Full wwPDB X-ray Structure Validation Report ⓘ

Jul 10, 2024 – 01:51 am BST

PDB ID	:	9FST
Title	:	Yeast 20S proteasome with human beta1i (1-51) in complex with epoxyketone inhibitor LU-001i
Authors	:	Maurits, E.; Huber, E.M.; Dekker, P.M.; Wang, X.; Heinemeyer, W.; Florea, B.I.; Groll, M.; Overkleeft, H.S.
Deposited on	:	2024-06-21
Resolution	:	2.75 Å(reported)

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

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

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

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

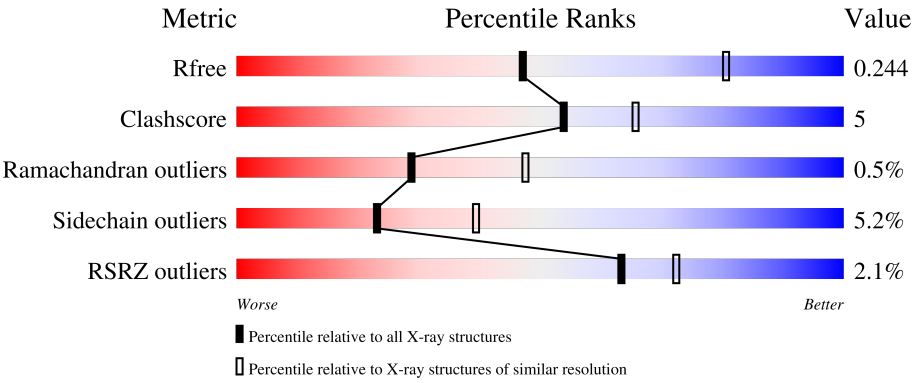
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	90% 9% •
1	O	250	2% 92% 8%
2	B	258	3% 73% 20% • 5%
2	P	258	4% 76% 18% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	254	5% 82% 11% 6%
3	Q	254	7% 83% 10% 6%
4	D	260	% 77% 13% 10%
4	R	260	% 77% 12% 10%
5	E	234	% 86% 12%
5	S	234	2% 86% 11%
6	F	288	2% 75% 8% 16%
6	T	288	3% 75% 9% 16%
7	G	252	% 81% 14%
7	U	252	2% 82% 12%
8	H	232	3% 82% 14%
8	V	232	2% 80% 15%
9	I	205	% 89% 11%
9	W	205	2% 88% 11%
10	J	198	% 83% 13%
10	X	198	% 78% 18%
11	K	211	% 85% 13%
11	Y	211	% 82% 16%
12	L	222	% 80% 18%
12	Z	222	% 83% 15%
13	M	246	% 80% 10% 9%
13	a	246	% 88% 7%
14	N	195	% 86% 14%
14	b	195	% 97%

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 49773 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	1	0
			1914	1207	324	380	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	1	0
			1767	1121	306	336	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	225	Total	C	N	O	S	0	0	0
			1761	1114	301	339	7			
13	a	228	Total	C	N	O	S	0	0	0
			1786	1131	305	343	7			

- Molecule 14 is a protein called Proteasome subunit beta type-9,Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	195	Total	C	N	O	S	0	0	0
			1495	946	243	299	7			
14	b	195	Total	C	N	O	S	0	0	0
			1495	946	243	299	7			

- Molecule 15 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Cl	0	0
			1	1		

Continued on next page...

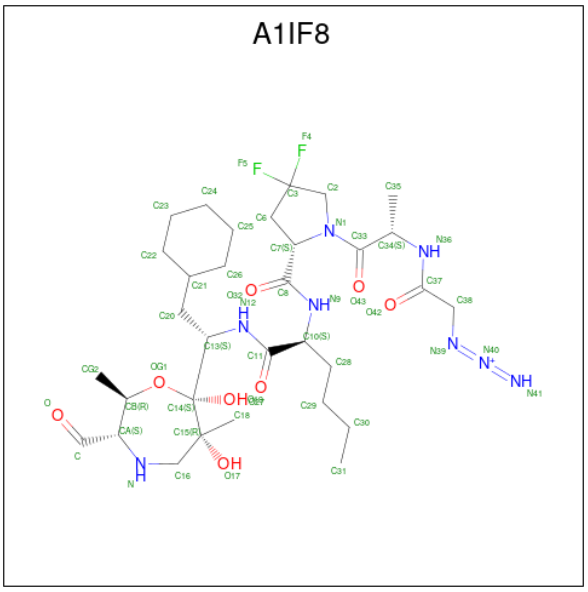
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	1	Total Cl 1 1	0	0
15	U	1	Total Cl 1 1	0	0
15	V	1	Total Cl 1 1	0	0

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

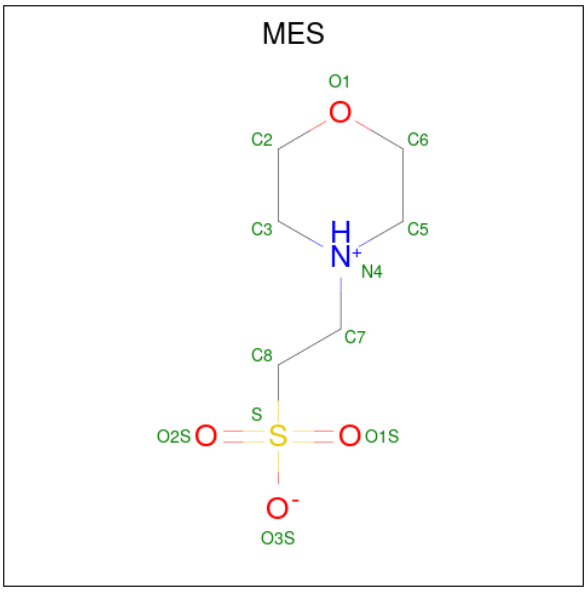
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Mg 1 1	0	0
16	I	1	Total Mg 1 1	0	0
16	K	1	Total Mg 1 1	0	0
16	N	1	Total Mg 1 1	0	0
16	W	1	Total Mg 1 1	0	0
16	X	1	Total Mg 1 1	0	0
16	Y	1	Total Mg 1 1	0	0
16	Z	1	Total Mg 1 1	0	0

- Molecule 17 is azanylidene-[2-[[(2S)-1-[(2S)-2-[[(2S)-1-[[(1S)-2-cyclohexyl-1-[(2R,3S,6R,7S)-3-methanoyl-2,6-dimethyl-6,7-bis(oxidanyl)-1,4-oxazepan-7-yl]ethyl]amino]-1-oxidanylidene-hexan-2-yl]carbamoyl]-4,4-bis(fluoranyl)pyrrolidin-1-yl]-1-oxidanylidene-propan-2-yl]amino]-2-oxidanylidene-ethyl]imino-azanium (three-letter code: A1IF8) (formula: $C_{32}H_{53}F_2N_8O_8$) (labeled as "Ligand of Interest" by depositor).



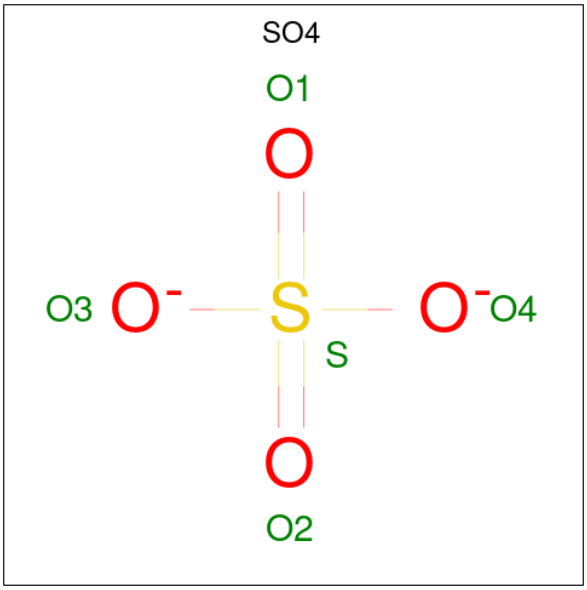
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	K	1	Total	C	F	N	O	0	0
			50	32	2	8	8		
17	N	1	Total	C	F	N	O	0	0
			50	32	2	8	8		
17	Y	1	Total	C	F	N	O	0	0
			50	32	2	8	8		
17	b	1	Total	C	F	N	O	0	0
			50	32	2	8	8		

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



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

- Molecule 19 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	N	1	Total	O	S	0	0
			5	4	1		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	6	Total	O	0	0
			6	6		
20	B	9	Total	O	0	0
			9	9		
20	C	7	Total	O	0	0
			7	7		
20	D	7	Total	O	0	0
			7	7		
20	E	4	Total	O	0	0
			4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	F	6	Total O 6 6	0	0
20	G	17	Total O 17 17	0	0
20	H	10	Total O 10 10	0	0
20	I	10	Total O 10 10	0	0
20	J	11	Total O 11 11	0	0
20	K	11	Total O 11 11	0	0
20	L	10	Total O 10 10	0	0
20	M	17	Total O 17 17	0	0
20	N	4	Total O 4 4	0	0
20	O	3	Total O 3 3	0	0
20	P	5	Total O 5 5	0	0
20	Q	9	Total O 9 9	0	0
20	R	5	Total O 5 5	0	0
20	S	4	Total O 4 4	0	0
20	T	11	Total O 11 11	0	0
20	U	11	Total O 11 11	0	0
20	V	13	Total O 13 13	0	0
20	W	11	Total O 11 11	0	0
20	X	13	Total O 13 13	0	0
20	Y	14	Total O 14 14	0	0
20	Z	13	Total O 13 13	0	0

Continued on next page...

Continued from previous page...

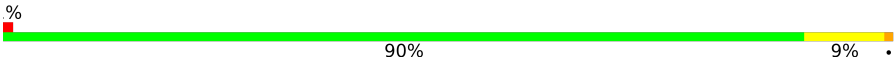
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	a	12	Total O 12 12	0	0
20	b	18	Total O 18 18	0	0

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.

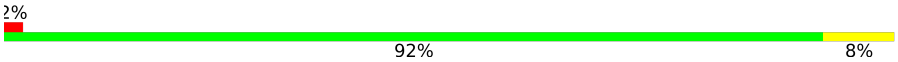
• Molecule 1: Proteasome subunit alpha type-2

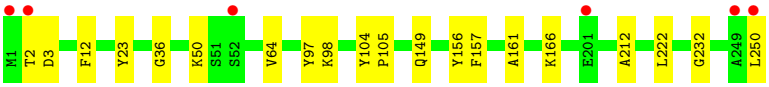
Chain A:



• Molecule 1: Proteasome subunit alpha type-2

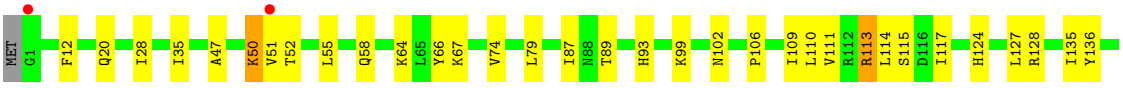
Chain O:

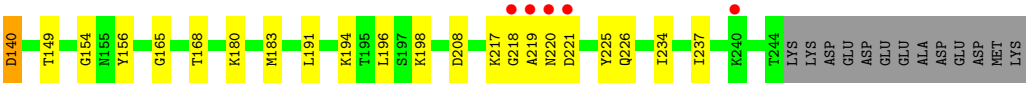




• Molecule 2: Proteasome subunit alpha type-3

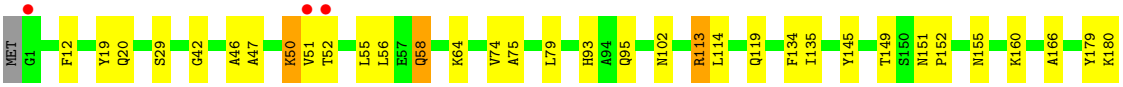
Chain B:

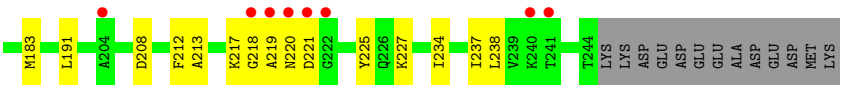




• Molecule 2: Proteasome subunit alpha type-3

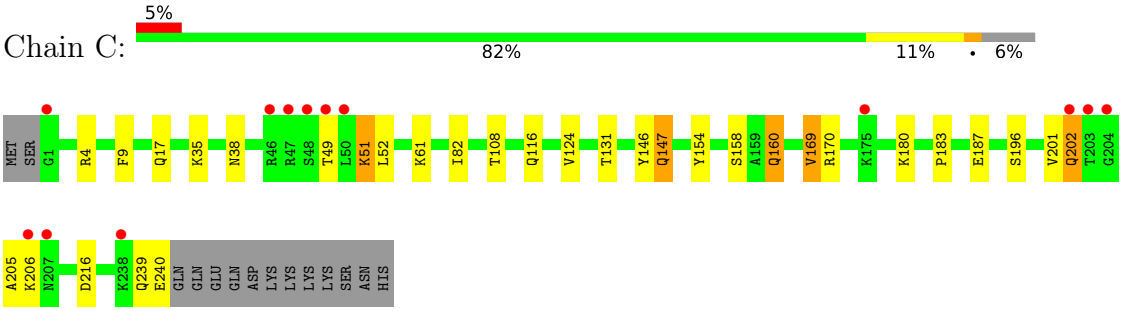
Chain P:





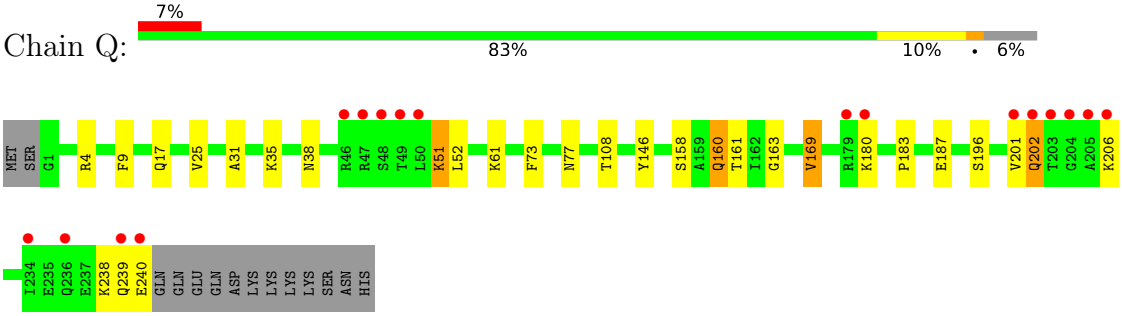
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



