46
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.99	0.45
12:Z:62:ASP:O	12:Z:66:LYS:HB2	2.16	0.45
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:101:PRO:HB3	9:W:126:ILE:CD1	2.46	0.45
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.99	0.45
14:N:20:THR:HG23	14:N:28:ASN:HB3	1.98	0.45
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.99	0.45
2:B:180:LYS:O	2:B:183:MET:HB2	2.17	0.45
13:M:165:ILE:HB	13:M:166:PRO:HD3	1.99	0.45
8:H:52:THR:O	8:H:56:THR:HB	2.17	0.45
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.52	0.45
13:M:17:ASP:OD1	13:M:18:ASN:N	2.50	0.44
6:T:14:ASP:OD2	6:T:14:ASP:N	2.40	0.44
6:T:156:TYR:CE2	7:U:55:LEU:HD23	2.51	0.44
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.97	0.44
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.99	0.44
12:L:62:ASP:O	12:L:66:LYS:HB2	2.16	0.44
4:R:185:LEU:O	4:R:189:GLU:HG3	2.17	0.44
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.52	0.44
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.99	0.44
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.99	0.44
13:M:96:LEU:O	13:M:100:MET:HG2	2.18	0.44
6:F:123:ASN:C	6:F:123:ASN:HD22	2.21	0.44
1:O:55:LEU:HB3	7:U:159:ALA:O	2.18	0.43
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.48	0.43
4:D:185:LEU:O	4:D:189:GLU:HG3	2.18	0.43
6:T:155:GLY:HA3	7:U:59:THR:HG21	2.01	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.48	0.43
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.01	0.43
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.54	0.43
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.34	0.43
8:V:52:THR:O	8:V:56:THR:HB	2.18	0.43
2:P:180:LYS:O	2:P:183:MET:HB2	2.18	0.42
11:Y:18:SER:O	11:Y:31:VAL:HG22	2.19	0.42
5:S:136:TYR:CE1	5:S:217:LYS:HA	2.54	0.42
5:E:136:TYR:CE1	5:E:217:LYS:HA	2.54	0.42
14:N:20:THR:CG2	14:N:28:ASN:HB3	2.49	0.42
6:T:123:ASN:C	6:T:123:ASN:HD22	2.23	0.42
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.54	0.42
11:K:12:ILE:HB	11:K:180:VAL:HB	2.01	0.42
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.54	0.42
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	2.02	0.42
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.54	0.42
14:N:175:MET:HB2	14:N:186:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLN:O	1:A:156:TYR:HA	2.20	0.41
11:K:4:LEU:HD13	11:K:161:ILE:HD11	2.02	0.41
5:S:38:ARG:HD2	5:S:39:SER:O	2.20	0.41
10:J:3:ILE:HD12	10:J:176:PHE:CG	2.54	0.41
8:H:80:LEU:HD12	8:H:113:ILE:HD11	2.02	0.41
5:E:38:ARG:HD2	5:E:39:SER:O	2.20	0.41
12:L:136:CYS:SG	12:L:150:LEU:HB3	2.61	0.41
12:L:147:MET:N	12:L:148:PRO:HD2	2.35	0.41
7:U:34:LEU:HD23	7:U:35:ALA:N	2.36	0.41
8:V:31:CYS:HB2	19:W:308:HOH:O	2.20	0.41
8:V:80:LEU:HD12	8:V:113:ILE:HD11	2.02	0.41
3:C:35:LYS:HG2	3:C:158:SER:O	2.21	0.41
3:Q:201:VAL:HG13	3:Q:202:GLN:H	1.86	0.41
3:C:202:GLN:CG	3:C:203:THR:H	2.33	0.41
11:K:100:MET:HE3	11:K:127:PHE:HB2	2.03	0.41
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.68	0.41
2:B:139:TYR:CE2	2:B:144:GLY:HA2	2.56	0.41
8:H:218:VAL:CG2	9:I:196:LYS:HB2	2.51	0.41
10:J:3:ILE:HD12	10:J:176:PHE:CD2	2.56	0.41
12:L:195:HIS:HD2	12:L:197:GLN:H	1.68	0.41
10:X:3:ILE:HD12	10:X:176:PHE:CD2	2.56	0.41
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.68	0.41
7:G:78:ILE:N	7:G:79:PRO:CD	2.84	0.41
1:O:149:GLN:O	1:O:156:TYR:HA	2.21	0.41
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.21	0.40
11:Y:4:LEU:HD13	11:Y:161:ILE:HD11	2.02	0.40
2:B:155:ASN:ND2	3:C:77:ASN:HB2	2.36	0.40
7:G:34:LEU:HD23	7:G:35:ALA:N	2.36	0.40
1:O:115:ALA:HB1	1:O:154:GLY:O	2.21	0.40
7:G:73:VAL:CG1	7:G:133:THR:HB	2.51	0.40
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.52	0.40
7:U:78:ILE:N	7:U:79:PRO:CD	2.84	0.40
12:L:4:PRO:O	13:M:104:ARG:NH1	2.44	0.40
11:Y:107:LYS:HE2	11:Y:108:GLU:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	240 (97%)	8 (3%)	0	100	100
1	O	248/250 (99%)	240 (97%)	8 (3%)	0	100	100
2	B	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	19	49
2	P	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	19	49
3	C	238/254 (94%)	227 (95%)	7 (3%)	4 (2%)	9	29
3	Q	238/254 (94%)	227 (95%)	7 (3%)	4 (2%)	9	29
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	F	241/288 (84%)	236 (98%)	4 (2%)	1 (0%)	34	66
6	T	241/288 (84%)	236 (98%)	4 (2%)	1 (0%)	34	66
7	G	239/252 (95%)	236 (99%)	2 (1%)	1 (0%)	34	66
7	U	239/252 (95%)	235 (98%)	3 (1%)	1 (0%)	34	66
8	H	220/232 (95%)	212 (96%)	8 (4%)	0	100	100
8	V	220/232 (95%)	212 (96%)	8 (4%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	2 (1%)	2 (1%)	15	44
10	X	193/198 (98%)	190 (98%)	1 (0%)	2 (1%)	15	44
11	K	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
11	Y	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
12	L	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
12	Z	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
All	All	6276/6614 (95%)	6085 (97%)	171 (3%)	20 (0%)	41	72

