



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 01:18 AM UTC

PDB ID : 3WQP / pdb_00003wqp
Title : Crystal structure of Rubisco T289D mutant from *Thermococcus kodakarensis*
Authors : Fujihashi, M.; Nishitani, Y.; Kiriyaama, T.; Miki, K.
Deposited on : 2014-01-29
Resolution : 2.25 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

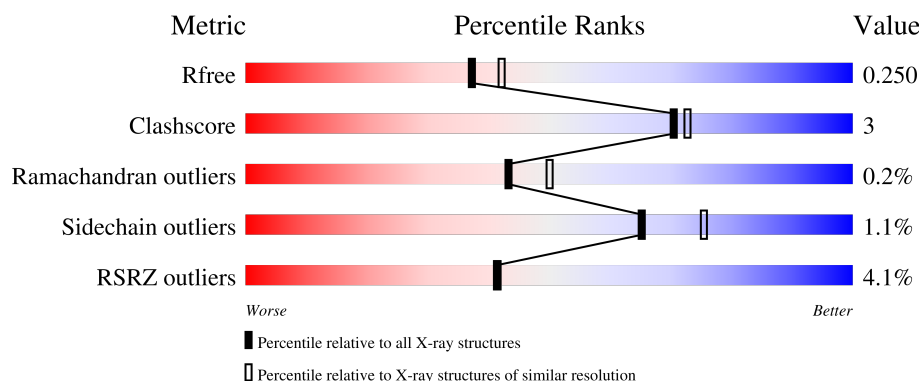
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	444	2% 90% 8%
1	B	444	7% 90% 9%
1	C	444	2% 91% 7%
1	D	444	3% 88% 10%
1	E	444	2% 91% 7%

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Mol	Chain	Length	Quality of chain
1	F	444	9% 86% 12%
1	G	444	5% 90% 8%
1	H	444	3% 89% 10%
1	I	444	3% 87% 11%
1	J	444	2% 92% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36577 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 Ribulose biphosphate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3425	2200	584	631	10			
1	B	438	Total	C	N	O	S	0	0	0
			3440	2207	587	636	10			
1	C	438	Total	C	N	O	S	0	0	0
			3443	2209	588	636	10			
1	D	436	Total	C	N	O	S	0	0	0
			3441	2209	587	635	10			
1	E	438	Total	C	N	O	S	0	0	0
			3438	2206	586	636	10			
1	F	436	Total	C	N	O	S	0	0	0
			3408	2185	584	629	10			
1	G	436	Total	C	N	O	S	0	0	0
			3416	2192	581	633	10			
1	H	437	Total	C	N	O	S	0	0	0
			3423	2200	586	627	10			
1	I	436	Total	C	N	O	S	0	0	0
			3434	2204	587	633	10			
1	J	437	Total	C	N	O	S	0	0	0
			3438	2209	586	633	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	ASP	THR	engineered mutation	UNP O93627
B	289	ASP	THR	engineered mutation	UNP O93627
C	289	ASP	THR	engineered mutation	UNP O93627
D	289	ASP	THR	engineered mutation	UNP O93627
E	289	ASP	THR	engineered mutation	UNP O93627
F	289	ASP	THR	engineered mutation	UNP O93627
G	289	ASP	THR	engineered mutation	UNP O93627
H	289	ASP	THR	engineered mutation	UNP O93627
I	289	ASP	THR	engineered mutation	UNP O93627

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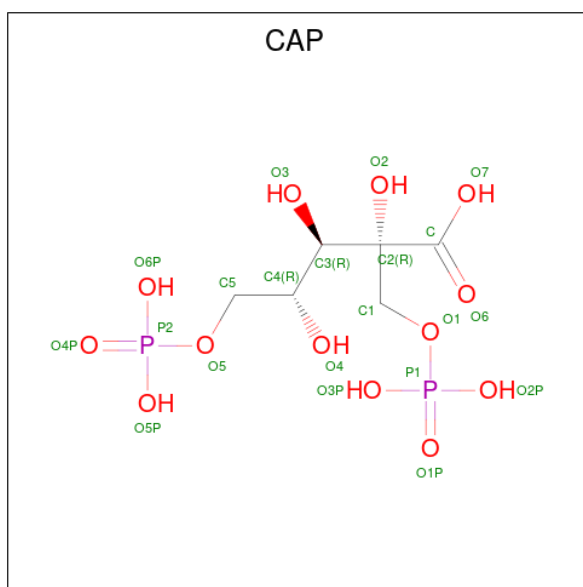
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Chain	Residue	Modelled	Actual	Comment	Reference
J	289	ASP	THR	engineered mutation	UNP O93627

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0
2	E	1	Total 1	Mg 1	0	0
2	F	1	Total 1	Mg 1	0	0
2	G	1	Total 1	Mg 1	0	0
2	H	1	Total 1	Mg 1	0	0
2	I	1	Total 1	Mg 1	0	0
2	J	1	Total 1	Mg 1	0	0

- Molecule 3 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (CCD ID: CAP) (formula: $C_6H_{14}O_{13}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			21	6	13	2		
3	B	1	Total	C	O	P	0	0
			21	6	13	2		
3	C	1	Total	C	O	P	0	0
			21	6	13	2		
3	D	1	Total	C	O	P	0	0
			21	6	13	2		
3	E	1	Total	C	O	P	0	0
			21	6	13	2		
3	F	1	Total	C	O	P	0	0
			21	6	13	2		
3	G	1	Total	C	O	P	0	0
			21	6	13	2		
3	H	1	Total	C	O	P	0	0
			21	6	13	2		
3	I	1	Total	C	O	P	0	0
			21	6	13	2		
3	J	1	Total	C	O	P	0	0
			21	6	13	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	183	Total O 183 183	0	0
5	B	127	Total O 127 127	0	0

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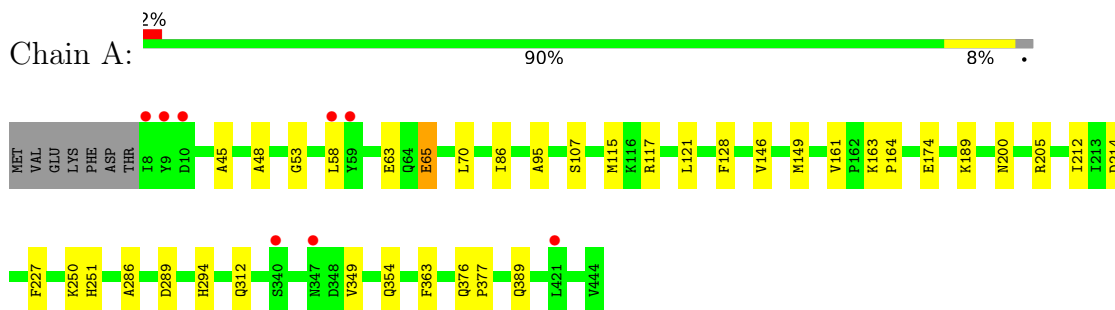
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	223	Total 223	O 223	0	0
5	D	240	Total 240	O 240	0	0
5	E	252	Total 252	O 252	0	0
5	F	170	Total 170	O 170	0	0
5	G	133	Total 133	O 133	0	0
5	H	184	Total 184	O 184	0	0
5	I	244	Total 244	O 244	0	0
5	J	255	Total 255	O 255	0	0

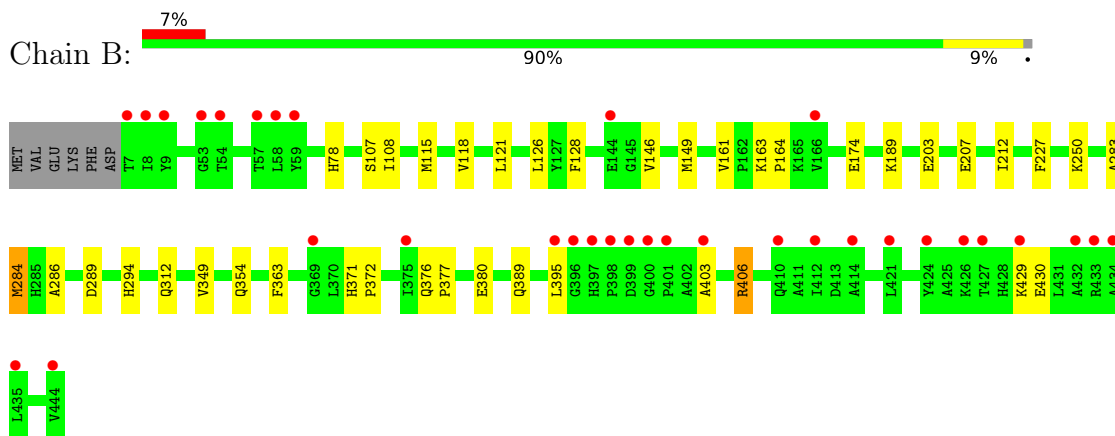
3 Residue-property plots [i](#)

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.

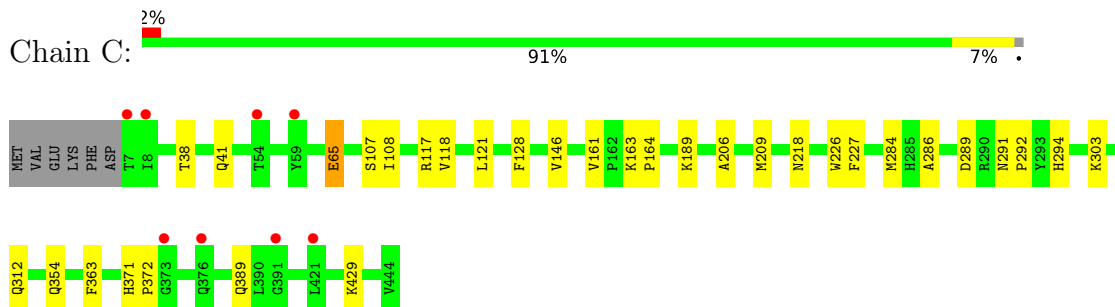
- Molecule 1: Ribulose biphosphate carboxylase



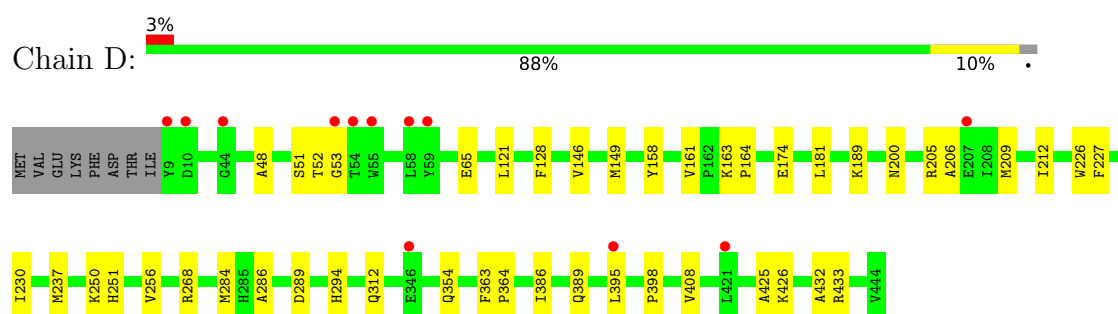
- Molecule 1: Ribulose biphosphate carboxylase



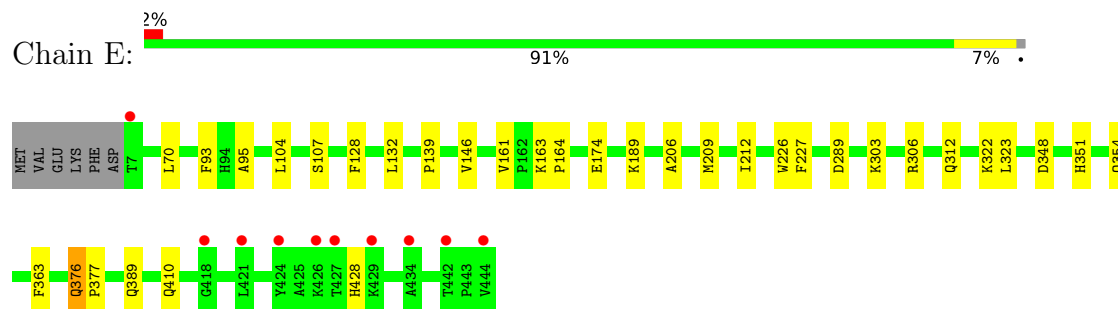
- Molecule 1: Ribulose biphosphate carboxylase



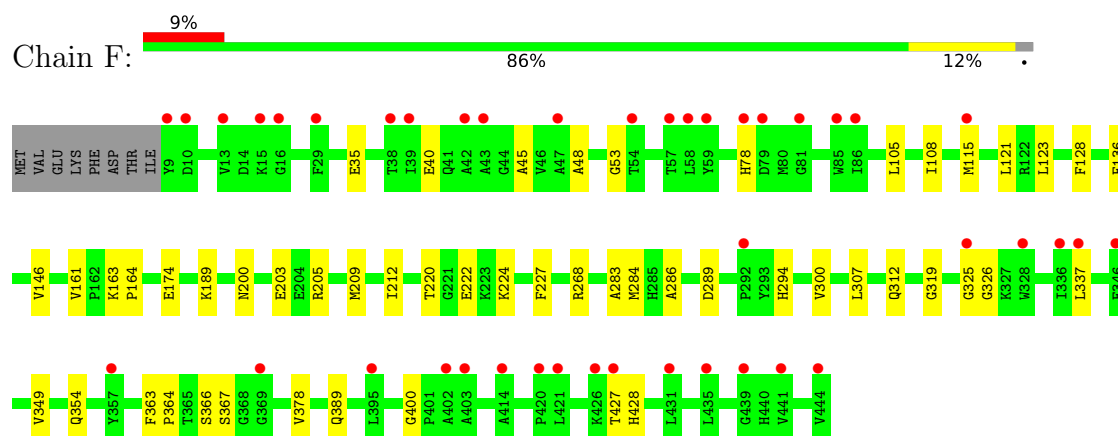
- Molecule 1: Ribulose biphosphate carboxylase



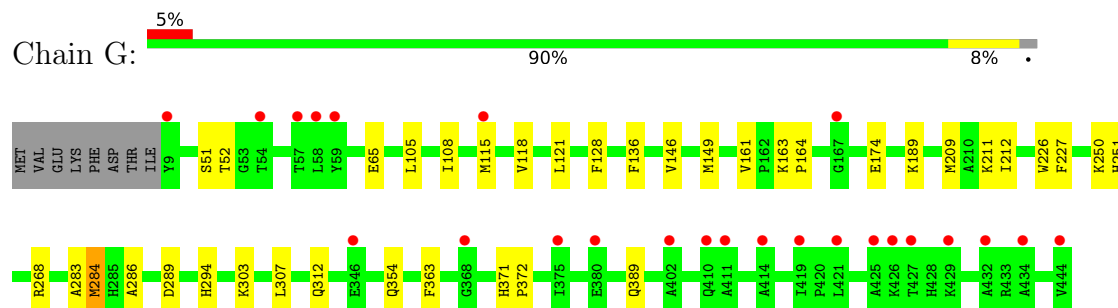
- Molecule 1: Ribulose biphosphate carboxylase



