Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2026 – 08:52 pm BST

PDB ID	:	5A8R / pdb_00005a8r
Title	:	METHYL-COENZYME M REDUCTASE II FROM METHANOTHERMOBACTER MARBURGENSIS AT 2.15 A RESOLUTION
Authors	:	Wagner, T.; Ermler, U.
Deposited on	:	2015-07-16
Resolution	:	2.15 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:

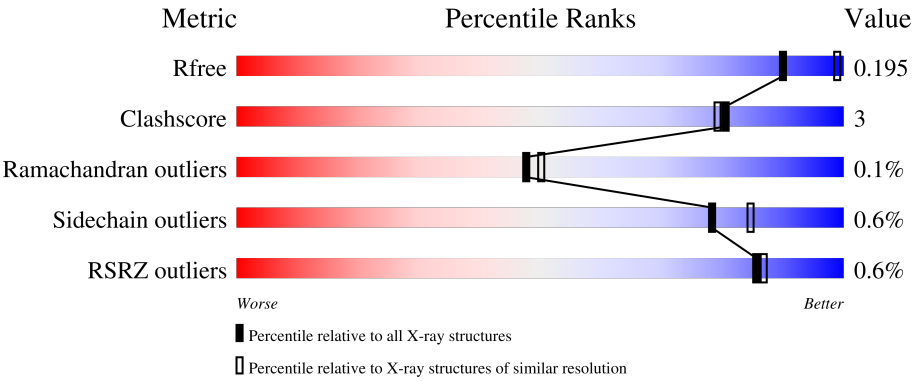
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	553	92% 7%
1	D	553	91% 8%
1	G	553	90% 8%
1	J	553	92% 7%
2	B	443	92% 7%

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Mol	Chain	Length	Quality of chain
2	E	443	93% 6%
2	H	443	92% 8%
2	K	443	94% 5%
3	C	265	91% 8%
3	F	265	89% 9%
3	I	265	91% 8%
3	L	265	92% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	COM	G	601	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 40798 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 METHYL-COENZYME M REDUCTASE II SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4235	2676	714	822	23			
1	D	548	Total	C	N	O	S	0	0	0
			4235	2676	714	822	23			
1	G	548	Total	C	N	O	S	0	0	0
			4235	2676	714	822	23			
1	J	548	Total	C	N	O	S	0	1	0
			4238	2678	714	823	23			

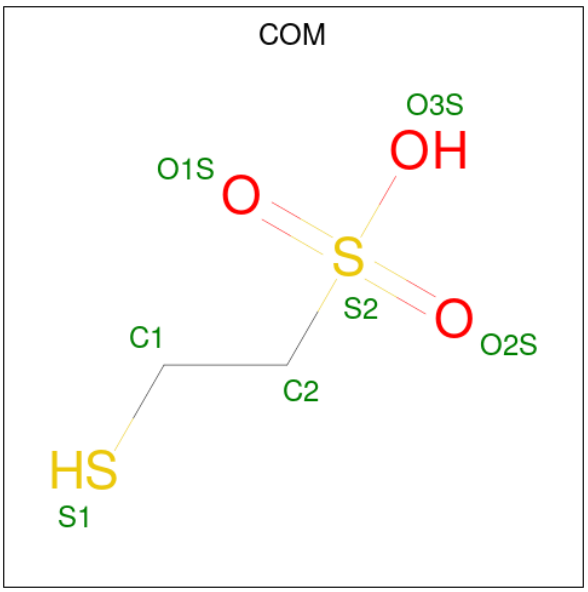
- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE II SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	0	0	0
			3296	2087	557	639	13			
2	E	442	Total	C	N	O	S	0	0	0
			3296	2087	557	639	13			
2	H	442	Total	C	N	O	S	0	0	0
			3296	2087	557	639	13			
2	K	442	Total	C	N	O	S	0	0	0
			3296	2087	557	639	13			

- Molecule 3 is a protein called METHYL-COENZYME M REDUCTASE II, SUBUNIT BETA.

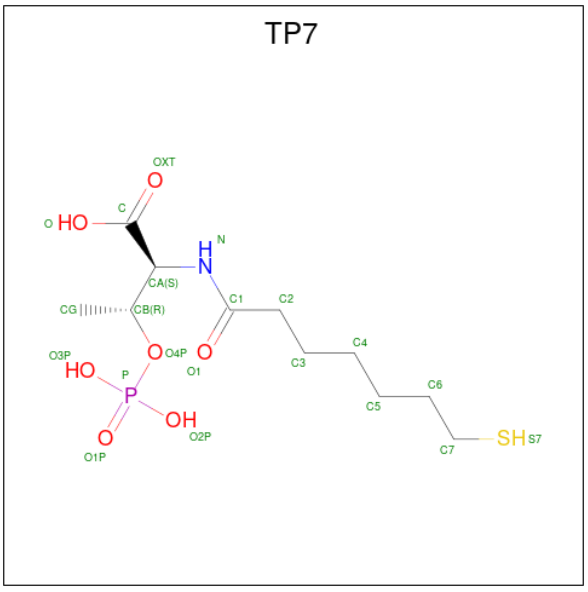
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	262	Total	C	N	O	S	0	0	0
			2122	1321	376	415	10			
3	F	261	Total	C	N	O	S	0	0	0
			2114	1317	375	412	10			
3	I	262	Total	C	N	O	S	0	0	0
			2120	1320	376	414	10			
3	L	263	Total	C	N	O	S	0	0	0
			2128	1324	377	417	10			

- Molecule 4 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $C_2H_6O_3S_2$).



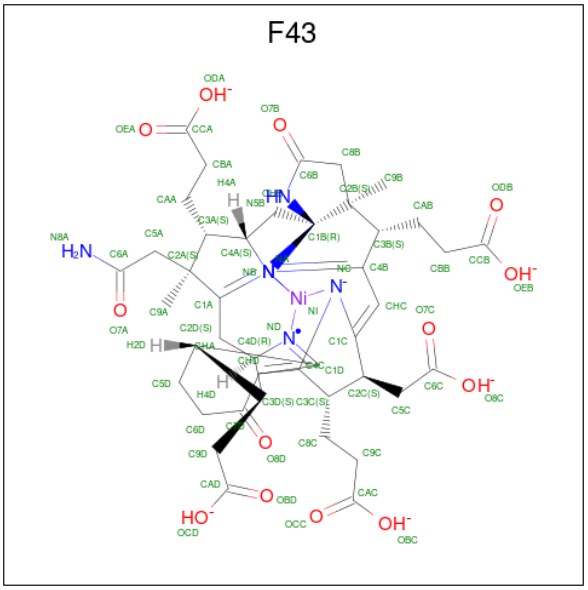
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			7	2	3	2		
4	D	1	Total	C	O	S	0	0
			7	2	3	2		
4	G	1	Total	C	O	S	0	0
			7	2	3	2		
4	J	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 5 is Coenzyme B (CCD ID: TP7) (formula: $C_{11}H_{22}NO_7PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
5	D	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
5	G	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
5	J	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		

- Molecule 6 is FACTOR 430 (CCD ID: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
6	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
6	G	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
6	J	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	K	0	0
			1	1		
7	D	2	Total	K	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total K 1 1	0	0
7	J	3	Total K 3 3	0	0

- Molecule 8 is water.

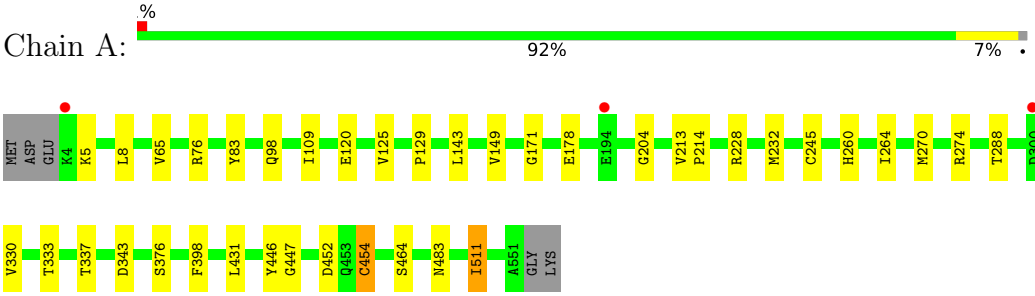
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	297	Total O 297 297	0	0
8	B	146	Total O 146 146	0	0
8	C	72	Total O 72 72	0	0
8	D	208	Total O 208 208	0	0
8	E	110	Total O 110 110	0	0
8	F	71	Total O 71 71	0	0
8	G	260	Total O 260 260	0	0
8	H	158	Total O 158 158	0	0
8	I	45	Total O 45 45	0	0
8	J	220	Total O 220 220	0	0
8	K	137	Total O 137 137	0	0
8	L	96	Total O 96 96	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.

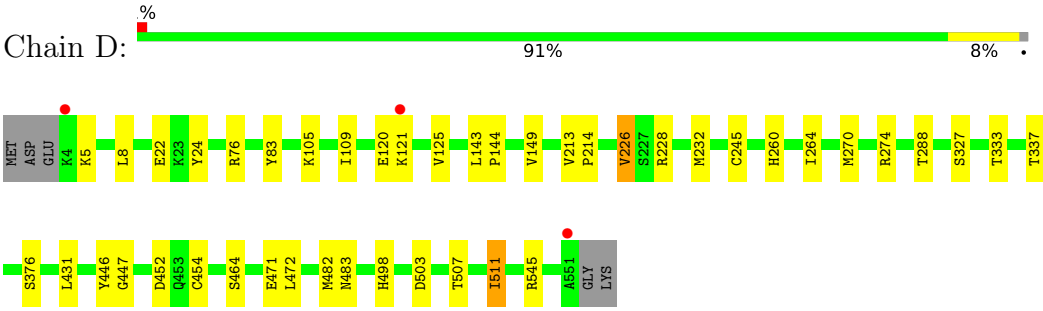
• Molecule 1: METHYL-COENZYME M REDUCTASE II SUBUNIT ALPHA

Chain A:



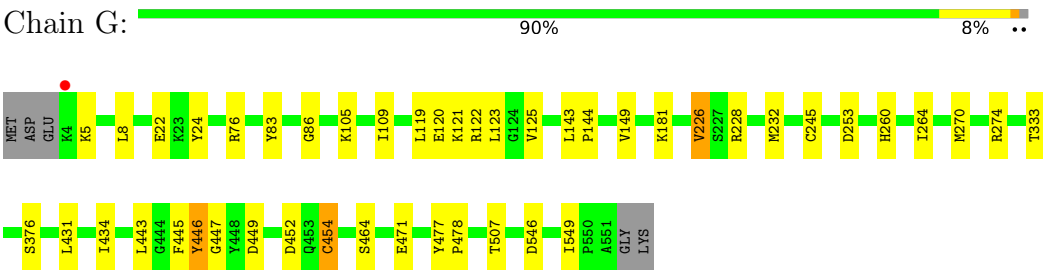
• Molecule 1: METHYL-COENZYME M REDUCTASE II SUBUNIT ALPHA

Chain D:



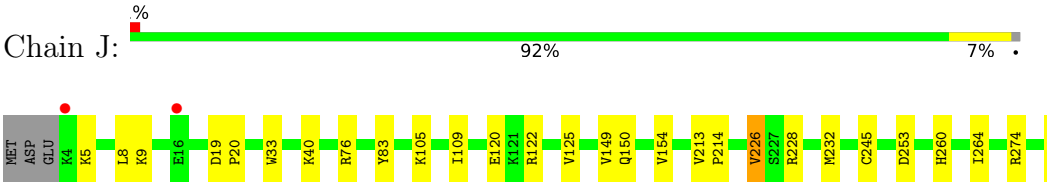
• Molecule 1: METHYL-COENZYME M REDUCTASE II SUBUNIT ALPHA

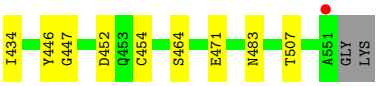
Chain G:



• Molecule 1: METHYL-COENZYME M REDUCTASE II SUBUNIT ALPHA

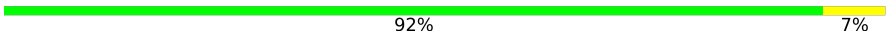
Chain J:

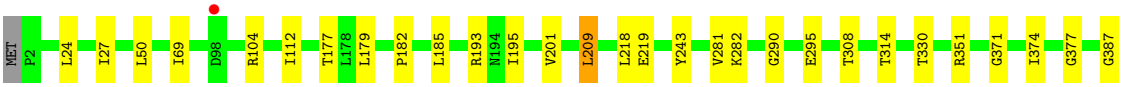




• Molecule 2: METHYL-COENZYME M REDUCTASE II SUBUNIT GAMMA

Chain B:

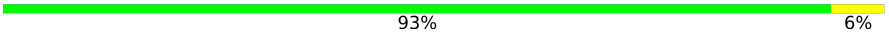


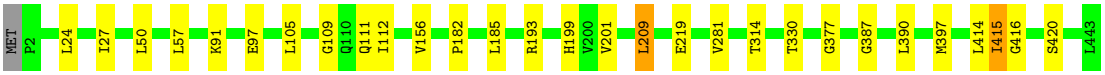




• Molecule 2: METHYL-COENZYME M REDUCTASE II SUBUNIT GAMMA

Chain E:

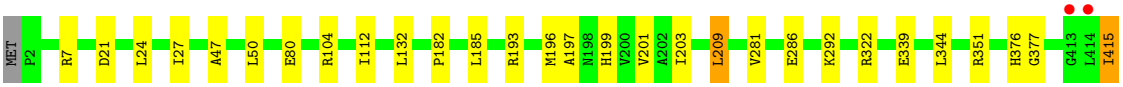


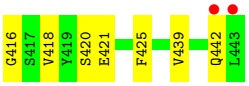


• Molecule 2: METHYL-COENZYME M REDUCTASE II SUBUNIT GAMMA

Chain H:

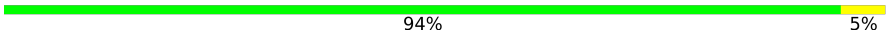


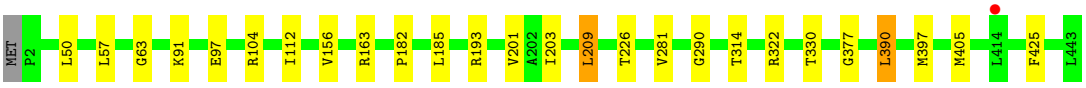




• Molecule 2: METHYL-COENZYME M REDUCTASE II SUBUNIT GAMMA

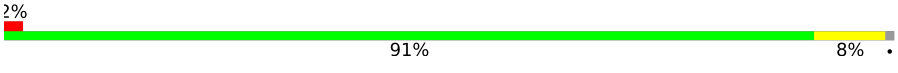
Chain K:

