



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:47 PM UTC

PDB ID : 6U44 / pdb_00006u44
Title : Crystal structure of Methanoperedens nitroreducens elongation factor 2 H595N bound to GMPPCP and magnesium (monoclinic crystal form)
Authors : Fenwick, M.K.; Ealick, S.E.
Deposited on : 2019-08-22
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

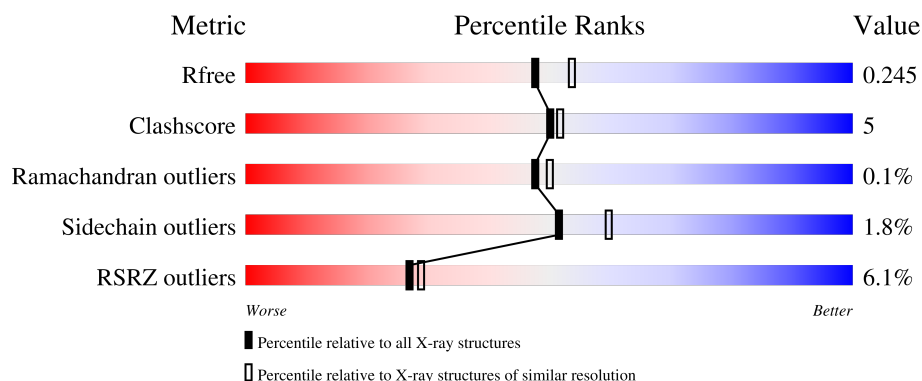
1 Overall quality at a glance

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	753	
1	B	753	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11854 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 Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	0	8	0
			5488	3460	966	1025	37			
1	B	715	Total	C	N	O	S	0	5	0
			5436	3423	959	1018	36			

There are 50 discrepancies between the modelled and reference sequences:

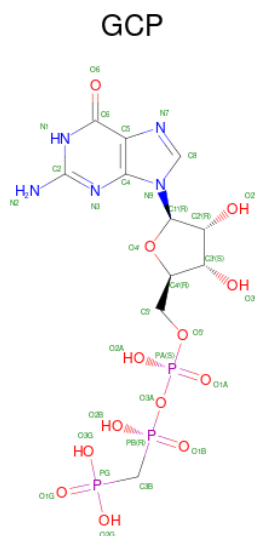
Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP A0A062V290
A	-22	GLY	-	expression tag	UNP A0A062V290
A	-21	SER	-	expression tag	UNP A0A062V290
A	-20	ASP	-	expression tag	UNP A0A062V290
A	-19	LYS	-	expression tag	UNP A0A062V290
A	-18	ILE	-	expression tag	UNP A0A062V290
A	-17	HIS	-	expression tag	UNP A0A062V290
A	-16	HIS	-	expression tag	UNP A0A062V290
A	-15	HIS	-	expression tag	UNP A0A062V290
A	-14	HIS	-	expression tag	UNP A0A062V290
A	-13	HIS	-	expression tag	UNP A0A062V290
A	-12	HIS	-	expression tag	UNP A0A062V290
A	-11	SER	-	expression tag	UNP A0A062V290
A	-10	SER	-	expression tag	UNP A0A062V290
A	-9	GLY	-	expression tag	UNP A0A062V290
A	-8	GLU	-	expression tag	UNP A0A062V290
A	-7	ASN	-	expression tag	UNP A0A062V290
A	-6	LEU	-	expression tag	UNP A0A062V290
A	-5	TYR	-	expression tag	UNP A0A062V290
A	-4	PHE	-	expression tag	UNP A0A062V290
A	-3	GLN	-	expression tag	UNP A0A062V290
A	-2	GLY	-	expression tag	UNP A0A062V290
A	-1	SER	-	expression tag	UNP A0A062V290
A	0	GLY	-	expression tag	UNP A0A062V290
A	595	ASN	HIS	engineered mutation	UNP A0A062V290

