



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:27 PM UTC

PDB ID : 8J83 / pdb_00008j83
Title : Crystal structure of formate dehydrogenase from *Methylobacterium extorquens* AM1
Authors : Kobayashi, A.; Taketa, M.; Sowa, K.; Kano, K.; Higuchi, Y.; Ogata, H.
Deposited on : 2023-04-29
Resolution : 2.40 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

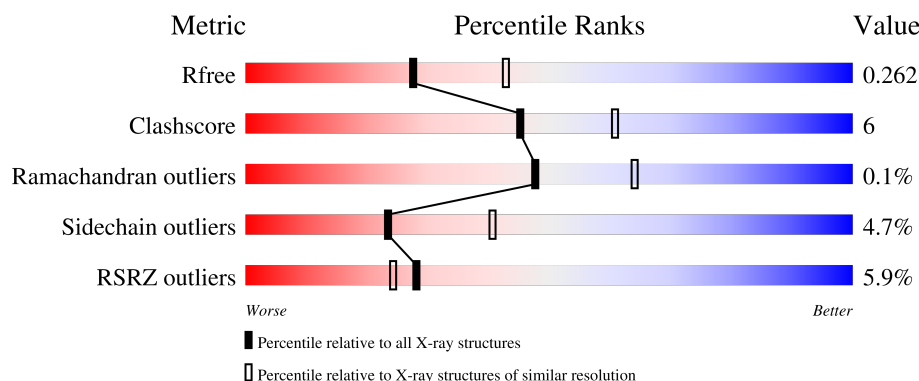
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	989	5% 76% 15% 8%
2	B	572	6% 80% 17% • •

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 11489 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.

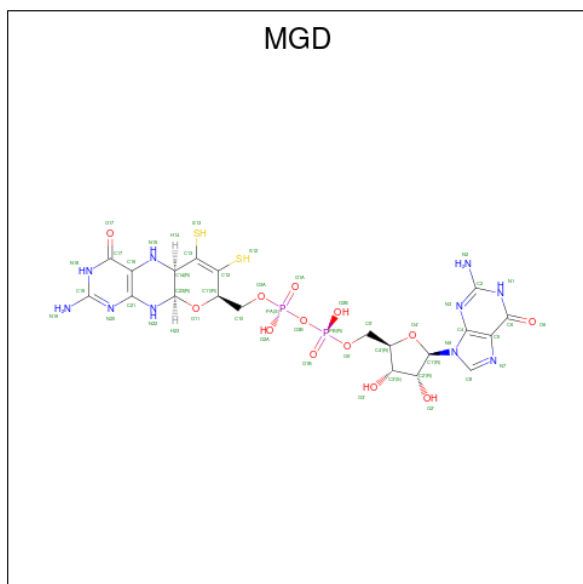
- Molecule 1 is a protein called Tungsten-containing formate dehydrogenase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	911	7007	4405	1253	1301	48	0	0	0

- Molecule 2 is a protein called Tungsten-containing formate dehydrogenase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	557	4278	2690	763	804	21	0	0	0

- Molecule 3 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	A	1	47	20	10	13	2	2	0	0

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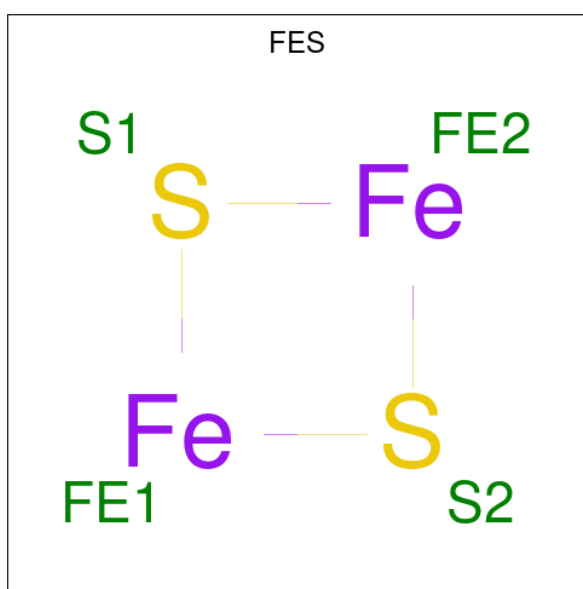
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 4 is TUNGSTEN ION (CCD ID: W) (formula: W).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	W	0	0
			1	1		

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			4	2	2		
5	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



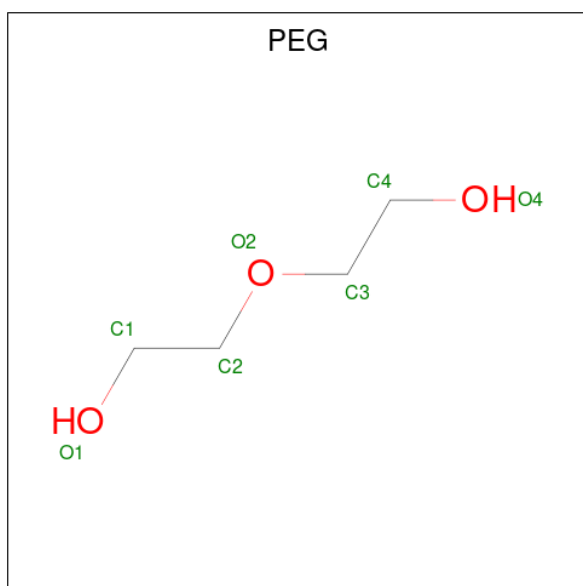
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



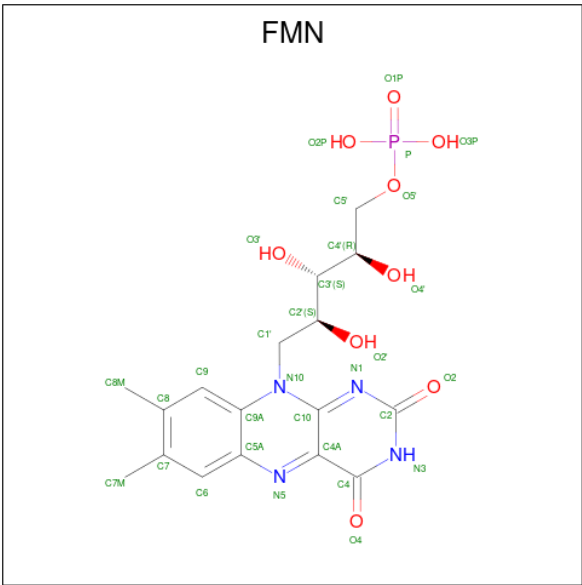
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