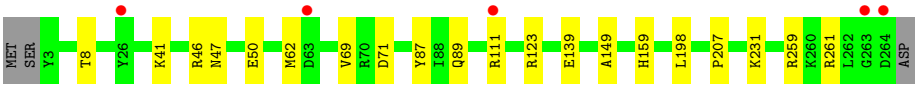




• Molecule 3: METHYL-COENZYME M REDUCTASE II, SUBUNIT BETA

Chain C:

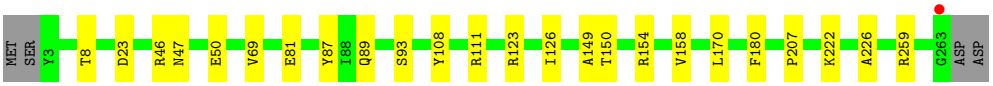




• Molecule 3: METHYL-COENZYME M REDUCTASE II, SUBUNIT BETA

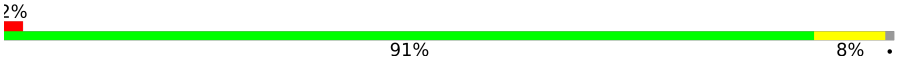
Chain F:

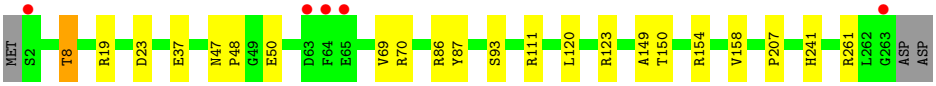




• Molecule 3: METHYL-COENZYME M REDUCTASE II, SUBUNIT BETA

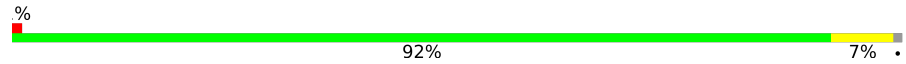
Chain I:

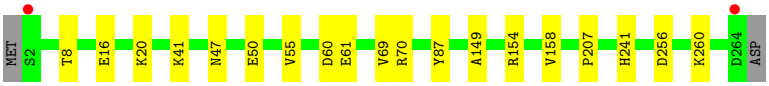




• Molecule 3: METHYL-COENZYME M REDUCTASE II, SUBUNIT BETA

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	216.66Å 246.61Å 103.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.36 – 2.15 55.36 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (55.36-2.15) 99.9 (55.36-2.15)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.14Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.156 , 0.196 0.158 , 0.195	Depositor DCC
R_{free} test set	15162 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 35.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	40798	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: F43, SMC, K, AGM, MHS, COM, TP7, MGN, DYA, GL3

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	0.39	0/4270	0.77	5/5779 (0.1%)
1	D	0.39	0/4270	0.77	3/5779 (0.1%)
1	G	0.37	0/4270	0.78	2/5779 (0.0%)
1	J	0.38	0/4276	0.77	4/5787 (0.1%)
2	B	0.37	0/3350	0.77	1/4552 (0.0%)
2	E	0.37	0/3350	0.77	0/4552
2	H	0.38	0/3350	0.77	0/4552
2	K	0.38	0/3350	0.78	1/4552 (0.0%)
3	C	0.36	0/2162	0.75	0/2913
3	F	0.37	0/2154	0.76	0/2902
3	I	0.34	0/2160	0.77	0/2910
3	L	0.36	0/2168	0.75	1/2921 (0.0%)
All	All	0.37	0/39130	0.77	17/52978 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	149	VAL	N-CA-C	7.80	118.27	111.56
1	G	149	VAL	N-CA-C	7.03	117.61	111.56
1	A	149	VAL	N-CA-C	6.82	117.42	111.56
1	J	149	VAL	N-CA-C	6.32	117.00	111.56
1	A	143	LEU	CA-C-N	-6.20	114.50	120.83
1	A	143	LEU	C-N-CA	-6.20	114.50	120.83
1	A	483	ASN	N-CA-C	5.58	118.57	109.59
2	B	290	GLY	N-CA-C	-5.49	106.95	114.64
1	J	483	ASN	N-CA-C	5.48	118.41	109.59
1	D	226	VAL	N-CA-C	5.45	115.66	110.53
2	K	290	GLY	N-CA-C	-5.41	107.06	114.64
1	G	226	VAL	N-CA-C	5.33	115.54	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	226	VAL	N-CA-C	5.29	115.50	110.53
1	J	150	GLN	N-CA-C	5.27	118.52	110.20
1	D	483	ASN	N-CA-C	5.07	117.66	109.40
3	L	55	VAL	N-CA-C	-5.05	107.91	112.96
1	A	65	VAL	N-CA-C	5.01	114.42	108.96

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	4235	0	4075	21	0
1	D	4235	0	4076	24	0
1	G	4235	0	4076	27	0
1	J	4238	0	4081	21	0
2	B	3296	0	3299	19	0
2	E	3296	0	3299	15	0
2	H	3296	0	3299	23	0
2	K	3296	0	3299	16	0
3	C	2122	0	2058	13	0
3	F	2114	0	2054	15	0
3	I	2120	0	2059	13	0
3	L	2128	0	2063	11	0
4	A	7	0	6	3	0
4	D	7	0	6	3	0
4	G	7	0	6	5	0
4	J	7	0	6	3	0
5	A	21	0	19	1	0
5	D	21	0	19	0	0
5	G	21	0	19	0	0
5	J	21	0	19	0	0
6	A	62	0	43	2	0
6	D	62	0	43	2	0
6	G	62	0	43	3	0
6	J	62	0	43	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
7	D	2	0	0	0	0
7	G	1	0	0	0	0
7	J	3	0	0	0	0
8	A	297	0	0	0	0
8	B	146	0	0	0	0
8	C	72	0	0	2	0
8	D	208	0	0	1	0
8	E	110	0	0	0	0
8	F	71	0	0	1	0
8	G	260	0	0	1	0
8	H	158	0	0	1	0
8	I	45	0	0	0	0
8	J	220	0	0	2	0
8	K	137	0	0	0	1
8	L	96	0	0	1	0
All	All	40798	0	38010	202	1