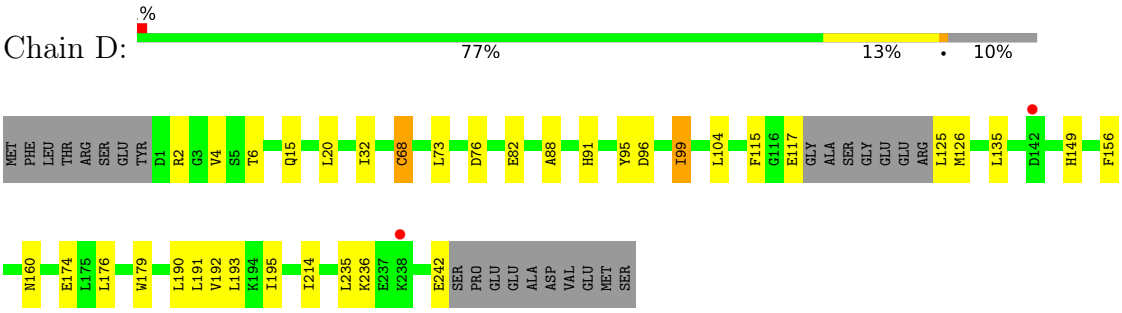
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



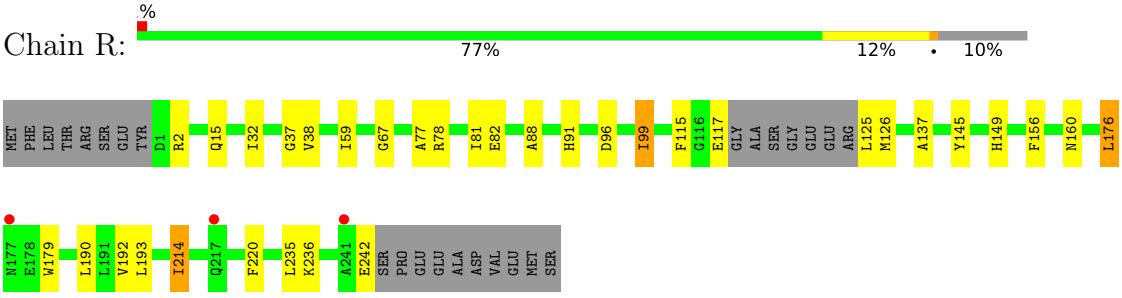
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



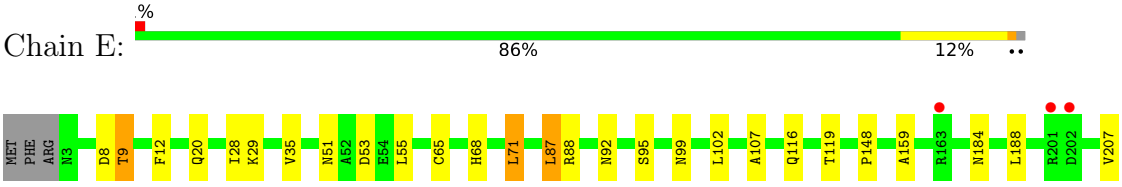
• Molecule 4: Proteasome subunit alpha type-5

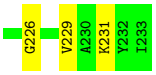
Chain R:



• Molecule 5: Proteasome subunit alpha type-6

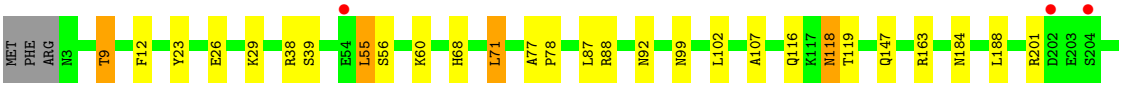
Chain E:





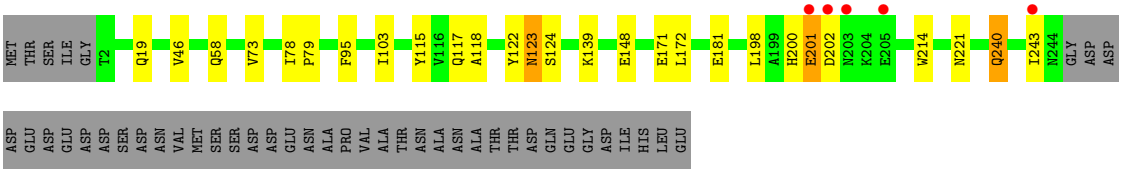
• Molecule 5: Proteasome subunit alpha type-6

Chain S:



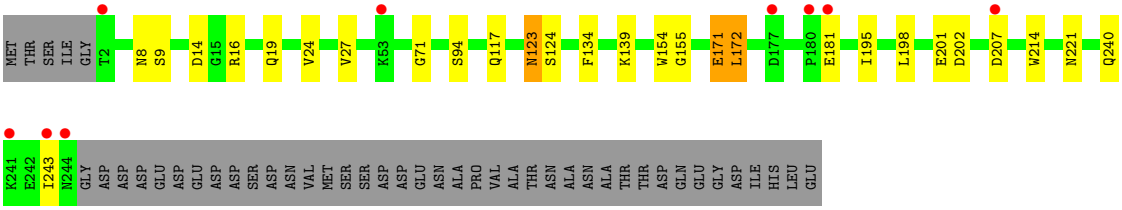
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



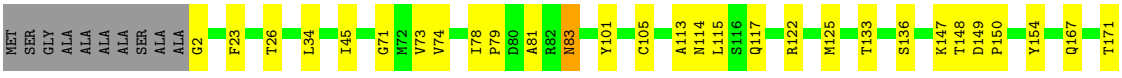
• Molecule 6: Probable proteasome subunit alpha type-7

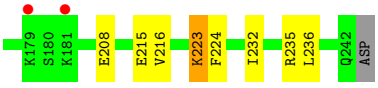
Chain T:



• Molecule 7: Proteasome subunit alpha type-1

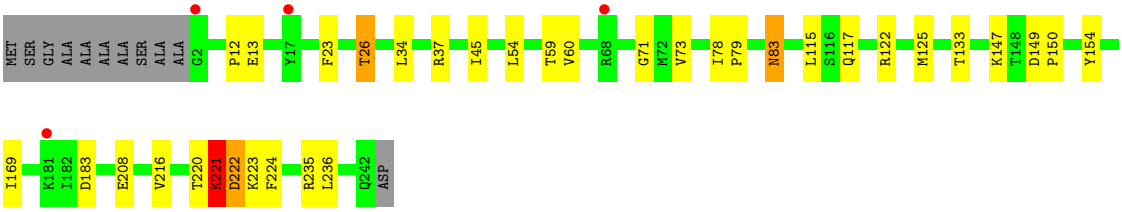
Chain G:



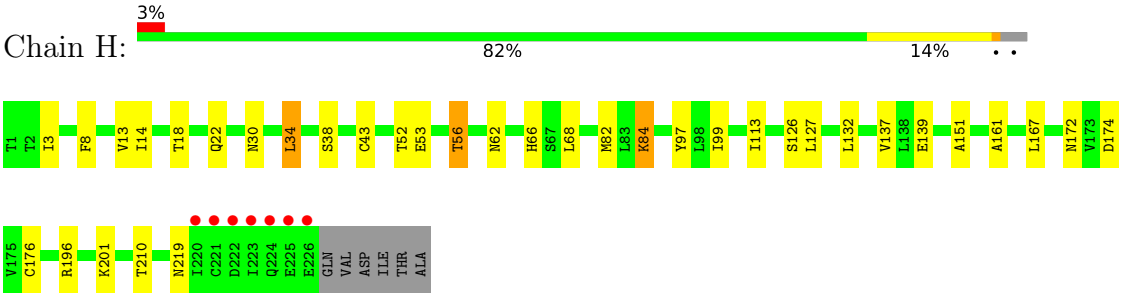


• Molecule 7: Proteasome subunit alpha type-1

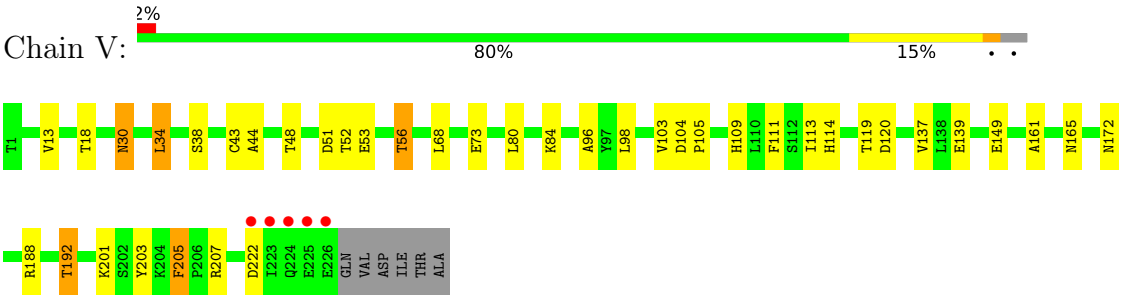
Chain U:



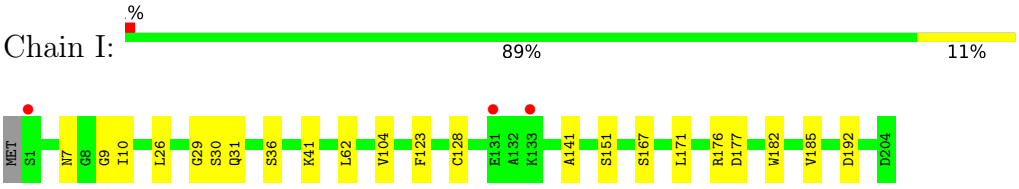
• Molecule 8: Proteasome subunit beta type-2



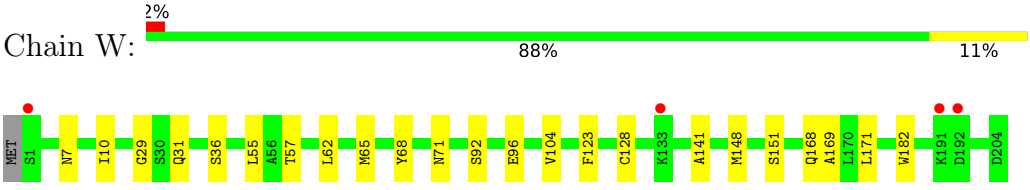
• Molecule 8: Proteasome subunit beta type-2



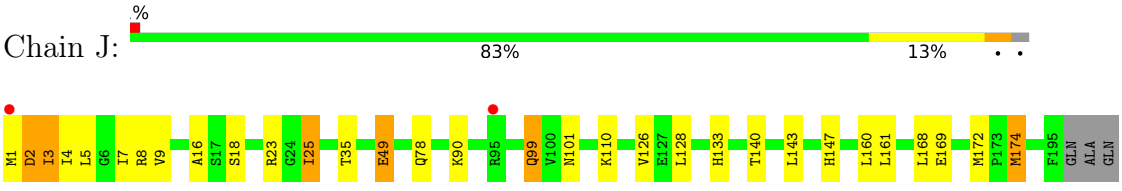
• Molecule 9: Proteasome subunit beta type-3



• Molecule 9: Proteasome subunit beta type-3

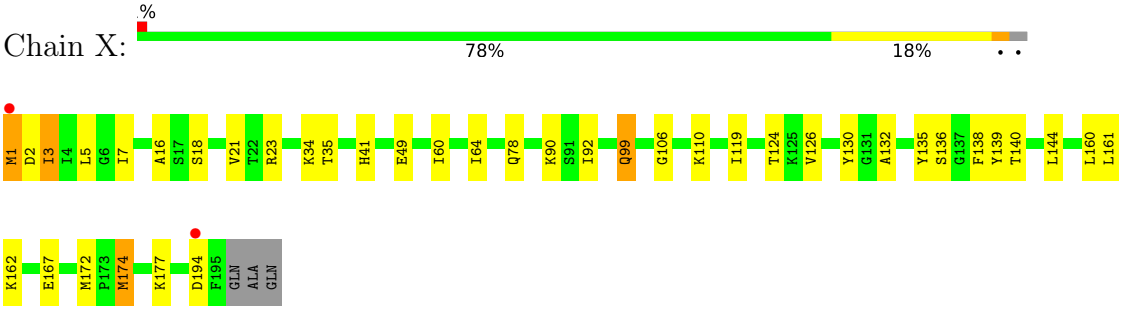


• Molecule 10: Proteasome subunit beta type-4



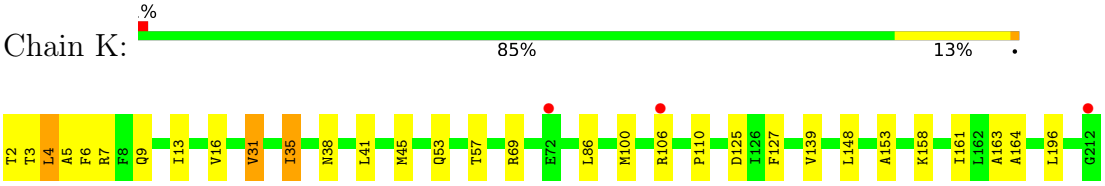
• Molecule 10: Proteasome subunit beta type-4

Chain X:



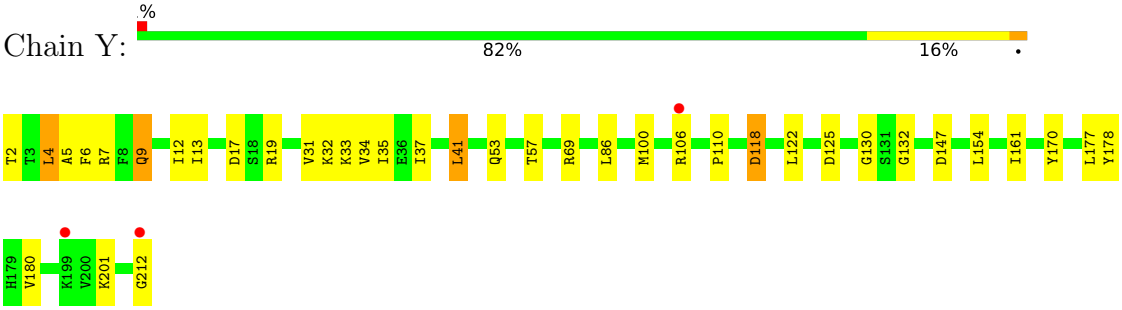
• Molecule 11: Proteasome subunit beta type-5

Chain K:



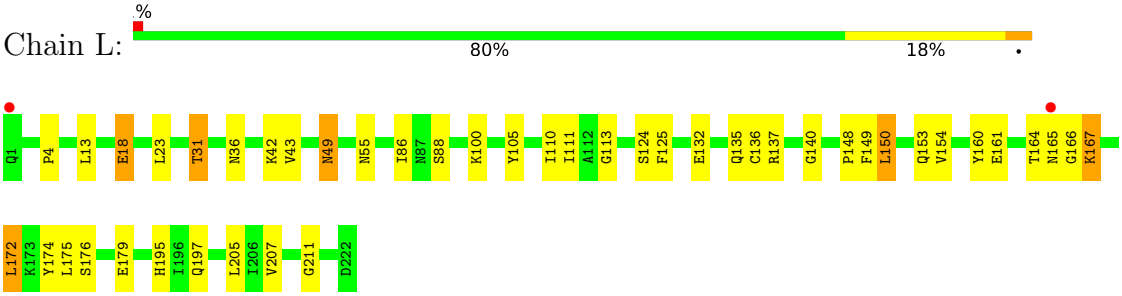
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



