Full wwPDB EM Validation Report ⓘ

Feb 24, 2025 – 12:14 pm GMT

PDB ID	:	9HMN
EMDB ID	:	EMD-52296
Title	:	CryoEM structure of human 20S proteasome in complex with proteasome inhibitor Salinosporamid A
Authors	:	Suelzen, H.; Boura, E.; Silhan, J.
Deposited on	:	2024-12-09
Resolution	:	2.55 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

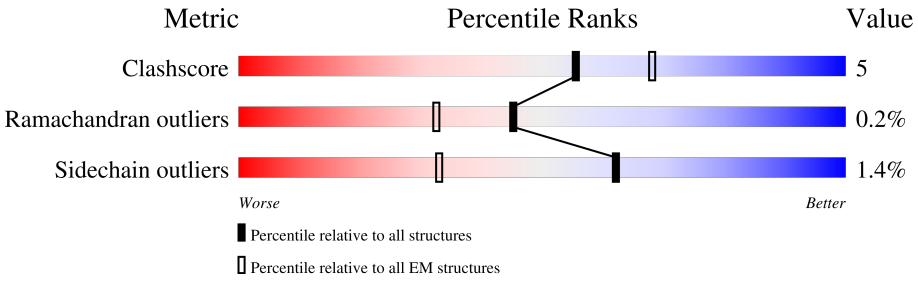
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.55 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	246	84% 14% .
1	O	246	83% 15% .
2	B	233	89% 9% .
2	P	233	89% 10% .
3	C	261	84% 13% .
3	Q	261	84% 13% .
4	E	241	83% 15% .
4	R	241	83% 15% .
5	F	263	75% 15% 10%

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Mol	Chain	Length	Quality of chain
5	S	263	75% 15% 10%
6	G	254	85% 10% 6%
6	T	254	84% 11% 6%
7	J	204	94% 6%
7	U	204	94% 6%
8	K	201	87% 11%
8	V	201	86% 12%
9	M	213	91% 9%
9	W	213	90% 10%
10	N	219	84% 14%
10	X	219	84% 14%
11	D	248	80% 15% 5%
11	Y	248	79% 16% 5%
12	H	205	90% 8%
12	Z	205	89% 9%
13	I	234	82% 11% 6%
13	a	234	92% 6%
14	L	204	91% 7%
14	b	204	96%

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 48800 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	242	Total	C	N	O	S	0	0
			1886	1197	315	361	13		
1	O	242	Total	C	N	O	S	0	0
			1886	1197	315	361	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	230	Total	C	N	O	S	0	0
			1792	1147	302	337	6		
2	P	230	Total	C	N	O	S	0	0
			1792	1147	302	337	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	255	Total	C	N	O	S	0	0
			2016	1272	347	387	10		
3	Q	255	Total	C	N	O	S	0	0
			2016	1272	347	387	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	236	Total	C	N	O	S	0	0
			1804	1133	297	363	11		
4	R	236	Total	C	N	O	S	0	0
			1804	1133	297	363	11		

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	237	Total	C	N	O	S	0	0
			1864	1167	335	351	11		
5	S	237	Total	C	N	O	S	0	0
			1864	1167	335	351	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		
6	T	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

- Molecule 7 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	204	Total	C	N	O	S	0	0
			1590	1013	265	293	19		
7	U	204	Total	C	N	O	S	0	0
			1590	1013	265	293	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	197	Total	C	N	O	S	0	0
			1578	1011	268	290	9		
8	V	197	Total	C	N	O	S	0	0
			1578	1011	268	290	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	212	Total	C	N	O	S	0	0
			1642	1041	280	311	10		
9	W	212	Total	C	N	O	S	0	0
			1642	1041	280	311	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

- Molecule 11 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	236	Total	C	N	O	S	0	0
			1864	1168	330	361	5		
11	Y	236	Total	C	N	O	S	0	0
			1864	1168	330	361	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		
12	Z	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		

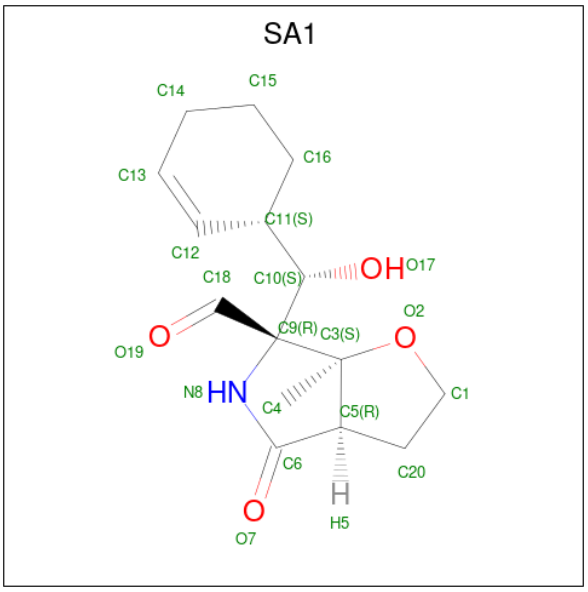
- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	221	Total	C	N	O	S	0	0
			1667	1050	284	321	12		
13	a	221	Total	C	N	O	S	0	0
			1667	1050	284	321	12		

- Molecule 14 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	200	Total	C	N	O	S	0	0
			1555	980	273	293	9		
14	b	200	Total	C	N	O	S	0	0
			1555	980	273	293	9		

- Molecule 15 is (3AR,6R,6AS)-6-((S)-((S)-CYCLOHEX-2-ENYL)(HYDROXY)METHYL)-6A-METHYL-4-OXO-HEXAHYDRO-2H-FURO[3,2-C]PYRROLE-6-CARBALDEHYDE (three-letter code: SA1) (formula: $C_{15}H_{21}NO_4$) (labeled as "Ligand of Interest" by depositor).



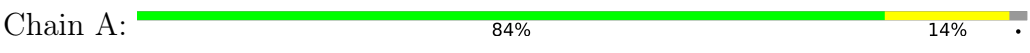
Mol	Chain	Residues	Atoms				AltConf
15	H	1	Total	C	N	O	0
			20	15	1	4	
15	I	1	Total	C	N	O	0
			20	15	1	4	
15	L	1	Total	C	N	O	0
			20	15	1	4	
15	Z	1	Total	C	N	O	0
			20	15	1	4	
15	a	1	Total	C	N	O	0
			20	15	1	4	
15	b	1	Total	C	N	O	0
			20	15	1	4	

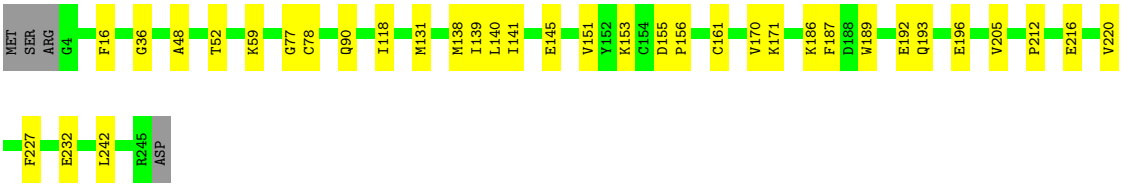
3 Residue-property plots (i)

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. 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. 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-6

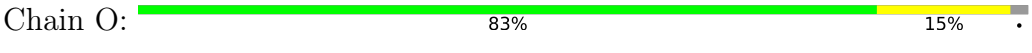
Chain A:

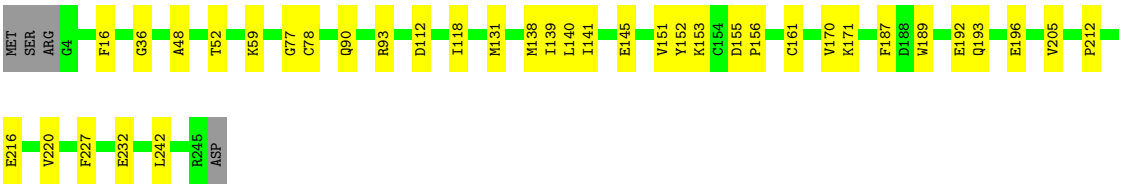




• Molecule 1: Proteasome subunit alpha type-6

Chain O:





• Molecule 2: Proteasome subunit alpha type-2

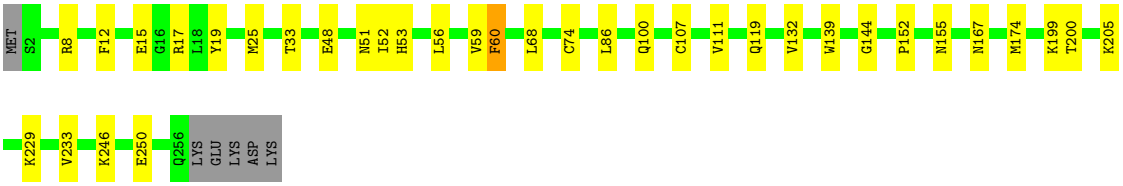
Chain B:

• Molecule 2: Proteasome subunit alpha type-2

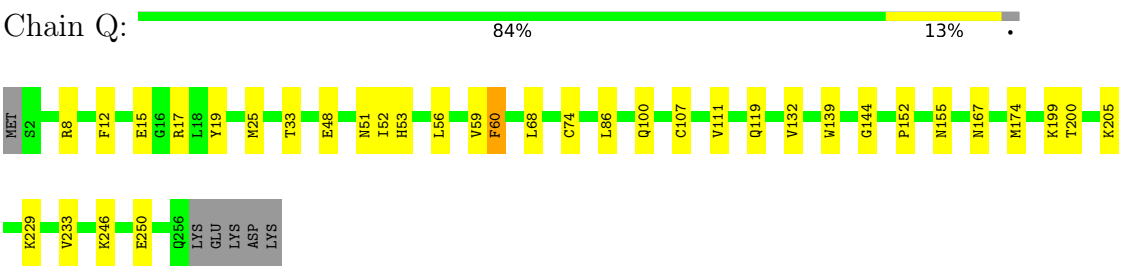
Chain P:

• Molecule 3: Proteasome subunit alpha type-4

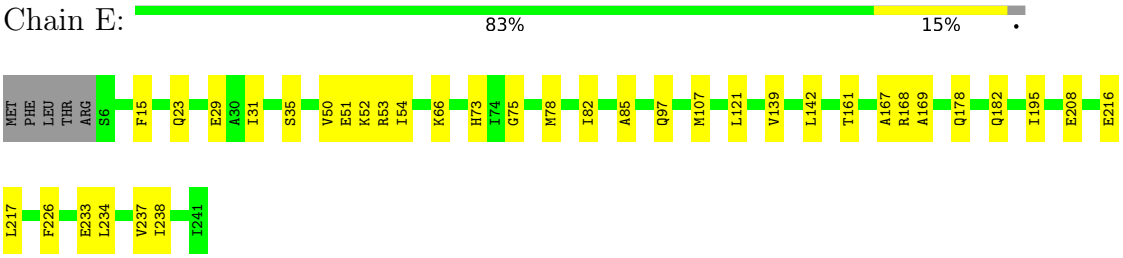
Chain C:



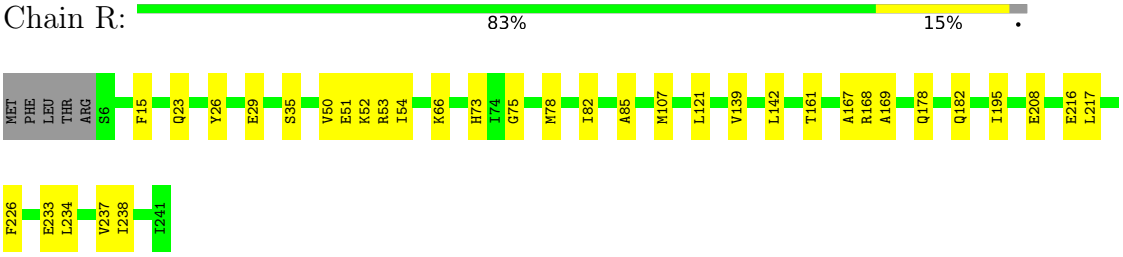
• Molecule 3: Proteasome subunit alpha type-4