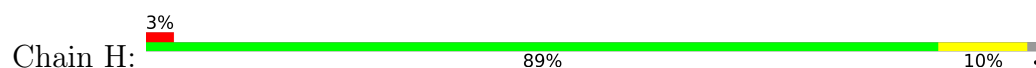
- Molecule 1: Ribulose biphosphate carboxylase



- Molecule 1: Ribulose biphosphate carboxylase



- Molecule 1: Ribulose biphosphate carboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	170.57Å 246.24Å 144.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 50.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.25) 99.7 (50.00-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.24Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.220 , 0.258 0.215 , 0.250	Depositor DCC
R_{free} test set	14440 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtrriage
Anisotropy	1.150	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36577	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2523e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KCX, EDO, CAP, 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	0.62	0/3502	0.77	0/4753
1	B	0.61	0/3517	0.77	0/4770
1	C	0.62	0/3520	0.76	0/4773
1	D	0.64	0/3517	0.79	1/4766 (0.0%)
1	E	0.63	0/3515	0.79	0/4767
1	F	0.63	0/3483	0.78	2/4724 (0.0%)
1	G	0.61	0/3493	0.77	0/4742
1	H	0.62	0/3500	0.77	0/4748
1	I	0.64	0/3510	0.79	0/4757
1	J	0.63	0/3515	0.78	0/4766
All	All	0.62	0/35072	0.78	3/47566 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	256	VAL	N-CA-C	5.30	116.07	110.72
1	F	400	GLY	CA-C-N	5.17	124.34	118.97
1	F	400	GLY	C-N-CA	5.17	124.34	118.97

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	3425	0	3321	20	0
1	B	3440	0	3335	26	0
1	C	3443	0	3344	20	0
1	D	3441	0	3368	27	0
1	E	3438	0	3328	19	0
1	F	3408	0	3301	30	0
1	G	3416	0	3299	22	0
1	H	3423	0	3328	23	0
1	I	3434	0	3355	34	0
1	J	3438	0	3346	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	21	0	8	0	0
3	B	21	0	9	0	0
3	C	21	0	9	0	0
3	D	21	0	8	0	0
3	E	21	0	9	0	0
3	F	21	0	9	0	0
3	G	21	0	8	0	0
3	H	21	0	9	0	0
3	I	21	0	7	0	0
3	J	21	0	9	0	0
4	A	4	0	6	1	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
4	E	4	0	6	0	0
4	H	8	0	12	0	0
4	I	8	0	12	0	0
4	J	4	0	6	1	0
5	A	183	0	0	0	0
5	B	127	0	0	0	0
5	C	223	0	0	2	0
5	D	240	0	0	0	0
5	E	252	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	170	0	0	3	0
5	G	133	0	0	1	0
5	H	184	0	0	0	0
5	I	244	0	0	2	0
5	J	255	0	0	0	0
All	All	36577	0	33470	234	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 3.

All (234) 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:B:406:ARG:HG2	1:B:406:ARG:HH11	1.06	1.06
1:F:174:GLU:HG3	1:F:212:ILE:HD11	1.52	0.90
1:B:108:ILE:HD12	1:B:126:LEU:HD11	1.52	0.90
1:A:128:PHE:H	1:A:354:GLN:HE22	1.24	0.86
1:B:406:ARG:HG2	1:B:406:ARG:NH1	1.86	0.86
1:C:38:THR:H	1:C:41:GLN:HE21	1.30	0.80
1:C:128:PHE:H	1:C:354:GLN:HE22	1.30	0.78
1:F:209:MET:HE2	1:F:209:MET:HA	1.66	0.78
1:J:128:PHE:H	1:J:354:GLN:HE22	1.32	0.76
1:B:174:GLU:HG3	1:B:212:ILE:HD11	1.68	0.75
1:J:173:PHE:CE2	1:J:209:MET:HE3	2.23	0.73
1:B:128:PHE:H	1:B:354:GLN:HE22	1.36	0.73
1:A:174:GLU:HG3	1:A:212:ILE:HD11	1.69	0.72
1:D:149:MET:HE1	1:D:251:HIS:CE1	2.25	0.71
1:H:128:PHE:H	1:H:354:GLN:HE22	1.39	0.71
1:B:403:ALA:HA	1:B:406:ARG:CD	2.21	0.70
1:J:149:MET:HE1	1:J:251:HIS:CE1	2.27	0.69
1:I:115:MET:HB2	1:I:118:VAL:HG22	1.74	0.69
1:D:128:PHE:H	1:D:354:GLN:HE22	1.38	0.68
1:C:121:LEU:H	1:C:294:HIS:HD2	1.41	0.68
1:I:161:VAL:H	1:I:389:GLN:NE2	1.90	0.68
1:E:189:KCX:HG2	1:E:227:PHE:HB2	1.76	0.68
1:G:174:GLU:HG3	1:G:212:ILE:HD11	1.75	0.68
1:H:149:MET:HE1	1:H:251:HIS:CE1	2.29	0.68
1:H:38:THR:H	1:H:41:GLN:HE21	1.42	0.67
1:G:128:PHE:H	1:G:354:GLN:HE22	1.42	0.67
1:I:128:PHE:H	1:I:354:GLN:HE22	1.40	0.67
1:D:174:GLU:HG3	1:D:212:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:389:GLN:C	1:I:390:LEU:HD12	2.20	0.66
1:E:128:PHE:H	1:E:354:GLN:HE22	1.45	0.65
1:I:161:VAL:H	1:I:389:GLN:HE21	1.46	0.64
1:I:191:ASP:HB2	5:I:658:HOH:O	1.97	0.64
1:B:403:ALA:HA	1:B:406:ARG:HD2	1.81	0.63
1:F:128:PHE:H	1:F:354:GLN:HE22	1.44	0.63
1:H:149:MET:HE3	1:H:250:LYS:HD3	1.80	0.63
1:D:121:LEU:H	1:D:294:HIS:HD2	1.47	0.63
1:D:163:LYS:H	1:D:395:LEU:HD22	1.64	0.62
1:B:403:ALA:HA	1:B:406:ARG:HD3	1.82	0.62
1:A:161:VAL:H	1:A:389:GLN:NE2	1.98	0.61
1:F:78:HIS:CD2	1:F:349:VAL:HG21	2.36	0.61
1:F:121:LEU:H	1:F:294:HIS:HD2	1.49	0.60
1:A:48:ALA:HB1	1:A:53:GLY:HA3	1.83	0.60
1:H:174:GLU:HG3	1:H:212:ILE:HD11	1.84	0.60
1:H:189:KCX:HG2	1:H:227:PHE:HB2	1.84	0.60
1:G:115:MET:HB2	1:G:118:VAL:HG22	1.84	0.60
1:I:406:ARG:O	1:I:410:GLN:HG3	2.02	0.59
1:F:222:GLU:HG3	1:F:224:LYS:HE2	1.84	0.59
1:F:161:VAL:H	1:F:389:GLN:NE2	1.99	0.59
1:C:121:LEU:H	1:C:294:HIS:CD2	2.20	0.59
1:H:406:ARG:HH11	1:H:430:GLU:HG2	1.67	0.58
1:F:337:LEU:HD22	1:F:364:PRO:HG3	1.85	0.58
1:G:189:KCX:HG2	1:G:227:PHE:HB2	1.84	0.58
1:G:65:GLU:HB2	5:G:689:HOH:O	2.04	0.58
1:D:149:MET:HE3	1:D:250:LYS:HD2	1.86	0.57
1:C:38:THR:H	1:C:41:GLN:NE2	2.02	0.57
1:G:163:LYS:HA	1:G:164:PRO:C	2.29	0.57
1:F:189:KCX:HG2	1:F:227:PHE:HB2	1.86	0.57
1:B:189:KCX:HG2	1:B:227:PHE:HB2	1.86	0.57
1:F:146:VAL:HG21	1:F:312:GLN:HE21	1.69	0.56
1:D:181:LEU:HD11	1:D:209:MET:HE1	1.88	0.56
1:F:121:LEU:H	1:F:294:HIS:CD2	2.24	0.55
1:I:146:VAL:HG21	1:I:312:GLN:HE21	1.70	0.55
1:D:161:VAL:H	1:D:389:GLN:NE2	2.04	0.55
1:D:163:LYS:HA	1:D:164:PRO:C	2.32	0.55
1:B:406:ARG:HH11	1:B:406:ARG:CG	1.97	0.55
1:A:121:LEU:H	1:A:294:HIS:HD2	1.54	0.54
1:A:189:KCX:HG2	1:A:227:PHE:HB2	1.89	0.54
1:G:149:MET:HE1	1:G:251:HIS:CE1	2.42	0.54
1:G:161:VAL:H	1:G:389:GLN:NE2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:MET:HE1	1:D:251:HIS:ND1	2.23	0.54
1:A:121:LEU:H	1:A:294:HIS:CD2	2.25	0.54
1:I:121:LEU:H	1:I:294:HIS:HD2	1.55	0.54
1:B:146:VAL:HG21	1:B:312:GLN:HE21	1.72	0.53
1:B:121:LEU:H	1:B:294:HIS:HD2	1.55	0.53
1:E:410:GLN:NE2	1:E:428:HIS:HB3	2.23	0.53
1:J:161:VAL:H	1:J:389:GLN:NE2	2.07	0.53
1:F:367:SER:HB2	1:F:389:GLN:HB3	1.91	0.52
1:H:163:LYS:HA	1:H:164:PRO:C	2.35	0.52
1:A:45:ALA:HB1	1:A:115:MET:HE1	1.91	0.52
1:C:161:VAL:H	1:C:389:GLN:NE2	2.08	0.52
1:E:376:GLN:HG3	1:E:377:PRO:HD3	1.91	0.52
1:J:149:MET:HE3	1:J:250:LYS:HD2	1.91	0.52
1:J:163:LYS:HA	1:J:164:PRO:C	2.33	0.52
1:J:202:PHE:CD2	1:J:240:ARG:HG2	2.44	0.52
1:B:163:LYS:HA	1:B:164:PRO:C	2.34	0.52
1:I:163:LYS:HA	1:I:164:PRO:C	2.34	0.52
1:G:105:LEU:HD23	1:G:108:ILE:HD11	1.90	0.52
1:H:406:ARG:NH1	1:H:430:GLU:HG2	2.25	0.52
1:I:389:GLN:O	1:I:390:LEU:HD12	2.09	0.51
1:H:330:VAL:HG12	1:H:382:LEU:HD21	1.92	0.51
1:F:161:VAL:H	1:F:389:GLN:HE21	1.58	0.51
1:D:121:LEU:H	1:D:294:HIS:CD2	2.25	0.51
1:F:286:ALA:HA	1:F:289:ASP:OD1	2.11	0.51
1:A:146:VAL:HG21	1:A:312:GLN:HE21	1.75	0.51
1:F:48:ALA:HB1	1:F:53:GLY:HA3	1.92	0.51
1:H:209:MET:HE2	1:H:226:TRP:HB2	1.92	0.51
1:I:159:GLY:HA3	1:I:187:TYR:CZ	2.45	0.51
1:I:201:ARG:HB2	1:I:204:GLU:HG3	1.93	0.51
1:I:286:ALA:HA	1:I:289:ASP:OD1	2.10	0.51
1:I:303:LYS:NZ	1:I:354:GLN:HE21	2.09	0.51
1:C:118:VAL:HG11	1:C:121:LEU:HB2	1.93	0.51
1:I:189:KCX:HG2	1:I:227:PHE:HB2	1.94	0.50
1:F:45:ALA:HB1	1:F:115:MET:HE1	1.94	0.50
1:F:203:GLU:HB2	5:F:624:HOH:O	2.10	0.50
1:G:209:MET:HE2	1:G:226:TRP:HB2	1.92	0.50
1:H:161:VAL:H	1:H:389:GLN:NE2	2.09	0.50
1:E:146:VAL:HG21	1:E:312:GLN:HE21	1.77	0.50
1:C:209:MET:HE2	1:C:226:TRP:HB2	1.93	0.49
1:I:161:VAL:N	1:I:389:GLN:HE21	2.10	0.49
1:B:163:LYS:H	1:B:395:LEU:HD22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:LEU:H	1:G:294:HIS:CD2	2.30	0.49
1:C:146:VAL:HG21	1:C:312:GLN:HE21	1.77	0.49
1:F:123:LEU:HG	1:F:300:VAL:HG21	1.94	0.49
1:G:146:VAL:HG21	1:G:312:GLN:HE21	1.77	0.49
1:C:163:LYS:HA	1:C:164:PRO:C	2.37	0.49
1:J:189:KCX:HG2	1:J:227:PHE:HB2	1.94	0.49
1:A:200:ASN:OD1	1:A:205:ARG:HD3	2.13	0.48
1:D:230:ILE:O	1:D:237:MET:HG2	2.14	0.48
1:B:121:LEU:H	1:B:294:HIS:CD2	2.31	0.48
1:I:427:THR:HG22	5:I:827:HOH:O	2.12	0.48
1:E:163:LYS:HA	1:E:164:PRO:C	2.38	0.48
1:G:121:LEU:H	1:G:294:HIS:HD2	1.60	0.48
1:B:108:ILE:CD1	1:B:126:LEU:HD11	2.35	0.48
1:E:161:VAL:H	1:E:389:GLN:NE2	2.11	0.48
1:C:189:KCX:HG2	1:C:227:PHE:HB2	1.94	0.48
1:H:358:SER:HB3	1:I:171:GLU:OE2	2.13	0.48
1:C:218:ASN:HB2	5:C:787:HOH:O	2.14	0.48
1:D:426:LYS:HG3	1:F:220:THR:O	2.13	0.48
1:F:105:LEU:HD23	1:F:108:ILE:HD11	1.96	0.48
1:D:206:ALA:HA	1:D:226:TRP:CZ3	2.49	0.47
1:I:256:VAL:HG12	1:I:264:LEU:HD11	1.95	0.47
1:J:303:LYS:NZ	1:J:354:GLN:HE21	2.12	0.47
1:B:78:HIS:CD2	1:B:349:VAL:HG21	2.49	0.47
1:H:286:ALA:HA	1:H:289:ASP:OD2	2.14	0.47
1:I:121:LEU:H	1:I:294:HIS:CD2	2.31	0.47
1:B:161:VAL:H	1:B:389:GLN:NE2	2.12	0.47
1:D:48:ALA:HB1	1:D:53:GLY:HA3	1.97	0.47
1:F:366:SER:OG	1:F:378:VAL:HG11	2.15	0.47
1:J:100:ASN:H	4:J:503:EDO:H12	1.79	0.47
1:D:398:PRO:HG2	1:D:433:ARG:O	2.15	0.46
1:E:174:GLU:HG3	1:E:212:ILE:HD11	1.97	0.46
1:F:163:LYS:HA	1:F:164:PRO:C	2.39	0.46
1:E:303:LYS:NZ	1:E:354:GLN:HE21	2.13	0.46
1:A:45:ALA:HB2	1:A:117:ARG:HD2	1.97	0.46
1:H:136:PHE:HB3	1:H:307:LEU:O	2.14	0.46
1:B:115:MET:HB2	1:B:118:VAL:HG12	1.98	0.46
1:D:189:KCX:HG2	1:D:227:PHE:HB2	1.98	0.46
1:G:51:SER:OG	1:G:52:THR:N	2.47	0.46
1:A:149:MET:HE1	1:A:251:HIS:CE1	2.51	0.46
1:E:209:MET:HE2	1:E:226:TRP:HB2	1.98	0.45
1:F:326:GLY:HA3	5:F:732:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:206:ALA:HA	1:J:226:TRP:CZ3	2.51	0.45
1:A:149:MET:HE3	1:A:250:LYS:HD2	1.99	0.45
1:G:303:LYS:HE2	1:G:354:GLN:HG2	1.98	0.45
1:H:163:LYS:H	1:H:395:LEU:HD22	1.81	0.45
1:E:348:ASP:OD2	1:E:351:HIS:HD2	1.99	0.45
1:B:283:ALA:O	1:B:284:MET:CB	2.64	0.44
1:C:65:GLU:CD	1:C:65:GLU:H	2.25	0.44
1:I:397:HIS:HA	1:I:398:PRO:HD2	1.75	0.44
1:F:427:THR:HG23	1:F:428:HIS:ND1	2.31	0.44
1:I:159:GLY:HA3	1:I:187:TYR:CE1	2.52	0.44
1:G:136:PHE:HB3	1:G:307:LEU:O	2.18	0.44
1:H:322:LYS:HA	1:H:443:PRO:O	2.17	0.44
1:C:286:ALA:HA	1:C:289:ASP:OD1	2.18	0.44
1:I:159:GLY:HA3	1:I:187:TYR:CE2	2.53	0.44
1:J:108:ILE:C	1:J:108:ILE:HD12	2.42	0.44
1:A:70:LEU:HD22	1:A:95:ALA:HA	2.00	0.43
1:J:209:MET:HG2	1:J:226:TRP:CG	2.52	0.43
1:A:286:ALA:HA	1:A:289:ASP:OD2	2.18	0.43
1:B:376:GLN:N	1:B:377:PRO:HD2	2.33	0.43
1:I:70:LEU:HD22	1:I:95:ALA:HA	2.01	0.43
1:H:105:LEU:HD23	1:H:108:ILE:HD11	2.01	0.43
1:I:200:ASN:OD1	1:I:205:ARG:HD3	2.18	0.43
1:H:202:PHE:CD2	1:H:240:ARG:HG2	2.54	0.43
1:I:28:VAL:HG22	1:I:88:ARG:HG2	2.01	0.43
1:I:389:GLN:HE22	1:I:391:GLY:N	2.17	0.43
1:D:425:ALA:HB1	1:D:432:ALA:HB2	2.01	0.43
1:D:200:ASN:OD1	1:D:205:ARG:CG	2.67	0.43
1:F:220:THR:OG1	1:F:222:GLU:HG2	2.18	0.43
1:I:93:PHE:CE1	1:I:131:LYS:HE3	2.54	0.43
1:I:251:HIS:NE2	1:I:312:GLN:NE2	2.65	0.43
1:F:268:ARG:HD3	1:F:268:ARG:C	2.44	0.43
1:A:214:ASP:OD1	4:A:503:EDO:H21	2.18	0.43
1:H:303:LYS:NZ	1:H:354:GLN:HE21	2.17	0.43
1:I:303:LYS:HZ3	1:I:354:GLN:HE21	1.66	0.43
1:A:86:ILE:HG21	1:A:349:VAL:O	2.19	0.43
1:I:181:LEU:HD21	1:I:188:MET:HG2	2.01	0.43
1:B:203:GLU:O	1:B:207:GLU:HG2	2.18	0.42
1:E:289:ASP:OD1	1:E:289:ASP:C	2.62	0.42
1:G:268:ARG:HD3	1:G:268:ARG:C	2.43	0.42
1:H:371:HIS:HB2	1:H:372:PRO:HD2	2.01	0.42
1:D:364:PRO:HB2	1:D:386:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:PHE:CD1	1:E:93:PHE:C	2.97	0.42
1:G:283:ALA:O	1:G:284:MET:CB	2.67	0.42
1:D:286:ALA:HA	1:D:289:ASP:OD1	2.19	0.42
1:D:51:SER:OG	1:D:52:THR:N	2.51	0.42
1:E:139:PRO:HD3	1:E:306:ARG:O	2.19	0.42
1:A:376:GLN:HB3	1:A:377:PRO:HD3	2.01	0.42
1:E:351:HIS:HE1	5:E:709:HOH:O	2.02	0.42
1:A:163:LYS:HA	1:A:164:PRO:C	2.45	0.42
1:I:158:TYR:CE1	1:I:408:VAL:HG11	2.55	0.42
1:B:371:HIS:HB2	1:B:372:PRO:HD2	2.02	0.41
1:C:291:ASN:HA	1:C:292:PRO:HD3	1.94	0.41
1:E:70:LEU:HD22	1:E:95:ALA:HA	2.01	0.41
1:F:136:PHE:HB3	1:F:307:LEU:O	2.20	0.41
1:H:146:VAL:HG21	1:H:312:GLN:HE21	1.84	0.41
1:D:149:MET:HE1	1:D:251:HIS:HD1	1.85	0.41
1:G:303:LYS:NZ	1:G:354:GLN:HE21	2.18	0.41
1:C:303:LYS:NZ	1:C:354:GLN:HE21	2.18	0.41
1:C:206:ALA:HA	1:C:226:TRP:CZ3	2.56	0.41
1:E:93:PHE:HB2	1:E:132:LEU:HD11	2.01	0.41
1:C:117:ARG:NH2	5:C:718:HOH:O	2.53	0.41
1:C:371:HIS:HB2	1:C:372:PRO:HD2	2.03	0.41
1:D:146:VAL:HG21	1:D:312:GLN:HE21	1.85	0.41
1:G:149:MET:HE3	1:G:250:LYS:HD2	2.02	0.41
1:E:206:ALA:HA	1:E:226:TRP:CZ3	2.55	0.41
1:G:286:ALA:HA	1:G:289:ASP:OD1	2.20	0.41
1:A:63:GLU:HG2	1:A:65:GLU:HG2	2.03	0.41
1:B:149:MET:HE3	1:B:250:LYS:HD2	2.02	0.41
1:B:286:ALA:HA	1:B:289:ASP:OD1	2.21	0.41
1:F:319:GLY:HA2	5:F:679:HOH:O	2.19	0.41
1:J:391:GLY:O	1:J:395:LEU:HD12	2.21	0.41
1:C:108:ILE:HD12	1:C:108:ILE:C	2.47	0.40
1:D:268:ARG:C	1:D:268:ARG:HD3	2.46	0.40
1:B:406:ARG:HD3	1:B:430:GLU:HG2	2.02	0.40
1:F:283:ALA:O	1:F:284:MET:CB	2.68	0.40
1:D:149:MET:CE	1:D:251:HIS:CE1	3.02	0.40
1:E:322:LYS:HG3	1:E:323:LEU:HG	2.03	0.40
1:G:371:HIS:HB2	1:G:372:PRO:CD	2.52	0.40
1:D:158:TYR:CD1	1:D:408:VAL:HG11	2.57	0.40
1:F:200:ASN:OD1	1:F:205:ARG:HG3	2.21	0.40
1:J:146:VAL:HG21	1:J:312:GLN:HE21	1.85	0.40
1:H:376:GLN:HB3	1:H:377:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:158:TYR:CD1	1:I:408:VAL:HG11	2.55	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	434/444 (98%)	415 (96%)	19 (4%)	0	100	100
1	B	435/444 (98%)	414 (95%)	20 (5%)	1 (0%)	43	50
1	C	435/444 (98%)	419 (96%)	15 (3%)	1 (0%)	43	50
1	D	433/444 (98%)	416 (96%)	16 (4%)	1 (0%)	43	50
1	E	435/444 (98%)	420 (97%)	15 (3%)	0	100	100
1	F	433/444 (98%)	417 (96%)	15 (4%)	1 (0%)	43	50
1	G	433/444 (98%)	416 (96%)	16 (4%)	1 (0%)	43	50
1	H	434/444 (98%)	417 (96%)	17 (4%)	0	100	100
1	I	433/444 (98%)	415 (96%)	16 (4%)	2 (0%)	24	24
1	J	434/444 (98%)	419 (96%)	14 (3%)	1 (0%)	43	50
All	All	4339/4440 (98%)	4168 (96%)	163 (4%)	8 (0%)	43	50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	284	MET
1	D	284	MET
1	I	284	MET
1	C	284	MET
1	G	284	MET
1	I	398	PRO

