WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 07:32 AM EDT

PDB ID	:	4IOM
Title	:	N10-formyltetrahydrofolate synthetase from Moorella thermoacetica with folate
Authors	:	Stec, B.
Deposited on	:	2013-01-08
Resolution	:	3.00 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

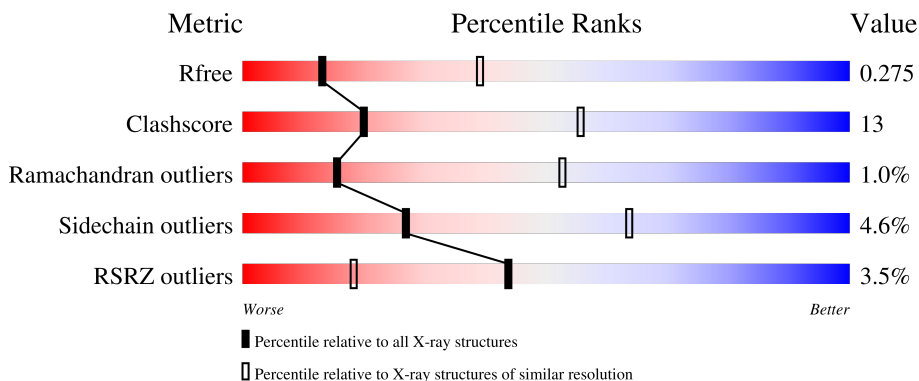|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.00 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	Percentile Ranks	Value
Rfree		0.275
Clashscore		13
Ramachandran outliers		1.0%
Sidechain outliers		4.6%
RSRZ outliers		3.5%

Worse　　　　　*Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	559	79% 　 19% 　 •
1	B	559	7%　62% 　 34% 　 •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FOL	A	608	-	-	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 8677 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 Formate--tetrahydrofolate ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4195	2661	721	792	21			
1	B	557	Total	C	N	O	S	0	0	0
			4195	2661	721	792	21			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

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

- Molecule 3 is 2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXYL (three-letter code: TOE) (formula: $C_7H_{16}O_4$).
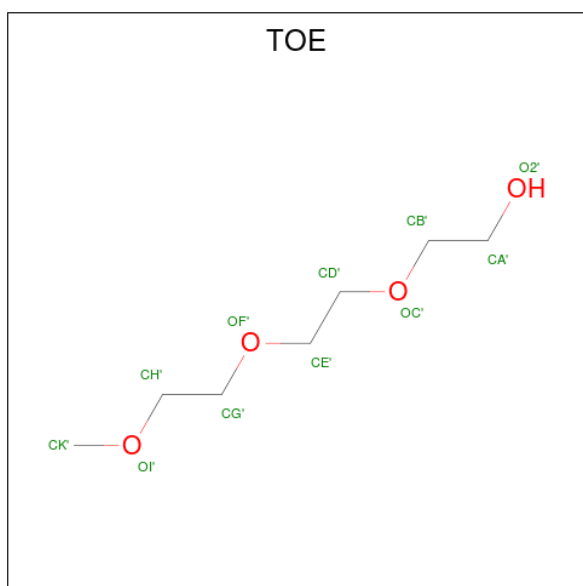
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 11	C 7	O 4	0	0
3	A	1	Total 11	C 7	O 4	0	0
3	B	1	Total 11	C 7	O 4	0	0

- Molecule 4 is FOLIC ACID (three-letter code: FOL) (formula: $C_{19}H_{19}N_7O_6$).

FOL
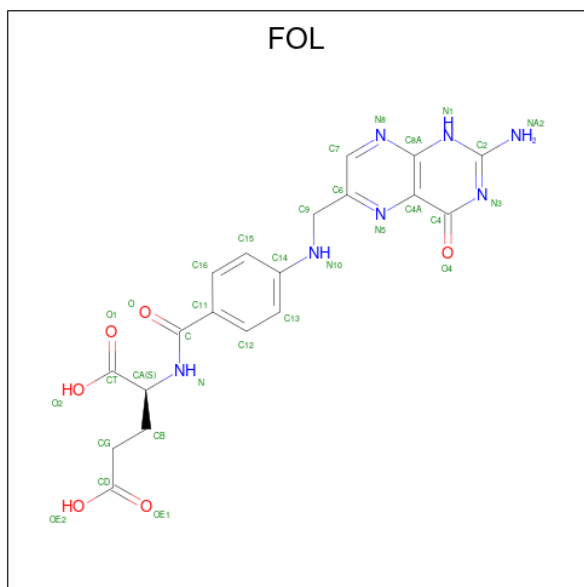
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			32	19	7	6		

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	133	Total	O	0	0
			133	133		
5	B	54	Total	O	0	0
			54	54		

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: Formate--tetrahydrofolate ligase

Chain A:

- Molecule 1: Formate--tetrahydrofolate ligase

Chain B:
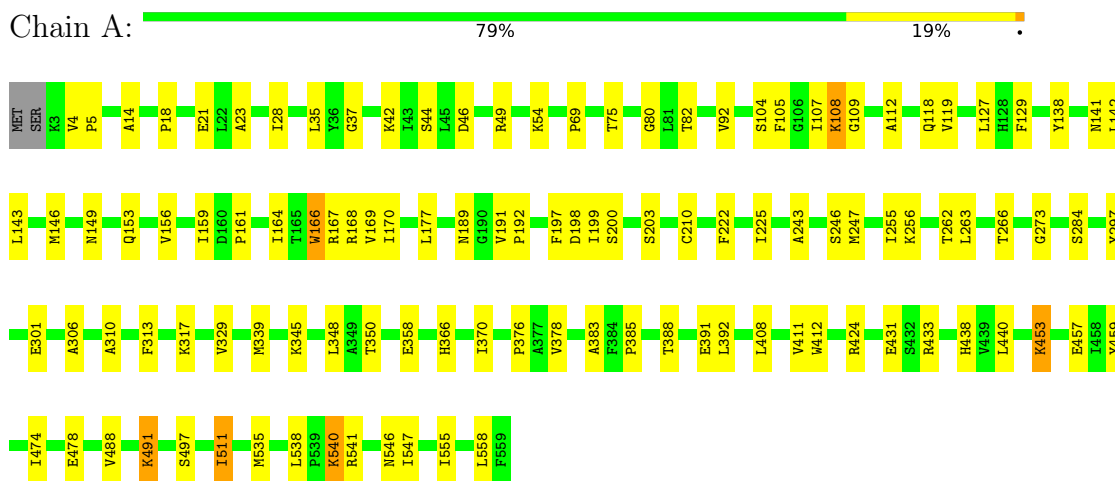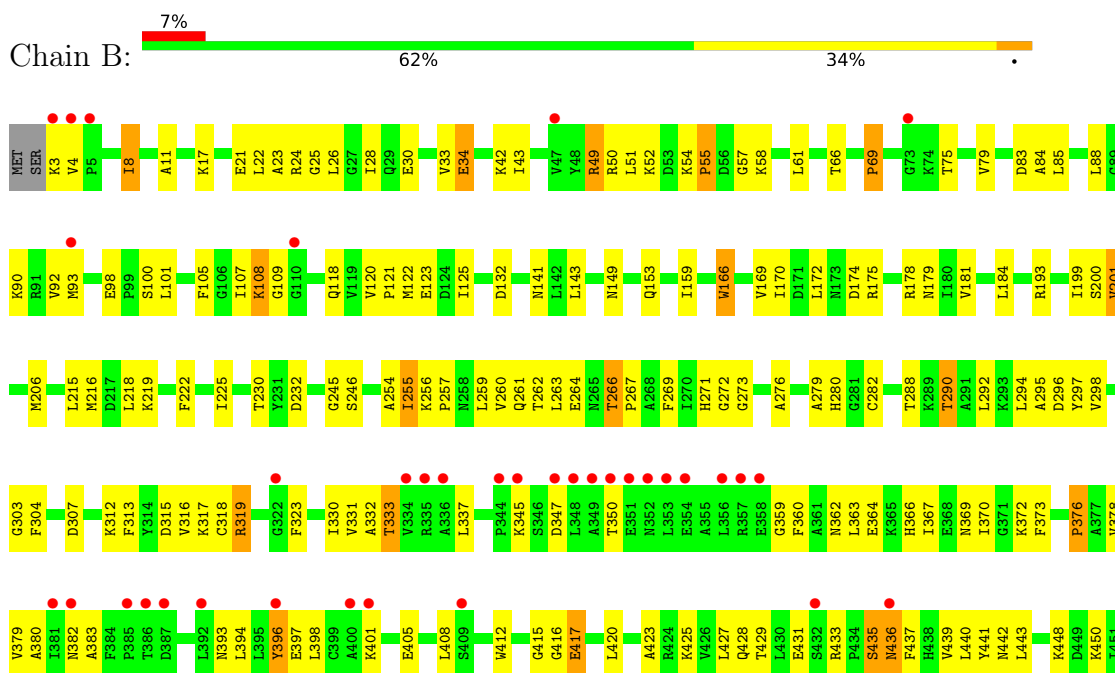
4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	160.99Å 160.99Å 256.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	122.51 – 3.00 48.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.9 (122.51-3.00) 91.0 (48.75-3.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	7.63 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.213 , 0.291 0.203 , 0.275	Depositor DCC
R_{free} test set	2524 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.5	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8677	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FOL, TOE, SO4

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	0.59	2/4266 (0.0%)	0.76	0/5778
1	B	0.51	2/4266 (0.0%)	0.70	0/5778
All	All	0.55	4/8532 (0.0%)	0.73	0/11556

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	TRP	CD2-CE2	5.72	1.48	1.41
1	B	412	TRP	CD2-CE2	5.46	1.48	1.41
1	A	166	TRP	CD2-CE2	5.33	1.47	1.41
1	A	412	TRP	CD2-CE2	5.01	1.47	1.41

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	4195	0	4278	79	0
1	B	4195	0	4278	150	0
2	A	25	0	0	0	0
2	B	10	0	0	2	0
3	A	22	0	32	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	16	0	0
4	A	32	0	17	6	0
5	A	133	0	0	9	0
5	B	54	0	0	2	0
All	All	8677	0	8621	216	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 13.