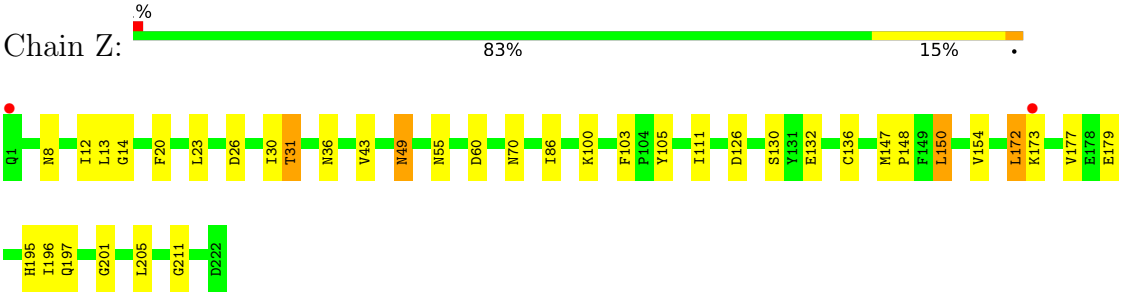
• Molecule 12: Proteasome subunit beta type-6

Chain L:



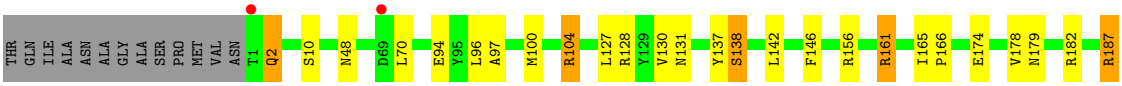
• Molecule 12: Proteasome subunit beta type-6

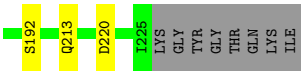
Chain Z:



• Molecule 13: Proteasome subunit beta type-7

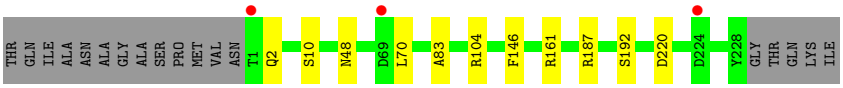
Chain M:





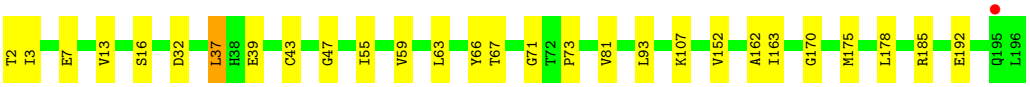
• Molecule 13: Proteasome subunit beta type-7

Chain a:



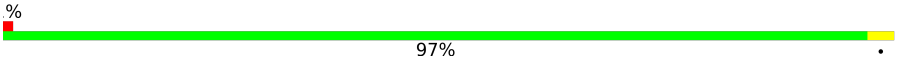
• Molecule 14: Proteasome subunit beta type-9,Proteasome subunit beta type-1

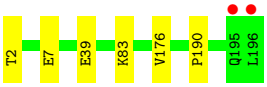
Chain N:



• Molecule 14: Proteasome subunit beta type-9,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	135.37Å 300.16Å 143.97Å 90.00° 112.78° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 29.95 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.00-2.75) 96.9 (29.95-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.205 , 0.245 0.209 , 0.244	Depositor DCC
R_{free} test set	13235 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	63.6	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 31.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	49773	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL, MES, A1IF8, MG

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	0.68	0/1952	0.77	0/2642
1	O	0.67	0/1952	0.77	0/2642
2	B	0.67	0/1945	0.78	0/2633
2	P	0.68	0/1934	0.79	0/2618
3	C	0.69	0/1910	0.79	0/2586
3	Q	0.70	0/1910	0.78	0/2586
4	D	0.70	0/1837	0.80	0/2475
4	R	0.69	0/1837	0.76	0/2475
5	E	0.68	0/1800	0.79	0/2433
5	S	0.68	0/1800	0.78	0/2433
6	F	0.66	0/1932	0.78	0/2609
6	T	0.71	0/1932	0.78	0/2609
7	G	0.66	0/1945	0.80	0/2634
7	U	0.69	0/1945	0.82	1/2634 (0.0%)
8	H	0.67	0/1750	0.81	0/2373
8	V	0.66	0/1750	0.81	0/2373
9	I	0.68	0/1611	0.80	0/2174
9	W	0.68	0/1611	0.79	0/2174
10	J	0.65	0/1589	0.77	0/2142
10	X	0.64	0/1589	0.81	0/2142
11	K	0.68	0/1674	0.82	0/2264
11	Y	0.68	0/1674	0.80	0/2264
12	L	0.64	0/1795	0.80	0/2420
12	Z	0.66	0/1806	0.80	0/2435
13	M	0.66	0/1791	0.83	0/2431
13	a	0.67	0/1817	0.81	0/2465
14	N	0.66	0/1524	0.78	0/2063
14	b	0.68	0/1524	0.80	0/2063
All	All	0.67	0/50136	0.79	1/67792 (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})
7	U	222	ASP	C-N-CA	5.30	134.94	121.70

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	14	0
1	O	1915	0	1929	8	0
2	B	1914	0	1910	32	0
2	P	1904	0	1904	23	0
3	C	1881	0	1895	14	0
3	Q	1881	0	1895	12	0
4	D	1813	0	1797	20	0
4	R	1813	0	1797	21	0
5	E	1773	0	1775	17	0
5	S	1773	0	1775	18	0
6	F	1892	0	1883	15	0
6	T	1892	0	1883	13	0
7	G	1907	0	1901	20	0
7	U	1907	0	1901	17	0
8	H	1719	0	1719	18	0
8	V	1719	0	1719	28	0
9	I	1581	0	1574	11	0
9	W	1581	0	1574	14	0
10	J	1561	0	1569	21	0
10	X	1561	0	1569	26	0
11	K	1637	0	1585	26	0
11	Y	1637	0	1585	24	0
12	L	1757	0	1711	34	0
12	Z	1767	0	1717	27	0
13	M	1761	0	1765	17	0
13	a	1786	0	1790	0	0
14	N	1495	0	1450	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	b	1495	0	1450	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	U	1	0	0	0	0
15	V	1	0	0	1	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	K	1	0	0	0	0
16	N	1	0	0	0	0
16	W	1	0	0	0	0
16	X	1	0	0	0	0
16	Y	1	0	0	0	0
16	Z	1	0	0	0	0
17	K	50	0	0	2	0
17	N	50	0	0	1	0
17	Y	50	0	0	2	0
17	b	50	0	0	0	0
18	K	12	0	13	0	0
18	M	12	0	13	0	0
18	Y	12	0	13	1	0
18	a	12	0	13	0	0
19	N	5	0	0	1	0
20	A	6	0	0	0	0
20	B	9	0	0	0	0
20	C	7	0	0	0	0
20	D	7	0	0	0	0
20	E	4	0	0	0	0
20	F	6	0	0	0	0
20	G	17	0	0	1	0
20	H	10	0	0	0	0
20	I	10	0	0	0	0
20	J	11	0	0	1	0
20	K	11	0	0	0	0
20	L	10	0	0	0	0
20	M	17	0	0	1	0
20	N	4	0	0	0	0
20	O	3	0	0	0	0
20	P	5	0	0	0	0
20	Q	9	0	0	0	0
20	R	5	0	0	0	0
20	S	4	0	0	0	0
20	T	11	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	U	11	0	0	0	0
20	V	13	0	0	0	0
20	W	11	0	0	0	0
20	X	13	0	0	1	0
20	Y	14	0	0	0	0
20	Z	13	0	0	1	0
20	a	12	0	0	0	0
20	b	18	0	0	0	0
All	All	49773	0	49003	459	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 5.

