



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:13 PM UTC

PDB ID : 3SQG / pdb_00003sqg
Title : Crystal structure of a methyl-coenzyme M reductase purified from Black Sea mats
Authors : Shima, S.; Krueger, M.; Weinert, T.; Demmer, U.; Thauer, R.K.; Ermler, U.
Deposited on : 2011-07-05
Resolution : 2.10 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

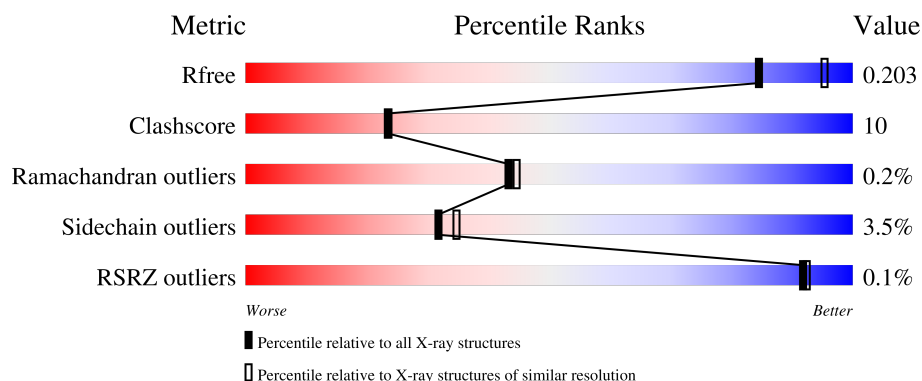
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

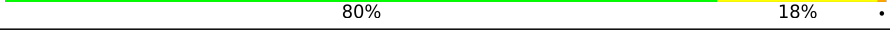
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	579	
1	D	579	
1	G	579	
2	B	433	
2	E	433	

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Mol	Chain	Length	Quality of chain
2	H	433	 79% 18% .
3	C	279	 87% 12% .
3	F	279	 79% 19% .
3	I	279	 84% 14% .

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
1	GL3	A	464	-	-	X	-
10	CL	A	586	-	-	X	-
12	P6G	B	434	-	-	X	-
5	COM	A	1003	-	X	X	-
6	M43	D	1001	X	-	-	-
6	M43	G	1001	X	-	-	-
7	1PE	D	580	-	-	X	-
7	1PE	G	580	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 32144 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, alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4467	2814	761	855	37			
1	D	578	Total	C	N	O	S	0	1	0
			4475	2819	764	855	37			
1	G	578	Total	C	N	O	S	0	0	0
			4467	2814	761	855	37			

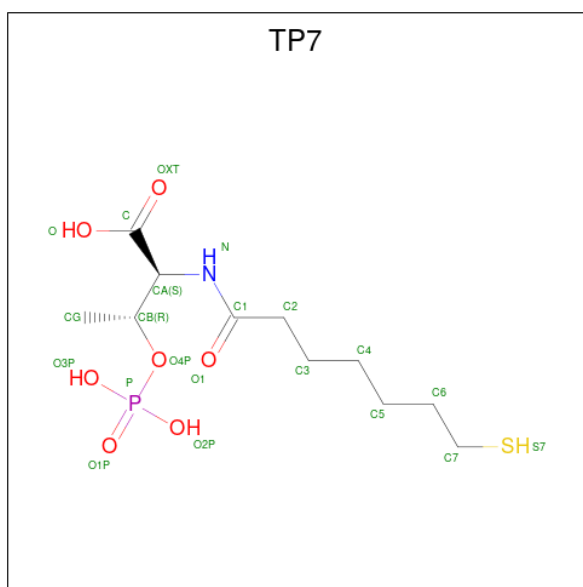
- Molecule 2 is a protein called Methyl-coenzyme M reductase, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	431	Total	C	N	O	S	0	0	0
			3197	2013	552	600	32			
2	E	431	Total	C	N	O	S	0	0	0
			3197	2013	552	600	32			
2	H	431	Total	C	N	O	S	0	1	0
			3205	2018	555	600	32			

- Molecule 3 is a protein called Methyl-coenzyme M reductase, gamma subunit.

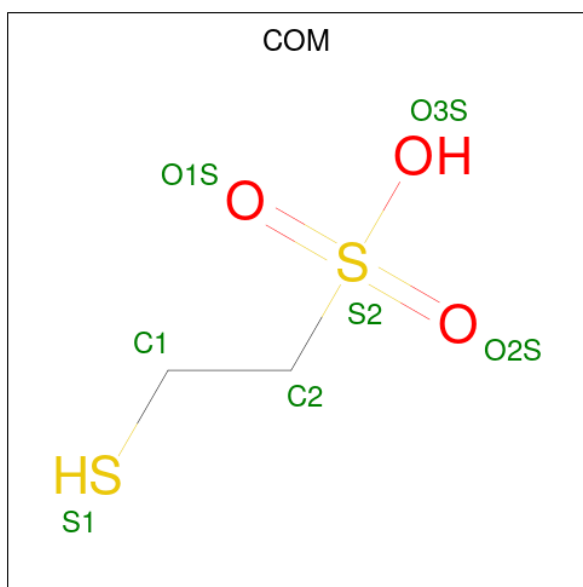
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	278	Total	C	N	O	S	0	0	0
			2205	1379	400	414	12			
3	F	278	Total	C	N	O	S	0	1	0
			2210	1382	401	415	12			
3	I	278	Total	C	N	O	S	0	0	0
			2205	1379	400	414	12			

- Molecule 4 is Coenzyme B (CCD ID: TP7) (formula: C₁₁H₂₂NO₇PS).



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

- Molecule 5 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $C_2H_6O_3S_2$).



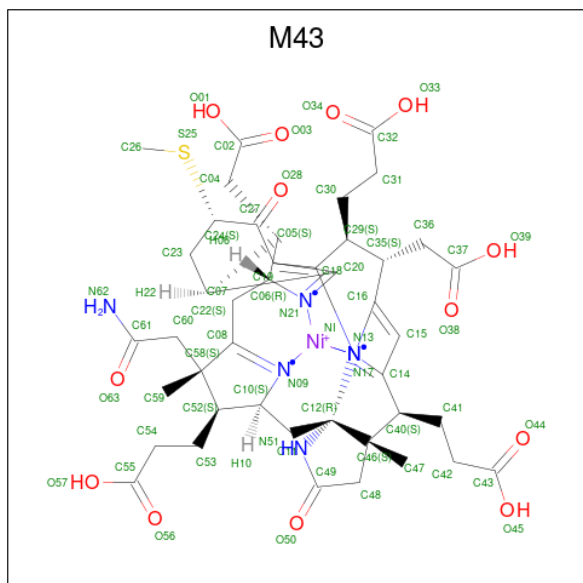
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			7	2	3	2		

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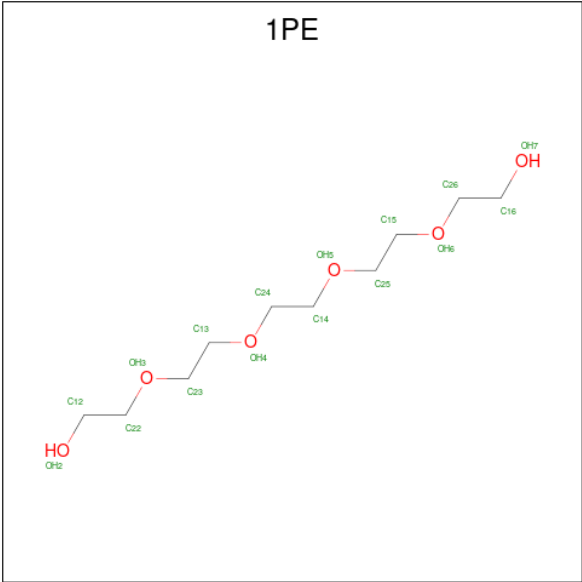
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	O	S	0	0
			7	2	3	2		
5	G	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 6 is (17[2]S)-17[2]-methylthio-coenzyme F43 (CCD ID: M43) (formula: $C_{43}H_{53}N_6NiO_{13}S$).



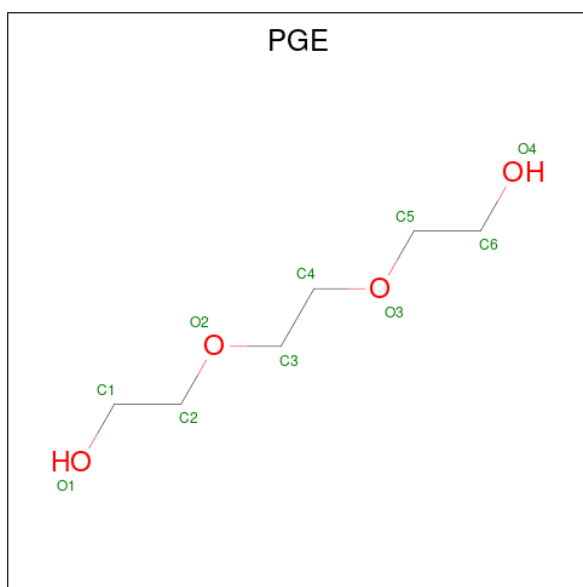
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	Ni	O	S	0	0
			64	43	6	1	13	1		
6	D	1	Total	C	N	Ni	O	S	0	0
			64	43	6	1	13	1		
6	G	1	Total	C	N	Ni	O	S	0	0
			64	43	6	1	13	1		

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



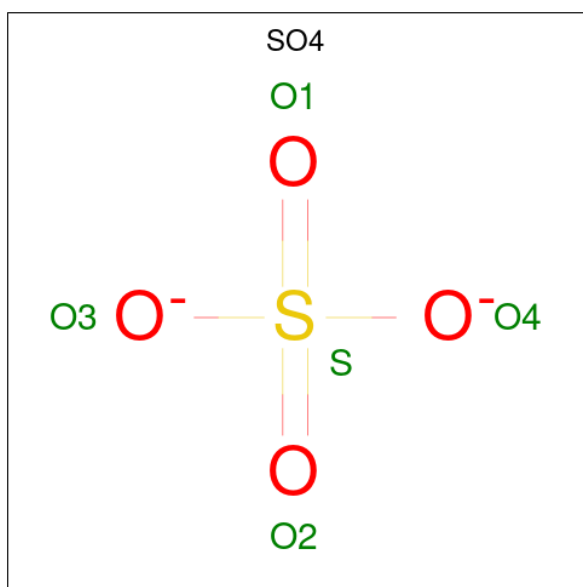
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			16	10	6		
7	D	1	Total	C	O	0	0
			16	10	6		
7	E	1	Total	C	O	0	0
			16	10	6		
7	F	1	Total	C	O	0	0
			16	10	6		
7	G	1	Total	C	O	0	0
			16	10	6		
7	H	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		
8	A	1	Total	C	O	0	0
			10	6	4		
8	D	1	Total	C	O	0	0
			10	6	4		
8	D	1	Total	C	O	0	0
			10	6	4		
8	G	1	Total	C	O	0	0
			10	6	4		
8	G	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	H	1	Total	O	S	0	0
			5	4	1		
9	I	1	Total	O	S	0	0
			5	4	1		

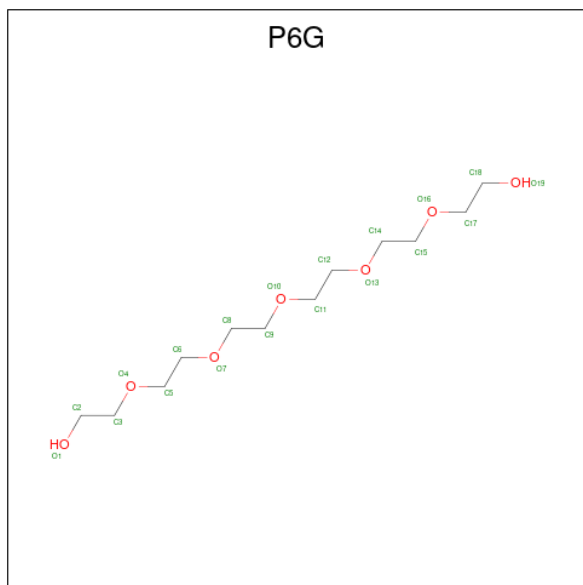
- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Cl	0	0
			1	1		

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

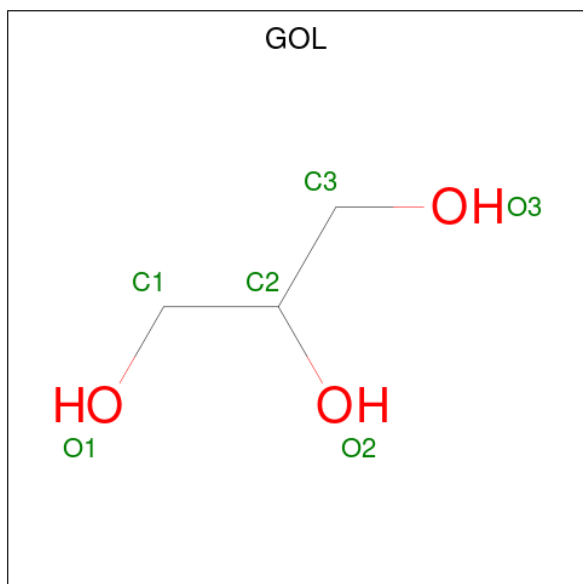
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Ca	0	0
			1	1		
11	G	1	Total	Ca	0	0
			1	1		

- Molecule 12 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 13 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			6	3	3		
13	E	1	Total	C	O	0	0
			6	3	3		

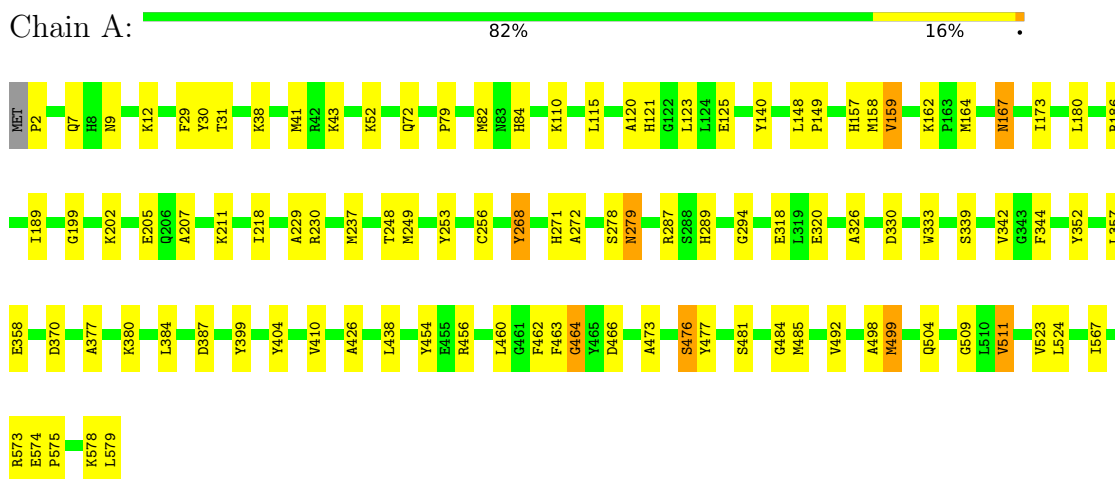
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	391	Total	O	0	0
			391	391		
14	B	173	Total	O	0	0
			173	173		
14	C	178	Total	O	0	0
			178	178		
14	D	341	Total	O	0	0
			341	341		
14	E	142	Total	O	0	0
			142	142		
14	F	120	Total	O	0	0
			120	120		
14	G	364	Total	O	0	0
			364	364		
14	H	140	Total	O	0	0
			140	140		
14	I	156	Total	O	0	0
			156	156		

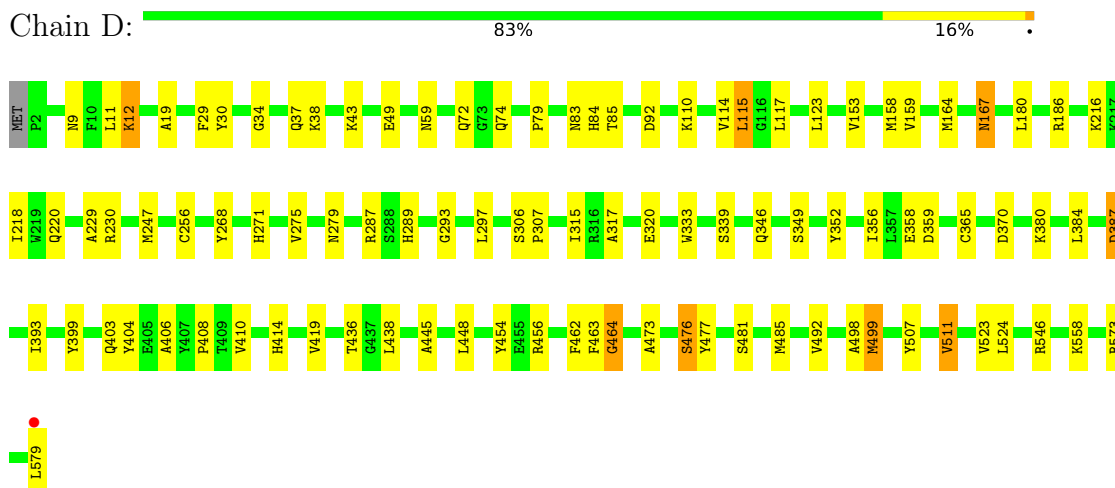
3 Residue-property plots

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.