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Mol	Chain	Res	Type
1	J	284	MET
1	F	325	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/355 (96%)	335 (99%)	4 (1%)	63	74
1	B	341/355 (96%)	336 (98%)	5 (2%)	57	68
1	C	342/355 (96%)	338 (99%)	4 (1%)	63	74
1	D	345/355 (97%)	343 (99%)	2 (1%)	78	84
1	E	340/355 (96%)	336 (99%)	4 (1%)	63	74
1	F	336/355 (95%)	333 (99%)	3 (1%)	70	79
1	G	338/355 (95%)	336 (99%)	2 (1%)	78	84
1	H	338/355 (95%)	334 (99%)	4 (1%)	63	74
1	I	343/355 (97%)	339 (99%)	4 (1%)	63	74
1	J	341/355 (96%)	337 (99%)	4 (1%)	63	74
All	All	3403/3550 (96%)	3367 (99%)	36 (1%)	65	75

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	65	GLU
1	A	107	SER
1	A	363	PHE
1	B	107	SER
1	B	363	PHE
1	B	380	GLU
1	B	406	ARG
1	B	429	LYS
1	C	65	GLU
1	C	107	SER

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Mol	Chain	Res	Type
1	C	363	PHE
1	C	429	LYS
1	D	65	GLU
1	D	363	PHE
1	E	104	LEU
1	E	107	SER
1	E	363	PHE
1	E	376	GLN
1	F	35	GLU
1	F	40	GLU
1	F	363	PHE
1	G	211	LYS
1	G	363	PHE
1	H	25	ILE
1	H	107	SER
1	H	175	LYS
1	H	363	PHE
1	I	65	GLU
1	I	115	MET
1	I	363	PHE
1	I	395	LEU
1	J	65	GLU
1	J	107	SER
1	J	363	PHE
1	J	427	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	HIS
1	A	312	GLN
1	A	354	GLN
1	A	389	GLN
1	B	64	GLN
1	B	78	HIS
1	B	279	HIS
1	B	294	HIS
1	B	312	GLN
1	B	354	GLN
1	C	41	GLN
1	C	294	HIS
1	C	312	GLN

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Mol	Chain	Res	Type
1	C	354	GLN
1	C	389	GLN
1	D	294	HIS
1	D	312	GLN
1	D	354	GLN
1	D	389	GLN
1	E	312	GLN
1	E	351	HIS
1	E	354	GLN
1	E	389	GLN
1	E	410	GLN
1	E	428	HIS
1	F	78	HIS
1	F	218	ASN
1	F	294	HIS
1	F	312	GLN
1	F	354	GLN
1	F	389	GLN
1	G	218	ASN
1	G	279	HIS
1	G	294	HIS
1	G	312	GLN
1	G	354	GLN
1	G	428	HIS
1	H	41	GLN
1	H	218	ASN
1	H	279	HIS
1	H	294	HIS
1	H	312	GLN
1	H	354	GLN
1	H	389	GLN
1	I	64	GLN
1	I	294	HIS
1	I	312	GLN
1	I	354	GLN
1	I	389	GLN
1	J	312	GLN
1	J	354	GLN
1	J	389	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	KCX	G	189	1,2	10,11,12	0.48	0	6,12,14	0.64	0
1	KCX	E	189	1,2	10,11,12	0.55	0	6,12,14	0.73	0
1	KCX	B	189	1,2	10,11,12	0.50	0	6,12,14	0.66	0
1	KCX	D	189	1,2	10,11,12	0.63	0	6,12,14	0.62	0
1	KCX	I	189	1,2	10,11,12	0.58	0	6,12,14	0.58	0
1	KCX	H	189	1,2	10,11,12	0.53	0	6,12,14	0.69	0
1	KCX	F	189	1,2	10,11,12	0.58	0	6,12,14	0.62	0
1	KCX	C	189	1,2	10,11,12	0.52	0	6,12,14	0.56	0
1	KCX	A	189	1,2	10,11,12	0.53	0	6,12,14	0.73	0
1	KCX	J	189	1,2	10,11,12	0.52	0	6,12,14	0.64	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
1	KCX	G	189	1,2	-	0/9/10/12	-
1	KCX	E	189	1,2	-	0/9/10/12	-
1	KCX	B	189	1,2	-	0/9/10/12	-
1	KCX	D	189	1,2	-	0/9/10/12	-
1	KCX	I	189	1,2	-	0/9/10/12	-
1	KCX	H	189	1,2	-	0/9/10/12	-
1	KCX	F	189	1,2	-	0/9/10/12	-
1	KCX	C	189	1,2	-	0/9/10/12	-
1	KCX	A	189	1,2	-	0/9/10/12	-
1	KCX	J	189	1,2	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	189	KCX	1	0
1	E	189	KCX	1	0
1	B	189	KCX	1	0
1	D	189	KCX	1	0
1	I	189	KCX	1	0
1	H	189	KCX	1	0
1	F	189	KCX	1	0
1	C	189	KCX	1	0
1	A	189	KCX	1	0
1	J	189	KCX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 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	$\# Z > 2$
3	CAP	G	502	2	18,20,20	0.80	0	23,31,31	1.04	1 (4%)
3	CAP	B	502	2	18,20,20	0.80	0	23,31,31	1.01	1 (4%)
3	CAP	H	502	2	18,20,20	0.75	0	23,31,31	0.98	1 (4%)
4	EDO	J	503	-	3,3,3	0.66	0	2,2,2	0.21	0
4	EDO	D	503	-	3,3,3	0.42	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CAP	J	502	2	18,20,20	0.78	0	23,31,31	0.95	0
4	EDO	E	503	-	3,3,3	0.52	0	2,2,2	0.20	0
3	CAP	I	502	2	18,20,20	0.80	0	23,31,31	1.10	1 (4%)
3	CAP	E	502	2	18,20,20	0.78	0	23,31,31	1.03	1 (4%)
4	EDO	A	503	-	3,3,3	0.48	0	2,2,2	0.18	0
4	EDO	C	503	-	3,3,3	0.48	0	2,2,2	0.29	0
4	EDO	H	504	-	3,3,3	0.49	0	2,2,2	0.25	0
3	CAP	D	502	2	18,20,20	0.87	0	23,31,31	0.91	0
4	EDO	H	503	-	3,3,3	0.45	0	2,2,2	0.31	0
4	EDO	I	503	-	3,3,3	0.46	0	2,2,2	0.25	0
3	CAP	F	502	2	18,20,20	0.75	0	23,31,31	1.09	2 (8%)
4	EDO	I	504	-	3,3,3	0.51	0	2,2,2	0.20	0
3	CAP	A	502	2	18,20,20	0.71	0	23,31,31	1.04	1 (4%)
4	EDO	B	503	-	3,3,3	0.40	0	2,2,2	0.40	0
3	CAP	C	502	2	18,20,20	0.78	0	23,31,31	0.97	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
3	CAP	G	502	2	-	6/29/29/29	-
3	CAP	B	502	2	-	7/29/29/29	-
3	CAP	H	502	2	-	8/29/29/29	-
4	EDO	J	503	-	-	0/1/1/1	-
4	EDO	D	503	-	-	0/1/1/1	-
3	CAP	J	502	2	-	9/29/29/29	-
4	EDO	E	503	-	-	1/1/1/1	-
3	CAP	I	502	2	-	6/29/29/29	-
3	CAP	E	502	2	-	9/29/29/29	-
4	EDO	A	503	-	-	1/1/1/1	-
4	EDO	C	503	-	-	0/1/1/1	-
4	EDO	H	504	-	-	1/1/1/1	-
3	CAP	D	502	2	-	8/29/29/29	-
4	EDO	H	503	-	-	0/1/1/1	-
4	EDO	I	503	-	-	0/1/1/1	-
3	CAP	F	502	2	-	7/29/29/29	-
4	EDO	I	504	-	-	0/1/1/1	-
3	CAP	A	502	2	-	7/29/29/29	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	503	-	-	1/1/1/1	-
3	CAP	C	502	2	-	6/29/29/29	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	502	CAP	O7-C-C2	2.60	118.41	114.06
3	F	502	CAP	O6P-P2-O5P	2.40	116.81	107.80
3	E	502	CAP	O7-C-C2	2.29	117.89	114.06
3	A	502	CAP	O7-C-C2	2.18	117.71	114.06
3	H	502	CAP	O7-C-C2	2.14	117.64	114.06
3	B	502	CAP	O7-C-C2	2.11	117.59	114.06
3	I	502	CAP	O6P-P2-O5P	2.10	115.69	107.80
3	G	502	CAP	O7-C-C2	2.07	117.53	114.06