All (459) 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)
12:L:164:THR:O	12:L:167:LYS:HD2	1.61	1.00
10:J:25:ILE:HD11	10:X:135:TYR:CD1	2.03	0.93
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.52	0.91
14:N:2:THR:HG21	14:N:162:ALA:CB	2.06	0.86
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.43	0.83
7:U:23:PHE:O	7:U:26:THR:HB	1.81	0.81
12:L:164:THR:O	12:L:167:LYS:CD	2.30	0.79
14:N:2:THR:HG21	14:N:162:ALA:HB3	1.64	0.78
10:J:25:ILE:HD11	10:X:135:TYR:CE1	2.19	0.77
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.69	0.75
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.68	0.74
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.53	0.74
1:O:12:PHE:H	2:P:20:GLN:HE22	1.34	0.73
5:E:12:PHE:HB2	6:F:19:GLN:HE22	1.54	0.73
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.54	0.72
2:B:12:PHE:H	3:C:17:GLN:HE22	1.38	0.72
7:U:221:LYS:O	7:U:221:LYS:HD3	1.88	0.72
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.90	0.71
3:C:35:LYS:HG2	3:C:158:SER:O	1.91	0.70
13:M:2:GLN:NE2	20:M:401:HOH:O	2.25	0.69
14:N:152:VAL:HA	14:N:175:MET:HE1	1.73	0.69
11:K:5:ALA:HB3	11:K:100:MET:HE1	1.74	0.69
8:H:201:LYS:HE2	12:Z:179:GLU:OE2	1.93	0.68
3:Q:35:LYS:HG2	3:Q:158:SER:O	1.94	0.68
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.07	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:5:ALA:CB	11:K:100:MET:HE1	2.23	0.67
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.07	0.67
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.40	0.67
12:Z:43:VAL:HG12	12:Z:205:LEU:HD22	1.76	0.67
11:K:53:GLN:O	11:K:57:THR:HG23	1.95	0.66
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.43	0.66
6:F:123:ASN:C	6:F:123:ASN:HD22	1.99	0.66
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.95	0.65
4:R:176:LEU:HD22	5:S:55:LEU:HD22	1.77	0.65
3:C:9:PHE:H	4:D:15:GLN:HE22	1.44	0.65
7:G:23:PHE:O	7:G:26:THR:HB	1.97	0.65
3:C:51:LYS:O	3:C:52:LEU:HB2	1.97	0.65
2:B:67:LYS:HG3	2:B:226:GLN:OE1	1.97	0.64
8:H:3:ILE:HG22	8:H:99:ILE:HD12	1.78	0.64
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.80	0.64
11:Y:34:VAL:HG11	11:Y:178:TYR:CE1	2.32	0.64
2:B:180:LYS:O	2:B:183:MET:HB2	1.98	0.63
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.64	0.63
4:R:176:LEU:HA	5:S:55:LEU:HD21	1.79	0.62
8:V:203:TYR:O	8:V:205:PHE:CD2	2.53	0.62
10:J:147:HIS:HB3	10:J:160:LEU:HD11	1.81	0.61
8:H:84:LYS:HA	8:H:113:ILE:HD11	1.81	0.61
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.83	0.61
14:N:2:THR:HG21	14:N:162:ALA:HB1	1.81	0.61
8:V:84:LYS:HA	8:V:113:ILE:HD11	1.81	0.61
7:G:45:ILE:HG22	7:G:216:VAL:HG13	1.83	0.61
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.83	0.60
2:B:93[B]:HIS:CD2	2:B:113:ARG:HD3	2.36	0.60
7:G:147:LYS:O	7:G:154:TYR:HA	2.01	0.60
4:R:176:LEU:HD22	5:S:55:LEU:CD2	2.31	0.60
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.66	0.60
12:Z:172:LEU:N	12:Z:172:LEU:HD23	2.17	0.60
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.84	0.60
7:G:73:VAL:HG12	7:G:133:THR:HB	1.82	0.59
5:S:12:PHE:H	6:T:19:GLN:HE22	1.48	0.59
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.85	0.59
11:K:5:ALA:HB3	11:K:100:MET:CE	2.32	0.59
10:X:139:TYR:CE2	10:X:172:MET:HE2	2.38	0.59
8:H:139:GLU:OE2	8:H:139:GLU:HA	2.03	0.59
11:Y:2:THR:OG1	11:Y:132:GLY:HA3	2.02	0.59
8:H:43:CYS:SG	8:H:56:THR:HG23	2.42	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:134:PHE:O	2:P:149:THR:HA	2.03	0.59
7:G:83:ASN:C	7:G:83:ASN:HD22	2.06	0.58
4:R:77:ALA:O	4:R:81:ILE:HG12	2.03	0.58
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.84	0.58
12:L:4:PRO:O	13:M:104:ARG:NH1	2.36	0.58
11:Y:7:ARG:NH1	11:Y:110:PRO:O	2.36	0.58
8:V:203:TYR:O	8:V:205:PHE:CE2	2.57	0.58
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.69	0.58
8:V:80:LEU:HD12	8:V:111:PHE:CG	2.39	0.58
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.68	0.58
12:L:164:THR:O	12:L:165:ASN:C	2.42	0.57
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.03	0.57
6:F:123:ASN:HD22	6:F:124:SER:N	2.03	0.57
7:U:45:ILE:HG22	7:U:216:VAL:HG22	1.87	0.57
10:X:7:ILE:CD1	10:X:160:LEU:HD23	2.35	0.57
7:U:71:GLY:HA3	7:U:224:PHE:CE1	2.40	0.57
5:E:68:HIS:HE1	5:E:102:LEU:O	1.88	0.56
8:H:52:THR:O	8:H:56:THR:OG1	2.23	0.56
9:I:26:LEU:HD21	9:I:185:VAL:HG23	1.87	0.56
2:P:93:HIS:CE1	2:P:113:ARG:HG2	2.39	0.56
2:B:217:LYS:C	2:B:219:ALA:H	2.08	0.56
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.40	0.56
2:P:213:ALA:HA	2:P:227:LYS:O	2.05	0.56
8:V:205:PHE:CD2	8:V:205:PHE:N	2.72	0.56
6:F:198:LEU:HD12	6:F:243:ILE:HG22	1.87	0.56
4:D:91:HIS:HB3	4:D:99:ILE:HG21	1.86	0.56
9:I:176:ARG:NH2	12:Z:147:MET:CE	2.69	0.56
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.54	0.56
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.70	0.56
17:Y:301:A1IF8:C2	17:Y:301:A1IF8:C35	2.84	0.56
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.41	0.56
12:L:164:THR:C	12:L:167:LYS:HD2	2.25	0.55
10:J:7:ILE:CD1	10:J:160:LEU:HD23	2.36	0.55
1:A:12:PHE:H	2:B:20:GLN:HE22	1.55	0.55
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.88	0.55
2:B:93[B]:HIS:CG	2:B:113:ARG:HD3	2.41	0.55
5:S:163:ARG:HD3	5:S:201:ARG:NH1	2.21	0.55
8:V:114:HIS:HB3	15:V:301:CL:CL	2.44	0.55
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.41	0.55
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.35	0.55
13:M:165:ILE:HB	13:M:166:PRO:HD3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	1.88	0.55
9:W:62:LEU:CD1	9:W:104:VAL:HG21	2.36	0.55
10:X:5:LEU:HD23	10:X:132:ALA:HB2	1.88	0.55
6:T:14:ASP:CB	6:T:16:ARG:HD3	2.37	0.54
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.90	0.54
7:G:34:LEU:C	7:G:34:LEU:HD23	2.26	0.54
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.07	0.54
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.38	0.54
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.38	0.54
6:T:8:ASN:O	6:T:9:SER:OG	2.26	0.54
8:H:43:CYS:SG	8:H:56:THR:CG2	2.97	0.53
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.91	0.53
11:K:100:MET:HE3	11:K:127:PHE:O	2.09	0.53
5:E:88:ARG:O	5:E:92:ASN:HB2	2.08	0.53
2:P:219:ALA:HB2	2:P:225:TYR:HB2	1.91	0.53
1:A:29:LYS:HE2	1:A:29:LYS:HA	1.91	0.53
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.89	0.53
8:V:80:LEU:HD23	8:V:80:LEU:C	2.28	0.53
14:N:2:THR:CG2	14:N:162:ALA:CB	2.85	0.52
11:Y:201:LYS:HE2	11:Y:212:GLY:HA2	1.91	0.52
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.91	0.52
2:P:42:GLY:HA2	2:P:145:TYR:CE1	2.44	0.52
11:K:3:THR:HG22	11:K:16:VAL:HG12	1.91	0.52
4:R:149:HIS:O	4:R:156:PHE:HA	2.09	0.52
12:L:179:GLU:OE2	8:V:201:LYS:HE2	2.10	0.52
6:T:123:ASN:C	6:T:123:ASN:HD22	2.13	0.52
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.92	0.51
10:J:5:LEU:HD21	10:J:140:THR:HG21	1.92	0.51
14:N:37:LEU:HB3	14:N:63:LEU:HD12	1.93	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
14:N:55:ILE:HD11	14:N:93:LEU:HD13	1.93	0.51
1:O:97:TYR:CE1	1:O:105:PRO:HA	2.46	0.51
1:A:64:VAL:HG11	1:A:212:ALA:HB3	1.93	0.51
14:N:66:TYR:CD1	14:N:73:PRO:HB3	2.46	0.51
8:V:205:PHE:N	8:V:205:PHE:HD2	2.08	0.51
7:G:101:TYR:OH	8:H:66:HIS:HE1	1.94	0.51
7:U:78:ILE:N	7:U:79:PRO:CD	2.74	0.51
10:X:5:LEU:HD21	10:X:140:THR:HG21	1.92	0.51
10:J:147:HIS:CB	10:J:160:LEU:HD11	2.41	0.51
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.06	0.51
14:N:37:LEU:HD21	14:N:43:CYS:HB3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:200:HIS:CG	6:F:200:HIS:O	2.65	0.50
14:N:3:ILE:HG22	14:N:16:SER:HB2	1.92	0.50
7:U:147:LYS:O	7:U:154:TYR:HA	2.11	0.50
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.58	0.50
7:G:73:VAL:CG1	7:G:133:THR:HB	2.41	0.50
1:O:149:GLN:O	1:O:156:TYR:HA	2.11	0.50
5:S:38:ARG:NH1	5:S:39:SER:O	2.44	0.50
6:T:198:LEU:HD12	6:T:243:ILE:HG22	1.93	0.50
8:H:18:THR:HG21	8:H:172:ASN:HB2	1.93	0.50
10:J:2:ASP:OD1	10:J:2:ASP:N	2.44	0.50
8:V:205:PHE:CE1	9:W:168:GLN:HG3	2.46	0.50
8:H:137:VAL:HG21	8:H:161:ALA:HB2	1.94	0.50
11:K:7:ARG:NH1	11:K:110:PRO:O	2.44	0.50
4:R:38:VAL:HG11	4:R:137:ALA:HB1	1.93	0.50
8:V:34:LEU:HD12	8:V:44:ALA:HB2	1.93	0.50
13:M:161:ARG:HH11	13:M:161:ARG:CG	2.24	0.50
14:N:2:THR:CG2	14:N:162:ALA:HB1	2.41	0.50
7:U:34:LEU:HD12	7:U:169:ILE:CG2	2.41	0.49
5:E:9:THR:HG21	5:E:119:THR:HA	1.94	0.49
5:S:77:ALA:N	5:S:78:PRO:CD	2.75	0.49
10:X:119:ILE:HA	10:X:124:THR:O	2.11	0.49
11:Y:130:GLY:HA2	18:Y:302:MES:O3S	2.12	0.49
5:E:28:ILE:HD11	5:E:148:PRO:HD3	1.95	0.49
9:I:7:ASN:HA	9:I:29:GLY:O	2.12	0.49
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.94	0.49
12:L:148:PRO:HB2	9:W:148:MET:SD	2.53	0.49
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.47	0.49
13:M:127:LEU:O	13:M:138:SER:OG	2.25	0.49
5:S:68:HIS:HE1	5:S:102:LEU:O	1.94	0.49
12:Z:20:PHE:CZ	12:Z:177:VAL:HA	2.47	0.49
12:L:160:TYR:CD2	12:L:166:GLY:HA2	2.48	0.49
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.94	0.49
4:D:82:GLU:OE2	11:K:69:ARG:NH1	2.46	0.49
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.95	0.49
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.95	0.49
2:B:28:ILE:O	2:B:165:GLY:HA2	2.13	0.49
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.95	0.49
12:L:136:CYS:SG	12:L:154:VAL:HG11	2.53	0.49
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.60	0.49
14:N:13:VAL:HG11	14:N:175:MET:CE	2.43	0.48
3:Q:25:VAL:O	3:Q:163:GLY:HA2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:136:CYS:SG	12:Z:154:VAL:HG11	2.53	0.48
2:P:74:VAL:HA	2:P:135:ILE:O	2.13	0.48
4:D:4:VAL:HG13	4:D:15:GLN:HG3	1.95	0.48
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.96	0.48
11:K:6:PHE:HA	11:K:125:ASP:O	2.12	0.48
4:R:82:GLU:OE2	11:Y:69:ARG:NH1	2.46	0.48
8:V:98:LEU:HB2	8:V:113:ILE:HG22	1.95	0.48
7:G:105:CYS:HB2	7:G:136:SER:OG	2.13	0.48
9:I:123:PHE:HA	9:I:128:CYS:O	2.12	0.48
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.95	0.48
1:A:98:LYS:HA	1:A:103:GLU:O	2.13	0.48
11:K:13:ILE:HG13	11:K:153:ALA:HB1	1.95	0.48
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.49	0.48
3:Q:238:LYS:O	3:Q:240:GLU:N	2.47	0.48
12:Z:12:ILE:HG23	12:Z:55:ASN:HD22	1.79	0.48
4:D:115:PHE:HA	4:D:126:MET:O	2.13	0.48
1:A:83:ARG:HE	7:G:114:ASN:ND2	2.12	0.48
14:N:3:ILE:HG22	14:N:16:SER:CB	2.44	0.48
2:B:111:VAL:HG22	2:B:136:TYR:CG	2.49	0.48
8:V:84:LYS:HE2	8:V:119:THR:HG23	1.95	0.48
12:Z:173:LYS:C	20:Z:402:HOH:O	2.51	0.48
1:A:115:ALA:HB1	1:A:154:GLY:O	2.14	0.47
11:K:4:LEU:HD13	11:K:161:ILE:HD11	1.96	0.47
14:N:47:GLY:N	19:N:202:SO4:O4	2.47	0.47
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.76	0.47
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.50	0.47
7:U:83:ASN:C	7:U:83:ASN:HD22	2.17	0.47
17:Y:301:A1IF8:C11	17:Y:301:A1IF8:C18	2.91	0.47
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.96	0.47
10:X:167:GLU:OE2	10:X:167:GLU:HA	2.15	0.47
10:X:194:ASP:HA	20:X:303:HOH:O	2.14	0.47
11:Y:12:ILE:HB	11:Y:180:VAL:HB	1.96	0.47
11:K:31:VAL:HG23	12:L:132:GLU:HG3	1.96	0.47
5:S:23:TYR:O	5:S:26:GLU:HB3	2.13	0.47
11:Y:17:ASP:O	11:Y:33:LYS:HD2	2.14	0.47
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.15	0.47
7:G:71:GLY:HA3	7:G:224:PHE:CZ	2.49	0.47
2:P:46:ALA:HB2	2:P:212:PHE:CE1	2.50	0.47
7:U:224:PHE:CD2	7:U:224:PHE:C	2.87	0.47
10:X:135:TYR:O	10:X:138:PHE:HB2	2.15	0.47
5:E:99:ASN:HB2	13:M:94:GLU:HG2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1:MET:O	20:J:201:HOH:O	2.20	0.47
17:K:301:A1IF8:C11	17:K:301:A1IF8:C18	2.93	0.47
2:B:219:ALA:HB2	2:B:225:TYR:HB2	1.96	0.47
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.49	0.47
10:X:23:ARG:NH1	11:Y:118:ASP:OD1	2.47	0.47
2:B:165:GLY:O	2:B:168:THR:HG23	2.15	0.47
8:H:97:TYR:HB3	8:H:127:LEU:HD21	1.97	0.47