All (20) 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
2	B	221	ASP
2	P	221	ASP
3	C	205	ALA
6	F	203	ASN
3	Q	183	PRO
3	Q	205	ALA
6	T	203	ASN
3	C	183	PRO
3	C	201	VAL
10	J	9	VAL
3	Q	201	VAL
7	U	51	PRO
10	X	9	VAL
7	G	51	PRO

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%)	204 (98%)	5 (2%)	49	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	209/209 (100%)	204 (98%)	5 (2%)	49	81
2	B	203/216 (94%)	189 (93%)	14 (7%)	15	41
2	P	203/216 (94%)	189 (93%)	14 (7%)	15	41
3	C	212/226 (94%)	195 (92%)	17 (8%)	12	34
3	Q	212/226 (94%)	195 (92%)	17 (8%)	12	34
4	D	194/215 (90%)	180 (93%)	14 (7%)	14	38
4	R	194/215 (90%)	180 (93%)	14 (7%)	14	38
5	E	190/193 (98%)	172 (90%)	18 (10%)	8	25
5	S	190/193 (98%)	172 (90%)	18 (10%)	8	25
6	F	201/239 (84%)	186 (92%)	15 (8%)	13	37
6	T	201/239 (84%)	186 (92%)	15 (8%)	13	37
7	G	206/210 (98%)	194 (94%)	12 (6%)	20	50
7	U	206/210 (98%)	194 (94%)	12 (6%)	20	50
8	H	181/190 (95%)	173 (96%)	8 (4%)	28	61
8	V	181/190 (95%)	173 (96%)	8 (4%)	28	61
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	82
9	W	172/173 (99%)	166 (96%)	6 (4%)	36	70
10	J	173/175 (99%)	163 (94%)	10 (6%)	20	50
10	X	173/175 (99%)	163 (94%)	10 (6%)	20	50
11	K	169/169 (100%)	162 (96%)	7 (4%)	30	64
11	Y	169/169 (100%)	162 (96%)	7 (4%)	30	64
12	L	185/185 (100%)	175 (95%)	10 (5%)	22	53
12	Z	185/185 (100%)	176 (95%)	9 (5%)	25	57
13	M	199/208 (96%)	187 (94%)	12 (6%)	19	48
13	a	199/208 (96%)	187 (94%)	12 (6%)	19	48
14	N	162/162 (100%)	156 (96%)	6 (4%)	34	68
14	b	162/162 (100%)	156 (96%)	6 (4%)	34	68
All	All	5312/5540 (96%)	5007 (94%)	305 (6%)	20	50

All (305) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS

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Mol	Chain	Res	Type
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	52	THR
2	B	54	THR
2	B	55	LEU
2	B	58	GLN
2	B	62	THR
2	B	119	GLN
2	B	173	THR
2	B	180	LYS
2	B	184	LYS
2	B	191	LEU
2	B	197	SER
2	B	209	ARG
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	49	THR
3	C	51	LYS
3	C	55	THR
3	C	61	LYS
3	C	77	ASN
3	C	116	GLN
3	C	124	VAL
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	187	GLU
3	C	203	THR
3	C	239	GLN
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	60	VAL
4	D	117	GLU
4	D	125	LEU
4	D	176	LEU

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Mol	Chain	Res	Type
4	D	190	LEU
4	D	193	LEU
4	D	214	ILE
4	D	224	ASP
4	D	235	LEU
4	D	236	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	71	LEU
5	E	87	LEU
5	E	116	GLN
5	E	144	LEU
5	E	184	ASN
5	E	188	LEU
5	E	207	VAL
5	E	219	THR
5	E	229	VAL
5	E	231	LYS
6	F	14	ASP
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	163	LYS
6	F	165	ARG
6	F	172	LEU
6	F	181	GLU
6	F	198	LEU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
6	F	228	LYS
6	F	240	GLN
7	G	26	THR
7	G	28	GLN