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	CAP	O6-C-C2-C1
3	A	502	CAP	O7-C-C2-C1
3	A	502	CAP	O6-C-C2-O2
3	A	502	CAP	O7-C-C2-O2
3	A	502	CAP	O3-C3-C4-O4
3	B	502	CAP	O6-C-C2-O2
3	B	502	CAP	O7-C-C2-O2
3	B	502	CAP	O3-C3-C4-O4
3	C	502	CAP	O6-C-C2-C1
3	C	502	CAP	O7-C-C2-C1
3	C	502	CAP	O6-C-C2-O2
3	C	502	CAP	O7-C-C2-O2
3	C	502	CAP	O3-C3-C4-O4
3	D	502	CAP	O6-C-C2-C3
3	D	502	CAP	O6-C-C2-O2
3	D	502	CAP	O3-C3-C4-O4
3	E	502	CAP	O6-C-C2-C1
3	E	502	CAP	O7-C-C2-C1
3	E	502	CAP	O6-C-C2-O2
3	E	502	CAP	O7-C-C2-O2
3	E	502	CAP	C2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	E	502	CAP	O3-C3-C4-O4
3	F	502	CAP	O6-C-C2-C1
3	F	502	CAP	O7-C-C2-C1
3	F	502	CAP	O6-C-C2-O2
3	F	502	CAP	O7-C-C2-O2
3	F	502	CAP	C2-C3-C4-O4
3	F	502	CAP	O3-C3-C4-O4
3	G	502	CAP	O6-C-C2-C1
3	G	502	CAP	O7-C-C2-C1
3	G	502	CAP	O6-C-C2-O2
3	G	502	CAP	O7-C-C2-O2
3	H	502	CAP	O6-C-C2-C1
3	H	502	CAP	O7-C-C2-C1
3	H	502	CAP	O6-C-C2-O2
3	H	502	CAP	O7-C-C2-O2
3	H	502	CAP	O3-C3-C4-O4
3	I	502	CAP	O6-C-C2-C1
3	I	502	CAP	O7-C-C2-C1
3	I	502	CAP	O6-C-C2-O2
3	I	502	CAP	O7-C-C2-O2
3	I	502	CAP	O3-C3-C4-O4
3	J	502	CAP	O6-C-C2-O2
3	J	502	CAP	O7-C-C2-O2
3	J	502	CAP	O3-C3-C4-O4
3	B	502	CAP	O6-C-C2-C1
3	B	502	CAP	O7-C-C2-C1
3	D	502	CAP	O6-C-C2-C1
3	J	502	CAP	O6-C-C2-C1
3	J	502	CAP	O7-C-C2-C1
3	D	502	CAP	O7-C-C2-O2
3	A	502	CAP	C2-C3-C4-O4
3	G	502	CAP	O3-C3-C4-O4
3	D	502	CAP	O7-C-C2-C1
3	J	502	CAP	O1-C1-C2-O2
3	A	502	CAP	O2-C2-C3-C4
3	B	502	CAP	O2-C2-C3-C4
3	C	502	CAP	O2-C2-C3-C4
3	D	502	CAP	O2-C2-C3-C4
3	E	502	CAP	O2-C2-C3-C4
3	F	502	CAP	O2-C2-C3-C4
3	G	502	CAP	O2-C2-C3-C4
3	H	502	CAP	O2-C2-C3-C4

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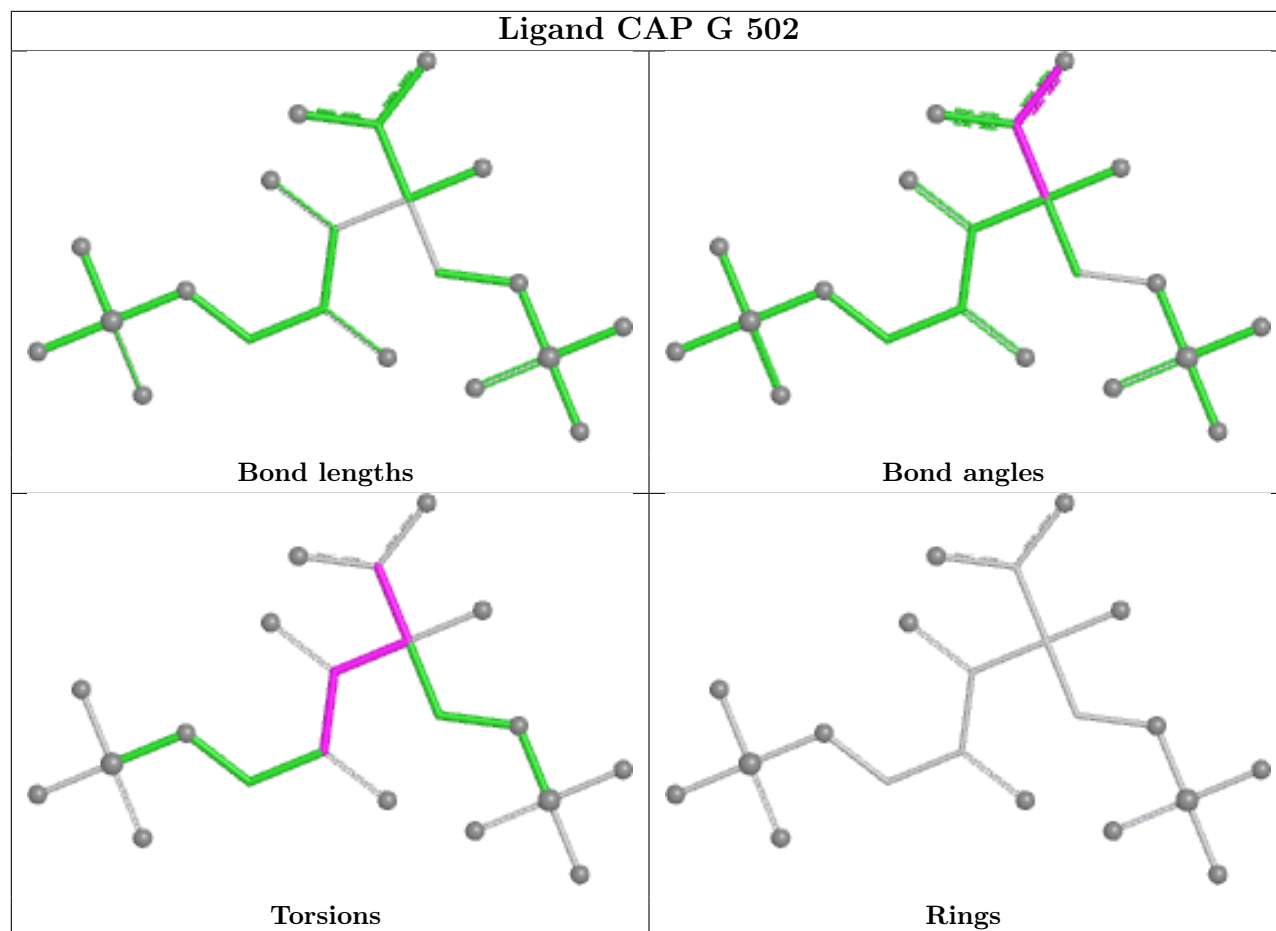
Mol	Chain	Res	Type	Atoms
3	I	502	CAP	O2-C2-C3-C4
3	J	502	CAP	O2-C2-C3-C4
3	J	502	CAP	C2-C3-C4-O4
3	H	502	CAP	C5-O5-P2-O4P
3	B	502	CAP	O7-C-C2-C3
3	D	502	CAP	O7-C-C2-C3
4	H	504	EDO	O1-C1-C2-O2
3	H	502	CAP	C2-C3-C4-O4
3	E	502	CAP	C4-C5-O5-P2
3	E	502	CAP	C5-O5-P2-O4P
4	B	503	EDO	O1-C1-C2-O2
3	J	502	CAP	O4-C4-C5-O5
4	E	503	EDO	O1-C1-C2-O2
4	A	503	EDO	O1-C1-C2-O2

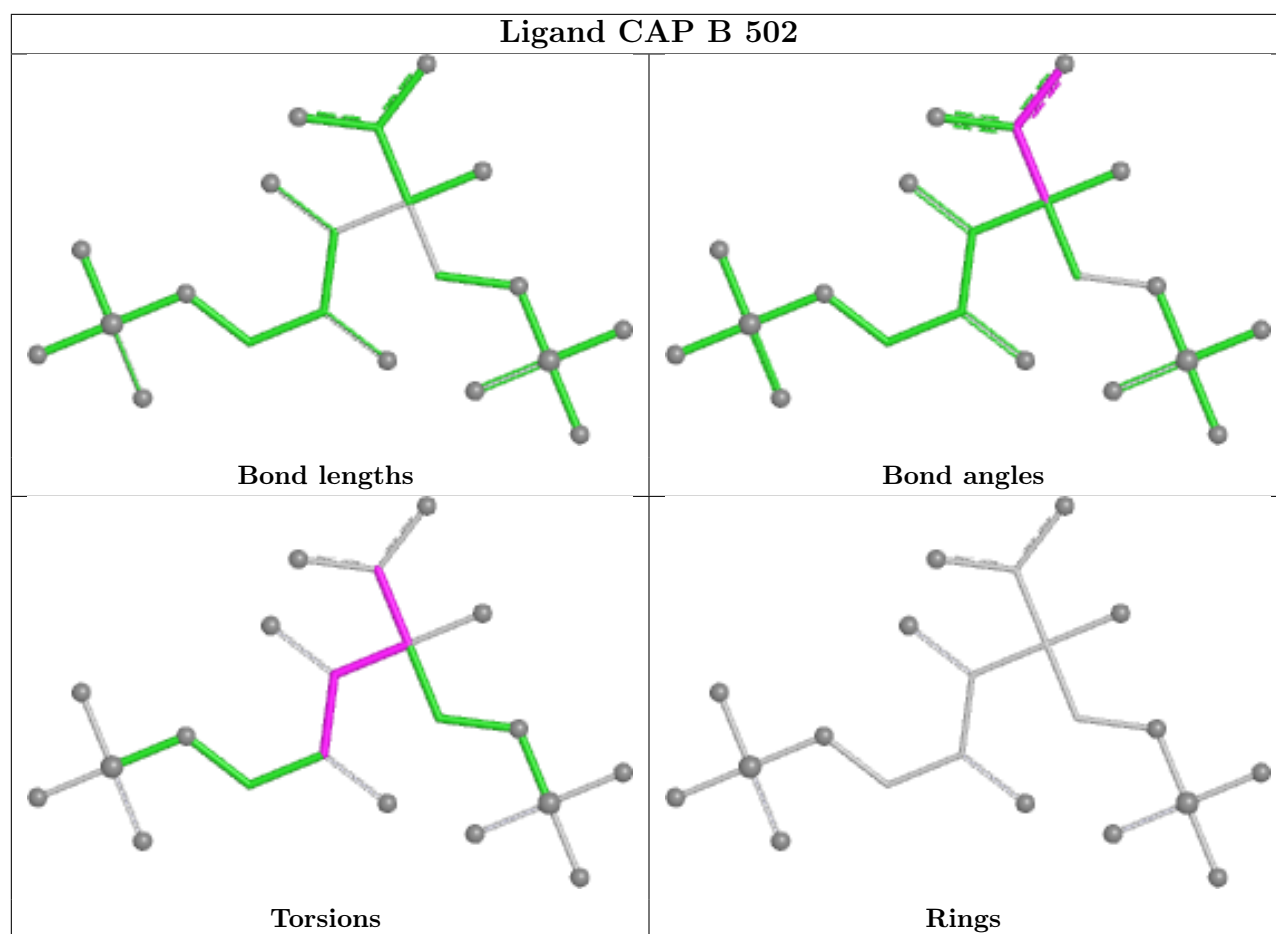
There are no ring outliers.