12:L:172:LEU:H	12:L:172:LEU:HD23	1.79	0.47
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.97	0.47
2:P:217:LYS:C	2:P:219:ALA:H	2.17	0.46
7:G:216:VAL:CG2	7:G:232:ILE:HG12	2.44	0.46
11:K:5:ALA:HA	11:K:13:ILE:O	2.15	0.46
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.63	0.46
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	1.98	0.46
11:K:5:ALA:N	11:K:100:MET:HE1	2.31	0.46
12:L:110:ILE:HD11	12:L:137:ARG:HG3	1.96	0.46
2:P:93:HIS:NE2	2:P:113:ARG:HG2	2.30	0.46
8:V:137:VAL:HG21	8:V:161:ALA:HB2	1.97	0.46
4:D:104:LEU:C	4:D:104:LEU:HD13	2.36	0.46
5:E:12:PHE:H	6:F:19:GLN:HE22	1.64	0.46
2:P:52:THR:OG1	2:P:56:LEU:HD22	2.15	0.46
6:T:123:ASN:HD22	6:T:124:SER:N	2.14	0.46
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.98	0.46
8:V:48:THR:HB	8:V:51:ASP:HB2	1.98	0.46
2:B:110:LEU:HD23	2:B:110:LEU:C	2.36	0.46
9:I:176:ARG:NH2	12:Z:147:MET:HE2	2.31	0.46
2:P:114:LEU:HD23	2:P:114:LEU:HA	1.83	0.46
11:Y:4:LEU:CD1	11:Y:161:ILE:HD11	2.46	0.46
12:Z:13:LEU:HD12	12:Z:14:GLY:N	2.30	0.46
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.51	0.46
2:P:180:LYS:O	2:P:183:MET:HB2	2.16	0.46
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.45	0.46
12:L:31:THR:HG22	12:L:36:ASN:HD21	1.78	0.46
2:B:234:ILE:O	2:B:237:ILE:HG22	2.15	0.46
6:F:115:TYR:O	6:F:118:ALA:HB3	2.16	0.46
10:J:25:ILE:CD1	10:X:135:TYR:CD1	2.87	0.46
11:K:3:THR:CG2	11:K:16:VAL:HG12	2.46	0.46
14:N:32:ASP:OD2	14:N:185:ARG:NH1	2.48	0.45
1:O:36:GLY:O	1:O:161:ALA:HA	2.16	0.45
17:K:301:A1IF8:C29	17:K:301:A1IF8:C8	2.94	0.45
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:71:LEU:C	5:S:71:LEU:CD2	2.85	0.45
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.46	0.45
5:E:71:LEU:C	5:E:71:LEU:HD22	2.36	0.45
2:B:35:ILE:HD12	2:B:196:LEU:HG	1.97	0.45
4:D:6:THR:HG23	5:E:20:GLN:NE2	2.31	0.45
8:H:210:THR:HG21	9:I:167:SER:HB3	1.98	0.45
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.27	0.45
4:D:149:HIS:O	4:D:156:PHE:HA	2.16	0.45
4:D:82:GLU:OE1	11:K:69:ARG:HD3	2.16	0.45
7:G:78:ILE:HG22	7:G:79:PRO:HD3	1.98	0.45
8:H:167:LEU:HD22	12:Z:196:ILE:O	2.17	0.45
6:T:14:ASP:HB2	6:T:16:ARG:HD3	1.97	0.45
2:B:111:VAL:HG22	2:B:136:TYR:CD2	2.52	0.45
13:M:128:ARG:HH11	13:M:138:SER:HB2	1.82	0.45
2:B:89:THR:HG21	2:B:117:ILE:HD13	1.98	0.45
2:B:114:LEU:HD23	2:B:114:LEU:HA	1.83	0.45
11:K:86:LEU:C	11:K:86:LEU:HD13	2.36	0.45
3:Q:73:PHE:HE2	3:Q:77:ASN:HD22	1.64	0.45
10:J:168:LEU:O	10:J:172:MET:HB2	2.17	0.44
5:S:60:LYS:O	5:S:60:LYS:HG3	2.16	0.44
9:W:92:SER:O	9:W:96:GLU:HG3	2.17	0.44
10:X:7:ILE:HD13	10:X:160:LEU:HD23	2.00	0.44
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.48	0.44
6:T:172:LEU:HB3	7:U:54:LEU:HD21	1.98	0.44
8:V:30:ASN:O	8:V:188:ARG:NH2	2.41	0.44
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.65	0.44
10:J:4:ILE:HG13	10:J:4:ILE:O	2.18	0.44
10:J:174:MET:HA	10:X:174:MET:HA	1.99	0.44
10:X:1:MET:H1	10:X:34:LYS:HE3	1.82	0.44
2:B:58:GLN:NE2	2:B:208:ASP:HA	2.33	0.44
5:E:35:VAL:HG22	5:E:159:ALA:HB2	1.99	0.44
7:G:78:ILE:N	7:G:79:PRO:CD	2.80	0.44
8:H:34:LEU:HD22	8:H:174:ASP:HB3	1.98	0.44
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.98	0.44
6:T:71:GLY:O	6:T:134:PHE:HA	2.17	0.44
2:B:149:THR:O	2:B:156:TYR:HA	2.17	0.44
12:L:86:ILE:HD11	12:L:111:ILE:HG13	1.99	0.44
12:L:124:SER:CB	12:L:137:ARG:HG2	2.48	0.44
14:N:59:VAL:HG22	14:N:81:VAL:HG12	1.99	0.44
5:S:88:ARG:O	5:S:92:ASN:HB2	2.17	0.44
11:Y:154:LEU:HD23	11:Y:177:LEU:HD22	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:123:ASN:C	6:F:123:ASN:ND2	2.68	0.44
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.48	0.44
8:V:84:LYS:HE2	8:V:119:THR:CG2	2.48	0.44
1:A:1:MET:O	1:A:2:THR:O	2.36	0.44
4:D:96:ASP:CG	4:D:96:ASP:O	2.56	0.44
10:X:7:ILE:HD11	10:X:160:LEU:HD23	2.00	0.44
10:J:147:HIS:HB3	10:J:160:LEU:CD1	2.47	0.44
12:L:18:GLU:HG3	12:L:174:TYR:CD2	2.52	0.44
4:R:115:PHE:HA	4:R:126:MET:O	2.18	0.44
8:V:109:HIS:HB3	8:V:111:PHE:CE2	2.53	0.44
3:C:82:ILE:N	3:C:82:ILE:HD12	2.32	0.43
5:E:12:PHE:HB2	6:F:19:GLN:NE2	2.25	0.43
5:E:71:LEU:C	5:E:71:LEU:CD2	2.86	0.43
11:K:4:LEU:CD1	11:K:161:ILE:HD11	2.48	0.43
9:W:7:ASN:HA	9:W:29:GLY:O	2.18	0.43
10:X:3:ILE:HB	10:X:18:SER:HB3	2.00	0.43
2:B:217:LYS:C	2:B:219:ALA:N	2.72	0.43
14:N:13:VAL:HG11	14:N:175:MET:HE2	1.99	0.43
9:W:62:LEU:HD12	9:W:104:VAL:HG11	2.00	0.43
7:G:113:ALA:HB2	7:G:148:THR:HG23	2.00	0.43
7:U:37:ARG:NH2	7:U:183:ASP:HB3	2.34	0.43
3:C:108:THR:HG21	3:C:146:TYR:HB3	2.01	0.43
11:K:4:LEU:HD22	11:K:4:LEU:C	2.39	0.43
9:W:148:MET:HB3	9:W:169:ALA:HA	2.00	0.43
1:A:110:LEU:O	1:A:114:VAL:HG23	2.18	0.43
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.32	0.43
4:D:73:LEU:O	4:D:76:ASP:HB2	2.18	0.43
12:L:195:HIS:HD2	12:L:197:GLN:H	1.66	0.43
12:Z:31:THR:HG23	12:Z:36:ASN:ND2	2.22	0.43
2:B:140:ASP:OD1	2:B:140:ASP:C	2.57	0.43
7:U:78:ILE:HG22	7:U:79:PRO:HD3	1.98	0.43
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.01	0.43
12:L:43:VAL:HG12	12:L:205:LEU:HD22	2.01	0.43
11:Y:5:ALA:N	11:Y:100:MET:CE	2.82	0.43
12:Z:86:ILE:HD11	12:Z:111:ILE:HG13	2.00	0.43
7:G:2:GLY:N	20:G:401:HOH:O	2.51	0.43
10:J:169:GLU:O	10:X:177:LYS:NZ	2.51	0.43
1:O:64:VAL:HG11	1:O:212:ALA:CB	2.49	0.43
8:V:43:CYS:SG	8:V:56:THR:CG2	3.06	0.43
10:X:60:ILE:O	10:X:64:ILE:HG12	2.19	0.43
2:P:58:GLN:NE2	2:P:208:ASP:HA	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:35:ILE:HB	11:K:45:MET:HE3	2.01	0.43
11:K:158:LYS:HD3	11:K:196:LEU:HD11	2.01	0.43
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.00	0.42
9:W:62:LEU:HD11	9:W:104:VAL:HG21	2.01	0.42
12:Z:147:MET:N	12:Z:148:PRO:CD	2.82	0.42
3:C:131:THR:O	3:C:147:GLN:HA	2.20	0.42
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.49	0.42
1:A:8:SER:OG	2:B:127:LEU:HA	2.20	0.42
2:B:194:LYS:O	2:B:198:LYS:HG3	2.20	0.42
12:L:113:GLY:HA2	12:L:207:VAL:HG11	2.01	0.42
7:U:73:VAL:HG12	7:U:133:THR:HB	2.01	0.42
8:V:52:THR:HG22	8:V:96:ALA:HA	2.01	0.42
10:X:49:GLU:HB2	10:X:99:GLN:HB3	2.00	0.42
11:K:3:THR:HB	11:K:16:VAL:HG12	2.02	0.42
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.54	0.42
6:T:24:VAL:O	6:T:27:VAL:HB	2.19	0.42
12:L:55:ASN:OD1	12:L:140:GLY:HA3	2.19	0.42
1:A:113:GLU:HA	1:A:113:GLU:OE1	2.19	0.42
12:L:125:PHE:N	12:L:125:PHE:CD1	2.88	0.42
4:R:91:HIS:HB3	4:R:99:ILE:HG21	2.02	0.42
8:V:84:LYS:CA	8:V:113:ILE:HD11	2.47	0.42
4:R:78:ARG:HA	4:R:78:ARG:HD3	1.92	0.42
6:T:171:GLU:HB3	6:T:195:ILE:HG12	2.02	0.42
8:H:14:ILE:HG22	8:H:176:CYS:HB3	2.02	0.42
8:V:18:THR:HG23	8:V:172:ASN:O	2.20	0.42
10:X:92:ILE:HD12	10:X:92:ILE:HA	1.85	0.42
12:Z:26:ASP:OD1	12:Z:26:ASP:N	2.52	0.42
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.84	0.42
5:S:9:THR:HG21	5:S:119:THR:HA	2.01	0.42
6:F:201:GLU:N	6:F:201:GLU:OE1	2.52	0.42
8:H:62:ASN:HB3	8:H:82:MET:CE	2.50	0.42
10:J:49:GLU:HB2	10:J:99:GLN:HB3	2.02	0.42
4:R:59:ILE:HG22	4:R:220:PHE:HZ	1.83	0.42
5:S:118:ASN:N	5:S:118:ASN:HD22	2.17	0.42
8:V:192:THR:HG23	8:V:192:THR:O	2.20	0.42
10:X:130:TYR:HB2	10:X:144:LEU:HD13	2.02	0.42
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.19	0.42
11:K:38:ASN:C	11:K:38:ASN:OD1	2.58	0.41
12:L:149:PHE:CE1	12:L:153:GLN:HG3	2.55	0.41
12:L:164:THR:CA	12:L:167:LYS:HD2	2.49	0.41
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:PRO:HG2	2:B:109:ILE:HD12	2.00	0.41
10:J:101:ASN:HB3	10:J:133:HIS:CE1	2.55	0.41
4:R:38:VAL:HB	4:R:214:ILE:HG23	2.02	0.41
11:Y:5:ALA:N	11:Y:100:MET:HE1	2.35	0.41
2:B:89:THR:HG21	2:B:117:ILE:CD1	2.50	0.41
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.01	0.41
3:C:147:GLN:O	3:C:154:TYR:HA	2.20	0.41
5:E:226:GLY:O	5:E:229:VAL:HG22	2.21	0.41
2:P:75:ALA:HB3	2:P:135:ILE:HB	2.02	0.41
9:I:62:LEU:CD1	9:I:104:VAL:HG21	2.50	0.41
12:L:49:ASN:HD22	12:L:49:ASN:HA	1.72	0.41
9:W:123:PHE:HA	9:W:128:CYS:O	2.20	0.41
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.03	0.41
2:B:115:SER:HB3	2:B:154:GLY:O	2.21	0.41
6:F:95:PHE:CE1	6:F:103:ILE:HA	2.56	0.41
10:J:143:LEU:HD23	10:J:143:LEU:C	2.41	0.41
12:Z:60:ASP:OD2	12:Z:105:TYR:HA	2.21	0.41
2:B:74:VAL:HA	2:B:135:ILE:O	2.21	0.41
6:F:78:ILE:N	6:F:79:PRO:CD	2.84	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.02	0.41
2:P:234:ILE:O	2:P:237:ILE:HG22	2.20	0.41
12:Z:100:LYS:HD3	12:Z:105:TYR:CZ	2.56	0.41
7:G:78:ILE:CG2	7:G:79:PRO:HD3	2.50	0.41
8:H:3:ILE:O	8:H:126:SER:HA	2.21	0.41
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.03	0.41
11:K:139:VAL:HG21	11:K:163:ALA:HB2	2.02	0.41
4:R:67:GLY:HA3	4:R:220:PHE:CD1	2.56	0.41
1:A:64:VAL:HG11	1:A:212:ALA:CB	2.50	0.41
6:F:240:GLN:HE21	6:F:240:GLN:HA	1.85	0.41
8:V:34:LEU:HD12	8:V:34:LEU:HA	1.90	0.41
11:Y:4:LEU:HD22	11:Y:4:LEU:C	2.41	0.41
11:Y:5:ALA:HB3	11:Y:100:MET:HE3	2.03	0.41
12:Z:26:ASP:HA	12:Z:201:GLY:O	2.21	0.41
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.76	0.41
2:B:66:TYR:CG	2:B:87:ILE:HD13	2.56	0.41
4:D:174:GLU:HG2	4:D:195:ILE:HG12	2.03	0.41
14:N:67:THR:HA	14:N:71:GLY:O	2.21	0.41
1:O:98:LYS:HE3	1:O:104:TYR:CZ	2.56	0.41
3:Q:31:ALA:O	3:Q:161:THR:HA	2.21	0.41
4:R:96:ASP:CG	4:R:96:ASP:O	2.59	0.41
9:W:65:MET:O	9:W:68:TYR:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:41:HIS:O	10:X:106:GLY:HA2	2.21	0.41
4:D:68:CYS:HA	4:D:135:LEU:O	2.20	0.40
5:E:65:CYS:SG	5:E:71:LEU:CD1	3.09	0.40
7:G:74:VAL:HG11	7:G:81:ALA:HB2	2.03	0.40
11:Y:86:LEU:HD13	11:Y:86:LEU:C	2.42	0.40
4:D:95:TYR:O	12:L:88:SER:HA	2.20	0.40
8:V:192:THR:O	8:V:192:THR:CG2	2.69	0.40
4:D:191:LEU:HD12	4:D:191:LEU:HA	1.96	0.40
5:E:51:ASN:ND2	5:E:53:ASP:O	2.54	0.40
13:M:131:ASN:C	13:M:131:ASN:OD1	2.59	0.40
13:M:174:GLU:O	13:M:178:VAL:HG23	2.21	0.40
17:N:201:A1IF8:O42	17:N:201:A1IF8:C35	2.69	0.40
2:P:29:SER:O	2:P:166:ALA:HA	2.21	0.40
2:P:160:LYS:HB3	2:P:179:TYR:CZ	2.56	0.40
9:W:55:LEU:HG	9:W:57:THR:HG22	2.03	0.40
11:Y:4:LEU:HD11	11:Y:161:ILE:HG12	2.04	0.40
11:Y:19:ARG:HD2	11:Y:170:TYR:O	2.22	0.40
1:A:149:GLN:O	1:A:156:TYR:HA	2.21	0.40
6:F:46:VAL:HB	6:F:73:VAL:HG21	2.04	0.40
11:K:2:THR:HG21	11:K:164:ALA:CB	2.51	0.40
12:L:36:ASN:HB3	13:M:137:TYR:CD1	2.56	0.40
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.69	0.40
11:K:139:VAL:HG21	11:K:163:ALA:CB	2.52	0.40
13:M:96:LEU:O	13:M:100:MET:HG2	2.22	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%)	239 (96%)	7 (3%)	2 (1%)	19 34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	O	248/250 (99%)	238 (96%)	6 (2%)	4 (2%)	9 16
2	B	243/258 (94%)	231 (95%)	7 (3%)	5 (2%)	7 12
2	P	242/258 (94%)	231 (96%)	6 (2%)	5 (2%)	7 12
3	C	238/254 (94%)	228 (96%)	6 (2%)	4 (2%)	9 16
3	Q	238/254 (94%)	226 (95%)	9 (4%)	3 (1%)	12 21
4	D	231/260 (89%)	225 (97%)	5 (2%)	1 (0%)	34 53
4	R	231/260 (89%)	224 (97%)	6 (3%)	1 (0%)	34 53
5	E	229/234 (98%)	218 (95%)	11 (5%)	0	100 100
5	S	229/234 (98%)	218 (95%)	11 (5%)	0	100 100
6	F	241/288 (84%)	235 (98%)	6 (2%)	0	100 100
6	T	241/288 (84%)	234 (97%)	7 (3%)	0	100 100
7	G	239/252 (95%)	230 (96%)	8 (3%)	1 (0%)	34 53
7	U	239/252 (95%)	228 (95%)	9 (4%)	2 (1%)	19 34
8	H	224/232 (97%)	214 (96%)	10 (4%)	0	100 100
8	V	224/232 (97%)	217 (97%)	7 (3%)	0	100 100
9	I	202/205 (98%)	192 (95%)	10 (5%)	0	100 100
9	W	202/205 (98%)	192 (95%)	10 (5%)	0	100 100
10	J	193/198 (98%)	187 (97%)	5 (3%)	1 (0%)	29 47
10	X	193/198 (98%)	184 (95%)	9 (5%)	0	100 100
11	K	209/211 (99%)	198 (95%)	11 (5%)	0	100 100
11	Y	209/211 (99%)	199 (95%)	9 (4%)	1 (0%)	29 47
12	L	220/222 (99%)	211 (96%)	9 (4%)	0	100 100
12	Z	221/222 (100%)	213 (96%)	8 (4%)	0	100 100
13	M	223/246 (91%)	215 (96%)	8 (4%)	0	100 100
13	a	226/246 (92%)	216 (96%)	9 (4%)	1 (0%)	34 53
14	N	193/195 (99%)	185 (96%)	8 (4%)	0	100 100
14	b	193/195 (99%)	183 (95%)	10 (5%)	0	100 100
All	All	6269/6610 (95%)	6011 (96%)	227 (4%)	31 (0%)	29 47