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Mol	Chain	Res	Type
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	125	MET
7	G	166	GLN
7	G	171	THR
7	G	181	LYS
7	G	201	MET
7	G	235	ARG
7	G	236	LEU
8	H	13	VAL
8	H	22	GLN
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	56	THR
8	H	68	LEU
8	H	113	ILE
9	I	37	ASN
9	I	133	LYS
9	I	171	LEU
9	I	182	TRP
10	J	2	ASP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	78	GLN
10	J	91	SER
10	J	95	ARG
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	57	THR
11	K	106	ARG
11	K	118	ASP
11	K	148	LEU
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN

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Mol	Chain	Res	Type
12	L	106	TYR
12	L	132	GLU
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
12	L	173	LYS
12	L	210	ASP
13	M	10	SER
13	M	43	ILE
13	M	48	ASN
13	M	68	LYS
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	204	THR
13	M	212	LEU
13	M	215	GLU
13	M	233	ILE
14	N	9	LYS
14	N	20	THR
14	N	36	ARG
14	N	119	VAL
14	N	144	GLU
14	N	178	LEU
1	O	17	LYS
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	52	THR
2	P	54	THR
2	P	55	LEU
2	P	58	GLN
2	P	62	THR
2	P	119	GLN
2	P	173	THR
2	P	180	LYS
2	P	184	LYS
2	P	191	LEU
2	P	197	SER

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Mol	Chain	Res	Type
2	P	209	ARG
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	49	THR
3	Q	51	LYS
3	Q	55	THR
3	Q	61	LYS
3	Q	77	ASN
3	Q	116	GLN
3	Q	124	VAL
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	239	GLN
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	60	VAL
4	R	117	GLU
4	R	125	LEU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	214	ILE
4	R	224	ASP
4	R	235	LEU
4	R	236	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	71	LEU

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Mol	Chain	Res	Type
5	S	87	LEU
5	S	116	GLN
5	S	144	LEU
5	S	184	ASN
5	S	188	LEU
5	S	207	VAL
5	S	219	THR
5	S	229	VAL
5	S	231	LYS
6	T	14	ASP
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	163	LYS
6	T	165	ARG
6	T	172	LEU
6	T	181	GLU
6	T	198	LEU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
6	T	228	LYS
6	T	240	GLN
7	U	26	THR
7	U	28	GLN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	125	MET
7	U	166	GLN
7	U	171	THR
7	U	181	LYS
7	U	201	MET
7	U	235	ARG
7	U	236	LEU
8	V	13	VAL
8	V	22	GLN
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	56	THR

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Mol	Chain	Res	Type
8	V	68	LEU
8	V	113	ILE
9	W	37	ASN
9	W	126	ILE
9	W	131	GLU
9	W	133	LYS
9	W	171	LEU
9	W	182	TRP
10	X	2	ASP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	78	GLN
10	X	91	SER
10	X	95	ARG
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	57	THR
11	Y	106	ARG
11	Y	118	ASP
11	Y	148	LEU
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	132	GLU
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
12	Z	173	LYS
12	Z	210	ASP
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	161	ARG
13	a	187	ARG

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Mol	Chain	Res	Type
13	a	204	THR
13	a	212	LEU
13	a	215	GLU
13	a	233	ILE
14	b	9	LYS
14	b	20	THR
14	b	36	ARG
14	b	119	VAL
14	b	144	GLU
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
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	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	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
8	H	30	ASN
8	H	57	GLN
8	H	66	HIS
8	H	172	ASN
8	H	189	ASN
9	I	31	GLN
10	J	55	GLN
10	J	147	HIS
10	J	191	GLN
11	K	85	ASN
11	K	143	ASN
11	K	176	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	108	HIS
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	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN

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Mol	Chain	Res	Type
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	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
7	U	167	GLN
7	U	175	ASN
8	V	30	ASN
8	V	57	GLN
8	V	66	HIS
8	V	172	ASN
8	V	189	ASN
9	W	31	GLN
10	X	55	GLN
10	X	146	HIS
10	X	147	HIS
10	X	191	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	108	HIS