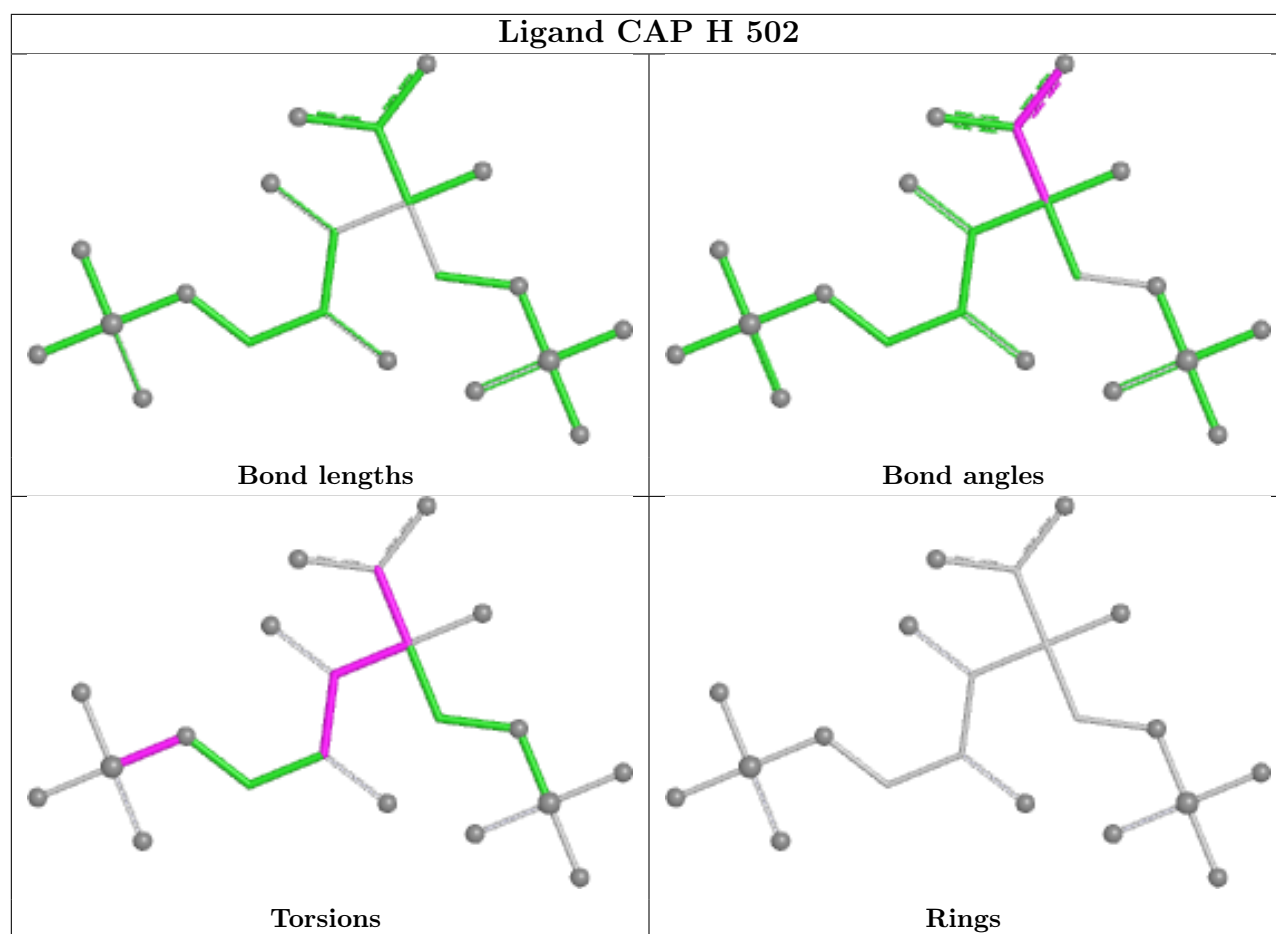
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	503	EDO	1	0
4	A	503	EDO	1	0

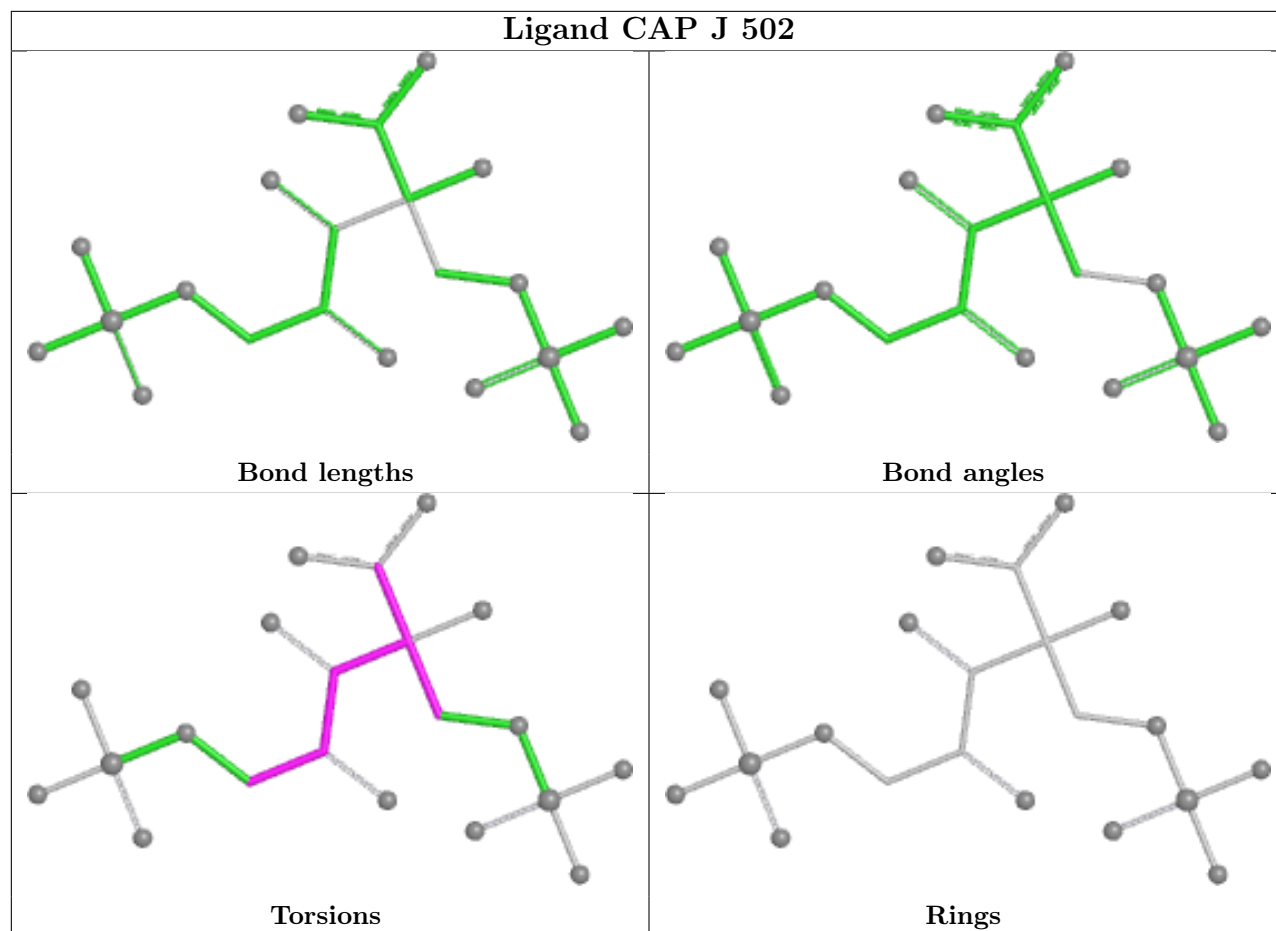
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