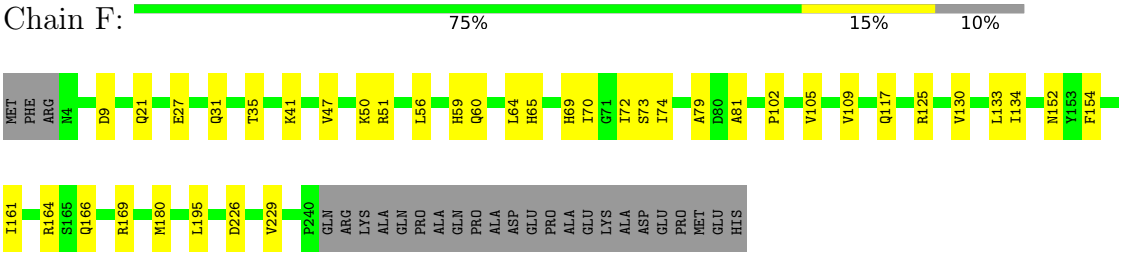
• Molecule 4: Proteasome subunit alpha type-5



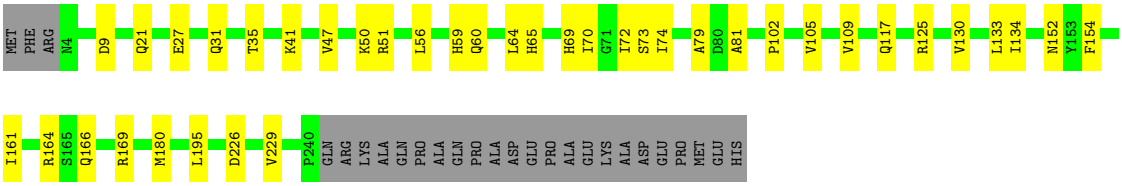
• Molecule 4: Proteasome subunit alpha type-5



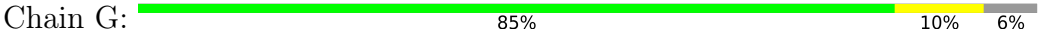
• Molecule 5: Proteasome subunit alpha type-1



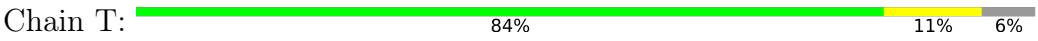
• Molecule 5: Proteasome subunit alpha type-1

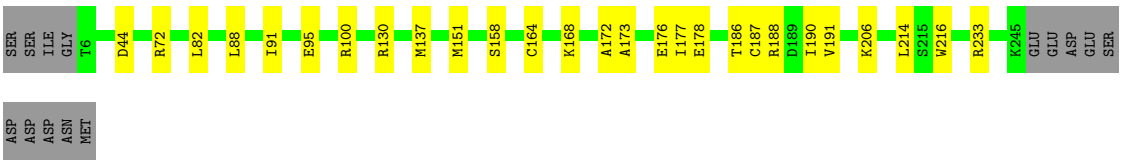


• Molecule 6: Proteasome subunit alpha type-3

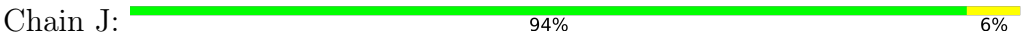


• Molecule 6: Proteasome subunit alpha type-3



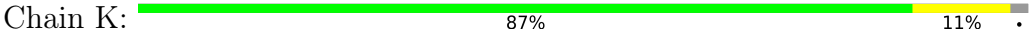


• Molecule 7: Proteasome subunit beta type-3

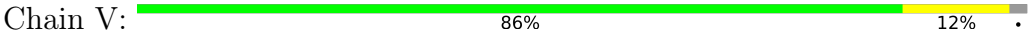


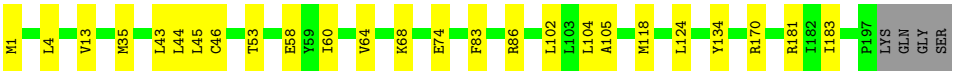
• Molecule 7: Proteasome subunit beta type-3

• Molecule 8: Proteasome subunit beta type-2

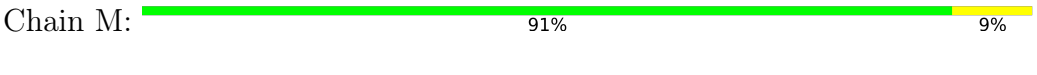


• Molecule 8: Proteasome subunit beta type-2

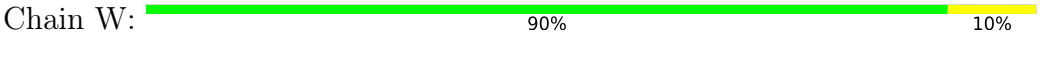




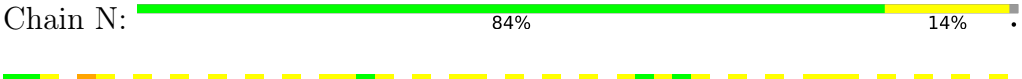
• Molecule 9: Proteasome subunit beta type-1

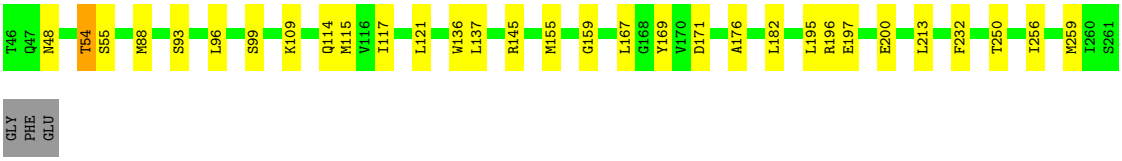


• Molecule 9: Proteasome subunit beta type-1

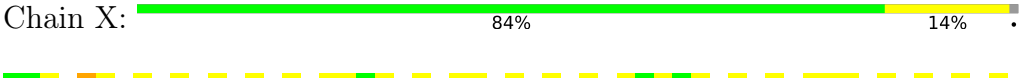


• Molecule 10: Proteasome subunit beta type-4

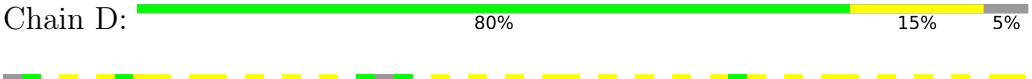


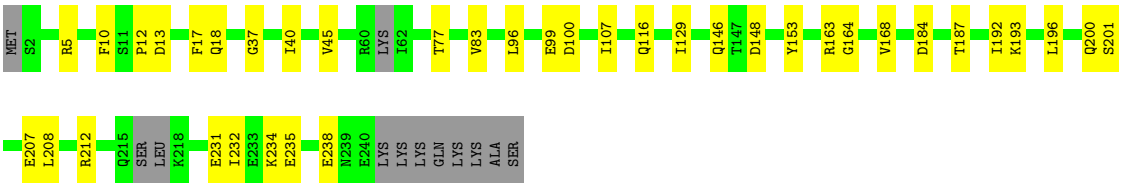


• Molecule 10: Proteasome subunit beta type-4

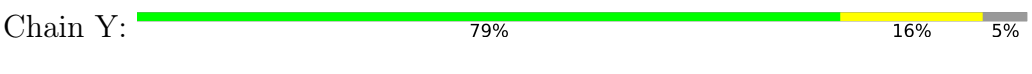


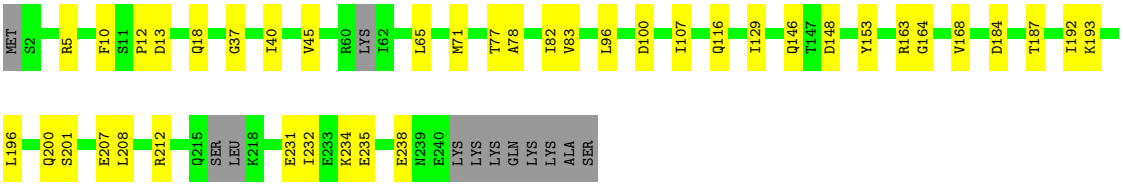
• Molecule 11: Proteasome subunit alpha type-7





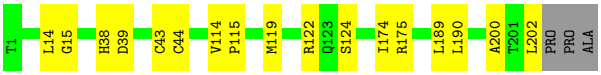
• Molecule 11: Proteasome subunit alpha type-7





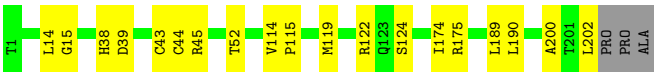
• Molecule 12: Proteasome subunit beta type-6

Chain H:



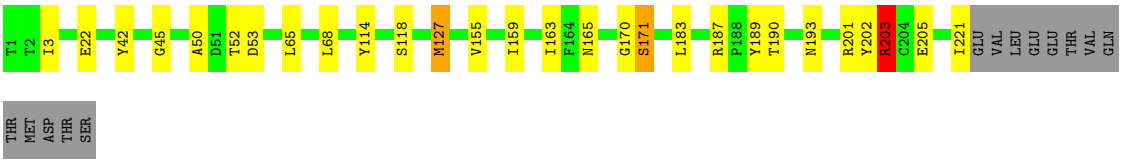
• Molecule 12: Proteasome subunit beta type-6

Chain Z:



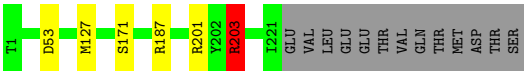
• Molecule 13: Proteasome subunit beta type-7

Chain I:



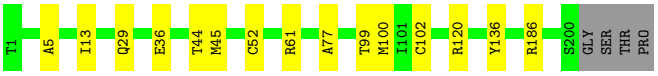
• Molecule 13: Proteasome subunit beta type-7

Chain a:



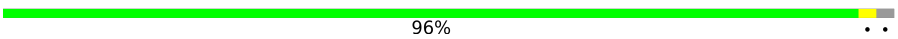
• Molecule 14: Proteasome subunit beta type-5

Chain L:



• Molecule 14: Proteasome subunit beta type-5

Chain b:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	209737	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

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: SA1

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	0.37	0/1920	0.53	0/2595
1	O	0.37	0/1920	0.53	0/2595
2	B	0.37	0/1831	0.52	0/2481
2	P	0.37	0/1831	0.52	0/2481
3	C	0.37	0/2046	0.54	0/2752
3	Q	0.37	0/2046	0.54	0/2752
4	E	0.37	0/1832	0.51	0/2475
4	R	0.37	0/1832	0.51	0/2475
5	F	0.37	0/1899	0.57	0/2567
5	S	0.37	0/1899	0.57	0/2567
6	G	0.38	0/1916	0.54	0/2580
6	T	0.38	0/1916	0.54	0/2580
7	J	0.37	0/1619	0.57	0/2184
7	U	0.37	0/1619	0.57	0/2184
8	K	0.36	0/1611	0.55	0/2180
8	V	0.36	0/1611	0.55	0/2180
9	M	0.37	0/1672	0.56	0/2254
9	W	0.37	0/1672	0.56	0/2254
10	N	0.37	0/1720	0.57	0/2328
10	X	0.37	0/1720	0.57	0/2328
11	D	0.37	0/1888	0.55	0/2545
11	Y	0.37	0/1888	0.55	0/2545
12	H	0.36	0/1540	0.55	0/2085
12	Z	0.36	0/1540	0.55	0/2085
13	I	0.37	0/1694	0.57	0/2293
13	a	0.37	0/1694	0.57	0/2293
14	L	0.38	0/1586	0.58	0/2142
14	b	0.38	0/1586	0.58	0/2142
All	All	0.37	0/49548	0.55	0/66922

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	F	0	1
5	S	0	1
6	G	0	1
6	T	0	1
11	D	0	1
11	Y	0	1
13	I	0	3
13	a	0	4
All	All	0	13

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	D	163	ARG	Sidechain
5	F	164	ARG	Sidechain
6	G	130	ARG	Sidechain
13	I	187	ARG	Peptide,Sidechain
13	I	201	ARG	Sidechain
5	S	164	ARG	Sidechain
6	T	130	ARG	Sidechain
11	Y	163	ARG	Sidechain
13	a	187	ARG	Peptide,Sidechain
13	a	201	ARG	Sidechain
13	a	203	ARG	Sidechain