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	51	VAL
2	B	220	ASN
2	B	221	ASP
3	C	202	GLN
3	C	205	ALA
3	C	239	GLN
7	G	223	LYS
1	O	2	THR
2	P	51	VAL
2	P	221	ASP
3	Q	202	GLN
3	Q	239	GLN
7	U	223	LYS
11	Y	9	GLN
1	A	3	ASP
2	B	218	GLY
1	O	3	ASP
2	P	218	GLY
4	D	2	ARG
1	O	50	LYS
3	Q	183	PRO
13	a	83	ALA
1	O	166	LYS
2	P	19	TYR
2	P	220	ASN
4	R	2	ARG
7	U	221	LYS
2	B	52	THR
3	C	183	PRO
10	J	9	VAL

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%)	203 (97%)	6 (3%)	42 62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	209/209 (100%)	207 (99%)	2 (1%)	76 85
2	B	204/216 (94%)	196 (96%)	8 (4%)	32 52
2	P	203/216 (94%)	193 (95%)	10 (5%)	25 43
3	C	212/226 (94%)	198 (93%)	14 (7%)	16 29
3	Q	212/226 (94%)	203 (96%)	9 (4%)	30 49
4	D	194/215 (90%)	182 (94%)	12 (6%)	18 32
4	R	194/215 (90%)	184 (95%)	10 (5%)	23 39
5	E	190/193 (98%)	178 (94%)	12 (6%)	18 31
5	S	190/193 (98%)	178 (94%)	12 (6%)	18 31
6	F	201/239 (84%)	188 (94%)	13 (6%)	17 30
6	T	201/239 (84%)	188 (94%)	13 (6%)	17 30
7	G	206/210 (98%)	196 (95%)	10 (5%)	25 43
7	U	206/210 (98%)	193 (94%)	13 (6%)	18 31
8	H	185/190 (97%)	173 (94%)	12 (6%)	17 30
8	V	185/190 (97%)	170 (92%)	15 (8%)	11 21
9	I	172/173 (99%)	166 (96%)	6 (4%)	36 56
9	W	172/173 (99%)	168 (98%)	4 (2%)	50 69
10	J	173/175 (99%)	161 (93%)	12 (7%)	15 27
10	X	173/175 (99%)	162 (94%)	11 (6%)	17 31
11	K	168/168 (100%)	161 (96%)	7 (4%)	30 49
11	Y	168/168 (100%)	159 (95%)	9 (5%)	22 38
12	L	185/185 (100%)	174 (94%)	11 (6%)	19 34
12	Z	186/185 (100%)	177 (95%)	9 (5%)	25 44
13	M	193/208 (93%)	181 (94%)	12 (6%)	18 32
13	a	195/208 (94%)	185 (95%)	10 (5%)	24 41
14	N	160/160 (100%)	154 (96%)	6 (4%)	33 53
14	b	160/160 (100%)	154 (96%)	6 (4%)	33 53
All	All	5306/5534 (96%)	5032 (95%)	274 (5%)	23 39

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	201	GLU
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	79	LEU
2	B	99	LYS
2	B	102	ASN
2	B	113	ARG
2	B	140	ASP
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	49	THR
3	C	51	LYS
3	C	61	LYS
3	C	116	GLN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	187	GLU
3	C	206	LYS
3	C	216	ASP
3	C	240	GLU
4	D	20	LEU
4	D	68	CYS
4	D	99	ILE
4	D	117	GLU
4	D	125	LEU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	8	ASP
5	E	9	THR
5	E	29	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	55	LEU
5	E	71	LEU
5	E	87	LEU
5	E	95	SER
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	207	VAL
5	E	231	LYS
6	F	58	GLN
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	148	GLU
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	214	TRP
6	F	221	ASN
6	F	240	GLN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	215	GLU
7	G	223	LYS
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	38	SER
8	H	53	GLU
8	H	56	THR
8	H	68	LEU
8	H	84	LYS
8	H	132	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	196	ARG
8	H	219	ASN
9	I	30	SER
9	I	31	GLN
9	I	151	SER
9	I	171	LEU
9	I	182	TRP
9	I	192	ASP
10	J	2	ASP
10	J	3	ILE
10	J	8	ARG
10	J	23	ARG
10	J	25	ILE
10	J	35	THR
10	J	49	GLU
10	J	78	GLN
10	J	90	LYS
10	J	99	GLN
10	J	110	LYS
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	31	VAL
11	K	35	ILE
11	K	41	LEU
11	K	106	ARG
11	K	148	LEU
12	L	18	GLU
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	135	GLN
12	L	150	LEU
12	L	161	GLU
12	L	167	LYS
12	L	172	LEU
12	L	175	LEU
12	L	176	SER
13	M	2	GLN
13	M	10	SER
13	M	48	ASN
13	M	70	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	104	ARG
13	M	138	SER
13	M	146	PHE
13	M	161	ARG
13	M	187	ARG
13	M	192	SER
13	M	213	GLN
13	M	220	ASP
14	N	7	GLU
14	N	37	LEU
14	N	39	GLU
14	N	107	LYS
14	N	178	LEU
14	N	192	GLU
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	58	GLN
2	P	79	LEU
2	P	102	ASN
2	P	113	ARG
2	P	119	GLN
2	P	155	ASN
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	61	LYS
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	187	GLU
3	Q	206	LYS
4	R	99	ILE
4	R	117	GLU
4	R	125	LEU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	214	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	56	SER
5	S	71	LEU
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	147	GLN
5	S	184	ASN
5	S	188	LEU
5	S	208	ASP
6	T	94	SER
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	207	ASP
6	T	214	TRP
6	T	221	ASN
6	T	240	GLN
7	U	13	GLU
7	U	26	THR
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	220	THR
7	U	221	LYS
7	U	222	ASP
7	U	235	ARG
7	U	236	LEU
8	V	13	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	V	30	ASN
8	V	34	LEU
8	V	38	SER
8	V	53	GLU
8	V	56	THR
8	V	68	LEU
8	V	73	GLU
8	V	103	VAL
8	V	120	ASP
8	V	149	GLU
8	V	192	THR
8	V	205	PHE
8	V	207	ARG
8	V	222	ASP
9	W	31	GLN
9	W	151	SER
9	W	171	LEU
9	W	182	TRP
10	X	1	MET
10	X	2	ASP
10	X	3	ILE
10	X	35	THR
10	X	78	GLN
10	X	90	LYS
10	X	99	GLN
10	X	110	LYS
10	X	136	SER
10	X	162	LYS
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	31	VAL
11	Y	32	LYS
11	Y	35	ILE
11	Y	41	LEU
11	Y	106	ARG
11	Y	118	ASP
11	Y	147	ASP
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	103	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	Z	126	ASP
12	Z	130	SER
12	Z	132	GLU
12	Z	150	LEU
12	Z	172	LEU
13	a	2	GLN
13	a	10	SER
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	146	PHE
13	a	161	ARG
13	a	187	ARG
13	a	192	SER
13	a	220	ASP
14	b	2	THR
14	b	7	GLU
14	b	39	GLU
14	b	83	LYS
14	b	176	VAL
14	b	190	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) 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
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	146	GLN
4	D	160	ASN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
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	22	GLN
8	H	66	HIS
8	H	200	GLN
9	I	172	ASN
10	J	55	GLN
10	J	118	GLN
10	J	147	HIS
10	J	191	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	165	ASN
12	L	195	HIS
13	M	48	ASN
13	M	102	GLN
13	M	171	GLN
13	M	179	ASN
14	N	69	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
3	Q	14	HIS
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	143	HIS
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	166	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
8	V	22	GLN
8	V	30	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	V	66	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	71	ASN
9	W	88	GLN
10	X	55	GLN
10	X	78	GLN
10	X	118	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	135	GLN
12	Z	195	HIS
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	69	GLN
14	b	106	ASN
14	b	161	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 12 are monoatomic - leaving 9 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	0.73	0	14,16,16	0.48	0
17	A1IF8	N	201	14	42,52,52	6.66	11 (26%)	43,75,75	1.46	8 (18%)
18	MES	a	301	-	12,12,12	0.68	0	14,16,16	0.55	0
19	SO4	N	202	-	4,4,4	0.40	0	6,6,6	0.05	0
18	MES	K	302	-	12,12,12	0.76	0	14,16,16	0.30	0
17	A1IF8	K	301	11	42,52,52	3.97	9 (21%)	43,75,75	1.33	5 (11%)
17	A1IF8	b	201	14	42,52,52	5.78	9 (21%)	43,75,75	1.53	8 (18%)
17	A1IF8	Y	301	11	42,52,52	4.42	6 (14%)	43,75,75	1.60	8 (18%)
18	MES	M	301	-	12,12,12	0.70	0	14,16,16	0.40	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MES	Y	302	-	-	3/6/14/14	0/1/1/1
17	A1IF8	N	201	14	-	6/40/94/94	0/2/3/3
18	MES	a	301	-	-	0/6/14/14	0/1/1/1
18	MES	K	302	-	-	2/6/14/14	0/1/1/1
17	A1IF8	K	301	11	-	6/40/94/94	0/2/3/3
17	A1IF8	b	201	14	-	13/40/94/94	0/2/3/3
17	A1IF8	Y	301	11	-	10/40/94/94	0/2/3/3
18	MES	M	301	-	-	0/6/14/14	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	201	A1IF8	F4-C3	-30.10	0.84	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	201	A1IF8	F5-C3	-28.72	0.87	1.38
17	b	201	A1IF8	F5-C3	-26.62	0.91	1.38
17	b	201	A1IF8	F4-C3	-23.62	0.96	1.38
17	Y	301	A1IF8	F5-C3	-19.46	1.03	1.38
17	Y	301	A1IF8	F4-C3	-17.12	1.07	1.38
17	K	301	A1IF8	F4-C3	-15.94	1.10	1.38
17	K	301	A1IF8	F5-C3	-14.49	1.12	1.38
17	K	301	A1IF8	C7-C8	-7.84	1.34	1.52
17	Y	301	A1IF8	C7-C8	-7.77	1.34	1.52
17	b	201	A1IF8	C7-C8	-7.07	1.36	1.52
17	N	201	A1IF8	C7-C8	-6.86	1.36	1.52
17	K	301	A1IF8	OG1-CB	-6.01	1.35	1.43
17	b	201	A1IF8	N40-N39	4.85	1.36	1.23
17	K	301	A1IF8	O17-C15	-4.70	1.37	1.44
17	Y	301	A1IF8	OG1-CB	-4.56	1.37	1.43
17	K	301	A1IF8	N40-N39	4.45	1.35	1.23
17	N	201	A1IF8	N40-N39	4.08	1.34	1.23
17	b	201	A1IF8	OG1-CB	-4.03	1.38	1.43
17	Y	301	A1IF8	N40-N39	3.81	1.33	1.23
17	K	301	A1IF8	OG1-C14	-3.67	1.36	1.43
17	Y	301	A1IF8	O17-C15	-3.58	1.39	1.44
17	N	201	A1IF8	OG1-CB	-3.04	1.39	1.43
17	N	201	A1IF8	C6-C7	-2.93	1.46	1.53
17	N	201	A1IF8	O17-C15	-2.74	1.40	1.44
17	K	301	A1IF8	C6-C7	-2.65	1.46	1.53
17	b	201	A1IF8	C34-C33	-2.60	1.48	1.53
17	b	201	A1IF8	C6-C7	-2.59	1.47	1.53
17	K	301	A1IF8	C26-C21	-2.32	1.46	1.52
17	N	201	A1IF8	C26-C21	-2.26	1.46	1.52
17	N	201	A1IF8	C34-C33	-2.18	1.49	1.53
17	N	201	A1IF8	C25-C26	-2.15	1.47	1.53
17	b	201	A1IF8	OG1-C14	-2.14	1.39	1.43
17	b	201	A1IF8	C22-C21	-2.02	1.46	1.52
17	N	201	A1IF8	C28-C10	-2.02	1.48	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	201	A1IF8	F5-C3-C6	3.77	121.85	112.91
17	b	201	A1IF8	C28-C10-C11	-3.60	101.80	110.20
17	b	201	A1IF8	C34-N36-C37	3.57	126.70	121.34
17	N	201	A1IF8	C25-C26-C21	-3.44	105.65	112.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Y	301	A1IF8	C2-N1-C7	-3.29	105.84	112.91
17	b	201	A1IF8	C13-N12-C11	-3.14	118.49	123.22
17	Y	301	A1IF8	C13-N12-C11	-3.11	118.54	123.22
17	Y	301	A1IF8	C2-N1-C33	2.99	137.47	126.69
17	Y	301	A1IF8	C7-C8-N9	-2.87	110.19	116.58
17	Y	301	A1IF8	C33-C34-N36	2.87	116.33	109.14
17	K	301	A1IF8	C29-C28-C10	-2.83	105.19	113.92
17	b	201	A1IF8	C20-C13-N12	2.78	115.84	109.46
17	K	301	A1IF8	F5-C3-C6	2.74	119.41	112.91
17	N	201	A1IF8	F5-C3-F4	-2.55	95.63	105.81
17	N	201	A1IF8	C28-C10-C11	-2.55	104.25	110.20
17	K	301	A1IF8	C13-N12-C11	-2.50	119.45	123.22
17	Y	301	A1IF8	C34-N36-C37	2.49	125.08	121.34
17	K	301	A1IF8	C7-C8-N9	-2.48	111.07	116.58
17	K	301	A1IF8	C20-C21-C22	-2.47	106.38	111.73
17	Y	301	A1IF8	C20-C21-C22	-2.42	106.48	111.73
17	b	201	A1IF8	F5-C3-C6	2.37	118.54	112.91
17	N	201	A1IF8	C7-N1-C33	2.36	129.55	121.41
17	b	201	A1IF8	C20-C21-C26	-2.27	106.79	111.73
17	N	201	A1IF8	C18-C15-C16	-2.21	103.95	109.02
17	N	201	A1IF8	C33-C34-N36	-2.09	103.89	109.14
17	b	201	A1IF8	C20-C21-C22	-2.08	107.21	111.73
17	N	201	A1IF8	O43-C33-N1	2.02	124.97	121.38
17	b	201	A1IF8	F4-C3-C6	2.00	117.66	112.91
17	Y	301	A1IF8	F5-C3-C6	2.00	117.66	112.91

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	301	A1IF8	C37-C38-N39-N40
17	K	301	A1IF8	O42-C37-C38-N39
17	K	301	A1IF8	N36-C37-C38-N39
17	Y	301	A1IF8	N1-C33-C34-C35
17	Y	301	A1IF8	O43-C33-C34-C35
17	b	201	A1IF8	C20-C13-N12-C11
17	b	201	A1IF8	N12-C13-C20-C21
17	b	201	A1IF8	C13-C20-C21-C22
17	b	201	A1IF8	C13-C20-C21-C26
18	K	302	MES	C8-C7-N4-C3
18	K	302	MES	C8-C7-N4-C5
18	Y	302	MES	C7-C8-S-O2S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	Y	302	MES	C7-C8-S-O3S
17	N	201	A1IF8	C35-C34-N36-C37
17	b	201	A1IF8	C35-C34-N36-C37
17	Y	301	A1IF8	N1-C33-C34-N36
17	b	201	A1IF8	C28-C29-C30-C31
17	Y	301	A1IF8	O43-C33-C34-N36
17	N	201	A1IF8	C38-N39-N40-N41
17	b	201	A1IF8	N1-C33-C34-N36
17	Y	301	A1IF8	C33-C34-N36-C37
17	Y	301	A1IF8	C28-C29-C30-C31
17	K	301	A1IF8	N9-C10-C11-O27
17	b	201	A1IF8	N9-C10-C11-N12
17	b	201	A1IF8	C14-C13-C20-C21
17	b	201	A1IF8	N9-C10-C11-O27
17	N	201	A1IF8	N9-C10-C11-N12
18	Y	302	MES	C7-C8-S-O1S
17	K	301	A1IF8	N9-C10-C11-N12
17	b	201	A1IF8	N1-C33-C34-C35
17	N	201	A1IF8	N9-C10-C11-O27
17	b	201	A1IF8	O43-C33-C34-N36
17	Y	301	A1IF8	N9-C10-C11-O27
17	N	201	A1IF8	C13-C20-C21-C26
17	K	301	A1IF8	C28-C10-C11-O27
17	Y	301	A1IF8	N9-C10-C11-N12
17	Y	301	A1IF8	C37-C38-N39-N40
17	N	201	A1IF8	C13-C20-C21-C22
17	Y	301	A1IF8	C6-C7-C8-O32
17	b	201	A1IF8	O43-C33-C34-C35

There are no ring outliers.