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Mol	Chain	Res	Type
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	MES	Y	302	-	12,12,12	2.21	1 (8%)	14,16,16	1.33	2 (14%)
18	MES	K	303	-	12,12,12	2.24	1 (8%)	14,16,16	1.35	2 (14%)
17	79P	Y	301	11	45,46,46	2.22	10 (22%)	56,62,62	1.78	14 (25%)
17	79P	K	301	11	45,46,46	2.17	10 (22%)	56,62,62	1.77	13 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MES	Y	302	-	-	0/6/14/14	0/1/1/1
18	MES	K	303	-	-	0/6/14/14	0/1/1/1
17	79P	Y	301	11	-	9/41/50/50	0/4/4/4
17	79P	K	301	11	-	10/41/50/50	0/4/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	303	MES	C8-S	-7.46	1.66	1.77
18	Y	302	MES	C8-S	-7.36	1.67	1.77
17	Y	301	79P	C60-C68	-6.69	1.30	1.41
17	K	301	79P	C60-C68	-6.64	1.30	1.41
17	K	301	79P	C63-C67	-6.14	1.29	1.42
17	Y	301	79P	C63-C67	-6.12	1.29	1.42
17	K	301	79P	C30-C41	-5.21	1.38	1.51
17	Y	301	79P	C30-C41	-4.95	1.39	1.51
17	Y	301	79P	C67-C68	-4.75	1.29	1.42
17	K	301	79P	C67-C68	-4.73	1.29	1.42
17	Y	301	79P	O32-C31	-4.02	1.33	1.43
17	K	301	79P	O32-C31	-4.02	1.33	1.43
17	Y	301	79P	C39-C37	-3.90	1.48	1.52
17	Y	301	79P	C37-C31	3.87	1.60	1.53
17	K	301	79P	C39-C37	-3.36	1.49	1.52
17	K	301	79P	C56-C2	-2.76	1.48	1.52
17	Y	301	79P	C65-N69	-2.73	1.31	1.36
17	K	301	79P	C68-N69	-2.43	1.31	1.38
17	Y	301	79P	C68-N69	-2.42	1.31	1.38
17	K	301	79P	C65-N69	-2.40	1.31	1.36
17	K	301	79P	C65-C66	-2.30	1.31	1.37
17	Y	301	79P	C65-C66	-2.06	1.31	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	K	301	79P	C30-C29-N28	-5.50	102.05	110.07
17	Y	301	79P	C30-C29-N28	-4.62	103.33	110.07
17	Y	301	79P	C56-N55-C50	-4.04	104.83	111.09
17	Y	301	79P	C54-N55-C50	3.88	117.55	108.83
17	K	301	79P	C56-N55-C50	-3.72	105.33	111.09
17	K	301	79P	C38-C37-C39	-3.60	105.15	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Y	301	79P	C63-C67-C68	3.44	122.73	118.17
17	Y	301	79P	O40-C39-C37	-3.27	104.64	111.33
17	K	301	79P	C63-C67-C68	3.16	122.36	118.17
17	K	301	79P	C66-C17-C16	-3.16	107.27	113.45
17	Y	301	79P	C56-N55-C54	-3.15	106.22	111.09
17	K	301	79P	C41-C30-C29	3.12	118.75	113.33
18	K	303	MES	O3S-S-C8	3.07	110.74	105.77
17	Y	301	79P	C41-C30-C29	3.06	118.66	113.33
17	K	301	79P	C13-C11-N1	-3.00	104.18	111.60
17	K	301	79P	C54-N55-C50	2.79	115.11	108.83
17	K	301	79P	C56-N55-C54	-2.77	106.79	111.09
18	Y	302	MES	O3S-S-C8	2.77	110.25	105.77
18	Y	302	MES	O2S-S-C8	2.76	110.23	106.92
17	Y	301	79P	C38-C37-C39	-2.71	106.31	109.88
17	Y	301	79P	O52-C51-C50	-2.71	105.83	111.80
17	Y	301	79P	C17-C16-N15	-2.55	105.41	110.79
17	K	301	79P	C17-C16-N15	-2.45	105.64	110.79
17	K	301	79P	O52-C53-C54	-2.31	106.70	111.80
17	Y	301	79P	C63-C67-C66	-2.26	130.27	134.42
17	K	301	79P	O52-C51-C50	-2.22	106.92	111.80
17	K	301	79P	C63-C67-C66	-2.20	130.38	134.42
18	K	303	MES	O2S-S-C8	2.14	109.49	106.92
17	Y	301	79P	C53-C54-N55	2.14	113.35	110.10
17	Y	301	79P	C12-C11-N1	-2.06	106.51	110.38
17	Y	301	79P	C66-C17-C16	-2.04	109.45	113.45

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	301	79P	C29-C31-C37-C38
17	Y	301	79P	C29-C31-C37-C38
17	Y	301	79P	C29-C30-C41-C42
17	Y	301	79P	C29-C30-C41-C46
17	K	301	79P	C29-C30-C41-C42
17	K	301	79P	C29-C30-C41-C46
17	K	301	79P	O32-C31-C37-C38
17	Y	301	79P	O32-C31-C37-C38
17	Y	301	79P	C29-C31-C37-C39
17	K	301	79P	N1-C11-C13-N15
17	Y	301	79P	O32-C31-C37-C39
17	K	301	79P	N28-C29-C30-C41

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Mol	Chain	Res	Type	Atoms
17	K	301	79P	N15-C16-C26-O27
17	Y	301	79P	N1-C11-C13-N15
17	K	301	79P	C13-C11-N1-C2
17	K	301	79P	N15-C16-C26-N28
17	Y	301	79P	C13-C11-N1-C2
17	K	301	79P	N1-C11-C13-O14
17	Y	301	79P	N1-C11-C13-O14