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	1886	0	1893	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1886	0	1893	28	0
2	B	1792	0	1787	17	0
2	P	1792	0	1787	15	0
3	C	2016	0	2038	30	0
3	Q	2016	0	2038	30	0
4	E	1804	0	1784	35	0
4	R	1804	0	1784	35	0
5	F	1864	0	1852	31	0
5	S	1864	0	1852	30	0
6	G	1881	0	1868	15	0
6	T	1881	0	1868	16	0
7	J	1590	0	1609	12	0
7	U	1590	0	1609	9	0
8	K	1578	0	1580	17	0
8	V	1578	0	1580	18	0
9	M	1642	0	1640	11	0
9	W	1642	0	1640	15	0
10	N	1687	0	1663	15	0
10	X	1687	0	1663	16	0
11	D	1864	0	1874	28	0
11	Y	1864	0	1874	27	0
12	H	1514	0	1486	13	0
12	Z	1514	0	1486	14	0
13	I	1667	0	1691	23	0
13	a	1667	0	1691	0	0
14	L	1555	0	1519	7	0
14	b	1555	0	1519	0	0
15	H	20	0	20	0	0
15	I	20	0	20	1	0
15	L	20	0	20	0	0
15	Z	20	0	20	0	0
15	a	20	0	20	0	0
15	b	20	0	20	0	0
All	All	48800	0	48688	443	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 (443) 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)
1:A:187:PHE:CE2	1:A:193:GLN:OE1	1.66	1.45
1:O:187:PHE:CE2	1:O:193:GLN:OE1	1.65	1.44
4:R:167:ALA:HB3	5:S:56:LEU:CD2	1.62	1.28
4:E:167:ALA:HB3	5:F:56:LEU:CD2	1.62	1.27
1:O:187:PHE:HE2	1:O:193:GLN:OE1	1.06	1.13
4:E:167:ALA:N	5:F:56:LEU:HD23	1.65	1.11
3:Q:59:VAL:HG23	3:Q:60:PHE:CD2	1.86	1.10
3:C:59:VAL:HG23	3:C:60:PHE:CD2	1.86	1.09
4:R:167:ALA:HB3	5:S:56:LEU:HD21	1.28	1.08
4:R:167:ALA:N	5:S:56:LEU:HD23	1.65	1.08
4:E:167:ALA:HB3	5:F:56:LEU:HD21	1.28	1.06
4:R:167:ALA:H	5:S:56:LEU:HD23	1.23	1.00
4:E:167:ALA:H	5:F:56:LEU:HD23	1.23	1.00
1:A:187:PHE:HE2	1:A:193:GLN:OE1	1.06	0.99
4:E:167:ALA:CA	5:F:56:LEU:HD23	1.93	0.97
4:R:167:ALA:CA	5:S:56:LEU:HD23	1.93	0.96
1:A:187:PHE:CD2	1:A:193:GLN:OE1	2.18	0.96
1:O:187:PHE:CD2	1:O:193:GLN:OE1	2.18	0.96
4:E:167:ALA:CB	5:F:56:LEU:CD2	2.43	0.95
4:R:167:ALA:CB	5:S:56:LEU:CD2	2.43	0.95
11:D:99:GLU:OE2	14:L:120:ARG:NH2	2.03	0.90
1:O:90:GLN:HE21	1:O:118:ILE:HG21	1.36	0.88
1:A:90:GLN:HE21	1:A:118:ILE:HG21	1.36	0.87
8:K:35:MET:SD	8:K:181:ARG:NH1	2.48	0.87
3:C:59:VAL:HG23	3:C:60:PHE:HD2	1.40	0.87
8:V:35:MET:SD	8:V:181:ARG:NH1	2.48	0.87
4:R:167:ALA:CB	5:S:56:LEU:HD23	2.06	0.85
3:Q:59:VAL:HG23	3:Q:60:PHE:HD2	1.40	0.84
4:E:167:ALA:CB	5:F:56:LEU:HD23	2.06	0.82
2:P:32:GLY:O	2:P:165:LYS:HG3	1.81	0.81
4:E:29:GLU:OE1	11:D:12:PRO:O	1.99	0.81
4:R:29:GLU:OE1	11:Y:12:PRO:O	1.99	0.80
9:M:173:LEU:HG	9:M:206:VAL:HG22	1.63	0.80
2:B:32:GLY:O	2:B:165:LYS:HG3	1.81	0.79
9:W:173:LEU:HG	9:W:206:VAL:HG22	1.63	0.79
13:I:193:ASN:CG	9:W:241:ASP:OD2	2.22	0.78
14:L:36:GLU:OE2	14:L:186:ARG:NH2	2.15	0.78
1:O:187:PHE:CE2	1:O:193:GLN:CD	2.56	0.78
1:A:187:PHE:CE2	1:A:193:GLN:CD	2.56	0.77
5:F:152:ASN:ND2	5:F:154:PHE:CZ	2.56	0.74
5:S:152:ASN:ND2	5:S:154:PHE:CZ	2.56	0.73
8:K:68:LYS:HD3	8:K:74:GLU:HG2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:58:GLU:HB3	11:Y:96:LEU:HD11	1.70	0.73
8:V:68:LYS:HD3	8:V:74:GLU:HG2	1.69	0.73
8:K:58:GLU:HB3	11:D:96:LEU:HD11	1.70	0.72
7:U:61:GLN:HE22	8:V:124:LEU:H	1.37	0.72
9:M:173:LEU:HD11	9:M:210:ALA:HB2	1.72	0.72
11:D:40:ILE:CD1	11:D:187:THR:HG21	2.20	0.72
11:Y:40:ILE:CD1	11:Y:187:THR:HG21	2.20	0.72
4:R:23:GLN:HE22	11:Y:10:PHE:H	1.37	0.71
4:E:23:GLN:HE22	11:D:10:PHE:H	1.37	0.71
7:J:61:GLN:HE22	8:K:124:LEU:H	1.37	0.70
9:W:173:LEU:HD11	9:W:210:ALA:HB2	1.72	0.70
11:Y:13:ASP:O	11:Y:13:ASP:OD1	2.10	0.70
11:D:40:ILE:HD11	11:D:187:THR:HG21	1.74	0.70
11:Y:40:ILE:HD11	11:Y:187:THR:HG21	1.74	0.70
11:D:13:ASP:OD1	11:D:13:ASP:O	2.10	0.70
13:I:42:TYR:CE1	13:I:183:LEU:HD11	2.28	0.68
4:R:50:VAL:HG11	4:R:66:LYS:HB2	1.76	0.68
4:E:195:ILE:HG23	4:E:217:LEU:HD11	1.76	0.67
11:D:200:GLN:O	11:D:201:SER:OG	2.10	0.67
9:M:173:LEU:HG	9:M:206:VAL:CG2	2.24	0.67
5:S:50:LYS:HB3	5:S:59:HIS:HB3	1.76	0.67
4:E:50:VAL:HG11	4:E:66:LYS:HB2	1.76	0.67
4:R:195:ILE:HG23	4:R:217:LEU:HD11	1.76	0.67
3:Q:155:ASN:HD21	11:Y:77:THR:HB	1.60	0.66
9:W:173:LEU:HG	9:W:206:VAL:CG2	2.24	0.66
11:Y:184:ASP:O	11:Y:187:THR:HG22	1.96	0.66
11:Y:200:GLN:O	11:Y:201:SER:OG	2.10	0.66
3:C:155:ASN:HD21	11:D:77:THR:HB	1.60	0.66
4:E:15:PHE:H	5:F:21:GLN:HE22	1.43	0.66
5:F:50:LYS:HB3	5:F:59:HIS:HB3	1.76	0.66
7:J:127:ILE:CD1	13:I:50:ALA:HB3	2.26	0.66
1:O:90:GLN:NE2	1:O:118:ILE:HG21	2.10	0.66
11:D:184:ASP:O	11:D:187:THR:HG22	1.96	0.65
1:A:90:GLN:NE2	1:A:118:ILE:HG21	2.10	0.65
9:M:176:LEU:HD22	7:U:152:SER:OG	1.97	0.64
4:R:15:PHE:H	5:S:21:GLN:HE22	1.43	0.64
4:R:167:ALA:CB	5:S:56:LEU:HD21	2.17	0.64
7:J:152:SER:OG	9:W:176:LEU:HD22	1.97	0.64
10:N:196:ARG:O	10:N:200:GLU:HG2	1.98	0.64
4:R:52:LYS:HE2	4:R:216:GLU:HG3	1.81	0.64
10:X:196:ARG:O	10:X:200:GLU:HG2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:52:LYS:HE2	4:E:216:GLU:HG3	1.81	0.62
5:S:64:LEU:HD22	5:S:74:ILE:HD11	1.82	0.62
5:F:64:LEU:HD22	5:F:74:ILE:HD11	1.82	0.61
3:C:12:PHE:H	11:D:18:GLN:HE22	1.48	0.61
5:F:47:VAL:HG12	5:F:195:LEU:HD22	1.81	0.61
3:Q:246:LYS:O	3:Q:250:GLU:HG2	2.01	0.61
2:B:143:ARG:HH21	3:C:59:VAL:CG1	2.13	0.60
4:E:50:VAL:HG12	4:E:216:GLU:HB2	1.83	0.60
4:E:167:ALA:CB	5:F:56:LEU:HD21	2.17	0.60
12:H:124:SER:OG	12:Z:200:ALA:HB1	2.02	0.60
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.81	0.60
2:P:143:ARG:HH21	3:Q:59:VAL:CG1	2.13	0.60
2:B:95:GLN:HG3	13:I:65:LEU:HG	1.83	0.60
3:Q:12:PHE:H	11:Y:18:GLN:HE22	1.48	0.59
4:E:178:GLN:O	4:E:182:GLN:HG2	2.03	0.59
1:A:90:GLN:HE21	1:A:118:ILE:CG2	2.12	0.59
12:H:200:ALA:HB1	12:Z:124:SER:OG	2.02	0.59
3:C:246:LYS:O	3:C:250:GLU:HG2	2.01	0.59
4:R:178:GLN:O	4:R:182:GLN:HG2	2.03	0.59
5:F:35:THR:HG21	5:F:73:SER:OG	2.03	0.59
2:P:143:ARG:HH21	3:Q:59:VAL:HG12	1.68	0.58
5:S:35:THR:HG21	5:S:73:SER:OG	2.03	0.58
2:B:143:ARG:HH21	3:C:59:VAL:HG12	1.68	0.58
4:R:50:VAL:HG12	4:R:216:GLU:HB2	1.83	0.58
2:B:111:VAL:HG22	2:B:136:ILE:HD13	1.85	0.58
12:H:202:LEU:HD11	12:Z:122:ARG:HG2	1.86	0.58
2:P:111:VAL:HG22	2:P:136:ILE:HD13	1.85	0.58
5:S:27:GLU:O	5:S:31:GLN:HG2	2.05	0.57
5:F:27:GLU:O	5:F:31:GLN:HG2	2.05	0.57
11:D:193:LYS:HG3	11:D:232:ILE:HD13	1.85	0.57
11:Y:193:LYS:HG3	11:Y:232:ILE:HD13	1.85	0.57
3:Q:100:GLN:HE21	8:V:83:PHE:HE1	1.52	0.57
11:Y:146:GLN:NE2	11:Y:148:ASP:OD1	2.38	0.57
12:H:122:ARG:HG2	12:Z:202:LEU:HD11	1.86	0.57
1:O:90:GLN:HE21	1:O:118:ILE:CG2	2.12	0.56
3:C:100:GLN:HE21	8:K:83:PHE:HE1	1.52	0.56
3:Q:52:ILE:O	3:Q:52:ILE:HD12	2.05	0.56
3:C:52:ILE:HD12	3:C:52:ILE:O	2.05	0.56
4:E:142:LEU:HD21	4:E:168:ARG:HG2	1.88	0.56
7:J:127:ILE:HD12	13:I:50:ALA:HB3	1.88	0.56
10:N:54:THR:HG23	10:N:55:SER:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:142:LEU:HD21	4:R:168:ARG:HG2	1.88	0.56
11:D:146:GLN:NE2	11:D:148:ASP:OD1	2.38	0.56
10:X:54:THR:HG23	10:X:55:SER:H	1.70	0.56
10:X:232:PHE:HE1	10:X:250:THR:HG23	1.71	0.56
10:N:232:PHE:HE1	10:N:250:THR:HG23	1.71	0.56
8:V:4:LEU:HD22	8:V:45:LEU:HB3	1.88	0.56
1:A:90:GLN:HG2	1:A:138:MET:HE1	1.89	0.55
3:C:15:GLU:HB2	3:C:17:ARG:HD3	1.89	0.55
8:K:4:LEU:HD22	8:K:45:LEU:HB3	1.88	0.54
3:Q:59:VAL:HG23	3:Q:60:PHE:CE2	2.40	0.54
3:Q:15:GLU:HB2	3:Q:17:ARG:HD3	1.89	0.54
7:J:87:LEU:O	7:J:91:VAL:HG23	2.08	0.54
1:O:90:GLN:HG2	1:O:138:MET:HE1	1.89	0.54
8:V:35:MET:SD	8:V:181:ARG:HD2	2.48	0.54
1:O:212:PRO:HB2	1:O:232:GLU:HG2	1.90	0.54
3:C:59:VAL:HG23	3:C:60:PHE:CE2	2.40	0.54
3:C:167:ASN:HB2	3:C:200:THR:HG23	1.89	0.53
9:M:38:GLY:HA3	9:M:70:LYS:HE3	1.90	0.53
11:D:231:GLU:O	11:D:235:GLU:HG2	2.08	0.53
11:D:234:LYS:O	11:D:238:GLU:HG2	2.08	0.53
1:O:192:GLU:O	1:O:196:GLU:HG3	2.08	0.53
4:R:35:SER:HB3	4:R:51:GLU:HG3	1.90	0.53
8:K:35:MET:SD	8:K:181:ARG:HD2	2.48	0.53
11:Y:231:GLU:O	11:Y:235:GLU:HG2	2.08	0.53
11:D:40:ILE:HG22	11:D:212:ARG:HG2	1.89	0.53
3:Q:167:ASN:HB2	3:Q:200:THR:HG23	1.89	0.53
11:D:40:ILE:HD13	11:D:187:THR:HG21	1.90	0.53
1:A:90:GLN:HG2	1:A:138:MET:CE	2.39	0.53
9:W:38:GLY:HA3	9:W:70:LYS:HE3	1.90	0.53
11:Y:234:LYS:O	11:Y:238:GLU:HG2	2.08	0.53
1:A:141:ILE:HG22	1:A:151:VAL:HG22	1.91	0.53
4:E:169:ALA:H	4:E:178:GLN:HE22	1.57	0.53
11:Y:40:ILE:HG22	11:Y:212:ARG:HG2	1.89	0.53
7:U:87:LEU:O	7:U:91:VAL:HG23	2.08	0.53
4:E:35:SER:HB3	4:E:51:GLU:HG3	1.90	0.53
12:H:14:LEU:HD23	12:H:44:CYS:SG	2.49	0.53
12:Z:115:PRO:HD2	12:Z:119:MET:HG3	1.91	0.53
1:A:212:PRO:HB2	1:A:232:GLU:HG2	1.90	0.52
9:W:57:LEU:HB3	9:W:65:THR:HG22	1.91	0.52
1:A:192:GLU:O	1:A:196:GLU:HG3	2.08	0.52
1:O:90:GLN:HG2	1:O:138:MET:CE	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:14:LEU:HD23	12:Z:44:CYS:SG	2.49	0.52
4:R:169:ALA:H	4:R:178:GLN:HE22	1.57	0.52
9:M:57:LEU:HB3	9:M:65:THR:HG22	1.91	0.52
12:H:115:PRO:HD2	12:H:119:MET:HG3	1.91	0.52
13:I:203:ARG:NH2	13:I:205:GLU:OE2	2.43	0.52
4:R:167:ALA:CA	5:S:56:LEU:CD2	2.75	0.52
4:E:78:MET:HG3	4:E:82:ILE:HD12	1.92	0.52
13:I:202:TYR:O	13:I:203:ARG:C	2.47	0.52
1:O:141:ILE:HG22	1:O:151:VAL:HG22	1.91	0.51
5:S:41:LYS:HG3	5:S:180:MET:HG3	1.93	0.51
1:O:155:ASP:HB2	1:O:156:PRO:HD2	1.93	0.51
5:S:72:ILE:HG22	5:S:134:ILE:HG13	1.93	0.51
4:E:85:ALA:HB2	4:E:139:VAL:HG11	1.93	0.51
1:O:48:ALA:HB3	1:O:220:VAL:HG12	1.92	0.51
3:Q:139:TRP:HA	3:Q:144:GLY:O	2.11	0.51
6:T:173:ALA:O	6:T:177:ILE:HG13	2.11	0.51
1:A:48:ALA:HB3	1:A:220:VAL:HG12	1.92	0.51
1:A:155:ASP:HB2	1:A:156:PRO:HD2	1.93	0.50
1:A:139:ILE:HG12	1:A:153:LYS:HG3	1.94	0.50
2:B:184:LEU:O	2:B:188:ILE:HG13	2.12	0.50
13:I:3:ILE:HD11	13:I:127:MET:HB2	1.94	0.50
6:G:173:ALA:O	6:G:177:ILE:HG13	2.11	0.50
12:H:202:LEU:CD1	12:Z:122:ARG:HG2	2.41	0.50
11:Y:40:ILE:HD13	11:Y:187:THR:HG21	1.90	0.50
3:C:139:TRP:HA	3:C:144:GLY:O	2.11	0.50
1:O:139:ILE:HG12	1:O:153:LYS:HG3	1.94	0.50
12:H:122:ARG:HG2	12:Z:202:LEU:CD1	2.41	0.50
4:R:85:ALA:HB2	4:R:139:VAL:HG11	1.93	0.50
5:F:41:LYS:HG3	5:F:180:MET:HG3	1.93	0.50
2:P:184:LEU:O	2:P:188:ILE:HG13	2.12	0.50
4:R:78:MET:HG3	4:R:82:ILE:HD12	1.92	0.50
3:Q:174:MET:HE1	3:Q:199:LYS:HB2	1.94	0.49
4:R:167:ALA:H	5:S:56:LEU:CD2	2.11	0.49
5:F:69:HIS:CE1	5:F:102:PRO:HB3	2.47	0.49
7:J:107:PRO:HD2	7:J:124:LEU:HB2	1.95	0.49
5:S:69:HIS:CE1	5:S:102:PRO:HB3	2.47	0.49
5:S:166:GLN:NE2	5:S:169:ARG:HH21	2.10	0.49
5:F:72:ILE:HG22	5:F:134:ILE:HG13	1.93	0.49
14:L:5:ALA:HA	14:L:13:ILE:O	2.12	0.49
3:C:174:MET:HE1	3:C:199:LYS:HB2	1.94	0.49
10:N:115:MET:HE1	10:N:136:TRP:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:203:ARG:NH2	9:W:189:VAL:HG13	2.28	0.49
5:F:105:VAL:O	5:F:109:VAL:HG23	2.13	0.49
7:J:65:GLN:NE2	8:K:86:ARG:HH21	2.11	0.49
3:C:229:LYS:O	3:C:233:VAL:HG23	2.13	0.48
5:F:166:GLN:NE2	5:F:169:ARG:HH21	2.10	0.48