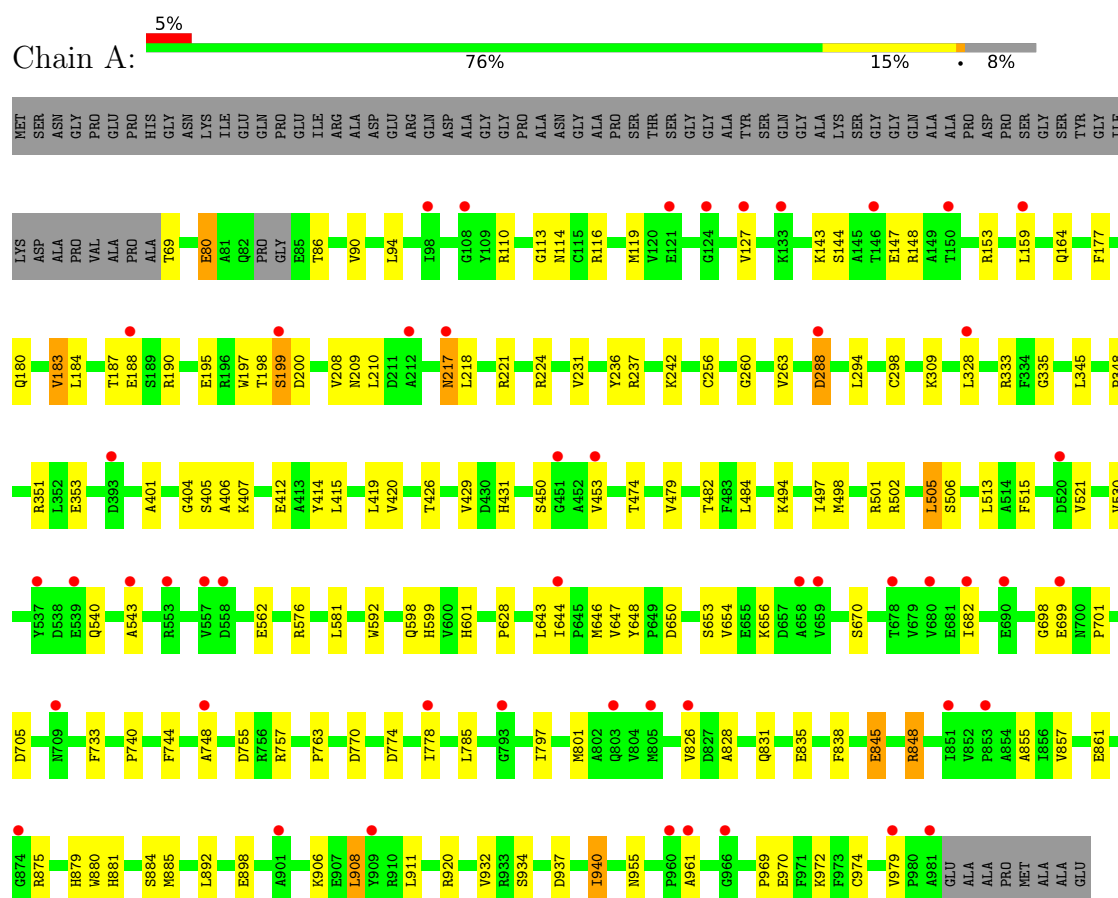
- Molecule 10 is water.

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

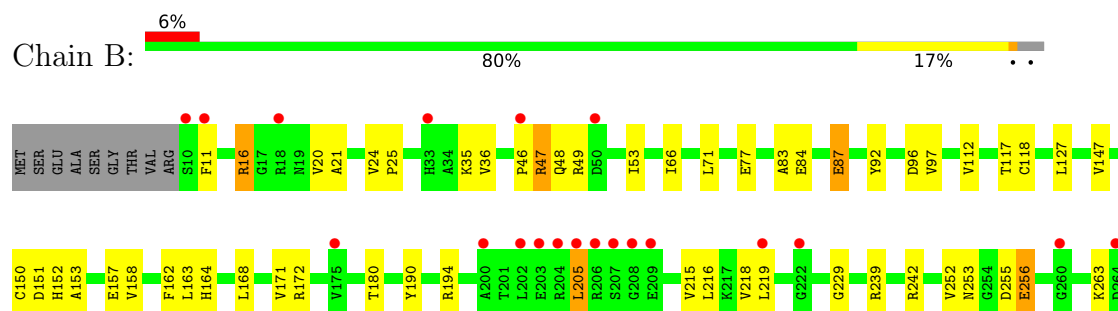
3 Residue-property plots

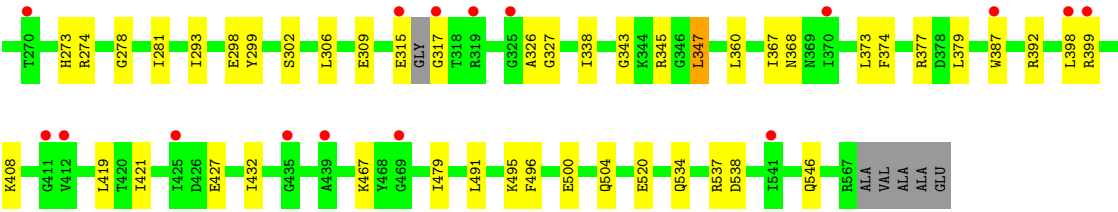
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Tungsten-containing formate dehydrogenase alpha subunit



- Molecule 2: Tungsten-containing formate dehydrogenase beta subunit





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	232.86Å 73.95Å 95.74Å 90.00° 106.72° 90.00°	Depositor
Resolution (Å)	47.48 – 2.40 47.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.6 (47.48-2.40) 93.6 (47.48-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.219 , 0.259 0.226 , 0.262	Depositor DCC
R_{free} test set	2868 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11489	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: W, FES, PEG, GOL, MGD, SF4, FMN

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	0.20	0/7166	0.39	0/9744
2	B	0.17	0/4371	0.35	0/5924
All	All	0.19	0/11537	0.37	0/15668

There are no bond length outliers.

There are no bond angle outliers.

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	7007	0	6878	83	0
2	B	4278	0	4180	57	0
3	A	94	0	42	9	0
4	A	1	0	0	0	0
5	A	4	0	0	1	0
5	B	4	0	0	0	0
6	A	24	0	0	0	0
6	B	8	0	0	0	0
7	A	18	0	24	0	0
7	B	12	0	16	2	0
8	A	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	31	0	19	2	0
10	A	1	0	0	0	0
All	All	11489	0	11169	133	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 6.