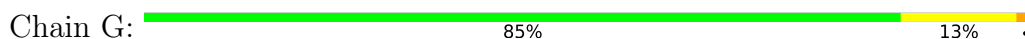
- Molecule 1: Methyl coenzyme M reductase, alpha subunit

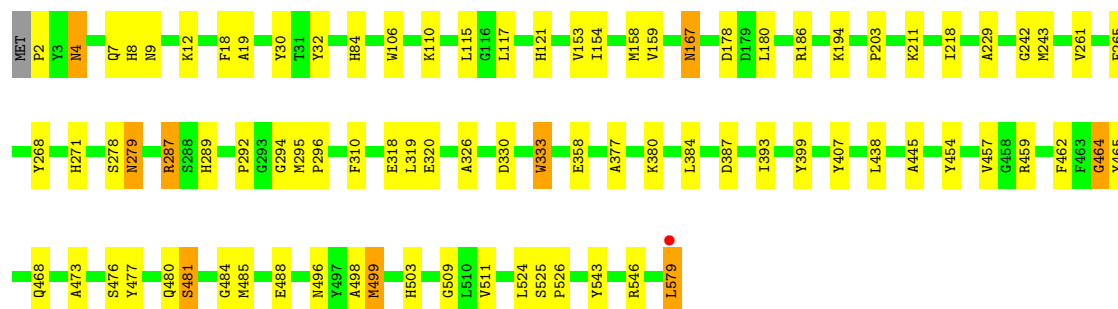


- Molecule 1: Methyl coenzyme M reductase, alpha subunit



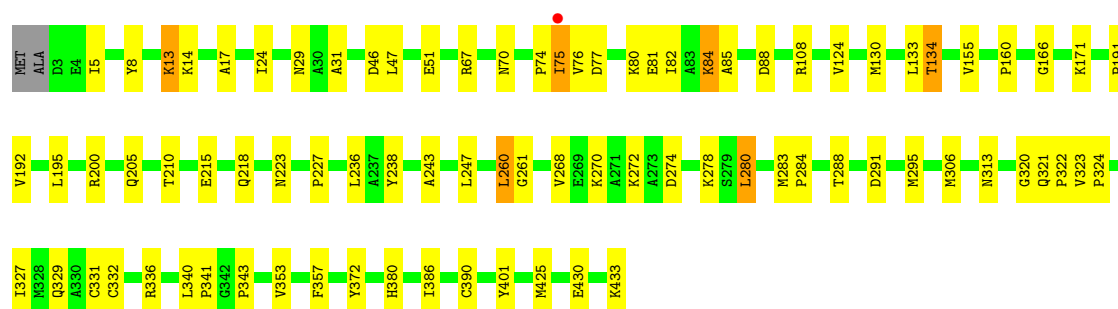
- Molecule 1: Methyl coenzyme M reductase, alpha subunit





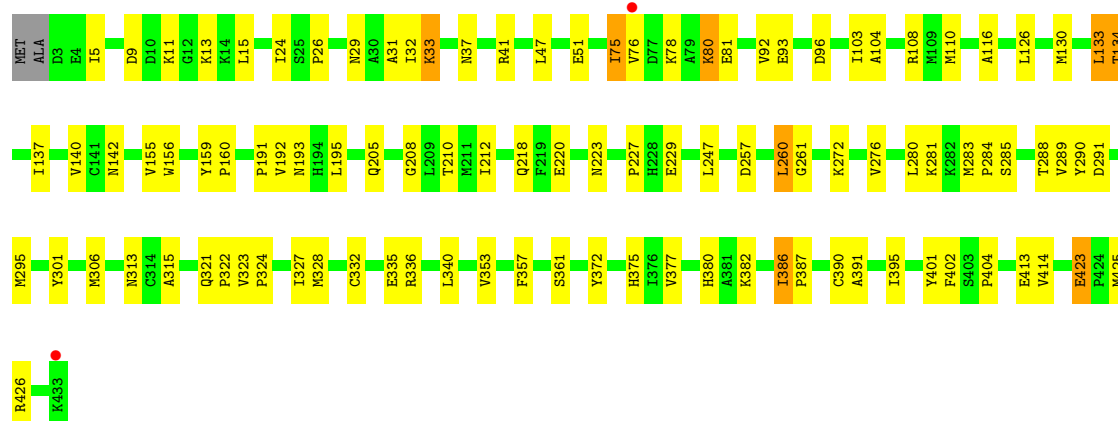
- Molecule 2: Methyl-coenzyme M reductase, beta subunit

Chain B: 80% 18%



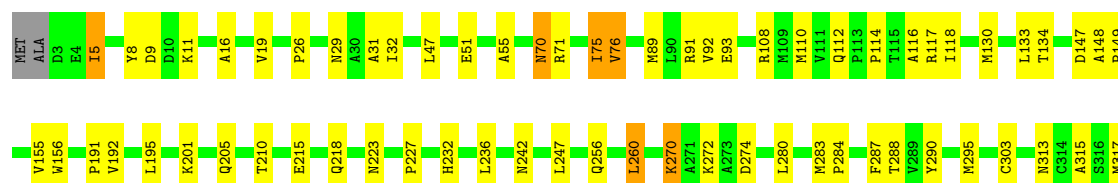
- Molecule 2: Methyl-coenzyme M reductase, beta subunit

Chain E: 76% 22%



- Molecule 2: Methyl-coenzyme M reductase, beta subunit

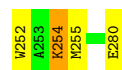
Chain H: 79% 18%





- Molecule 3: Methyl-coenzyme M reductase, gamma subunit

Chain C: 87% 12% .



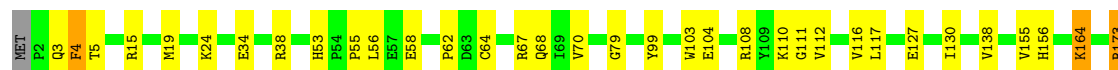
- Molecule 3: Methyl-coenzyme M reductase, gamma subunit

Chain F: 79% 19% .



- Molecule 3: Methyl-coenzyme M reductase, gamma subunit

Chain I: 84% 14% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	128.86Å 412.49Å 165.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.58 – 2.10 47.58 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.2 (47.58-2.10) 95.3 (47.58-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.161 , 0.206 0.157 , 0.203	Depositor DCC
R_{free} test set	12184 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	32144	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TP7, M43, 0AF, CA, CL, 1PE, GOL, P6G, GL3, COM, MHO, SO4, PGE, MHS

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	0.54	0/4528	0.79	1/6126 (0.0%)
1	D	0.50	0/4539	0.77	0/6140
1	G	0.49	0/4528	0.78	2/6126 (0.0%)
2	B	0.46	0/3258	0.77	1/4410 (0.0%)
2	E	0.42	0/3258	0.78	3/4410 (0.1%)
2	H	0.45	1/3269 (0.0%)	0.80	2/4424 (0.0%)
3	C	0.48	0/2251	0.78	0/3034
3	F	0.38	0/2259	0.74	2/3045 (0.1%)
3	I	0.45	0/2251	0.76	0/3034
All	All	0.47	1/30141 (0.0%)	0.78	11/40749 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	323	VAL	CA-CB	5.88	1.57	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	118	ILE	N-CA-C	6.24	112.89	106.21
3	F	250	GLN	CA-C-N	6.14	126.33	119.32
3	F	250	GLN	C-N-CA	6.14	126.33	119.32
2	B	380	HIS	N-CA-C	5.48	117.34	111.36
1	G	310	PHE	CA-C-N	5.37	125.19	119.28
1	G	310	PHE	C-N-CA	5.37	125.19	119.28
2	H	380	HIS	N-CA-C	5.35	117.12	111.28
1	A	237	MET	N-CA-C	5.24	116.68	110.97
2	E	380	HIS	N-CA-C	5.10	116.92	111.36
2	E	423	GLU	CA-C-N	5.08	124.39	118.85
2	E	423	GLU	C-N-CA	5.08	124.39	118.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4467	0	4267	91	0
1	D	4475	0	4280	102	0
1	G	4467	0	4267	80	0
2	B	3197	0	3195	85	0
2	E	3197	0	3195	105	0
2	H	3205	0	3208	98	0
3	C	2205	0	2187	40	0
3	F	2210	0	2193	56	0
3	I	2205	0	2187	44	0
4	A	42	0	38	1	0
4	G	21	0	19	1	0
5	A	7	0	5	4	0
5	D	7	0	5	3	0
5	G	7	0	5	3	0
6	A	64	0	48	3	0
6	D	64	0	48	1	0
6	G	64	0	48	3	0
7	A	16	0	22	5	0
7	D	16	0	22	8	0
7	E	16	0	22	2	0
7	F	16	0	22	4	0
7	G	16	0	22	9	0
7	H	16	0	22	5	0
8	A	20	0	28	5	0
8	D	20	0	28	5	0
8	G	20	0	28	1	0
9	A	10	0	0	0	0
9	B	10	0	0	0	0
9	C	5	0	0	0	0
9	D	10	0	0	0	0
9	H	5	0	0	0	0
9	I	5	0	0	0	0
10	A	1	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	1	0	0	0	0
11	G	1	0	0	0	0
12	B	19	0	26	11	0
13	C	6	0	8	0	0
13	E	6	0	8	0	0
14	A	391	0	0	6	0
14	B	173	0	0	7	0
14	C	178	0	0	4	0
14	D	341	0	0	9	0
14	E	142	0	0	7	0
14	F	120	0	0	4	0
14	G	364	0	0	2	0
14	H	140	0	0	2	0
14	I	156	0	0	1	0
All	All	32144	0	29453	609	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 10.