3:Q:33:THR:HG21	3:Q:200:THR:HG21	1.95	0.48
4:R:195:ILE:HG23	4:R:217:LEU:CD1	2.43	0.48
5:S:105:VAL:O	5:S:109:VAL:HG23	2.13	0.48
1:A:90:GLN:NE2	1:A:118:ILE:CG2	2.74	0.48
8:K:44:LEU:HD11	8:K:102:LEU:HD22	1.95	0.48
3:Q:229:LYS:O	3:Q:233:VAL:HG23	2.13	0.48
2:B:75:VAL:HG12	2:B:135:LEU:HB2	1.95	0.48
4:E:167:ALA:CA	5:F:56:LEU:CD2	2.75	0.48
6:G:137:MET:SD	6:G:164:CYS:HB3	2.53	0.48
4:R:234:LEU:O	4:R:238:ILE:HG12	2.14	0.48
6:T:137:MET:SD	6:T:164:CYS:HB3	2.53	0.48
7:U:107:PRO:HD2	7:U:124:LEU:HB2	1.95	0.48
4:E:167:ALA:H	5:F:56:LEU:CD2	2.11	0.48
2:P:75:VAL:HG12	2:P:135:LEU:HB2	1.95	0.48
4:E:234:LEU:O	4:E:238:ILE:HG12	2.14	0.48
3:Q:68:LEU:HD11	3:Q:74:CYS:HB3	1.96	0.48
2:B:143:ARG:NH2	3:C:59:VAL:CG1	2.76	0.48
10:N:96:LEU:HD11	10:N:137:LEU:HD11	1.96	0.48
2:P:143:ARG:NH2	3:Q:59:VAL:CG1	2.76	0.48
5:S:226:ASP:O	5:S:229:VAL:HG22	2.14	0.48
12:Z:38:HIS:CD2	12:Z:39:ASP:H	2.32	0.48
7:U:65:GLN:NE2	8:V:86:ARG:HH21	2.11	0.47
3:C:33:THR:HG21	3:C:200:THR:HG21	1.95	0.47
3:C:33:THR:H	3:C:48:GLU:HG2	1.79	0.47
3:C:68:LEU:HD11	3:C:74:CYS:HB3	1.96	0.47
8:K:118:MET:HE2	8:K:124:LEU:HD13	1.96	0.47
5:F:65:HIS:ND1	9:M:105:HIS:HE1	2.13	0.47
12:H:38:HIS:CD2	12:H:39:ASP:H	2.32	0.47
3:Q:86:LEU:HD12	3:Q:132:VAL:HG11	1.96	0.47
10:X:96:LEU:HD11	10:X:137:LEU:HD11	1.96	0.47
5:F:226:ASP:O	5:F:229:VAL:HG22	2.14	0.47
6:T:188:ARG:HE	6:T:188:ARG:HB3	1.61	0.47
8:V:44:LEU:HD11	8:V:102:LEU:HD22	1.95	0.47
1:O:90:GLN:NE2	1:O:118:ILE:CG2	2.74	0.47
13:I:45:GLY:HA3	13:I:52:THR:HG21	1.97	0.47
3:C:205:LYS:HA	3:C:205:LYS:HD3	1.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:195:ILE:HG23	4:E:217:LEU:CD1	2.43	0.47
11:Y:146:GLN:O	11:Y:153:TYR:HA	2.16	0.47
8:V:1:MET:HE3	8:V:134:TYR:CE2	2.49	0.46
8:V:118:MET:HE2	8:V:124:LEU:HD13	1.95	0.46
1:A:187:PHE:HD2	1:A:189:TRP:HD1	1.63	0.46
3:Q:33:THR:H	3:Q:48:GLU:HG2	1.79	0.46
11:Y:107:ILE:HD12	11:Y:107:ILE:HA	1.78	0.46
1:A:36:GLY:HA2	1:A:170:VAL:HG21	1.98	0.46
2:B:76:TYR:HB3	2:B:83:TYR:CD1	2.50	0.46
2:P:143:ARG:NH2	3:Q:59:VAL:HG12	2.30	0.46
1:A:16:PHE:H	2:B:21:GLN:HE22	1.63	0.46
1:O:77:GLY:HA3	1:O:227:PHE:CD2	2.50	0.46
2:P:76:TYR:HB3	2:P:83:TYR:CD1	2.50	0.46
1:A:59:LYS:CE	6:G:178:GLU:HB3	2.46	0.46
1:A:77:GLY:HA3	1:A:227:PHE:CD2	2.50	0.46
13:I:165:ASN:ND2	10:X:196:ARG:HH11	2.13	0.46
1:O:16:PHE:H	2:P:21:GLN:HE22	1.63	0.46
1:A:52:THR:HG22	1:A:216:GLU:HB2	1.98	0.46
3:C:51:ASN:HB3	3:C:56:LEU:HD13	1.98	0.46
9:M:151:SER:O	9:M:158:TYR:HA	2.16	0.46
5:S:65:HIS:ND1	9:W:105:HIS:HE1	2.13	0.46
2:B:42:ASN:OD1	2:B:42:ASN:N	2.49	0.46
3:C:86:LEU:HD12	3:C:132:VAL:HG11	1.96	0.46
8:K:1:MET:HE3	8:K:134:TYR:CE2	2.51	0.46
11:Y:164:GLY:O	11:Y:168:VAL:HG23	2.16	0.46
3:Q:8:ARG:HH21	11:Y:5:ARG:HD2	1.81	0.46
6:G:44:ASP:OD1	6:G:44:ASP:N	2.50	0.45
1:O:59:LYS:CE	6:T:178:GLU:HB3	2.46	0.45
13:I:163:ILE:HG23	13:I:170:GLY:HA2	1.98	0.45
3:Q:51:ASN:HB3	3:Q:56:LEU:HD13	1.98	0.45
3:Q:100:GLN:NE2	8:V:83:PHE:HE1	2.13	0.45
11:D:83:VAL:HG21	11:D:129:ILE:HD11	1.98	0.45
11:D:164:GLY:O	11:D:168:VAL:HG23	2.16	0.45
13:I:114:TYR:HB2	13:I:118:SER:OG	2.16	0.45
14:L:45:MET:HG2	14:L:52:CYS:HB3	1.99	0.45
1:O:52:THR:HG22	1:O:216:GLU:HB2	1.98	0.45
10:X:169:TYR:O	10:X:176:ALA:HA	2.16	0.45
2:P:42:ASN:OD1	2:P:42:ASN:N	2.49	0.45
6:T:44:ASP:OD1	6:T:44:ASP:N	2.50	0.45
10:X:115:MET:HE1	10:X:136:TRP:CE2	2.51	0.45
7:J:117:PHE:CD2	7:J:192:LYS:HE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:112:THR:O	9:M:116:ILE:HG13	2.17	0.45
11:D:146:GLN:O	11:D:153:TYR:HA	2.16	0.45
6:T:91:ILE:O	6:T:95:GLU:HG2	2.17	0.45
10:N:54:THR:O	10:N:99:SER:HB2	2.16	0.45
13:I:170:GLY:O	13:I:171:SER:HB2	2.14	0.45
1:O:36:GLY:HA2	1:O:170:VAL:HG21	1.98	0.45
2:B:143:ARG:NH2	3:C:59:VAL:HG12	2.30	0.45
4:R:161:THR:HG23	5:S:60:GLN:NE2	2.32	0.45
2:B:107:THR:O	2:B:111:VAL:HG23	2.17	0.45
10:N:169:TYR:O	10:N:176:ALA:HA	2.16	0.45
8:V:46:CYS:SG	8:V:53:THR:HG23	2.57	0.45
4:E:161:THR:HG23	5:F:60:GLN:NE2	2.32	0.45
5:F:51:ARG:HA	5:F:59:HIS:CD2	2.52	0.45
2:P:107:THR:O	2:P:111:VAL:HG23	2.17	0.45
9:W:112:THR:O	9:W:116:ILE:HG13	2.17	0.45
11:D:107:ILE:HD12	11:D:107:ILE:HA	1.78	0.44
1:O:187:PHE:HD2	1:O:189:TRP:HD1	1.62	0.44
3:Q:86:LEU:HD12	3:Q:132:VAL:CG1	2.47	0.44
4:R:233:GLU:O	4:R:237:VAL:HG23	2.18	0.44
5:S:51:ARG:HA	5:S:59:HIS:CD2	2.52	0.44
9:W:151:SER:O	9:W:158:TYR:HA	2.16	0.44
4:R:121:LEU:HD12	5:S:79:ALA:HB3	2.00	0.44
5:S:69:HIS:CD2	5:S:70:ILE:HG13	2.53	0.44
8:K:46:CYS:SG	8:K:53:THR:HG23	2.57	0.44
13:I:155:VAL:O	13:I:159:ILE:HG12	2.17	0.44
4:E:121:LEU:HD12	5:F:79:ALA:HB3	2.00	0.44
4:E:233:GLU:O	4:E:237:VAL:HG23	2.18	0.44
11:Y:83:VAL:HG21	11:Y:129:ILE:HD11	1.98	0.44
3:C:25:MET:SD	3:C:152:PRO:HD2	2.58	0.44
2:P:71:HIS:ND1	2:P:139:TRP:HB3	2.33	0.44
7:U:117:PHE:CD2	7:U:192:LYS:HE2	2.52	0.44
10:X:54:THR:O	10:X:99:SER:HB2	2.16	0.44
3:C:100:GLN:NE2	8:K:83:PHE:HE1	2.13	0.44
3:C:8:ARG:HH21	11:D:5:ARG:HD2	1.81	0.44
13:I:165:ASN:HD22	10:X:196:ARG:HH11	1.66	0.44
6:G:91:ILE:O	6:G:95:GLU:HG2	2.17	0.44
13:I:193:ASN:ND2	9:W:241:ASP:OD2	2.50	0.44
3:Q:25:MET:SD	3:Q:152:PRO:HD2	2.58	0.44
5:F:69:HIS:CD2	5:F:70:ILE:HG13	2.53	0.43
3:C:86:LEU:HD12	3:C:132:VAL:CG1	2.47	0.43
6:G:168:LYS:HB3	6:G:168:LYS:HE2	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:205:LYS:HA	3:Q:205:LYS:HD3	1.65	0.43
9:M:127:ARG:HG3	9:M:132:TYR:CE2	2.54	0.43
2:B:71:HIS:ND1	2:B:139:TRP:HB3	2.33	0.43
3:Q:53:HIS:H	3:Q:56:LEU:HD12	1.84	0.43
6:T:168:LYS:HB3	6:T:168:LYS:HE2	1.80	0.43
2:B:177:ARG:HE	2:B:177:ARG:HB3	1.58	0.43
10:N:195:LEU:HD23	10:N:213:LEU:HG	2.01	0.43
10:N:256:ILE:HA	10:N:259:MET:HG3	2.00	0.43
13:I:203:ARG:CZ	9:W:189:VAL:HG13	2.47	0.43
7:U:65:GLN:HE21	8:V:86:ARG:HH21	1.67	0.43
11:D:99:GLU:OE1	14:L:77:ALA:HB1	2.18	0.43
7:J:65:GLN:HE21	8:K:86:ARG:HH21	1.67	0.43
10:N:232:PHE:CE1	10:N:250:THR:HG23	2.53	0.43
1:O:59:LYS:HE2	6:T:178:GLU:OE1	2.19	0.43
10:X:256:ILE:HA	10:X:259:MET:HG3	2.00	0.43
6:G:151:MET:O	6:G:158:SER:HA	2.19	0.43
6:T:151:MET:O	6:T:158:SER:HA	2.19	0.43
9:W:127:ARG:HG3	9:W:132:TYR:CE2	2.54	0.43
11:Y:45:VAL:HG22	11:Y:207:GLU:HB3	2.00	0.43
8:K:60:ILE:O	8:K:64:VAL:HG23	2.19	0.42
6:G:186:THR:O	6:G:190:ILE:HG12	2.20	0.42
11:D:45:VAL:HG22	11:D:207:GLU:HB3	2.00	0.42
4:R:73:HIS:H	4:R:73:HIS:CD2	2.37	0.42
8:V:60:ILE:O	8:V:64:VAL:HG23	2.19	0.42
12:Z:15:GLY:HA2	12:Z:175:ARG:O	2.19	0.42
6:G:88:LEU:HD23	6:G:88:LEU:HA	1.81	0.42
7:J:125:ASP:CG	13:I:22:GLU:OE2	2.57	0.42
2:P:92:LYS:HE3	2:P:92:LYS:HB3	1.78	0.42
6:T:206:LYS:HE3	6:T:206:LYS:HB3	1.84	0.42
6:T:214:LEU:HD12	6:T:233:ARG:HG3	2.02	0.42
1:A:186:LYS:HA	1:A:186:LYS:HD2	1.89	0.42
5:F:133:LEU:HD11	5:F:161:ILE:HG12	2.02	0.42
1:A:59:LYS:HE2	6:G:178:GLU:OE1	2.19	0.42
3:C:53:HIS:H	3:C:56:LEU:HD12	1.84	0.42
4:E:73:HIS:HE1	4:E:107:MET:O	2.03	0.42
6:G:214:LEU:HD12	6:G:233:ARG:HG3	2.02	0.42
10:N:167:LEU:HG	10:N:182:LEU:HD12	2.01	0.42
10:X:195:LEU:HD23	10:X:213:LEU:HG	2.01	0.42
14:L:44:THR:O	14:L:99:THR:HG23	2.20	0.42
4:R:234:LEU:HD23	4:R:234:LEU:HA	1.90	0.42
2:B:91:ARG:HD3	13:I:68:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:73:HIS:H	4:E:73:HIS:CD2	2.37	0.42
6:T:187:CYS:O	6:T:191:VAL:HG23	2.20	0.42
12:Z:174:ILE:HB	12:Z:189:LEU:HB2	2.02	0.42
6:G:100:ARG:HH11	10:N:114:GLN:HE22	1.68	0.42
6:G:187:CYS:O	6:G:191:VAL:HG23	2.20	0.42
12:H:15:GLY:HA2	12:H:175:ARG:O	2.19	0.42
12:H:174:ILE:HB	12:H:189:LEU:HB2	2.02	0.42
13:I:189:TYR:CD2	13:I:190:THR:HG23	2.54	0.42
6:T:88:LEU:HD23	6:T:88:LEU:HA	1.81	0.42
3:C:107:CYS:O	3:C:111:VAL:HG23	2.20	0.41
6:G:206:LYS:HE3	6:G:206:LYS:HB3	1.84	0.41
7:J:192:LYS:NZ	13:I:221:ILE:HD13	2.35	0.41
5:S:133:LEU:HD11	5:S:161:ILE:HG12	2.02	0.41
12:Z:190:LEU:C	12:Z:190:LEU:HD12	2.41	0.41
1:O:78:CYS:HB3	1:O:140:LEU:HD23	2.02	0.41
1:O:171:LYS:HB3	1:O:205:VAL:CG1	2.50	0.41
4:E:75:GLY:HA3	4:E:226:PHE:CE1	2.56	0.41
7:J:127:ILE:HD11	13:I:50:ALA:HB3	2.02	0.41
10:N:93:SER:O	10:N:159:GLY:HA2	2.20	0.41
4:R:75:GLY:HA3	4:R:226:PHE:CE1	2.56	0.41
5:S:81:ALA:HB2	5:S:130:VAL:HG21	2.02	0.41
10:X:93:SER:O	10:X:159:GLY:HA2	2.20	0.41
1:A:78:CYS:HB3	1:A:140:LEU:HD23	2.02	0.41
4:E:52:LYS:O	4:E:54:ILE:HD12	2.20	0.41
11:D:17:PHE:HD2	11:D:17:PHE:HA	1.76	0.41
11:D:192:ILE:O	11:D:196:LEU:HG	2.20	0.41
11:D:96:LEU:HD12	11:D:96:LEU:HA	1.94	0.41
3:Q:107:CYS:O	3:Q:111:VAL:HG23	2.20	0.41
4:R:52:LYS:O	4:R:54:ILE:HD12	2.20	0.41
10:X:88:MET:SD	10:X:109:LYS:HG3	2.61	0.41
11:Y:37:GLY:HA3	11:Y:40:ILE:HD12	2.03	0.41
11:D:37:GLY:HA3	11:D:40:ILE:HD12	2.03	0.41
15:I:301:SA1:H12	15:I:301:SA1:HN8	1.86	0.41
4:R:73:HIS:HE1	4:R:107:MET:O	2.03	0.41
11:Y:192:ILE:O	11:Y:196:LEU:HG	2.20	0.41
10:N:88:MET:SD	10:N:109:LYS:HG3	2.61	0.41
12:H:114:VAL:HA	12:H:119:MET:O	2.21	0.41
11:Y:65:LEU:HD21	11:Y:71:MET:HE2	2.02	0.41
2:B:92:LYS:HE3	2:B:92:LYS:HB3	1.78	0.41
4:E:31:ILE:HD13	4:E:31:ILE:HA	1.85	0.41
4:E:167:ALA:C	5:F:56:LEU:HD23	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:42:CYS:SG	6:G:44:ASP:OD1	2.64	0.41
1:O:93:ARG:HD2	1:O:93:ARG:HA	1.83	0.41
1:O:187:PHE:HD2	1:O:189:TRP:CD1	2.39	0.41
6:T:172:ALA:O	6:T:176:GLU:HG2	2.21	0.41
7:U:131:MET:HE2	7:U:131:MET:HB2	1.91	0.41
8:V:44:LEU:HD13	8:V:104:LEU:HD12	2.03	0.41
10:X:167:LEU:HG	10:X:182:LEU:HD12	2.01	0.41
1:A:171:LYS:HB3	1:A:205:VAL:CG1	2.50	0.41
4:E:97:GLN:HB3	14:L:61:ARG:HG2	2.03	0.41
8:K:13:VAL:HG11	8:K:105:ALA:HB1	2.03	0.41
12:H:190:LEU:HD12	12:H:190:LEU:C	2.41	0.41
4:R:26:TYR:CD1	11:Y:12:PRO:HA	2.56	0.41
8:V:13:VAL:HG11	8:V:105:ALA:HB1	2.03	0.41
11:Y:78:ALA:O	11:Y:82:ILE:HG12	2.21	0.41
10:N:117:ILE:O	10:N:121:LEU:HG	2.20	0.40
6:T:186:THR:O	6:T:190:ILE:HG12	2.20	0.40
7:U:106:GLU:HA	7:U:107:PRO:HD3	1.84	0.40
12:Z:114:VAL:HA	12:Z:119:MET:O	2.21	0.40
1:A:187:PHE:HD2	1:A:189:TRP:CD1	2.39	0.40
3:C:59:VAL:CG2	3:C:60:PHE:CD2	2.80	0.40
8:K:44:LEU:HD13	8:K:104:LEU:HD12	2.03	0.40
2:P:74:LEU:HD23	2:P:87:VAL:HG22	2.04	0.40
3:Q:59:VAL:CG2	3:Q:60:PHE:CD2	2.80	0.40
4:R:52:LYS:HB2	4:R:54:ILE:HD11	2.03	0.40
8:V:43:LEU:HD12	8:V:183:ILE:HD11	2.03	0.40
1:O:112:ASP:HB3	1:O:152:TYR:CZ	2.57	0.40
6:T:100:ARG:HH11	10:X:114:GLN:HE22	1.68	0.40
10:X:117:ILE:O	10:X:121:LEU:HG	2.20	0.40
12:Z:45:ARG:HB3	12:Z:52:THR:HB	2.02	0.40
9:M:90:LEU:O	9:M:94:LYS:HG3	2.22	0.40
9:W:90:LEU:O	9:W:94:LYS:HG3	2.22	0.40
5:F:81:ALA:HB2	5:F:130:VAL:HG21	2.02	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 PDB entries followed by that with respect to all EM