All (133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:VAL:HG12	1:A:628:PRO:HD2	1.71	0.70
1:A:236:TYR:O	2:B:345:ARG:NH2	2.27	0.68
2:B:495:LYS:NZ	2:B:520:GLU:OE2	2.27	0.68
2:B:315:GLU:O	2:B:317:GLY:N	2.27	0.67
2:B:47:ARG:HD3	2:B:77:GLU:HG3	1.76	0.67
1:A:885:MET:SD	3:A:1001:MGD:H8	2.35	0.66
1:A:200:ASP:HB3	1:A:208:VAL:HB	1.76	0.66
1:A:755:ASP:HB2	1:A:757:ARG:HG3	1.77	0.66
1:A:908:LEU:HD21	1:A:932:VAL:HG21	1.78	0.65
1:A:351:ARG:NH2	1:A:733:PHE:O	2.31	0.64
1:A:294:LEU:HB2	1:A:744:PHE:HZ	1.61	0.64
2:B:152:HIS:HB3	2:B:164:HIS:HB3	1.80	0.64
2:B:49:ARG:NH1	2:B:343:GLY:O	2.31	0.63
1:A:199:SER:OG	1:A:209:ASN:OD1	2.16	0.62
1:A:757:ARG:NH2	1:A:835:GLU:OE2	2.34	0.61
1:A:881:HIS:NE2	3:A:1002:MGD:S13	2.73	0.61
2:B:392:ARG:NH2	2:B:427:GLU:OE1	2.34	0.60
1:A:920:ARG:HB3	1:A:979:VAL:HG23	1.82	0.60
1:A:875:ARG:NH2	3:A:1001:MGD:S13	2.75	0.59
2:B:205:LEU:HD13	2:B:215:VAL:HG21	1.84	0.59
2:B:46:PRO:HB2	2:B:48:GLN:HG2	1.84	0.58
1:A:599:HIS:HA	1:A:970:GLU:HG3	1.85	0.58
1:A:875:ARG:HE	3:A:1002:MGD:H15	1.51	0.58
1:A:592:TRP:CZ2	1:A:628:PRO:HG3	2.39	0.57
2:B:274:ARG:HD2	2:B:374:PHE:CZ	2.40	0.56
1:A:543:ALA:O	1:A:848:ARG:NH2	2.36	0.56
2:B:83:ALA:O	2:B:87:GLU:HB2	2.05	0.56
1:A:217:ASN:ND2	1:A:221:ARG:HE	2.03	0.56
1:A:404:GLY:HA3	1:A:643:LEU:HD21	1.87	0.55
2:B:147:VAL:HG12	2:B:298:GLU:HG2	1.88	0.55
1:A:498:MET:HE2	1:A:513:LEU:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TRP:CD1	1:A:242:LYS:HD2	2.44	0.53
1:A:407:LYS:HE2	1:A:885:MET:HE1	1.91	0.52
2:B:219:LEU:HD23	2:B:379:LEU:HD23	1.91	0.52
1:A:113:GLY:HA2	5:A:1004:FES:S1	2.49	0.52
1:A:224:ARG:HH12	2:B:87:GLU:CD	2.16	0.52
1:A:406:ALA:HB2	1:A:431:HIS:CD2	2.45	0.51
1:A:875:ARG:HH22	3:A:1001:MGD:H15	1.59	0.51
2:B:421:ILE:HD11	2:B:479:ILE:HD11	1.93	0.51
2:B:537:ARG:HA	2:B:546:GLN:HA	1.92	0.51
1:A:231:VAL:HG21	1:A:256:CYS:HA	1.93	0.51
1:A:294:LEU:HB2	1:A:744:PHE:CZ	2.43	0.51
2:B:190:TYR:CZ	2:B:194:ARG:HD2	2.46	0.50
2:B:168:LEU:HD21	2:B:172:ARG:HH21	1.77	0.50
2:B:392:ARG:HG3	2:B:419:LEU:HD23	1.94	0.49
2:B:216:LEU:HD13	2:B:239:ARG:HG2	1.95	0.49
1:A:501:ARG:HD3	3:A:1002:MGD:O2'	2.13	0.48
2:B:96:ASP:HA	7:B:605:GOL:H2	1.95	0.48
1:A:86:THR:O	1:A:90:VAL:HG23	2.13	0.48
1:A:419:LEU:HD11	1:A:785:LEU:HD12	1.97	0.47
1:A:197:TRP:NE1	1:A:242:LYS:HD2	2.30	0.47
2:B:534:GLN:O	2:B:538:ASP:HB2	2.14	0.47
1:A:415:LEU:HB3	1:A:778:ILE:HG21	1.97	0.47
1:A:497:ILE:HD12	1:A:506:SER:HA	1.96	0.47
1:A:401:ALA:HB1	1:A:682:ILE:HD13	1.97	0.46
1:A:880:TRP:CD1	1:A:885:MET:HE2	2.51	0.46
1:A:699:GLU:HG2	1:A:701:PRO:HD3	1.98	0.46
2:B:158:VAL:HG12	2:B:180:THR:HG22	1.98	0.46
2:B:273:HIS:CE1	2:B:309:GLU:HB3	2.51	0.46
1:A:224:ARG:NH2	2:B:84:GLU:HG2	2.31	0.45
1:A:335:GLY:HA3	1:A:892:LEU:HD11	1.98	0.45
1:A:210:LEU:HD12	1:A:242:LYS:NZ	2.31	0.45
2:B:118:CYS:HA	2:B:153:ALA:HB1	1.98	0.45
2:B:229:GLY:HA3	7:B:604:GOL:O2	2.17	0.45
2:B:491:LEU:HG	2:B:495:LYS:HE2	1.98	0.45
1:A:562:GLU:OE2	1:A:576:ARG:NH2	2.31	0.45
2:B:496:PHE:CZ	2:B:500:GLU:HG3	2.51	0.44
1:A:479:VAL:O	1:A:482:THR:OG1	2.35	0.44
2:B:163:LEU:HD12	2:B:171:VAL:HG22	2.00	0.44
1:A:180:GLN:O	1:A:183:VAL:HG22	2.18	0.44
1:A:405:SER:HB2	1:A:698:GLY:HA3	1.99	0.44
1:A:116:ARG:O	1:A:119:MET:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:TYR:HB3	2:B:302:SER:HB2	2.00	0.43
1:A:348:PRO:HA	1:A:740:PRO:HD3	2.00	0.43
2:B:338:ILE:HG23	2:B:360:LEU:HA	2.00	0.43
1:A:217:ASN:ND2	1:A:217:ASN:O	2.51	0.43
1:A:502:ARG:HB3	1:A:937:ASP:CG	2.43	0.43
2:B:347:LEU:HD13	2:B:504:GLN:HB2	2.00	0.43
1:A:69:THR:HB	1:A:80:GLU:HG2	2.00	0.43
1:A:515:PHE:HZ	3:A:1002:MGD:N2	2.17	0.43
1:A:598:GLN:OE1	1:A:972:LYS:NZ	2.28	0.43
1:A:114:ASN:HB2	2:B:504:GLN:O	2.19	0.43
1:A:210:LEU:HD12	1:A:242:LYS:HZ2	1.83	0.43
2:B:151:ASP:OD1	2:B:151:ASP:N	2.46	0.43
1:A:345:LEU:HB3	1:A:740:PRO:HB3	2.01	0.43
1:A:647:VAL:HG12	1:A:653:SER:HA	2.00	0.43
2:B:117:THR:HG22	2:B:153:ALA:HB2	2.01	0.43
1:A:237:ARG:NH2	2:B:327:GLY:O	2.51	0.42
1:A:474:THR:HG23	1:A:505:LEU:HG	2.01	0.42
1:A:828:ALA:HB3	1:A:831:GLN:HG3	2.01	0.42
1:A:148:ARG:HD3	2:B:538:ASP:OD2	2.20	0.42
2:B:252:VAL:HB	2:B:293:ILE:HA	2.01	0.42
1:A:748:ALA:HB2	1:A:763:PRO:HD3	2.01	0.42
2:B:112:VAL:HB	2:B:127:LEU:HD13	2.01	0.42
2:B:253:ASN:ND2	9:B:601:FMN:O4'	2.50	0.42
1:A:494:LYS:HD3	1:A:581:LEU:HD21	2.01	0.42
2:B:368:ASN:HA	9:B:601:FMN:O1P	2.20	0.42
1:A:164:GLN:HG3	1:A:177:PHE:CE2	2.55	0.42
2:B:306:LEU:HD23	2:B:306:LEU:HA	1.84	0.42
1:A:906:LYS:HG2	1:A:940:ILE:HD11	2.02	0.41
1:A:934:SER:O	2:B:25:PRO:HD3	2.20	0.41
2:B:157:GLU:HB2	2:B:162:PHE:CE1	2.54	0.41
2:B:205:LEU:HD22	2:B:281:ILE:HG23	2.01	0.41
2:B:338:ILE:HD11	2:B:367:ILE:HD11	2.02	0.41
2:B:408:LYS:HE3	2:B:432:ILE:O	2.20	0.41
2:B:16:ARG:N	2:B:16:ARG:HD3	2.35	0.41
1:A:288:ASP:OD1	1:A:309:LYS:HD2	2.21	0.41
1:A:879:HIS:O	3:A:1002:MGD:N18	2.42	0.41
3:A:1002:MGD:H8	3:A:1002:MGD:H2'	1.86	0.41
2:B:53:ILE:HG12	2:B:343:GLY:HA2	2.02	0.41
1:A:260:GLY:HA3	1:A:333:ARG:CD	2.50	0.41
1:A:521:VAL:HG11	1:A:855:ALA:O	2.19	0.41
1:A:845:GLU:H	1:A:845:GLU:HG3	1.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:TRP:CH2	2:B:398:LEU:HB2	2.55	0.41
1:A:705:ASP:O	1:A:955:ASN:HB3	2.21	0.41
2:B:255:ASP:O	2:B:256:GLU:C	2.64	0.41
1:A:530:VAL:HG21	1:A:576:ARG:HA	2.02	0.41
1:A:656:LYS:HD2	1:A:656:LYS:HA	1.89	0.41
1:A:898:GLU:HB3	2:B:21:ALA:HB2	2.02	0.41
1:A:601:HIS:HB3	1:A:857:VAL:HB	2.03	0.41
2:B:66:ILE:O	2:B:97:VAL:HA	2.21	0.41
2:B:218:VAL:HG12	2:B:379:LEU:HG	2.03	0.41
2:B:278:GLY:HA3	2:B:373:LEU:O	2.21	0.41
1:A:414:TYR:CG	1:A:801:MET:HG2	2.57	0.40
1:A:861:GLU:OE1	1:A:974:CYS:HB2	2.21	0.40
1:A:144:SER:O	1:A:153:ARG:NH2	2.54	0.40
1:A:648:TYR:CE2	1:A:654:VAL:HA	2.56	0.40
1:A:412:GLU:OE2	1:A:774:ASP:HB2	2.20	0.40
1:A:420:VAL:HG11	1:A:429:VAL:HB	2.04	0.40
1:A:450:SER:HB2	1:A:838:PHE:CZ	2.57	0.40
1:A:961:ALA:O	1:A:969:PRO:HA	2.21	0.40
2:B:92:TYR:HB3	2:B:326:ALA:O	2.21	0.40
1:A:797:ILE:O	1:A:801:MET:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	907/989 (92%)	879 (97%)	28 (3%)	0	100	100
2	B	553/572 (97%)	540 (98%)	12 (2%)	1 (0%)	43	58
All	All	1460/1561 (94%)	1419 (97%)	40 (3%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	256	GLU