All (216) 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:383:ALA:HB1	4:A:608:FOL:H12	1.24	1.10
1:B:49:ARG:HG2	1:B:49:ARG:HH11	1.27	0.97
1:B:262:THR:HG22	1:B:264:GLU:H	1.29	0.96
1:A:383:ALA:HB1	4:A:608:FOL:C12	1.97	0.94
1:B:83:ASP:OD2	1:B:262:THR:HG21	1.71	0.91
1:B:429:THR:HG23	1:B:433:ARG:HD3	1.54	0.89
1:B:330:ILE:HD11	1:B:370:ILE:HD13	1.55	0.89
1:A:107:ILE:O	1:A:108:LYS:HB2	1.72	0.88
1:B:455:ALA:HA	1:B:459:TYR:HD2	1.37	0.88
1:B:292:LEU:HD23	1:B:298:VAL:HG21	1.58	0.85
1:A:169:VAL:HG11	1:A:203:SER:HB2	1.60	0.80
1:B:312:LYS:O	1:B:316:VAL:HG12	1.86	0.74
1:A:488:VAL:HA	5:A:704:HOH:O	1.85	0.73
1:B:455:ALA:HA	1:B:459:TYR:CD2	2.25	0.70
1:B:394:LEU:O	1:B:398:LEU:HG	1.90	0.70
1:B:376:PRO:HD2	1:B:435:SER:HB2	1.74	0.69
1:B:49:ARG:HG2	1:B:49:ARG:NH1	2.00	0.69
1:B:456:THR:HG23	1:B:457:GLU:N	2.08	0.68
1:B:383:ALA:HB2	1:B:408:LEU:HD11	1.75	0.68
1:A:385:PRO:HG3	4:A:608:FOL:H91	1.74	0.68
1:B:143:LEU:HD23	1:B:166:TRP:CE2	2.30	0.67
1:B:330:ILE:HD11	1:B:370:ILE:CD1	2.24	0.67
1:B:330:ILE:CD1	1:B:370:ILE:HD13	2.26	0.64
1:A:392:LEU:HD13	4:A:608:FOL:HG1	1.79	0.64
1:B:262:THR:HB	1:B:266:THR:H	1.63	0.64
1:A:538:LEU:HD12	1:B:149:ASN:HB2	1.79	0.63
1:B:456:THR:HG23	1:B:457:GLU:H	1.63	0.63
1:A:49:ARG:NH2	5:A:825:HOH:O	2.30	0.62
1:B:66:THR:H	1:B:362:ASN:HD21	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:HIS:HD2	1:B:282:CYS:SG	2.22	0.62
1:B:450:LYS:O	1:B:454:ILE:HG13	1.99	0.62
1:B:318:CYS:HA	1:B:323:PHE:HB2	1.83	0.61
1:B:58:LYS:N	1:B:296:ASP:O	2.27	0.61
1:B:448:LYS:HG2	1:B:466:TYR:CZ	2.36	0.61
1:B:33:VAL:HG12	1:B:34:GLU:H	1.66	0.60
1:B:132:ASP:OD2	1:B:254:ALA:HA	2.00	0.60
1:B:83:ASP:HB3	1:B:416:GLY:HA3	1.84	0.60
1:B:490:ALA:HB1	1:B:532:ILE:HD11	1.85	0.59
1:A:18:PRO:O	1:A:21:GLU:HB2	2.03	0.58
1:A:54:LYS:HB3	5:A:766:HOH:O	2.03	0.58
1:B:441:TYR:C	1:B:442:ASN:HD22	2.08	0.57
1:B:363:LEU:O	1:B:367:ILE:HG13	2.04	0.57
1:B:469:GLU:HA	1:B:472:LYS:HB3	1.87	0.57
1:B:26:LEU:HD11	1:B:267:PRO:HB3	1.87	0.56
1:A:474:ILE:O	1:A:478:GLU:HG3	2.05	0.56
1:B:312:LYS:HE2	1:B:489:MET:H	1.70	0.56
1:B:376:PRO:CD	1:B:435:SER:HB2	2.36	0.56
1:B:448:LYS:HG2	1:B:466:TYR:OH	2.05	0.56
1:A:491:LYS:HE3	1:A:497:SER:O	2.06	0.55
1:B:61:LEU:HD22	1:B:313:PHE:CD2	2.40	0.55
1:B:107:ILE:O	1:B:108:LYS:HB2	2.07	0.55
1:B:373:PHE:CE2	1:B:440:LEU:HB2	2.41	0.55
1:A:170:ILE:O	1:A:199:ILE:HA	2.07	0.55
1:A:161:PRO:HA	1:A:164:ILE:HD12	1.88	0.55
1:B:498:ASP:OD1	1:B:498:ASP:N	2.40	0.54
1:B:466:TYR:HB3	1:B:471:ASP:OD2	2.08	0.54
1:B:121:PRO:O	1:B:125:ILE:HG12	2.08	0.54
1:B:315:ASP:O	1:B:319:ARG:HD2	2.06	0.54
1:B:467:THR:OG1	1:B:514:ARG:O	2.25	0.54
1:A:138:TYR:HD2	1:B:172:LEU:HD21	1.73	0.54
1:A:4:VAL:HG12	1:A:5:PRO:O	2.07	0.54
1:B:215:LEU:HA	1:B:255:ILE:HD13	1.90	0.54
1:A:82:THR:HG22	1:A:266:THR:HG21	1.89	0.53
1:A:141:ASN:HD22	1:B:170:ILE:HD11	1.72	0.53
1:B:379:VAL:HG12	1:B:380:ALA:N	2.22	0.53
1:B:276:ALA:HB3	1:B:304:PHE:CD2	2.44	0.53
1:B:105:PHE:HB3	1:B:544:ALA:HB2	1.91	0.53
1:A:69:PRO:HB2	1:A:345:LYS:HD3	1.91	0.53
1:A:189:ASN:HD22	1:B:179:ASN:HD22	1.57	0.53
1:B:443:LEU:HA	1:B:450:LYS:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LYS:CB	5:A:766:HOH:O	2.57	0.52
1:B:11:ALA:HB3	1:B:122:MET:HE1	1.91	0.52