entries.

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	240/246 (98%)	236 (98%)	4 (2%)	0	100	100
1	O	240/246 (98%)	235 (98%)	5 (2%)	0	100	100
2	B	228/233 (98%)	225 (99%)	3 (1%)	0	100	100
2	P	228/233 (98%)	225 (99%)	3 (1%)	0	100	100
3	C	253/261 (97%)	247 (98%)	5 (2%)	1 (0%)	30	40
3	Q	253/261 (97%)	247 (98%)	5 (2%)	1 (0%)	30	40
4	E	234/241 (97%)	231 (99%)	3 (1%)	0	100	100
4	R	234/241 (97%)	231 (99%)	3 (1%)	0	100	100
5	F	235/263 (89%)	231 (98%)	4 (2%)	0	100	100
5	S	235/263 (89%)	231 (98%)	4 (2%)	0	100	100
6	G	238/254 (94%)	236 (99%)	2 (1%)	0	100	100
6	T	238/254 (94%)	236 (99%)	2 (1%)	0	100	100
7	J	202/204 (99%)	193 (96%)	8 (4%)	1 (0%)	25	34
7	U	202/204 (99%)	193 (96%)	8 (4%)	1 (0%)	25	34
8	K	195/201 (97%)	190 (97%)	5 (3%)	0	100	100
8	V	195/201 (97%)	190 (97%)	5 (3%)	0	100	100
9	M	210/213 (99%)	206 (98%)	3 (1%)	1 (0%)	25	34
9	W	210/213 (99%)	206 (98%)	3 (1%)	1 (0%)	25	34
10	N	214/219 (98%)	209 (98%)	4 (2%)	1 (0%)	25	34
10	X	214/219 (98%)	209 (98%)	4 (2%)	1 (0%)	25	34
11	D	230/248 (93%)	225 (98%)	5 (2%)	0	100	100
11	Y	230/248 (93%)	225 (98%)	5 (2%)	0	100	100
12	H	200/205 (98%)	198 (99%)	2 (1%)	0	100	100
12	Z	200/205 (98%)	198 (99%)	2 (1%)	0	100	100
13	I	219/234 (94%)	215 (98%)	2 (1%)	2 (1%)	14	21
13	a	219/234 (94%)	215 (98%)	2 (1%)	2 (1%)	14	21
14	L	198/204 (97%)	194 (98%)	4 (2%)	0	100	100
14	b	198/204 (97%)	194 (98%)	4 (2%)	0	100	100
All	All	6192/6452 (96%)	6071 (98%)	109 (2%)	12 (0%)	45	56