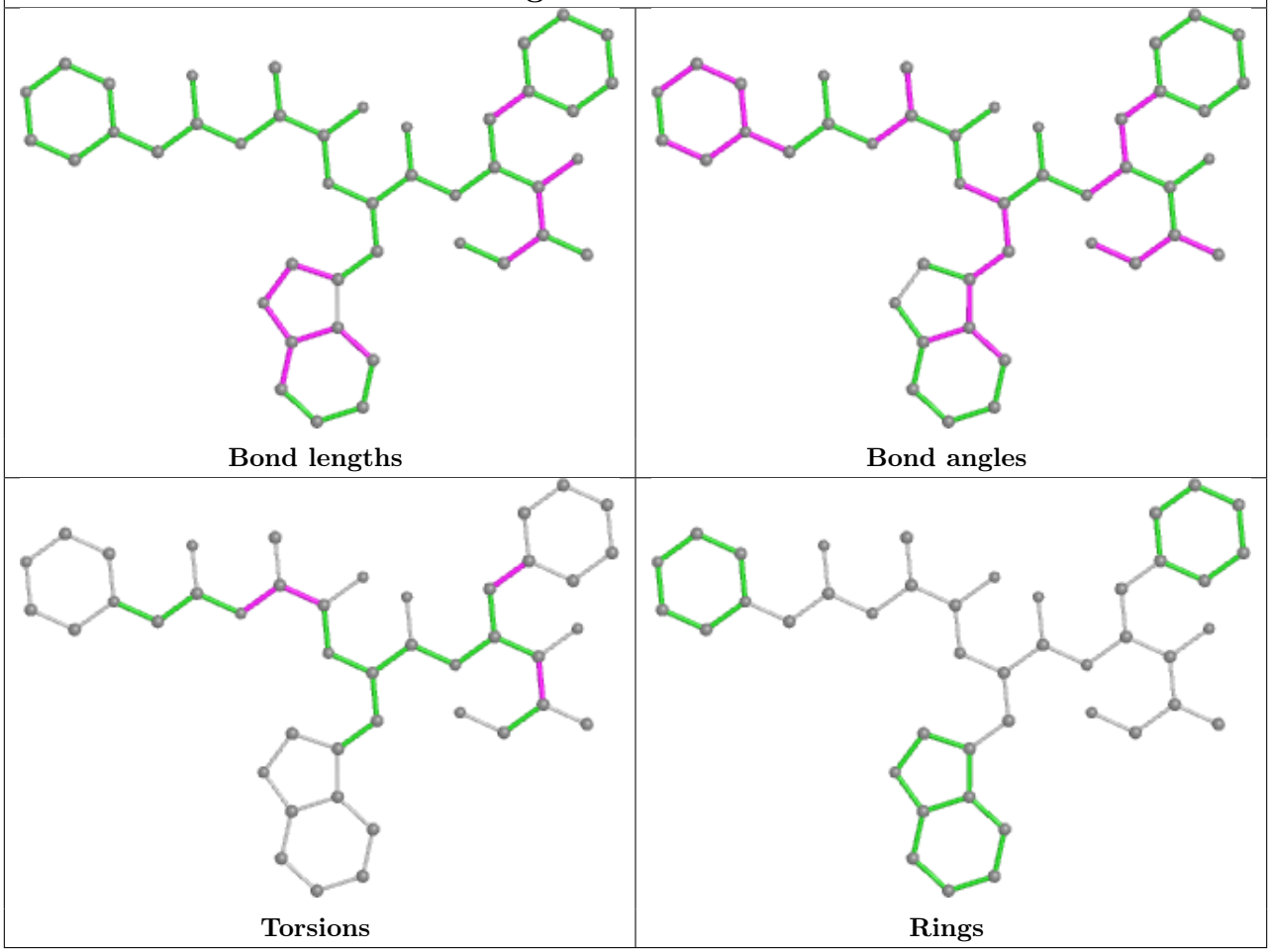
There are no ring outliers.

1 monomer is involved in 1 short contact:

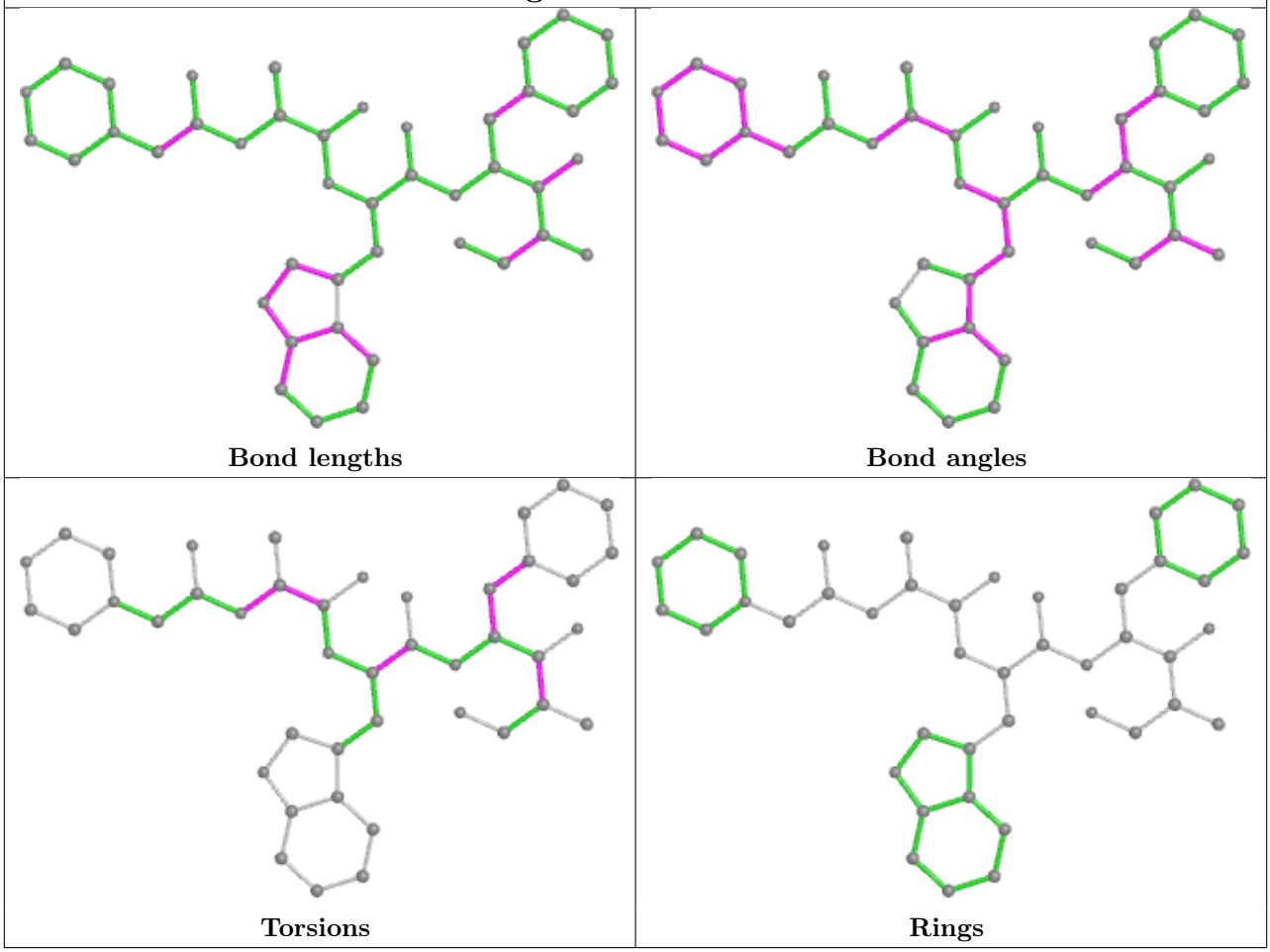
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	301	79P	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 79P Y 301