All (609) 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)
2:B:51:GLU:HB2	2:B:75:ILE:CD1	1.77	1.15
1:D:186:ARG:HH12	7:G:580:1PE:H221	1.16	1.10
2:B:14:LYS:CE	2:B:17:ALA:HB2	1.86	1.06
1:A:186:ARG:HH12	7:A:581:1PE:H121	1.20	1.03
7:D:580:1PE:H141	1:G:186:ARG:HH11	1.25	1.02
2:B:288:THR:H	3:C:3:GLN:HE22	1.09	1.00
2:H:288:THR:H	3:I:3:GLN:HE22	1.06	0.99
2:E:257:ASP:HA	3:F:110:LYS:HD2	1.43	0.98
1:D:546[B]:ARG:NH2	14:D:1849:HOH:O	1.98	0.95
2:E:288:THR:H	3:F:3:GLN:HE22	1.16	0.93
2:E:323:VAL:HG13	2:E:324:PRO:HD3	1.48	0.93
2:H:130:MET:O	2:H:134:THR:HG23	1.69	0.92
1:D:463:PHE:HB2	5:D:1003:COM:O2S	1.72	0.90
2:H:288:THR:H	3:I:3:GLN:NE2	1.72	0.88
2:B:14:LYS:HE3	2:B:17:ALA:HB2	1.52	0.87
1:D:186:ARG:HH11	7:G:580:1PE:H242	1.37	0.87
1:D:167:ASN:H	1:D:167:ASN:HD22	1.19	0.86
1:A:186:ARG:HH11	7:A:581:1PE:H242	1.41	0.86
2:H:47:LEU:HD22	2:H:75:ILE:HD11	1.54	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:GLU:HB2	2:B:75:ILE:HD12	1.59	0.84
2:B:191:PRO:HG3	12:B:434:P6G:H142	1.57	0.84
1:A:511:VAL:HG13	1:A:523:VAL:HG11	1.59	0.84
1:A:463:PHE:HB2	5:A:1003:COM:O2S	1.78	0.83
2:E:323:VAL:CG1	2:E:324:PRO:HD3	2.09	0.82
2:E:47:LEU:O	2:E:75:ILE:HD11	1.80	0.82
2:H:92:VAL:HG23	2:H:93:GLU:HG2	1.62	0.81
2:E:272:LYS:HE2	2:E:290:TYR:CZ	2.16	0.81
2:E:336:ARG:HE	3:F:5:THR:HG22	1.45	0.81
1:D:511:VAL:HG13	1:D:523:VAL:HG11	1.61	0.81
2:H:47:LEU:HD22	2:H:75:ILE:CD1	2.10	0.81
2:E:336:ARG:HB3	3:F:5:THR:HG22	1.64	0.80
2:H:51:GLU:OE1	2:H:76:VAL:HG22	1.81	0.80
1:A:121:HIS:HE1	10:A:586:CL:CL	2.02	0.80
2:B:191:PRO:HD3	12:B:434:P6G:H111	1.63	0.80
1:D:186:ARG:HH12	7:G:580:1PE:C22	1.93	0.80
14:B:1926:HOH:O	3:C:67:ARG:HD2	1.81	0.80
1:A:462:PHE:HB2	5:A:1003:COM:H22	1.63	0.79
2:B:313:ASN:HD21	3:C:112:VAL:H	1.31	0.79
1:A:473:ALA:O	1:A:476:SER:HB2	1.81	0.79
3:C:254:LYS:HD3	3:C:255:MET:H	1.47	0.79
1:G:167:ASN:HD22	1:G:167:ASN:H	1.28	0.78
1:A:167:ASN:H	1:A:167:ASN:HD22	1.27	0.78
3:C:15:ARG:O	3:C:19:MET:HG3	1.83	0.78
2:B:51:GLU:OE1	2:B:76:VAL:HG22	1.84	0.78
7:D:580:1PE:H162	1:G:186:ARG:HH12	1.49	0.77
2:H:323:VAL:CG1	2:H:324:PRO:HD3	2.14	0.77
2:B:130:MET:O	2:B:134:THR:HG23	1.83	0.77
2:B:14:LYS:NZ	2:B:17:ALA:HB2	2.00	0.77
2:B:336:ARG:HB3	3:C:5:THR:HG22	1.66	0.76
1:D:186:ARG:NH1	7:G:580:1PE:H242	2.00	0.75
7:D:580:1PE:C14	1:G:186:ARG:HD3	2.15	0.75
7:D:580:1PE:H141	1:G:186:ARG:NH1	2.01	0.74
1:G:180:LEU:HD22	1:G:218:ILE:HD11	1.68	0.74
1:G:2:PRO:HD2	3:I:280:GLU:HG2	1.69	0.74
2:H:108:ARG:HH21	2:H:108:ARG:HG3	1.53	0.74
1:D:186:ARG:HH11	7:G:580:1PE:C24	2.00	0.74
2:H:323:VAL:HG13	2:H:324:PRO:HD3	1.69	0.74
2:B:336:ARG:HE	3:C:5:THR:HG22	1.53	0.73
2:E:313:ASN:HD21	3:F:112:VAL:H	1.35	0.73
1:A:186:ARG:NH1	7:A:581:1PE:H121	2.01	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:295:MET:CE	3:I:243:LYS:HE3	2.19	0.72
1:D:84:HIS:HD2	1:D:358:GLU:OE1	1.72	0.72
1:A:84:HIS:HD2	1:A:358:GLU:OE1	1.73	0.72
2:H:9:ASP:OD1	2:H:11:LYS:HE2	1.89	0.71
2:E:280:LEU:C	2:E:280:LEU:HD23	2.15	0.71
1:D:511:VAL:CG1	1:D:523:VAL:HG11	2.21	0.71
2:E:283:MET:HB3	2:E:284:PRO:HD2	1.73	0.71
1:D:180:LEU:HD13	8:D:582:PGE:H22	1.72	0.70
1:A:256:CYS:HB2	3:F:84:TYR:CZ	2.26	0.70
2:B:280:LEU:HD23	2:B:280:LEU:O	1.90	0.70
1:D:546[B]:ARG:NH1	14:D:1227:HOH:O	2.24	0.70
2:B:134:THR:HG22	2:B:155:VAL:HG11	1.72	0.70
3:F:46:GLY:HA2	7:F:281:1PE:H251	1.73	0.70
1:D:186:ARG:NH1	7:G:580:1PE:H221	2.01	0.70
1:D:546[B]:ARG:NH2	1:G:543:TYR:CE1	2.60	0.69
2:B:288:THR:H	3:C:3:GLN:NE2	1.86	0.69
2:E:11:LYS:HE2	2:E:426:ARG:HH22	1.58	0.69
2:H:295:MET:HE3	3:I:243:LYS:HE3	1.73	0.69
2:E:51:GLU:OE1	2:E:76:VAL:HG22	1.93	0.68
3:I:5:THR:HG21	3:I:103:TRP:CZ3	2.28	0.68
3:I:34:GLU:HG2	3:I:38:ARG:NH1	2.08	0.68
2:H:288:THR:N	3:I:3:GLN:HE22	1.87	0.68
2:B:280:LEU:HD23	2:B:280:LEU:C	2.19	0.68
1:D:167:ASN:HD22	1:D:167:ASN:N	1.92	0.67
1:G:30:TYR:CE2	3:I:173:ARG:HD3	2.29	0.67
1:D:546[B]:ARG:HH22	1:G:543:TYR:HE1	1.42	0.67
3:F:132:LYS:HE2	14:F:1269:HOH:O	1.95	0.67
2:B:47:LEU:O	2:B:75:ILE:HD11	1.95	0.67
2:E:75:ILE:HG13	2:E:76:VAL:N	2.10	0.67
2:E:81:GLU:HG3	14:E:1829:HOH:O	1.95	0.67
2:E:288:THR:H	3:F:3:GLN:NE2	1.88	0.67
1:G:84:HIS:HE1	1:G:320:GLU:OE2	1.78	0.67
2:H:201:LYS:NZ	2:H:396:ASP:O	2.27	0.67
1:D:387:ASP:OD2	14:D:1408:HOH:O	2.12	0.66
2:H:110:MET:HE3	2:H:112:GLN:CD	2.19	0.66
3:I:127:GLU:O	3:I:130:ILE:HG22	1.96	0.66
2:H:313:ASN:HD21	3:I:112:VAL:H	1.44	0.65
2:H:108:ARG:HG3	2:H:108:ARG:NH2	2.10	0.65
1:D:473:ALA:O	1:D:476:SER:HB2	1.95	0.65
2:E:291:ASP:HA	2:E:340:LEU:HD21	1.79	0.65
1:G:243:MET:HE2	1:G:243:MET:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:336:ARG:HB3	3:I:5:THR:HG22	1.79	0.64
2:E:51:GLU:HB2	2:E:75:ILE:HG12	1.79	0.64
2:H:295:MET:HE1	2:H:340:LEU:HD23	1.80	0.64
2:H:91[A]:ARG:HG3	2:H:91[A]:ARG:HH11	1.63	0.64
2:E:280:LEU:HD23	2:E:280:LEU:O	1.98	0.64
3:F:15:ARG:O	3:F:19:MET:HG3	1.97	0.64
2:H:47:LEU:HB3	2:H:75:ILE:HD11	1.79	0.63
2:E:134:THR:HG22	2:E:155:VAL:HG11	1.80	0.63
1:G:499:MHO:O	4:G:1002:TP7:H72C	1.98	0.63
2:B:67:ARG:NH2	14:B:439:HOH:O	2.30	0.63
2:E:193:ASN:OD1	2:E:404:PRO:HD3	1.99	0.63
3:I:205:LEU:HD22	3:I:209:GLU:HG2	1.81	0.63
1:A:164:MET:HE3	1:D:573:ARG:HD2	1.80	0.63
2:H:134:THR:HG22	2:H:155:VAL:CB	2.28	0.63
12:B:434:P6G:H22	14:B:1577:HOH:O	1.99	0.63
3:F:254:LYS:NZ	3:F:255:MET:H	1.96	0.62
2:B:372:TYR:CE2	12:B:434:P6G:H141	2.34	0.62
2:E:80:LYS:HB2	14:E:1442:HOH:O	1.99	0.62
1:A:573:ARG:HD2	1:D:164:MET:CE	2.28	0.62
14:E:455:HOH:O	3:F:67:ARG:HD2	1.99	0.62
1:D:511:VAL:HG13	1:D:523:VAL:CG1	2.30	0.62
1:G:180:LEU:HD22	1:G:218:ILE:CD1	2.30	0.62
7:D:580:1PE:H162	1:G:186:ARG:NH1	2.15	0.62
1:D:84:HIS:O	1:D:546[B]:ARG:NH1	2.33	0.62
1:A:167:ASN:HD22	1:A:167:ASN:N	1.98	0.61
2:B:51:GLU:HB2	2:B:75:ILE:HD13	1.77	0.61
7:D:580:1PE:H151	1:G:186:ARG:NH1	2.16	0.61
7:D:580:1PE:H142	1:G:186:ARG:HD3	1.80	0.61
1:D:462:PHE:HB2	5:D:1003:COM:H22	1.81	0.61
1:A:52:LYS:NZ	14:A:783:HOH:O	2.25	0.61
2:E:130:MET:O	2:E:134:THR:CG2	2.48	0.61
2:E:295:MET:HE1	2:E:340:LEU:HD22	1.83	0.61
1:A:164:MET:HE1	1:D:573:ARG:HG3	1.82	0.60
2:E:336:ARG:HB3	3:F:5:THR:CG2	2.30	0.60
2:H:89:MET:O	2:H:117:ARG:NH1	2.34	0.60
2:E:375:HIS:CE1	2:E:377:VAL:HG23	2.36	0.60
1:A:256:CYS:HB2	3:F:84:TYR:CE2	2.37	0.60
3:F:95:PRO:HD2	14:F:1087:HOH:O	2.02	0.60
2:H:92:VAL:HG21	2:H:116:ALA:CB	2.30	0.60
2:E:218:GLN:HE22	2:E:223:ASN:HD22	1.50	0.60
1:G:84:HIS:HD2	1:G:358:GLU:OE1	1.85	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:270:LYS:NZ	2:H:274:ASP:OD2	2.24	0.59
1:G:318:GLU:HG2	1:G:509:GLY:O	2.03	0.59
2:B:210:THR:HG21	2:B:386:ILE:HG22	1.85	0.59
1:G:167:ASN:HD22	1:G:167:ASN:N	1.99	0.59
2:B:51:GLU:HB2	2:B:75:ILE:HD11	1.77	0.59
1:G:457:VAL:HG12	1:G:459:ARG:HG2	1.85	0.59
2:H:260:LEU:CD1	2:H:260:LEU:C	2.76	0.59
2:E:323:VAL:HG13	2:E:324:PRO:CD	2.28	0.59
3:F:254:LYS:HZ2	3:F:255:MET:H	1.50	0.58
3:I:15:ARG:O	3:I:19:MET:HG3	2.02	0.58
1:A:253:TYR:OH	10:A:586:CL:CL	2.55	0.58
14:A:804:HOH:O	1:D:43:LYS:HE3	2.02	0.58
1:A:120:ALA:HB1	1:A:249:MET:HE3	1.86	0.58
3:C:84:TYR:CE2	1:D:256:CYS:HB2	2.37	0.58
2:B:268:VAL:HG12	2:B:272:LYS:HE3	1.86	0.58
1:G:121:HIS:HE1	14:G:1981:HOH:O	1.86	0.58
1:D:84:HIS:HE1	1:D:320:GLU:OE2	1.87	0.58
1:A:38:LYS:HE3	8:A:583:PGE:H5	1.86	0.58
2:E:227:PRO:HB2	3:F:252:TRP:CZ3	2.38	0.58
1:G:180:LEU:CD2	1:G:218:ILE:CD1	2.81	0.57
2:H:191:PRO:HB3	7:H:434:1PE:H262	1.87	0.57
2:E:33:LYS:HB2	14:E:1864:HOH:O	2.04	0.57
2:E:288:THR:N	3:F:3:GLN:HE22	1.96	0.57
1:A:123:LEU:HD13	2:E:401:TYR:HB2	1.86	0.57
2:B:130:MET:O	2:B:134:THR:CG2	2.52	0.57
1:G:19:ALA:H	7:G:580:1PE:C16	2.17	0.57
2:H:315:ALA:HB3	3:I:70:VAL:HG11	1.87	0.57
1:A:2:PRO:HD2	3:C:280:GLU:CG	2.35	0.57
1:A:289:HIS:CD2	1:A:289:HIS:H	2.22	0.57
2:B:13:LYS:NZ	2:B:13:LYS:HB3	2.19	0.57
7:D:580:1PE:H141	1:G:186:ARG:HD3	1.87	0.56
2:E:272:LYS:HE2	2:E:290:TYR:CE1	2.40	0.56
2:E:280:LEU:HD12	2:E:291:ASP:HB2	1.87	0.56
2:H:16:ALA:CB	2:H:433:LYS:HE3	2.35	0.56
2:H:47:LEU:CD2	2:H:75:ILE:HD11	2.30	0.56
3:C:231:PRO:HG2	14:C:1960:HOH:O	2.05	0.56
2:E:92:VAL:HG23	2:E:93:GLU:N	2.21	0.56
1:G:180:LEU:CD2	1:G:218:ILE:HD11	2.35	0.56
2:B:321:GLN:N	2:B:322:PRO:CD	2.69	0.56
3:F:181:ASP:OD1	3:F:203:LYS:HE2	2.05	0.56
2:H:70:ASN:H	2:H:70:ASN:ND2	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:464:GL3:HA1	2:E:357:PHE:HB2	1.88	0.56
2:H:260:LEU:C	2:H:260:LEU:HD12	2.31	0.56
2:B:288:THR:N	3:C:3:GLN:HE22	1.91	0.56
6:G:1001:M43:C14	5:G:1003:COM:H22	2.36	0.56
2:B:192:VAL:HG13	2:B:390:CYS:HA	1.88	0.56
2:E:315:ALA:HB3	3:F:70:VAL:HG11	1.88	0.56
2:E:328:MET:HE2	2:E:353:VAL:HG22	1.87	0.55
2:B:323:VAL:HG13	2:B:324:PRO:HD3	1.87	0.55
1:G:488:GLU:HA	1:G:511:VAL:HG21	1.89	0.55
12:B:434:P6G:H112	14:B:952:HOH:O	2.06	0.55
1:A:164:MET:CE	1:D:573:ARG:HD2	2.36	0.55
12:B:434:P6G:H52	14:B:1691:HOH:O	2.07	0.55
1:D:74:GLN:HG2	14:D:1877:HOH:O	2.07	0.55
2:E:291:ASP:OD2	3:F:254:LYS:HE3	2.07	0.55
1:G:393:ILE:CD1	1:G:445:ALA:HA	2.37	0.55
1:A:79:PRO:HG3	8:A:583:PGE:H6	1.88	0.54
3:C:254:LYS:HD3	3:C:255:MET:N	2.19	0.54
2:E:321:GLN:N	2:E:322:PRO:CD	2.70	0.54
1:D:79:PRO:HB3	8:D:581:PGE:H6	1.90	0.54
2:B:295:MET:HE3	3:C:243:LYS:HE3	1.90	0.54
2:E:205:GLN:HG3	2:E:425:MET:HE1	1.89	0.54
3:F:46:GLY:HA3	7:F:281:1PE:H262	1.89	0.54
3:C:175:TRP:NE1	14:C:1265:HOH:O	2.30	0.54
2:H:70:ASN:H	2:H:70:ASN:HD22	1.56	0.54
2:E:321:GLN:N	2:E:322:PRO:HD3	2.22	0.54
2:H:29:ASN:OD1	2:H:31:ALA:HB3	2.07	0.54
2:E:130:MET:O	2:E:134:THR:HG22	2.08	0.54
1:A:30:TYR:CE2	3:C:173:ARG:HD3	2.43	0.54
3:F:173:ARG:NH1	14:F:1659:HOH:O	2.41	0.54
2:H:423:GLU:HG3	2:H:426:ARG:HD2	1.90	0.54
7:A:581:1PE:H231	1:D:59:ASN:HD22	1.72	0.53
1:D:216:LYS:NZ	14:D:1543:HOH:O	2.41	0.53
3:F:46:GLY:HA2	7:F:281:1PE:C25	2.38	0.53
2:H:134:THR:HG22	2:H:155:VAL:HG11	1.89	0.53
2:B:51:GLU:OE1	2:B:75:ILE:HD13	2.08	0.53
2:E:260:LEU:C	2:E:260:LEU:HD13	2.34	0.53
1:G:2:PRO:HD2	3:I:280:GLU:CG	2.39	0.53
1:A:268:TYR:HA	1:A:272:ALA:HB3	1.91	0.53
1:D:393:ILE:HG21	1:D:448:LEU:HB3	1.89	0.53
2:H:92:VAL:CG2	2:H:93:GLU:HG2	2.36	0.53
1:G:462:PHE:HB2	5:G:1003:COM:O2S	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:191:PRO:CG	7:H:434:1PE:H242	2.39	0.53
2:B:280:LEU:C	2:B:280:LEU:CD2	2.82	0.53
2:H:134:THR:CG2	2:H:155:VAL:HG11	2.39	0.53
2:H:318:ARG:HG3	3:I:56:LEU:HD11	1.90	0.53
2:E:257:ASP:CA	3:F:110:LYS:HD2	2.27	0.52
1:D:11:LEU:CD1	1:G:203:PRO:HB3	2.40	0.52
1:D:85:THR:HG22	1:D:546[B]:ARG:HD2	1.90	0.52
1:D:110:LYS:HD2	1:D:229:ALA:HB1	1.91	0.52
2:E:280:LEU:C	2:E:280:LEU:CD2	2.83	0.52
3:I:249:PHE:CE2	3:I:250:GLN:HG3	2.45	0.52
2:E:92:VAL:HG22	2:E:96:ASP:OD2	2.10	0.52
2:H:321:GLN:N	2:H:322:PRO:CD	2.73	0.52
1:A:511:VAL:HG13	1:A:523:VAL:CG1	2.37	0.52
3:I:64:CYS:HB3	3:I:67:ARG:CD	2.39	0.52
1:D:19:ALA:HA	1:G:186:ARG:NH2	2.24	0.52
1:D:43:LYS:HG3	14:D:598:HOH:O	2.10	0.52
1:G:464:GL3:CA	2:H:357:PHE:HB2	2.39	0.52
1:G:468:GLN:HB3	1:G:496:ASN:O	2.10	0.52
2:H:55:ALA:HB2	14:H:1667:HOH:O	2.09	0.52
3:I:64:CYS:HB3	3:I:67:ARG:HD3	1.90	0.52
3:F:46:GLY:HA2	7:F:281:1PE:C15	2.40	0.52
3:F:242:TRP:O	3:F:246:VAL:HG23	2.09	0.52
2:E:130:MET:O	2:E:134:THR:HG23	2.09	0.52
2:E:306:MET:SD	2:E:327:ILE:HG23	2.50	0.52
3:C:117:LEU:HD12	3:C:117:LEU:N	2.25	0.52
2:E:26:PRO:HA	2:E:32:ILE:HG21	1.92	0.52
3:F:82:ILE:O	3:F:83:ARG:HD2	2.09	0.52
2:H:218:GLN:HE21	2:H:232:HIS:HE1	1.56	0.52
14:A:1616:HOH:O	1:D:558:LYS:HE2	2.09	0.51
2:H:134:THR:HG22	2:H:155:VAL:HB	1.91	0.51
3:I:249:PHE:CD2	3:I:250:GLN:HG3	2.46	0.51
3:C:84:TYR:CZ	1:D:256:CYS:HB2	2.45	0.51
2:B:171:LYS:NZ	12:B:434:P6G:H21	2.25	0.51
1:G:289:HIS:H	1:G:289:HIS:CD2	2.26	0.51
1:A:72:GLN:NE2	1:D:158:MET:H	2.07	0.51
1:D:19:ALA:HA	1:G:186:ARG:HH21	1.75	0.51
3:F:27:LYS:HA	3:F:140:CYS:HA	1.92	0.51
1:G:30:TYR:CD2	3:I:173:ARG:HD3	2.46	0.51
2:H:191:PRO:HG3	7:H:434:1PE:H152	1.92	0.51
2:H:227:PRO:HB2	3:I:252:TRP:CZ3	2.45	0.51
2:E:78:LYS:HD3	2:E:140:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:GLY:O	1:A:485:MET:HB3	2.11	0.51
1:D:289:HIS:CD2	1:D:289:HIS:H	2.29	0.51
1:G:106:TRP:CZ2	1:G:292:PRO:HD3	2.45	0.51
6:G:1001:M43:N13	5:G:1003:COM:H22	2.26	0.51
2:E:210:THR:HG21	2:E:386:ILE:HG22	1.92	0.51
2:B:320:GLY:C	2:B:322:PRO:HD2	2.36	0.50
1:D:546[A]:ARG:HD3	1:G:546:ARG:HD3	1.93	0.50
2:E:218:GLN:NE2	2:E:223:ASN:HD22	2.08	0.50
2:B:227:PRO:HB2	3:C:252:TRP:CZ3	2.46	0.50
3:C:35:ASP:OD1	3:C:197:LYS:HE3	2.11	0.50
1:D:315:ILE:HD11	1:D:365:CYS:HB2	1.93	0.50
2:E:133:LEU:O	2:E:137:ILE:HG13	2.11	0.50
2:H:8:TYR:HB2	2:H:242:ASN:ND2	2.27	0.50
2:B:13:LYS:HB3	2:B:13:LYS:HZ3	1.77	0.50
3:C:58:GLU:HG3	3:C:58:GLU:O	2.10	0.50
3:I:104:GLU:HG2	3:I:108:ARG:HD2	1.93	0.50
3:C:254:LYS:HA	3:C:254:LYS:HZ2	1.76	0.50
1:A:578:LYS:HD2	1:A:578:LYS:N	2.27	0.50
2:B:331:CYS:SG	2:B:343:PRO:HD2	2.52	0.50
2:B:84:LYS:HG3	2:B:85:ALA:N	2.25	0.50
1:A:318:GLU:HG2	1:A:509:GLY:O	2.12	0.50
2:B:323:VAL:CG1	2:B:324:PRO:HD3	2.41	0.50
3:F:40:LEU:HB3	3:F:42:HIS:CD2	2.47	0.50
2:H:210:THR:HG21	2:H:386:ILE:HG22	1.93	0.50
2:B:191:PRO:CD	12:B:434:P6G:H111	2.39	0.49
3:F:19:MET:O	3:F:21:PRO:HD3	2.12	0.49
2:H:280:LEU:O	2:H:280:LEU:HD23	2.12	0.49
2:H:323:VAL:HG12	2:H:324:PRO:HD3	1.92	0.49
1:D:476:SER:HB3	1:D:477:TYR:CD2	2.47	0.49
1:A:121:HIS:CE1	10:A:586:CL:CL	2.93	0.49
2:E:295:MET:HE1	2:E:340:LEU:CD2	2.43	0.49
2:H:323:VAL:HG13	2:H:324:PRO:CD	2.38	0.49
2:B:200:ARG:HG3	14:B:445:HOH:O	2.13	0.49
2:B:215:GLU:OE2	2:B:215:GLU:HA	2.12	0.49
1:D:180:LEU:O	1:D:180:LEU:HG	2.12	0.49
1:D:380:LYS:HE2	1:D:436:THR:O	2.13	0.49
3:F:35:ASP:OD1	3:F:197:LYS:HE3	2.13	0.49
1:A:278:SER:HB2	1:A:294:GLY:C	2.38	0.49
1:G:399:TYR:HD1	3:I:274:THR:HG22	1.78	0.49
2:H:321:GLN:N	2:H:322:PRO:HD3	2.27	0.49
2:B:210:THR:CG2	2:B:386:ILE:HG22	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:226:GLN:NE2	14:F:1278:HOH:O	2.45	0.49
1:A:72:GLN:HE22	1:D:158:MET:H	1.59	0.48
1:G:19:ALA:H	7:G:580:1PE:H161	1.77	0.48