1:A:23:ALA:HA	1:A:28:ILE:HD12	1.92	0.52
1:A:383:ALA:HB1	4:A:608:FOL:C13	2.40	0.52
1:B:49:ARG:HH11	1:B:49:ARG:CG	2.13	0.52
1:B:169:VAL:HB	1:B:200:SER:HA	1.90	0.52
1:B:292:LEU:HD23	1:B:298:VAL:CG2	2.36	0.52
1:B:149:ASN:O	1:B:153:GLN:HG2	2.09	0.51
1:B:490:ALA:HB1	1:B:532:ILE:CD1	2.40	0.51
1:B:118:GLN:HB2	1:B:263:LEU:HG	1.93	0.51
1:B:181:VAL:CG1	1:B:184:LEU:HD21	2.41	0.51
1:A:383:ALA:HB2	1:A:408:LEU:HD11	1.91	0.51
1:A:392:LEU:CD1	4:A:608:FOL:HG1	2.40	0.51
1:B:264:GLU:HG3	5:B:746:HOH:O	2.10	0.51
1:A:42:LYS:HD3	1:A:256:LYS:HB2	1.93	0.51
1:A:149:ASN:O	1:A:153:GLN:HG2	2.11	0.50
1:A:149:ASN:HB2	1:B:538:LEU:HD12	1.93	0.50
1:B:175:ARG:NH2	1:B:538:LEU:O	2.45	0.50
1:B:456:THR:CG2	1:B:457:GLU:H	2.24	0.50
1:B:26:LEU:HD11	1:B:267:PRO:CB	2.42	0.50
1:A:35:LEU:HD22	1:A:37:GLY:O	2.12	0.49
1:B:23:ALA:HA	1:B:28:ILE:HD12	1.94	0.49
1:B:88:LEU:O	1:B:90:LYS:HG2	2.11	0.49
1:B:17:LYS:HB2	1:B:22:LEU:HD21	1.95	0.49
1:B:425:LYS:O	1:B:428:GLN:HB2	2.12	0.49
1:A:453:LYS:HE3	1:A:457:GLU:OE1	2.13	0.49
1:B:75:THR:O	1:B:79:VAL:HG23	2.13	0.49
1:B:8:ILE:HA	1:B:122:MET:CE	2.43	0.49
1:B:319:ARG:HE	1:B:443:LEU:HG	1.78	0.49
1:B:24:ARG:C	1:B:26:LEU:H	2.16	0.49
1:B:181:VAL:HG12	1:B:184:LEU:HD21	1.95	0.49
1:A:142:LEU:O	1:A:146:MET:HG3	2.13	0.49
1:B:415:GLY:C	1:B:417:GLU:H	2.16	0.49
1:A:159:ILE:O	1:A:161:PRO:HD3	2.13	0.48
1:A:440:LEU:O	1:A:453:LYS:HE2	2.13	0.48
1:B:472:LYS:HE3	1:B:476:ARG:HH22	1.78	0.48
1:B:109:GLY:O	1:B:559:PHE:HD1	1.96	0.48
1:B:257:PRO:HA	1:B:271:HIS:CD2	2.48	0.48
1:B:378:VAL:HG13	1:B:405:GLU:HB2	1.96	0.48
1:B:313:PHE:O	1:B:317:LYS:HB3	2.12	0.48
1:B:69:PRO:O	1:B:345:LYS:HE3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLY:O	1:B:559:PHE:CD1	2.67	0.48
1:B:11:ALA:CB	1:B:122:MET:HE1	2.43	0.48
1:A:339:MET:HG2	1:A:348:LEU:HD21	1.96	0.48
1:A:156:VAL:HG23	5:A:718:HOH:O	2.14	0.47
1:B:369:ASN:O	1:B:372:LYS:HB2	2.14	0.47
1:B:100:SER:HB2	1:B:201:VAL:HG21	1.96	0.47
1:A:453:LYS:O	1:A:457:GLU:HB2	2.14	0.47
1:B:17:LYS:N	1:B:261:GLN:OE1	2.47	0.47
1:B:452:ALA:O	1:B:456:THR:HG22	2.15	0.47
1:B:193:ARG:HD2	5:B:703:HOH:O	2.13	0.47
1:A:329:VAL:HA	1:A:378:VAL:O	2.15	0.47
1:B:84:ALA:HB1	1:B:423:ALA:HB2	1.97	0.47
1:B:333:THR:HG23	1:B:382:ASN:HB3	1.97	0.47
1:A:301:GLU:HG3	5:A:752:HOH:O	2.14	0.47
1:A:540:LYS:CD	1:A:540:LYS:H	2.28	0.47
1:B:92:VAL:HA	1:B:297:TYR:O	2.15	0.46
1:A:104:SER:HA	1:A:109:GLY:N	2.30	0.46
1:B:42:LYS:HD3	1:B:256:LYS:HB2	1.97	0.46
1:A:141:ASN:HD22	1:B:170:ILE:CD1	2.29	0.46
1:B:218:LEU:HD22	1:B:255:ILE:HD12	1.98	0.46
1:B:222:PHE:HA	1:B:225:ILE:CD1	2.46	0.46
1:B:456:THR:CG2	1:B:457:GLU:N	2.74	0.46
1:A:555:ILE:O	5:A:818:HOH:O	2.21	0.46
1:A:119:VAL:HA	1:A:262:THR:HA	1.98	0.46
1:A:167:ARG:HB2	5:A:714:HOH:O	2.14	0.46
1:A:200:SER:O	1:A:203:SER:HB3	2.16	0.46
1:B:337:LEU:O	1:B:359:GLY:HA3	2.16	0.46
1:B:288:THR:HG23	1:B:298:VAL:HG11	1.98	0.45
1:A:189:ASN:ND2	1:B:179:ASN:ND2	2.64	0.45
1:B:257:PRO:HB2	1:B:269:PHE:CE1	2.51	0.45
1:B:466:TYR:CB	1:B:471:ASP:OD2	2.64	0.45
1:B:393:ASN:HA	1:B:396:TYR:HB2	1.98	0.45
1:B:440:LEU:HG	1:B:440:LEU:O	2.15	0.45
1:B:379:VAL:CG1	1:B:380:ALA:N	2.78	0.45
1:A:105:PHE:CE2	1:B:246:SER:HB3	2.51	0.45
1:A:143:LEU:HD23	1:A:166:TRP:CE2	2.52	0.45
1:A:376:PRO:HG3	1:A:433:ARG:O	2.17	0.45