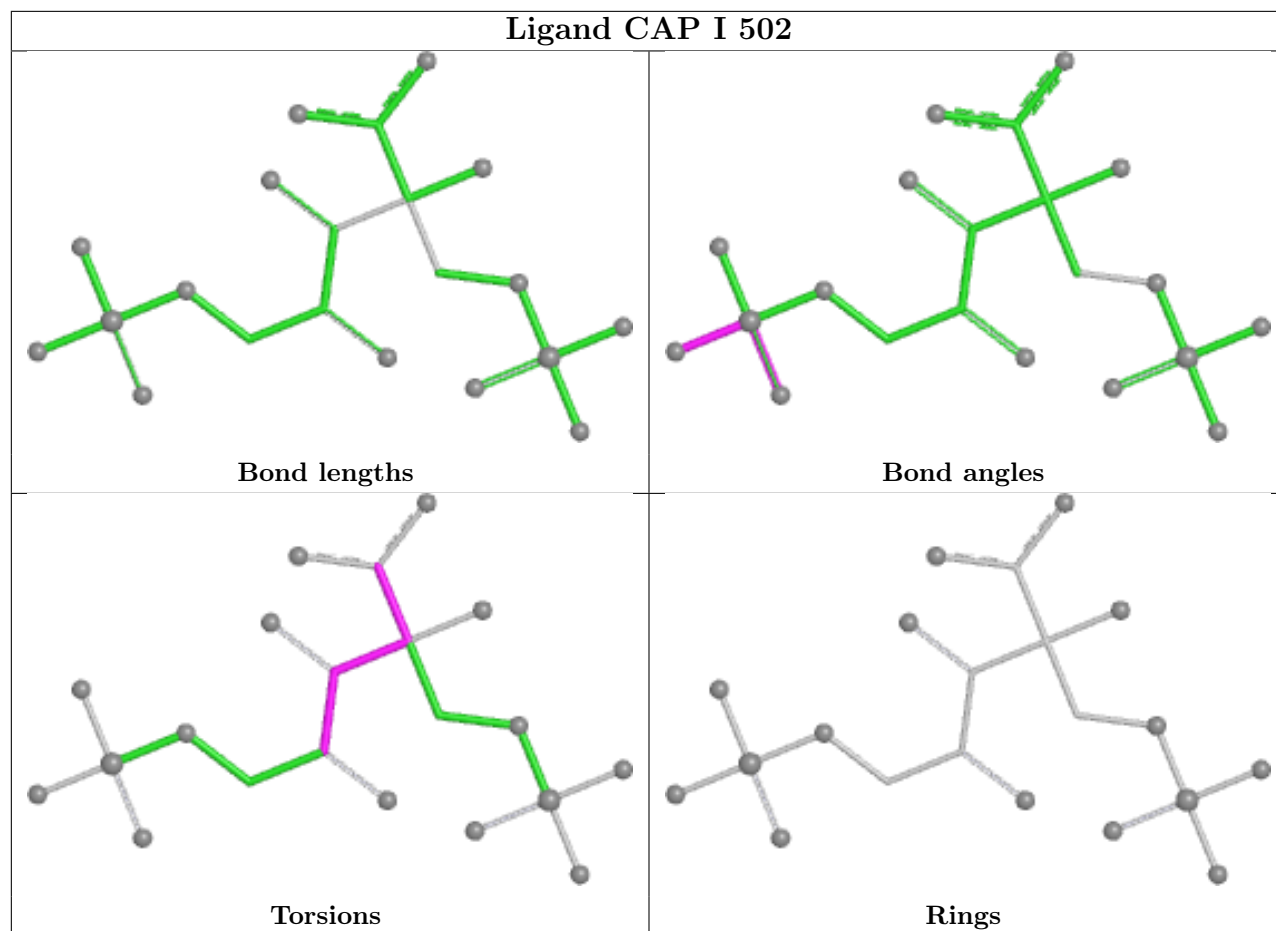


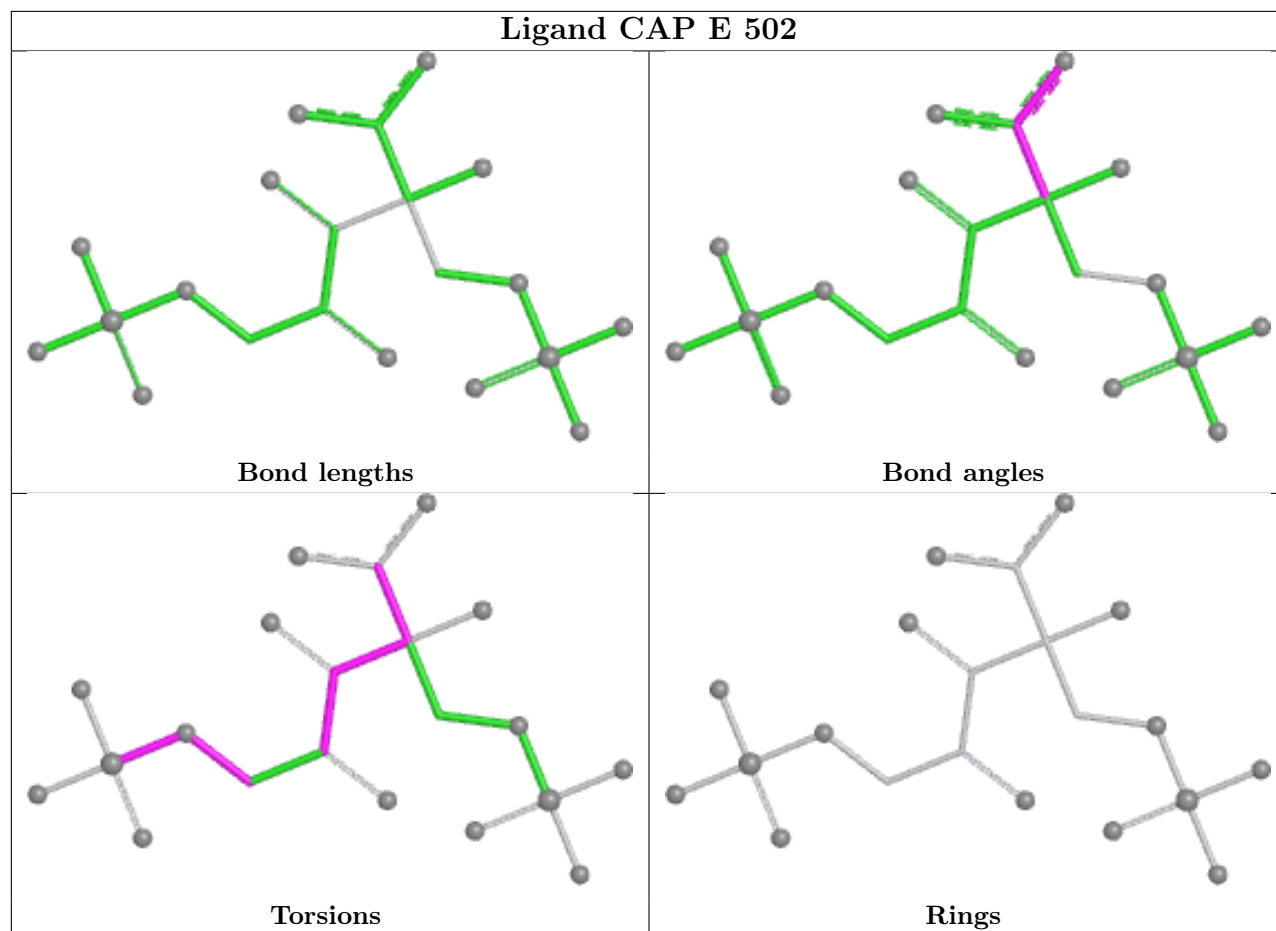


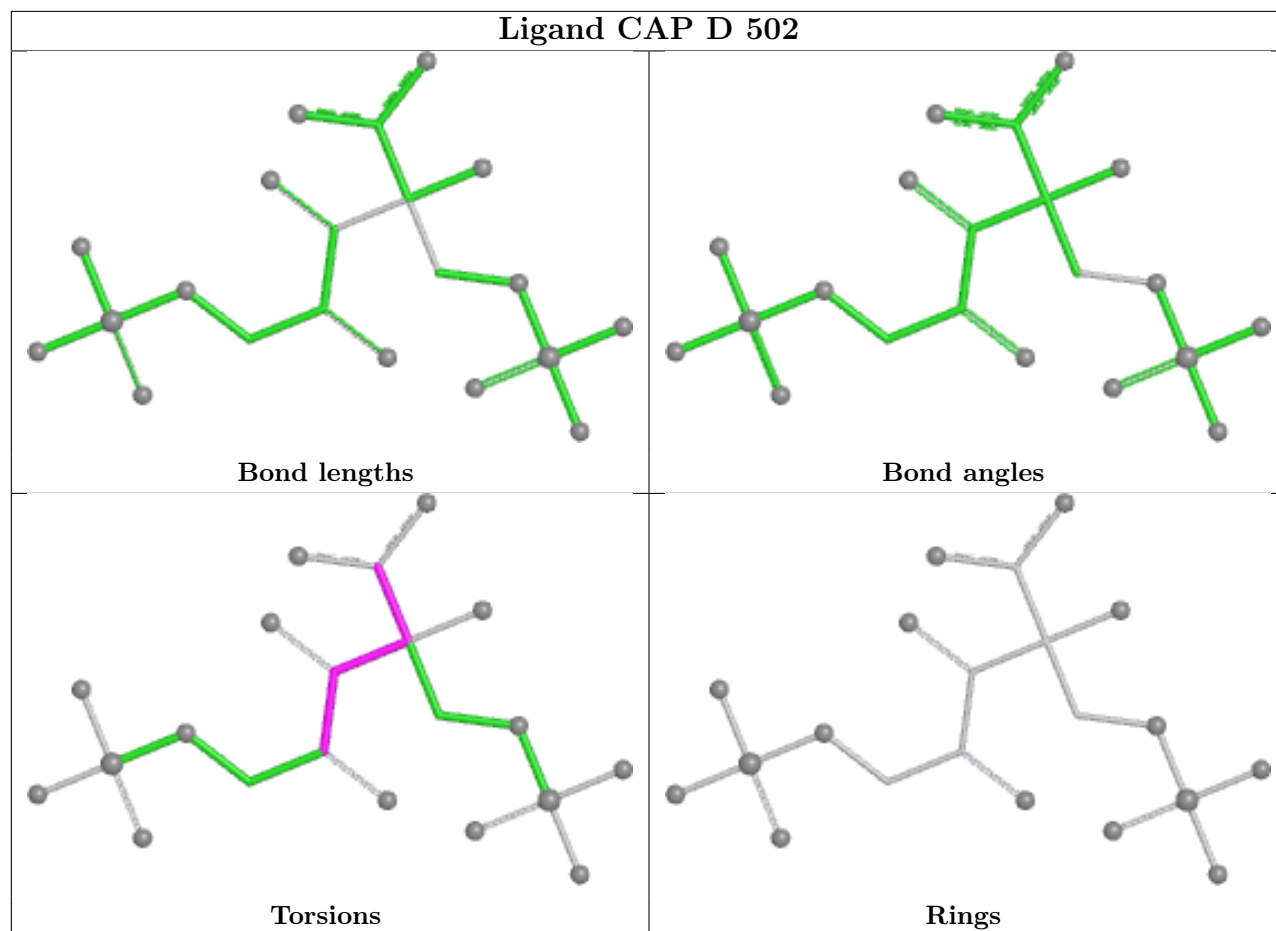
Ligand CAP J 502



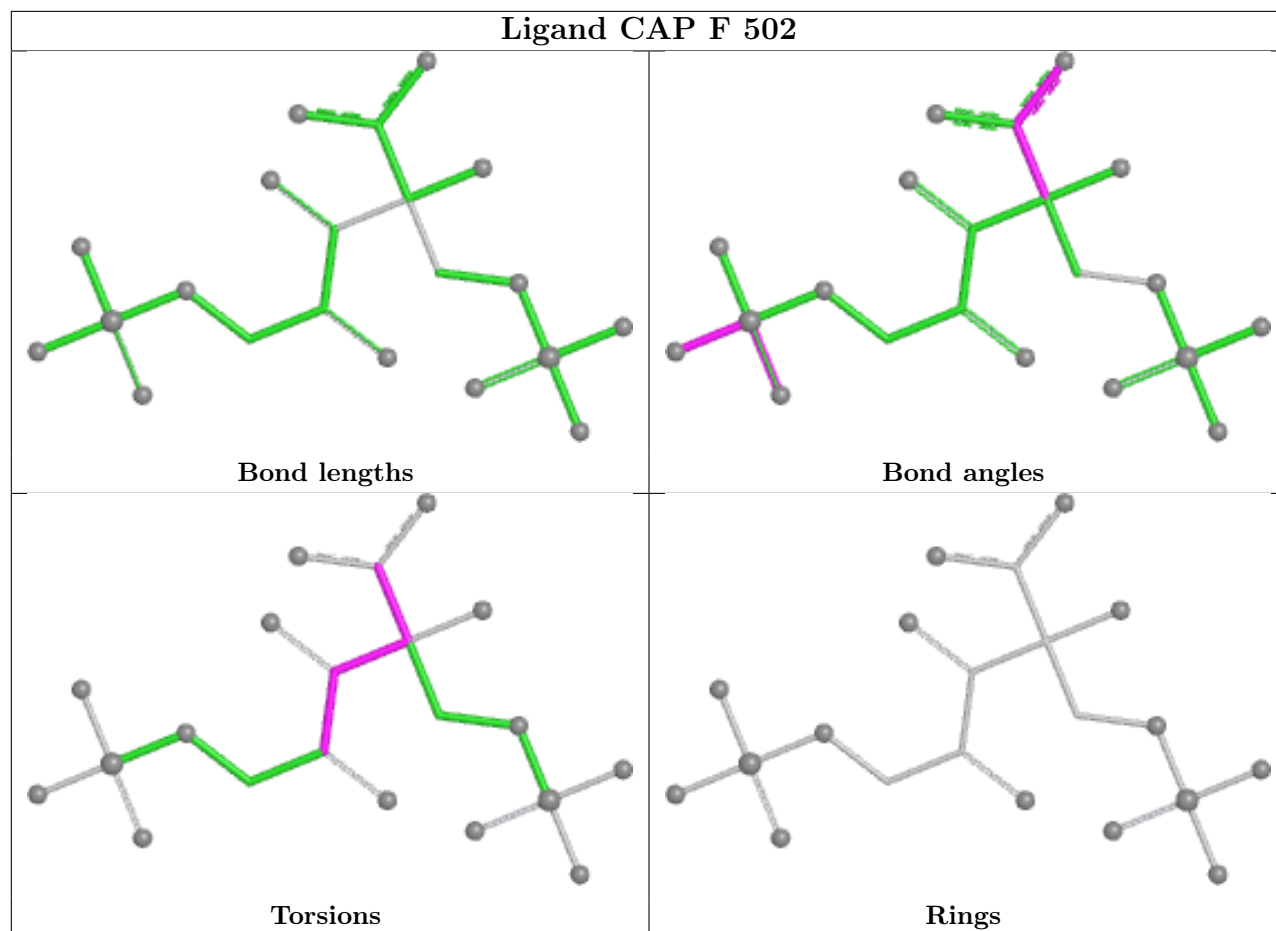
Ligand CAP I 502

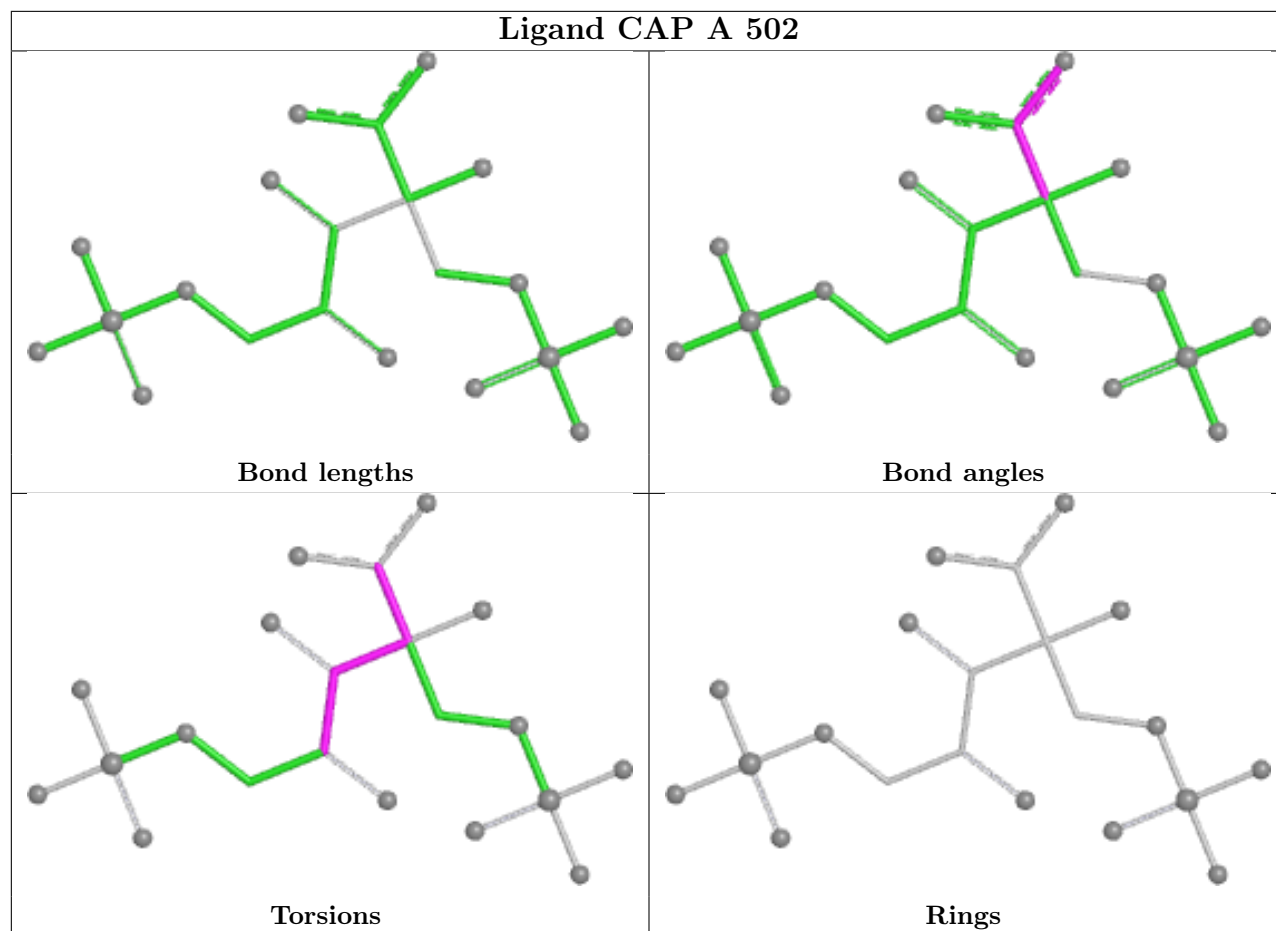


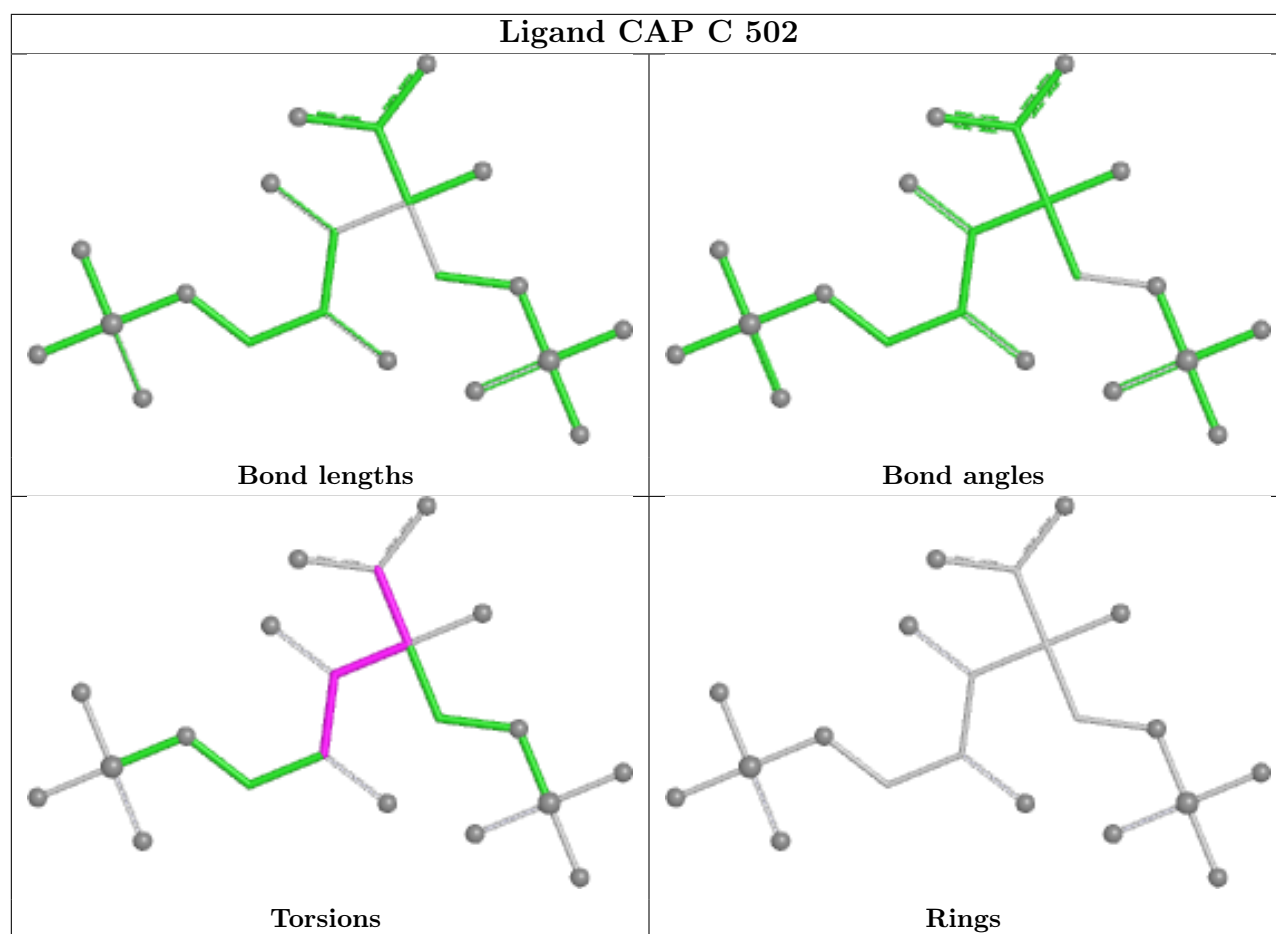




Ligand CAP F 502







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	436/444 (98%)	0.22	8 (1%) 67 68	30, 49, 71, 89	0
1	B	437/444 (98%)	0.56	33 (7%) 20 18	38, 58, 90, 108	0
1	C	437/444 (98%)	0.14	8 (1%) 67 68	28, 43, 76, 95	0
1	D	435/444 (97%)	0.38	12 (2%) 55 55	26, 50, 80, 93	0
1	E	437/444 (98%)	0.14	10 (2%) 61 61	24, 42, 84, 101	0
1	F	435/444 (97%)	0.77	42 (9%) 13 12	32, 62, 94, 123	0
1	G	435/444 (97%)	0.55	24 (5%) 30 29	40, 58, 87, 109	0
1	H	436/444 (98%)	0.45	15 (3%) 48 48	32, 53, 95, 122	0
1	I	435/444 (97%)	0.23	15 (3%) 48 48	25, 46, 77, 92	0
1	J	436/444 (98%)	0.13	10 (2%) 61 61	25, 40, 79, 96	0
All	All	4359/4440 (98%)	0.36	177 (4%) 41 41	24, 50, 85, 123	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	9	TYR	6.0
1	H	421	LEU	5.6
1	D	9	TYR	5.3
1	D	54	THR	5.0
1	B	7	THR	4.9
1	I	9	TYR	4.9
1	D	59	TYR	4.8
1	E	7	THR	4.7
1	F	57	THR	4.5
1	F	58	LEU	4.5
1	I	54	THR	4.4
1	I	59	TYR	4.2
1	A	59	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	H	8	ILE	4.1
1	F	59	TYR	4.0
1	I	58	LEU	4.0
1	F	421	LEU	3.9
1	B	426	LYS	3.9
1	D	58	LEU	3.8
1	B	427	THR	3.8
1	F	10	ASP	3.7
1	E	442	THR	3.7
1	I	347	ASN	3.7
1	H	422	ASP	3.6
1	C	7	THR	3.6
1	J	421	LEU	3.5
1	E	427	THR	3.5
1	G	421	LEU	3.4
1	G	9	TYR	3.4
1	F	43	ALA	3.4
1	A	8	ILE	3.4
1	D	55	TRP	3.3
1	H	58	LEU	3.3
1	I	60	PRO	3.3
1	D	10	ASP	3.3
1	G	58	LEU	3.3
1	G	414	ALA	3.2
1	F	403	ALA	3.2
1	J	424	TYR	3.2
1	J	444	VAL	3.2
1	G	54	THR	3.1
1	B	59	TYR	3.1
1	J	414	ALA	3.1
1	C	59	TYR	3.1
1	B	399	ASP	3.0
1	E	421	LEU	3.0
1	F	42	ALA	3.0
1	C	421	LEU	3.0
1	D	395	LEU	3.0
1	B	414	ALA	2.9
1	G	59	TYR	2.9
1	A	58	LEU	2.9
1	B	58	LEU	2.9
1	B	375	ILE	2.9
1	F	427	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	346	GLU	2.9
1	H	115	MET	2.9
1	E	426	LYS	2.9
1	E	429	LYS	2.9
1	I	55	TRP	2.9
1	G	429	LYS	2.8
1	H	59	TYR	2.8
1	J	59	TYR	2.8
1	B	395	LEU	2.8
1	F	85	TRP	2.8
1	B	369	GLY	2.7
1	F	115	MET	2.7
1	E	434	ALA	2.7
1	G	419	ILE	2.7
1	I	10	ASP	2.6
1	B	54	THR	2.6
1	J	376	GLN	2.6
1	F	81	GLY	2.6
1	B	398	PRO	2.6
1	B	424	TYR	2.6
1	F	414	ALA	2.6
1	G	411	ALA	2.6
1	F	79	ASP	2.6
1	B	57	THR	2.6
1	H	427	THR	2.6
1	B	429	LYS	2.5
1	B	412	ILE	2.5
1	B	403	ALA	2.5
1	G	402	ALA	2.5
1	B	166	VAL	2.5
1	I	346	GLU	2.5
1	F	431	LEU	2.5
1	F	78	HIS	2.5
1	F	426	LYS	2.4
1	F	292	PRO	2.4
1	G	425	ALA	2.4
1	E	444	VAL	2.4
1	F	346	GLU	2.4
1	A	421	LEU	2.4
1	H	424	TYR	2.4
1	F	439	GLY	2.4
1	B	433	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	9	TYR	2.3
1	I	53	GLY	2.3
1	G	434	ALA	2.3
1	G	375	ILE	2.3
1	J	8	ILE	2.3
1	B	144	GLU	2.3
1	B	401	PRO	2.3
1	B	396	GLY	2.3
1	F	325	GLY	2.3
1	H	391	GLY	2.3
1	B	410	GLN	2.3
1	G	426	LYS	2.3
1	C	373	GLY	2.3
1	I	400	GLY	2.3
1	J	440	HIS	2.3
1	B	444	VAL	2.3
1	G	444	VAL	2.3
1	D	207	GLU	2.2
1	F	47	ALA	2.2
1	F	38	THR	2.2
1	I	427	THR	2.2
1	F	39	ILE	2.2
1	F	444	VAL	2.2
1	F	420	PRO	2.2
1	B	53	GLY	2.2