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 (202) 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)
3:F:47:ASN:N	3:F:50:GLU:OE2	2.05	0.87
2:K:91:LYS:NZ	2:K:97:GLU:OE2	2.09	0.86
3:L:256:ASP:OD1	3:L:260:LYS:NZ	2.15	0.79
3:F:46:ARG:HB2	3:F:50:GLU:OE2	1.83	0.77
2:H:281:VAL:HG21	2:H:344:LEU:HD11	1.73	0.70
2:E:91:LYS:NZ	2:E:97:GLU:OE2	2.24	0.69
2:H:209:LEU:HG	3:I:69:VAL:HG21	1.76	0.67
1:J:388:GLU:OE2	8:J:2160:HOH:O	2.12	0.67
1:G:22:GLU:HG3	1:G:24:TYR:H	1.60	0.67
3:C:46:ARG:HB2	3:C:50:GLU:OE2	1.94	0.67
3:C:231:LYS:NZ	8:C:2067:HOH:O	2.30	0.64
3:I:23:ASP:O	3:I:111:ARG:NH2	2.32	0.63
3:C:71:ASP:OD2	8:C:2016:HOH:O	2.15	0.62
1:D:5:LYS:HB2	1:D:8:LEU:HG	1.81	0.62
2:K:209:LEU:HG	3:L:69:VAL:HG21	1.80	0.61
3:C:47:ASN:N	3:C:50:GLU:OE2	2.26	0.61
3:F:47:ASN:O	3:F:50:GLU:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:149:ALA:HB2	3:L:207:PRO:HB3	1.83	0.60
2:B:209:LEU:HG	3:C:69:VAL:HG21	1.84	0.60
1:A:5:LYS:HB2	1:A:8:LEU:HG	1.82	0.59
2:B:282:LYS:NZ	2:B:295:GLU:OE2	2.36	0.59
1:A:288:THR:HG23	1:A:511:ILE:HD12	1.85	0.59
3:C:47:ASN:O	3:C:50:GLU:HG2	2.04	0.58
1:G:121:LYS:HD3	2:K:405:MET:HE1	1.86	0.58
2:K:50:LEU:HD11	2:K:112:ILE:HD11	1.86	0.57
2:B:50:LEU:HD11	2:B:112:ILE:HD11	1.87	0.56
1:G:434:ILE:HD11	3:I:241:HIS:HB2	1.88	0.56
1:J:76:ARG:NH1	1:J:343:ASP:OD2	2.38	0.56
3:I:87:TYR:CZ	1:J:245:CYS:HB2	2.41	0.56
2:E:111:GLN:HG2	2:E:414:LEU:HD11	1.88	0.56
1:J:122:ARG:NH1	1:J:253:ASP:OD2	2.40	0.55
2:E:209:LEU:HG	3:F:69:VAL:HG21	1.89	0.54
1:D:288:THR:HG23	1:D:511:ILE:HD12	1.88	0.54
2:K:314:THR:HA	2:K:330:THR:HG21	1.90	0.54
1:J:5:LYS:HB2	1:J:8:LEU:HG	1.90	0.54
1:D:228:ARG:O	1:D:232:MET:HG2	2.08	0.53
2:H:182:PRO:HB2	2:K:182:PRO:HB2	1.91	0.53
2:B:182:PRO:HA	2:B:185:LEU:HG	1.90	0.53
2:H:104:ARG:NH2	2:H:421:GLU:HG3	2.24	0.52
1:A:76:ARG:NH1	1:A:343:ASP:OD2	2.42	0.52
1:G:109:ILE:HB	1:G:264:ILE:HB	1.92	0.52
1:A:109:ILE:HB	1:A:264:ILE:HB	1.91	0.52
2:B:314:THR:HA	2:B:330:THR:HG21	1.92	0.52
4:G:601:COM:H22	6:G:603:F43:C6B	2.40	0.51
2:E:50:LEU:HD11	2:E:112:ILE:HD11	1.92	0.51
3:C:41:LYS:HG2	3:C:198:LEU:HD22	1.93	0.51
1:G:5:LYS:HB2	1:G:8:LEU:HG	1.93	0.50
1:D:359:LYS:NZ	8:D:2143:HOH:O	2.42	0.50
2:H:24:LEU:O	2:H:27:ILE:HG13	2.12	0.50
1:J:446:TYR:HB2	4:J:601:COM:O1S	2.12	0.50
4:J:601:COM:H22	6:J:603:F43:N5B	2.28	0.49
1:G:120:GLU:HG2	1:G:125:VAL:O	2.13	0.49
3:L:47:ASN:O	3:L:50:GLU:HG2	2.12	0.49
4:J:601:COM:H22	6:J:603:F43:C6B	2.42	0.49
3:F:149:ALA:HB2	3:F:207:PRO:HB3	1.95	0.49
2:B:219:GLU:HB3	2:B:387:GLY:HA2	1.95	0.49
2:E:314:THR:HA	2:E:330:THR:HG21	1.93	0.49
1:D:76:ARG:NH1	1:D:343:ASP:OD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HB2	1:A:83:TYR:CE2	2.48	0.49
2:B:104:ARG:NH1	2:B:421:GLU:HG3	2.28	0.48
1:D:446:TYR:HB2	4:D:601:COM:O2S	2.13	0.48
1:D:76:ARG:HB2	1:D:83:TYR:CE2	2.48	0.48
4:G:601:COM:H22	6:G:603:F43:N5B	2.29	0.48
2:K:57:LEU:HD21	2:K:156:VAL:HA	1.95	0.48
1:D:471:GLU:HB3	1:D:507:THR:HG22	1.96	0.48
3:F:154:ARG:HD3	3:F:158:VAL:HA	1.95	0.48
1:J:20:PRO:O	8:J:2008:HOH:O	2.20	0.48
1:D:22:GLU:HG3	1:D:24:TYR:H	1.79	0.48
2:H:50:LEU:HD11	2:H:112:ILE:HD11	1.95	0.48
1:G:76:ARG:HB2	1:G:83:TYR:CE2	2.49	0.48
2:H:439:VAL:O	2:H:442:GLN:HG2	2.13	0.48
2:E:57:LEU:HD21	2:E:156:VAL:HA	1.96	0.47
1:G:181:LYS:HE2	8:G:2090:HOH:O	2.14	0.47
2:H:322:ARG:NH2	3:I:70:ARG:HD2	2.29	0.47
3:I:87:TYR:CE1	1:J:245:CYS:HB2	2.50	0.47
1:A:333:THR:O	1:A:337:THR:HG23	2.14	0.47
3:C:87:TYR:CZ	1:D:245:CYS:HB2	2.49	0.47
2:E:416:GLY:O	2:E:420:SER:OG	2.27	0.47
2:H:416:GLY:O	2:H:420:SER:OG	2.20	0.47
3:I:8:THR:HG22	3:I:19:ARG:HG3	1.96	0.47
1:A:245:CYS:HB2	3:F:87:TYR:CZ	2.49	0.47
1:G:228:ARG:O	1:G:232:MET:HG2	2.14	0.47
1:A:446:TYR:HB2	4:A:601:COM:HOS3	1.80	0.47
2:E:105:LEU:HD22	2:E:109:GLY:HA2	1.97	0.47
3:F:170:LEU:HD11	3:F:180:PHE:HB2	1.97	0.47
1:A:446:TYR:HB2	4:A:601:COM:O3S	2.15	0.46
6:A:603:F43:CHC	4:D:601:COM:H12	2.45	0.46
2:H:7:ARG:NE	8:H:2007:HOH:O	2.45	0.46
3:I:149:ALA:HB2	3:I:207:PRO:HB3	1.98	0.46
1:J:109:ILE:HB	1:J:264:ILE:HB	1.96	0.46
1:J:434:ILE:HD11	3:L:241:HIS:HB2	1.97	0.46
1:G:376:SER:HB3	1:G:431:LEU:HD23	1.98	0.46
3:L:60:ASP:OD1	3:L:61:GLU:HG3	2.15	0.46
4:G:601:COM:H12	6:G:603:F43:CHC	2.46	0.46
2:B:195:ILE:HD12	2:B:218:LEU:HD13	1.98	0.46
2:B:405:MET:HE1	1:D:121:LYS:HD3	1.97	0.46
3:C:149:ALA:HB2	3:C:207:PRO:HB3	1.97	0.46
2:E:182:PRO:HA	2:E:185:LEU:HG	1.98	0.46
2:H:104:ARG:HH22	2:H:421:GLU:HG3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:120:GLU:HG2	1:J:125:VAL:O	2.16	0.46
1:A:228:ARG:O	1:A:232:MET:HG2	2.16	0.46
2:H:199:HIS:CG	2:H:415:ILE:HD12	2.51	0.46
1:A:376:SER:HB3	1:A:431:LEU:HD23	1.97	0.45
2:E:219:GLU:HB3	2:E:387:GLY:HA2	1.98	0.45
3:F:222:LYS:HA	3:F:226:ALA:HB2	1.96	0.45
2:B:182:PRO:HB2	2:E:182:PRO:HB2	1.98	0.45
1:G:333:THR:O	1:G:337:THR:HG23	2.15	0.45
1:G:443:LEU:HD23	1:G:449:ASP:HB3	1.99	0.45
2:B:193:ARG:HB3	2:B:377:GLY:HA3	1.98	0.45
2:H:286:GLU:HG2	2:H:292:LYS:HG2	1.99	0.45
2:K:201:VAL:HG21	2:K:397:MET:HB2	1.99	0.45
1:A:213:VAL:HG13	1:A:214:PRO:HD2	1.99	0.45
1:J:105:LYS:O	1:J:226:VAL:HG21	2.16	0.45
1:D:109:ILE:HB	1:D:264:ILE:HB	1.99	0.45
1:G:245:CYS:HB2	3:L:87:TYR:CZ	2.52	0.44
1:A:454:SMC:SG	2:B:351:ARG:HA	2.57	0.44
2:B:201:VAL:HG21	2:B:397:MET:HB2	1.98	0.44
1:A:327:SER:OG	1:A:328:GLY:N	2.49	0.44
2:H:132:LEU:HD13	2:K:226:THR:HA	1.99	0.44
2:H:203:ILE:CG2	2:H:425:PHE:HB3	2.48	0.44
2:H:47:ALA:HB2	2:H:418:VAL:HG11	2.00	0.44
3:F:81:GLU:O	8:F:2024:HOH:O	2.21	0.44
1:D:120:GLU:HG2	1:D:125:VAL:O	2.18	0.44
1:D:213:VAL:HG13	1:D:214:PRO:HD2	1.98	0.44
2:E:24:LEU:O	2:E:27:ILE:HG13	2.17	0.44
1:G:105:LYS:O	1:G:226:VAL:HG21	2.18	0.44
3:I:47:ASN:HB2	3:I:50:GLU:CD	2.42	0.44
2:H:7:ARG:HD3	2:H:21:ASP:OD1	2.18	0.44
1:A:270:MET:HA	1:A:270:MET:HE2	2.00	0.43
2:B:24:LEU:O	2:B:27:ILE:HG13	2.18	0.43
2:K:203:ILE:CG2	2:K:425:PHE:HB3	2.48	0.43
1:D:333:THR:O	1:D:337:THR:HG23	2.18	0.43
2:B:243:TYR:HB3	2:B:308:THR:OG1	2.18	0.43
1:G:76:ARG:NH1	1:G:343:ASP:OD2	2.51	0.43
1:G:446:TYR:HB2	4:G:601:COM:O2S	2.18	0.43
1:J:76:ARG:HB2	1:J:83:TYR:CE2	2.53	0.43
1:J:471:GLU:HB3	1:J:507:THR:HG22	2.01	0.43
1:J:19:ASP:HA	1:J:20:PRO:HD3	1.85	0.43
1:J:33:TRP:HZ3	1:J:40:LYS:HG2	1.83	0.43
1:G:471:GLU:HB3	1:G:507:THR:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:193:ARG:HB3	2:E:377:GLY:HA3	2.01	0.43
1:G:471:GLU:HB3	1:G:507:THR:HG22	1.99	0.43
3:F:93:SER:HB3	3:F:150:THR:HB	2.01	0.43
3:F:259:ARG:HD3	3:F:259:ARG:HA	1.62	0.43
3:C:89:GLN:OE1	3:C:123:ARG:HD2	2.19	0.43
2:K:193:ARG:HB3	2:K:377:GLY:HA3	2.01	0.43
1:A:120:GLU:HG2	1:A:125:VAL:O	2.19	0.42
1:G:122:ARG:NH1	1:G:253:ASP:OD2	2.50	0.42
1:G:445:PHE:HB2	4:G:601:COM:O2S	2.19	0.42
2:H:339:GLU:HG2	2:H:344:LEU:O	2.19	0.42
3:I:120:LEU:HD13	3:I:123:ARG:HG3	2.01	0.42
1:J:213:VAL:HG13	1:J:214:PRO:HD2	2.00	0.42
2:K:182:PRO:HA	2:K:185:LEU:HG	2.01	0.42
1:J:228:ARG:O	1:J:232:MET:HG2	2.19	0.42
3:L:154:ARG:HD3	3:L:158:VAL:HA	2.01	0.42
2:B:401:ALA:HB1	3:C:62:MET:HE1	2.00	0.42
2:E:199:HIS:CD2	2:E:415:ILE:HD12	2.54	0.42
3:I:37:GLU:HG3	3:I:48:PRO:HG2	2.01	0.42
1:D:471:GLU:HB3	1:D:507:THR:CG2	2.50	0.42
1:G:270:MET:HE2	1:G:270:MET:HA	2.01	0.42
3:I:154:ARG:HD3	3:I:158:VAL:HA	2.01	0.42
2:K:104:ARG:HE	2:K:104:ARG:HB3	1.50	0.42
1:D:498:HIS:HB3	1:D:503:ASP:HB2	2.02	0.42
1:A:330:VAL:HB	6:D:603:F43:H9A1	2.00	0.42
2:H:196:MET:HA	2:H:376:HIS:HB3	2.02	0.42
3:L:41:LYS:HE3	8:L:2077:HOH:O	2.19	0.42
1:A:171:GLY:HA3	1:A:204:GLY:O	2.19	0.41
1:D:376:SER:HB3	1:D:431:LEU:HD23	2.02	0.41
2:K:63:GLY:HA2	2:K:163:ARG:HG3	2.02	0.41
1:G:119:LEU:HD23	1:G:123:LEU:HD12	2.02	0.41
1:G:546:ASP:HA	1:G:549:ILE:HG12	2.03	0.41
2:B:371:GLY:O	2:B:374:ILE:HG13	2.20	0.41
1:D:105:LYS:O	1:D:226:VAL:HG21	2.20	0.41
1:D:143:LEU:HB3	1:D:144:PRO:HD3	2.03	0.41
2:K:390:LEU:HD13	2:K:390:LEU:HA	1.88	0.41
5:A:602:TP7:H32C	1:D:482:MET:O	2.20	0.41
1:D:270:MET:HA	1:D:270:MET:HE2	2.02	0.41
3:F:23:ASP:O	3:F:111:ARG:NH2	2.53	0.41
1:G:143:LEU:HB3	1:G:144:PRO:HD3	2.02	0.41
2:B:69:ILE:HD11	1:D:472:LEU:HD13	2.03	0.41
1:G:477:TYR:HA	1:G:478:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:182:PRO:HA	2:H:185:LEU:HG	2.02	0.41
3:I:93:SER:HB3	3:I:150:THR:HB	2.03	0.41
1:A:98:GLN:OE1	1:D:545:ARG:HD3	2.21	0.41
3:F:89:GLN:OE1	3:F:123:ARG:HD2	2.20	0.41
3:C:111:ARG:NE	3:C:139:GLU:OE2	2.54	0.41
1:G:86:GLY:HA3	1:J:154:VAL:HG11	2.03	0.41
2:H:193:ARG:HB3	2:H:377:GLY:HA3	2.03	0.40
2:K:322:ARG:NH2	3:L:70:ARG:HD2	2.37	0.40
1:A:398:PHE:CD1	3:C:159:HIS:HE1	2.40	0.40
4:A:601:COM:H12	6:D:603:F43:C1C	2.51	0.40
2:B:177:THR:OG1	2:B:179:LEU:O	2.37	0.40
3:F:108:TYR:CZ	3:F:126:ILE:HD11	2.57	0.40
1:J:9:LYS:HE3	1:J:9:LYS:HB2	1.77	0.40
6:J:603:F43:HN5	6:J:603:F43:H4A	1.75	0.40
6:A:603:F43:C6B	4:D:601:COM:H22	2.51	0.40
2:H:197:ALA:O	2:H:201:VAL:HG23	2.21	0.40
1:J:471:GLU:HB3	1:J:507:THR:CG2	2.52	0.40
3:L:16:GLU:O	3:L:20:LYS:HG3	2.21	0.40
1:A:129:PRO:HG2	1:A:178:GLU:OE1	2.20	0.40
2:E:201:VAL:HG21	2:E:397:MET:HB2	2.03	0.40
1:G:454:SMC:SG	2:H:351:ARG:HA	2.61	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:2104:HOH:O	8:K:2104:HOH:O[2_555]	2.04	0.16

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	540/553 (98%)	521 (96%)	18 (3%)	1 (0%)	43	44
1	D	540/553 (98%)	521 (96%)	17 (3%)	2 (0%)	30	26
1	G	540/553 (98%)	521 (96%)	18 (3%)	1 (0%)	43	44
1	J	541/553 (98%)	522 (96%)	18 (3%)	1 (0%)	43	44
2	B	440/443 (99%)	433 (98%)	7 (2%)	0	100	100
2	E	440/443 (99%)	432 (98%)	8 (2%)	0	100	100
2	H	440/443 (99%)	432 (98%)	8 (2%)	0	100	100
2	K	440/443 (99%)	431 (98%)	9 (2%)	0	100	100
3	C	260/265 (98%)	253 (97%)	7 (3%)	0	100	100
3	F	259/265 (98%)	252 (97%)	7 (3%)	0	100	100
3	I	260/265 (98%)	253 (97%)	7 (3%)	0	100	100
3	L	261/265 (98%)	254 (97%)	7 (3%)	0	100	100
All	All	4961/5044 (98%)	4825 (97%)	131 (3%)	5 (0%)	48	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	464	SER
1	D	464	SER
1	G	464	SER
1	J	464	SER
1	D	327	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/434 (99%)	429 (100%)	1 (0%)	87	92
1	D	430/434 (99%)	429 (100%)	1 (0%)	87	92
1	G	430/434 (99%)	429 (100%)	1 (0%)	87	92
1	J	431/434 (99%)	431 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	344/345 (100%)	342 (99%)	2 (1%)	78 84
2	E	344/345 (100%)	340 (99%)	4 (1%)	63 70
2	H	344/345 (100%)	341 (99%)	3 (1%)	70 77
2	K	344/345 (100%)	341 (99%)	3 (1%)	70 77
3	C	228/231 (99%)	225 (99%)	3 (1%)	61 68
3	F	227/231 (98%)	226 (100%)	1 (0%)	84 89
3	I	228/231 (99%)	225 (99%)	3 (1%)	61 68
3	L	229/231 (99%)	228 (100%)	1 (0%)	84 89
All	All	4009/4040 (99%)	3986 (99%)	23 (1%)	78 84

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	511	ILE
2	B	209	LEU
2	B	281	VAL
3	C	8	THR
3	C	259	ARG
3	C	261	ARG
1	D	511	ILE
2	E	209	LEU
2	E	281	VAL
2	E	390	LEU
2	E	415	ILE
3	F	8	THR
1	G	446	TYR
2	H	80	GLU
2	H	209	LEU
2	H	415	ILE
3	I	8	THR
3	I	86	ARG
3	I	261	ARG
2	K	209	LEU
2	K	281	VAL
2	K	390	LEU
3	L	8	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
2	B	37	ASN
2	B	102	ASN
1	D	487	GLN
2	E	37	ASN
1	G	304	ASN
1	G	458	ASN
1	G	479	ASN
2	H	37	ASN
2	H	431	ASN
3	I	13	GLN
1	J	304	ASN
2	K	37	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

24 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	GL3	G	447	1	2,3,4	5.79	1 (50%)	1,2,4	0.11	0
1	DYA	J	452	1	7,7,8	1.51	2 (28%)	5,8,10	2.30	2 (40%)
1	MHS	A	260	1	10,11,12	1.71	2 (20%)	6,14,16	1.37	1 (16%)
1	SMC	J	454	1	5,6,7	1.18	1 (20%)	2,6,8	0.87	0
1	SMC	D	454	1	5,6,7	1.41	1 (20%)	2,6,8	1.76	1 (50%)
1	MGN	D	402	1	6,9,10	0.92	0	5,12,14	0.72	0
1	MHS	D	260	1	10,11,12	1.77	2 (20%)	6,14,16	1.48	2 (33%)
1	MHS	G	260	1	10,11,12	1.68	1 (10%)	6,14,16	1.83	2 (33%)
1	AGM	J	274	1	10,11,12	1.25	1 (10%)	6,13,15	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	AGM	D	274	1	10,11,12	1.27	1 (10%)	6,13,15	0.92	0
1	GL3	A	447	1	2,3,4	5.53	1 (50%)	1,2,4	0.26	0
1	SMC	A	454	1	5,6,7	1.52	1 (20%)	2,6,8	2.59	1 (50%)
1	DYA	D	452	1	7,7,8	1.51	1 (14%)	5,8,10	2.58	2 (40%)
1	MHS	J	260	1	10,11,12	1.72	2 (20%)	6,14,16	1.42	2 (33%)
1	AGM	G	274	1	10,11,12	1.37	1 (10%)	6,13,15	1.06	0
1	DYA	A	452	1	7,7,8	1.45	1 (14%)	5,8,10	2.52	2 (40%)
1	GL3	D	447	1	2,3,4	4.98	1 (50%)	1,2,4	0.13	0
1	MGN	A	402	1	6,9,10	0.87	0	5,12,14	0.98	0
1	AGM	A	274	1	10,11,12	1.29	1 (10%)	6,13,15	0.79	0
1	DYA	G	452	1	7,7,8	1.50	1 (14%)	5,8,10	2.47	2 (40%)
1	GL3	J	447	1	2,3,4	4.80	1 (50%)	1,2,4	0.30	0
1	SMC	G	454	1	5,6,7	1.25	1 (20%)	2,6,8	1.16	0
1	MGN	J	402	1	6,9,10	0.87	0	5,12,14	0.95	0
1	MGN	G	402	1	6,9,10	0.88	0	5,12,14	0.74	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	GL3	G	447	1	-	1/1/1/2	-
1	DYA	J	452	1	-	3/4/6/8	-
1	MHS	A	260	1	-	0/5/6/8	0/1/1/1
1	SMC	J	454	1	-	1/3/5/7	-
1	SMC	D	454	1	-	1/3/5/7	-
1	MGN	D	402	1	-	0/7/9/12	-
1	MHS	D	260	1	-	0/5/6/8	0/1/1/1
1	MHS	G	260	1	-	0/5/6/8	0/1/1/1
1	AGM	J	274	1	-	1/10/11/13	-
1	AGM	D	274	1	-	1/10/11/13	-
1	GL3	A	447	1	-	1/1/1/2	-
1	SMC	A	454	1	-	1/3/5/7	-
1	DYA	D	452	1	-	3/4/6/8	-
1	MHS	J	260	1	-	0/5/6/8	0/1/1/1
1	AGM	G	274	1	-	2/10/11/13	-
1	DYA	A	452	1	-	3/4/6/8	-
1	GL3	D	447	1	-	1/1/1/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MGN	A	402	1	-	0/7/9/12	-
1	AGM	A	274	1	-	0/10/11/13	-
1	DYA	G	452	1	-	3/4/6/8	-
1	GL3	J	447	1	-	1/1/1/2	-
1	SMC	G	454	1	-	1/3/5/7	-
1	MGN	J	402	1	-	0/7/9/12	-
1	MGN	G	402	1	-	0/7/9/12	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	447	GL3	C-S	-8.19	1.52	1.80
1	A	447	GL3	C-S	-7.81	1.53	1.80
1	D	447	GL3	C-S	-7.05	1.56	1.80
1	J	447	GL3	C-S	-6.79	1.57	1.80
1	D	260	MHS	CD2-CG	3.67	1.41	1.36
1	A	260	MHS	CD2-CG	3.53	1.41	1.36
1	G	260	MHS	CD2-CG	3.45	1.41	1.36
1	J	260	MHS	CD2-CG	3.43	1.41	1.36
1	G	274	AGM	CZ-NE1	3.29	1.38	1.33
1	A	454	SMC	CB-SG	-3.07	1.76	1.80
1	J	274	AGM	CZ-NE1	2.94	1.38	1.33
1	D	274	AGM	CZ-NE1	2.92	1.38	1.33
1	A	274	AGM	CZ-NE1	2.91	1.38	1.33
1	G	452	DYA	CA-N	2.82	1.42	1.35
1	J	452	DYA	CA-N	2.79	1.42	1.35
1	D	452	DYA	CA-N	2.79	1.42	1.35
1	D	454	SMC	CB-SG	-2.71	1.77	1.80
1	A	452	DYA	CA-N	2.52	1.41	1.35
1	G	454	SMC	CB-SG	-2.34	1.77	1.80
1	J	260	MHS	CG-ND1	2.08	1.41	1.38
1	A	260	MHS	CG-ND1	2.06	1.41	1.38
1	J	452	DYA	OD1-CG	-2.06	1.25	1.30
1	D	260	MHS	CG-ND1	2.06	1.41	1.38
1	J	454	SMC	CB-SG	-2.03	1.78	1.80