1:A:547:ILE:O	1:B:245:GLY:HA3	2.17	0.45
1:B:178:ARG:NH2	2:B:601:SO4:O4	2.46	0.45
1:B:506:PRO:O	1:B:509:PHE:HE2	2.00	0.45
1:A:92:VAL:HA	1:A:297:TYR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LYS:HB3	1:B:52:LYS:HE2	1.78	0.44
1:B:502:LYS:HB3	1:B:506:PRO:HG3	1.98	0.44
1:B:93:MET:HG3	1:B:295:ALA:HB2	1.99	0.44
1:B:83:ASP:CB	1:B:416:GLY:HA3	2.47	0.44
1:B:373:PHE:O	1:B:437:PHE:HA	2.17	0.44
1:A:541:ARG:HH11	1:A:546:ASN:HD21	1.65	0.44
1:B:366:HIS:O	1:B:370:ILE:HD12	2.17	0.44
1:A:459:TYR:HD2	1:A:511:ILE:CD1	2.30	0.44
1:B:470:ALA:O	1:B:474:ILE:HG13	2.18	0.44
1:A:108:LYS:HG3	1:A:558:LEU:O	2.17	0.44
1:A:112:ALA:O	1:A:118:GLN:HA	2.17	0.44
1:B:262:THR:HG22	1:B:263:LEU:N	2.32	0.44
1:B:25:GLY:O	1:B:26:LEU:HG	2.18	0.44
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.82	0.44
1:A:105:PHE:HE2	1:B:246:SER:HB3	1.83	0.43
1:B:22:LEU:O	1:B:26:LEU:HD12	2.19	0.43
1:B:43:ILE:HD11	1:B:259:LEU:HD23	1.99	0.43
1:B:269:PHE:CE2	1:B:290:THR:HG22	2.54	0.43
1:B:101:LEU:HD21	1:B:105:PHE:HE1	1.81	0.43
1:B:303:GLY:HA2	2:B:602:SO4:O1	2.18	0.43
1:B:427:LEU:O	1:B:431:GLU:HG2	2.19	0.43
1:A:168:ARG:NH2	1:B:174:ASP:OD1	2.42	0.43
1:B:417:GLU:O	1:B:420:LEU:HB2	2.18	0.43
1:A:255:ILE:HG13	1:A:255:ILE:O	2.18	0.43
1:B:8:ILE:HA	1:B:122:MET:HE1	2.01	0.43
1:B:50:ARG:HG3	1:B:51:LEU:N	2.33	0.43
1:B:543:ALA:O	1:B:547:ILE:HG13	2.19	0.43
1:A:14:ALA:HB2	1:A:263:LEU:HD22	2.01	0.42
1:A:44:SER:OG	1:A:46:ASP:HB2	2.19	0.42
1:A:189:ASN:ND2	1:B:179:ASN:HD22	2.17	0.42
1:B:219:LYS:HE2	1:B:219:LYS:HB3	1.87	0.42
1:B:54:LYS:HG3	1:B:55:PRO:HD2	2.01	0.42
1:B:429:THR:O	1:B:433:ARG:HB2	2.20	0.42
1:A:170:ILE:HD11	1:B:141:ASN:HD22	1.84	0.42
1:B:159:ILE:HA	1:B:230:THR:HA	2.01	0.42
1:A:177:LEU:HB3	1:A:197:PHE:HB2	2.01	0.42
1:A:198:ASP:HA	1:A:535:MET:HB2	2.02	0.42
1:A:366:HIS:O	1:A:370:ILE:HD12	2.20	0.42
1:B:107:ILE:H	1:B:107:ILE:HG13	1.67	0.42
1:A:222:PHE:HA	1:A:225:ILE:HD12	2.02	0.41
1:A:191:VAL:HA	1:A:192:PRO:HD3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ALA:O	1:A:247:MET:HG3	2.20	0.41
1:A:424:ARG:HD2	5:A:751:HOH:O	2.20	0.41
1:B:397:GLU:O	1:B:401:LYS:HB2	2.20	0.41
1:B:477:TYR:O	1:B:478:GLU:C	2.58	0.41
1:B:276:ALA:HB3	1:B:304:PHE:CE2	2.55	0.41
1:A:210:CYS:HA	1:A:284:SER:HA	2.02	0.41
1:B:279:ALA:HA	1:B:488:VAL:HG11	2.02	0.41
1:B:280:HIS:CD2	1:B:282:CYS:SG	3.10	0.41
1:B:331:VAL:HG12	1:B:332:ALA:N	2.35	0.41
1:B:360:PHE:CE1	1:B:364:GLU:HB2	2.56	0.41
1:A:306:ALA:O	1:A:310:ALA:HB3	2.20	0.41
1:B:57:GLY:HA3	1:B:296:ASP:HA	2.02	0.41
1:B:216:MET:CE	1:B:216:MET:HA	2.51	0.41
1:A:168:ARG:O	1:A:197:PHE:HA	2.21	0.41
1:B:98:GLU:N	1:B:272:GLY:O	2.43	0.41
1:A:80:GLY:HA3	1:A:411:VAL:HG11	2.03	0.41
1:A:75:THR:HA	1:A:301:GLU:OE2	2.21	0.41
1:A:313:PHE:O	1:A:317:LYS:HB3	2.21	0.40
1:B:436:ASN:OD1	1:B:436:ASN:N	2.54	0.40
1:A:388:THR:OG1	1:A:391:GLU:HG3	2.22	0.40
1:B:462:ASP:OD2	1:B:508:ASN:HA	2.21	0.40
1:A:169:VAL:HB	1:A:200:SER:HA	2.04	0.40
1:B:123:GLU:OE1	1:B:555:ILE:HD12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	555/559 (99%)	515 (93%)	37 (7%)	3 (0%)	29	68
1	B	555/559 (99%)	470 (85%)	77 (14%)	8 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1110/1118 (99%)	985 (89%)	114 (10%)	11 (1%)	15 53

