Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 08:27 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
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:

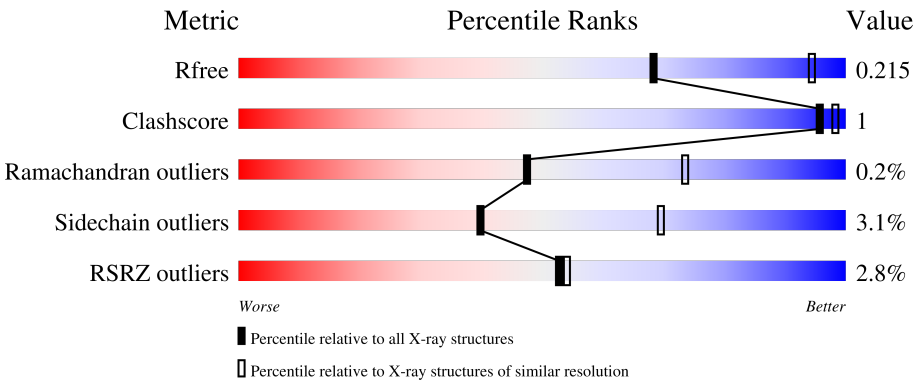
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 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	3% 98% •
1	O	250	4% 99% •
2	B	258	5% 90% • • 5%
2	P	258	5% 90% • • 5%
3	C	254	6% 90% • • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	9% 89% 6%
4	D	260	2% 86% 10%
4	R	260	3% 86% 10%
5	E	234	3% 94% 5%
5	S	234	6% 94% 5%
6	F	288	3% 81% 16%
6	T	288	4% 81% 16%
7	G	252	3% 90% 5%
7	U	252	2% 92%
8	H	232	% 93%
8	V	232	% 91%
9	I	205	93% 6%
9	W	205	% 93% 6%
10	J	198	2% 93%
10	X	198	2% 93%
11	K	212	92% 7%
11	Y	212	% 92% 6%
12	L	222	94% 6%
12	Z	222	% 94% 6%
13	M	246	% 88% 9%
13	a	246	% 89% 9%
14	N	196	% 96%
14	b	196	% 99%

2 Entry composition (i)

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
			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	225	1761	1114	301	339	7	0	0	0
			Total	C	N	O	S			
13	a	225	1761	1114	301	339	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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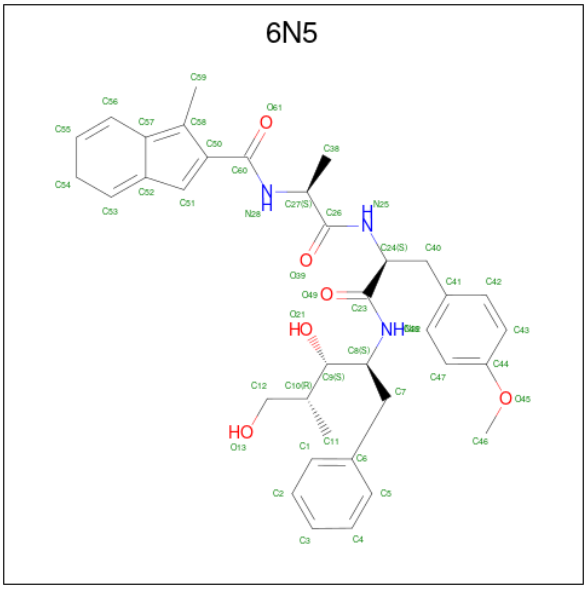
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	2	Total Mg 2 2	0	0
15	L	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	X	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

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

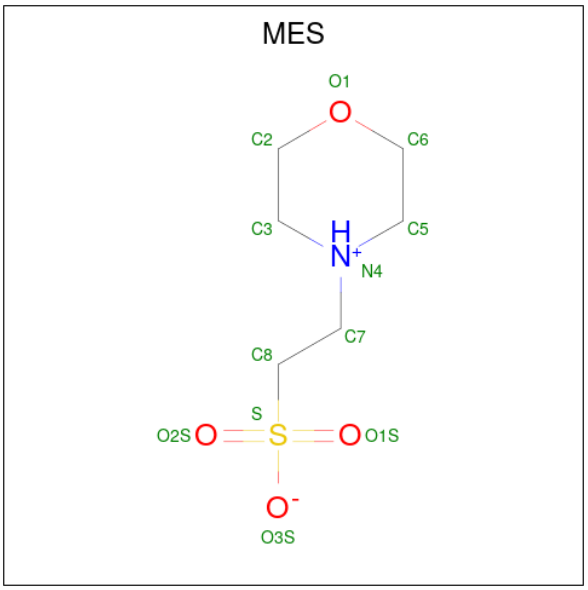
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is {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: $C_{36}H_{43}N_3O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
17	K	1	45	36	3	6	0	0
			Total	C	N	O		
17	N	1	45	36	3	6	0	0
			Total	C	N	O		
17	Y	1	45	36	3	6	0	0
			Total	C	N	O		
17	b	1	45	36	3	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	21	21	21	0	0
			Total	O		
19	C	13	13	13	0	0

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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

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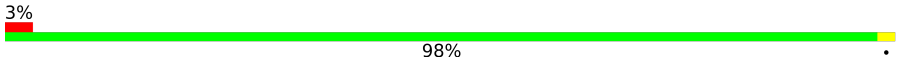
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
19	Y	14	14	14	0	0
			Total	O		
19	Z	26	26	26	0	0
			Total	O		
19	a	22	22	22	0	0
			Total	O		
19	b	15	15	15	0	0

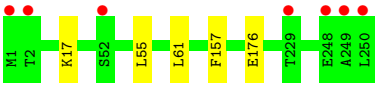
3 Residue-property plots (i)

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

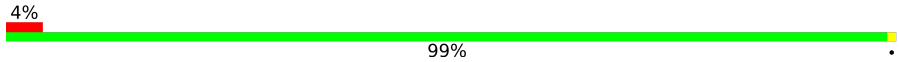
Chain A:

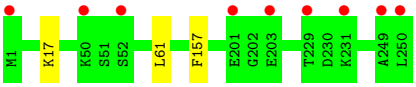




• Molecule 1: Proteasome subunit alpha type-2

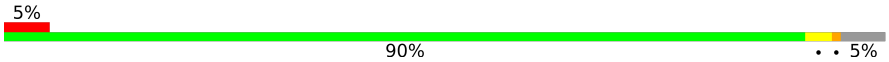
Chain O:

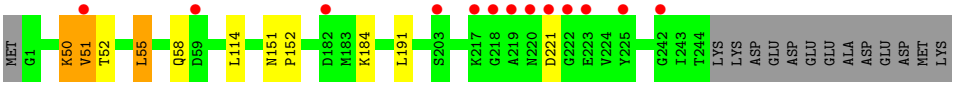




• Molecule 2: Proteasome subunit alpha type-3

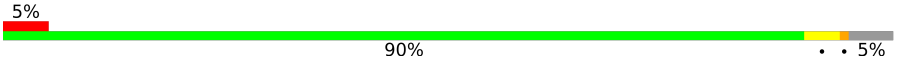
Chain B:

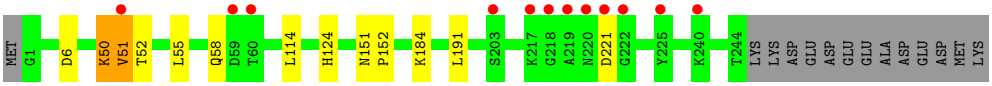




• Molecule 2: Proteasome subunit alpha type-3

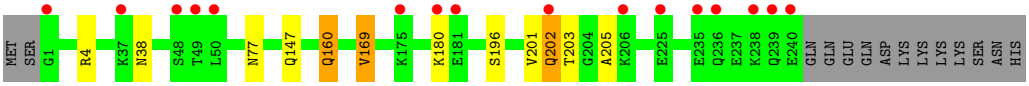
Chain P:





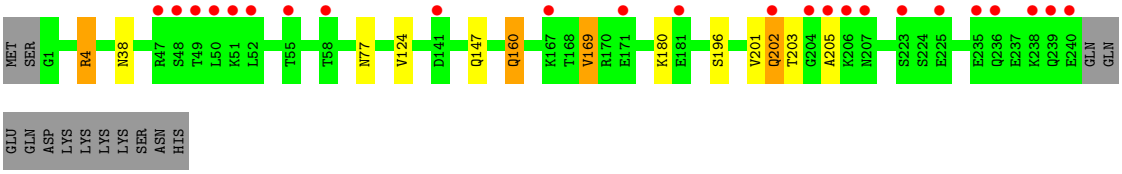
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



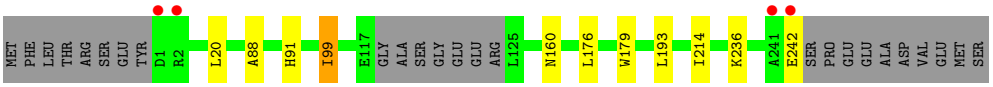
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



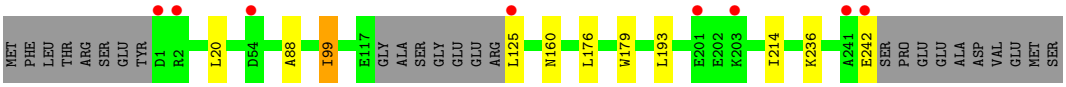
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



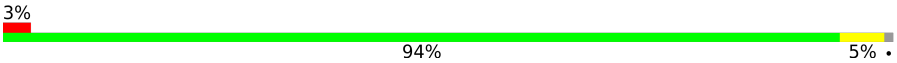
• Molecule 4: Proteasome subunit alpha type-5

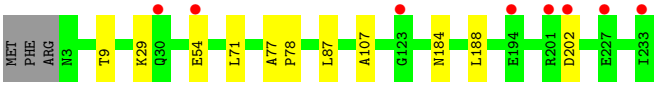
Chain R:



• Molecule 5: Proteasome subunit alpha type-6

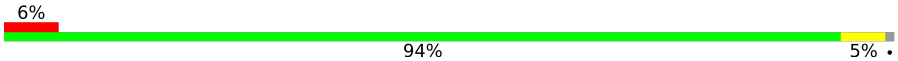
Chain E:

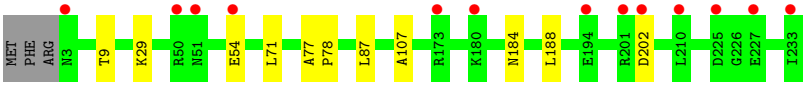




• Molecule 5: Proteasome subunit alpha type-6

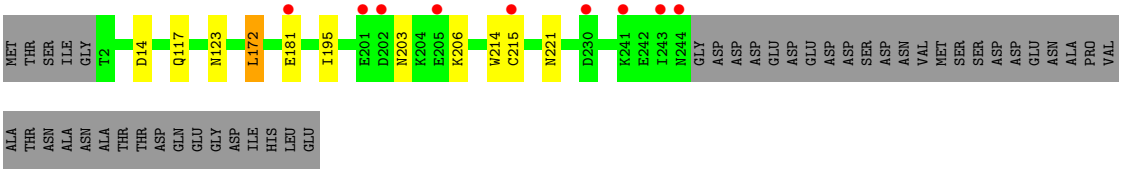
Chain S:





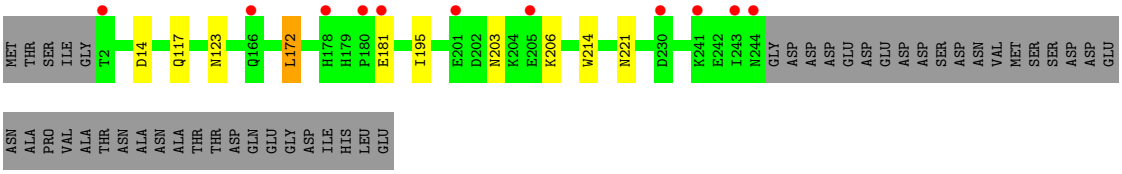
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



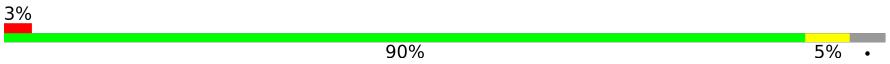
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



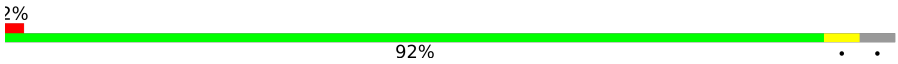
- Molecule 7: Proteasome subunit alpha type-1

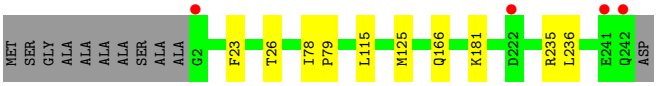
Chain G:



- Molecule 7: Proteasome subunit alpha type-1

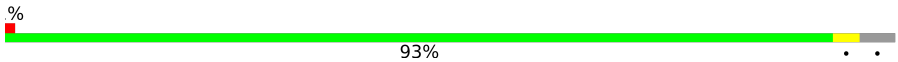
Chain U:

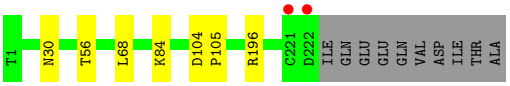




- Molecule 8: Proteasome subunit beta type-2

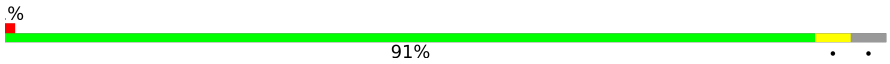
Chain H:

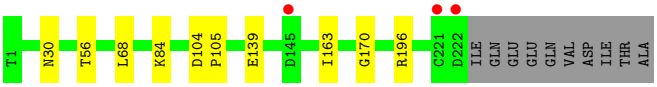




- Molecule 8: Proteasome subunit beta type-2

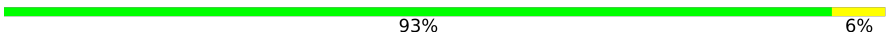
Chain V:

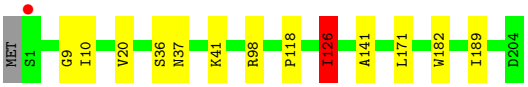




- Molecule 9: Proteasome subunit beta type-3

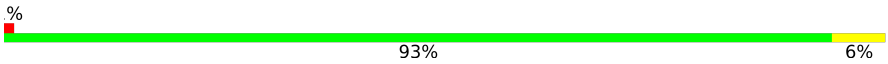
Chain I:





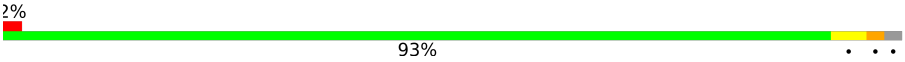
- Molecule 9: Proteasome subunit beta type-3

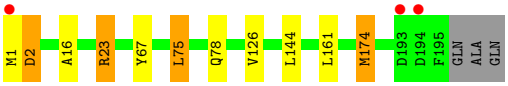
Chain W:



• Molecule 10: Proteasome subunit beta type-4

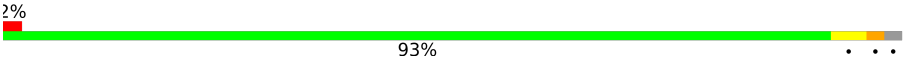
Chain J:





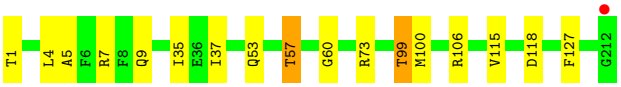
• Molecule 10: Proteasome subunit beta type-4