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	452	DYA	O-C-CA	-4.12	120.15	125.39
1	G	452	DYA	O-C-CA	-3.93	120.39	125.39
1	A	452	DYA	CA-CB-CG	-3.80	117.59	126.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	454	SMC	CA-CB-SG	-3.65	108.14	114.04
1	J	452	DYA	O-C-CA	-3.45	121.01	125.39
1	A	452	DYA	O-C-CA	-3.18	121.34	125.39
1	G	452	DYA	CA-CB-CG	-3.17	119.12	126.82
1	G	260	MHS	CB-CA-C	-3.16	105.55	111.47
1	D	452	DYA	CA-CB-CG	-3.15	119.16	126.82
1	J	452	DYA	CA-CB-CG	-2.99	119.55	126.82
1	G	260	MHS	ND1-CE1-NE2	-2.88	111.25	112.93
1	D	260	MHS	ND1-CE1-NE2	-2.79	111.30	112.93
1	A	260	MHS	ND1-CE1-NE2	-2.70	111.35	112.93
1	J	260	MHS	ND1-CE1-NE2	-2.57	111.42	112.93
1	D	454	SMC	CA-CB-SG	-2.47	110.04	114.04
1	J	260	MHS	CB-CA-C	-2.07	107.60	111.47
1	D	260	MHS	CB-CA-C	-2.00	107.71	111.47

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	452	DYA	O-C-CA-CB
1	A	452	DYA	CA-CB-CG-OD2
1	A	454	SMC	CA-CB-SG-CS
1	D	452	DYA	O-C-CA-CB
1	D	452	DYA	CA-CB-CG-OD1
1	D	454	SMC	CA-CB-SG-CS
1	G	452	DYA	O-C-CA-CB
1	G	452	DYA	CA-CB-CG-OD1
1	G	452	DYA	CA-CB-CG-OD2
1	G	454	SMC	CA-CB-SG-CS
1	J	452	DYA	O-C-CA-CB
1	J	452	DYA	CA-CB-CG-OD1
1	J	454	SMC	CA-CB-SG-CS
1	A	452	DYA	CA-CB-CG-OD1
1	D	452	DYA	CA-CB-CG-OD2
1	J	452	DYA	CA-CB-CG-OD2
1	G	447	GL3	S-C-CA-N
1	A	447	GL3	S-C-CA-N
1	D	447	GL3	S-C-CA-N
1	D	274	AGM	NE1-CD-CG-CB
1	J	447	GL3	S-C-CA-N
1	G	274	AGM	NE1-CD-CG-CB
1	G	274	AGM	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	J	274	AGM	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	454	SMC	1	0
1	G	454	SMC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 7 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
5	TP7	A	602	-	19,20,20	0.64	0	24,26,26	0.91	1 (4%)
6	F43	A	603	1	61,71,71	2.09	5 (8%)	64,118,118	1.40	11 (17%)
4	COM	A	601	-	6,6,6	1.42	2 (33%)	7,8,8	2.67	4 (57%)
5	TP7	D	602	-	19,20,20	0.65	0	24,26,26	0.93	0
5	TP7	G	602	-	19,20,20	0.63	0	24,26,26	1.00	1 (4%)
5	TP7	J	602	-	19,20,20	0.66	0	24,26,26	0.88	1 (4%)
4	COM	G	601	-	6,6,6	1.37	2 (33%)	7,8,8	2.97	3 (42%)
6	F43	D	603	1	61,71,71	2.08	5 (8%)	64,118,118	1.35	9 (14%)
4	COM	J	601	-	6,6,6	1.31	2 (33%)	7,8,8	2.81	4 (57%)
6	F43	J	603	1	61,71,71	2.05	6 (9%)	64,118,118	1.41	9 (14%)
6	F43	G	603	1	61,71,71	2.04	5 (8%)	64,118,118	1.34	11 (17%)
4	COM	D	601	-	6,6,6	1.40	2 (33%)	7,8,8	2.66	3 (42%)

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
5	TP7	A	602	-	-	1/24/24/24	-
6	F43	A	603	1	-	8/28/185/185	-
4	COM	A	601	-	-	0/4/4/4	-
5	TP7	D	602	-	-	1/24/24/24	-
5	TP7	G	602	-	-	3/24/24/24	-
5	TP7	J	602	-	-	1/24/24/24	-
4	COM	G	601	-	-	0/4/4/4	-
6	F43	D	603	1	-	6/28/185/185	-
4	COM	J	601	-	-	1/4/4/4	-
6	F43	J	603	1	-	8/28/185/185	-
6	F43	G	603	1	-	5/28/185/185	-
4	COM	D	601	-	-	0/4/4/4	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	F43	NI-NA	7.82	2.06	1.89
6	D	603	F43	NI-NA	7.78	2.06	1.89
6	G	603	F43	NI-NA	7.69	2.06	1.89
6	J	603	F43	NI-NA	7.50	2.05	1.89
6	A	603	F43	NI-NB	7.50	2.05	1.89
6	D	603	F43	NI-NB	7.49	2.05	1.89
6	J	603	F43	NI-NB	7.28	2.05	1.89
6	G	603	F43	NI-NB	7.02	2.04	1.89
6	A	603	F43	NI-ND	6.90	2.04	1.89
6	J	603	F43	CHD-C1D	-6.72	1.34	1.43
6	A	603	F43	CHD-C1D	-6.70	1.34	1.43
6	G	603	F43	NI-ND	6.68	2.03	1.89
6	D	603	F43	CHD-C1D	-6.56	1.34	1.43
6	D	603	F43	NI-ND	6.47	2.03	1.89
6	G	603	F43	CHD-C1D	-6.47	1.34	1.43
6	J	603	F43	NI-ND	6.10	2.02	1.89
6	A	603	F43	CHC-C4B	2.94	1.47	1.39
6	D	603	F43	CHC-C4B	2.87	1.47	1.39
6	J	603	F43	CHC-C4B	2.85	1.47	1.39
6	G	603	F43	CHC-C4B	2.73	1.46	1.39
4	A	601	COM	O1S-S2	2.47	1.52	1.45
6	J	603	F43	CHB-C1B	-2.18	1.51	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	601	COM	O1S-S2	2.14	1.51	1.45
4	D	601	COM	O2S-S2	2.14	1.51	1.45
4	D	601	COM	O1S-S2	2.10	1.51	1.45
4	A	601	COM	O2S-S2	2.08	1.51	1.45
4	G	601	COM	O2S-S2	2.05	1.51	1.45
4	J	601	COM	O2S-S2	2.04	1.51	1.45
4	J	601	COM	O1S-S2	2.03	1.51	1.45

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	601	COM	O1S-S2-C2	5.97	114.10	106.92
4	A	601	COM	O2S-S2-C2	4.86	112.77	106.92
4	J	601	COM	O2S-S2-C2	4.84	112.74	106.92
4	D	601	COM	O1S-S2-C2	4.74	112.62	106.92
6	J	603	F43	O7B-C6B-C8B	-4.15	121.53	126.59
6	D	603	F43	O7B-C6B-C8B	-3.83	121.91	126.59
6	G	603	F43	O7B-C6B-C8B	-3.75	122.01	126.59
4	D	601	COM	O2S-S2-O1S	-3.67	101.25	113.95
6	D	603	F43	CAB-C3B-C2B	-3.64	111.39	119.09
6	A	603	F43	O7B-C6B-C8B	-3.63	122.16	126.59
4	G	601	COM	O2S-S2-O1S	-3.59	101.53	113.95
6	J	603	F43	CAB-C3B-C2B	-3.51	111.67	119.09
6	A	603	F43	O8D-C7D-C6D	-3.43	115.24	120.86
4	J	601	COM	O3S-S2-O1S	-3.40	102.97	111.27
6	J	603	F43	O8D-C7D-C6D	-3.37	115.34	120.86
4	A	601	COM	O2S-S2-O1S	-3.17	102.98	113.95
6	A	603	F43	CAB-C3B-C2B	-3.16	112.41	119.09
4	J	601	COM	O1S-S2-C2	3.15	110.71	106.92
6	G	603	F43	CAB-C3B-C2B	-3.05	112.63	119.09
4	D	601	COM	O2S-S2-C2	3.01	110.54	106.92
6	D	603	F43	O8D-C7D-C6D	-2.96	116.02	120.86
6	A	603	F43	C6D-C5D-C2D	-2.87	105.67	111.46
4	A	601	COM	O3S-S2-C2	2.84	110.36	105.77
6	G	603	F43	O8D-C7D-C6D	-2.78	116.30	120.86
6	A	603	F43	C9A-C2A-C3A	2.74	117.03	112.98
4	G	601	COM	O3S-S2-C2	2.60	109.97	105.77
6	G	603	F43	C4D-ND-C1D	2.57	111.89	108.51
6	D	603	F43	C2B-C1B-NB	2.55	105.65	101.84
6	J	603	F43	C4D-ND-C1D	2.47	111.77	108.51
6	D	603	F43	C9A-C2A-C3A	2.44	116.58	112.98
6	G	603	F43	C9A-C2A-C3A	2.37	116.48	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	601	COM	O3S-S2-C2	2.37	109.60	105.77
6	D	603	F43	ODA-CCA-CBA	2.33	121.53	114.03
6	J	603	F43	C9A-C2A-C3A	2.28	116.35	112.98
6	D	603	F43	C4D-ND-C1D	2.26	111.48	108.51
6	A	603	F43	C4D-ND-C1D	2.25	111.47	108.51
6	J	603	F43	C6D-C7D-CHD	2.22	121.12	116.95
6	G	603	F43	ODA-CCA-CBA	2.20	121.11	114.03
6	A	603	F43	OEA-CCA-CBA	-2.16	116.13	123.08
6	G	603	F43	C6D-C5D-C2D	-2.16	107.10	111.46
6	D	603	F43	C5D-C6D-C7D	-2.15	107.90	113.55
6	D	603	F43	OEA-CCA-CBA	-2.13	116.22	123.08
6	A	603	F43	ODA-CCA-CBA	2.13	120.87	114.03
6	J	603	F43	ODA-CCA-CBA	2.13	120.87	114.03
6	A	603	F43	C1B-C2B-C3B	2.12	104.65	101.51
6	J	603	F43	C2B-C1B-NB	2.11	105.00	101.84
6	J	603	F43	C1B-C2B-C3B	2.10	104.62	101.51
6	A	603	F43	C2B-C1B-NB	2.10	104.98	101.84
6	G	603	F43	OBC-CAC-C9C	2.10	120.78	114.03
5	A	602	TP7	O3P-P-O2P	2.09	115.63	107.64
4	A	601	COM	O1S-S2-C2	2.09	109.43	106.92
6	G	603	F43	C5D-C6D-C7D	-2.07	108.11	113.55
6	G	603	F43	OEA-CCA-CBA	-2.05	116.48	123.08
5	J	602	TP7	O4P-P-O1P	-2.03	101.55	109.39
6	G	603	F43	C2B-C1B-NB	2.02	104.87	101.84
5	G	602	TP7	O4P-P-O1P	-2.01	101.64	109.39
6	A	603	F43	OCD-CAD-C9D	2.00	120.49	114.07

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	TP7	C2-C3-C4-C5
5	D	602	TP7	C2-C3-C4-C5
4	J	601	COM	C1-C2-S2-O3S
6	G	603	F43	C2C-C5C-C6C-O7C
6	G	603	F43	C2C-C5C-C6C-O8C
5	G	602	TP7	O1-C1-N-CA
5	J	602	TP7	C2-C3-C4-C5
6	J	603	F43	C2C-C5C-C6C-O7C
6	J	603	F43	C2C-C5C-C6C-O8C
6	J	603	F43	CAB-CBB-CCB-OEB
6	A	603	F43	C8C-C9C-CAC-OBC

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Mol	Chain	Res	Type	Atoms
6	J	603	F43	CAB-CBB-CCB-ODB
6	A	603	F43	CAB-CBB-CCB-OEB
6	A	603	F43	C8C-C9C-CAC-OCC
6	A	603	F43	CAB-CBB-CCB-ODB
6	A	603	F43	C3A-CAA-CBA-CCA
6	D	603	F43	CAB-CBB-CCB-OEB
6	J	603	F43	C8C-C9C-CAC-OBC
6	G	603	F43	CAB-CBB-CCB-OEB
6	D	603	F43	CAB-CBB-CCB-ODB
6	G	603	F43	CAB-CBB-CCB-ODB
6	J	603	F43	C8C-C9C-CAC-OCC
6	A	603	F43	CAA-CBA-CCA-ODA
6	D	603	F43	C3D-C9D-CAD-OCD
6	J	603	F43	C3D-C9D-CAD-OCD
5	G	602	TP7	C2-C3-C4-C5
6	A	603	F43	CAA-CBA-CCA-OEA
6	A	603	F43	C3D-C9D-CAD-OBD
6	D	603	F43	C3D-C9D-CAD-OBD
6	J	603	F43	C3D-C9D-CAD-OBD
5	G	602	TP7	C2-C1-N-CA
6	D	603	F43	CAA-CBA-CCA-ODA
6	D	603	F43	CAA-CBA-CCA-OEA
6	G	603	F43	C8C-C9C-CAC-OBC

There are no ring outliers.