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	LYS
1	B	108	LYS
1	B	273	GLY
1	B	551	ALA
1	A	129	PHE
1	B	34	GLU
1	A	273	GLY
1	B	376	PRO
1	B	482	TYR
1	B	69	PRO
1	B	55	PRO

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	439/441 (100%)	430 (98%)	9 (2%)	53 82
1	B	439/441 (100%)	408 (93%)	31 (7%)	14 46
All	All	878/882 (100%)	838 (95%)	40 (5%)	27 64

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	SER
1	A	350	THR
1	A	358	GLU
1	A	431	GLU
1	A	438	HIS
1	A	453	LYS
1	A	491	LYS

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Mol	Chain	Res	Type
1	A	511	ILE
1	A	540	LYS
1	B	3	LYS
1	B	4	VAL
1	B	8	ILE
1	B	21	GLU
1	B	30	GLU
1	B	49	ARG
1	B	85	LEU
1	B	120	VAL
1	B	199	ILE
1	B	201	VAL
1	B	206	MET
1	B	232	ASP
1	B	255	ILE
1	B	260	VAL
1	B	266	THR
1	B	290	THR
1	B	294	LEU
1	B	307	ASP
1	B	319	ARG
1	B	333	THR
1	B	347	ASP
1	B	350	THR
1	B	396	TYR
1	B	417	GLU
1	B	435	SER
1	B	436	ASN
1	B	439	VAL
1	B	462	ASP
1	B	475	GLN
1	B	498	ASP
1	B	546	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	ASN
1	A	465	ASN
1	B	179	ASN
1	B	280	HIS
1	B	283	ASN

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Mol	Chain	Res	Type
1	B	362	ASN
1	B	382	ASN
1	B	442	ASN
1	B	508	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	SO4	A	604	-	4,4,4	0.51	0	6,6,6	0.26	0
2	SO4	B	601	-	4,4,4	0.48	0	6,6,6	0.22	0
3	TOE	A	607	-	10,10,10	0.70	0	9,9,9	0.40	0
2	SO4	A	602	-	4,4,4	0.33	0	6,6,6	0.27	0
2	SO4	A	603	-	4,4,4	0.40	0	6,6,6	0.19	0
2	SO4	A	601	-	4,4,4	0.26	0	6,6,6	0.63	0
2	SO4	B	602	-	4,4,4	0.38	0	6,6,6	0.35	0
2	SO4	A	605	-	4,4,4	0.43	0	6,6,6	0.23	0
3	TOE	B	600	-	10,10,10	0.55	0	9,9,9	0.37	0
4	FOL	A	608	-	34,34,34	1.70	6 (17%)	44,47,47	2.50	15 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	TOE	A	606	-	10,10,10	0.77	0	9,9,9	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TOE	B	600	-	-	5/8/8/8	-
3	TOE	A	607	-	-	5/8/8/8	-
4	FOL	A	608	-	-	7/22/22/22	0/3/3/3
3	TOE	A	606	-	-	5/8/8/8	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	608	FOL	C4A-C4	5.51	1.50	1.41
4	A	608	FOL	C4A-C8A	4.79	1.49	1.40
4	A	608	FOL	C6-N5	2.95	1.37	1.32
4	A	608	FOL	C4A-N5	2.65	1.37	1.33
4	A	608	FOL	C7-N8	2.04	1.35	1.31
4	A	608	FOL	C4-N3	2.01	1.36	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	608	FOL	C2-N1-C8A	5.87	122.06	115.36
4	A	608	FOL	C4-C4A-N5	5.83	125.26	118.60
4	A	608	FOL	C8A-C4A-C4	-5.66	116.21	119.95
4	A	608	FOL	N8-C8A-N1	5.41	122.00	115.82
4	A	608	FOL	C4A-C4-N3	-3.91	118.08	123.43
4	A	608	FOL	C7-N8-C8A	3.76	120.47	116.69
4	A	608	FOL	C2-N3-C4	3.69	121.79	115.93
4	A	608	FOL	C8A-C4A-N5	-3.35	118.53	122.33
4	A	608	FOL	N1-C2-N3	-3.25	122.89	127.22
4	A	608	FOL	C13-C14-N10	-3.17	114.41	120.97
4	A	608	FOL	C15-C14-N10	3.11	127.43	120.97
4	A	608	FOL	CA-N-C	2.95	128.82	121.60
4	A	608	FOL	C9-C6-N5	2.80	121.64	116.66
4	A	608	FOL	C9-C6-C7	-2.22	117.67	121.55
4	A	608	FOL	O2-CT-CA	2.06	120.26	113.40