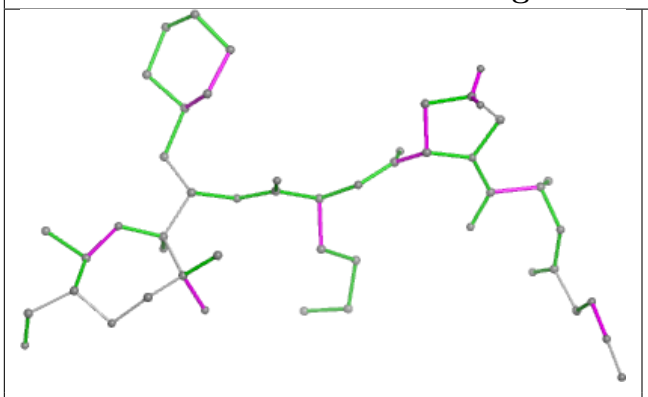
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	Y	302	MES	1	0
17	N	201	A1IF8	1	0
19	N	202	SO4	1	0
17	K	301	A1IF8	2	0
17	Y	301	A1IF8	2	0

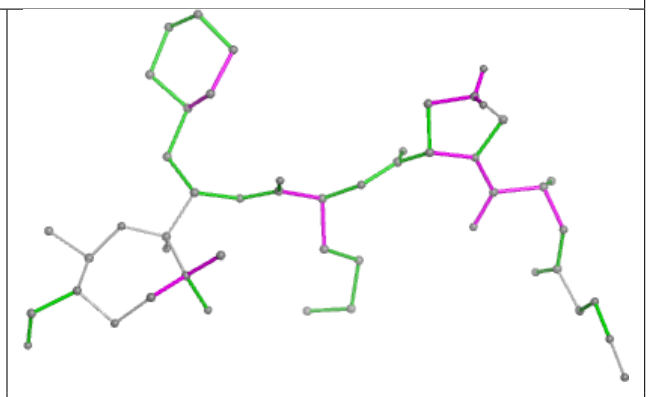
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