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	60	PHE
13	I	171	SER
13	I	203	ARG
3	Q	60	PHE
13	a	171	SER
13	a	203	ARG
9	M	219	ASP
9	W	219	ASP
7	J	31	GLN
7	U	31	GLN
10	N	54	THR
10	X	54	THR

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 PDB entries followed by that with respect to all EM entries.

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	206/210 (98%)	202 (98%)	4 (2%)	52	70
1	O	206/210 (98%)	202 (98%)	4 (2%)	52	70
2	B	188/190 (99%)	184 (98%)	4 (2%)	48	66
2	P	188/190 (99%)	184 (98%)	4 (2%)	48	66
3	C	215/221 (97%)	213 (99%)	2 (1%)	75	87
3	Q	215/221 (97%)	213 (99%)	2 (1%)	75	87
4	E	198/203 (98%)	196 (99%)	2 (1%)	73	84
4	R	198/203 (98%)	196 (99%)	2 (1%)	73	84
5	F	203/224 (91%)	200 (98%)	3 (2%)	60	76
5	S	203/224 (91%)	200 (98%)	3 (2%)	60	76
6	G	198/211 (94%)	195 (98%)	3 (2%)	60	76
6	T	198/211 (94%)	195 (98%)	3 (2%)	60	76
7	J	173/173 (100%)	172 (99%)	1 (1%)	84	92
7	U	173/173 (100%)	172 (99%)	1 (1%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	K	168/171 (98%)	167 (99%)	1 (1%)	84 92
8	V	168/171 (98%)	167 (99%)	1 (1%)	84 92
9	M	177/178 (99%)	176 (99%)	1 (1%)	84 92
9	W	177/178 (99%)	176 (99%)	1 (1%)	84 92
10	N	179/181 (99%)	174 (97%)	5 (3%)	38 55
10	X	179/181 (99%)	174 (97%)	5 (3%)	38 55
11	D	200/211 (95%)	197 (98%)	3 (2%)	60 76
11	Y	200/211 (95%)	197 (98%)	3 (2%)	60 76
12	H	157/159 (99%)	156 (99%)	1 (1%)	84 92
12	Z	157/159 (99%)	156 (99%)	1 (1%)	84 92
13	I	182/195 (93%)	179 (98%)	3 (2%)	58 75
13	a	182/195 (93%)	179 (98%)	3 (2%)	58 75
14	L	156/159 (98%)	152 (97%)	4 (3%)	41 59
14	b	156/159 (98%)	152 (97%)	4 (3%)	41 59
All	All	5200/5372 (97%)	5126 (99%)	74 (1%)	62 77

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	MET
1	A	145	GLU
1	A	161	CYS
1	A	242	LEU
2	B	77	SER
2	B	119	GLN
2	B	137	CYS
2	B	177	ARG
3	C	19	TYR
3	C	119	GLN
4	E	53	ARG
4	E	208	GLU
5	F	9	ASP
5	F	117	GLN
5	F	125	ARG
6	G	72	ARG
6	G	82	LEU
6	G	216	TRP

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Mol	Chain	Res	Type
7	J	34	MET
8	K	170	ARG
9	M	197	ASP
10	N	48	ASN
10	N	145	ARG
10	N	155	MET
10	N	171	ASP
10	N	197	GLU
11	D	100	ASP
11	D	116	GLN
11	D	208	LEU
12	H	43	CYS
13	I	53	ASP
13	I	127	MET
13	I	203	ARG
14	L	29	GLN
14	L	100	MET
14	L	102	CYS
14	L	136	TYR
1	O	131	MET
1	O	145	GLU
1	O	161	CYS
1	O	242	LEU
2	P	77	SER
2	P	119	GLN
2	P	137	CYS
2	P	177	ARG
3	Q	19	TYR
3	Q	119	GLN
4	R	53	ARG
4	R	208	GLU
5	S	9	ASP
5	S	117	GLN
5	S	125	ARG
6	T	72	ARG
6	T	82	LEU
6	T	216	TRP
7	U	34	MET
8	V	170	ARG
9	W	197	ASP
10	X	48	ASN
10	X	145	ARG

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Mol	Chain	Res	Type
10	X	155	MET
10	X	171	ASP
10	X	197	GLU
11	Y	100	ASP
11	Y	116	GLN
11	Y	208	LEU
12	Z	43	CYS
13	a	53	ASP
13	a	127	MET
13	a	203	ARG
14	b	29	GLN
14	b	100	MET
14	b	102	CYS
14	b	136	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	172	GLN
1	A	193	GLN
2	B	21	GLN
2	B	52	GLN
2	B	96	GLN
2	B	109	GLN
2	B	112	GLN
2	B	119	GLN
2	B	123	GLN
2	B	166	ASN
2	B	179	ASN
3	C	40	ASN
3	C	95	GLN
3	C	109	GLN
3	C	119	GLN
3	C	155	ASN
3	C	220	ASN
4	E	23	GLN
4	E	73	HIS
4	E	98	ASN
4	E	178	GLN
4	E	182	GLN
4	E	224	GLN

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Mol	Chain	Res	Type
5	F	21	GLN
5	F	43	HIS
5	F	60	GLN
5	F	69	HIS
5	F	117	GLN
5	F	121	GLN
5	F	143	HIS
5	F	166	GLN
5	F	183	ASN
6	G	69	ASN
6	G	98	ASN
6	G	102	ASN
6	G	106	ASN
6	G	202	HIS
7	J	7	ASN
7	J	40	GLN
7	J	61	GLN
7	J	65	GLN
7	J	188	HIS
8	K	65	GLN
8	K	168	GLN
8	K	189	HIS
8	K	193	ASN
9	M	105	HIS
9	M	136	ASN
9	M	159	GLN
9	M	174	GLN
9	M	179	ASN
10	N	106	GLN
10	N	114	GLN
10	N	134	HIS
10	N	149	ASN
10	N	207	GLN
11	D	15	HIS
11	D	18	GLN
11	D	92	GLN
11	D	94	HIS
11	D	116	GLN
11	D	120	GLN
12	H	7	GLN
12	H	38	HIS
12	H	53	GLN

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Mol	Chain	Res	Type
12	H	106	GLN
13	I	57	GLN
13	I	66	HIS
13	I	153	ASN
13	I	165	ASN
14	L	62	GLN
14	L	162	GLN
1	O	53	GLN
1	O	172	GLN
1	O	193	GLN
2	P	21	GLN
2	P	52	GLN
2	P	96	GLN
2	P	109	GLN
2	P	112	GLN
2	P	119	GLN
2	P	123	GLN
2	P	166	ASN
2	P	179	ASN
3	Q	40	ASN
3	Q	95	GLN
3	Q	109	GLN
3	Q	119	GLN
3	Q	155	ASN
3	Q	220	ASN
4	R	23	GLN
4	R	73	HIS
4	R	98	ASN
4	R	178	GLN
4	R	182	GLN
4	R	224	GLN
5	S	21	GLN
5	S	43	HIS
5	S	60	GLN
5	S	69	HIS
5	S	117	GLN
5	S	121	GLN
5	S	143	HIS
5	S	166	GLN
5	S	183	ASN
6	T	69	ASN
6	T	98	ASN