Chain X:



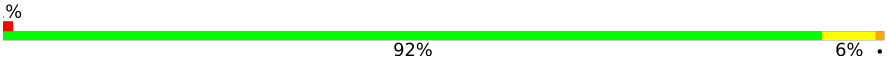
• Molecule 11: Proteasome subunit beta type-5

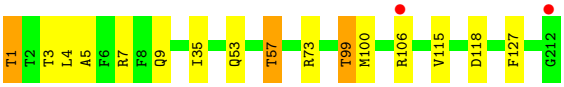
Chain K:



• Molecule 11: Proteasome subunit beta type-5

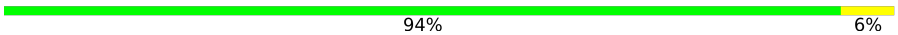
Chain Y:





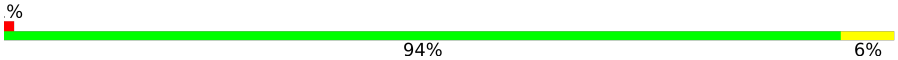
• Molecule 12: Proteasome subunit beta type-6

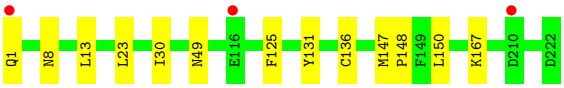
Chain L:



• Molecule 12: Proteasome subunit beta type-6

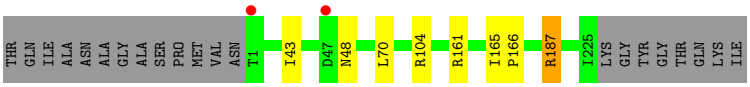
Chain Z:





• Molecule 13: Proteasome subunit beta type-7

Chain M:

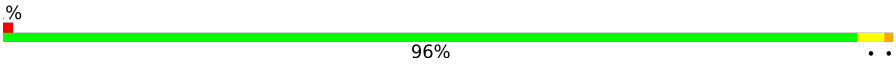


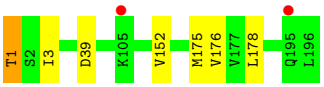
• Molecule 13: Proteasome subunit beta type-7

Chain a:

• Molecule 14: Proteasome subunit beta type-1

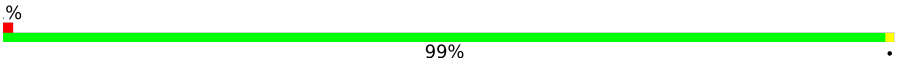
Chain N:

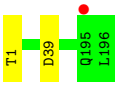




• Molecule 14: Proteasome subunit beta type-1

Chain b:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.44Å 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
$< I/\sigma(I) >$ [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 (5.00%)	wwPDB-VP
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]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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(^{o})	Ideal(^{o})
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 (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	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

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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

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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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:98:ARG:HD2	9:I:126:ILE:CD1	2.39	0.53
10:J:174:MET:HA	10:X:174:MET:HA	1.90	0.53
11:K:100:MET:HE3	11:K:127:PHE:HB2	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

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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:HE21	3:C:160:GLN:HA	1.85	0.41
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.02	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
17:K:301:6N5:C48	17:K:301:6N5:N25	2.84	0.41
2:P:6:ASP:OD2	3:Q:4:ARG:HG3	2.20	0.41
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.04	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 (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%)	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%)	19	43
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	19	43
3	C	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	19	43
3	Q	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	19	43
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%)	29	54
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	54
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

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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%)	47	73

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 (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%)	206 (99%)	3 (1%)	67	86
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	86
2	B	203/216 (94%)	196 (97%)	7 (3%)	37	66
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	66
3	C	212/226 (94%)	204 (96%)	8 (4%)	33	62
3	Q	212/226 (94%)	204 (96%)	8 (4%)	33	62
4	D	194/215 (90%)	187 (96%)	7 (4%)	35	64
4	R	194/215 (90%)	186 (96%)	8 (4%)	30	59
5	E	190/193 (98%)	183 (96%)	7 (4%)	34	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	190/193 (98%)	183 (96%)	7 (4%)	34	63
6	F	201/239 (84%)	192 (96%)	9 (4%)	27	55
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	55
7	G	206/210 (98%)	200 (97%)	6 (3%)	42	71
7	U	206/210 (98%)	200 (97%)	6 (3%)	42	71
8	H	181/190 (95%)	176 (97%)	5 (3%)	43	73
8	V	181/190 (95%)	176 (97%)	5 (3%)	43	73
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	78
9	W	172/173 (99%)	168 (98%)	4 (2%)	50	78
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	71
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	71
11	K	169/169 (100%)	161 (95%)	8 (5%)	26	54
11	Y	169/169 (100%)	161 (95%)	8 (5%)	26	54
12	L	185/185 (100%)	180 (97%)	5 (3%)	44	74
12	Z	185/185 (100%)	180 (97%)	5 (3%)	44	74
13	M	193/208 (93%)	187 (97%)	6 (3%)	40	69
13	a	193/208 (93%)	187 (97%)	6 (3%)	40	69
14	N	162/162 (100%)	161 (99%)	1 (1%)	86	95
14	b	162/162 (100%)	161 (99%)	1 (1%)	86	95
All	All	5300/5540 (96%)	5137 (97%)	163 (3%)	40	69

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

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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

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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

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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

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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

Sometimes 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

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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

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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 monosaccharides 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	b	201	14	48,48,48	1.82	9 (18%)	54,66,66	1.59	11 (20%)
18	MES	K	304	-	12,12,12	2.38	1 (8%)	14,16,16	1.33	2 (14%)
18	MES	Y	303	-	12,12,12	2.33	1 (8%)	14,16,16	1.46	2 (14%)
17	6N5	N	201	14	48,48,48	1.84	9 (18%)	54,66,66	1.58	11 (20%)
17	6N5	K	301	11	48,48,48	1.81	8 (16%)	54,66,66	1.41	9 (16%)
17	6N5	Y	301	11	48,48,48	1.83	9 (18%)	54,66,66	1.42	9 (16%)

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	b	201	14	-	12/44/67/67	0/4/4/4
18	MES	K	304	-	-	0/6/14/14	0/1/1/1
18	MES	Y	303	-	-	0/6/14/14	0/1/1/1
17	6N5	N	201	14	-	12/44/67/67	0/4/4/4
17	6N5	K	301	11	-	11/44/67/67	0/4/4/4
17	6N5	Y	301	11	-	11/44/67/67	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	-8.01	1.66	1.77
18	Y	303	MES	C8-S	-7.79	1.66	1.77
17	N	201	6N5	C10-C9	6.43	1.64	1.53
17	Y	301	6N5	C10-C9	6.41	1.64	1.53
17	K	301	6N5	C10-C9	6.17	1.64	1.53
17	b	201	6N5	C10-C9	5.96	1.64	1.53
17	Y	301	6N5	C50-C60	-4.41	1.35	1.49
17	K	301	6N5	C50-C60	-4.36	1.35	1.49
17	K	301	6N5	C40-C41	-4.29	1.41	1.51
17	Y	301	6N5	C40-C41	-4.26	1.41	1.51
17	b	201	6N5	C40-C41	-4.20	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	201	6N5	C40-C41	-4.17	1.41	1.51
17	Y	301	6N5	C57-C52	-4.15	1.34	1.47
17	K	301	6N5	C57-C52	-4.10	1.34	1.47
17	b	201	6N5	C57-C52	-4.06	1.34	1.47
17	N	201	6N5	C57-C52	-4.06	1.34	1.47
17	N	201	6N5	C50-C60	-3.96	1.37	1.49
17	b	201	6N5	C50-C60	-3.95	1.37	1.49
17	b	201	6N5	C7-C6	-3.65	1.42	1.51
17	N	201	6N5	C7-C6	-3.65	1.42	1.51
17	Y	301	6N5	C7-C6	-3.60	1.42	1.51
17	K	301	6N5	C7-C6	-3.60	1.42	1.51
17	N	201	6N5	C54-C53	-2.94	1.39	1.49
17	b	201	6N5	C54-C53	-2.94	1.39	1.49
17	Y	301	6N5	C54-C53	-2.93	1.39	1.49
17	K	301	6N5	C54-C53	-2.90	1.39	1.49
17	N	201	6N5	C56-C55	2.57	1.40	1.33
17	b	201	6N5	C56-C55	2.56	1.40	1.33
17	K	301	6N5	C56-C57	-2.49	1.34	1.40
17	Y	301	6N5	C56-C57	-2.48	1.34	1.40
17	K	301	6N5	C56-C55	2.31	1.39	1.33
17	Y	301	6N5	C56-C55	2.30	1.39	1.33
17	N	201	6N5	C56-C57	-2.24	1.35	1.40
17	b	201	6N5	C56-C57	-2.23	1.35	1.40
17	b	201	6N5	C27-N28	2.19	1.50	1.45
17	N	201	6N5	C27-N28	2.08	1.50	1.45
17	Y	301	6N5	C57-C58	-2.00	1.33	1.37