1	E	418	GLY	2.2
1	G	368	GLY	2.2
1	G	380	GLU	2.2
1	I	61	TRP	2.2
1	C	8	ILE	2.2
1	F	441	VAL	2.2
1	C	391	GLY	2.2
1	F	336	ILE	2.2
1	A	347	ASN	2.2
1	F	13	VAL	2.2
1	G	115	MET	2.2
1	G	167	GLY	2.2
1	B	434	ALA	2.2
1	G	57	THR	2.2
1	G	427	THR	2.2
1	G	432	ALA	2.2
1	J	427	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	16	GLY	2.1
1	H	396	GLY	2.1
1	C	54	THR	2.1
1	E	424	TYR	2.1
1	B	8	ILE	2.1
1	B	421	LEU	2.1
1	F	337	LEU	2.1
1	G	346	GLU	2.1
1	H	423	GLU	2.1
1	J	438	TRP	2.1
1	F	54	THR	2.1
1	B	435	LEU	2.1
1	F	357	TYR	2.1
1	B	397	HIS	2.1
1	C	376	GLN	2.1
1	F	29	PHE	2.1
1	B	400	GLY	2.1
1	D	44	GLY	2.1
1	B	432	ALA	2.1
1	F	15	LYS	2.1
1	F	395	LEU	2.1
1	F	435	LEU	2.1
1	A	10	ASP	2.1
1	F	86	ILE	2.1
1	G	410	GLN	2.1
1	A	9	TYR	2.1
1	D	53	GLY	2.1
1	F	369	GLY	2.1
1	H	418	GLY	2.1
1	F	328	TRP	2.1
1	A	340	SER	2.0
1	F	402	ALA	2.0
1	H	35	GLU	2.0
1	D	421	LEU	2.0
1	I	426	LYS	2.0
1	I	115	MET	2.0
1	H	54	THR	2.0
1	H	443	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	F	189	12/13	0.94	0.09	42,43,44,46	0
1	KCX	I	189	12/13	0.94	0.08	26,27,28,29	0
1	KCX	B	189	12/13	0.96	0.07	48,49,50,51	0
1	KCX	G	189	12/13	0.96	0.07	48,49,50,51	0
1	KCX	H	189	12/13	0.96	0.08	48,49,51,52	0
1	KCX	C	189	12/13	0.96	0.08	39,41,42,42	0
1	KCX	J	189	12/13	0.96	0.08	37,38,39,39	0
1	KCX	E	189	12/13	0.97	0.07	38,40,41,41	0
1	KCX	D	189	12/13	0.97	0.06	30,31,32,33	0
1	KCX	A	189	12/13	0.98	0.06	34,35,36,36	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	503	4/4	0.60	0.28	62,62,63,64	0
4	EDO	E	503	4/4	0.62	0.26	42,43,44,44	0
4	EDO	J	503	4/4	0.65	0.20	32,32,33,33	0
4	EDO	H	504	4/4	0.67	0.26	50,53,53,54	0
4	EDO	I	504	4/4	0.70	0.25	48,48,49,50	0
3	CAP	E	502	21/21	0.91	0.11	45,50,57,58	0
3	CAP	F	502	21/21	0.94	0.09	49,53,56,57	0
3	CAP	G	502	21/21	0.94	0.09	52,56,62,62	0
3	CAP	J	502	21/21	0.94	0.10	41,47,53,54	0
2	MG	C	501	1/1	0.94	0.05	46,46,46,46	0
4	EDO	C	503	4/4	0.95	0.07	24,25,25,26	0
3	CAP	B	502	21/21	0.95	0.09	55,59,65,66	0

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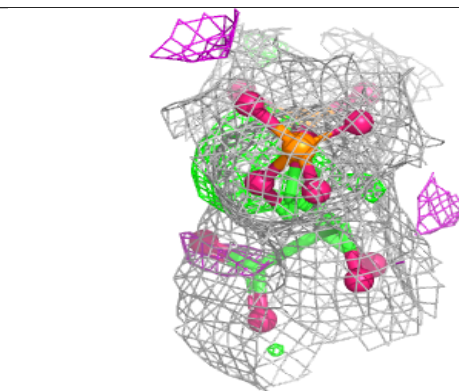
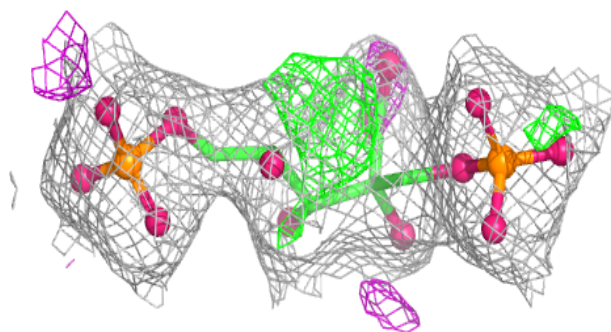
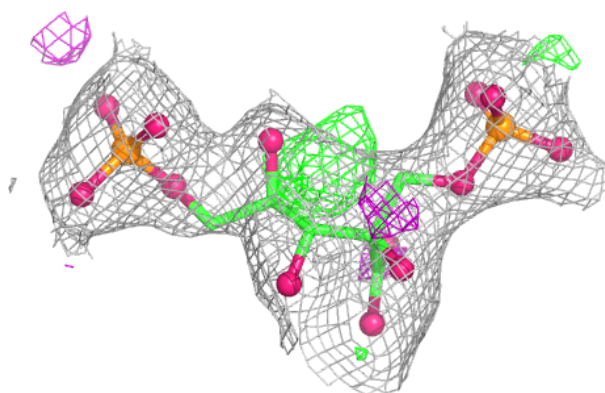
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CAP	H	502	21/21	0.95	0.08	56,60,67,68	0
4	EDO	I	503	4/4	0.95	0.07	26,26,26,28	0
2	MG	B	501	1/1	0.95	0.06	59,59,59,59	0
2	MG	H	501	1/1	0.95	0.06	58,58,58,58	0
4	EDO	D	503	4/4	0.96	0.09	28,28,29,30	0
3	CAP	C	502	21/21	0.96	0.07	43,47,51,52	0
2	MG	J	501	1/1	0.97	0.05	43,43,43,43	0
4	EDO	H	503	4/4	0.97	0.06	29,29,30,32	0
3	CAP	D	502	21/21	0.97	0.06	32,35,38,39	0
4	EDO	B	503	4/4	0.97	0.06	31,31,31,33	0
2	MG	E	501	1/1	0.97	0.06	45,45,45,45	0
3	CAP	I	502	21/21	0.97	0.06	31,33,35,36	0
3	CAP	A	502	21/21	0.98	0.06	37,39,42,43	0
2	MG	G	501	1/1	0.98	0.05	57,57,57,57	0
2	MG	A	501	1/1	0.98	0.04	36,36,36,36	0
2	MG	F	501	1/1	0.98	0.04	46,46,46,46	0
2	MG	I	501	1/1	0.99	0.03	28,28,28,28	0
2	MG	D	501	1/1	0.99	0.03	31,31,31,31	0

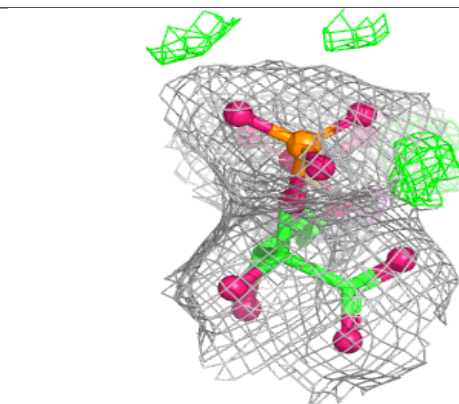
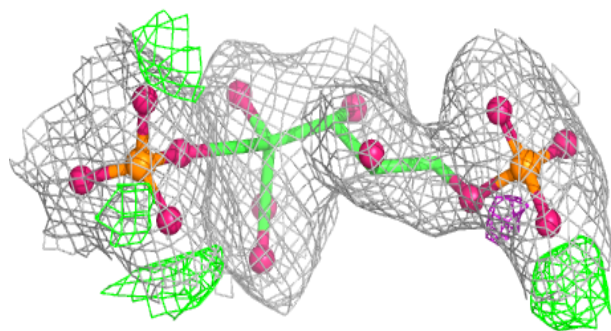
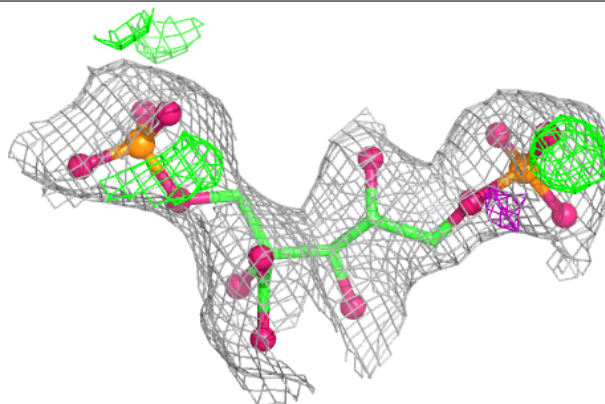
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CAP E 502:

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

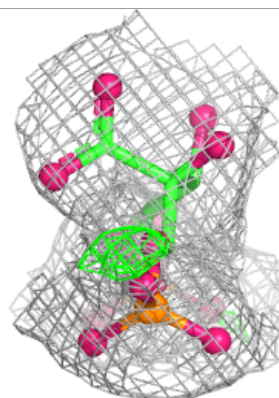
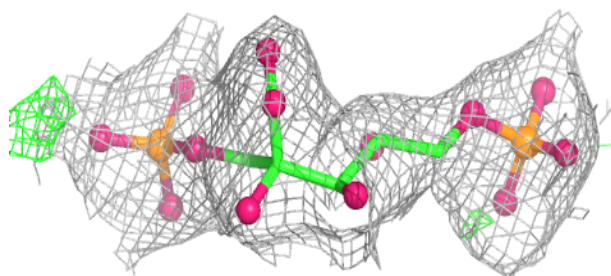
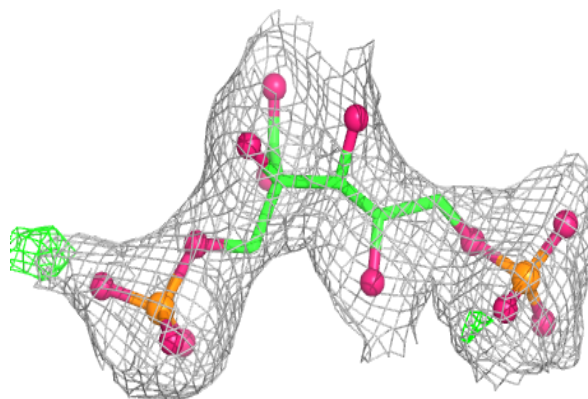
**Electron density around CAP F 502:**

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

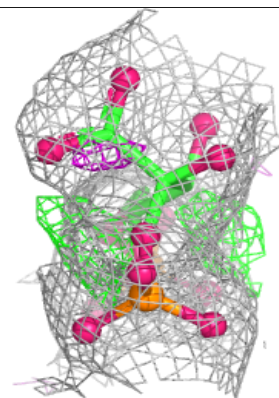
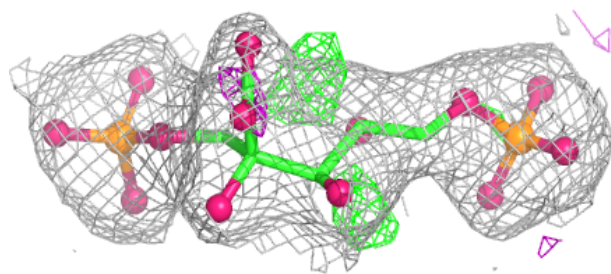
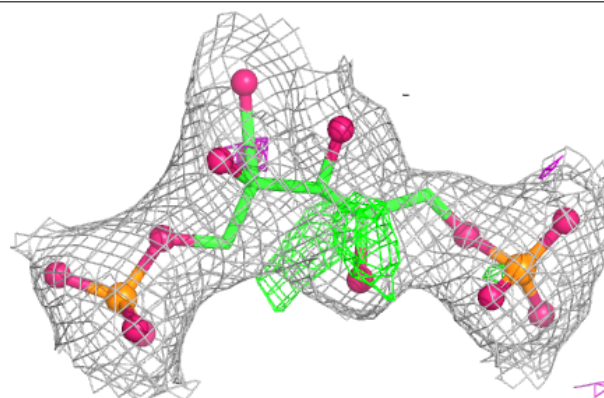


Electron density around CAP G 502:

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

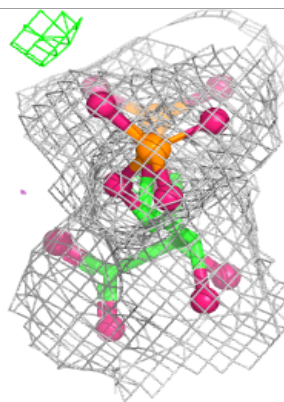
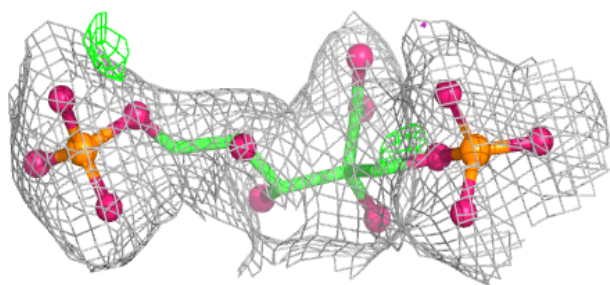
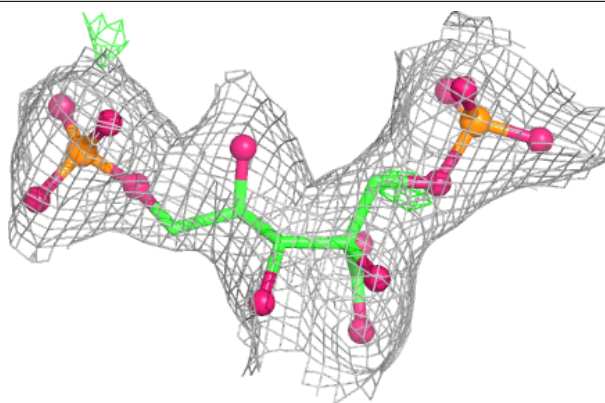
**Electron density around CAP J 502:**

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

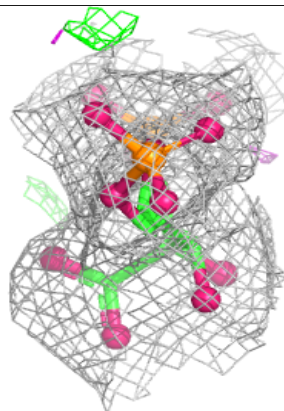
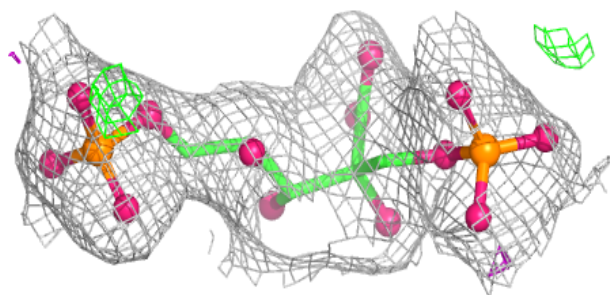
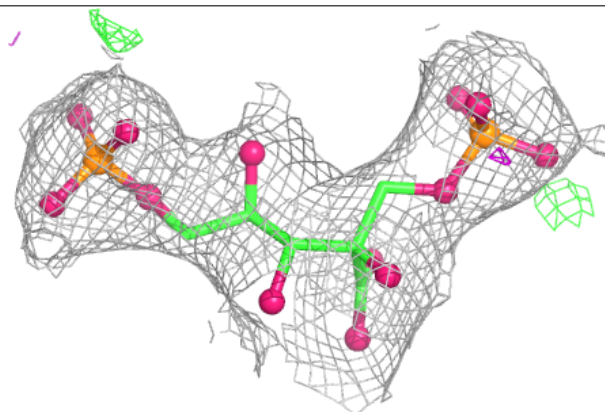


Electron density around CAP B 502:

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

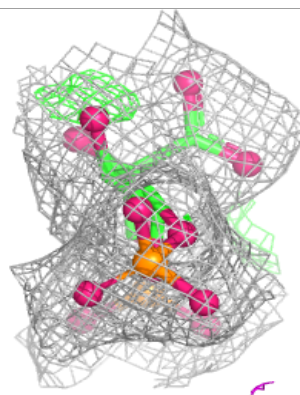
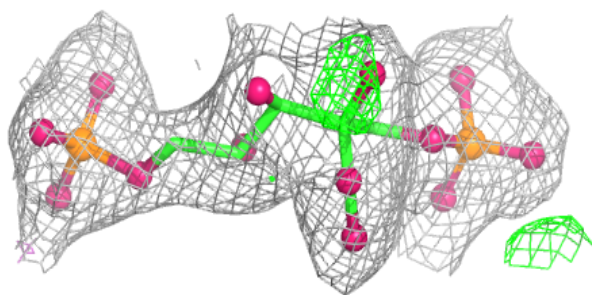
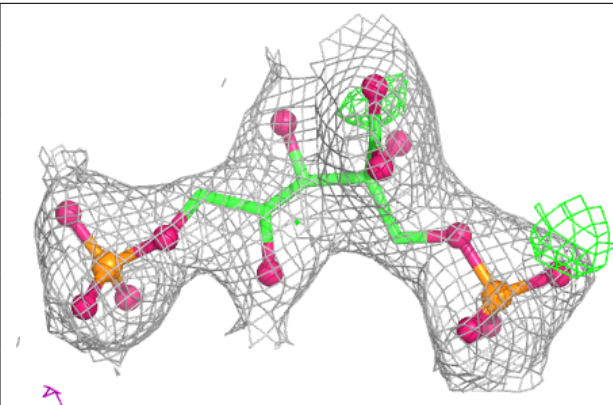
**Electron density around CAP H 502:**

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

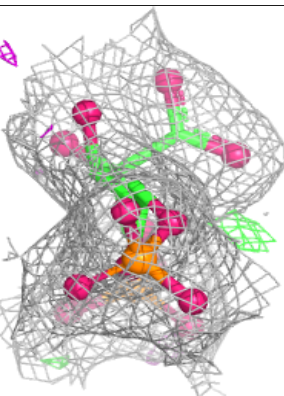
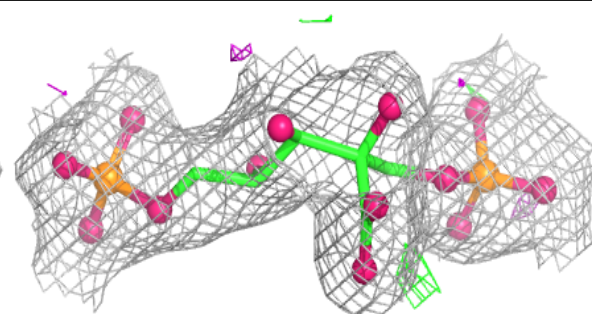
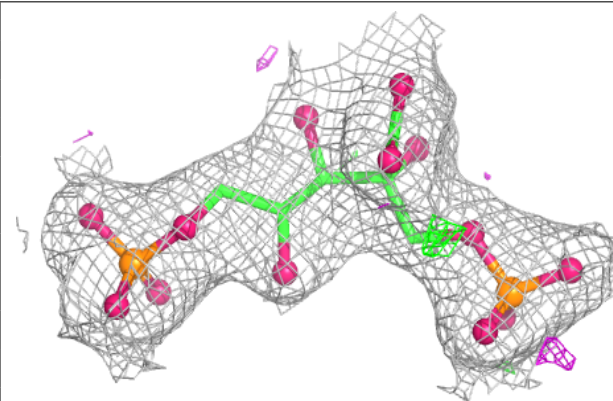


Electron density around CAP C 502:

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

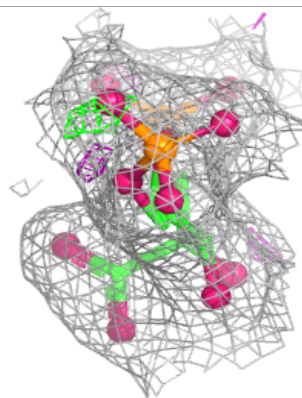
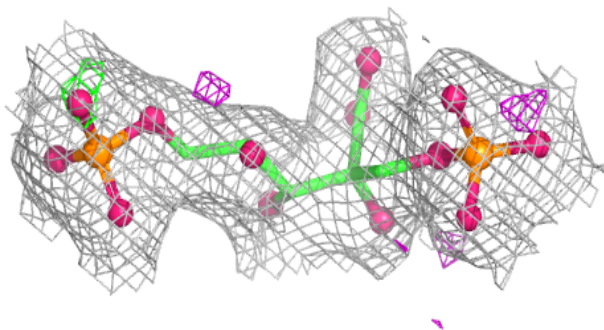
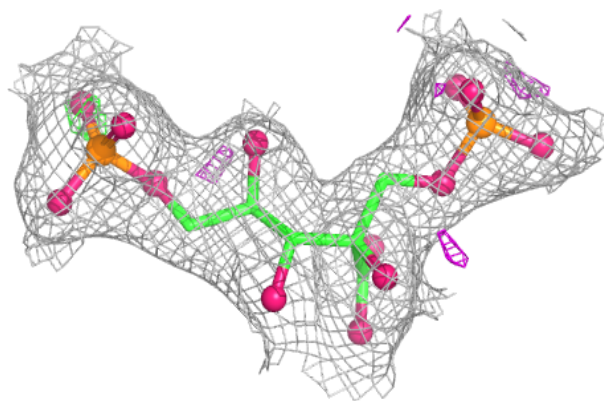
**Electron density around CAP D 502:**

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

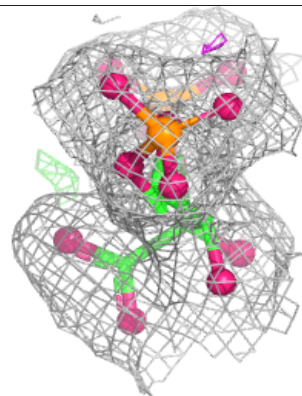
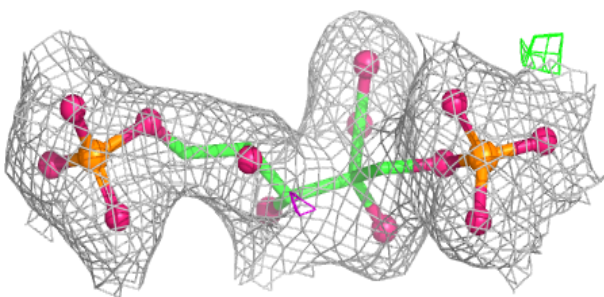
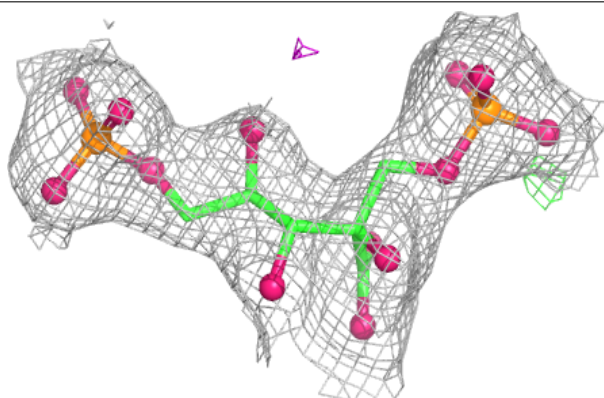


Electron density around CAP I 502:

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

**Electron density around CAP A 502:**

$2mF_o-DF_c$ (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.