1:G:153:VAL:HG23	1:G:154:ILE:HG12	1.95	0.48
1:D:158:MET:HE2	1:D:158:MET:HA	1.95	0.48
2:E:227:PRO:HB2	3:F:252:TRP:CH2	2.48	0.48
3:F:127:GLU:O	3:F:130:ILE:HG22	2.14	0.48
1:G:167:ASN:H	1:G:167:ASN:ND2	2.06	0.48
2:H:134:THR:HG22	2:H:155:VAL:HG21	1.95	0.48
3:I:34:GLU:HG2	3:I:38:ARG:HH12	1.79	0.48
2:B:205:GLN:HA	2:B:425:MET:HE1	1.96	0.48
1:D:180:LEU:HD22	1:D:218:ILE:HG12	1.95	0.48
2:E:336:ARG:HE	3:F:5:THR:CG2	2.22	0.48
1:D:464:GL3:CA	2:E:357:PHE:HB2	2.44	0.48
2:E:110:MET:HG3	2:E:414:VAL:CG1	2.44	0.48
1:G:326:ALA:O	1:G:330:ASP:HB2	2.13	0.48
2:H:134:THR:HG22	2:H:155:VAL:CG1	2.43	0.48
1:A:173:ILE:HG13	1:A:189:ILE:HD13	1.95	0.48
1:D:34:GLY:O	1:D:37:GLN:HG2	2.14	0.48
1:A:162:LYS:NZ	1:D:49:GLU:OE2	2.42	0.48
3:C:209:GLU:OE2	3:C:213:LYS:HE2	2.14	0.48
1:G:319:LEU:HD13	1:G:358:GLU:CD	2.39	0.48
2:H:210:THR:CG2	2:H:386:ILE:HG22	2.43	0.48
2:E:229:GLU:OE1	14:E:1940:HOH:O	2.19	0.48
1:A:2:PRO:HD2	3:C:280:GLU:HG2	1.95	0.48
1:A:344:PHE:CZ	4:A:1002:TP7:H71C	2.48	0.48
2:B:76:VAL:HG23	2:B:77:ASP:N	2.29	0.48
1:G:393:ILE:HD13	1:G:445:ALA:HA	1.96	0.48
2:H:114:PRO:HB2	14:H:1329:HOH:O	2.13	0.48
1:A:2:PRO:HA	1:A:399:TYR:OH	2.14	0.47
3:I:164:LYS:HE3	3:I:164:LYS:HB3	1.60	0.47
3:C:17:ASN:HB3	3:C:23:TYR:CD2	2.49	0.47
2:E:134:THR:HG21	2:E:156:TRP:HE1	1.78	0.47
2:E:210:THR:CG2	2:E:386:ILE:HG22	2.44	0.47
2:H:5:ILE:HD13	2:H:19:VAL:O	2.14	0.47
1:A:29:PHE:CE1	3:C:163:ASP:HB3	2.49	0.47
1:A:110:LYS:HD2	1:A:229:ALA:HB1	1.96	0.47
1:A:158:MET:H	1:D:72:GLN:NE2	2.11	0.47
5:A:1003:COM:O2S	3:C:117:LEU:HD23	2.14	0.47
1:G:319:LEU:HD13	1:G:358:GLU:OE1	2.15	0.47
3:I:53:HIS:CE1	3:I:79:GLY:HA2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:NH1	7:A:581:1PE:H232	2.29	0.47
2:E:108:ARG:HD2	2:E:413:GLU:OE2	2.14	0.47
1:G:473:ALA:O	1:G:476:SER:HB3	2.14	0.47
1:A:326:ALA:O	1:A:330:ASP:HB2	2.14	0.47
2:H:215:GLU:HG3	2:H:236:LEU:HB2	1.96	0.47
2:H:423:GLU:HB3	2:H:426:ARG:HB2	1.97	0.47
1:A:164:MET:CE	1:D:573:ARG:CG	2.93	0.47
6:A:1001:M43:O50	2:E:361:SER:HB2	2.15	0.47
2:E:29:ASN:OD1	2:E:31:ALA:HB3	2.14	0.47
2:H:423:GLU:OE2	2:H:423:GLU:HA	2.14	0.47
1:A:31:THR:OG1	8:A:582:PGE:H2	2.13	0.47
1:A:456:ARG:HB2	3:C:226:GLN:HE22	1.79	0.47
2:B:291:ASP:OD1	3:C:254:LYS:HE3	2.14	0.47
1:D:83:ASN:O	1:D:85:THR:HG23	2.14	0.47
1:D:414:HIS:HB3	1:D:419:VAL:HG23	1.96	0.47
7:E:434:1PE:H151	14:E:1309:HOH:O	2.15	0.47
3:F:208:ALA:O	3:F:212:LYS:HG3	2.14	0.47
1:G:2:PRO:HD3	1:G:407:TYR:CE2	2.50	0.47
2:H:381:ALA:HB3	2:H:385:PHE:HB2	1.96	0.47
1:A:30:TYR:CD2	3:C:173:ARG:HD3	2.50	0.47
1:D:30:TYR:CE2	3:F:173:ARG:HD3	2.49	0.47
1:G:287:ARG:HD3	1:G:333:0AF:HH2	1.96	0.47
1:G:488:GLU:HG3	1:G:511:VAL:CG2	2.45	0.47
1:A:38:LYS:HE3	8:A:583:PGE:C5	2.44	0.47
6:A:1001:M43:C59	6:A:1001:M43:C54	2.93	0.47
2:B:283:MET:HB3	2:B:284:PRO:HD2	1.96	0.47
1:A:511:VAL:CG1	1:A:523:VAL:HG11	2.38	0.47
1:D:153:VAL:CG2	1:D:247:MET:HB3	2.44	0.47
1:D:399:TYR:O	1:D:403:GLN:HG2	2.15	0.47
2:E:285:SER:HA	3:F:8:ASN:OD1	2.15	0.47
3:F:254:LYS:HD2	3:F:254:LYS:HA	1.49	0.47
1:A:159:VAL:HB	1:D:92:ASP:HA	1.97	0.46
2:B:321:GLN:HG2	2:B:322:PRO:HD3	1.97	0.46
3:I:67:ARG:HD2	14:I:1397:HOH:O	2.15	0.46
1:A:84:HIS:HE1	1:A:320:GLU:OE2	1.98	0.46
6:A:1001:M43:O28	6:A:1001:M43:H29	2.15	0.46
1:D:38:LYS:HE3	8:D:581:PGE:O4	2.15	0.46
2:E:218:GLN:NE2	2:E:382:LYS:HB3	2.30	0.46
3:F:116:VAL:C	3:F:117:LEU:HD12	2.40	0.46
1:A:464:GL3:HA2	2:B:353:VAL:HG12	1.97	0.46
2:B:134:THR:HG22	2:B:155:VAL:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:47:LEU:HD22	2:E:75:ILE:HD12	1.97	0.46
2:H:91[A]:ARG:HG3	2:H:91[A]:ARG:NH1	2.31	0.46
1:A:498:ALA:C	1:A:499:MHO:HG2	2.41	0.46
2:B:260:LEU:C	2:B:260:LEU:HD13	2.41	0.46
1:D:293:GLY:HA2	1:D:492:VAL:HG23	1.97	0.46
1:D:399:TYR:CD2	1:D:399:TYR:C	2.94	0.46
7:E:434:1PE:H141	14:E:1664:HOH:O	2.15	0.46
1:G:7:GLN:HG3	1:G:8:HIS:CD2	2.51	0.46
2:B:8:TYR:CE2	2:B:14:LYS:HB2	2.49	0.46
1:D:406:ALA:C	1:D:408:PRO:HD3	2.41	0.46
2:B:29:ASN:OD1	2:B:31:ALA:HB3	2.15	0.46
2:E:47:LEU:C	2:E:75:ILE:HD11	2.39	0.46
2:E:423:GLU:HA	2:E:423:GLU:OE2	2.15	0.46
1:G:178:ASP:OD2	1:G:211:LYS:NZ	2.49	0.46
2:E:272:LYS:HE2	2:E:290:TYR:OH	2.14	0.46
3:F:146:ALA:HB2	3:F:204:PRO:HB3	1.98	0.46
1:A:41:MET:HE3	14:A:606:HOH:O	2.16	0.46
2:H:26:PRO:HA	2:H:32:ILE:HG21	1.97	0.46
1:A:464:GL3:HA1	2:B:357:PHE:HB2	1.98	0.46
2:B:261:GLY:HA3	3:C:107:ASN:OD1	2.16	0.46
1:A:230:ARG:HA	1:D:230:ARG:O	2.15	0.45
2:E:92:VAL:HG23	2:E:93:GLU:H	1.80	0.45
2:E:192:VAL:HG13	2:E:390:CYS:HA	1.97	0.45
1:G:464:GL3:HA2	2:H:353:VAL:HG12	1.99	0.45
2:E:24:ILE:C	2:E:24:ILE:HD12	2.40	0.45
2:E:208:GLY:O	2:E:212:ILE:HG13	2.16	0.45
3:C:67:ARG:NH1	14:C:1593:HOH:O	2.48	0.45
2:E:134:THR:HG21	2:E:156:TRP:NE1	2.32	0.45
1:D:317:ALA:HB1	14:D:1473:HOH:O	2.16	0.45
1:A:377:ALA:O	1:A:380:LYS:HE2	2.17	0.45
2:H:303:CYS:SG	2:H:384:GLN:HG2	2.57	0.45
2:B:166:GLY:O	12:B:434:P6G:H32	2.17	0.45
2:H:280:LEU:HD23	2:H:280:LEU:C	2.42	0.45
2:B:401:TYR:HB2	1:D:123:LEU:HD13	1.99	0.45
1:D:306:SER:HB3	1:D:307:PRO:HD3	1.98	0.45
1:D:456:ARG:HB2	3:F:226:GLN:NE2	2.32	0.45
1:A:207:ALA:O	1:A:211:LYS:HG3	2.16	0.45
2:B:51:GLU:CB	2:B:75:ILE:HD12	2.39	0.45
2:B:336:ARG:HB3	3:C:5:THR:CG2	2.42	0.45
1:D:9:ASN:HB2	1:D:359:ASP:OD2	2.16	0.45
1:D:293:GLY:HA2	1:D:492:VAL:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:126:LEU:HD11	2:E:130:MET:HE3	1.99	0.45
2:H:318:ARG:HG3	3:I:56:LEU:CD1	2.47	0.45
1:A:121:HIS:HD2	14:A:666:HOH:O	1.99	0.44
1:A:202:LYS:O	1:A:205:GLU:HG3	2.17	0.44
2:B:74:PRO:HB2	2:B:77:ASP:HB2	1.98	0.44
1:G:480:GLN:O	1:G:481:SER:C	2.59	0.44
2:B:160:PRO:HD2	1:D:485:MET:CG	2.47	0.44
2:B:215:GLU:HG3	2:B:236:LEU:HB2	1.98	0.44
1:G:464:GL3:HA1	2:H:357:PHE:HB2	1.99	0.44
2:E:103:ILE:HG22	2:E:104:ALA:N	2.32	0.44
1:G:579:LEU:HD12	1:G:579:LEU:HA	1.77	0.44
1:A:123:LEU:HD13	2:E:401:TYR:CB	2.47	0.44
1:D:114:VAL:HB	1:D:275:VAL:HB	1.99	0.44
2:E:260:LEU:HD13	2:E:260:LEU:O	2.17	0.44
1:G:498:ALA:C	1:G:499:MHO:HG2	2.41	0.44
2:H:16:ALA:HB1	2:H:433:LYS:HE3	1.97	0.44
1:A:230:ARG:O	1:D:230:ARG:HA	2.17	0.44
1:A:279:ASN:HD22	1:A:279:ASN:HA	1.66	0.44
2:E:9:ASP:HB3	2:E:15:LEU:HD21	1.99	0.44
2:E:37:ASN:OD1	2:E:41:ARG:HD3	2.18	0.44
3:F:187:VAL:HG12	3:F:198:GLU:HG2	1.99	0.44
1:G:158:MET:HE2	1:G:158:MET:HA	1.99	0.44
2:H:192:VAL:HG13	2:H:390:CYS:HA	2.00	0.44
1:D:84:HIS:CD2	1:D:358:GLU:OE1	2.62	0.44
1:G:180:LEU:CD2	1:G:218:ILE:HG12	2.48	0.44
2:H:134:THR:HG22	2:H:155:VAL:CG2	2.48	0.44
1:A:573:ARG:HG3	1:D:164:MET:HE1	1.99	0.44
1:D:12:LYS:HE3	1:G:194:LYS:O	2.17	0.44
3:I:3:GLN:O	3:I:4:PHE:HB2	2.18	0.44
3:I:55:PRO:HD2	3:I:58:GLU:OE2	2.18	0.44
1:A:164:MET:CE	1:D:573:ARG:HG3	2.46	0.44
2:E:159:TYR:CD1	2:E:160:PRO:HA	2.53	0.44
1:G:18:PHE:HA	7:G:580:1PE:H162	1.99	0.44
1:G:399:TYR:CD1	3:I:274:THR:HG22	2.53	0.44
2:B:320:GLY:C	2:B:322:PRO:CD	2.91	0.43
3:C:5:THR:HG21	3:C:103:TRP:CZ3	2.52	0.43
1:G:261:VAL:HG12	1:G:265:PHE:CE1	2.52	0.43
2:E:281:LYS:NZ	3:F:264:ASP:OD2	2.47	0.43
1:G:110:LYS:HD2	1:G:229:ALA:HB1	2.01	0.43
2:H:260:LEU:CD1	2:H:260:LEU:O	2.66	0.43
1:A:476:SER:HB3	1:A:477:TYR:CD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:84:TYR:HB3	14:C:780:HOH:O	2.19	0.43
1:D:464:GL3:HA2	2:E:353:VAL:HG12	2.00	0.43
2:H:71:ARG:HE	2:H:147:ASP:CG	2.25	0.43
2:H:191:PRO:HG3	7:H:434:1PE:H242	2.00	0.43
3:I:155:VAL:O	3:I:156:HIS:C	2.61	0.43
2:B:84:LYS:HD3	2:B:88:ASP:OD2	2.18	0.43
2:B:124:VAL:HG22	2:E:220:GLU:HA	2.01	0.43
1:D:29:PHE:HZ	3:F:161:ARG:O	2.01	0.43
2:H:218:GLN:HE22	2:H:223:ASN:HD22	1.67	0.43
1:A:404:TYR:CD2	1:A:410:VAL:HG12	2.52	0.43
2:B:340:LEU:HB3	2:B:341:PRO:HD2	2.00	0.43
1:D:346:GLN:HA	1:D:349:SER:OG	2.18	0.43
2:E:335:GLU:HG2	2:E:340:LEU:O	2.19	0.43
1:G:242:GLY:C	1:G:243:MET:HE2	2.43	0.43
2:H:92:VAL:HG21	2:H:116:ALA:HB3	1.99	0.43
2:H:110:MET:CE	2:H:112:GLN:CD	2.90	0.43
2:H:317:MET:HE2	3:I:111:GLY:O	2.18	0.43
2:E:375:HIS:HE1	2:E:377:VAL:HG23	1.82	0.43
1:G:32:TYR:CZ	8:G:582:PGE:H3	2.54	0.43
6:G:1001:M43:O28	6:G:1001:M43:H29	2.18	0.43
2:H:134:THR:HG21	2:H:156:TRP:NE1	2.34	0.43
2:H:386:ILE:N	2:H:387:PRO:CD	2.82	0.43
1:A:342:VAL:HB	6:D:1001:M43:H59	2.00	0.43
1:G:279:ASN:HD22	1:G:279:ASN:HA	1.64	0.43
2:H:5:ILE:HD13	2:H:5:ILE:N	2.34	0.43
3:I:62:PRO:O	3:I:64:CYS:N	2.50	0.43
1:A:462:PHE:CB	5:A:1003:COM:H22	2.43	0.43
2:B:332:CYS:O	2:B:336:ARG:HG2	2.19	0.43
1:G:377:ALA:O	1:G:380:LYS:HE2	2.19	0.42
1:D:404:TYR:CD2	1:D:410:VAL:HG12	2.53	0.42
2:H:283:MET:HB3	2:H:284:PRO:HD2	2.01	0.42
3:C:163:ASP:C	3:C:163:ASP:OD1	2.62	0.42
3:F:53:HIS:CE1	3:F:79:GLY:HA2	2.53	0.42
3:F:227:GLU:OE2	3:F:227:GLU:HA	2.19	0.42
1:D:393:ILE:HD13	1:D:445:ALA:HA	2.01	0.42
2:E:276:VAL:HG21	2:E:301:TYR:CZ	2.54	0.42
1:G:9:ASN:OD1	1:G:9:ASN:C	2.62	0.42
3:I:64:CYS:O	3:I:68:GLN:HG3	2.19	0.42
1:A:167:ASN:H	1:A:167:ASN:ND2	2.05	0.42
2:E:280:LEU:HB3	2:E:289:VAL:O	2.20	0.42
1:G:84:HIS:CE1	1:G:320:GLU:OE2	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ALA:HB2	1:A:268:TYR:CZ	2.55	0.42
2:B:306:MET:SD	2:B:327:ILE:HG23	2.59	0.42
1:D:356:ILE:HD13	1:D:410:VAL:HG13	2.01	0.42
1:D:463:PHE:CB	5:D:1003:COM:O2S	2.55	0.42
1:G:4:ASN:ND2	1:G:4:ASN:C	2.77	0.42
3:C:116:VAL:C	3:C:117:LEU:HD12	2.45	0.42
2:E:33:LYS:HB2	2:E:33:LYS:HE2	1.73	0.42
2:E:92:VAL:HG21	2:E:116:ALA:HB3	2.01	0.42
2:E:386:ILE:N	2:E:387:PRO:CD	2.83	0.42
3:F:117:LEU:HD12	3:F:117:LEU:N	2.34	0.42
2:H:256:GLN:O	3:I:110:LYS:HE2	2.19	0.42
1:A:574:GLU:HA	1:A:575:PRO:HD3	1.93	0.42
2:B:321:GLN:N	2:B:322:PRO:HD3	2.33	0.42
1:D:180:LEU:CD2	1:D:218:ILE:HG12	2.50	0.42
2:E:9:ASP:CG	2:E:11:LYS:HG2	2.44	0.42
1:G:295:MET:HA	1:G:296:PRO:HD3	1.87	0.42
2:H:9:ASP:CG	2:H:11:LYS:HG2	2.44	0.42
2:E:191:PRO:HA	2:E:372:TYR:HB3	2.00	0.42
2:E:332:CYS:O	2:E:336:ARG:HG2	2.20	0.42
1:A:158:MET:H	1:D:72:GLN:HE22	1.68	0.42
2:B:75:ILE:HB	2:B:82:ILE:CD1	2.50	0.42
1:D:85:THR:HG22	1:D:546[B]:ARG:HH11	1.84	0.42
3:F:144:ASP:O	3:F:148:THR:HB	2.20	0.42
2:H:272:LYS:HE2	2:H:290:TYR:CZ	2.54	0.42
1:A:167:ASN:N	1:A:167:ASN:ND2	2.67	0.41
2:B:191:PRO:HB3	12:B:434:P6G:H172	2.01	0.41
12:B:434:P6G:H82	14:B:1691:HOH:O	2.18	0.41
1:D:164:MET:HE3	14:D:1005:HOH:O	2.19	0.41
1:D:218:ILE:HD11	8:D:582:PGE:H1	2.02	0.41
2:H:92:VAL:HG13	2:H:114:PRO:HG3	2.02	0.41
2:H:191:PRO:HD3	7:H:434:1PE:H242	2.02	0.41
1:A:140:TYR:CD1	1:A:248:THR:HG22	2.55	0.41
1:A:180:LEU:HD22	1:A:218:ILE:CD1	2.50	0.41
1:A:357:LEU:HD11	1:A:426:ALA:HB3	2.01	0.41
3:F:250:GLN:O	3:F:253:ALA:HB3	2.20	0.41
1:G:289:HIS:HD2	14:G:1190:HOH:O	2.03	0.41
2:H:205:GLN:NE2	2:H:423:GLU:OE1	2.50	0.41
3:I:138:VAL:O	3:I:138:VAL:HG12	2.20	0.41
1:A:148:LEU:N	1:A:149:PRO:CD	2.83	0.41
1:A:492:VAL:CG1	1:A:504:GLN:HG3	2.50	0.41
2:B:227:PRO:HB2	3:C:252:TRP:CH2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:LYS:NZ	2:B:274:ASP:OD1	2.51	0.41
2:H:320:GLY:C	2:H:322:PRO:CD	2.93	0.41
3:I:116:VAL:C	3:I:117:LEU:HD12	2.46	0.41
1:A:43:LYS:HE3	14:D:723:HOH:O	2.20	0.41
1:A:573:ARG:HD2	1:D:164:MET:HE2	2.01	0.41
2:E:295:MET:HE3	3:F:243:LYS:CE	2.50	0.41
1:G:278:SER:HB2	1:G:294:GLY:C	2.46	0.41
1:G:476:SER:OG	1:G:477:TYR:CE2	2.73	0.41
1:A:148:LEU:HB3	1:A:149:PRO:HD3	2.03	0.41
1:D:349:SER:HA	1:D:352:TYR:CZ	2.56	0.41
1:G:180:LEU:HD21	1:G:218:ILE:CD1	2.50	0.41
1:G:465:TYR:CE1	1:G:503:HIS:CE1	3.09	0.41
2:H:260:LEU:O	2:H:260:LEU:HD13	2.21	0.41
3:C:130:ILE:HD12	3:C:130:ILE:HA	1.91	0.41
2:E:260:LEU:C	2:E:260:LEU:CD1	2.93	0.41
2:E:295:MET:HE3	3:F:243:LYS:HE3	2.02	0.41
1:G:525:SER:HA	1:G:526:PRO:HD2	1.94	0.41
2:H:148:ALA:N	2:H:149:PRO:CD	2.83	0.41
1:D:297:LEU:HD13	1:D:507:TYR:HB3	2.03	0.41
3:F:262:LYS:HB3	3:F:262:LYS:HE2	1.91	0.41
1:G:484:GLY:O	1:G:485:MET:HB3	2.20	0.41
2:H:92:VAL:HG21	2:H:116:ALA:HB1	2.02	0.41
1:A:464:GL3:HA2	2:B:353:VAL:CG1	2.51	0.41
2:B:238:TYR:HA	2:B:243:ALA:HB3	2.03	0.41
2:B:329:GLN:OE1	2:B:329:GLN:HA	2.21	0.41
3:C:155:VAL:O	3:C:156:HIS:C	2.64	0.41
1:D:115:LEU:HD13	1:D:220:GLN:HE22	1.85	0.41
2:E:11:LYS:HG3	2:E:13:LYS:HG3	2.03	0.41
2:E:261:GLY:HA3	3:F:107:ASN:OD1	2.21	0.41
2:E:425:MET:HE2	2:E:425:MET:HB2	1.89	0.41
2:H:335:GLU:HG2	2:H:340:LEU:O	2.21	0.41
3:I:62:PRO:HD2	3:I:67:ARG:CZ	2.50	0.41
3:I:164:LYS:O	3:I:164:LYS:HG2	2.20	0.41
1:A:464:GL3:CA	2:B:357:PHE:HB2	2.50	0.41
14:A:1930:HOH:O	2:E:402:PHE:HB2	2.21	0.41
2:B:14:LYS:NZ	2:B:17:ALA:CB	2.78	0.41
1:D:79:PRO:CB	8:D:581:PGE:H6	2.50	0.41
8:A:583:PGE:H42	8:A:583:PGE:H22	1.86	0.40
1:D:498:ALA:C	1:D:499:MHO:HG2	2.45	0.40
3:I:249:PHE:O	3:I:250:GLN:HG2	2.21	0.40
1:A:199:GLY:HA3	1:A:202:LYS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:GLN:HE22	2:B:223:ASN:HD22	1.68	0.40
2:B:295:MET:HE1	2:B:340:LEU:CD2	2.51	0.40
1:D:393:ILE:CD1	1:D:445:ALA:HA	2.51	0.40
1:A:9:ASN:OD1	1:A:9:ASN:C	2.65	0.40
2:B:46:ASP:HA	2:B:108:ARG:HG2	2.04	0.40
2:E:391:ALA:O	2:E:395:ILE:HG13	2.21	0.40
1:A:460:LEU:HD23	1:A:466:ASP:HB3	2.03	0.40
2:B:24:ILE:C	2:B:24:ILE:HD12	2.47	0.40
2:B:430:GLU:HA	2:B:433:LYS:HD3	2.03	0.40
2:H:110:MET:HE3	2:H:112:GLN:NE2	2.36	0.40
2:H:227:PRO:HB2	3:I:252:TRP:CH2	2.56	0.40
2:H:287:PHE:CD2	2:H:287:PHE:C	2.99	0.40
1:A:82:MET:HE1	1:A:352:TYR:CD1	2.57	0.40
1:A:157:HIS:N	1:D:72:GLN:HE22	2.20	0.40
2:B:51:GLU:OE1	2:B:76:VAL:HG13	2.21	0.40
2:E:227:PRO:HB2	3:F:252:TRP:CE3	2.56	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	572/579 (99%)	547 (96%)	23 (4%)	2 (0%)	36	36
1	D	573/579 (99%)	545 (95%)	26 (4%)	2 (0%)	36	36
1	G	572/579 (99%)	547 (96%)	24 (4%)	1 (0%)	43	44
2	B	429/433 (99%)	421 (98%)	8 (2%)	0	100	100
2	E	429/433 (99%)	418 (97%)	11 (3%)	0	100	100
2	H	430/433 (99%)	417 (97%)	13 (3%)	0	100	100
3	C	276/279 (99%)	267 (97%)	8 (3%)	1 (0%)	30	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	277/279 (99%)	269 (97%)	8 (3%)	0	100	100
3	I	276/279 (99%)	267 (97%)	8 (3%)	1 (0%)	30	28
All	All	3834/3873 (99%)	3698 (96%)	129 (3%)	7 (0%)	43	44