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	201	6N5	C11-C10-C12	-4.75	103.64	109.88
17	b	201	6N5	C11-C10-C12	-4.70	103.70	109.88
17	N	201	6N5	C27-N28-C60	4.67	128.78	121.57
17	b	201	6N5	C27-N28-C60	4.55	128.59	121.57
17	Y	301	6N5	C50-C51-C52	-3.85	104.93	109.47
17	K	301	6N5	C50-C51-C52	-3.75	105.05	109.47
17	b	201	6N5	C51-C52-C57	3.58	109.82	106.64
17	N	201	6N5	C51-C52-C57	3.49	109.74	106.64
17	b	201	6N5	C50-C51-C52	-3.47	105.38	109.47
17	Y	301	6N5	C51-C52-C57	3.47	109.72	106.64
17	K	301	6N5	C51-C52-C57	3.46	109.71	106.64
18	Y	303	MES	O3S-S-C8	3.42	111.30	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	201	6N5	C50-C51-C52	-3.33	105.54	109.47
17	Y	301	6N5	C41-C40-C24	-3.20	104.55	113.39
17	K	301	6N5	C41-C40-C24	-3.19	104.58	113.39
17	b	201	6N5	C26-C27-N28	-3.19	103.71	111.60
17	N	201	6N5	C26-C27-N28	-3.18	103.73	111.60
18	K	304	MES	O3S-S-C8	3.16	110.89	105.77
17	Y	301	6N5	O13-C12-C10	-3.00	105.20	111.33
17	K	301	6N5	O13-C12-C10	-2.90	105.40	111.33
18	Y	303	MES	O2S-S-C8	2.89	110.39	106.92
17	b	201	6N5	C7-C6-C5	2.71	126.29	120.91
17	N	201	6N5	C7-C6-C5	2.64	126.14	120.91
17	N	201	6N5	C59-C58-C57	-2.60	121.93	128.30
17	Y	301	6N5	C7-C6-C5	2.59	126.05	120.91
17	b	201	6N5	C59-C58-C57	-2.58	121.98	128.30
17	K	301	6N5	C7-C6-C5	2.58	126.02	120.91
17	Y	301	6N5	C59-C58-C57	-2.52	122.14	128.30
17	K	301	6N5	C59-C58-C57	-2.50	122.19	128.30
17	b	201	6N5	C7-C6-C1	-2.42	116.10	120.91
17	b	201	6N5	O13-C12-C10	-2.41	106.40	111.33
17	N	201	6N5	C7-C6-C1	-2.39	116.16	120.91
17	K	301	6N5	C7-C6-C1	-2.28	116.38	120.91
17	Y	301	6N5	C50-C60-N28	2.27	119.15	116.31
17	b	201	6N5	C38-C27-N28	2.26	114.63	110.38
17	N	201	6N5	C38-C27-N28	2.25	114.61	110.38
18	K	304	MES	O2S-S-C8	2.21	109.58	106.92
17	Y	301	6N5	C7-C6-C1	-2.20	116.55	120.91
17	N	201	6N5	C40-C24-N25	-2.14	106.28	110.79
17	K	301	6N5	C50-C60-N28	2.10	118.94	116.31
17	N	201	6N5	O13-C12-C10	-2.10	107.05	111.33
17	b	201	6N5	C40-C24-N25	-2.08	106.41	110.79
17	Y	301	6N5	C46-O45-C44	-2.06	113.05	117.51
17	K	301	6N5	C46-O45-C44	-2.02	113.13	117.51

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	301	6N5	C11-C10-C9-C8
17	K	301	6N5	C12-C10-C9-C8
17	N	201	6N5	C11-C10-C9-C8
17	N	201	6N5	C12-C10-C9-C8
17	N	201	6N5	C9-C10-C12-O13

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Mol	Chain	Res	Type	Atoms
17	N	201	6N5	C11-C10-C12-O13
17	Y	301	6N5	C11-C10-C9-C8
17	Y	301	6N5	C12-C10-C9-C8
17	Y	301	6N5	C11-C10-C12-O13
17	b	201	6N5	C11-C10-C9-C8
17	b	201	6N5	C12-C10-C9-C8
17	b	201	6N5	C9-C10-C12-O13
17	b	201	6N5	C11-C10-C12-O13
17	Y	301	6N5	C43-C44-O45-C46
17	K	301	6N5	C47-C44-O45-C46
17	K	301	6N5	C43-C44-O45-C46
17	Y	301	6N5	C47-C44-O45-C46
17	N	201	6N5	C43-C44-O45-C46
17	b	201	6N5	C43-C44-O45-C46
17	N	201	6N5	C47-C44-O45-C46
17	b	201	6N5	C47-C44-O45-C46
17	N	201	6N5	C5-C6-C7-C8
17	b	201	6N5	C5-C6-C7-C8
17	N	201	6N5	C1-C6-C7-C8
17	b	201	6N5	C1-C6-C7-C8
17	N	201	6N5	C12-C10-C9-O21
17	b	201	6N5	C12-C10-C9-O21
17	Y	301	6N5	C5-C6-C7-C8
17	K	301	6N5	C5-C6-C7-C8
17	Y	301	6N5	C1-C6-C7-C8
17	K	301	6N5	C1-C6-C7-C8
17	K	301	6N5	C11-C10-C12-O13
17	K	301	6N5	C11-C10-C9-O21
17	K	301	6N5	C12-C10-C9-O21
17	N	201	6N5	C11-C10-C9-O21
17	Y	301	6N5	C11-C10-C9-O21
17	Y	301	6N5	C12-C10-C9-O21
17	b	201	6N5	C11-C10-C9-O21
17	Y	301	6N5	C9-C10-C12-O13
17	b	201	6N5	N25-C26-C27-N28
17	N	201	6N5	N25-C26-C27-N28
17	K	301	6N5	C9-C10-C12-O13
17	K	301	6N5	N22-C8-C9-C10
17	N	201	6N5	N22-C8-C9-C10
17	Y	301	6N5	N22-C8-C9-C10
17	b	201	6N5	N22-C8-C9-C10