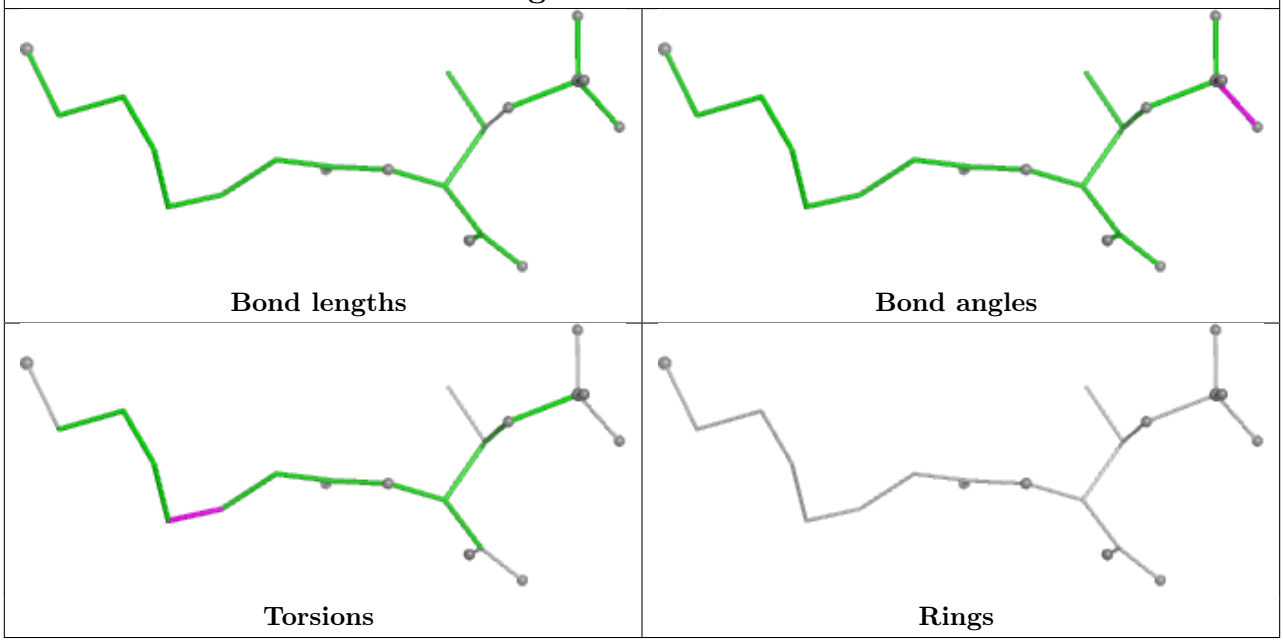
9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	TP7	1	0
6	A	603	F43	2	0
4	A	601	COM	3	0
4	G	601	COM	5	0
6	D	603	F43	2	0
4	J	601	COM	3	0
6	J	603	F43	3	0
6	G	603	F43	3	0
4	D	601	COM	3	0

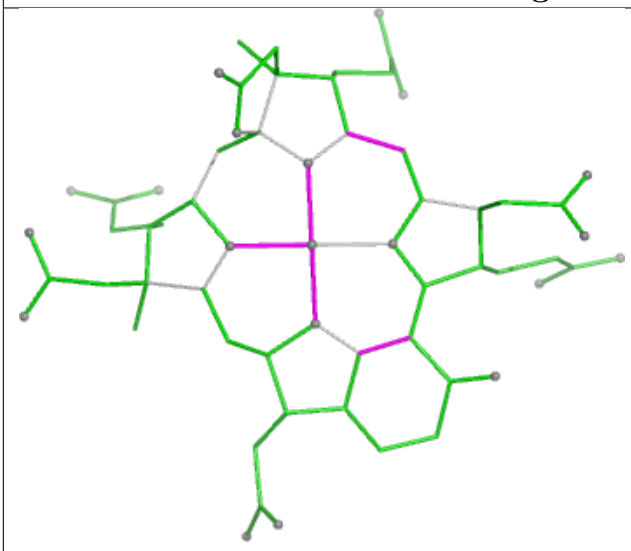
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