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	481	SER
1	A	481	SER
1	D	481	SER
3	I	4	PHE
1	A	339	SER
3	C	4	PHE
1	D	339	SER

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	453/454 (100%)	434 (96%)	19 (4%)	26	28
1	D	454/454 (100%)	437 (96%)	17 (4%)	30	33
1	G	453/454 (100%)	438 (97%)	15 (3%)	33	37
2	B	331/332 (100%)	317 (96%)	14 (4%)	26	28
2	E	331/332 (100%)	320 (97%)	11 (3%)	33	37
2	H	332/332 (100%)	322 (97%)	10 (3%)	36	41
3	C	231/232 (100%)	224 (97%)	7 (3%)	36	41
3	F	232/232 (100%)	224 (97%)	8 (3%)	32	35
3	I	231/232 (100%)	226 (98%)	5 (2%)	45	53
All	All	3048/3054 (100%)	2942 (96%)	106 (4%)	32	35

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	12	LYS
1	A	115	LEU
1	A	125	GLU
1	A	159	VAL
1	A	167	ASN
1	A	268	TYR
1	A	279	ASN
1	A	287	ARG
1	A	370	ASP
1	A	384	LEU
1	A	387	ASP
1	A	438	LEU
1	A	454	TYR
1	A	476	SER
1	A	511	VAL
1	A	524	LEU
1	A	567	ILE
1	A	579	LEU
2	B	5	ILE
2	B	13	LYS
2	B	70	ASN
2	B	75	ILE
2	B	80	LYS
2	B	81	GLU
2	B	84	LYS
2	B	133	LEU
2	B	134	THR
2	B	195	LEU
2	B	247	LEU
2	B	260	LEU
2	B	278	LYS
2	B	280	LEU
3	C	11	VAL
3	C	57	GLU
3	C	68	GLN
3	C	99	TYR
3	C	117	LEU
3	C	173	ARG
3	C	254	LYS
1	D	12	LYS
1	D	115	LEU
1	D	117	LEU

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Mol	Chain	Res	Type
1	D	159	VAL
1	D	167	ASN
1	D	268	TYR
1	D	279	ASN
1	D	287	ARG
1	D	370	ASP
1	D	384	LEU
1	D	387	ASP
1	D	438	LEU
1	D	454	TYR
1	D	476	SER
1	D	511	VAL
1	D	524	LEU
1	D	579	LEU
2	E	5	ILE
2	E	33	LYS
2	E	75	ILE
2	E	80	LYS
2	E	133	LEU
2	E	134	THR
2	E	142	ASN
2	E	195	LEU
2	E	247	LEU
2	E	260	LEU
2	E	386	ILE
3	F	5	THR
3	F	33	GLU
3	F	59	MET
3	F	60	GLU
3	F	99	TYR
3	F	173	ARG
3	F	254	LYS
3	F	268	LYS
1	G	4	ASN
1	G	12	LYS
1	G	115	LEU
1	G	117	LEU
1	G	159	VAL
1	G	167	ASN
1	G	268	TYR
1	G	279	ASN
1	G	287	ARG

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Mol	Chain	Res	Type
1	G	384	LEU
1	G	387	ASP
1	G	438	LEU
1	G	454	TYR
1	G	524	LEU
1	G	579	LEU
2	H	5	ILE
2	H	70	ASN
2	H	75	ILE
2	H	76	VAL
2	H	133	LEU
2	H	195	LEU
2	H	247	LEU
2	H	260	LEU
2	H	270	LYS
2	H	386	ILE
3	I	24	LYS
3	I	99	TYR
3	I	164	LYS
3	I	173	ARG
3	I	256	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	72	GLN
1	A	74	GLN
1	A	84	HIS
1	A	90	ASN
1	A	121	HIS
1	A	167	ASN
1	A	276	GLN
1	A	279	ASN
1	A	289	HIS
1	A	468	GLN
2	B	99	ASN
2	B	218	GLN
2	B	313	ASN
2	B	326	ASN
3	C	3	GLN
3	C	68	GLN

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Mol	Chain	Res	Type
3	C	226	GLN
1	D	59	ASN
1	D	72	GLN
1	D	84	HIS
1	D	121	HIS
1	D	167	ASN
1	D	279	ASN
1	D	289	HIS
2	E	218	GLN
2	E	313	ASN
2	E	326	ASN
3	F	3	GLN
3	F	226	GLN
3	F	250	GLN
1	G	74	GLN
1	G	84	HIS
1	G	121	HIS
1	G	167	ASN
1	G	279	ASN
1	G	289	HIS
1	G	468	GLN
1	G	480	GLN
2	H	70	ASN
2	H	218	GLN
2	H	256	GLN
2	H	313	ASN
2	H	326	ASN
3	I	3	GLN
3	I	68	GLN
3	I	226	GLN
3	I	250	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	D	464	1	2,3,4	2.80	1 (50%)	1,2,4	0.12	0
1	MHS	G	271	1	10,11,12	1.39	2 (20%)	5,14,16	3.08	1 (20%)
1	0AF	G	333	1	15,16,17	1.06	1 (6%)	14,22,24	1.11	2 (14%)
1	GL3	A	464	1	2,3,4	2.98	1 (50%)	1,2,4	0.47	0
1	0AF	A	333	1	15,16,17	1.02	2 (13%)	14,22,24	1.27	2 (14%)
1	0AF	D	333	1	15,16,17	1.03	1 (6%)	14,22,24	1.20	2 (14%)
1	MHO	D	499	1	6,8,9	0.74	0	3,9,11	1.69	1 (33%)
1	MHS	D	271	1	10,11,12	1.28	1 (10%)	5,14,16	3.02	1 (20%)
1	GL3	G	464	1	2,3,4	2.60	1 (50%)	1,2,4	0.25	0
1	MHO	G	499	1	6,8,9	0.76	0	3,9,11	2.38	2 (66%)
1	MHO	A	499	1	6,8,9	0.63	0	3,9,11	1.64	1 (33%)
1	MHS	A	271	1	10,11,12	1.07	0	5,14,16	3.89	2 (40%)

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	D	464	1	-	1/1/1/2	-
1	MHS	G	271	1	-	0/5/6/8	0/1/1/1
1	0AF	G	333	1	-	0/5/6/8	0/2/2/2
1	GL3	A	464	1	-	0/1/1/2	-
1	0AF	A	333	1	-	0/5/6/8	0/2/2/2
1	0AF	D	333	1	-	0/5/6/8	0/2/2/2
1	MHO	D	499	1	-	3/6/7/9	-
1	MHS	D	271	1	-	0/5/6/8	0/1/1/1
1	GL3	G	464	1	-	1/1/1/2	-
1	MHO	G	499	1	-	3/6/7/9	-
1	MHO	A	499	1	-	3/6/7/9	-
1	MHS	A	271	1	-	0/5/6/8	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	464	GL3	C-S	-4.17	1.63	1.80
1	D	464	GL3	C-S	-3.89	1.64	1.80
1	G	464	GL3	C-S	-3.57	1.66	1.80
1	D	333	0AF	CD1-NE1	2.65	1.41	1.37
1	G	271	MHS	CD2-CG	2.49	1.40	1.36
1	G	271	MHS	CG-ND1	-2.30	1.34	1.38
1	A	333	0AF	CD1-NE1	2.25	1.40	1.37
1	D	271	MHS	CD2-CG	2.25	1.39	1.36
1	G	333	0AF	O-C	2.23	1.28	1.20
1	A	333	0AF	O-C	2.09	1.27	1.20

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	MHS	ND1-CE1-NE2	-7.96	108.20	112.94
1	G	271	MHS	ND1-CE1-NE2	-6.47	109.09	112.94
1	D	271	MHS	ND1-CE1-NE2	-6.29	109.19	112.94
1	A	333	0AF	CE2-NE1-CD1	-2.97	106.37	108.93
1	G	499	MHO	CE-SD-CG	-2.97	90.04	97.45
1	G	333	0AF	CE2-NE1-CD1	-2.95	106.39	108.93
1	A	271	MHS	CD2-NE2-CE1	2.94	109.08	105.24
1	G	499	MHO	OD1-SD-CG	2.86	113.41	105.89
1	D	333	0AF	CE2-NE1-CD1	-2.84	106.48	108.93
1	A	499	MHO	CE-SD-CG	-2.64	90.85	97.45
1	A	333	0AF	CH2-CZ3-CE3	2.41	123.34	120.24
1	D	499	MHO	CE-SD-CG	-2.29	91.72	97.45
1	D	333	0AF	CH2-CZ3-CE3	2.20	123.07	120.24
1	G	333	0AF	CH2-CZ3-CE3	2.00	122.82	120.24

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	499	MHO	O-C-CA-CB
1	A	499	MHO	CB-CG-SD-CE
1	D	499	MHO	O-C-CA-CB
1	G	499	MHO	O-C-CA-CB
1	A	499	MHO	CB-CG-SD-OD1
1	D	499	MHO	CB-CG-SD-OD1
1	G	499	MHO	CB-CG-SD-OD1
1	D	464	GL3	S-C-CA-N
1	G	464	GL3	S-C-CA-N

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Mol	Chain	Res	Type	Atoms
1	D	499	MHO	CB-CG-SD-CE
1	G	499	MHO	CB-CG-SD-CE

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	464	GL3	3	0
1	G	333	0AF	1	0
1	A	464	GL3	4	0
1	D	499	MHO	1	0
1	G	464	GL3	3	0
1	G	499	MHO	2	0
1	A	499	MHO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 3 are monoatomic - leaving 33 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	$\# Z > 2$
12	P6G	B	434	-	18,18,18	0.71	0	17,17,17	1.52	0
7	1PE	A	581	-	15,15,15	0.65	0	14,14,14	1.52	0
7	1PE	G	580	-	15,15,15	0.58	0	14,14,14	1.65	3 (21%)
9	SO4	D	584	-	4,4,4	0.24	0	6,6,6	0.10	0
8	PGE	A	583	-	9,9,9	0.54	0	8,8,8	0.36	0
5	COM	G	1003	6	6,6,6	3.06	1 (16%)	8,8,8	1.59	2 (25%)
6	M43	G	1001	5	64,73,73	3.37	25 (39%)	71,121,121	2.18	12 (16%)
13	GOL	E	435	-	5,5,5	0.41	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	1PE	H	434	-	15,15,15	0.68	0	14,14,14	1.58	3 (21%)
9	SO4	A	584	-	4,4,4	0.24	0	6,6,6	0.15	0
7	1PE	D	580	-	15,15,15	0.67	0	14,14,14	1.55	2 (14%)
9	SO4	B	435	-	4,4,4	0.24	0	6,6,6	0.09	0
9	SO4	A	585	-	4,4,4	0.25	0	6,6,6	0.07	0
9	SO4	D	583	-	4,4,4	0.24	0	6,6,6	0.12	0
5	COM	D	1003	6	6,6,6	2.86	1 (16%)	8,8,8	2.01	2 (25%)
5	COM	A	1003	6	6,6,6	2.80	1 (16%)	8,8,8	3.12	3 (37%)
4	TP7	A	580	-	19,20,20	2.73	2 (10%)	24,26,26	2.38	5 (20%)
6	M43	A	1001	1,5	64,73,73	3.51	25 (39%)	71,121,121	2.38	15 (21%)
7	1PE	E	434	-	15,15,15	0.69	0	14,14,14	1.49	2 (14%)
9	SO4	C	282	-	4,4,4	0.24	0	6,6,6	0.20	0
8	PGE	G	581	-	9,9,9	0.51	0	8,8,8	0.21	0
8	PGE	G	582	-	9,9,9	0.51	0	8,8,8	0.18	0
7	1PE	F	281	-	15,15,15	0.65	0	14,14,14	1.58	3 (21%)
4	TP7	G	1002	-	19,20,20	2.79	2 (10%)	24,26,26	2.32	5 (20%)
13	GOL	C	281	-	5,5,5	0.44	0	5,5,5	0.50	0
6	M43	D	1001	1,5	64,73,73	3.67	26 (40%)	71,121,121	2.21	13 (18%)
8	PGE	D	581	-	9,9,9	0.53	0	8,8,8	0.28	0
4	TP7	A	1002	-	19,20,20	2.68	2 (10%)	24,26,26	2.38	2 (8%)
8	PGE	D	582	-	9,9,9	0.54	0	8,8,8	0.25	0
9	SO4	H	435	-	4,4,4	0.23	0	6,6,6	0.10	0
9	SO4	I	281	-	4,4,4	0.22	0	6,6,6	0.10	0
8	PGE	A	582	-	9,9,9	0.41	0	8,8,8	0.43	0
9	SO4	B	436	-	4,4,4	0.24	0	6,6,6	0.23	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
12	P6G	B	434	-	-	8/16/16/16	-
7	1PE	A	581	-	-	9/13/13/13	-
7	1PE	G	580	-	-	9/13/13/13	-
8	PGE	A	583	-	-	6/7/7/7	-
5	COM	G	1003	6	-	3/4/4/4	-
6	M43	G	1001	5	1/1/31/33	7/28/190/190	-
13	GOL	E	435	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	1PE	H	434	-	-	7/13/13/13	-
7	1PE	D	580	-	-	5/13/13/13	-
5	COM	D	1003	6	-	3/4/4/4	-
5	COM	A	1003	6	-	4/4/4/4	-
4	TP7	A	580	-	-	2/24/24/24	-
6	M43	A	1001	1,5	-	9/28/190/190	-
7	1PE	E	434	-	-	8/13/13/13	-
8	PGE	G	581	-	-	3/7/7/7	-
8	PGE	G	582	-	-	1/7/7/7	-
7	1PE	F	281	-	-	5/13/13/13	-
4	TP7	G	1002	-	-	3/24/24/24	-
13	GOL	C	281	-	-	0/4/4/4	-
6	M43	D	1001	1,5	1/1/31/33	10/28/190/190	-
8	PGE	D	581	-	-	2/7/7/7	-
4	TP7	A	1002	-	-	3/24/24/24	-
8	PGE	D	582	-	-	2/7/7/7	-
8	PGE	A	582	-	-	4/7/7/7	-

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1001	M43	NI-N13	13.23	2.21	1.89
6	A	1001	M43	NI-N13	12.78	2.20	1.89
6	D	1001	M43	NI-N21	11.42	2.16	1.89
6	G	1001	M43	NI-N21	11.32	2.16	1.89
4	G	1002	TP7	O1-C1	10.50	1.44	1.23
4	A	580	TP7	O1-C1	10.29	1.43	1.23
6	A	1001	M43	NI-N21	10.16	2.13	1.89
4	A	1002	TP7	O1-C1	9.95	1.43	1.23
6	G	1001	M43	NI-N13	9.43	2.12	1.89
6	D	1001	M43	C06-N21	-8.32	1.36	1.49
6	A	1001	M43	C06-N21	-7.89	1.37	1.49
6	D	1001	M43	C59-C58	7.46	1.66	1.54
5	G	1003	COM	C2-S2	-7.25	1.67	1.77
6	A	1001	M43	C52-C10	7.19	1.66	1.53
6	G	1001	M43	C59-C58	7.01	1.66	1.54
5	D	1003	COM	C2-S2	-6.80	1.68	1.77
6	A	1001	M43	C59-C58	6.72	1.65	1.54
6	D	1001	M43	C52-C10	6.66	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1003	COM	C2-S2	-6.64	1.68	1.77
6	G	1001	M43	NI-N09	6.46	2.05	1.89
6	A	1001	M43	NI-N09	6.41	2.05	1.89
6	G	1001	M43	C52-C10	6.38	1.65	1.53
6	D	1001	M43	NI-N09	6.35	2.04	1.89
6	G	1001	M43	C06-N21	-6.33	1.39	1.49
6	A	1001	M43	C05-C06	6.08	1.65	1.53
6	G	1001	M43	C05-C06	5.92	1.65	1.53
6	D	1001	M43	C05-C06	5.88	1.65	1.53
6	D	1001	M43	C24-S25	-5.35	1.77	1.83
4	G	1002	TP7	C1-N	5.34	1.45	1.34
6	D	1001	M43	C48-C49	-5.25	1.39	1.50
4	A	580	TP7	C1-N	5.15	1.44	1.34
6	G	1001	M43	C18-N17	5.13	1.44	1.35
4	A	1002	TP7	C1-N	4.96	1.44	1.34
6	G	1001	M43	C24-S25	-4.87	1.78	1.83
6	G	1001	M43	C15-C14	4.84	1.52	1.39
6	A	1001	M43	C15-C14	4.68	1.52	1.39
6	G	1001	M43	C48-C49	-4.68	1.40	1.50
6	D	1001	M43	C18-N17	4.67	1.43	1.35
6	A	1001	M43	C18-N17	4.63	1.43	1.35
6	A	1001	M43	C48-C49	-4.59	1.40	1.50
6	D	1001	M43	C15-C14	4.59	1.52	1.39
6	D	1001	M43	C58-C52	4.58	1.63	1.54
6	G	1001	M43	C14-N13	4.42	1.40	1.30
6	A	1001	M43	C19-C20	4.42	1.50	1.43
6	D	1001	M43	C19-C20	4.37	1.50	1.43
6	D	1001	M43	C47-C46	-4.36	1.45	1.54
6	A	1001	M43	C20-N21	4.24	1.40	1.30
6	G	1001	M43	C20-N21	4.13	1.40	1.30
6	G	1001	M43	C58-C52	4.10	1.62	1.54
6	A	1001	M43	C14-N13	4.07	1.40	1.30
6	G	1001	M43	C47-C46	-3.88	1.46	1.54
6	A	1001	M43	C58-C52	3.86	1.61	1.54
6	D	1001	M43	C48-C46	-3.85	1.48	1.54
6	D	1001	M43	C20-N21	3.84	1.39	1.30
6	G	1001	M43	C19-C20	3.84	1.49	1.43
6	D	1001	M43	C14-N13	3.81	1.39	1.30
6	A	1001	M43	C47-C46	-3.77	1.47	1.54
6	G	1001	M43	C61-N62	3.68	1.44	1.32
6	G	1001	M43	C48-C46	-3.66	1.49	1.54
6	D	1001	M43	C61-N62	3.52	1.44	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1001	M43	C10-N09	-3.49	1.44	1.49
6	A	1001	M43	C61-N62	3.45	1.44	1.32
6	A	1001	M43	C10-N09	-3.42	1.44	1.49
6	D	1001	M43	C23-C22	3.35	1.58	1.53
6	D	1001	M43	C16-N17	3.34	1.45	1.37
6	G	1001	M43	C23-C22	3.24	1.58	1.53
6	G	1001	M43	C10-N09	-3.24	1.44	1.49
6	A	1001	M43	C23-C22	3.19	1.58	1.53
6	A	1001	M43	C24-S25	-3.15	1.79	1.83
6	A	1001	M43	C48-C46	-3.09	1.49	1.54
6	D	1001	M43	C60-C58	2.96	1.65	1.56
6	A	1001	M43	C60-C58	2.87	1.65	1.56
6	G	1001	M43	C60-C58	2.86	1.65	1.56
6	G	1001	M43	C16-N17	2.82	1.44	1.37
6	A	1001	M43	C16-N17	2.78	1.43	1.37
6	A	1001	M43	C07-C06	-2.77	1.50	1.53
6	A	1001	M43	C04-C05	-2.55	1.49	1.53
6	A	1001	M43	C36-C35	-2.39	1.49	1.53
6	G	1001	M43	C07-C06	-2.27	1.50	1.53
6	G	1001	M43	C04-C05	-2.27	1.49	1.53
6	D	1001	M43	C11-C12	2.17	1.54	1.53
6	D	1001	M43	C07-C06	-2.15	1.51	1.53
6	G	1001	M43	C15-C16	2.12	1.41	1.36
6	D	1001	M43	C15-C16	2.06	1.40	1.36
6	D	1001	M43	C04-C05	-2.01	1.49	1.53