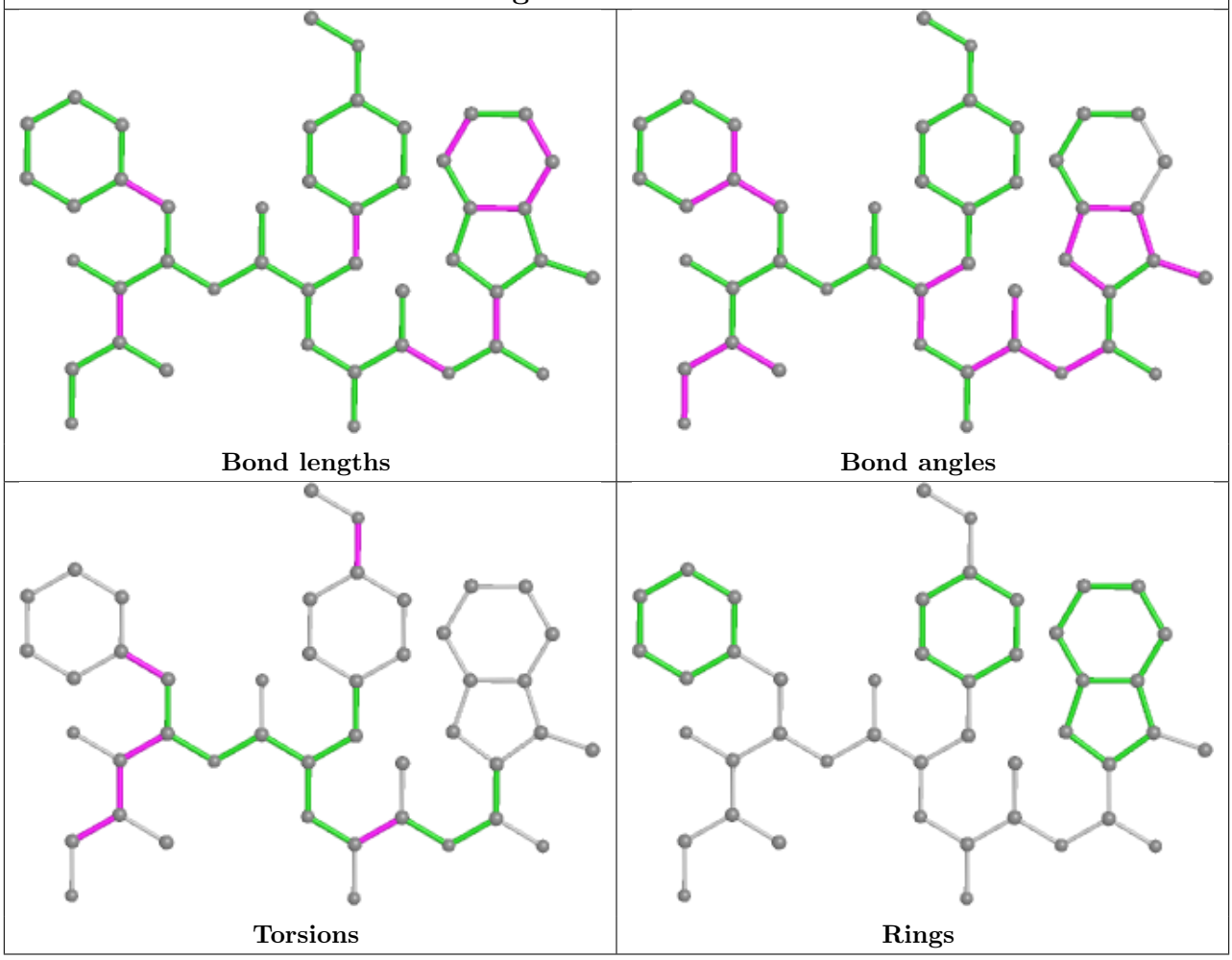
There are no ring outliers.

3 monomers are involved in 3 short contacts:

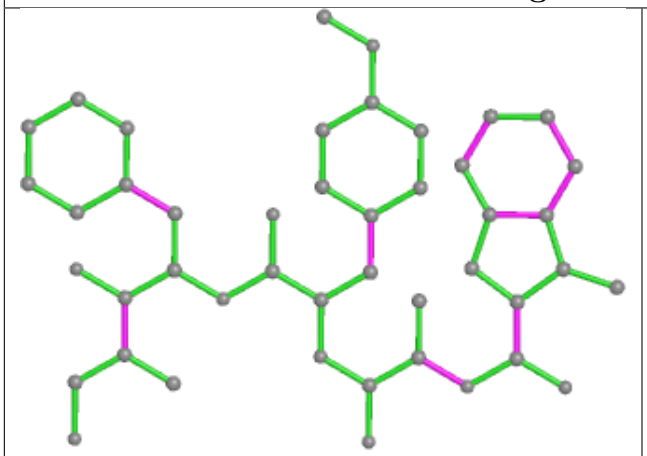
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	K	304	MES	1	0
18	Y	303	MES	1	0
17	K	301	6N5	1	0

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.