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	735/785 (94%)	697 (95%)	38 (5%)	21	36
2	B	443/454 (98%)	426 (96%)	17 (4%)	29	49
All	All	1178/1239 (95%)	1123 (95%)	55 (5%)	23	41

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	94	LEU
1	A	110	ARG
1	A	127	VAL
1	A	143	LYS
1	A	147	GLU
1	A	159	LEU
1	A	183	VAL
1	A	184	LEU
1	A	187	THR
1	A	188	GLU
1	A	190	ARG
1	A	195	GLU
1	A	198	THR
1	A	199	SER
1	A	217	ASN
1	A	218	LEU
1	A	263	VAL
1	A	288	ASP
1	A	298	CYS
1	A	328	LEU
1	A	353	GLU
1	A	426	THR

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Mol	Chain	Res	Type
1	A	484	LEU
1	A	505	LEU
1	A	540	GLN
1	A	644	ILE
1	A	646	MET
1	A	650	ASP
1	A	670	SER
1	A	770	ASP
1	A	826	VAL
1	A	845	GLU
1	A	848	ARG
1	A	884	SER
1	A	908	LEU
1	A	911	LEU
1	A	940	ILE
2	B	11	PHE
2	B	16	ARG
2	B	20	VAL
2	B	24	VAL
2	B	35	LYS
2	B	36	VAL
2	B	47	ARG
2	B	71	LEU
2	B	87	GLU
2	B	150	CYS
2	B	205	LEU
2	B	242	ARG
2	B	263	LYS
2	B	347	LEU
2	B	377	ARG
2	B	399	ARG
2	B	467	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
1	A	326	ASN
1	A	395	ASN
1	A	601	HIS
1	A	652	GLN
1	A	713	HIS

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Mol	Chain	Res	Type
2	B	29	GLN
2	B	492	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	FES	A	1004	1	0,4,4	-	-	-		
3	MGD	A	1002	4	47,52,52	4.92	29 (61%)	58,81,81	2.93	21 (36%)
7	GOL	B	605	-	5,5,5	0.84	0	5,5,5	1.07	0
5	FES	B	603	2	0,4,4	-	-	-		
8	PEG	A	1010	-	6,6,6	0.18	0	5,5,5	0.17	0
7	GOL	B	604	-	5,5,5	0.79	0	5,5,5	1.13	1 (20%)
6	SF4	A	1006	1	0,12,12	-	-	-		
3	MGD	A	1001	4	47,52,52	4.86	32 (68%)	58,81,81	2.47	21 (36%)
7	GOL	A	1009	-	5,5,5	0.80	0	5,5,5	1.17	0
9	FMN	B	601	-	33,33,33	2.39	6 (18%)	48,50,50	1.79	14 (29%)
7	GOL	A	1008	-	5,5,5	0.78	0	5,5,5	1.16	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SF4	B	602	2	0,12,12	-	-	-		
6	SF4	A	1007	1	0,12,12	-	-	-		
7	GOL	A	1011	-	5,5,5	0.95	0	5,5,5	1.01	0
6	SF4	A	1005	1	0,12,12	-	-	-		

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	FES	A	1004	1	-	-	0/1/1/1
3	MGD	A	1002	4	-	8/22/66/66	0/6/6/6
7	GOL	B	605	-	-	2/4/4/4	-
8	PEG	A	1010	-	-	1/4/4/4	-
5	FES	B	603	2	-	-	0/1/1/1
7	GOL	B	604	-	-	2/4/4/4	-
7	GOL	A	1009	-	-	4/4/4/4	-
3	MGD	A	1001	4	-	8/22/66/66	0/6/6/6
9	FMN	B	601	-	-	5/18/18/18	0/3/3/3
6	SF4	A	1006	1	-	-	0/6/5/5
7	GOL	A	1008	-	-	4/4/4/4	-
6	SF4	B	602	2	-	-	0/6/5/5
6	SF4	A	1007	1	-	-	0/6/5/5
7	GOL	A	1011	-	-	3/4/4/4	-
6	SF4	A	1005	1	-	-	0/6/5/5

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	MGD	C14-N15	-12.11	1.32	1.46
3	A	1002	MGD	C23-C14	-11.37	1.44	1.53
3	A	1002	MGD	C14-N15	-11.18	1.33	1.46
3	A	1001	MGD	C19-N18	10.57	1.63	1.37
3	A	1002	MGD	C19-N18	10.50	1.63	1.37
3	A	1001	MGD	C3'-C4'	-9.86	1.28	1.53
3	A	1001	MGD	C23-C14	-9.86	1.45	1.53
3	A	1002	MGD	C3'-C4'	-9.70	1.28	1.53
3	A	1002	MGD	C19-N20	9.17	1.55	1.33
3	A	1001	MGD	C19-N20	9.10	1.55	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	MGD	C2'-C1'	-8.70	1.26	1.53
3	A	1001	MGD	C2'-C1'	-8.34	1.27	1.53
3	A	1002	MGD	C23-N22	-7.93	1.32	1.45
3	A	1002	MGD	PA-O3B	7.64	1.67	1.59
3	A	1002	MGD	C17-N18	7.42	1.52	1.38
3	A	1001	MGD	C23-N22	-7.28	1.33	1.45
3	A	1001	MGD	C17-N18	7.22	1.52	1.38
3	A	1002	MGD	PB-O3B	7.17	1.67	1.59
3	A	1001	MGD	PB-O3B	7.07	1.67	1.59
3	A	1001	MGD	PA-O3B	7.04	1.67	1.59
9	B	601	FMN	O4-C4	6.65	1.36	1.23
9	B	601	FMN	O2-C2	6.33	1.36	1.24
3	A	1001	MGD	C4-N3	6.22	1.48	1.34
3	A	1002	MGD	C4-N3	6.14	1.48	1.34
9	B	601	FMN	C9-C8	6.04	1.47	1.39
3	A	1001	MGD	O4'-C1'	5.95	1.55	1.42
9	B	601	FMN	C9A-C5A	5.54	1.50	1.41
3	A	1002	MGD	O4'-C1'	5.32	1.54	1.42
3	A	1002	MGD	C19-N19	5.01	1.45	1.34
3	A	1001	MGD	C19-N19	4.90	1.45	1.34
3	A	1001	MGD	C2'-C3'	4.87	1.66	1.53
3	A	1002	MGD	C2-N3	4.82	1.44	1.33
3	A	1001	MGD	C2-N3	4.67	1.44	1.33
3	A	1002	MGD	C2'-C3'	4.60	1.65	1.53
3	A	1001	MGD	O4'-C4'	4.15	1.54	1.45
3	A	1001	MGD	C2-N2	3.90	1.43	1.34
3	A	1002	MGD	C10-C11	-3.88	1.46	1.51
3	A	1002	MGD	C2-N2	3.79	1.43	1.34
3	A	1002	MGD	O4'-C4'	3.75	1.53	1.45
3	A	1002	MGD	C16-C21	3.56	1.44	1.38
9	B	601	FMN	C8-C7	3.45	1.49	1.40
3	A	1001	MGD	C16-C21	3.38	1.44	1.38
3	A	1001	MGD	C10-C11	-3.26	1.47	1.51
3	A	1001	MGD	O11-C11	3.24	1.49	1.43
3	A	1002	MGD	C21-N20	3.11	1.41	1.36
3	A	1001	MGD	C2-N1	3.06	1.45	1.37
3	A	1001	MGD	C21-N20	3.03	1.40	1.36
3	A	1002	MGD	C4-N9	-3.01	1.30	1.38
3	A	1002	MGD	C2-N1	2.97	1.44	1.37
3	A	1001	MGD	C5-N7	-2.76	1.33	1.39
3	A	1002	MGD	C5-N7	-2.75	1.33	1.39
3	A	1002	MGD	O6-C6	-2.69	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	MGD	C16-C17	2.68	1.49	1.41
3	A	1001	MGD	C4-N9	-2.61	1.31	1.38
3	A	1002	MGD	O17-C17	-2.53	1.18	1.23
3	A	1001	MGD	O6-C6	-2.47	1.18	1.23
3	A	1002	MGD	O11-C11	2.47	1.48	1.43
3	A	1001	MGD	C16-C17	2.43	1.49	1.41
3	A	1001	MGD	C5-C6	2.39	1.53	1.44
3	A	1002	MGD	C5-C6	2.35	1.53	1.44
3	A	1001	MGD	O17-C17	-2.33	1.19	1.23
9	B	601	FMN	C4A-N5	2.29	1.35	1.30
3	A	1001	MGD	O11-C23	2.23	1.47	1.43
3	A	1001	MGD	C16-N15	-2.17	1.32	1.37
3	A	1001	MGD	C5'-C4'	2.05	1.57	1.51
3	A	1002	MGD	C6-N1	2.03	1.42	1.38
3	A	1001	MGD	C6-N1	2.02	1.42	1.38