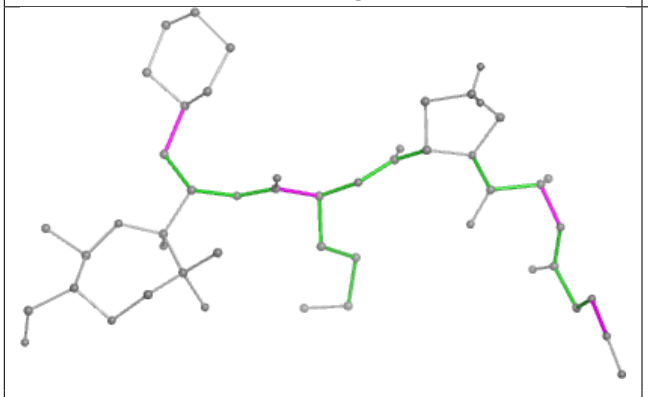
Ligand A1IF8 N 201



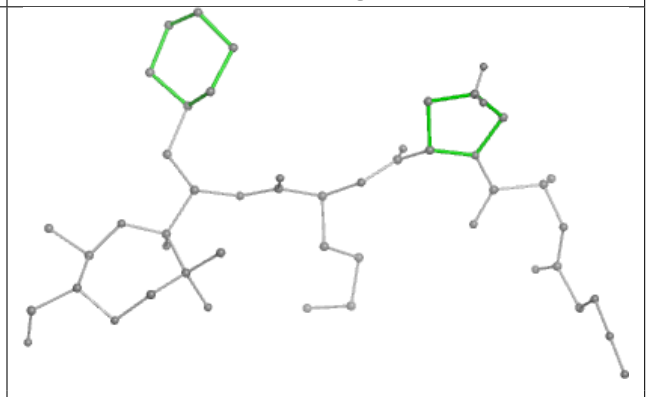
Bond lengths



Bond angles

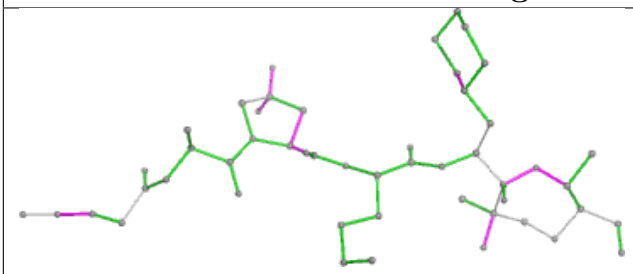


Torsions

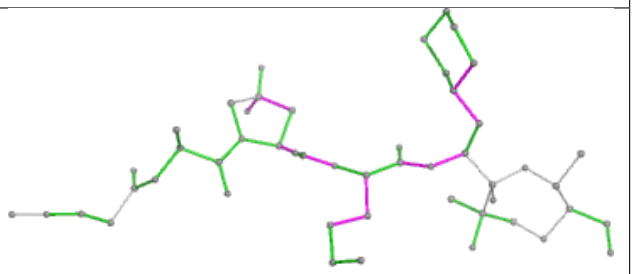


Rings

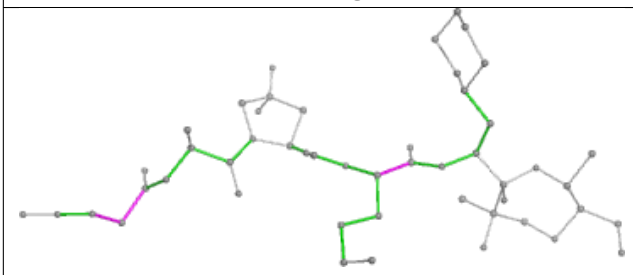
Ligand A1IF8 K 301



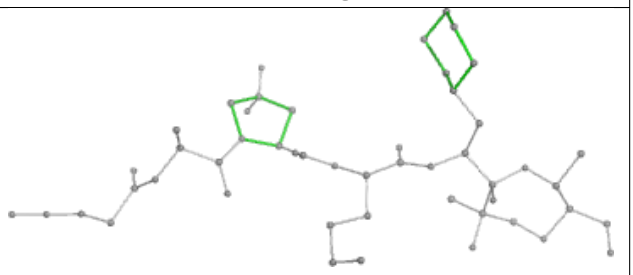
Bond lengths



Bond angles

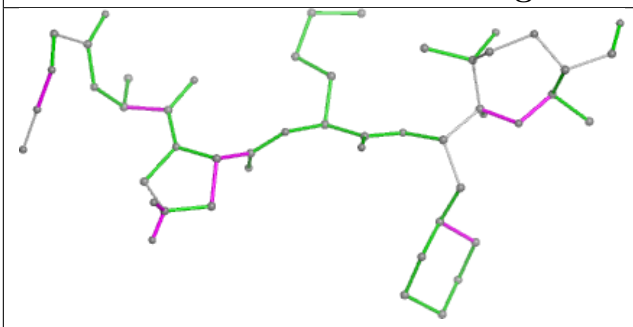


Torsions

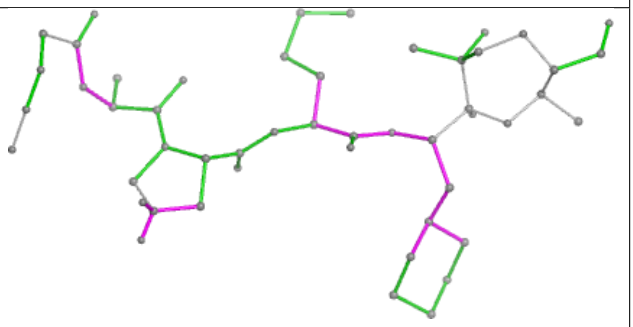


Rings

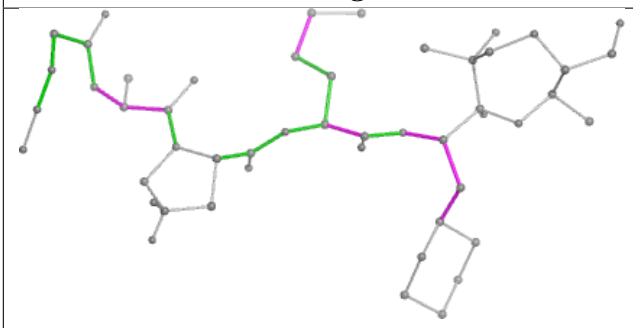
Ligand A1IF8 b 201



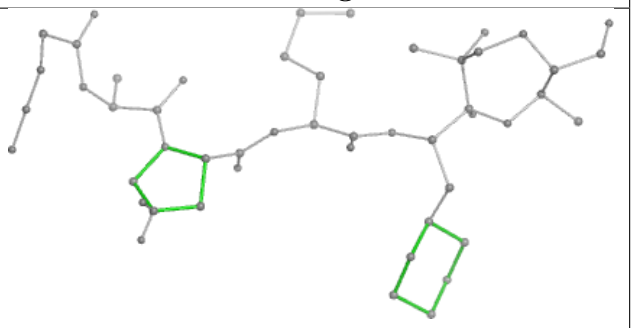
Bond lengths



Bond angles

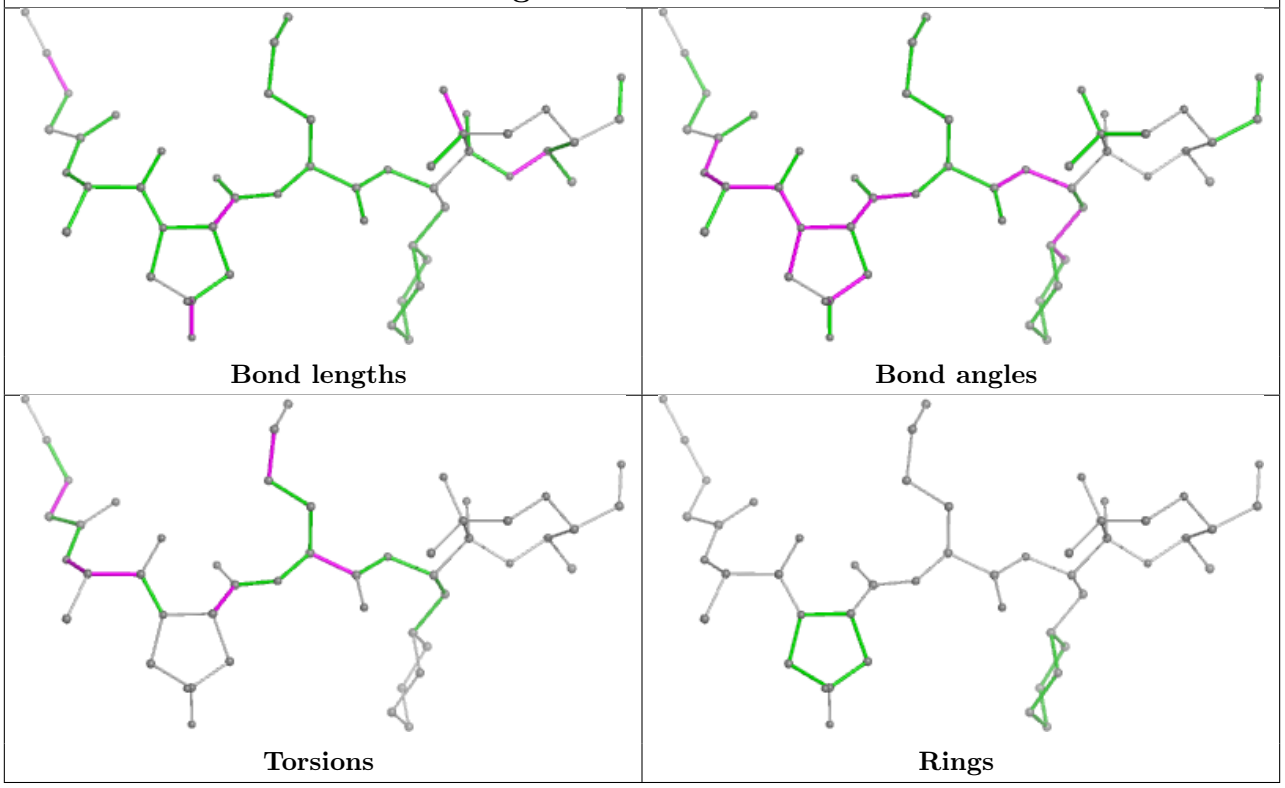


Torsions



Rings

Ligand A1IF8 Y 301



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.14	3 (1%)	79	85	58, 71, 102, 135	0
1	O	250/250 (100%)	-0.04	6 (2%)	59	68	63, 79, 111, 138	0
2	B	244/258 (94%)	0.00	7 (2%)	51	61	58, 75, 112, 172	0
2	P	244/258 (94%)	0.05	11 (4%)	33	39	63, 78, 123, 155	0
3	C	240/254 (94%)	0.07	13 (5%)	25	31	57, 79, 134, 147	0
3	Q	240/254 (94%)	0.31	17 (7%)	16	19	64, 91, 155, 176	0
4	D	235/260 (90%)	-0.18	2 (0%)	84	89	61, 79, 100, 135	0
4	R	235/260 (90%)	0.01	3 (1%)	77	84	65, 84, 114, 139	0
5	E	231/234 (98%)	-0.06	3 (1%)	77	84	62, 81, 108, 127	0
5	S	231/234 (98%)	0.16	5 (2%)	62	70	69, 89, 124, 139	0
6	F	243/288 (84%)	-0.14	5 (2%)	63	72	58, 74, 108, 137	0
6	T	243/288 (84%)	0.06	9 (3%)	41	49	64, 80, 117, 138	0
7	G	241/252 (95%)	-0.24	2 (0%)	86	90	56, 69, 99, 141	0
7	U	241/252 (95%)	-0.14	4 (1%)	70	78	61, 74, 100, 131	0
8	H	226/232 (97%)	-0.09	7 (3%)	49	58	56, 69, 92, 148	0
8	V	226/232 (97%)	-0.07	5 (2%)	62	70	59, 73, 95, 150	0
9	I	204/205 (99%)	-0.22	3 (1%)	73	81	54, 68, 89, 104	0
9	W	204/205 (99%)	-0.22	4 (1%)	65	73	53, 66, 89, 105	0
10	J	195/198 (98%)	-0.11	2 (1%)	82	87	56, 68, 91, 121	0
10	X	195/198 (98%)	-0.22	2 (1%)	82	87	59, 69, 88, 125	0
11	K	211/211 (100%)	-0.10	3 (1%)	75	82	53, 65, 85, 99	0
11	Y	211/211 (100%)	-0.13	3 (1%)	75	82	58, 70, 91, 111	0
12	L	222/222 (100%)	-0.18	2 (0%)	84	89	56, 69, 90, 112	0
12	Z	222/222 (100%)	-0.15	2 (0%)	84	89	56, 71, 95, 118	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	225/246 (91%)	-0.28	2 (0%)	84	89	54, 68, 86, 115	0
13	a	228/246 (92%)	-0.19	3 (1%)	77	84	54, 66, 87, 120	0
14	N	195/195 (100%)	-0.14	1 (0%)	91	94	54, 66, 89, 119	0
14	b	195/195 (100%)	-0.14	2 (1%)	82	87	56, 67, 89, 118	0
All	All	6327/6610 (95%)	-0.09	131 (2%)	63	72	53, 73, 111, 176	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	50	LEU	9.9
3	Q	49	THR	6.7
1	A	1	MET	6.1
3	Q	204	GLY	6.0
2	P	51	VAL	5.7
11	Y	212	GLY	5.6
12	Z	173	LYS	5.3
3	Q	206	LYS	5.1
3	Q	47	ARG	4.8
5	S	202	ASP	4.7
8	V	226	GLU	4.7
6	T	2	THR	4.6
8	V	223	ILE	4.6
2	B	51	VAL	4.6
13	a	1	THR	4.5
3	Q	203	THR	4.4
3	Q	48	SER	4.4
1	O	2	THR	4.3
4	R	241	ALA	4.3
10	J	1	MET	4.2
8	H	223	ILE	4.2
5	S	204	SER	4.0
14	b	195	GLN	4.0
2	B	221	ASP	3.9
1	O	1	MET	3.9
3	Q	234	ILE	3.9
8	V	225	GLU	3.9
3	Q	205	ALA	3.8
3	Q	202	GLN	3.8
5	E	202	ASP	3.8
5	S	233	ILE	3.8
13	M	1	THR	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	1	GLY	3.8
3	C	49	THR	3.6
8	H	224	GLN	3.6
1	A	2	THR	3.6
3	C	206	LYS	3.6
2	B	220	ASN	3.5
3	C	202	GLN	3.5
2	P	52	THR	3.5
2	B	219	ALA	3.5
1	O	249	ALA	3.5
8	H	222	ASP	3.4
2	P	221	ASP	3.3
10	X	194	ASP	3.3
2	B	218	GLY	3.3
9	W	1	SER	3.2
3	C	50	LEU	3.2
2	P	1	GLY	3.1
2	P	222	GLY	3.1
3	C	47	ARG	3.1
3	C	46	ARG	3.1
8	V	222	ASP	3.1
14	N	195	GLN	3.1
6	T	181	GLU	3.0
7	U	2	GLY	3.0
8	V	224	GLN	3.0
10	X	1	MET	3.0
3	C	48	SER	3.0
8	H	225	GLU	3.0
10	J	95	ARG	3.0
8	H	220	ILE	3.0
9	W	133	LYS	3.0
5	E	201	ARG	2.9
6	F	202	ASP	2.9
5	S	207	VAL	2.8
6	T	180	PRO	2.8
2	P	219	ALA	2.8
11	Y	106	ARG	2.8
2	P	218	GLY	2.8
3	Q	236	GLN	2.7
8	H	226	GLU	2.7
2	P	204	ALA	2.7
6	T	177	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	F	243	ILE	2.7
5	S	54	GLU	2.7
2	P	240	LYS	2.6
6	T	241	LYS	2.6
8	H	221	CYS	2.6
3	C	175	LYS	2.6
3	Q	201	VAL	2.6
3	Q	180	LYS	2.5
2	B	240	LYS	2.5
3	Q	46	ARG	2.5
2	P	220	ASN	2.5
1	O	201	GLU	2.5
6	F	205	GLU	2.5
13	M	69	ASP	2.5
14	b	196	LEU	2.5
11	K	212	GLY	2.5
9	I	1	SER	2.5
4	R	177	ASN	2.5
6	T	207	ASP	2.5
6	T	53	LYS	2.5
3	C	203	THR	2.4
7	G	181	LYS	2.4
6	T	244	ASN	2.4
9	I	133	LYS	2.4
6	F	203	ASN	2.3
4	R	217	GLN	2.3
13	a	224	ASP	2.3
1	O	52	SER	2.3
3	Q	239	GLN	2.3
3	Q	240	GLU	2.3
3	C	1	GLY	2.3
11	K	72	GLU	2.3
5	E	163	ARG	2.3
3	C	204	GLY	2.2
1	O	250	LEU	2.2
2	P	241	THR	2.2
13	a	69	ASP	2.2
6	T	243	ILE	2.2
6	F	201	GLU	2.2
4	D	142	ASP	2.2
7	G	179	LYS	2.2
3	C	238	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	207	ASN	2.1
12	Z	1	GLN	2.1
9	W	191	LYS	2.1
11	Y	199	LYS	2.1
12	L	1	GLN	2.1
3	Q	179	ARG	2.1
12	L	165	ASN	2.1
7	U	181	LYS	2.1
9	I	131	GLU	2.1
7	U	68	ARG	2.1
1	A	231	LYS	2.1
11	K	106	ARG	2.1
4	D	238	LYS	2.1
9	W	192	ASP	2.1
7	U	17	TYR	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	MES	a	301	12/12	0.82	0.45	125,130,140,141	0
18	MES	M	301	12/12	0.83	0.33	140,142,154,158	0
17	A1IF8	Y	301	50/50	0.86	0.22	65,74,97,100	0
15	CL	V	301	1/1	0.86	0.15	96,96,96,96	0
16	MG	Z	301	1/1	0.86	0.21	79,79,79,79	0
16	MG	N	203	1/1	0.88	0.21	55,55,55,55	0
15	CL	H	301	1/1	0.89	0.13	77,77,77,77	0
16	MG	W	301	1/1	0.91	0.17	72,72,72,72	0

Continued on next page...

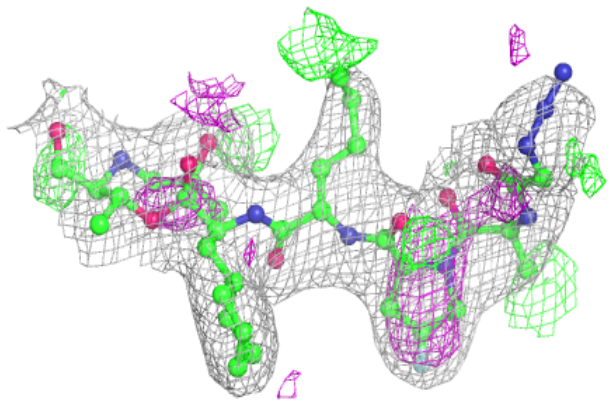
Continued from previous page...

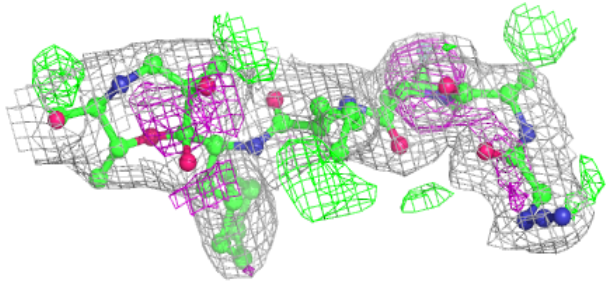
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	A1IF8	b	201	50/50	0.91	0.16	61,65,93,99	0
17	A1IF8	K	301	50/50	0.91	0.18	59,68,99,100	0
17	A1IF8	N	201	50/50	0.91	0.17	55,59,82,91	0
19	SO4	N	202	5/5	0.91	0.36	120,121,125,132	0
16	MG	I	301	1/1	0.93	0.42	95,95,95,95	0
18	MES	Y	302	12/12	0.93	0.19	89,90,97,101	0
15	CL	U	301	1/1	0.95	0.09	64,64,64,64	0
18	MES	K	302	12/12	0.95	0.18	81,86,94,104	0
16	MG	K	303	1/1	0.96	0.12	73,73,73,73	0
16	MG	X	201	1/1	0.96	0.35	38,38,38,38	0
15	CL	G	301	1/1	0.96	0.09	59,59,59,59	0
16	MG	G	302	1/1	0.98	0.09	67,67,67,67	0
16	MG	Y	303	1/1	0.98	0.10	80,80,80,80	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 A1IF8 Y 301:

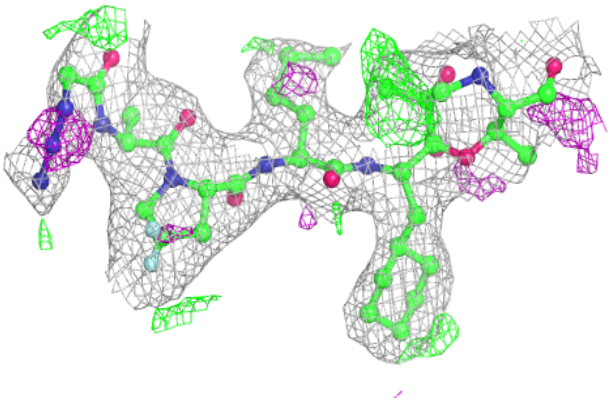
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

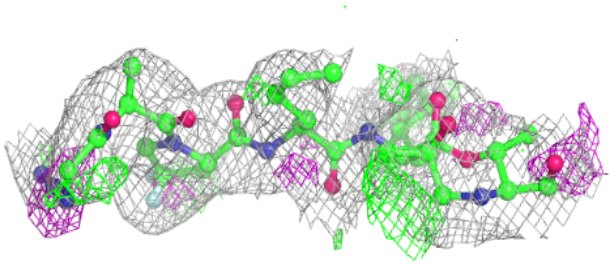


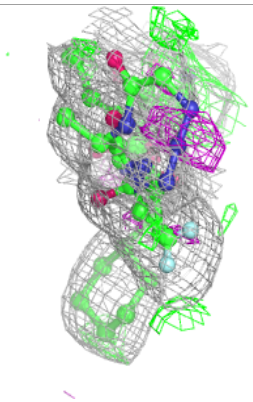


Electron density around A1IF8 b 201:

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

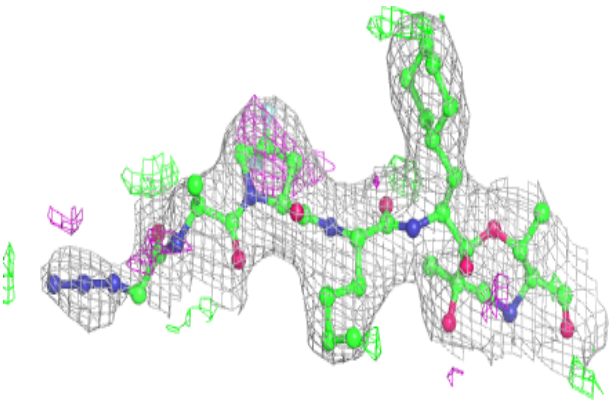


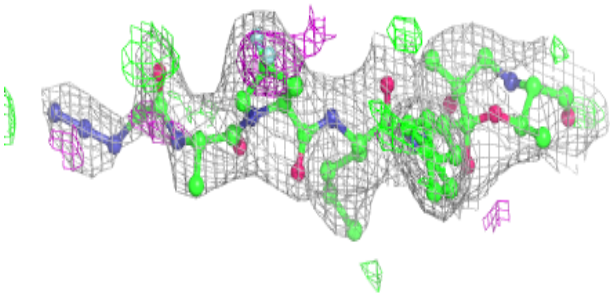


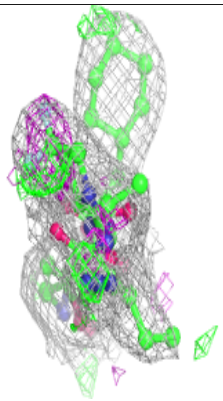


Electron density around A1IF8 K 301:

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

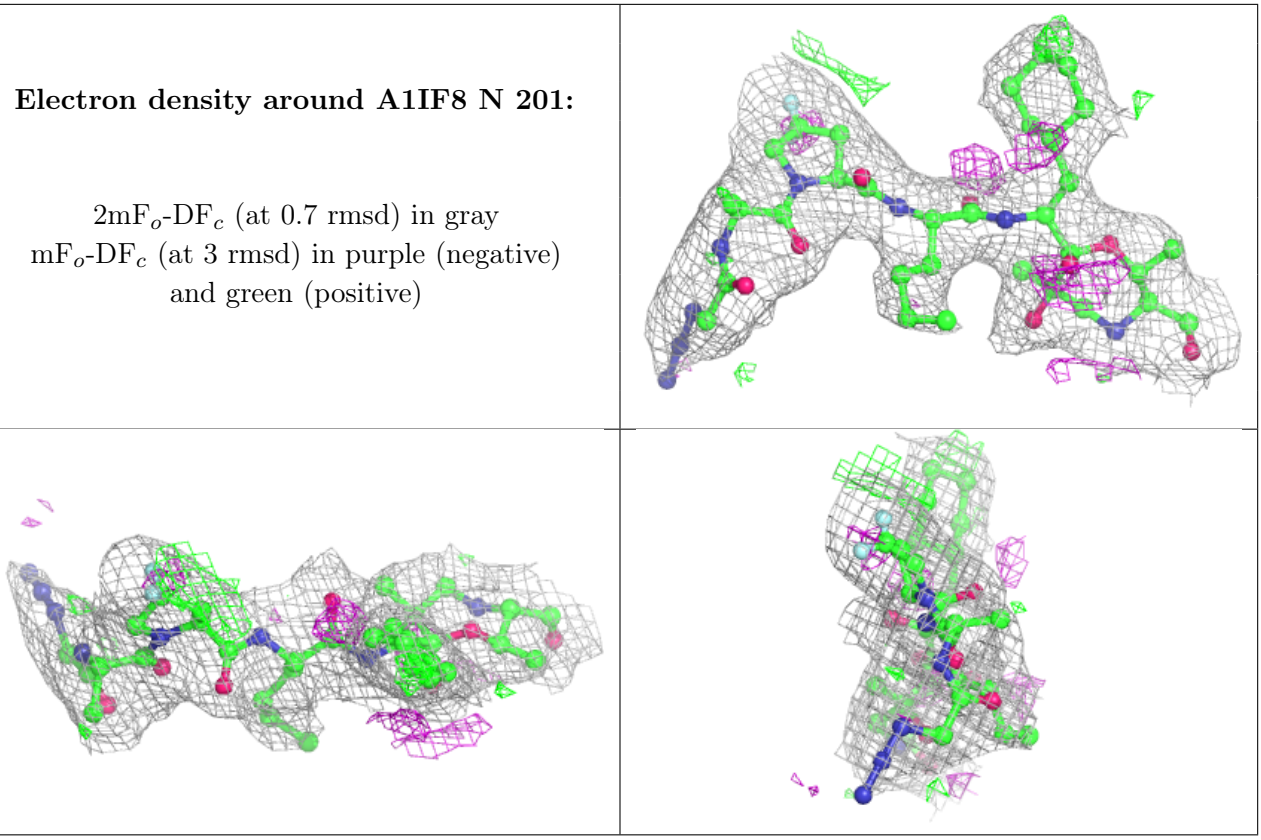






Electron density around A1IF8 N 201:

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



6.5 Other polymers (i)

There are no such residues in this entry.