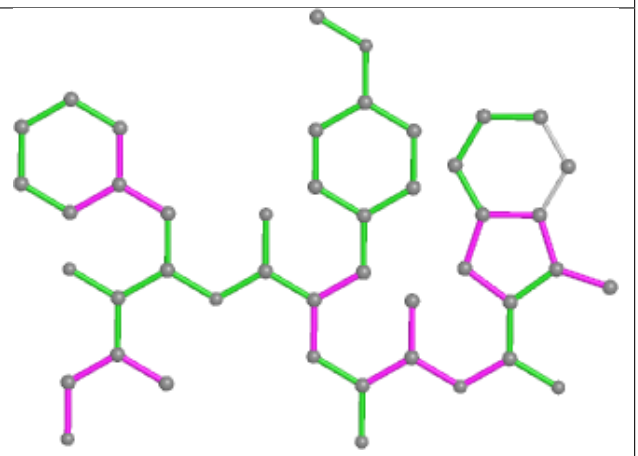
Ligand 6N5 b 201



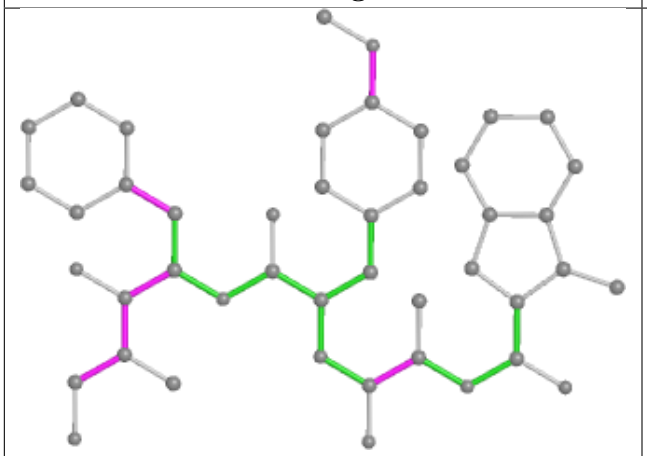
Ligand 6N5 N 201



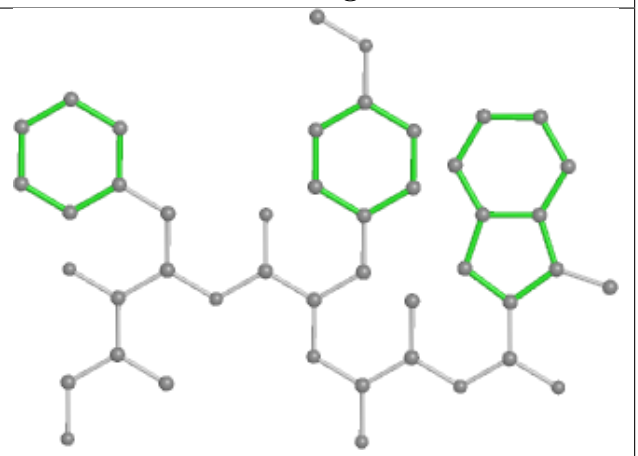
Bond lengths



Bond angles

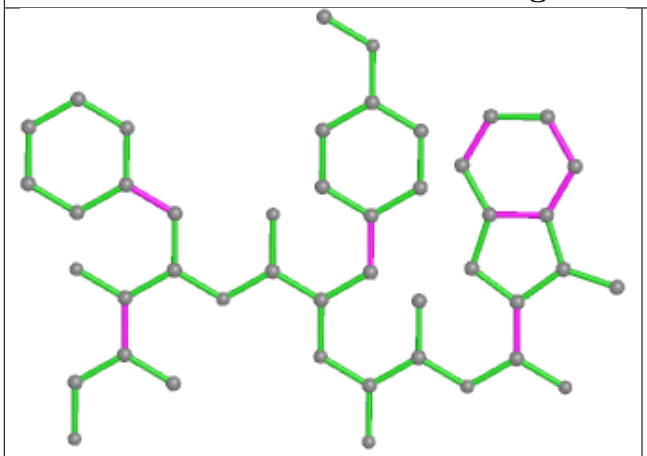


Torsions

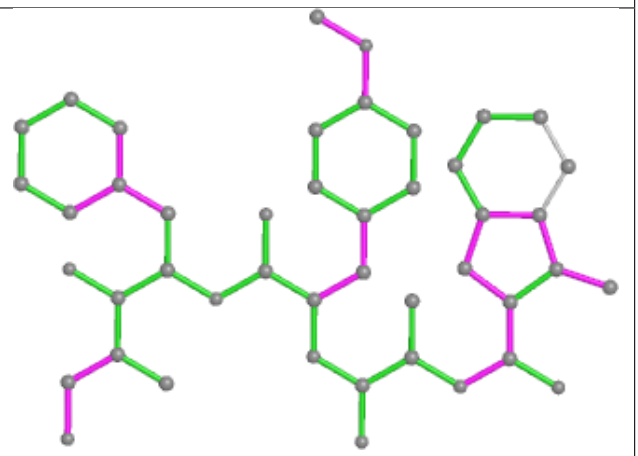


Rings

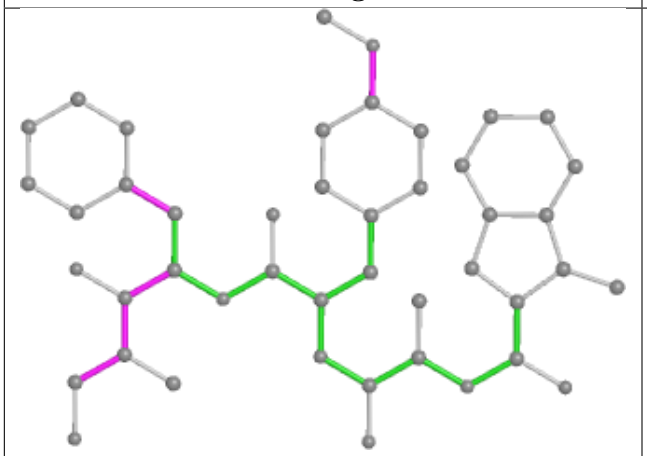
Ligand 6N5 K 301



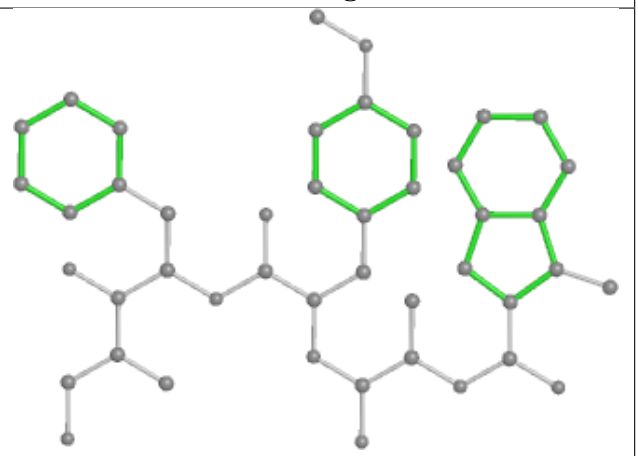
Bond lengths



Bond angles

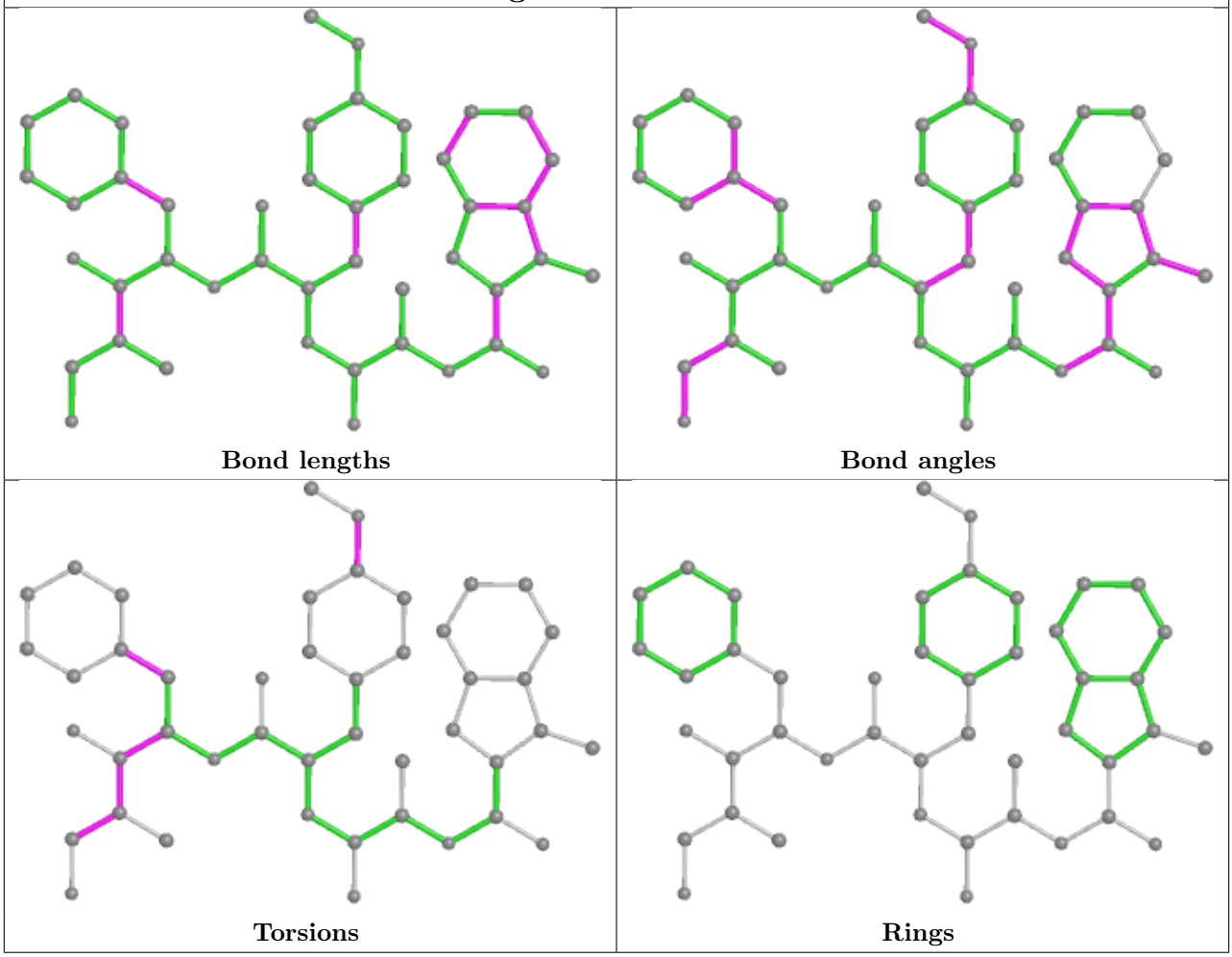


Torsions



Rings

Ligand 6N5 Y 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%)	-0.26	7 (2%)	53	54	42, 55, 98, 146	0
1	O	250/250 (100%)	-0.24	9 (3%)	42	42	45, 64, 105, 151	0
2	B	244/258 (94%)	-0.07	13 (5%)	26	25	40, 61, 111, 169	0
2	P	244/258 (94%)	-0.09	12 (4%)	29	28	42, 65, 110, 159	0
3	C	240/254 (94%)	-0.04	16 (6%)	17	16	39, 64, 126, 153	0
3	Q	240/254 (94%)	0.26	24 (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%)	45	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%)	24	23	49, 80, 133, 171	0
6	F	243/288 (84%)	-0.31	9 (3%)	41	41	38, 63, 113, 148	0
6	T	243/288 (84%)	-0.14	11 (4%)	33	31	43, 73, 132, 167	0
7	G	241/252 (95%)	-0.31	7 (2%)	51	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	77	45, 61, 89, 128	0
9	I	204/205 (99%)	-0.61	1 (0%)	91	92	35, 50, 80, 104	0
9	W	204/205 (99%)	-0.54	2 (0%)	82	83	36, 53, 82, 108	0
10	J	195/198 (98%)	-0.46	3 (1%)	73	76	35, 51, 80, 120	0
10	X	195/198 (98%)	-0.46	4 (2%)	63	65	37, 53, 84, 132	0
11	K	212/212 (100%)	-0.54	1 (0%)	91	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	77	34, 56, 85, 105	0