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	608	FOL	C6-C9-N10-C14
4	A	608	FOL	N-CA-CB-CG
3	A	607	TOE	OC'-CD'-CE'-OF'
3	A	607	TOE	OF'-CG'-CH'-OI'
3	A	606	TOE	OF'-CG'-CH'-OI'
4	A	608	FOL	CT-CA-CB-CG
3	A	607	TOE	O2'-CA'-CB'-OC'
3	A	606	TOE	OC'-CD'-CE'-OF'
3	B	600	TOE	OC'-CD'-CE'-OF'
3	B	600	TOE	OF'-CG'-CH'-OI'
3	A	606	TOE	O2'-CA'-CB'-OC'
4	A	608	FOL	N-C-C11-C12
3	A	606	TOE	CG'-CH'-OI'-CK'
3	A	606	TOE	CE'-CD'-OC'-CB'
4	A	608	FOL	O-C-C11-C12
3	A	607	TOE	CH'-CG'-OF'-CE'
4	A	608	FOL	N-C-C11-C16
3	A	607	TOE	CA'-CB'-OC'-CD'
3	B	600	TOE	CH'-CG'-OF'-CE'
4	A	608	FOL	O-C-C11-C16
3	B	600	TOE	CG'-CH'-OI'-CK'
3	B	600	TOE	CD'-CE'-OF'-CG'

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	SO4	1	0
2	B	602	SO4	1	0
4	A	608	FOL	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FOL A 608