Ligand 79P K 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.45	6 (2%)	59	49	39, 55, 91, 124	0
1	O	250/250 (100%)	-0.44	4 (1%)	72	66	41, 61, 102, 128	0
2	B	244/258 (94%)	-0.33	9 (3%)	41	31	38, 59, 106, 161	0
2	P	244/258 (94%)	-0.29	11 (4%)	33	23	41, 62, 116, 163	0
3	C	240/254 (94%)	-0.24	11 (4%)	32	22	41, 64, 128, 151	0
3	Q	240/254 (94%)	-0.05	12 (5%)	28	19	47, 76, 150, 165	0
4	D	235/260 (90%)	-0.43	2 (0%)	84	80	43, 66, 98, 140	0
4	R	235/260 (90%)	-0.39	3 (1%)	77	72	46, 70, 103, 151	0
5	E	231/234 (98%)	-0.30	4 (1%)	70	63	47, 71, 103, 144	0
5	S	231/234 (98%)	-0.24	3 (1%)	77	72	44, 75, 110, 140	0
6	F	243/288 (84%)	-0.45	2 (0%)	86	81	43, 63, 110, 142	0
6	T	243/288 (84%)	-0.37	5 (2%)	63	54	38, 67, 117, 145	0
7	G	241/252 (95%)	-0.45	5 (2%)	63	54	33, 57, 97, 136	0
7	U	241/252 (95%)	-0.49	4 (1%)	70	63	41, 58, 90, 122	0
8	H	222/232 (95%)	-0.48	2 (0%)	84	80	39, 56, 84, 129	0
8	V	222/232 (95%)	-0.45	2 (0%)	84	80	43, 60, 87, 130	0
9	I	204/205 (99%)	-0.60	3 (1%)	73	68	37, 52, 81, 116	0
9	W	204/205 (99%)	-0.56	5 (2%)	57	47	38, 55, 83, 109	0
10	J	195/198 (98%)	-0.64	2 (1%)	82	77	35, 50, 79, 122	0
10	X	195/198 (98%)	-0.59	3 (1%)	73	68	37, 54, 81, 145	0
11	K	212/212 (100%)	-0.64	1 (0%)	91	88	35, 52, 77, 104	0
11	Y	212/212 (100%)	-0.66	2 (0%)	84	80	28, 53, 78, 109	0
12	L	222/222 (100%)	-0.61	0	100	100	37, 56, 88, 103	0
12	Z	222/222 (100%)	-0.62	1 (0%)	91	88	37, 56, 82, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.53	6 (2%) 56 46	36, 56, 85, 126	0
13	a	233/246 (94%)	-0.56	1 (0%) 92 91	36, 55, 80, 115	0
14	N	196/196 (100%)	-0.61	1 (0%) 91 88	41, 53, 79, 105	0
14	b	196/196 (100%)	-0.62	0 100 100	37, 52, 81, 107	0
All	All	6336/6614 (95%)	-0.46	110 (1%) 70 63	28, 59, 102, 165	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	206	LYS	7.9
2	P	219	ALA	6.7
2	B	220	ASN	6.7
3	Q	49	THR	6.6
8	V	222	ASP	5.3
3	Q	206	LYS	5.3
8	H	221	CYS	5.3
2	B	219	ALA	4.9
3	Q	50	LEU	4.8
9	W	1	SER	4.6
8	V	221	CYS	4.5
6	F	202	ASP	4.2
2	P	51	VAL	4.1
2	B	218	GLY	4.1
2	P	222	GLY	4.1
2	B	221	ASP	4.1
8	H	222	ASP	4.1
5	S	202	ASP	4.0
3	Q	238	LYS	4.0
13	M	230	THR	3.9
3	C	239	GLN	3.8
1	O	249	ALA	3.8
3	Q	240	GLU	3.7
10	X	194	ASP	3.6
1	A	1	MET	3.6
3	C	238	LYS	3.6
6	T	205	GLU	3.6
10	X	1	MET	3.6
9	W	128	CYS	3.5
3	Q	239	GLN	3.5
3	Q	48	SER	3.5
2	P	221	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
9	I	1	SER	3.4
2	P	220	ASN	3.4
5	E	202	ASP	3.4
3	C	49	THR	3.3
6	F	205	GLU	3.2
11	K	212	GLY	3.2
4	D	242	GLU	3.2
13	a	1	THR	3.1
3	Q	236	GLN	3.1
2	P	218	GLY	3.1
6	T	244	ASN	3.1
6	T	2	THR	3.0
13	M	1	THR	3.0
9	I	128	CYS	3.0
3	C	202	GLN	3.0
7	G	242	GLN	3.0
3	Q	202	GLN	2.9
5	S	54	GLU	2.9
13	M	233	ILE	2.9
3	C	225	GLU	2.9
13	M	216	ASN	2.9
11	Y	212	GLY	2.8
1	A	250	LEU	2.8
3	C	216	ASP	2.7
2	B	51	VAL	2.7
10	J	1	MET	2.7
2	B	60	THR	2.7
2	B	222	GLY	2.7
2	B	203	SER	2.7
6	T	230	ASP	2.6
4	R	125	LEU	2.6
3	C	240	GLU	2.6
1	A	249	ALA	2.6
1	O	1	MET	2.5
9	W	127	GLY	2.5
1	A	201	GLU	2.4
4	R	242	GLU	2.4
4	D	125	LEU	2.4
3	Q	51	LYS	2.4
7	G	241	GLU	2.4
10	J	194	ASP	2.4
3	Q	203	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	Q	225	GLU	2.4
5	E	201	ARG	2.4
6	T	243	ILE	2.3
4	R	1	ASP	2.3
9	W	130	ASP	2.3
10	X	193	ASP	2.3
1	O	52	SER	2.3
3	C	37	LYS	2.3
7	G	240	ALA	2.3
3	C	236	GLN	2.2
11	Y	106	ARG	2.2
2	P	60	THR	2.2
3	C	50	LEU	2.2
7	U	242	GLN	2.2
13	M	232	LYS	2.2
7	G	2	GLY	2.2
9	W	131	GLU	2.2
9	I	130	ASP	2.2
14	N	104	ASP	2.2
13	M	231	GLN	2.2
2	P	203	SER	2.2
1	A	248	GLU	2.1
7	U	222	ASP	2.1
7	G	3	TYR	2.1
2	P	50	LYS	2.1
2	P	225	TYR	2.1
1	O	231	LYS	2.1
1	A	2	THR	2.1
5	E	122	TYR	2.1
12	Z	210	ASP	2.1
5	E	123	GLY	2.1
2	P	223	GLU	2.1
2	B	240	LYS	2.1
5	S	30	GLN	2.0
7	U	241	GLU	2.0
7	U	181	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