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Mol	Chain	Res	Type
6	T	102	ASN
6	T	106	ASN
6	T	202	HIS
7	U	7	ASN
7	U	40	GLN
7	U	61	GLN
7	U	65	GLN
7	U	169	GLN
7	U	188	HIS
8	V	65	GLN
8	V	168	GLN
8	V	189	HIS
8	V	193	ASN
9	W	105	HIS
9	W	136	ASN
9	W	159	GLN
9	W	174	GLN
9	W	179	ASN
9	W	191	HIS
10	X	106	GLN
10	X	114	GLN
10	X	134	HIS
10	X	149	ASN
10	X	207	GLN
11	Y	15	HIS
11	Y	18	GLN
11	Y	92	GLN
11	Y	94	HIS
11	Y	116	GLN
11	Y	120	GLN
12	Z	7	GLN
12	Z	38	HIS
12	Z	53	GLN
12	Z	106	GLN
13	a	57	GLN
13	a	66	HIS
13	a	153	ASN
13	a	165	ASN
14	b	62	GLN
14	b	162	GLN
14	b	196	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	SA1	L	301	14	18,22,22	0.93	1 (5%)	24,34,34	1.60	6 (25%)
15	SA1	b	301	14	18,22,22	0.93	1 (5%)	24,34,34	1.60	6 (25%)
15	SA1	H	301	12	18,22,22	0.95	2 (11%)	24,34,34	1.91	5 (20%)
15	SA1	I	301	13	18,22,22	0.99	2 (11%)	24,34,34	1.57	7 (29%)
15	SA1	Z	301	12	18,22,22	0.95	2 (11%)	24,34,34	1.91	5 (20%)
15	SA1	a	301	13	18,22,22	0.99	2 (11%)	24,34,34	1.57	7 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SA1	L	301	14	-	0/4/52/52	0/3/3/3
15	SA1	b	301	14	-	0/4/52/52	0/3/3/3
15	SA1	H	301	12	-	0/4/52/52	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SA1	I	301	13	-	0/4/52/52	0/3/3/3
15	SA1	Z	301	12	-	0/4/52/52	0/3/3/3
15	SA1	a	301	13	-	0/4/52/52	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	301	SA1	C5-C6	-2.28	1.49	1.52
15	a	301	SA1	C5-C6	-2.28	1.49	1.52
15	L	301	SA1	C5-C6	-2.22	1.49	1.52
15	b	301	SA1	C5-C6	-2.22	1.49	1.52
15	H	301	SA1	C5-C6	-2.18	1.49	1.52
15	Z	301	SA1	C5-C6	-2.18	1.49	1.52
15	I	301	SA1	O2-C3	-2.13	1.42	1.45
15	a	301	SA1	O2-C3	-2.13	1.42	1.45
15	H	301	SA1	O2-C3	-2.03	1.43	1.45
15	Z	301	SA1	O2-C3	-2.03	1.43	1.45

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	H	301	SA1	C9-C10-C11	4.35	119.56	114.09
15	Z	301	SA1	C9-C10-C11	4.35	119.56	114.09
15	H	301	SA1	O17-C10-C11	-3.56	101.94	109.98
15	Z	301	SA1	O17-C10-C11	-3.56	101.94	109.98
15	L	301	SA1	O17-C10-C11	-3.54	101.99	109.98
15	b	301	SA1	O17-C10-C11	-3.54	101.99	109.98
15	I	301	SA1	C14-C13-C12	-2.95	118.35	123.61
15	a	301	SA1	C14-C13-C12	-2.95	118.35	123.61
15	H	301	SA1	C14-C13-C12	-2.89	118.47	123.61
15	Z	301	SA1	C14-C13-C12	-2.89	118.47	123.61
15	L	301	SA1	O7-C6-C5	-2.87	122.97	126.13
15	b	301	SA1	O7-C6-C5	-2.87	122.97	126.13
15	H	301	SA1	O7-C6-C5	-2.82	123.02	126.13
15	Z	301	SA1	O7-C6-C5	-2.82	123.02	126.13
15	I	301	SA1	O7-C6-C5	-2.64	123.22	126.13
15	a	301	SA1	O7-C6-C5	-2.64	123.22	126.13
15	H	301	SA1	C3-C5-C6	-2.51	102.25	104.28
15	Z	301	SA1	C3-C5-C6	-2.51	102.25	104.28
15	I	301	SA1	C11-C12-C13	-2.32	118.05	123.28
15	a	301	SA1	C11-C12-C13	-2.32	118.05	123.28
15	L	301	SA1	C9-N8-C6	-2.29	113.08	115.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b	301	SA1	C9-N8-C6	-2.29	113.08	115.42
15	I	301	SA1	C1-C20-C5	2.28	105.63	102.69
15	a	301	SA1	C1-C20-C5	2.28	105.63	102.69
15	I	301	SA1	C9-N8-C6	-2.12	113.25	115.42
15	a	301	SA1	C9-N8-C6	-2.12	113.25	115.42
15	L	301	SA1	C3-C5-C6	-2.06	102.61	104.28
15	b	301	SA1	C3-C5-C6	-2.06	102.61	104.28
15	L	301	SA1	C20-C5-C6	-2.05	109.48	114.48
15	b	301	SA1	C20-C5-C6	-2.05	109.48	114.48
15	I	301	SA1	C20-C5-C6	-2.04	109.48	114.48
15	a	301	SA1	C20-C5-C6	-2.04	109.48	114.48
15	I	301	SA1	C20-C5-C3	2.04	107.10	103.78
15	a	301	SA1	C20-C5-C3	2.04	107.10	103.78
15	L	301	SA1	C5-C6-N8	2.01	111.69	108.78
15	b	301	SA1	C5-C6-N8	2.01	111.69	108.78

There are no chirality outliers.

There are no torsion outliers.

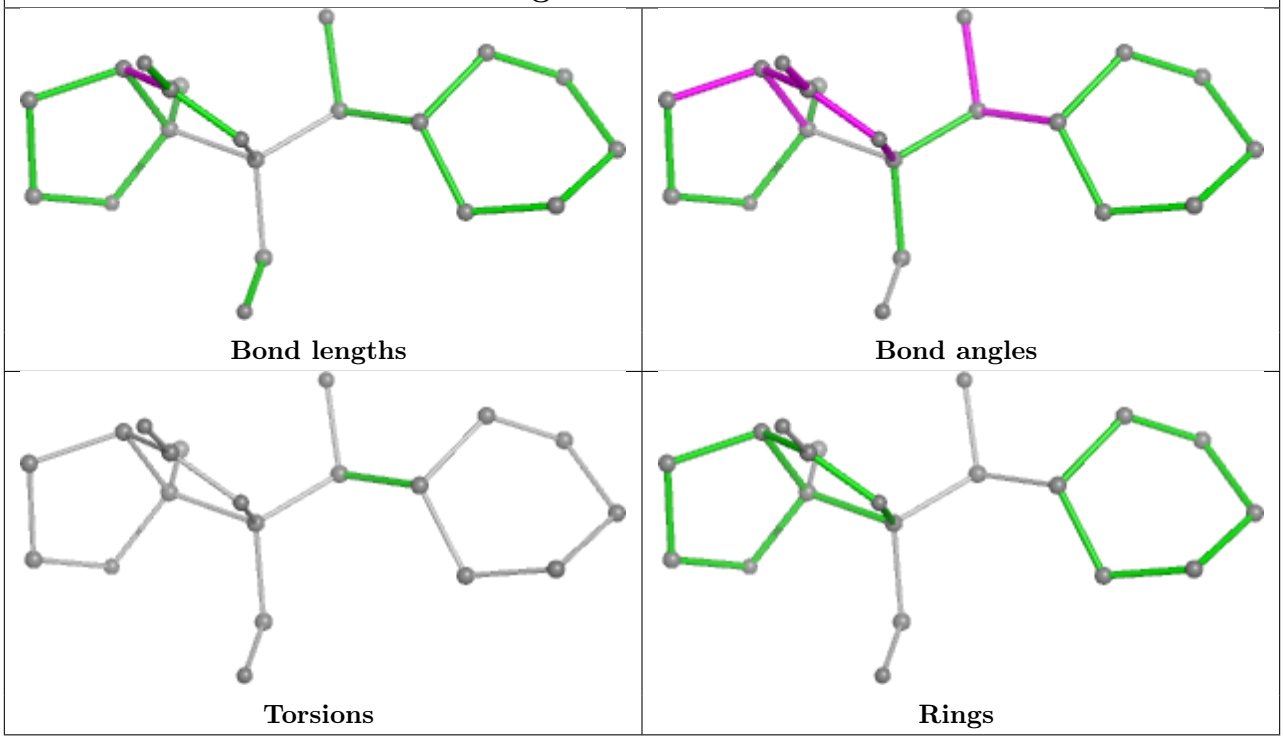
There are no ring outliers.

1 monomer is involved in 1 short contact:

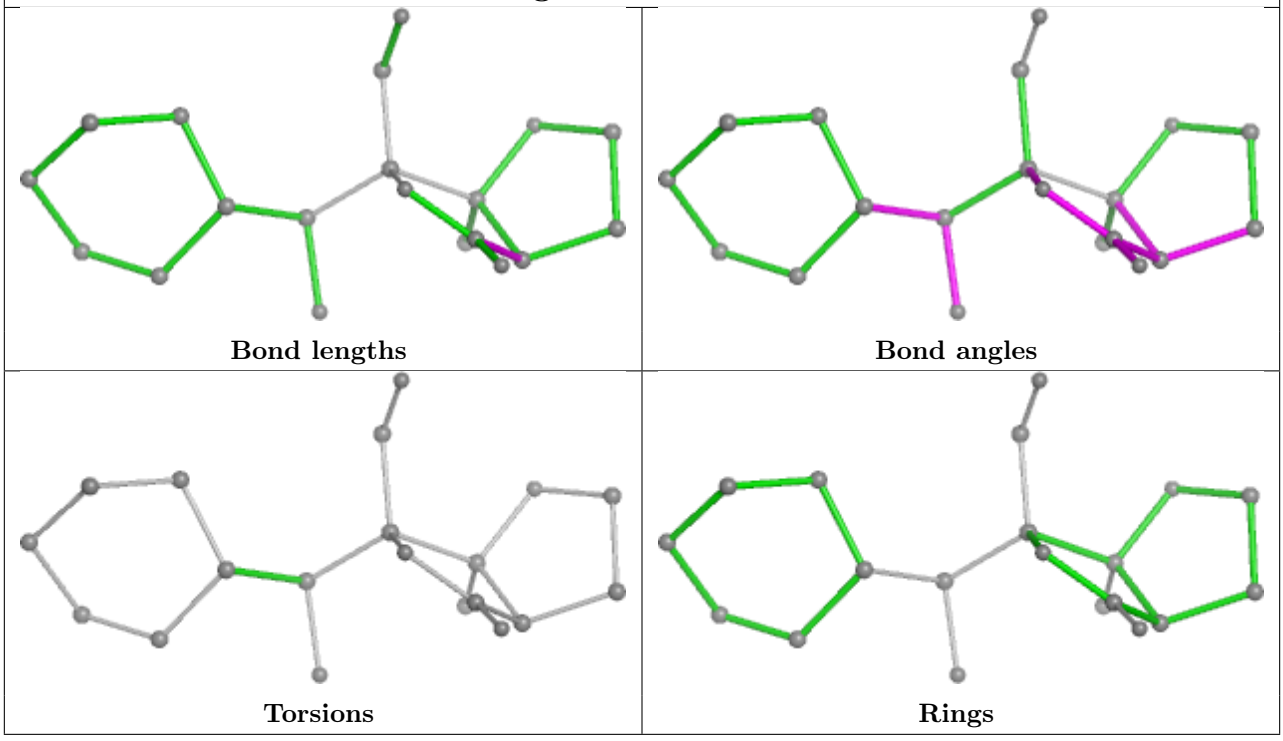
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	I	301	SA1	1	0

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.