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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	83	30, 52, 82, 107	0
14	b	196/196 (100%)	-0.49	1 (0%)	91	92	30, 53, 85, 109	0
All	All	6320/6614 (95%)	-0.29	174 (2%)	53	54	25, 60, 109, 208	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	10.7
2	B	219	ALA	10.6
8	V	222	ASP	10.3
2	B	220	ASN	9.7
8	H	222	ASP	8.6
2	B	221	ASP	8.1
2	P	220	ASN	7.8
3	Q	50	LEU	7.1
1	O	1	MET	6.4
2	P	218	GLY	6.3
3	Q	206	LYS	6.2
1	A	1	MET	5.9
2	P	222	GLY	5.9
1	O	249	ALA	5.8
10	X	1	MET	5.8
8	H	221	CYS	5.7
3	Q	49	THR	5.5
8	V	221	CYS	5.5
3	Q	48	SER	5.4
10	J	1	MET	5.4
2	P	221	ASP	5.3
5	E	202	ASP	5.3
3	Q	239	GLN	5.2
5	S	202	ASP	5.1
4	D	242	GLU	5.1
2	B	51	VAL	5.0
2	P	51	VAL	4.9
4	R	241	ALA	4.8
3	Q	223	SER	4.6
6	T	2	THR	4.6
3	Q	238	LYS	4.5
3	Q	51	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
3	Q	205	ALA	4.4
5	S	54	GLU	4.1
11	Y	212	GLY	4.1
3	C	206	LYS	4.1
3	Q	236	GLN	4.0
5	E	123	GLY	4.0
3	C	202	GLN	3.9
10	X	194	ASP	3.9
9	W	1	SER	3.9
2	B	222	GLY	3.9
3	C	238	LYS	3.8
3	Q	240	GLU	3.8
3	Q	202	GLN	3.7
5	S	51	ASN	3.6
3	C	49	THR	3.5
10	J	194	ASP	3.5
7	G	222	ASP	3.5
13	M	1	THR	3.4
7	U	222	ASP	3.4
3	Q	55	THR	3.3
6	F	202	ASP	3.3
2	B	242	GLY	3.2
1	A	250	LEU	3.2
7	U	242	GLN	3.2
3	C	239	GLN	3.2
5	S	233	ILE	3.2
7	G	242	GLN	3.2
6	T	243	ILE	3.2
5	S	225	ASP	3.2
6	T	181	GLU	3.2
6	T	244	ASN	3.1
5	S	3	ASN	3.1
6	F	181	GLU	3.0
13	a	1	THR	3.0
5	E	201	ARG	3.0
4	R	242	GLU	2.9
3	C	225	GLU	2.9
6	F	243	ILE	2.9
7	G	241	GLU	2.9
9	W	133	LYS	2.9
2	P	225	TYR	2.9
6	F	244	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
5	E	233	ILE	2.8
7	U	241	GLU	2.8
3	C	236	GLN	2.8
7	U	2	GLY	2.8
1	O	52	SER	2.8
4	D	241	ALA	2.8
11	Y	106	ARG	2.8
6	T	230	ASP	2.8
3	Q	204	GLY	2.8
6	T	180	PRO	2.7
3	C	50	LEU	2.7
6	T	241	LYS	2.7
4	D	2	ARG	2.7
3	C	235	GLU	2.7
10	J	193	ASP	2.7
10	X	193	ASP	2.7
1	A	249	ALA	2.6
5	S	173	ARG	2.6
3	C	37	LYS	2.6
2	B	218	GLY	2.6
1	A	2	THR	2.6
1	O	229	THR	2.6
3	C	180	LYS	2.6
7	G	240	ALA	2.6
6	T	178	HIS	2.6
6	T	166	GLN	2.6
1	O	201	GLU	2.6
3	Q	58	THR	2.6
4	R	201	GLU	2.6
2	B	225	TYR	2.6
14	N	105	LYS	2.5
13	a	225	ILE	2.5
3	C	48	SER	2.5
3	Q	207	ASN	2.5
11	K	212	GLY	2.5
4	R	125	LEU	2.5
4	R	1	ASP	2.5
3	Q	167	LYS	2.5
6	F	201	GLU	2.4
5	S	201	ARG	2.4
2	P	59	ASP	2.4
6	T	205	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
14	N	195	GLN	2.4
3	Q	52	LEU	2.4
9	I	1	SER	2.4
3	Q	225	GLU	2.4
13	a	224	ASP	2.4
2	B	203	SER	2.4
1	A	248	GLU	2.4
3	Q	181	GLU	2.4
4	R	54	ASP	2.4
1	O	203	GLU	2.4
2	B	223	GLU	2.4
2	B	182	ASP	2.4
13	M	47	ASP	2.4
6	F	230	ASP	2.3
12	Z	210	ASP	2.3
5	S	180	LYS	2.3
3	C	181	GLU	2.3
3	C	175	LYS	2.3
1	O	250	LEU	2.3
1	A	229	THR	2.3
5	E	30	GLN	2.3
4	D	1	ASP	2.3
7	G	3	TYR	2.3
12	Z	1	GLN	2.3
5	E	54	GLU	2.3
8	V	145	ASP	2.3
1	A	52	SER	2.3
2	P	203	SER	2.3
6	F	205	GLU	2.3
7	G	68	ARG	2.3
3	Q	171	GLU	2.2
2	B	59	ASP	2.2
3	Q	235	GLU	2.2
2	P	217	LYS	2.2
3	Q	141	ASP	2.2
2	B	217	LYS	2.2
6	F	215	CYS	2.2
3	C	1	GLY	2.2
5	S	194	GLU	2.2
6	F	241	LYS	2.2
12	Z	116	GLU	2.1
1	O	231	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
4	R	203	LYS	2.1
3	C	240	GLU	2.1
6	T	201	GLU	2.1
7	G	188	GLU	2.1
2	P	240	LYS	2.1
3	Q	47	ARG	2.1
1	O	50	LYS	2.1
5	E	227	GLU	2.1
4	R	2	ARG	2.1
5	E	194	GLU	2.1
10	X	72	ASP	2.1
5	S	50	ARG	2.0
5	S	227	GLU	2.0
2	P	60	THR	2.0
5	S	210	LEU	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 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
17	6N5	N	201	45/45	0.82	0.26	27,41,53,56	45
17	6N5	b	201	45/45	0.86	0.23	27,41,55,60	0
15	MG	G	301	1/1	0.89	0.15	61,61,61,61	0
15	MG	N	202	1/1	0.93	0.16	60,60,60,60	0
17	6N5	K	301	45/45	0.93	0.15	28,39,50,57	0
17	6N5	Y	301	45/45	0.94	0.14	24,36,49,56	0
15	MG	K	303	1/1	0.94	0.18	46,46,46,46	0