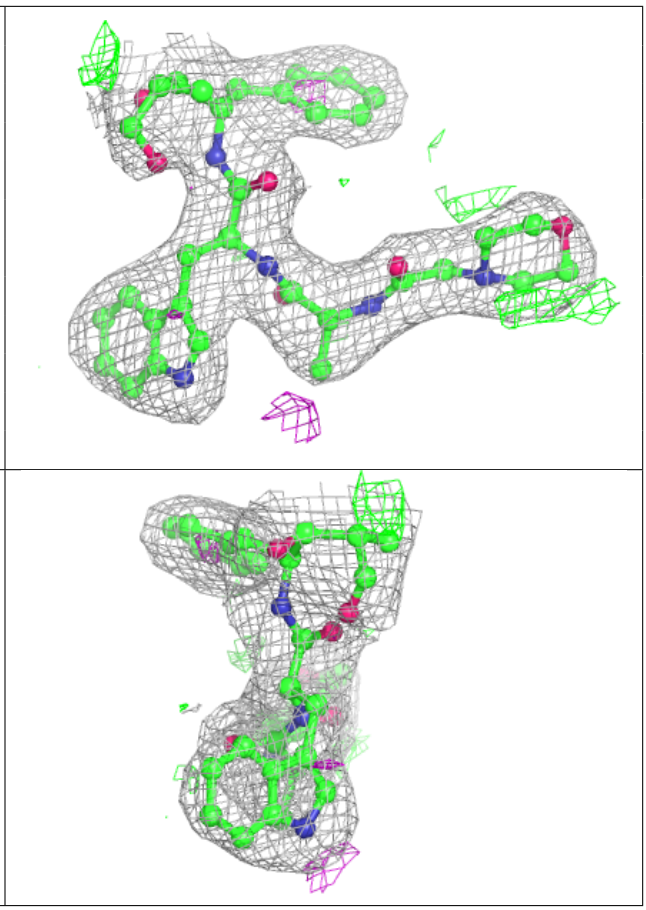
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	N	201	1/1	0.88	0.18	54,54,54,54	0
15	MG	Z	301	1/1	0.93	0.23	62,62,62,62	0
17	79P	Y	301	43/43	0.94	0.15	39,48,67,73	0
18	MES	Y	302	12/12	0.94	0.21	61,69,72,74	0
18	MES	K	303	12/12	0.95	0.25	61,66,73,75	0
17	79P	K	301	43/43	0.95	0.15	39,47,65,71	0
15	MG	I	301	1/1	0.96	0.21	62,62,62,62	0
16	CL	G	302	1/1	0.96	0.32	30,30,30,30	0
15	MG	G	301	1/1	0.96	0.08	47,47,47,47	0
15	MG	K	302	1/1	0.98	0.07	53,53,53,53	0
16	CL	U	301	1/1	0.98	0.23	30,30,30,30	0
15	MG	L	301	1/1	0.98	0.08	66,66,66,66	0
15	MG	I	302	1/1	1.00	0.04	38,38,38,38	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

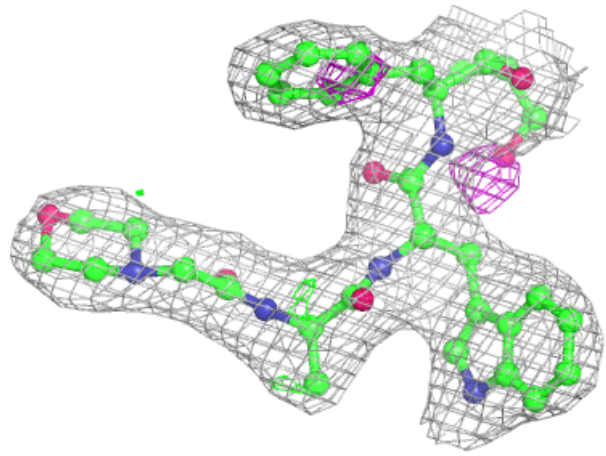
Electron density around 79P Y 301:

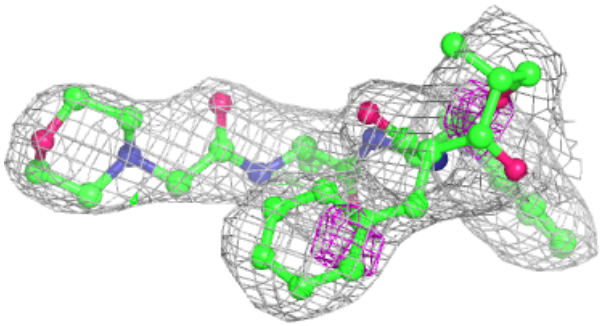
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

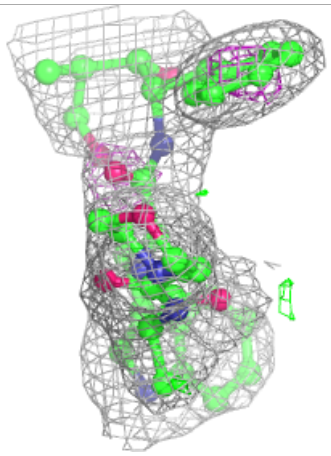


Electron density around 79P K 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.