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	MGD	O11-C23-N22	-14.92	95.07	108.61
3	A	1001	MGD	O11-C23-C14	9.73	115.45	108.96
3	A	1002	MGD	C23-C14-N15	5.75	113.52	107.87
3	A	1001	MGD	C23-C14-N15	5.40	113.17	107.87
3	A	1001	MGD	C19-N18-C17	-5.29	115.52	125.11
9	B	601	FMN	C8M-C8-C7	-5.20	110.14	120.76
3	A	1002	MGD	C19-N18-C17	-4.98	116.08	125.11
3	A	1002	MGD	C19-N20-C21	4.95	122.09	113.36
9	B	601	FMN	C8M-C8-C9	-4.37	111.88	119.57
3	A	1001	MGD	C19-N20-C21	4.33	121.00	113.36
3	A	1001	MGD	C5-C4-N3	-4.14	121.81	128.39
3	A	1001	MGD	C2-N3-C4	4.11	119.37	112.30
3	A	1002	MGD	N18-C19-N20	-3.82	116.33	123.32
3	A	1002	MGD	C2-N3-C4	3.81	118.87	112.30
3	A	1002	MGD	N9-C8-N7	-3.74	106.46	113.40
9	B	601	FMN	C9-C8-C7	-3.59	114.41	119.69
3	A	1001	MGD	N9-C8-N7	-3.55	106.83	113.40
3	A	1002	MGD	C5-C4-N3	-3.38	123.01	128.39
3	A	1002	MGD	C16-C17-N18	3.33	121.28	112.13
9	B	601	FMN	C4-C4A-N5	3.21	122.65	118.21
3	A	1001	MGD	N18-C19-N20	-3.11	117.62	123.32
3	A	1001	MGD	C16-C17-N18	3.06	120.52	112.13
3	A	1001	MGD	C2-N1-C6	-3.00	119.67	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	MGD	C2'-C3'-C4'	2.99	108.39	102.61
3	A	1002	MGD	N19-C19-N18	2.82	122.70	116.76
3	A	1001	MGD	O17-C17-C16	-2.81	120.50	127.26
3	A	1001	MGD	C2'-C3'-C4'	2.80	108.02	102.61
3	A	1002	MGD	C2-N1-C6	-2.66	120.28	125.11
3	A	1002	MGD	C5-C6-N1	2.62	119.93	113.25
3	A	1001	MGD	C5-C6-N1	2.62	119.92	113.25
3	A	1002	MGD	C4'-O4'-C1'	-2.60	103.73	109.47
3	A	1001	MGD	N19-C19-N18	2.58	122.21	116.76
3	A	1002	MGD	O17-C17-C16	-2.52	121.17	127.26
9	B	601	FMN	C4A-C10-N10	2.46	120.00	116.48
3	A	1002	MGD	O6-C6-C5	-2.46	120.05	126.53
3	A	1001	MGD	O3A-C10-C11	-2.45	102.53	108.58
9	B	601	FMN	C6-C7-C8	2.43	123.25	119.69
3	A	1001	MGD	C8-N7-C5	2.41	108.55	104.26
3	A	1001	MGD	O4'-C1'-N9	-2.39	102.94	108.36
3	A	1001	MGD	O6-C6-C5	-2.36	120.31	126.53
3	A	1002	MGD	N2-C2-N1	2.34	121.71	116.76
3	A	1001	MGD	N2-C2-N1	2.31	121.64	116.76
3	A	1001	MGD	C4-C5-N7	-2.29	107.04	110.67
9	B	601	FMN	O2-C2-N1	-2.29	118.00	121.80
3	A	1001	MGD	C1'-N9-C8	-2.28	120.27	126.73
3	A	1002	MGD	O5'-C5'-C4'	-2.27	101.26	108.99
3	A	1002	MGD	C6-C5-N7	2.24	134.37	130.29
3	A	1002	MGD	C8-N7-C5	2.23	108.23	104.26
9	B	601	FMN	O2P-P-O5'	-2.16	101.03	106.67
9	B	601	FMN	O3P-P-O2P	2.16	115.89	107.80
9	B	601	FMN	C10-N1-C2	2.15	121.49	116.85
9	B	601	FMN	O4-C4-C4A	-2.14	120.88	126.53
9	B	601	FMN	C4-N3-C2	-2.13	121.87	125.64
9	B	601	FMN	C4A-C10-N1	-2.13	119.38	124.59
7	A	1008	GOL	C3-C2-C1	-2.11	104.05	111.80
7	B	604	GOL	C3-C2-C1	-2.07	104.21	111.80
9	B	601	FMN	C4A-C4-N3	2.06	118.49	113.25
3	A	1002	MGD	C4-C5-N7	-2.04	107.44	110.67

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	MGD	C5'-O5'-PB-O1B
3	A	1001	MGD	C5'-O5'-PB-O3B

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Mol	Chain	Res	Type	Atoms
3	A	1002	MGD	PA-O3B-PB-O5'
3	A	1002	MGD	C5'-O5'-PB-O1B
3	A	1002	MGD	C5'-O5'-PB-O2B
3	A	1002	MGD	C5'-O5'-PB-O3B
3	A	1002	MGD	C10-O3A-PA-O1A
7	A	1008	GOL	C1-C2-C3-O3
7	A	1009	GOL	C1-C2-C3-O3
7	A	1011	GOL	C1-C2-C3-O3
7	B	605	GOL	O1-C1-C2-C3
9	B	601	FMN	C5'-O5'-P-O1P
9	B	601	FMN	C5'-O5'-P-O2P
9	B	601	FMN	C5'-O5'-P-O3P
7	A	1008	GOL	O1-C1-C2-C3
7	A	1009	GOL	O1-C1-C2-C3
7	B	604	GOL	O1-C1-C2-C3
7	A	1008	GOL	O2-C2-C3-O3
7	B	605	GOL	O1-C1-C2-O2
8	A	1010	PEG	O1-C1-C2-O2
7	A	1008	GOL	O1-C1-C2-O2
7	A	1009	GOL	O2-C2-C3-O3
7	A	1011	GOL	O2-C2-C3-O3
7	B	604	GOL	O1-C1-C2-O2
3	A	1001	MGD	PA-O3B-PB-O5'
3	A	1001	MGD	C10-O3A-PA-O1A
9	B	601	FMN	O2'-C2'-C3'-C4'
7	A	1011	GOL	O1-C1-C2-C3
3	A	1001	MGD	C3'-C4'-C5'-O5'
3	A	1001	MGD	O4'-C4'-C5'-O5'
7	A	1009	GOL	O1-C1-C2-O2
3	A	1001	MGD	O3A-C10-C11-O11
3	A	1002	MGD	C2'-C1'-N9-C8
9	B	601	FMN	O2'-C2'-C3'-O3'
3	A	1001	MGD	O3A-C10-C11-C12
3	A	1002	MGD	C2'-C1'-N9-C4
3	A	1002	MGD	PA-O3B-PB-O2B

There are no ring outliers.