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	MET	-	initiating methionine	UNP A0A062V290
B	-22	GLY	-	expression tag	UNP A0A062V290
B	-21	SER	-	expression tag	UNP A0A062V290
B	-20	ASP	-	expression tag	UNP A0A062V290
B	-19	LYS	-	expression tag	UNP A0A062V290
B	-18	ILE	-	expression tag	UNP A0A062V290
B	-17	HIS	-	expression tag	UNP A0A062V290
B	-16	HIS	-	expression tag	UNP A0A062V290
B	-15	HIS	-	expression tag	UNP A0A062V290
B	-14	HIS	-	expression tag	UNP A0A062V290
B	-13	HIS	-	expression tag	UNP A0A062V290
B	-12	HIS	-	expression tag	UNP A0A062V290
B	-11	SER	-	expression tag	UNP A0A062V290
B	-10	SER	-	expression tag	UNP A0A062V290
B	-9	GLY	-	expression tag	UNP A0A062V290
B	-8	GLU	-	expression tag	UNP A0A062V290
B	-7	ASN	-	expression tag	UNP A0A062V290
B	-6	LEU	-	expression tag	UNP A0A062V290
B	-5	TYR	-	expression tag	UNP A0A062V290
B	-4	PHE	-	expression tag	UNP A0A062V290
B	-3	GLN	-	expression tag	UNP A0A062V290
B	-2	GLY	-	expression tag	UNP A0A062V290
B	-1	SER	-	expression tag	UNP A0A062V290
B	0	GLY	-	expression tag	UNP A0A062V290
B	595	ASN	HIS	engineered mutation	UNP A0A062V290

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 32	C 11	N 5	O 13	P 3	0	0
2	B	1	Total 32	C 11	N 5	O 13	P 3	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0
4	B	2	Total Cl 2 2	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

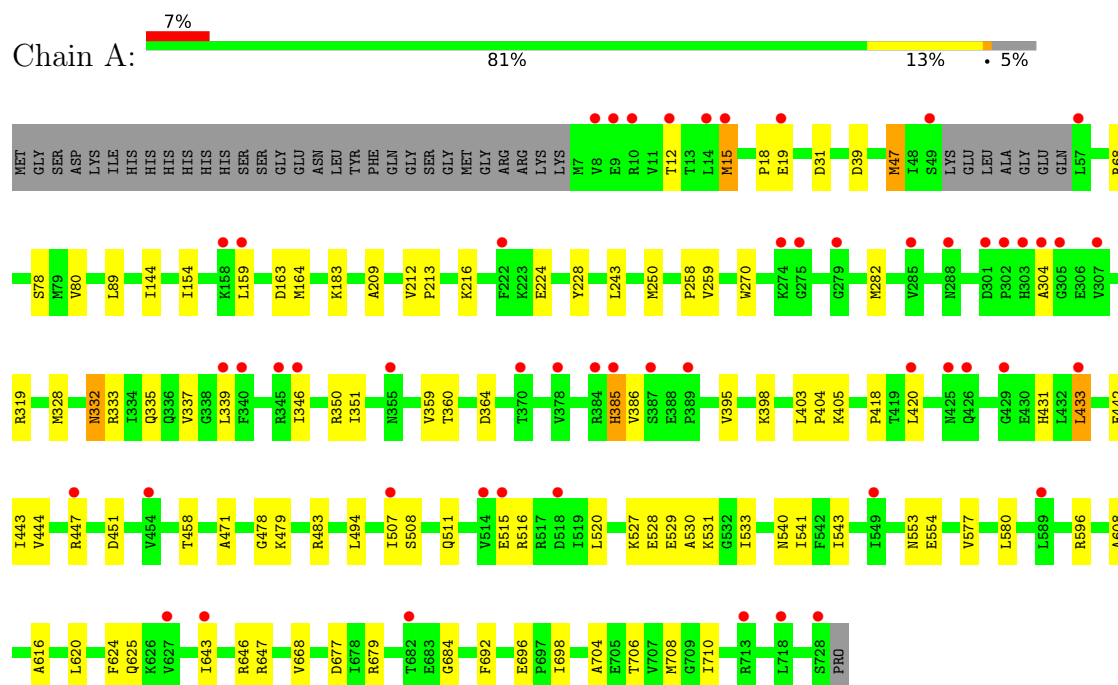
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	408	Total	O	0	3
			408	408		
6	B	422	Total	O	0	1
			422	422		