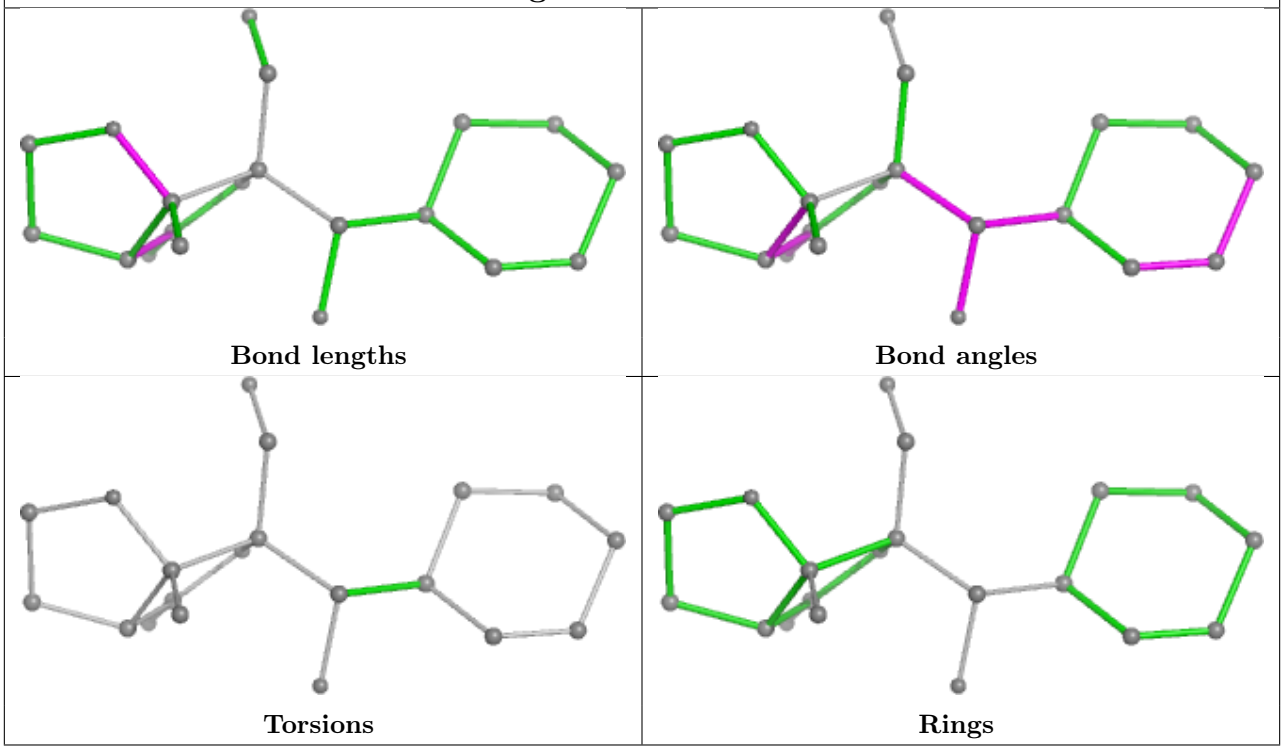
Ligand SA1 L 301



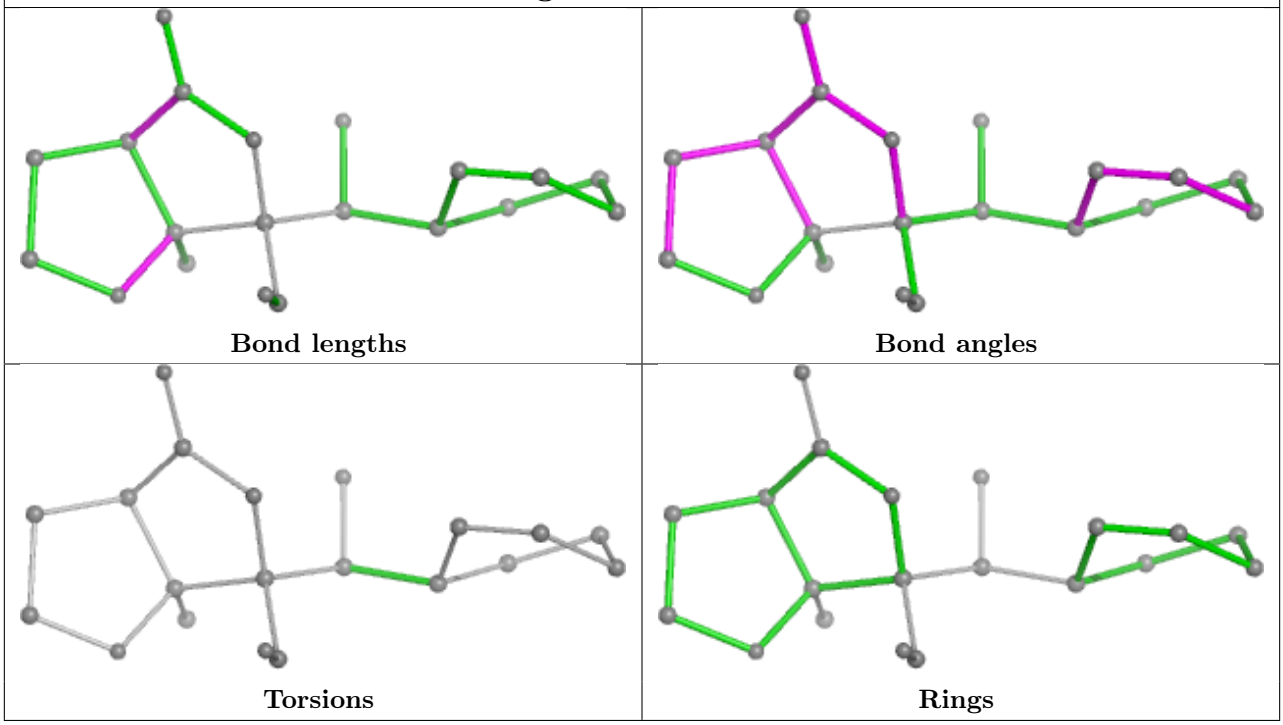
Ligand SA1 b 301



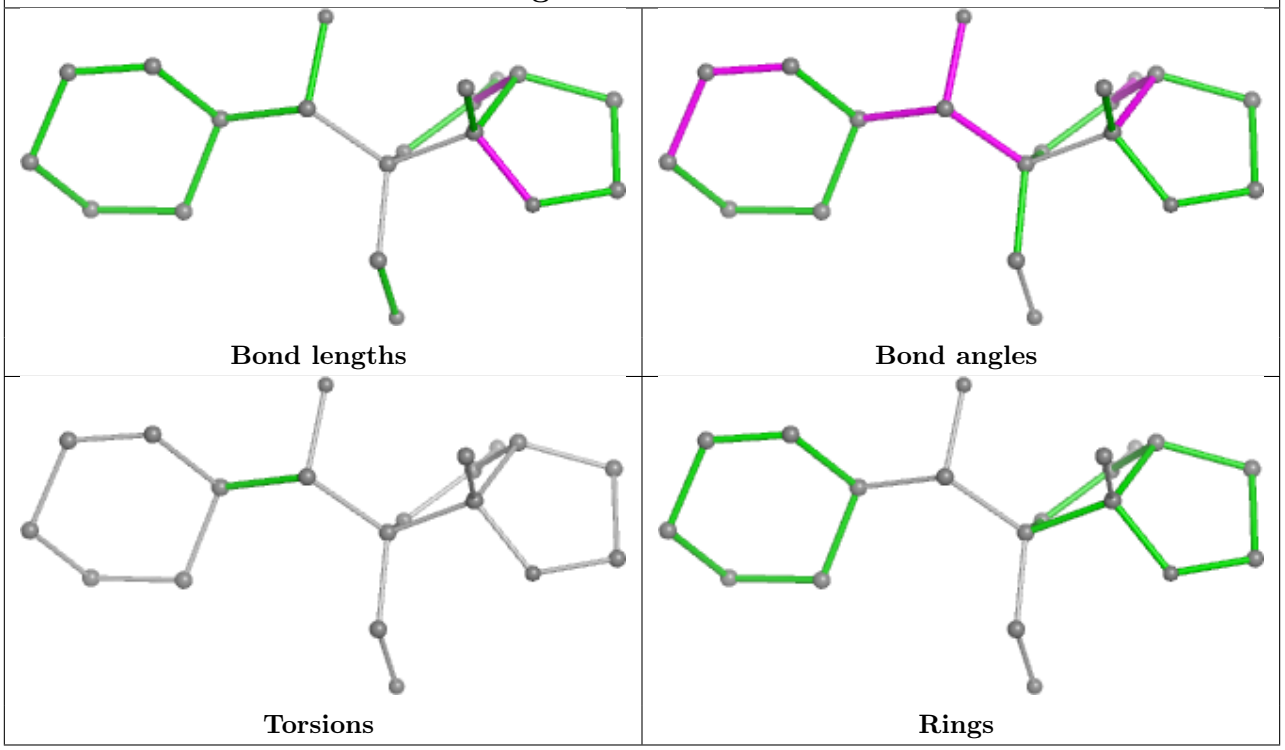
Ligand SA1 H 301



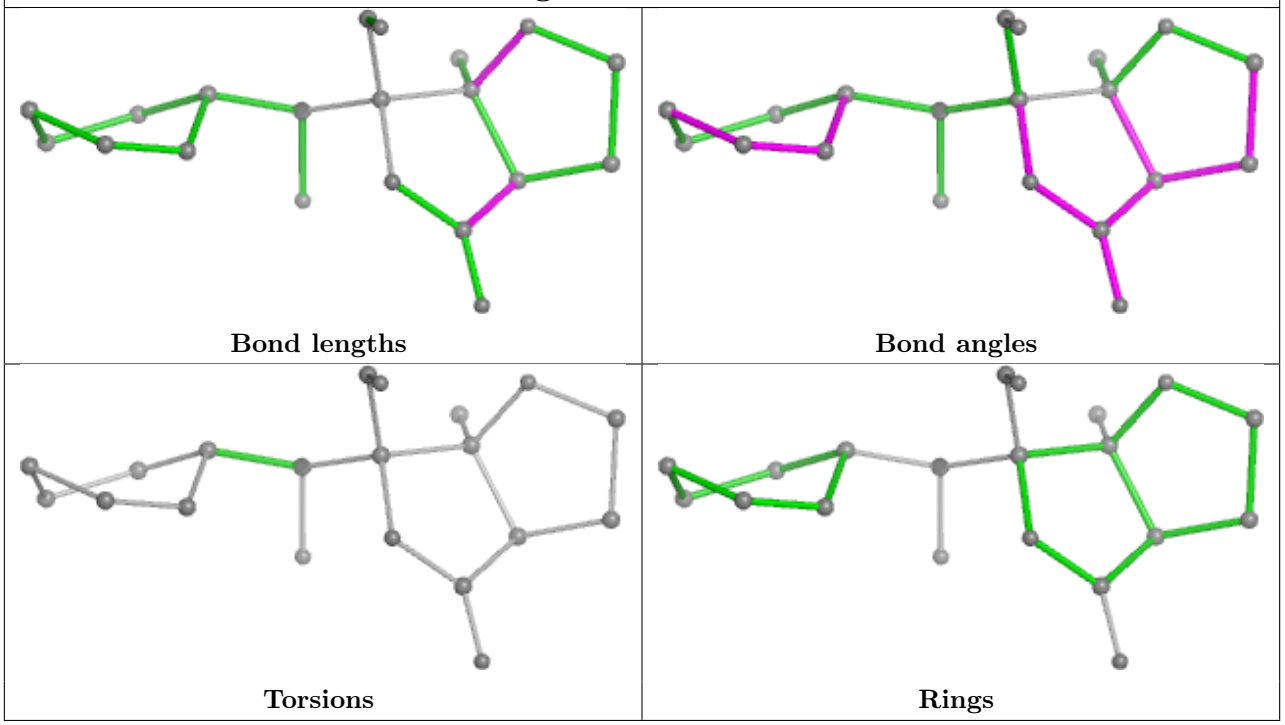
Ligand SA1 I 301



Ligand SA1 Z 301



Ligand SA1 a 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.