6 monomers are involved in 14 short contacts:

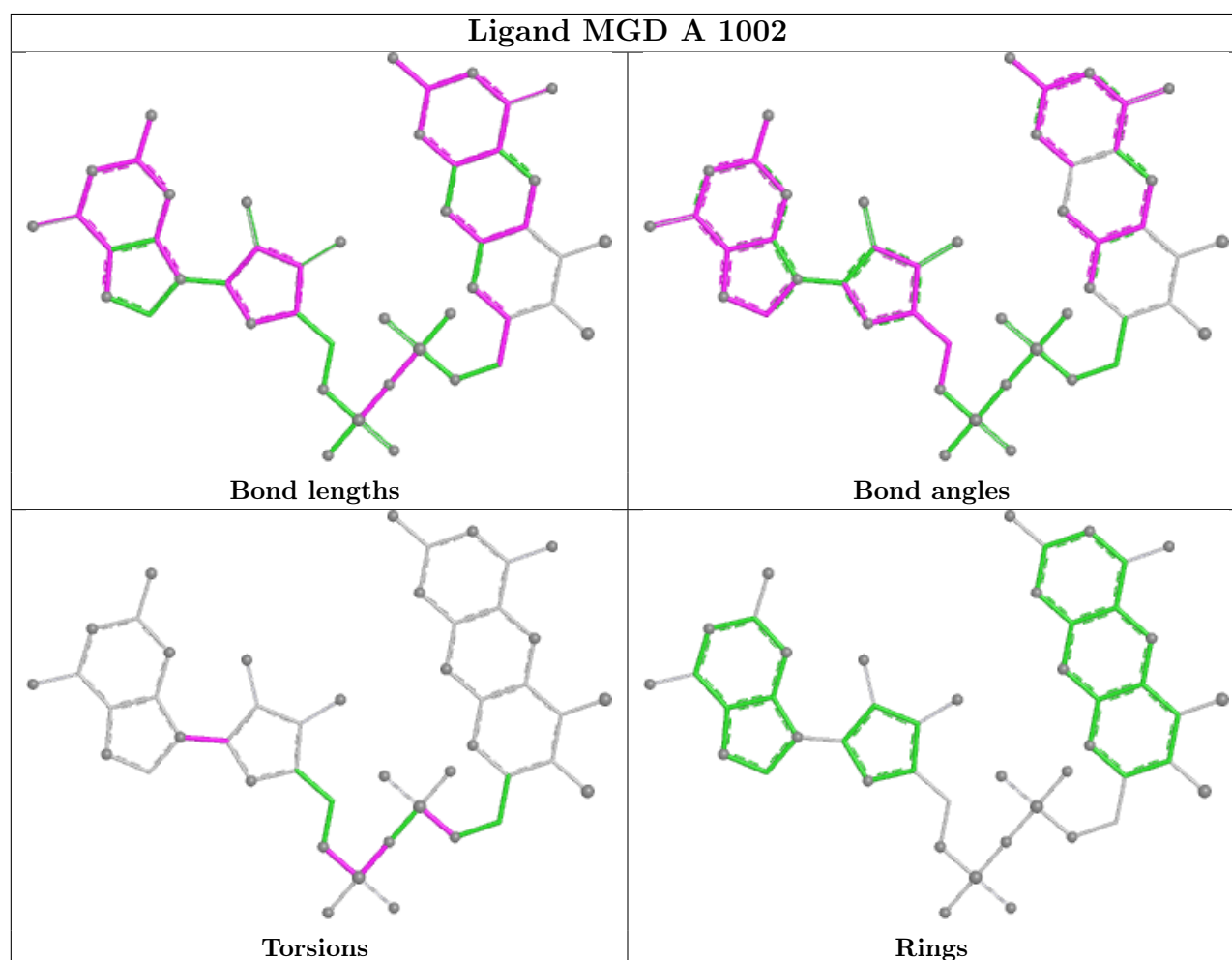
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1004	FES	1	0
3	A	1002	MGD	6	0