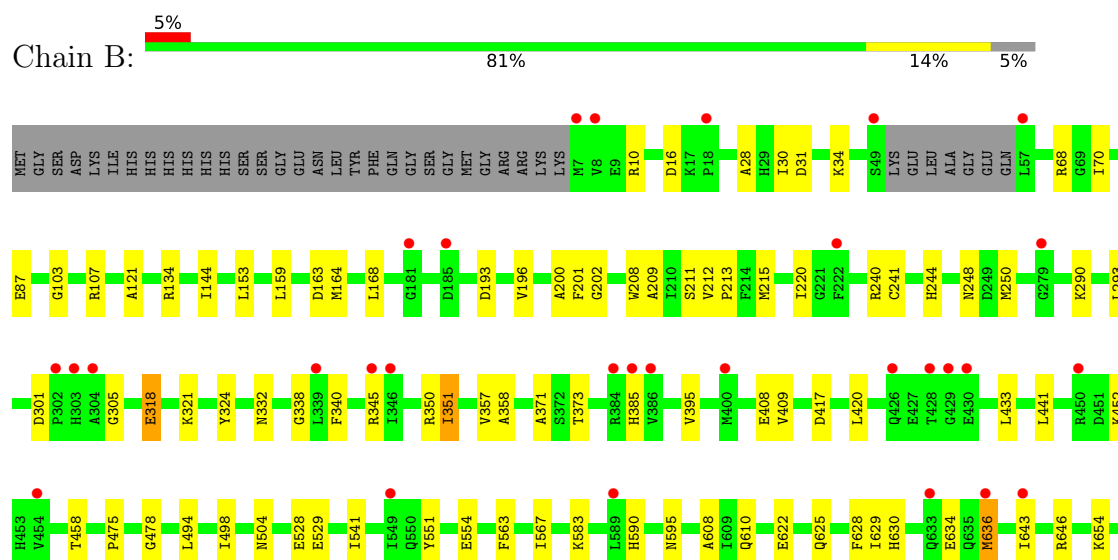
3 Residue-property plots [i](#)

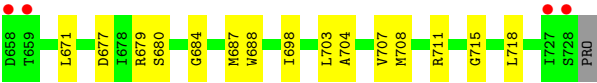
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Elongation factor 2



• Molecule 1: Elongation factor 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.32Å 106.81Å 98.06Å 90.00° 105.46° 90.00°	Depositor
Resolution (Å)	75.49 – 2.10 75.49 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (75.49-2.10) 98.3 (75.49-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.14_3211	Depositor
R, R_{free}	0.187 , 0.240 (Not available) , 0.245	Depositor DCC
R_{free} test set	4385 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.8	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	0.95	EDS
Total number of atoms	11854	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6995e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MG, CL, GCP

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	0.29	0/5577	0.48	0/7540
1	B	0.32	0/5524	0.50	0/7474
All	All	0.30	0/11101	0.49	0/15014

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	5488	0	5488	60	0
1	B	5436	0	5406	59	0
2	A	32	0	14	1	0
2	B	32	0	14	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	1	0
4	B	2	0	0	1	0
5	A	15	0	0	0	0
5	B	15	0	0	1	0
6	A	408	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	422	0	0	4	0
All	All	11854	0	10922	117	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 5.