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1001	M43	C59-C58-C60	13.84	134.26	110.74
6	G	1001	M43	C59-C58-C60	11.20	129.77	110.74
6	D	1001	M43	C59-C58-C60	9.80	127.39	110.74
4	A	580	TP7	O1-C1-N	-8.89	107.90	122.95
4	A	1002	TP7	O1-C1-N	-8.71	108.21	122.95
6	A	1001	M43	C59-C58-C52	-7.64	102.02	112.99
4	G	1002	TP7	O1-C1-N	-7.55	110.17	122.95
6	D	1001	M43	C59-C58-C52	-7.42	102.33	112.99
6	G	1001	M43	C59-C58-C52	-7.30	102.51	112.99
6	D	1001	M43	C52-C58-C08	-7.10	92.86	99.97
5	A	1003	COM	O1S-S2-C2	7.05	117.39	106.73
4	G	1002	TP7	O1-C1-C2	-6.57	110.12	122.02
4	A	1002	TP7	O1-C1-C2	-6.28	110.64	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	1001	M43	C52-C58-C08	-5.88	94.10	99.97
4	A	580	TP7	O1-C1-C2	-5.11	112.76	122.02
6	A	1001	M43	C52-C58-C08	-3.90	96.07	99.97
5	D	1003	COM	O3S-S2-C2	3.86	113.56	106.00
6	D	1001	M43	C06-N21-C20	3.51	113.72	108.46
6	D	1001	M43	C16-N17-C18	-3.51	99.96	107.50
6	G	1001	M43	C48-C49-N51	3.49	117.85	109.41
5	A	1003	COM	C2-C1-S1	-3.49	104.26	113.10
6	D	1001	M43	C48-C49-N51	3.48	117.81	109.41
6	A	1001	M43	C14-C15-C16	-3.40	120.34	125.84
6	A	1001	M43	C06-N21-C20	3.23	113.30	108.46
6	A	1001	M43	C16-N17-C18	-3.18	100.65	107.50
6	A	1001	M43	C48-C49-N51	3.12	116.94	109.41
6	D	1001	M43	O50-C49-C48	-3.03	120.82	126.92
7	D	580	1PE	C24-OH4-C13	2.98	126.32	113.26
6	G	1001	M43	C16-N17-C18	-2.97	101.11	107.50
6	G	1001	M43	O50-C49-C48	-2.93	121.03	126.92
5	D	1003	COM	C2-C1-S1	-2.92	105.70	113.10
7	E	434	1PE	OH6-C15-C25	2.82	123.20	110.35
5	G	1003	COM	C2-C1-S1	-2.76	106.11	113.10
7	G	580	1PE	C25-OH5-C14	2.60	124.63	113.26
6	D	1001	M43	C12-N51-C49	-2.58	105.14	112.40
6	A	1001	M43	C23-C22-C20	2.57	112.96	110.21
6	D	1001	M43	O39-C37-C36	2.53	121.86	114.00
6	A	1001	M43	O50-C49-C48	-2.48	121.94	126.92
4	A	580	TP7	C2-C1-N	-2.47	111.51	115.86
6	G	1001	M43	O39-C37-C36	2.47	121.68	114.00
6	G	1001	M43	C05-C06-N21	2.45	106.15	102.34
7	F	281	1PE	C24-OH4-C13	2.44	123.92	113.26
6	G	1001	M43	C46-C12-N13	2.43	105.47	101.86
6	G	1001	M43	C47-C46-C12	2.41	118.08	113.03
5	G	1003	COM	O2S-S2-C2	2.39	110.34	106.73
7	F	281	1PE	OH5-C25-C15	2.39	121.22	110.35
4	G	1002	TP7	CA-N-C1	-2.35	117.16	121.80
7	G	580	1PE	OH3-C22-C12	2.35	120.46	110.11
6	D	1001	M43	O01-C02-C04	2.31	121.19	114.00
4	G	1002	TP7	C3-C2-C1	-2.31	106.78	113.19
7	H	434	1PE	C24-OH4-C13	2.29	123.28	113.26
6	G	1001	M43	C26-S25-C24	2.28	103.85	100.72
4	A	580	TP7	CA-N-C1	-2.25	117.36	121.80
7	G	580	1PE	OH6-C15-C25	2.23	120.51	110.35
7	D	580	1PE	OH5-C14-C24	2.20	120.37	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	434	1PE	C26-OH6-C15	2.19	122.85	113.26
4	G	1002	TP7	O3P-P-O2P	2.18	115.99	107.80
7	F	281	1PE	C23-OH3-C22	2.18	122.80	113.26
7	H	434	1PE	OH5-C25-C15	2.17	120.24	110.35
6	G	1001	M43	C22-C20-C19	2.15	124.52	121.85
6	A	1001	M43	C46-C40-C14	2.15	104.05	101.64
6	D	1001	M43	C10-N09-C08	-2.13	106.19	109.08
6	D	1001	M43	C26-S25-C24	2.13	103.65	100.72
4	A	580	TP7	O4P-P-O1P	-2.13	101.75	109.33
6	A	1001	M43	C12-N51-C49	-2.11	106.47	112.40
7	E	434	1PE	OH5-C14-C24	2.10	119.92	110.35
6	D	1001	M43	C14-C15-C16	-2.09	122.46	125.84
6	A	1001	M43	O01-C02-C04	2.06	120.41	114.00
5	A	1003	COM	C1-C2-S2	2.04	116.33	111.77
6	A	1001	M43	C47-C46-C40	-2.03	107.74	112.91
6	A	1001	M43	C20-C19-C18	-2.00	119.65	125.28
6	A	1001	M43	O33-C32-C31	2.00	120.32	114.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	D	1001	M43	N17
6	G	1001	M43	N17

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	TP7	O1-C1-N-CA
4	A	580	TP7	O1-C1-N-CA
4	G	1002	TP7	O1-C1-N-CA
5	A	1003	COM	C1-C2-S2-O1S
5	A	1003	COM	C1-C2-S2-O2S
5	D	1003	COM	C1-C2-S2-O1S
5	D	1003	COM	C1-C2-S2-O2S
5	D	1003	COM	C1-C2-S2-O3S
5	G	1003	COM	C1-C2-S2-O1S
5	G	1003	COM	C1-C2-S2-O2S
5	G	1003	COM	C1-C2-S2-O3S
13	E	435	GOL	C1-C2-C3-O3
12	B	434	P6G	C5-C6-O7-C8
7	A	581	1PE	C23-C13-OH4-C24
7	A	581	1PE	C12-C22-OH3-C23

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Mol	Chain	Res	Type	Atoms
8	D	582	PGE	O2-C3-C4-O3
8	A	582	PGE	O2-C3-C4-O3
7	A	581	1PE	OH6-C15-C25-OH5
12	B	434	P6G	O10-C11-C12-O13
7	D	580	1PE	OH6-C15-C25-OH5
7	G	580	1PE	C24-C14-OH5-C25
7	E	434	1PE	OH4-C13-C23-OH3
7	A	581	1PE	OH5-C14-C24-OH4
7	G	580	1PE	OH5-C14-C24-OH4
8	A	582	PGE	O3-C5-C6-O4
7	H	434	1PE	OH5-C14-C24-OH4
12	B	434	P6G	O7-C8-C9-O10
7	E	434	1PE	OH6-C15-C25-OH5
8	G	581	PGE	O3-C5-C6-O4
7	G	580	1PE	OH4-C13-C23-OH3
6	A	1001	M43	C52-C53-C54-C55
6	G	1001	M43	C52-C53-C54-C55
8	D	582	PGE	O3-C5-C6-O4
13	E	435	GOL	O2-C2-C3-O3
6	D	1001	M43	C52-C53-C54-C55
8	A	583	PGE	C4-C3-O2-C2
8	D	581	PGE	O3-C5-C6-O4
7	F	281	1PE	OH5-C14-C24-OH4
7	H	434	1PE	OH4-C13-C23-OH3
7	E	434	1PE	OH7-C16-C26-OH6
4	A	580	TP7	C1-C2-C3-C4
7	F	281	1PE	OH4-C13-C23-OH3
12	B	434	P6G	O4-C5-C6-O7
4	G	1002	TP7	C1-C2-C3-C4
5	A	1003	COM	C1-C2-S2-O3S
7	D	580	1PE	OH5-C14-C24-OH4
7	A	581	1PE	C25-C15-OH6-C26
12	B	434	P6G	C18-C17-O16-C15
7	G	580	1PE	C23-C13-OH4-C24
7	D	580	1PE	C13-C23-OH3-C22
8	A	583	PGE	C6-C5-O3-C4
7	A	581	1PE	C15-C25-OH5-C14
8	G	581	PGE	C6-C5-O3-C4
6	A	1001	M43	C58-C52-C53-C54
4	A	1002	TP7	C1-C2-C3-C4
7	F	281	1PE	C25-C15-OH6-C26
7	F	281	1PE	C13-C23-OH3-C22

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Mol	Chain	Res	Type	Atoms
7	G	580	1PE	C15-C25-OH5-C14
8	A	582	PGE	C3-C4-O3-C5
8	A	583	PGE	C1-C2-O2-C3
6	D	1001	M43	C59-C58-C60-C61
7	H	434	1PE	C16-C26-OH6-C15
7	G	580	1PE	C14-C24-OH4-C13
7	A	581	1PE	OH4-C13-C23-OH3
12	B	434	P6G	C11-C12-O13-C14
7	H	434	1PE	OH2-C12-C22-OH3
7	G	580	1PE	C25-C15-OH6-C26
5	A	1003	COM	S1-C1-C2-S2
8	D	581	PGE	O2-C3-C4-O3
8	A	583	PGE	O1-C1-C2-O2
8	G	582	PGE	O2-C3-C4-O3
7	A	581	1PE	C24-C14-OH5-C25
6	G	1001	M43	C59-C58-C60-C61
6	D	1001	M43	C35-C36-C37-O39
7	H	434	1PE	OH7-C16-C26-OH6
7	A	581	1PE	C14-C24-OH4-C13
6	A	1001	M43	C53-C54-C55-O57
6	D	1001	M43	C35-C36-C37-O38
8	A	582	PGE	C4-C3-O2-C2
7	E	434	1PE	OH2-C12-C22-OH3
7	E	434	1PE	C16-C26-OH6-C15
6	A	1001	M43	C53-C54-C55-O56
7	G	580	1PE	OH2-C12-C22-OH3
6	G	1001	M43	C41-C42-C43-O45
6	G	1001	M43	C41-C42-C43-O44
7	G	580	1PE	OH6-C15-C25-OH5
7	H	434	1PE	OH6-C15-C25-OH5
6	D	1001	M43	C30-C31-C32-O33
7	E	434	1PE	C23-C13-OH4-C24
7	H	434	1PE	C15-C25-OH5-C14
4	A	1002	TP7	C2-C3-C4-C5
7	E	434	1PE	C14-C24-OH4-C13
6	G	1001	M43	C53-C54-C55-O57
6	D	1001	M43	C53-C54-C55-O57
4	G	1002	TP7	C4-C5-C6-C7
6	D	1001	M43	C30-C31-C32-O34
6	D	1001	M43	C53-C54-C55-O56
6	G	1001	M43	C53-C54-C55-O56
8	A	583	PGE	C3-C4-O3-C5

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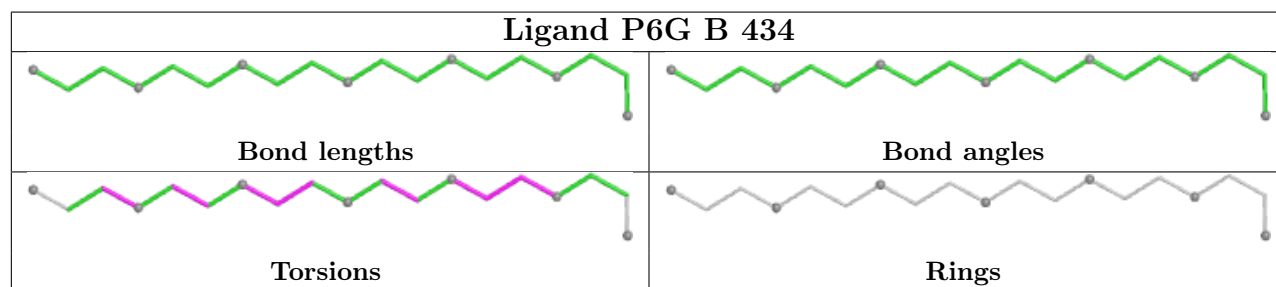
Mol	Chain	Res	Type	Atoms
13	E	435	GOL	O1-C1-C2-O2
6	D	1001	M43	C41-C42-C43-O44
8	G	581	PGE	C4-C3-O2-C2
6	A	1001	M43	C59-C58-C60-C61
12	B	434	P6G	C6-C5-O4-C3
7	E	434	1PE	OH5-C14-C24-OH4
6	A	1001	M43	C41-C42-C43-O44
7	D	580	1PE	C24-C14-OH5-C25
6	A	1001	M43	C02-C04-C05-C22
6	G	1001	M43	C18-C29-C30-C31
7	D	580	1PE	C14-C24-OH4-C13
6	A	1001	M43	C41-C42-C43-O45
7	F	281	1PE	OH6-C15-C25-OH5
6	D	1001	M43	C41-C42-C43-O45
12	B	434	P6G	O13-C14-C15-O16
6	A	1001	M43	C30-C31-C32-O33
8	A	583	PGE	O2-C3-C4-O3

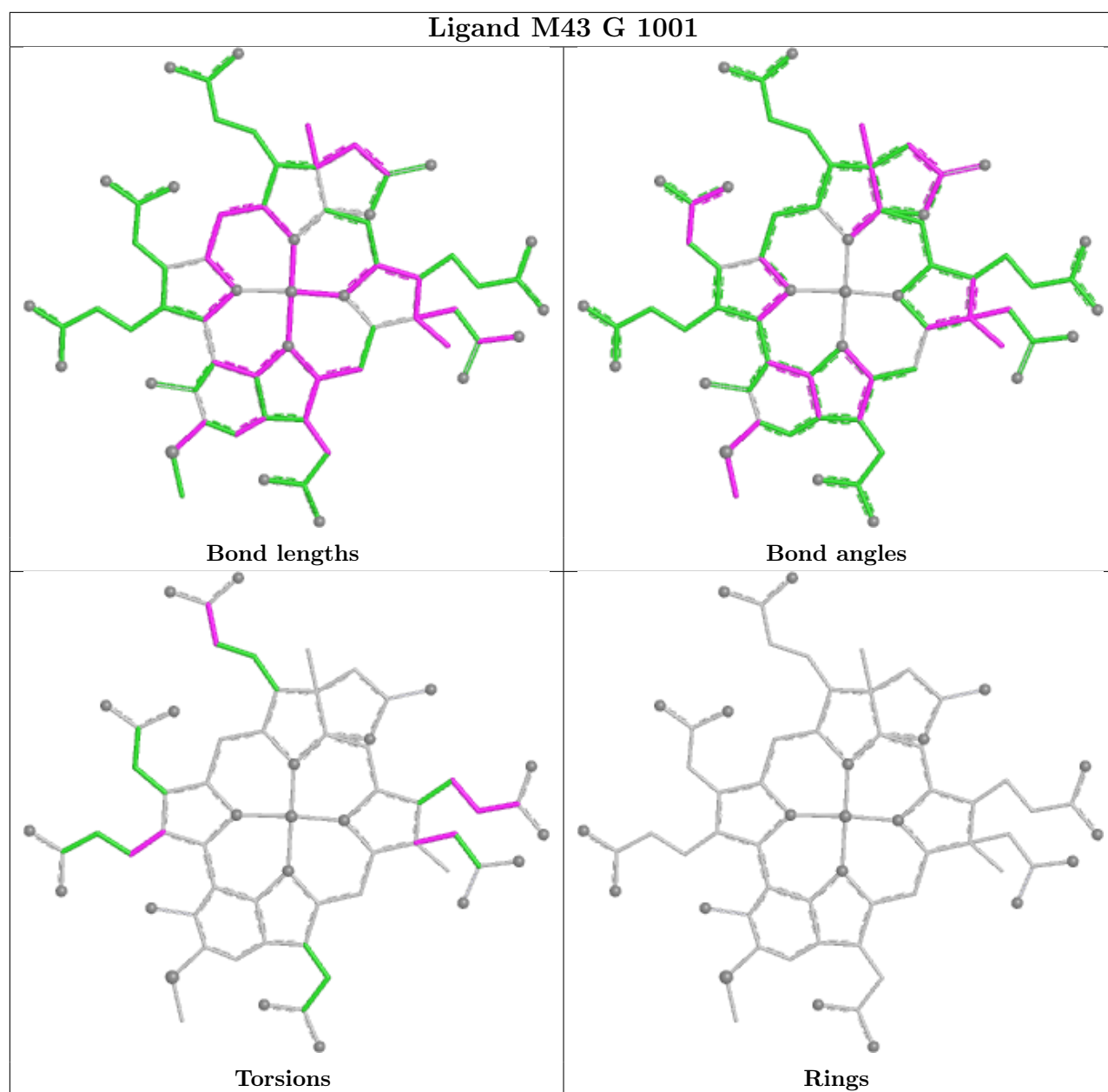
There are no ring outliers.