Bond lengths   Bond angles

Torsions   Rings
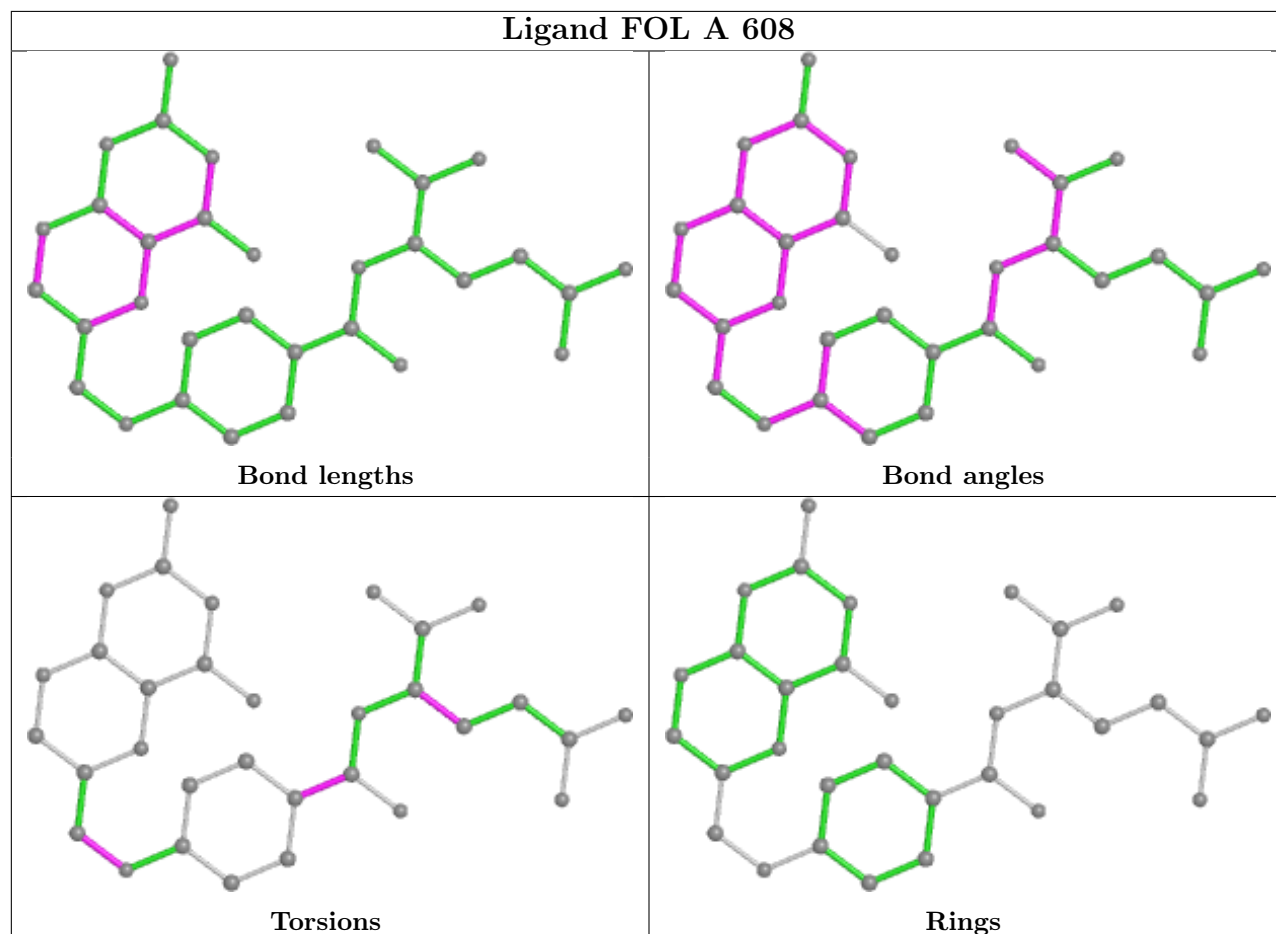
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	557/559 (99%)	-0.37	0	100	100	10, 19, 50, 74	0
1	B	557/559 (99%)	0.45	39 (7%)	16	5	14, 55, 97, 122	0
All	All	1114/1118 (99%)	0.04	39 (3%)	44	18	10, 32, 90, 122	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	409	SER	4.7
1	B	356	LEU	4.1
1	B	334	VAL	4.0
1	B	432	SER	3.5
1	B	4	VAL	3.5
1	B	345	LYS	3.4
1	B	385	PRO	3.2
1	B	353	LEU	3.2
1	B	396	TYR	3.0
1	B	387	ASP	3.0
1	B	349	ALA	2.9
1	B	352	ASN	2.9
1	B	358	GLU	2.9
1	B	344	PRO	2.7
1	B	348	LEU	2.7
1	B	401	LYS	2.7
1	B	357	ARG	2.7
1	B	3	LYS	2.6
1	B	351	GLU	2.5
1	B	381	ILE	2.5
1	B	436	ASN	2.4
1	B	347	ASP	2.4
1	B	93	MET	2.4
1	B	386	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	392	LEU	2.3
1	B	350	THR	2.3
1	B	354	GLU	2.3
1	B	506	PRO	2.2
1	B	382	ASN	2.2
1	B	5	PRO	2.2
1	B	400	ALA	2.2
1	B	475	GLN	2.1
1	B	322	GLY	2.1
1	B	73	GLY	2.1
1	B	335	ARG	2.1
1	B	336	ALA	2.0
1	B	47	VAL	2.0
1	B	110	GLY	2.0
1	B	559	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
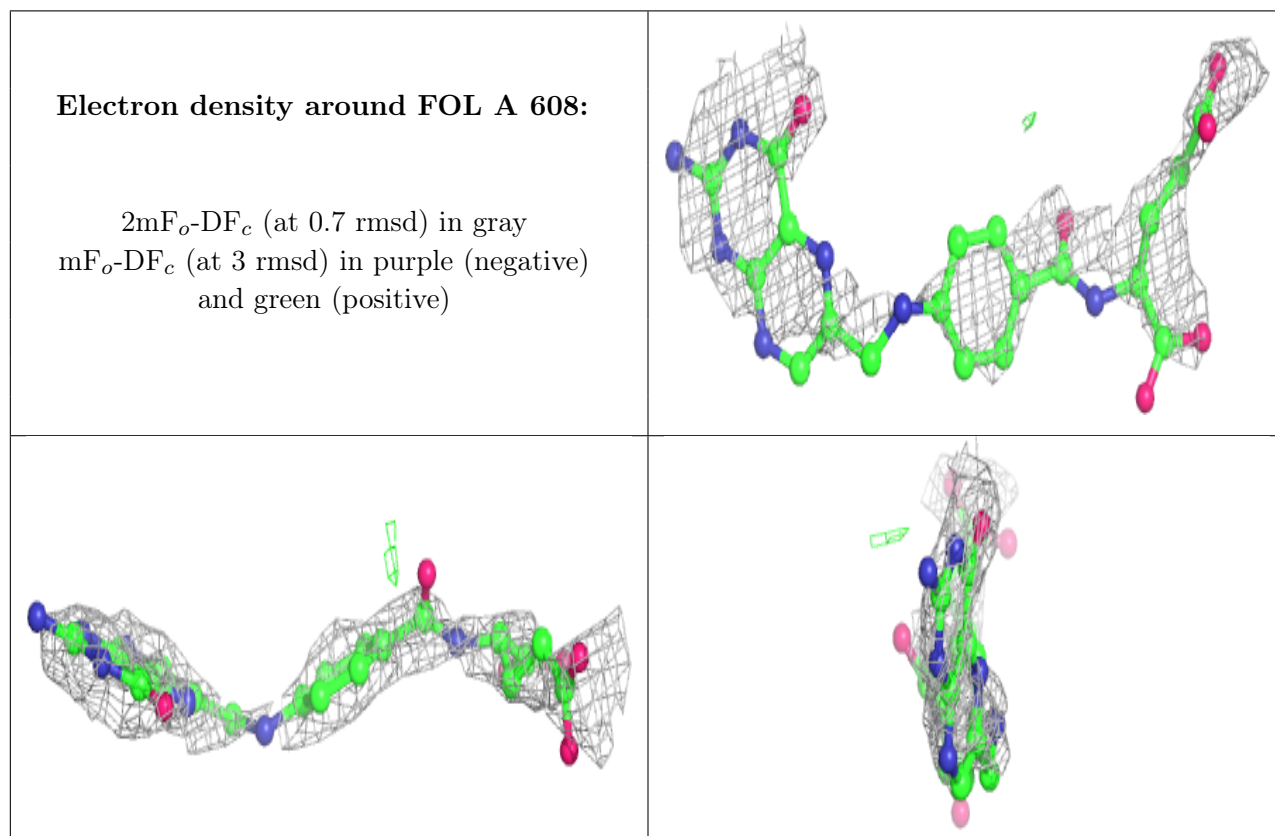
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	605	5/5	0.71	0.36	92,95,99,101	0
4	FOL	A	608	32/32	0.78	0.44	43,49,54,54	32
3	TOE	A	607	11/11	0.86	0.20	21,32,47,49	0
2	SO4	A	603	5/5	0.87	0.16	61,63,65,67	0
3	TOE	A	606	11/11	0.89	0.22	15,19,29,30	0
2	SO4	A	602	5/5	0.90	0.23	71,71,73,75	0
2	SO4	A	604	5/5	0.90	0.18	51,52,53,54	0
3	TOE	B	600	11/11	0.91	0.18	25,25,29,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	SO4	B	601	5/5	0.93	0.16	50,52,56,56	0
2	SO4	B	602	5/5	0.94	0.18	52,52,56,57	0
2	SO4	A	601	5/5	0.98	0.12	27,28,29,29	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 FOL A 608:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.