All (117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:VAL:HG22	1:B:458:THR:HG22	1.70	0.74
1:A:625[A]:GLN:HG2	1:A:668:VAL:HG22	1.73	0.70
1:B:212:VAL:HA	1:B:215:MET:HE3	1.80	0.64
1:B:679:ARG:HG3	1:B:684:GLY:HA2	1.79	0.64
1:A:511:GLN:NE2	1:A:515:GLU:OE1	2.25	0.61
1:A:444:VAL:HA	1:A:447[B]:ARG:HD2	1.82	0.60
1:B:193:ASP:HB3	1:B:196:VAL:HG22	1.85	0.59
1:B:698:ILE:HD11	1:B:703:LEU:HA	1.84	0.58
1:B:563:PHE:O	1:B:567:ILE:HG12	2.04	0.57
1:A:553:ASN:HB2	4:A:803:CL:CL	2.41	0.57
1:A:31:ASP:HA	2:A:801:GCP:H3B1	1.87	0.57
1:B:629:ILE:HD12	1:B:643:ILE:HD11	1.85	0.56
1:A:625[B]:GLN:HG3	1:A:668:VAL:HG22	1.86	0.56
1:B:417:ASP:HB3	1:B:420:LEU:HD12	1.87	0.56
1:B:494:LEU:HD21	1:B:541:ILE:HG12	1.86	0.55
1:A:19:GLU:HG2	1:A:259:VAL:HG21	1.88	0.55
1:A:18:PRO:O	1:A:258:PRO:HD2	2.06	0.54
1:A:328:MET:HG3	1:A:364:ASP:HB3	1.88	0.53
1:A:478:GLY:HA3	1:A:608:ALA:HB2	1.89	0.53
1:A:159:LEU:HB3	1:A:163:ASP:HB2	1.89	0.53
1:B:31:ASP:HA	2:B:801:GCP:H3B1	1.91	0.53
1:A:647:ARG:NH1	6:A:915:HOH:O	2.41	0.52
1:B:10:ARG:NH2	1:B:87:GLU:OE1	2.43	0.52
1:B:159:LEU:HB3	1:B:163:ASP:HB2	1.92	0.51
1:B:478:GLY:HA3	1:B:608:ALA:HB2	1.93	0.51
1:B:433:LEU:HG	1:B:441:LEU:HD22	1.91	0.51
1:A:479:LYS:NZ	1:A:483:ARG:HH21	2.09	0.50
1:B:68:ARG:HB2	1:B:70:ILE:HG22	1.92	0.50
1:B:590:HIS:CE1	1:B:595:ASN:HD22	2.29	0.50
1:B:134[A]:ARG:NH1	6:B:910[A]:HOH:O	2.37	0.50
1:B:338:GLY:N	1:B:351:ILE:HD11	2.27	0.50
1:B:646:ARG:NH2	1:B:677:ASP:OD2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:GLN:NE2	5:B:806:SO4:O3	2.45	0.50
1:A:335:GLN:HB3	1:B:305:GLY:HA3	1.95	0.49
1:A:507:ILE:HD13	1:A:520:LEU:HD21	1.94	0.49
1:B:340:PHE:CE2	1:B:358:ALA:HB2	2.48	0.49
1:A:431:HIS:ND1	6:A:909:HOH:O	2.35	0.48
1:A:443:ILE:O	1:A:447[A]:ARG:HG2	2.14	0.48
1:B:351:ILE:HG21	1:B:357:VAL:HG12	1.94	0.47
1:A:528:GLU:HB2	6:A:1192:HOH:O	2.14	0.47
1:B:715:GLY:HA2	6:B:1204:HOH:O	2.14	0.47
1:B:628:PHE:O	1:B:688:TRP:HA	2.14	0.47
1:A:47:MET:HE1	1:A:80:VAL:HG23	1.97	0.47
1:A:144:ILE:HD12	1:A:250:MET:HG2	1.96	0.47
1:B:636:MET:HE3	1:B:636:MET:HB3	1.58	0.47
1:B:103:GLY:O	1:B:107:ARG:HG3	2.15	0.47