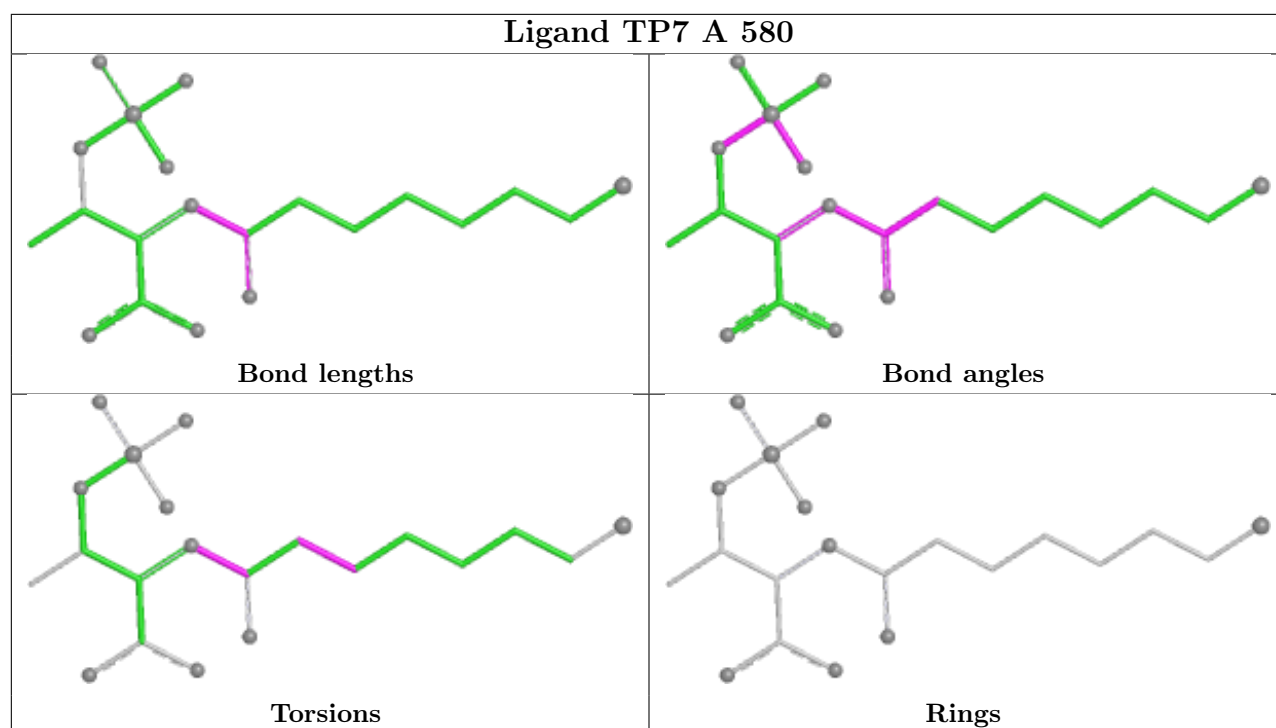
20 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	434	P6G	11	0
7	A	581	1PE	5	0
7	G	580	1PE	9	0
8	A	583	PGE	4	0
5	G	1003	COM	3	0
6	G	1001	M43	3	0
7	H	434	1PE	5	0
7	D	580	1PE	8	0
5	D	1003	COM	3	0
5	A	1003	COM	4	0
6	A	1001	M43	3	0
7	E	434	1PE	2	0
8	G	582	PGE	1	0
7	F	281	1PE	4	0
4	G	1002	TP7	1	0
6	D	1001	M43	1	0
8	D	581	PGE	3	0
4	A	1002	TP7	1	0
8	D	582	PGE	2	0
8	A	582	PGE	1	0

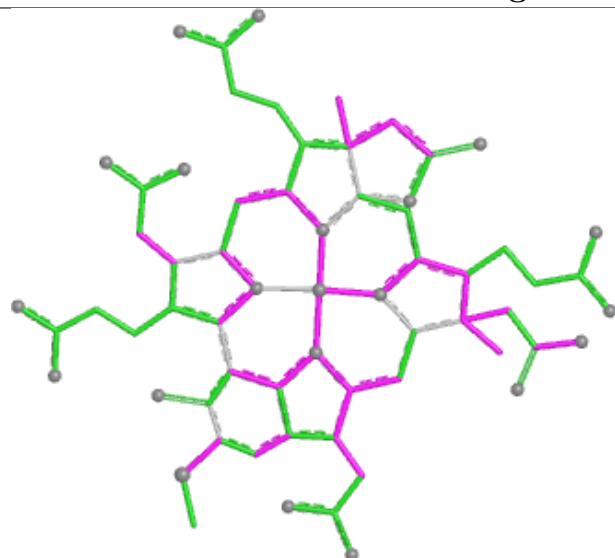
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



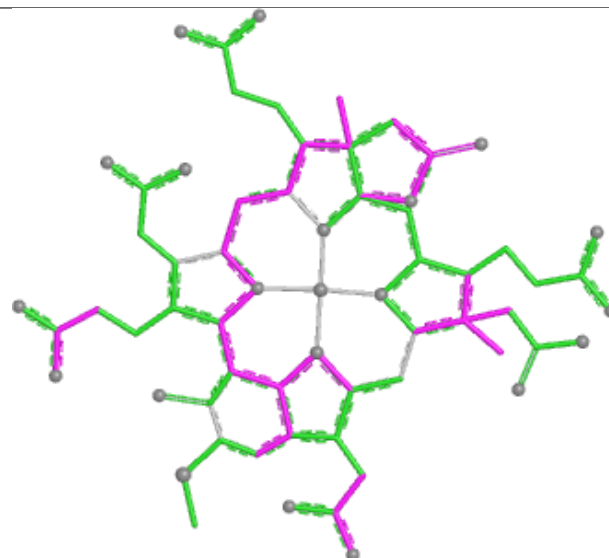




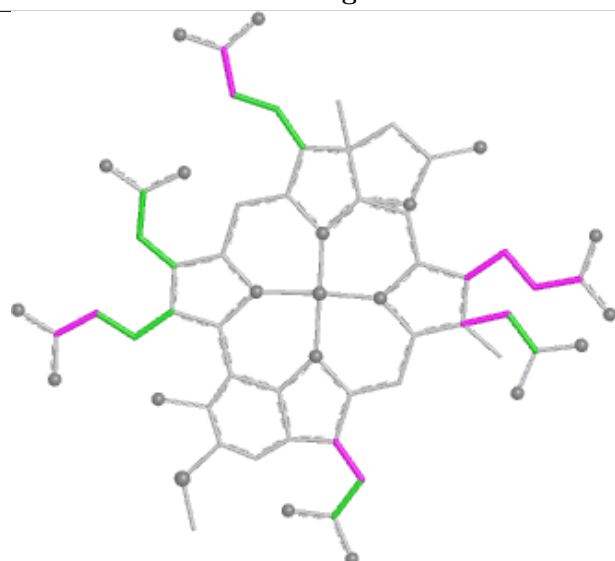
Ligand M43 A 1001



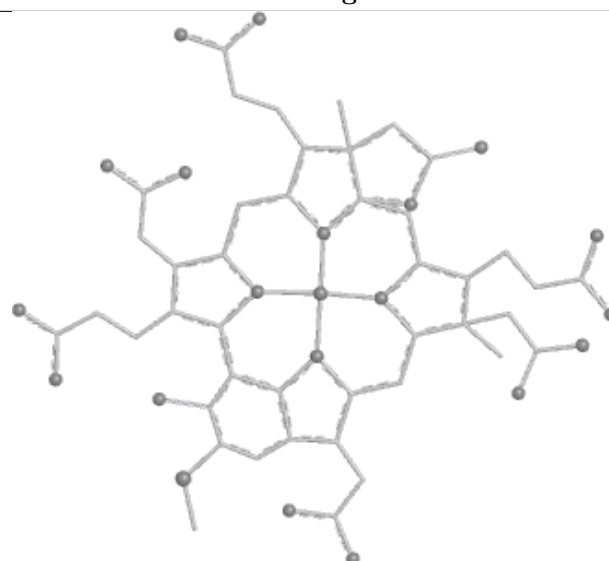
Bond lengths



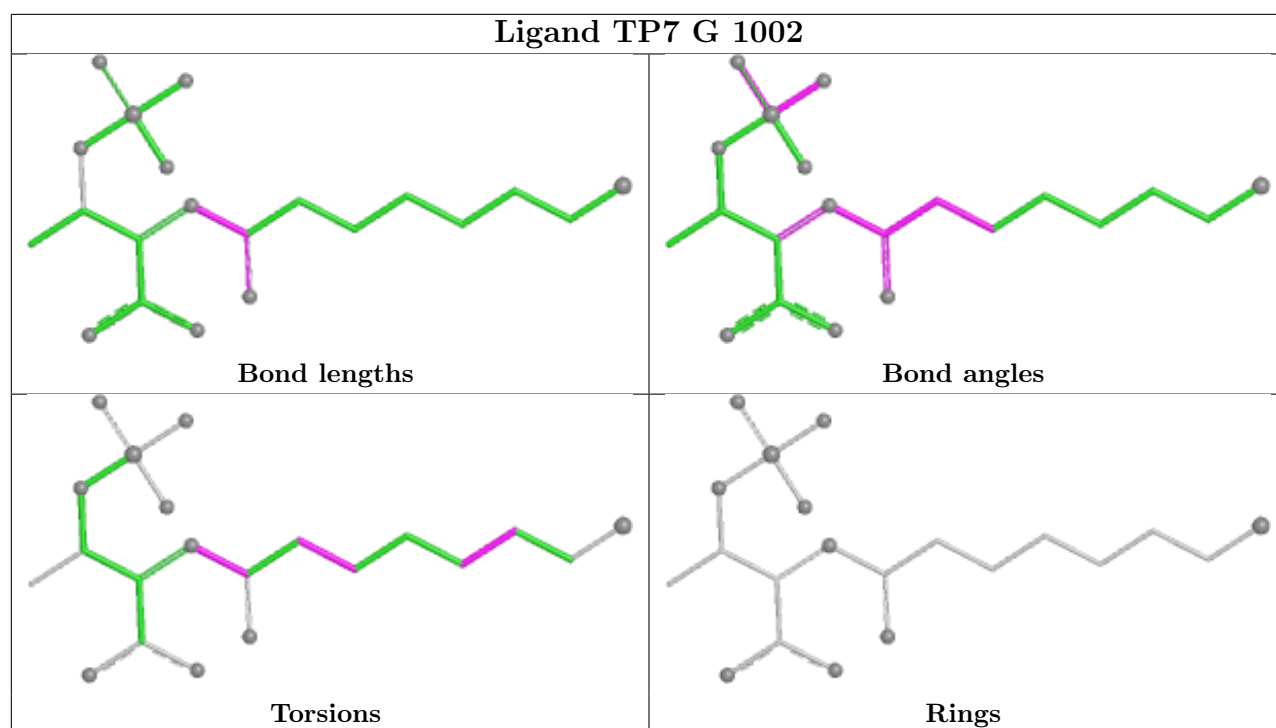
Bond angles

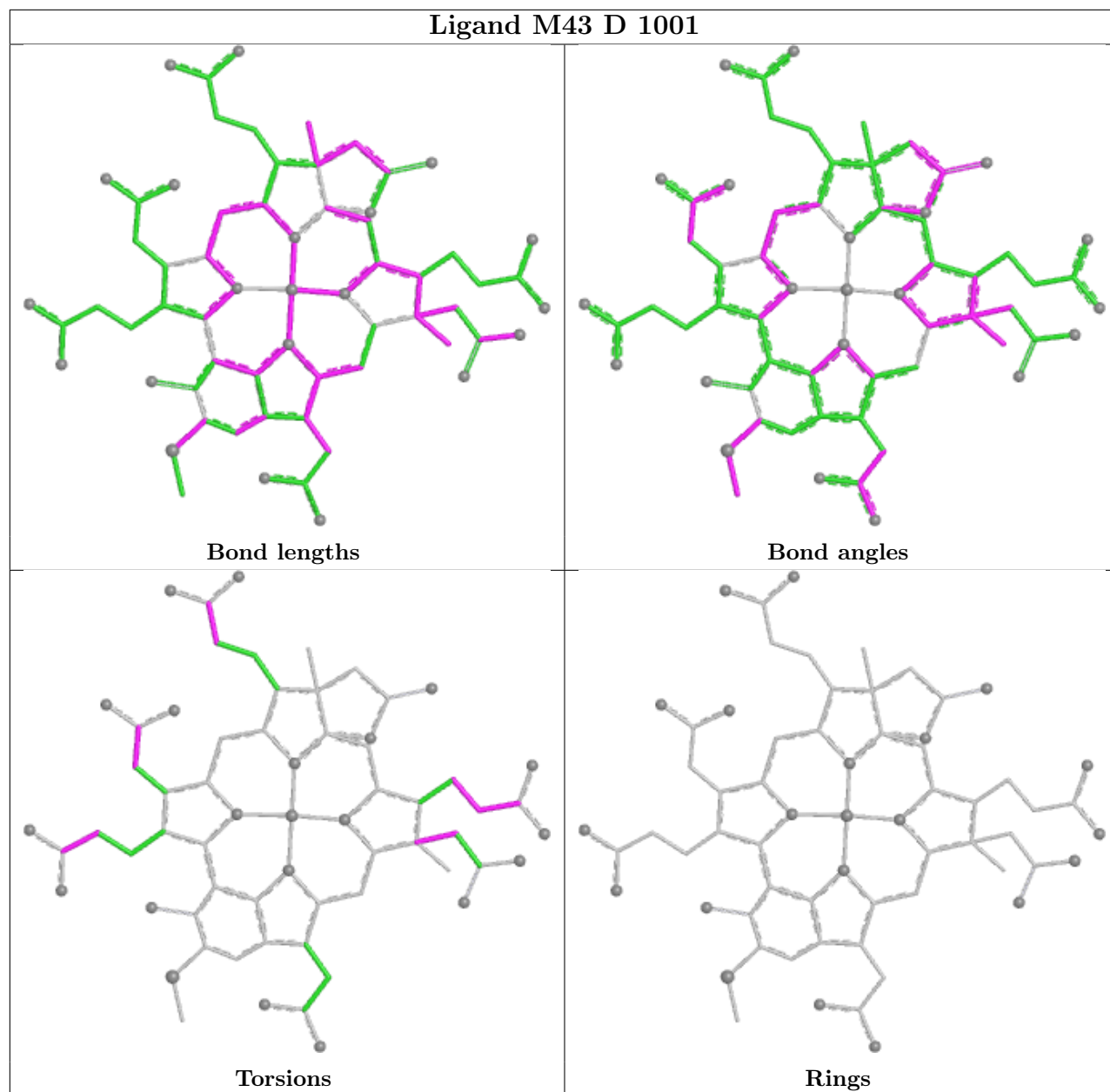


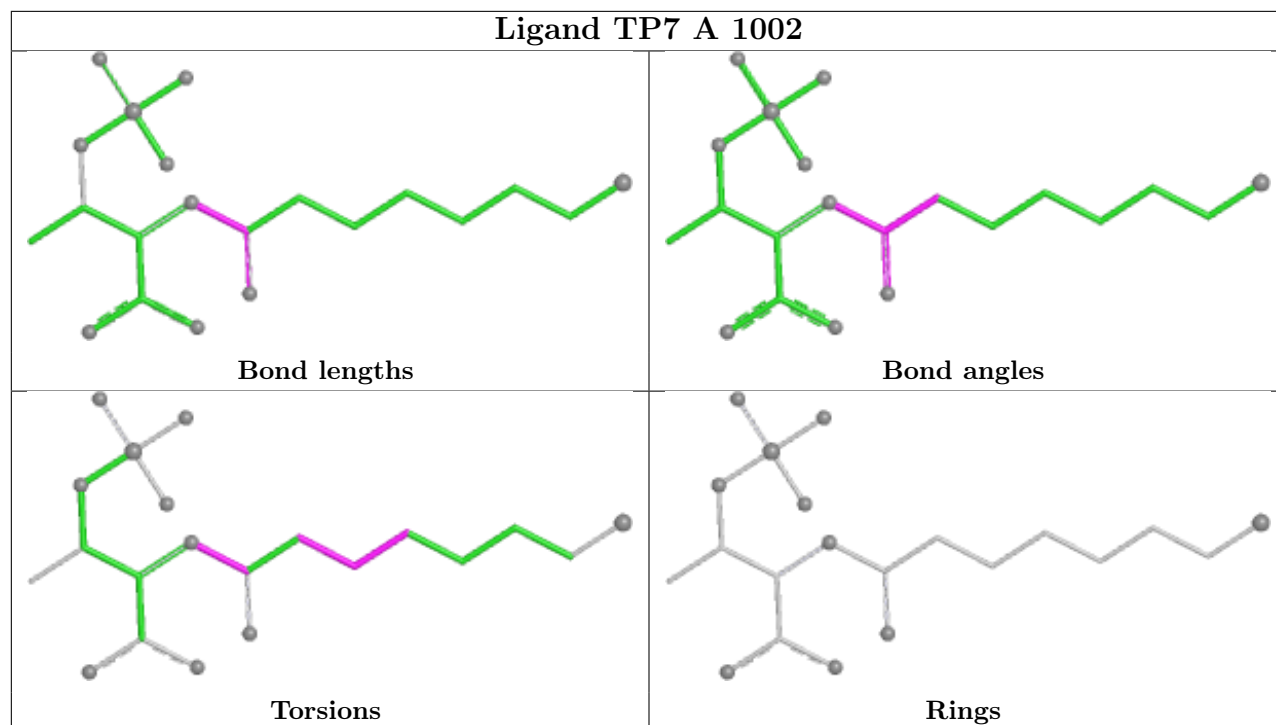
Torsions



Rings







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	574/579 (99%)	-0.74	0 100 100	16, 24, 36, 58	0
1	D	574/579 (99%)	-0.64	1 (0%) 91 92	17, 27, 40, 61	1 (0%)
1	G	574/579 (99%)	-0.61	1 (0%) 91 92	20, 28, 41, 68	0
2	B	431/433 (99%)	-0.25	1 (0%) 91 92	21, 37, 55, 79	0
2	E	431/433 (99%)	-0.02	2 (0%) 87 88	26, 42, 61, 83	0
2	H	431/433 (99%)	-0.09	0 100 100	26, 41, 58, 70	2 (0%)
3	C	278/279 (99%)	-0.41	0 100 100	20, 31, 48, 72	0
3	F	278/279 (99%)	-0.09	0 100 100	27, 42, 59, 96	1 (0%)
3	I	278/279 (99%)	-0.23	0 100 100	24, 38, 54, 96	0
All	All	3849/3873 (99%)	-0.39	5 (0%) 92 92	16, 33, 54, 96	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	579	LEU	2.9
2	E	76	VAL	2.7
2	B	75	ILE	2.5
2	E	433	LYS	2.1
1	D	579	LEU	2.0