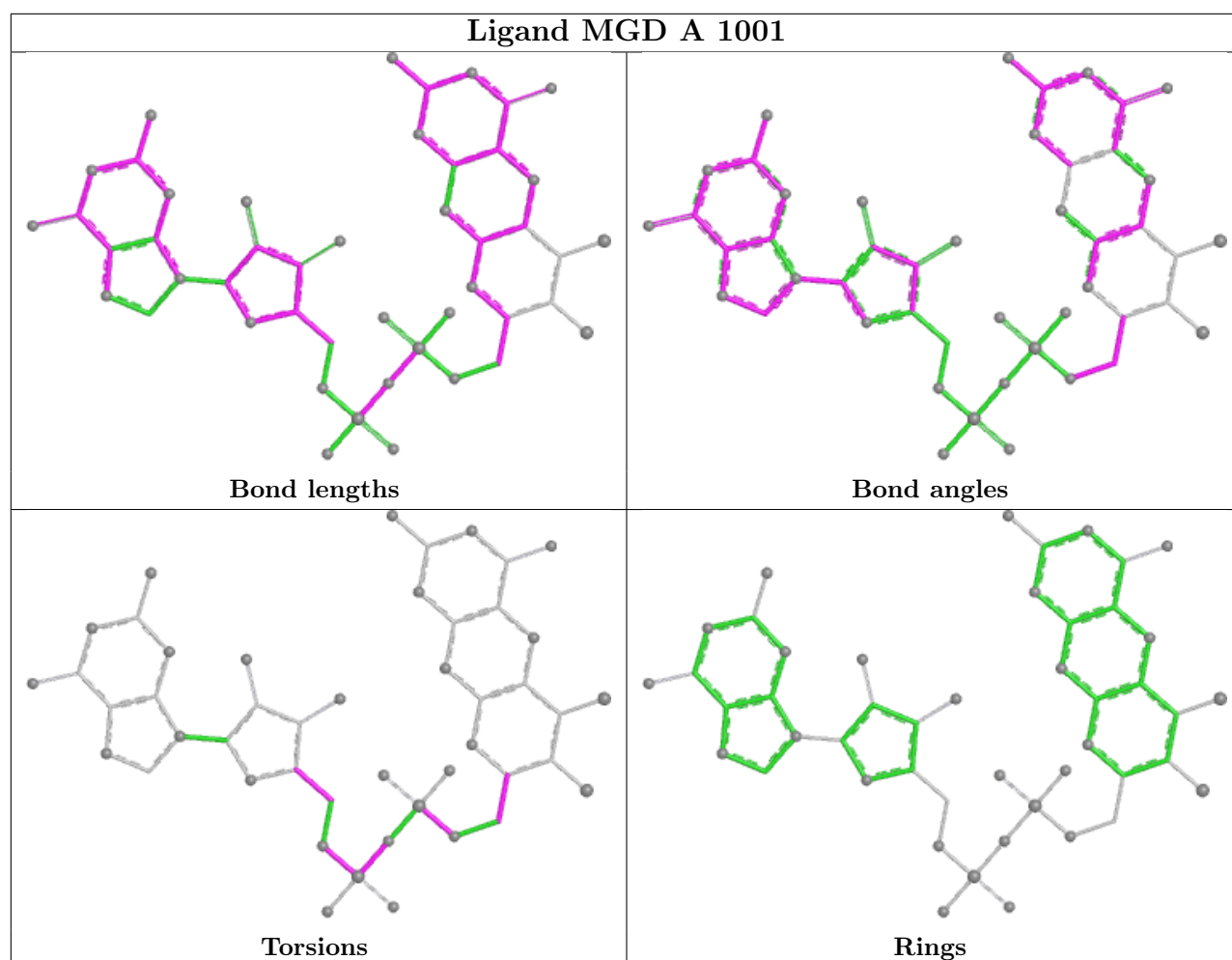
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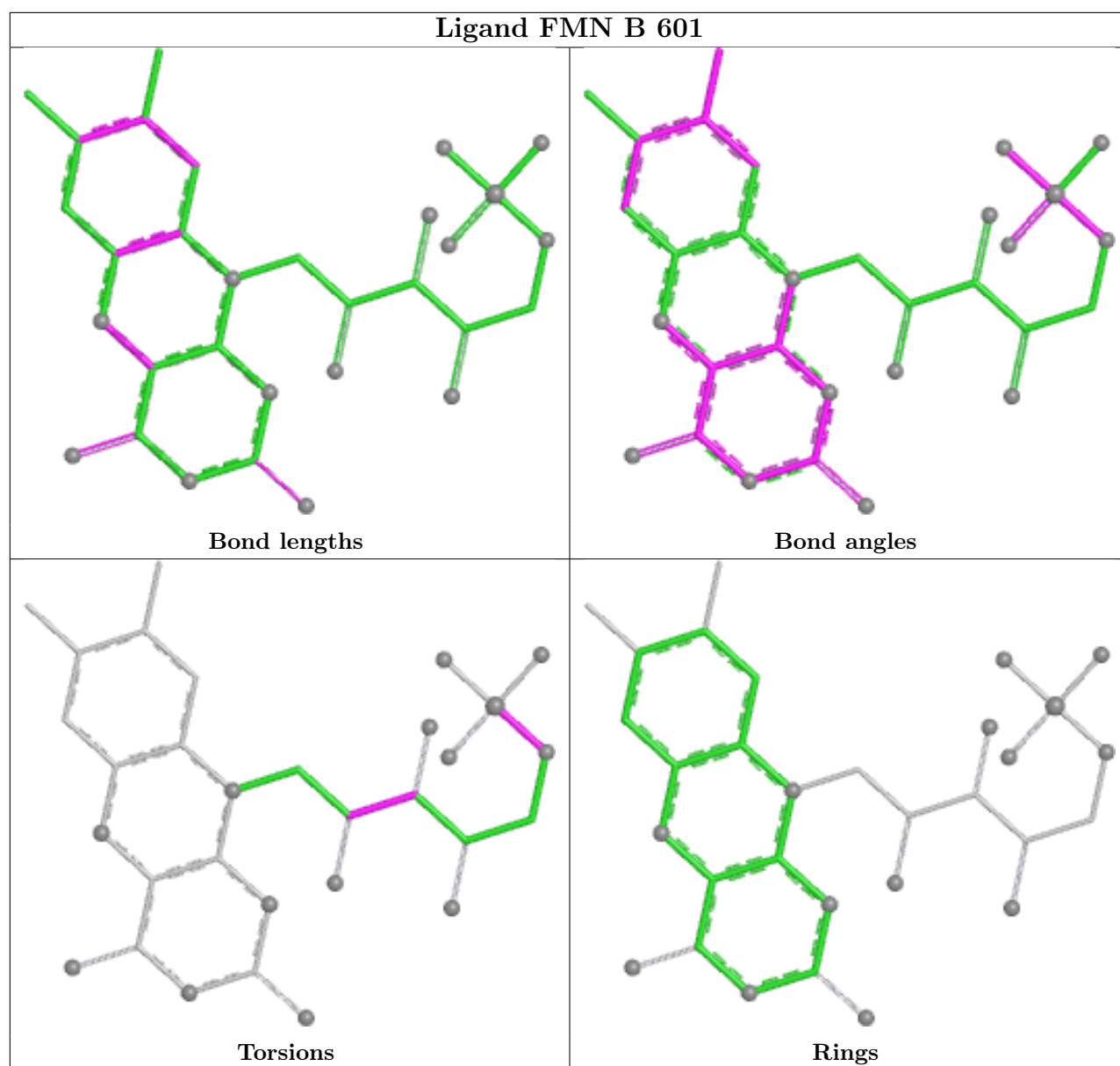
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	605	GOL	1	0
7	B	604	GOL	1	0
3	A	1001	MGD	3	0
9	B	601	FMN	2	0

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







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	911/989 (92%)	0.94	50 (5%)	30 27	38, 48, 63, 76	0
2	B	557/572 (97%)	0.96	36 (6%)	25 21	41, 53, 67, 95	0
All	All	1468/1561 (94%)	0.95	86 (5%)	28 24	38, 50, 65, 95	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	203	GLU	4.8
2	B	202	LEU	3.9
2	B	264	ASP	3.8
2	B	46	PRO	3.8
2	B	206	ARG	3.7
2	B	205	LEU	3.6
2	B	209	GLU	3.5
2	B	18	ARG	3.4
1	A	901	ALA	3.4
2	B	207	SER	3.4
1	A	981	ALA	3.3
2	B	204	ARG	3.3
1	A	874	GLY	3.1
1	A	520	ASP	3.0
1	A	451	GLY	3.0
2	B	10	SER	2.9
2	B	208	GLY	2.9
2	B	399	ARG	2.9
2	B	11	PHE	2.9
1	A	699	GLU	2.9
1	A	150	THR	2.8
2	B	317	GLY	2.8
1	A	127	VAL	2.8
2	B	33	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	260	GLY	2.8
1	A	979	VAL	2.7
1	A	557	VAL	2.6
2	B	469	GLY	2.6
2	B	370	ILE	2.5
1	A	133	LYS	2.5
1	A	851	ILE	2.5
1	A	690	GLU	2.5
2	B	175	VAL	2.5
1	A	146	THR	2.5
2	B	411	GLY	2.5
1	A	658	ALA	2.5
1	A	659	VAL	2.4
1	A	121	GLU	2.4
2	B	315	GLU	2.4
1	A	961	ALA	2.4
2	B	425	ILE	2.3
1	A	288	ASP	2.3
1	A	212	ALA	2.3
1	A	98	ILE	2.3
1	A	188	GLU	2.3
2	B	435	GLY	2.3
1	A	159	LEU	2.3
1	A	682	ILE	2.3
1	A	453	VAL	2.3
2	B	412	VAL	2.3
1	A	960	PRO	2.3
1	A	543	ALA	2.2
2	B	200	ALA	2.2
1	A	678	THR	2.2
1	A	966	GLY	2.2
2	B	541	ILE	2.2
2	B	319	ARG	2.2
2	B	50	ASP	2.2
2	B	439	ALA	2.2
1	A	803	GLN	2.2
1	A	909	TYR	2.2
1	A	199	SER	2.2
2	B	387	TRP	2.2
1	A	826	VAL	2.1
1	A	709	ASN	2.1
1	A	124	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	222	GLY	2.1
1	A	680	VAL	2.1
1	A	793	GLY	2.1
1	A	539	GLU	2.1
1	A	393	ASP	2.1
1	A	853	PRO	2.1
2	B	219	LEU	2.1
1	A	778	ILE	2.1
1	A	537	TYR	2.1
1	A	748	ALA	2.1
1	A	217	ASN	2.1
2	B	398	LEU	2.1
2	B	270	THR	2.1
1	A	644	ILE	2.1
1	A	553	ARG	2.0
1	A	328	LEU	2.0
1	A	108	GLY	2.0
2	B	325	GLY	2.0
1	A	558	ASP	2.0
1	A	805	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.