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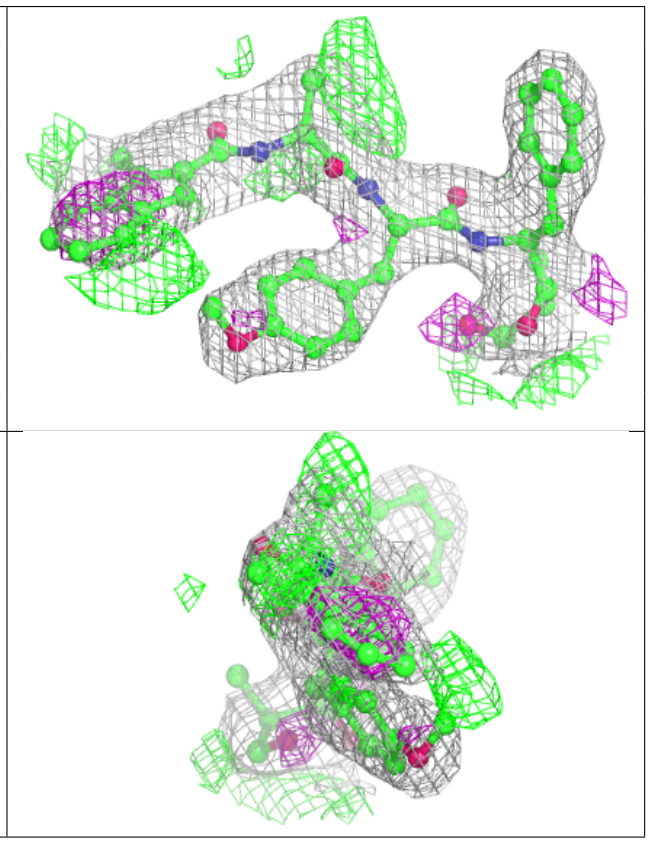
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	Z	301	1/1	0.95	0.40	66,66,66,66	0
15	MG	L	301	1/1	0.96	0.15	72,72,72,72	0
15	MG	I	301	1/1	0.97	0.17	60,60,60,60	0
18	MES	K	304	12/12	0.97	0.15	34,35,41,50	12
15	MG	X	201	1/1	0.98	0.34	34,34,34,34	0
15	MG	Y	302	1/1	0.98	0.08	37,37,37,37	0
15	MG	K	302	1/1	0.98	0.06	56,56,56,56	0
15	MG	I	302	1/1	0.98	0.07	55,55,55,55	0
18	MES	Y	303	12/12	0.98	0.12	32,35,36,39	12
16	CL	U	301	1/1	0.99	0.10	46,46,46,46	0
16	CL	G	302	1/1	1.00	0.11	44,44,44,44	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.

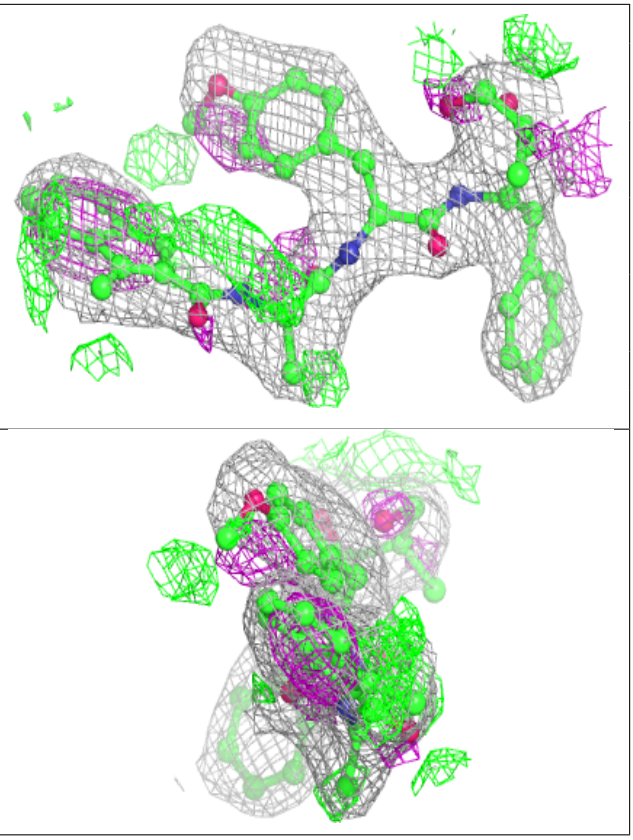
Electron density around 6N5 N 201:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



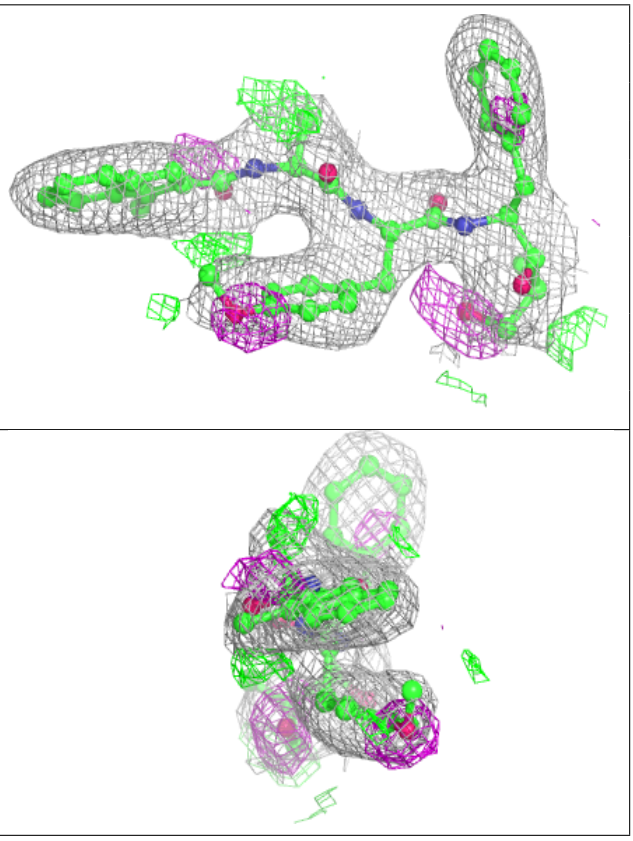
Electron density around 6N5 b 201:

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



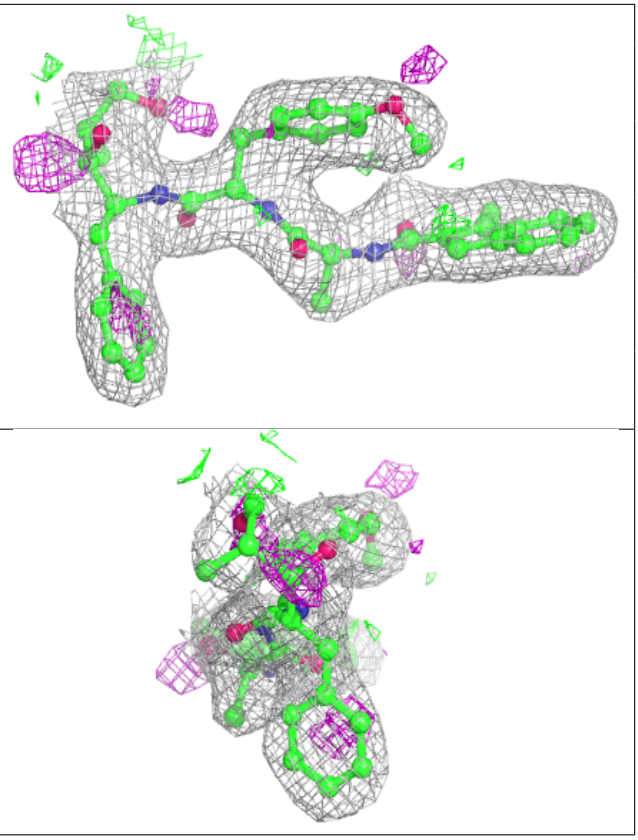
Electron density around 6N5 K 301:

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



Electron density around 6N5 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)



6.5 Other polymers (i)

There are no such residues in this entry.