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

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($\text{\AA}^2$)	Q<0.9
1	MHS	G	271	11/12	0.95	0.07	30,32,34,34	0
1	MHS	D	271	11/12	0.97	0.05	24,26,27,27	0
1	OAF	D	333	15/16	0.97	0.05	19,22,24,26	0
1	MHO	D	499	9/10	0.97	0.07	23,29,30,30	0
1	MHS	A	271	11/12	0.97	0.06	28,29,32,32	0
1	OAF	G	333	15/16	0.97	0.05	21,25,26,27	0
1	MHO	G	499	9/10	0.97	0.06	21,26,31,32	0
1	OAF	A	333	15/16	0.98	0.05	17,22,23,24	0
1	MHO	A	499	9/10	0.98	0.05	18,22,24,24	0
1	GL3	A	464	4/5	0.99	0.04	21,22,24,24	0
1	GL3	G	464	4/5	0.99	0.04	27,28,28,29	0
1	GL3	D	464	4/5	0.99	0.05	29,32,32,34	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($\text{\AA}^2$)	Q<0.9
9	SO4	A	585	5/5	0.72	0.10	110,110,110,110	0
13	GOL	C	281	6/6	0.76	0.16	37,44,45,46	0
7	1PE	F	281	16/16	0.77	0.17	56,63,68,68	0
8	PGE	D	582	10/10	0.79	0.17	58,62,68,69	0
9	SO4	D	584	5/5	0.85	0.11	98,98,99,99	0
7	1PE	D	580	16/16	0.86	0.16	42,61,62,63	0
9	SO4	H	435	5/5	0.86	0.10	65,66,67,68	5
5	COM	D	1003	7/7	0.86	0.22	17,23,45,46	7
9	SO4	C	282	5/5	0.87	0.12	62,63,63,66	0
9	SO4	I	281	5/5	0.87	0.11	64,64,65,67	5
9	SO4	B	435	5/5	0.87	0.09	63,64,64,65	5
9	SO4	B	436	5/5	0.88	0.14	71,72,72,73	5
9	SO4	A	584	5/5	0.88	0.14	53,54,56,58	5
8	PGE	G	582	10/10	0.89	0.12	49,51,57,58	0
7	1PE	H	434	16/16	0.89	0.12	43,47,51,52	0
5	COM	G	1003	7/7	0.89	0.16	17,28,33,35	7
9	SO4	D	583	5/5	0.89	0.10	85,85,86,86	0

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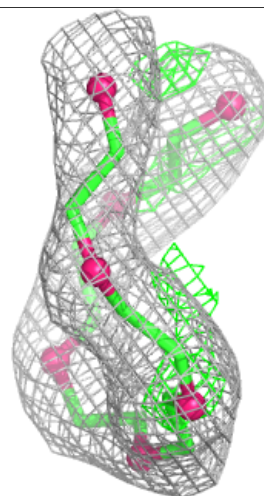
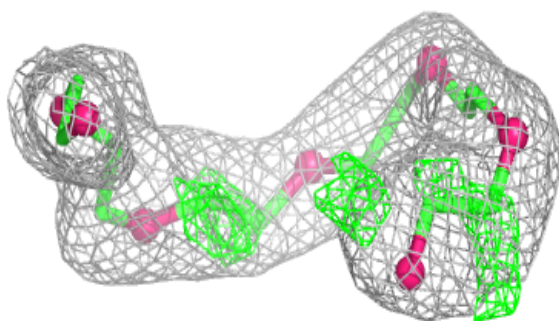
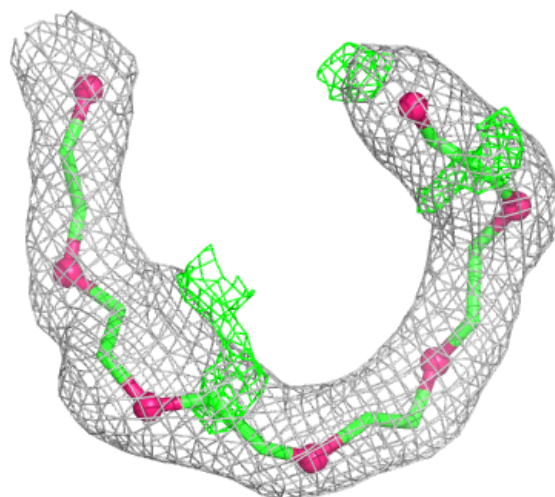
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	GOL	E	435	6/6	0.89	0.15	65,67,68,68	0
7	1PE	A	581	16/16	0.90	0.13	33,58,61,61	0
8	PGE	A	582	10/10	0.90	0.13	58,61,70,70	0
7	1PE	G	580	16/16	0.90	0.12	34,55,59,59	0
7	1PE	E	434	16/16	0.91	0.11	40,45,47,49	0
12	P6G	B	434	19/19	0.91	0.11	41,44,58,60	0
8	PGE	A	583	10/10	0.92	0.11	42,45,50,53	0
8	PGE	D	581	10/10	0.93	0.10	40,42,45,47	0
8	PGE	G	581	10/10	0.94	0.10	41,43,52,52	0
5	COM	A	1003	7/7	0.95	0.11	14,18,28,29	7
4	TP7	G	1002	21/21	0.97	0.06	21,26,33,37	0
4	TP7	A	580	21/21	0.98	0.06	24,29,30,31	0
6	M43	A	1001	64/64	0.98	0.06	20,28,33,36	0
6	M43	G	1001	64/64	0.98	0.06	16,26,31,33	0
11	CA	A	587	1/1	0.99	0.04	24,24,24,24	0
11	CA	G	583	1/1	0.99	0.07	22,22,22,22	1
4	TP7	A	1002	21/21	0.99	0.04	18,22,27,27	0
6	M43	D	1001	64/64	0.99	0.05	13,20,25,27	0
10	CL	A	586	1/1	0.99	0.16	47,47,47,47	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.

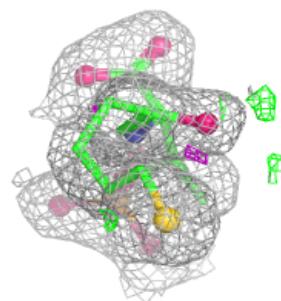
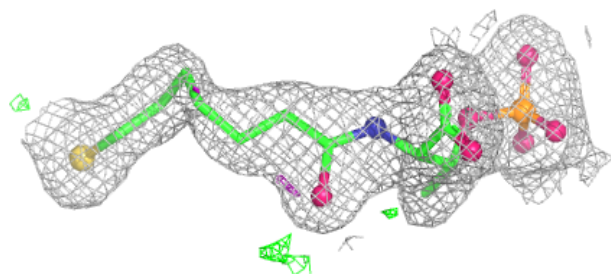
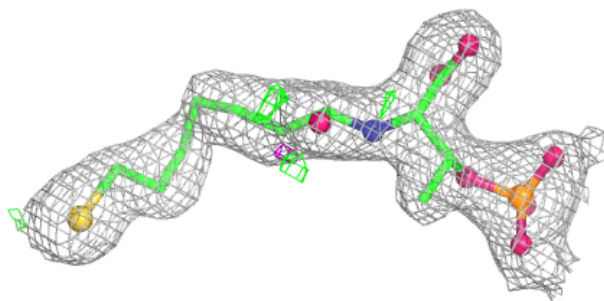
Electron density around P6G B 434:

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

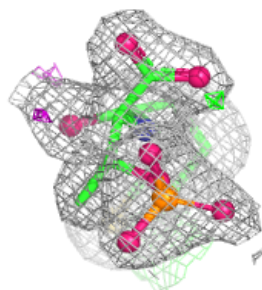
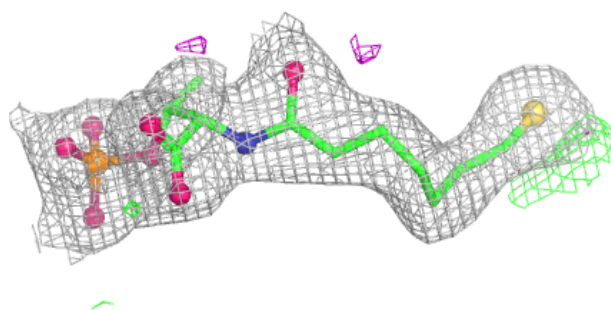
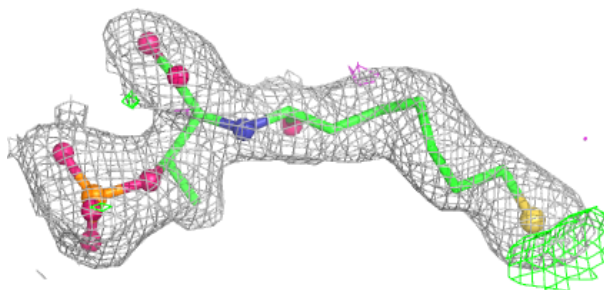


Electron density around TP7 G 1002:

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

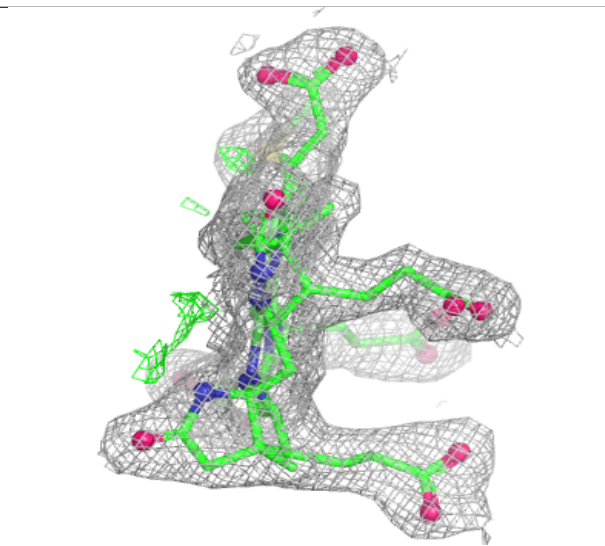
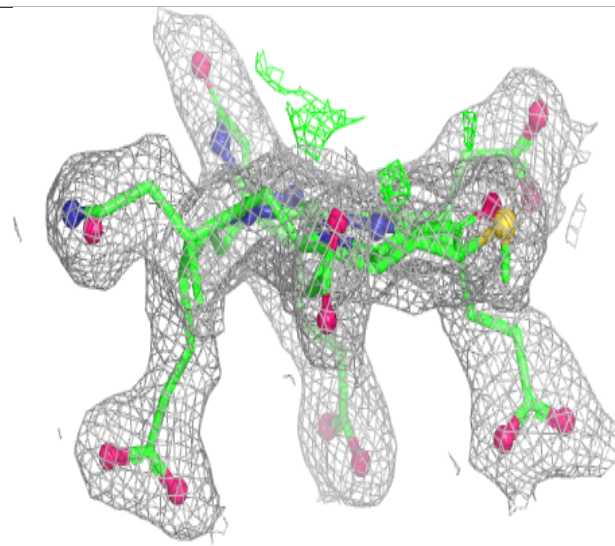
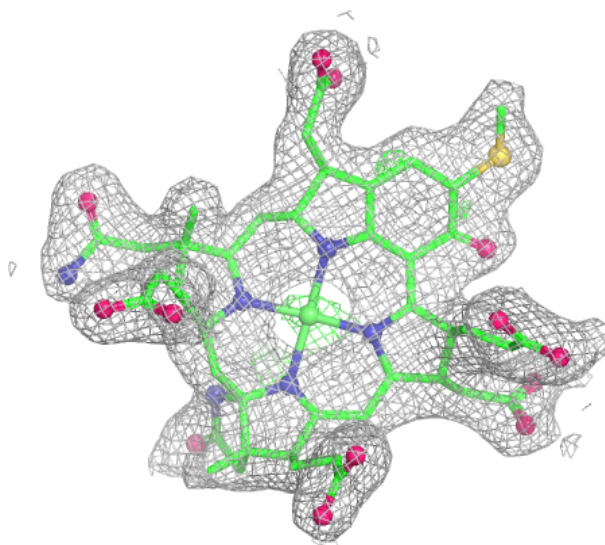
**Electron density around TP7 A 580:**

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



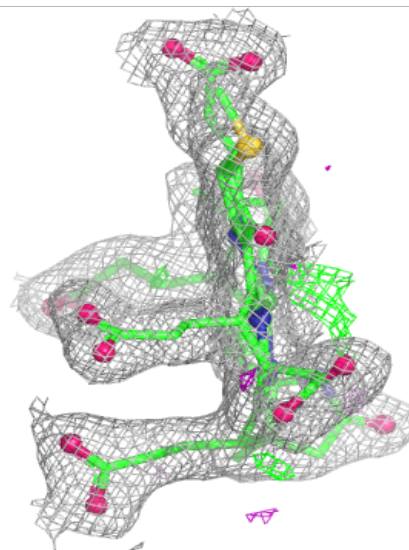
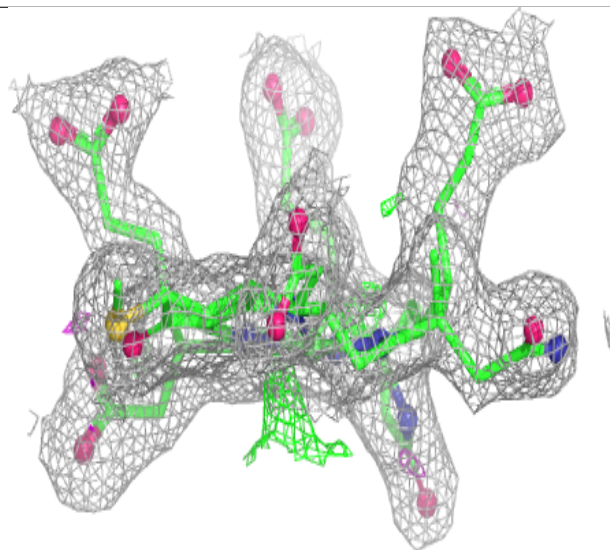
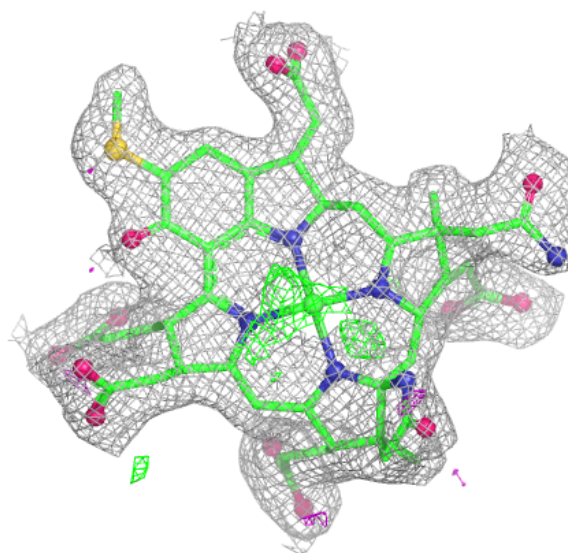
Electron density around M43 A 1001:

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



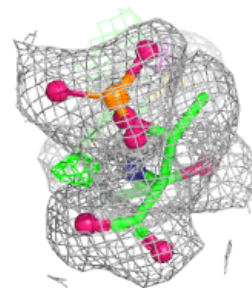
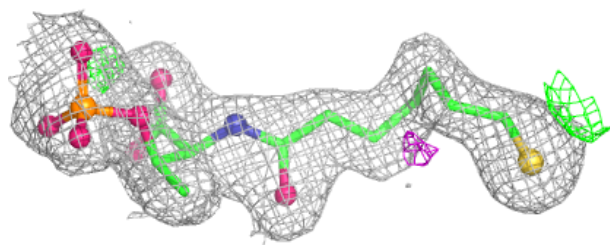
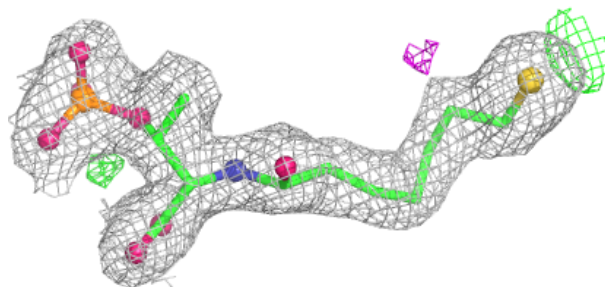
Electron density around M43 G 1001:

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



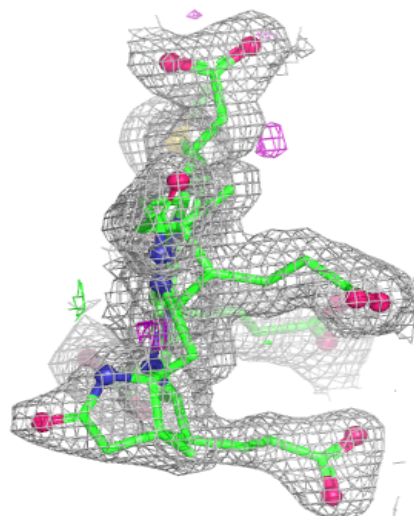
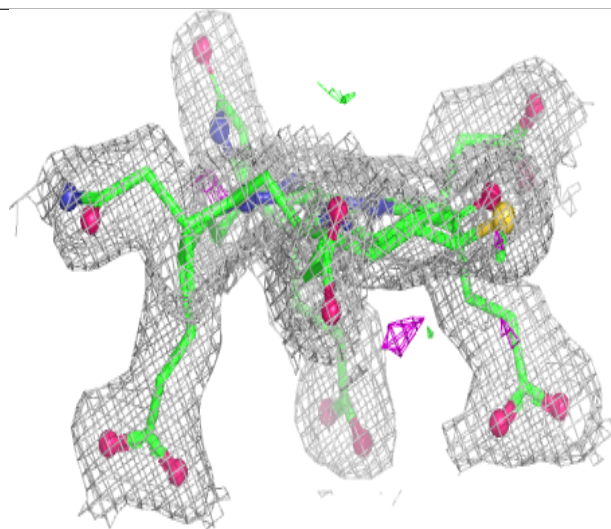
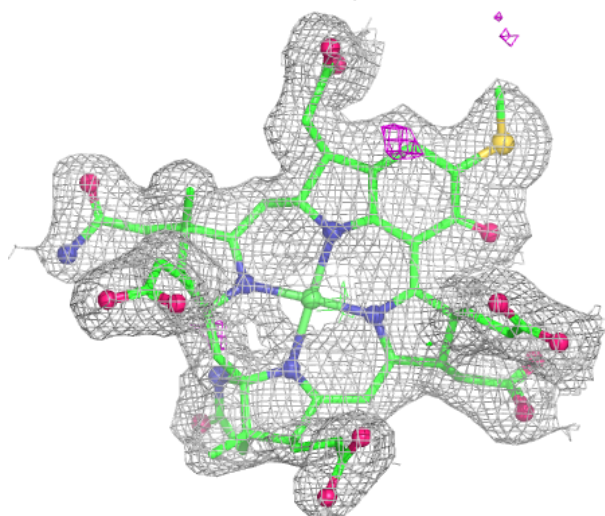
Electron density around TP7 A 1002:

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



Electron density around M43 D 1001:

$2mF_o-DF_c$ (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.