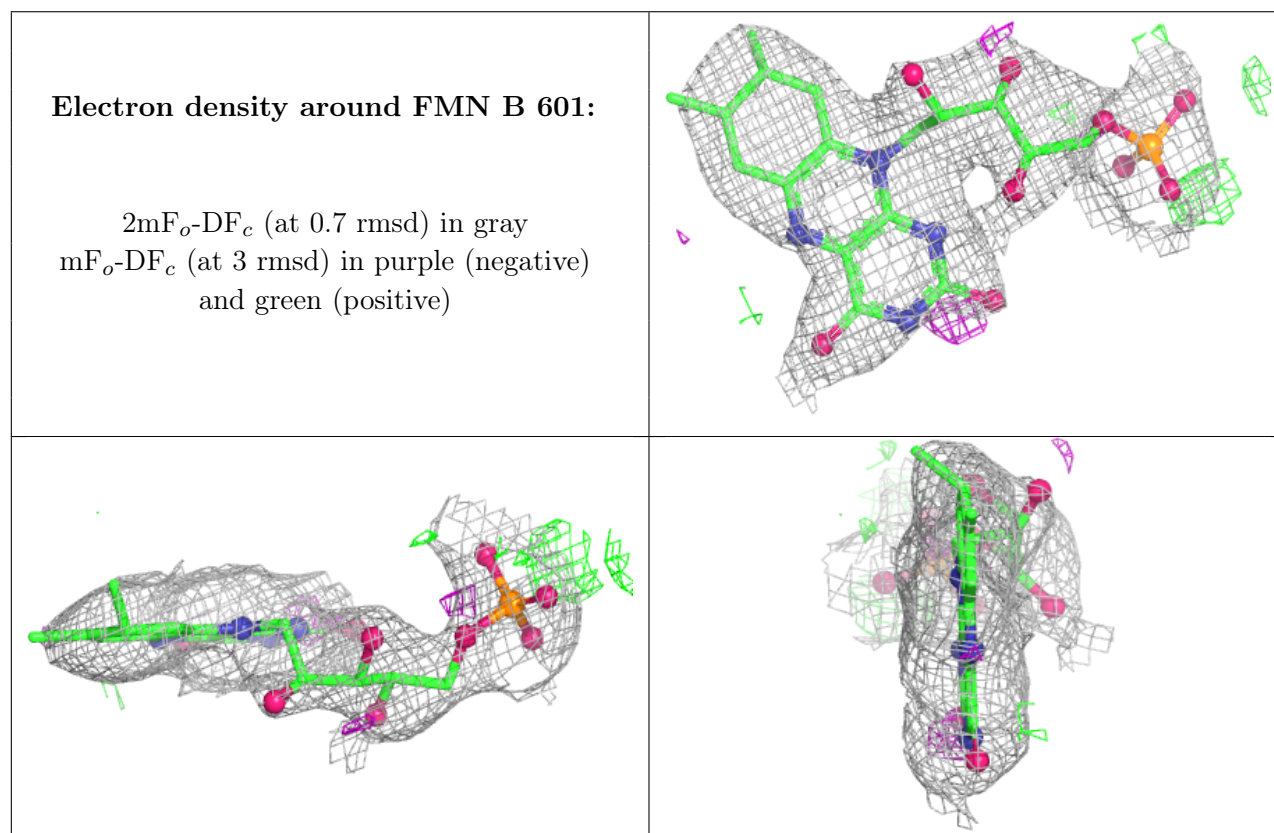
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	PEG	A	1010	7/7	0.62	0.18	53,56,61,63	0
7	GOL	B	605	6/6	0.75	0.16	46,49,50,50	0
7	GOL	A	1008	6/6	0.77	0.17	50,52,55,55	0

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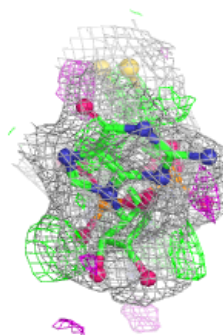
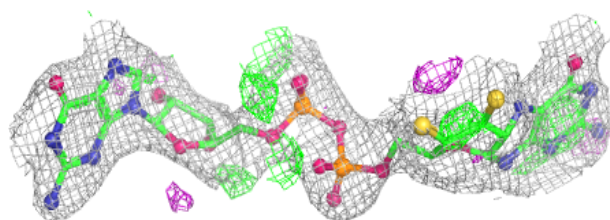
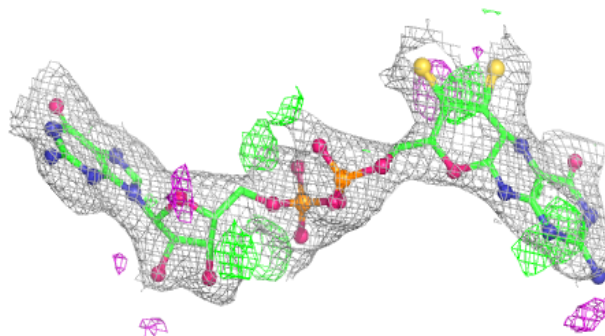
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	B	604	6/6	0.80	0.16	50,51,51,51	0
7	GOL	A	1011	6/6	0.85	0.16	44,45,45,45	0
7	GOL	A	1009	6/6	0.87	0.15	41,42,43,43	0
9	FMN	B	601	31/31	0.87	0.13	47,49,50,50	0
3	MGD	A	1001	47/47	0.92	0.12	40,43,44,45	0
5	FES	B	603	4/4	0.94	0.08	44,45,45,46	0
6	SF4	B	602	8/8	0.95	0.06	41,42,43,43	0
3	MGD	A	1002	47/47	0.95	0.10	40,41,45,46	0
6	SF4	A	1007	8/8	0.96	0.05	39,40,41,41	0
6	SF4	A	1005	8/8	0.96	0.06	38,40,41,41	0
6	SF4	A	1006	8/8	0.96	0.05	38,39,40,40	0
5	FES	A	1004	4/4	0.97	0.07	37,37,38,39	0
4	W	A	1003	1/1	1.00	0.02	44,44,44,44	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.

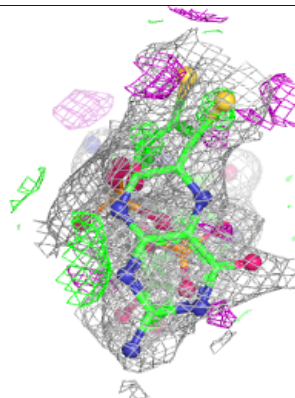
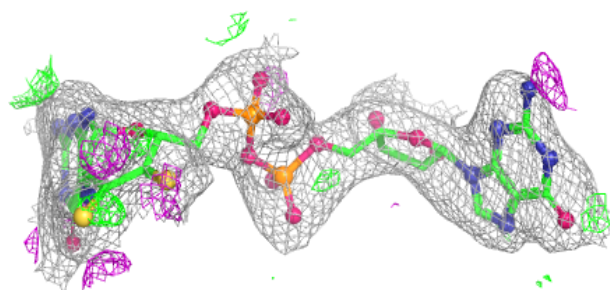
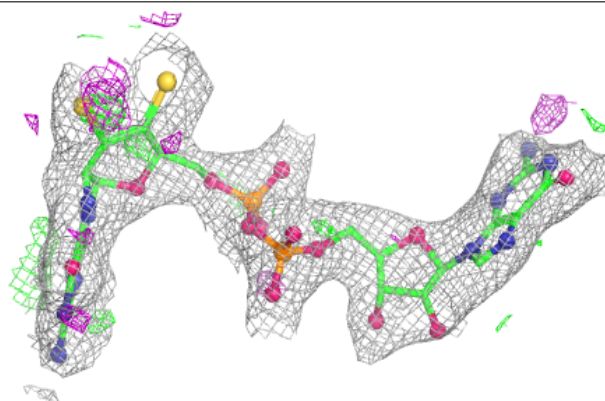


Electron density around MGD A 1001:

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

**Electron density around MGD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.