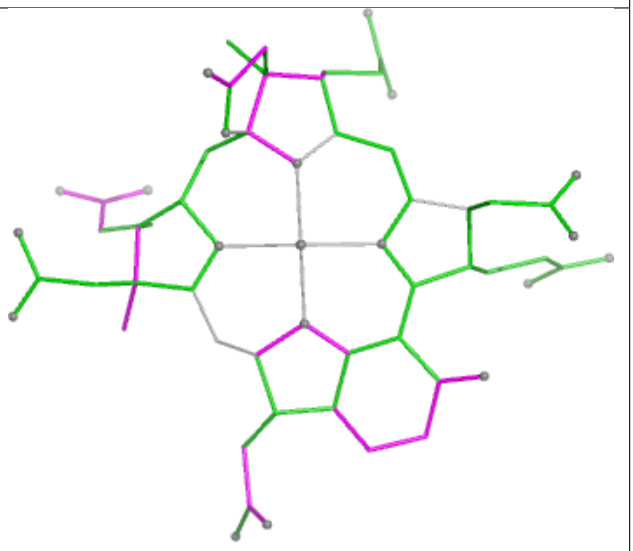
Ligand TP7 A 602



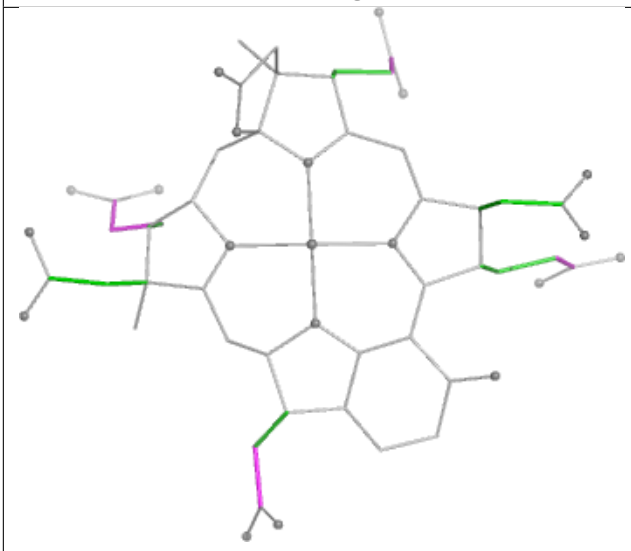
Ligand F43 A 603



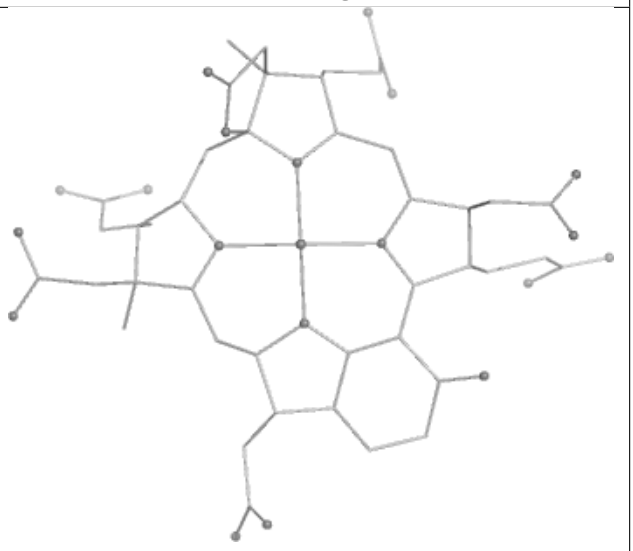
Bond lengths



Bond angles

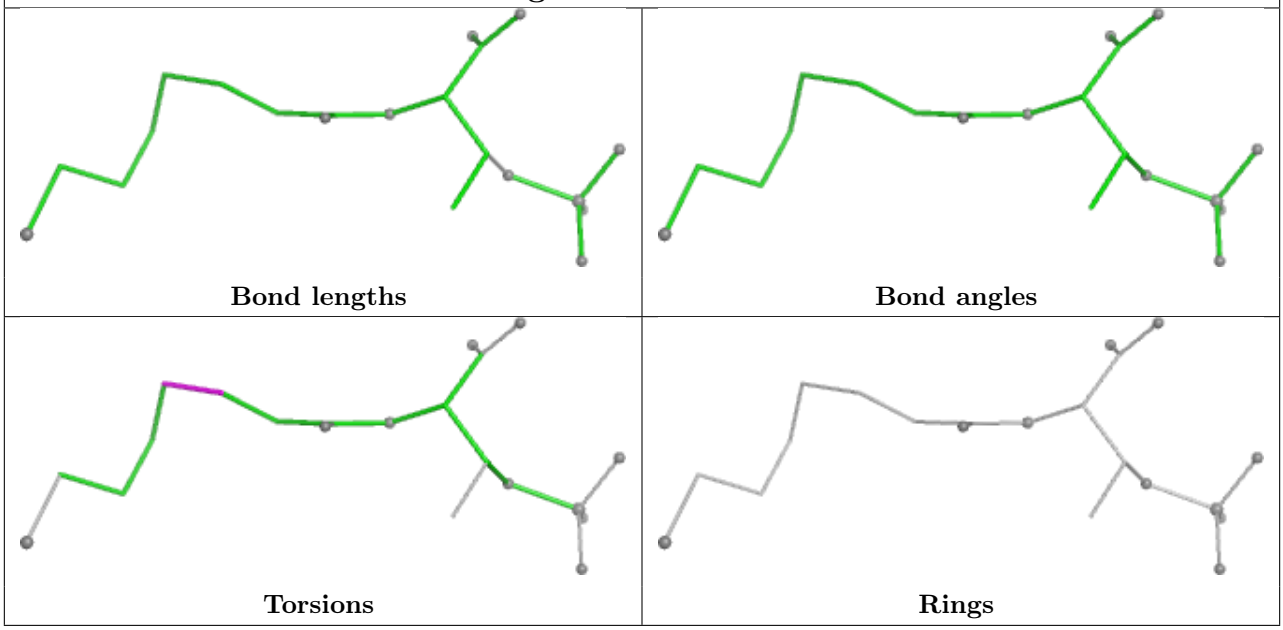


Torsions

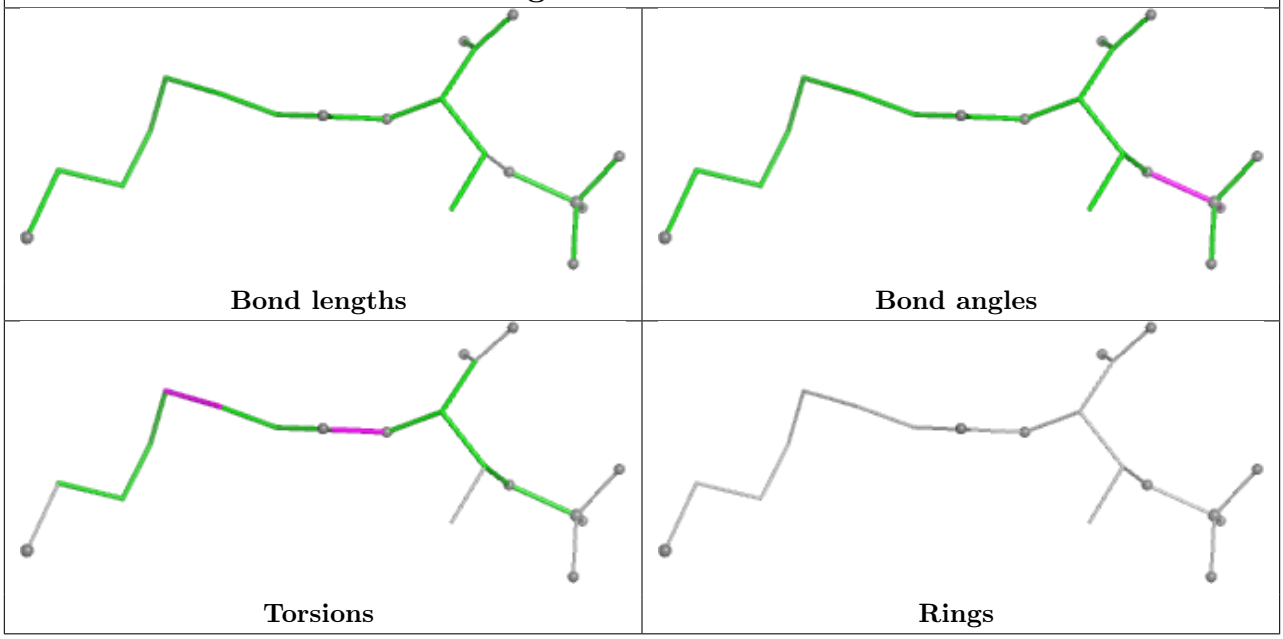


Rings

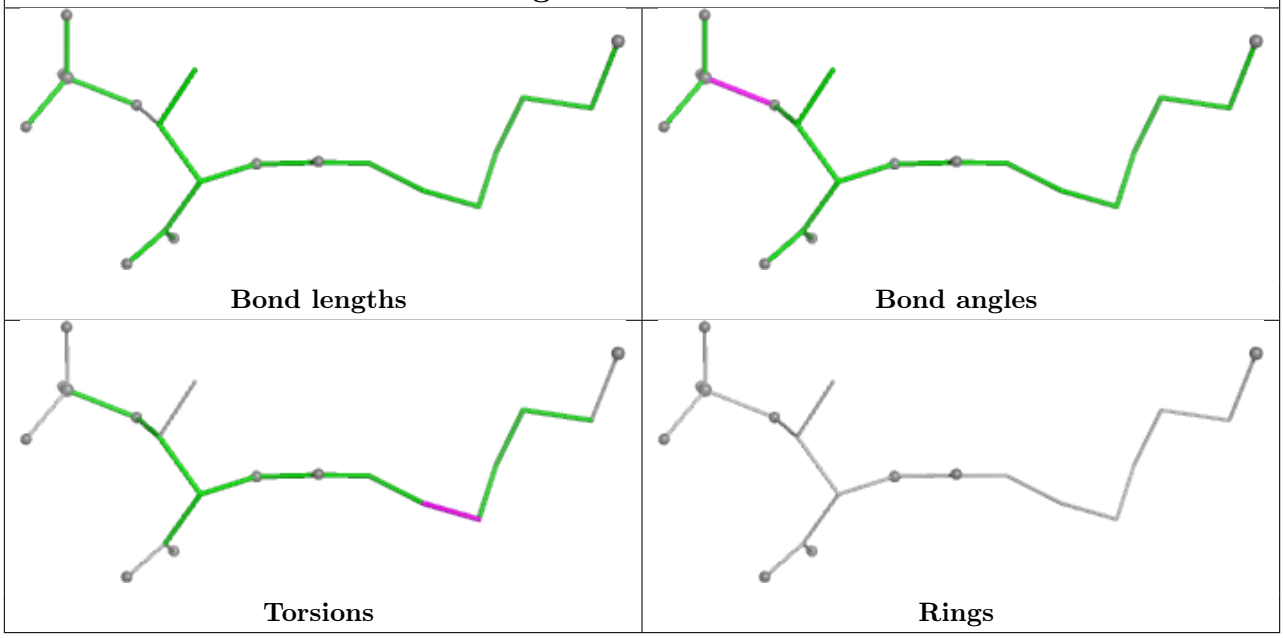
Ligand TP7 D 602



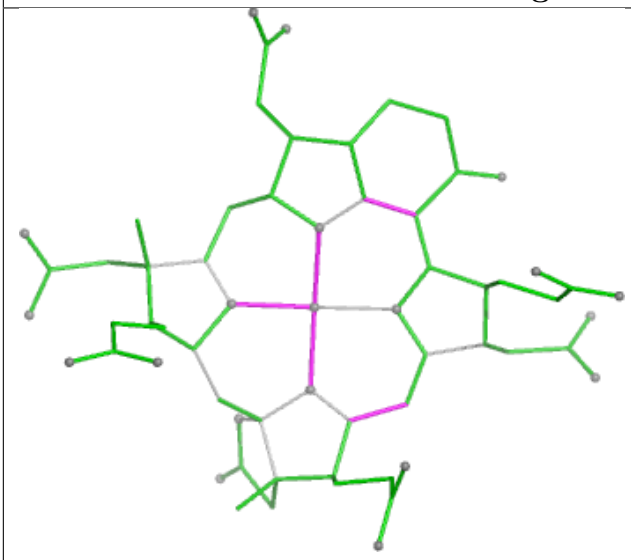
Ligand TP7 G 602



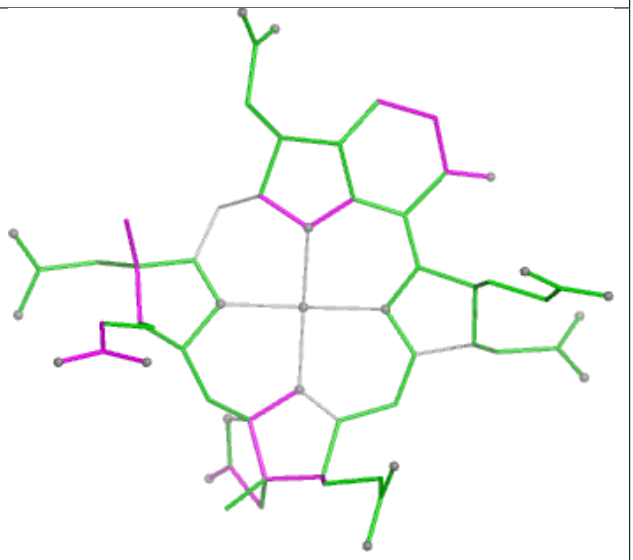
Ligand TP7 J 602



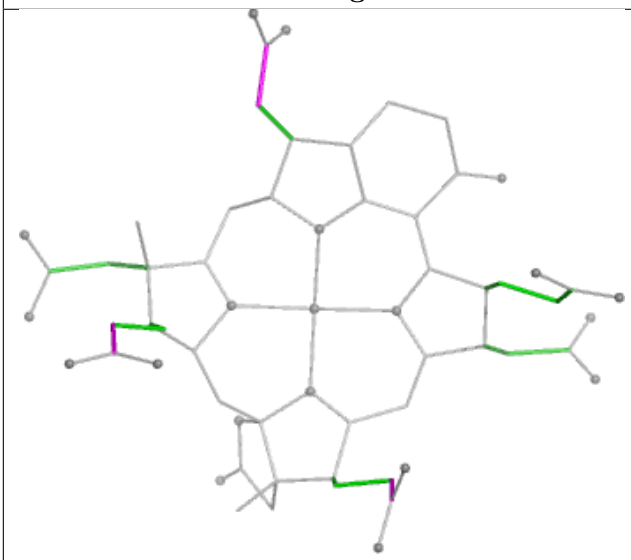
Ligand F43 D 603



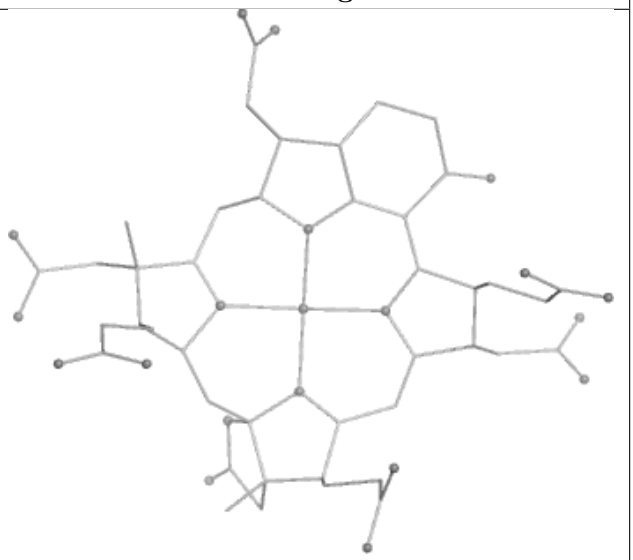
Bond lengths



Bond angles

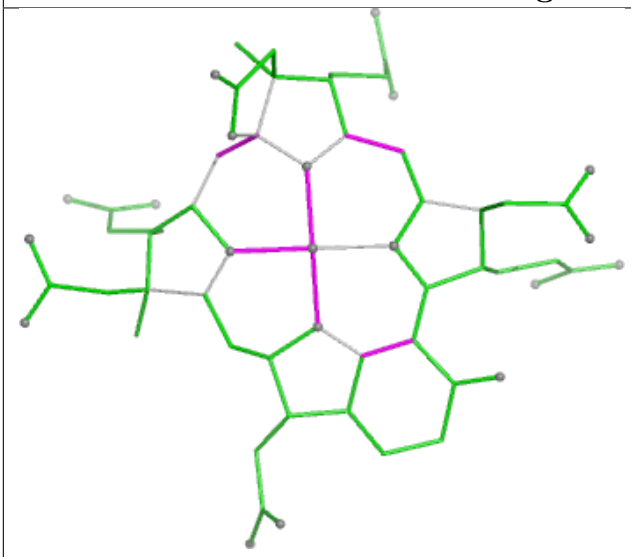


Torsions

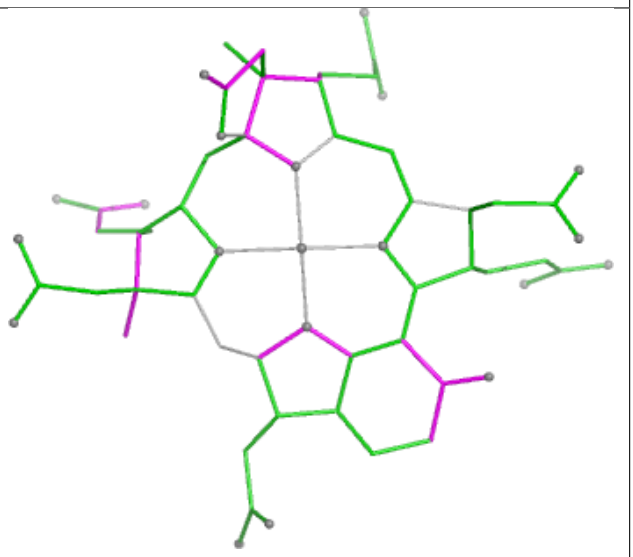


Rings

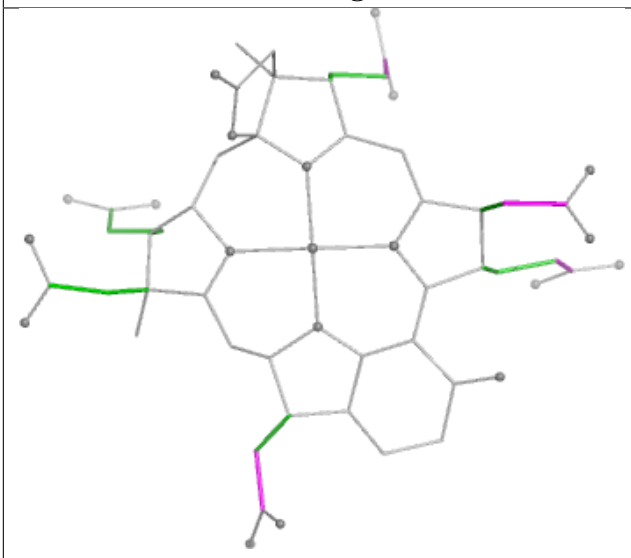
Ligand F43 J 603



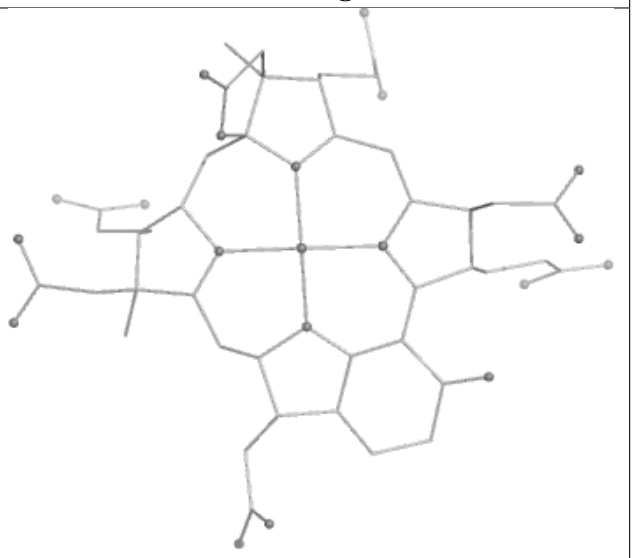
Bond lengths



Bond angles

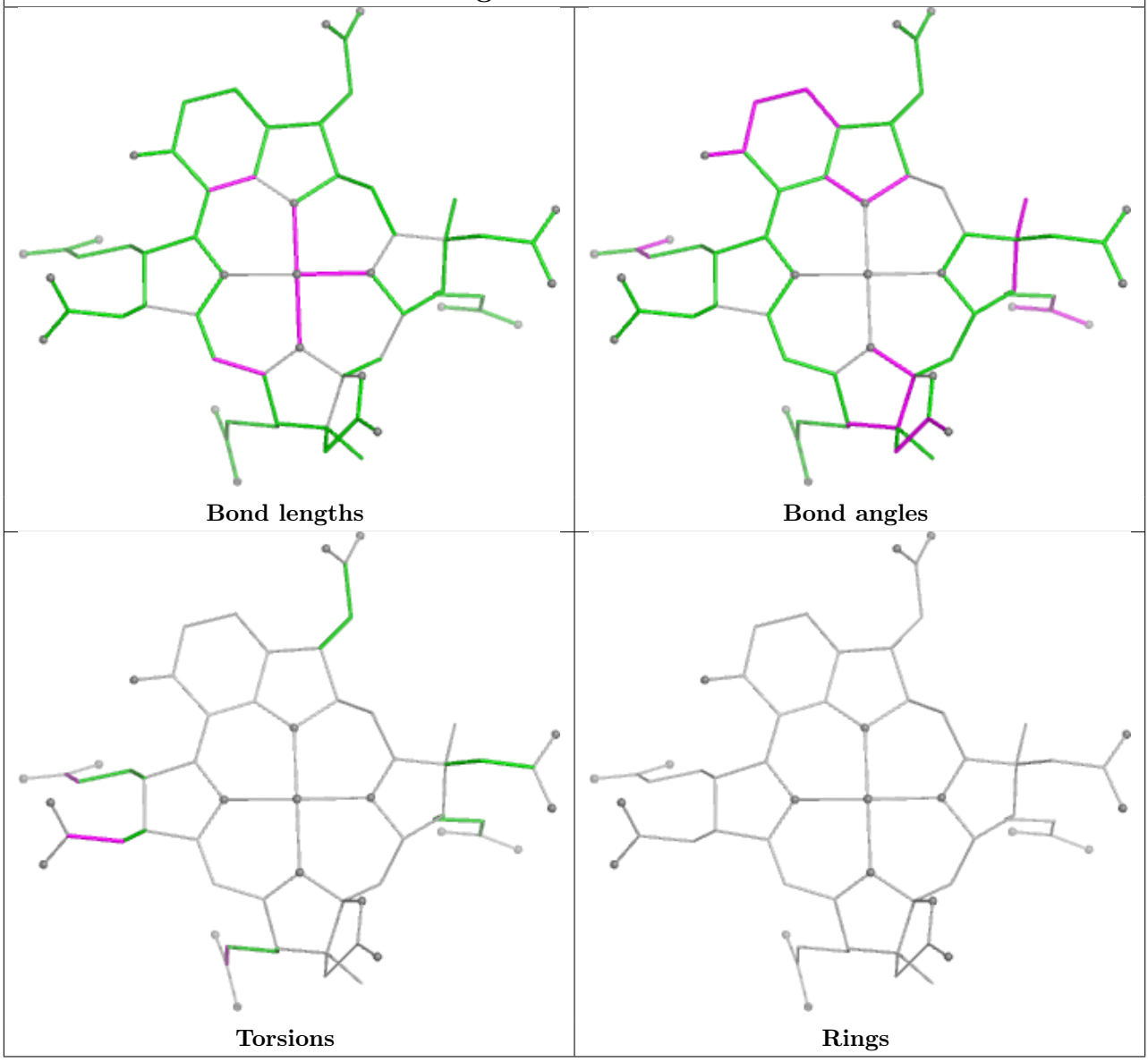


Torsions



Rings

Ligand F43 G 603



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	542/553 (98%)	-0.65	3 (0%) 85 87	9, 19, 40, 64	0
1	D	542/553 (98%)	-0.67	3 (0%) 85 87	9, 19, 40, 65	0
1	G	542/553 (98%)	-0.55	1 (0%) 91 92	12, 23, 45, 78	0
1	J	542/553 (98%)	-0.65	3 (0%) 85 87	9, 19, 42, 73	1 (0%)
2	B	442/443 (99%)	-0.45	1 (0%) 91 92	12, 26, 48, 82	0
2	E	442/443 (99%)	-0.50	0 100 100	11, 24, 48, 70	0
2	H	442/443 (99%)	-0.38	4 (0%) 81 83	11, 27, 47, 76	0
2	K	442/443 (99%)	-0.56	1 (0%) 91 92	11, 22, 43, 66	0
3	C	262/265 (98%)	-0.25	5 (1%) 66 70	17, 30, 59, 92	0
3	F	261/265 (98%)	-0.41	1 (0%) 88 90	14, 27, 54, 75	0
3	I	262/265 (98%)	-0.03	5 (1%) 66 70	22, 38, 62, 79	0
3	L	263/265 (99%)	-0.48	2 (0%) 82 84	11, 26, 54, 83	0
All	All	4984/5044 (98%)	-0.50	29 (0%) 85 87	9, 24, 49, 92	1 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	263	GLY	4.6
3	F	263	GLY	4.0
3	C	63	ASP	3.4
1	J	4	LYS	3.1
3	I	63	ASP	3.0
3	L	2	SER	2.9
3	C	263	GLY	2.8
3	C	111	ARG	2.7
3	L	264	ASP	2.7
1	G	4	LYS	2.7
1	A	300	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
3	I	2	SER	2.6
1	A	4	LYS	2.5
1	J	16	GLU	2.4
2	H	414	LEU	2.4
1	D	551	ALA	2.4
1	A	194	GLU	2.3
1	D	121	LYS	2.3
2	H	413	GLY	2.3
2	H	442	GLN	2.2
2	K	414	LEU	2.1
1	D	4	LYS	2.1
2	H	443	LEU	2.1
3	C	26	TYR	2.1
3	I	65	GLU	2.1
3	C	264	ASP	2.1
2	B	98	ASP	2.0
3	I	64	PHE	2.0
1	J	551	ALA	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MHS	J	260	11/12	0.93	0.08	18,31,39,39	0
1	MHS	D	260	11/12	0.96	0.07	15,26,38,38	0
1	MHS	G	260	11/12	0.96	0.07	21,26,32,34	0
1	MHS	A	260	11/12	0.96	0.08	19,21,28,29	0
1	MGN	D	402	10/11	0.97	0.05	9,14,18,19	0
1	DYA	D	452	8/9	0.97	0.05	12,15,19,20	0
1	DYA	A	452	8/9	0.97	0.05	12,16,20,23	0
1	AGM	G	274	12/13	0.97	0.05	12,18,20,21	0
1	DYA	G	452	8/9	0.97	0.05	17,22,28,29	0
1	SMC	G	454	7/8	0.97	0.04	17,18,23,27	0
1	AGM	A	274	12/13	0.97	0.06	10,15,22,22	0
1	AGM	J	274	12/13	0.97	0.05	8,16,18,20	0
1	MGN	A	402	10/11	0.98	0.04	11,12,17,18	0
1	AGM	D	274	12/13	0.98	0.04	7,14,16,20	0
1	MGN	G	402	10/11	0.98	0.04	15,18,24,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	GL3	G	447	4/5	0.98	0.08	18,18,19,20	0
1	MGN	J	402	10/11	0.98	0.04	8,10,18,21	0
1	DYA	J	452	8/9	0.98	0.04	7,12,16,27	0
1	SMC	A	454	7/8	0.99	0.03	11,11,22,23	0
1	SMC	D	454	7/8	0.99	0.04	9,13,16,18	0
1	GL3	A	447	4/5	0.99	0.04	15,16,17,20	0
1	GL3	J	447	4/5	0.99	0.05	12,12,14,14	0
1	GL3	D	447	4/5	0.99	0.04	13,18,19,22	0
1	SMC	J	454	7/8	0.99	0.04	6,12,15,19	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

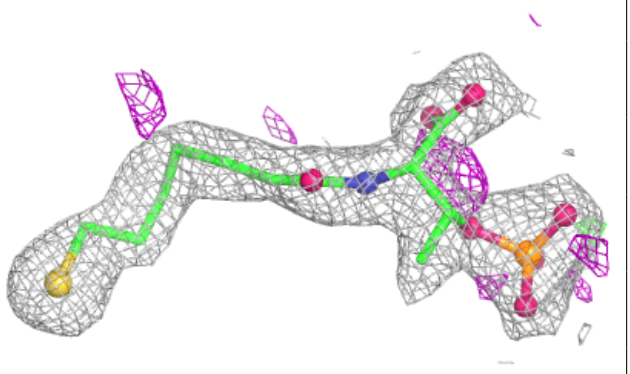
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

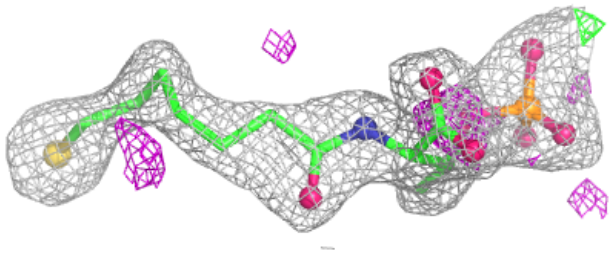
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	COM	A	601	7/7	0.95	0.07	19,25,28,29	0
5	TP7	G	602	21/21	0.95	0.08	19,31,39,44	0
5	TP7	J	602	21/21	0.95	0.08	17,29,38,43	0
4	COM	D	601	7/7	0.96	0.10	20,25,26,28	0
4	COM	G	601	7/7	0.96	0.08	25,31,34,34	0
5	TP7	D	602	21/21	0.97	0.06	10,24,30,33	0
4	COM	J	601	7/7	0.97	0.08	17,25,34,37	0
5	TP7	A	602	21/21	0.97	0.06	10,25,36,39	0
6	F43	G	603	62/62	0.97	0.06	9,22,31,35	0
6	F43	D	603	62/62	0.98	0.05	1,15,25,29	0
6	F43	A	603	62/62	0.98	0.05	5,13,20,25	0
6	F43	J	603	62/62	0.98	0.05	3,14,23,30	0
7	K	A	604	1/1	0.99	0.03	24,24,24,24	0
7	K	D	604	1/1	0.99	0.04	22,22,22,22	0
7	K	G	604	1/1	0.99	0.04	30,30,30,30	0
7	K	J	604	1/1	0.99	0.03	19,19,19,19	0
7	K	J	605	1/1	0.99	0.02	26,26,26,26	0
7	K	J	606	1/1	0.99	0.02	25,25,25,25	0
7	K	D	605	1/1	1.00	0.01	15,15,15,15	0

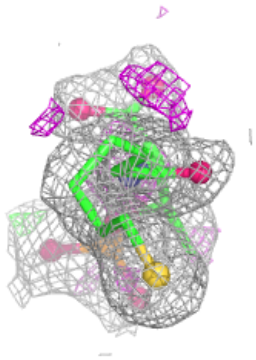
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TP7 G 602:

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

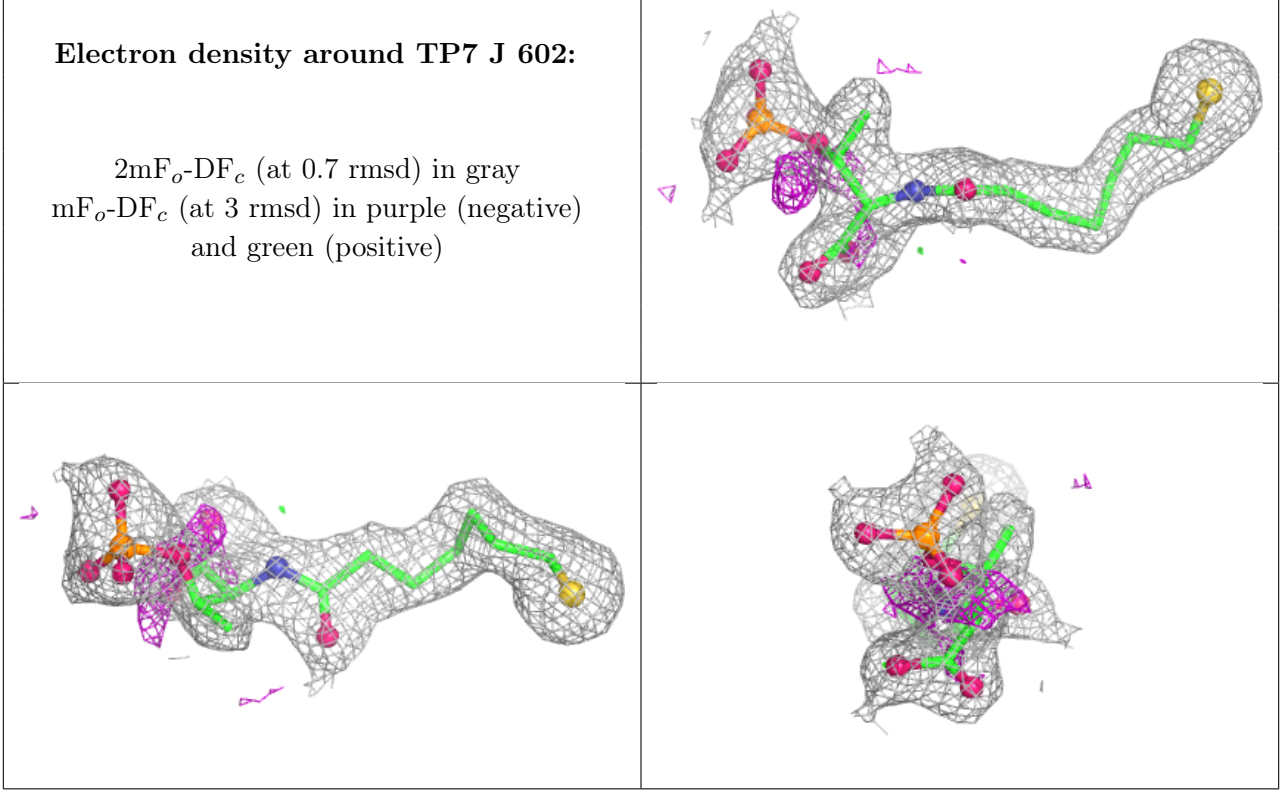






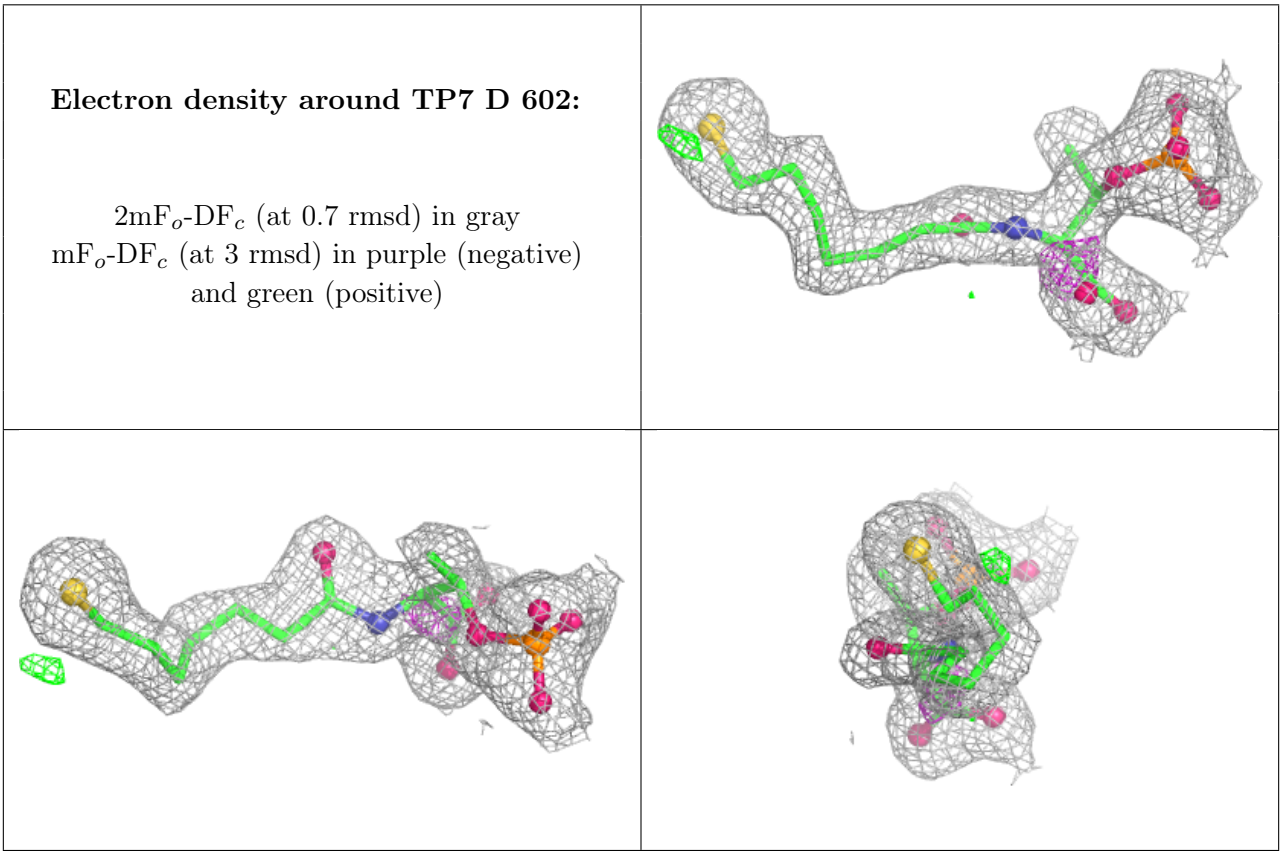
Electron density around TP7 J 602:

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



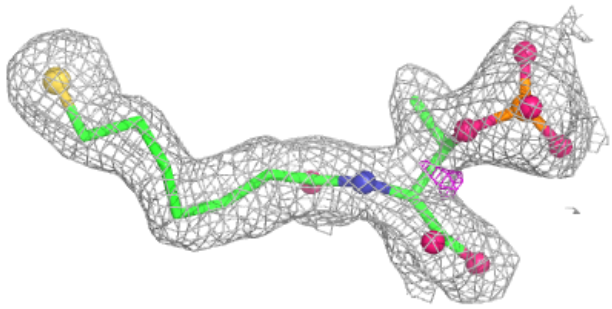
Electron density around TP7 D 602:

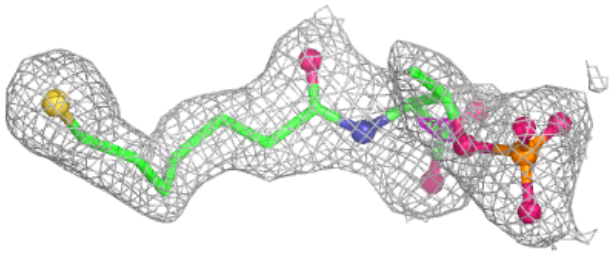
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

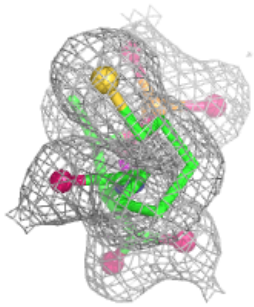


Electron density around TP7 A 602:

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

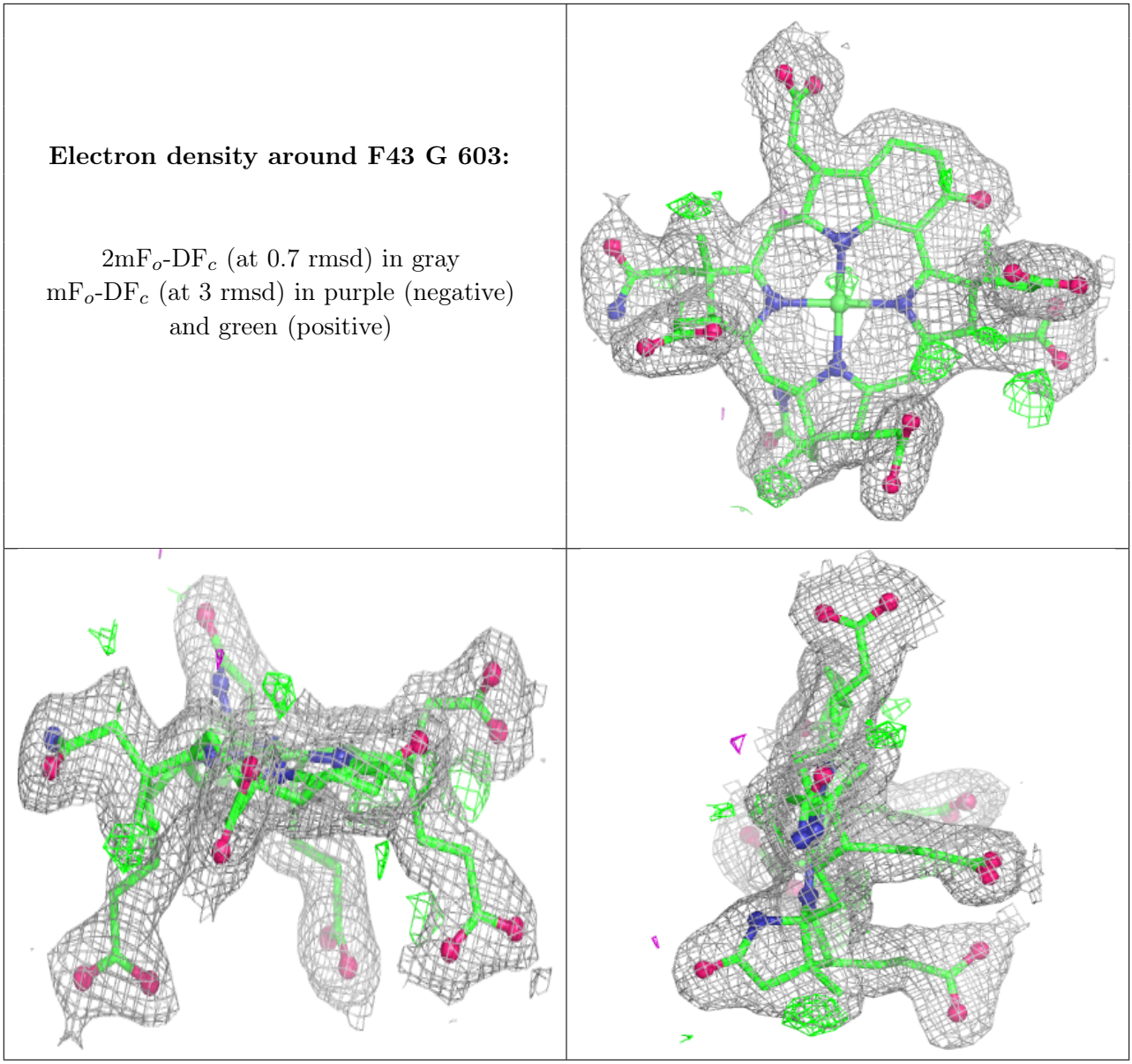






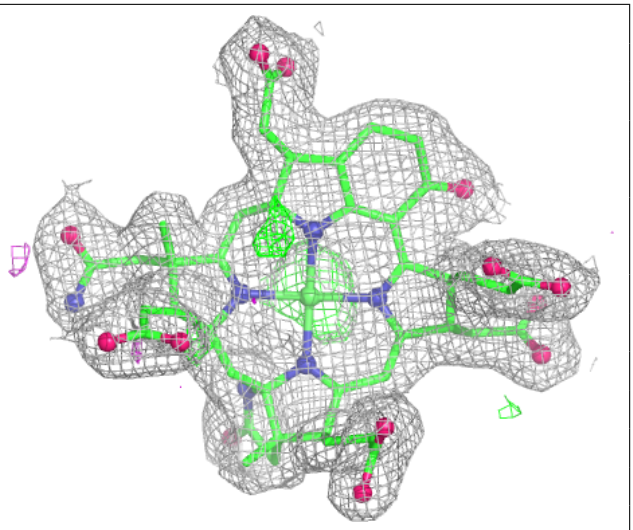
Electron density around F43 G 603:

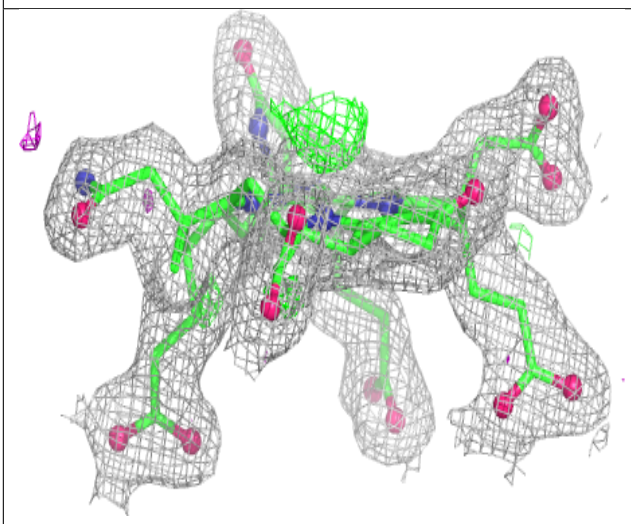
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

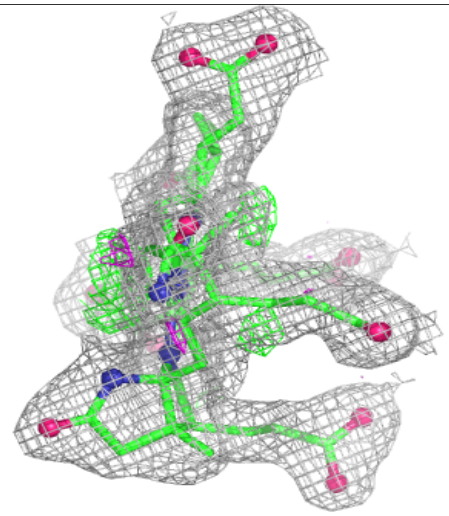


Electron density around F43 D 603:

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

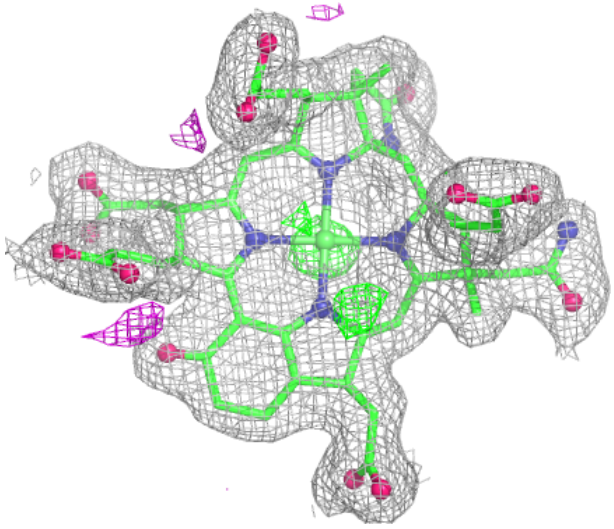


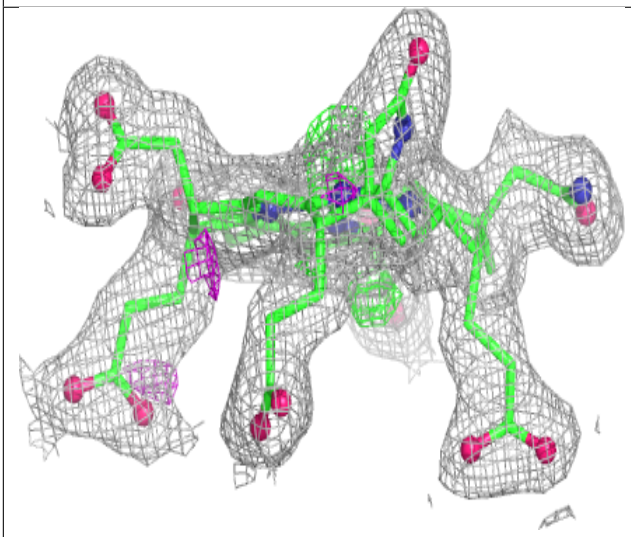


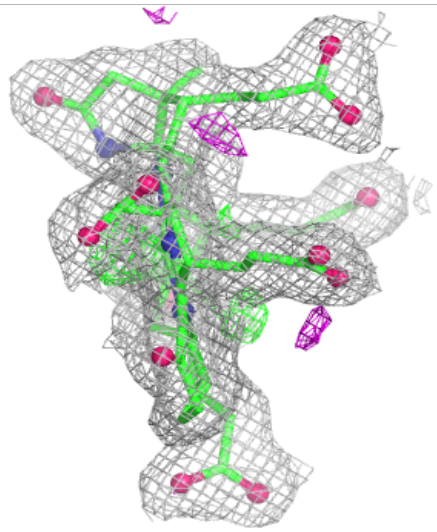


Electron density around F43 A 603:

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

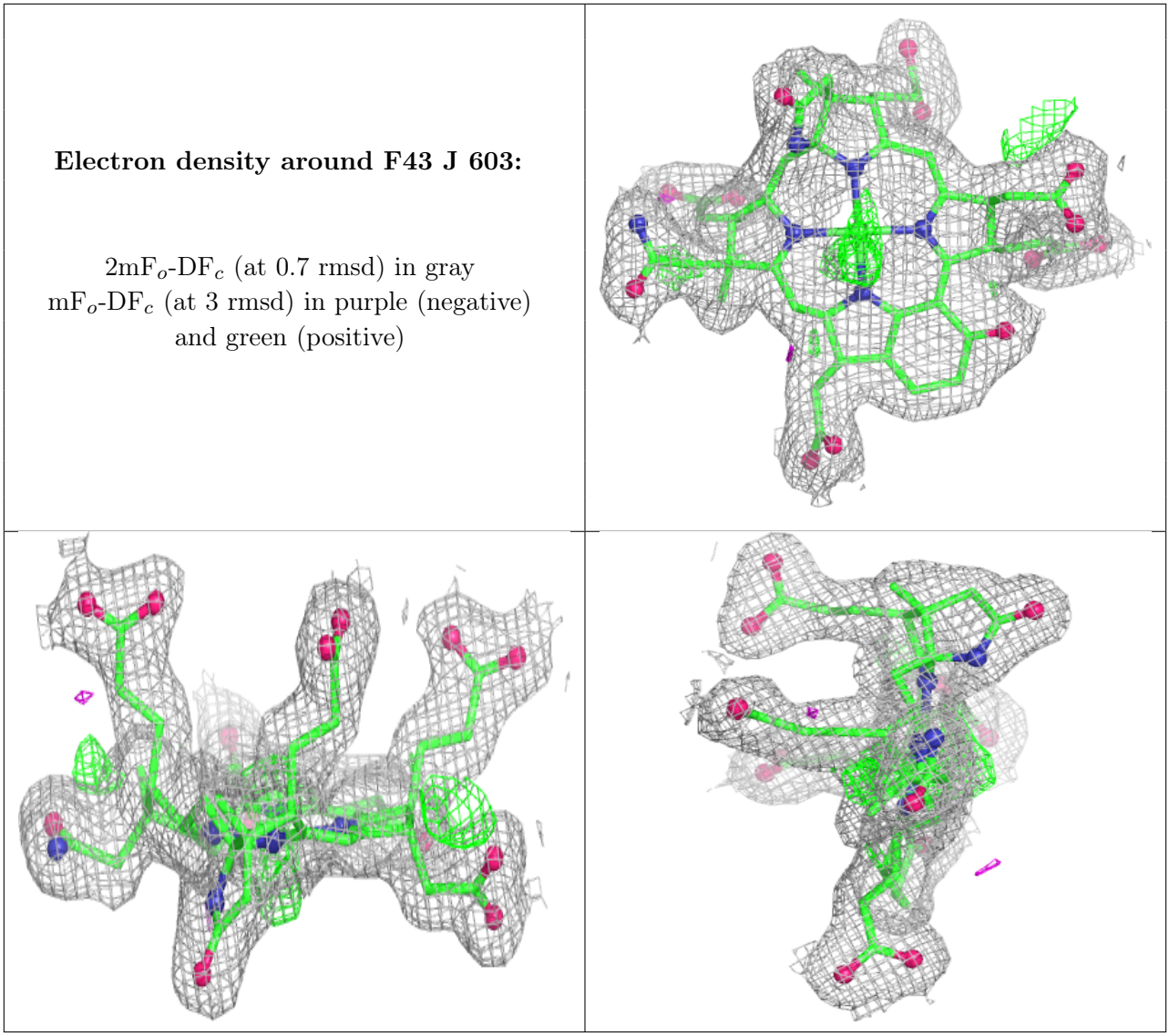






Electron density around F43 J 603:

$2mF_o$-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.