1:A:479:LYS:HZ3	1:A:483:ARG:HH21	1.61	0.46
1:B:475:PRO:HG3	6:B:962:HOH:O	2.14	0.46
1:B:528:GLU:HB2	6:B:1090:HOH:O	2.15	0.46
1:B:529:GLU:OE2	1:B:583:LYS:NZ	2.43	0.46
1:A:212:VAL:O	1:A:216:LYS:HG2	2.15	0.45
1:A:385:HIS:NE2	1:A:418:PRO:HB2	2.31	0.45
1:B:293:LEU:HB3	1:B:371:ALA:HB3	1.99	0.45
1:A:646:ARG:NH1	1:A:677:ASP:OD2	2.49	0.45
1:A:337:VAL:HG12	1:A:359:VAL:HG13	1.99	0.45
1:A:554:GLU:OE2	1:A:596:ARG:NH2	2.46	0.45
1:B:290:LYS:HB3	1:B:373:THR:HB	1.98	0.45
1:A:494:LEU:HD21	1:A:541:ILE:HG12	1.99	0.44
1:A:395:VAL:HG22	1:A:458:THR:HG22	1.99	0.44
1:B:409:VAL:HG13	1:B:452:LYS:HG2	1.98	0.44
1:A:679:ARG:HG3	1:A:684:GLY:HA2	1.98	0.44
1:A:398:LYS:HB2	1:A:398:LYS:HE2	1.78	0.44
1:A:68:ARG:HH22	1:A:442:GLU:CD	2.25	0.44
1:A:304:ALA:HB1	1:A:360:THR:HG21	1.99	0.44
1:B:144:ILE:HD12	1:B:250:MET:HE2	2.00	0.44
1:B:200:ALA:HB2	1:B:250:MET:SD	2.58	0.44
1:B:134[B]:ARG:NH1	1:B:504:ASN:HD21	2.16	0.44
1:A:339:LEU:O	1:A:346:ILE:N	2.51	0.44
1:B:704:ALA:O	1:B:708:MET:HG2	2.18	0.44
1:A:405:LYS:HD2	1:B:350[A]:ARG:HH12	1.83	0.43
1:B:630:HIS:HB2	1:B:687:MET:HB2	2.00	0.43
1:A:625[A]:GLN:OE1	1:A:692:PHE:HA	2.19	0.43
1:A:420:LEU:HD21	1:A:433:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:LYS:HE3	1:B:654:LYS:HB2	1.70	0.43
1:A:530:ALA:O	1:A:533:ILE:HG22	2.19	0.43
1:B:318:GLU:OE2	1:B:321:LYS:HD2	2.18	0.43
1:A:624:PHE:CE2	1:A:696:GLU:HB2	2.54	0.43
1:B:498:ILE:HG13	4:B:803:CL:CL	2.56	0.43
1:A:319:ARG:HD2	1:A:335:GLN:O	2.20	0.42
1:A:447[A]:ARG:O	1:A:451:ASP:HB2	2.19	0.42
1:B:211:SER:OG	1:B:213:PRO:HD2	2.19	0.42
1:A:183:LYS:NZ	6:A:934:HOH:O	2.52	0.42
1:B:164:MET:O	1:B:168:LEU:HG	2.19	0.42
1:A:332:ASN:HD22	1:A:332:ASN:N	2.18	0.42
1:A:704:ALA:O	1:A:708:MET:HG2	2.18	0.42
1:A:159:LEU:HB3	1:A:163:ASP:CB	2.49	0.42
1:A:270:TRP:CD2	1:A:282:MET:HE1	2.55	0.41
1:B:121:ALA:HB1	1:B:153:LEU:HD22	2.02	0.41
1:A:471:ALA:O	1:A:616:ALA:HB1	2.20	0.41
1:A:577:VAL:HG11	1:A:580:LEU:HD22	2.01	0.41
1:A:706:THR:O	1:A:710:ILE:HG13	2.20	0.41
1:B:634:GLU:H	1:B:634:GLU:CD	2.29	0.41
1:A:403:LEU:HB2	1:A:404:PRO:HD3	2.01	0.41
1:A:508:SER:O	1:A:516:ARG:HD3	2.20	0.41
1:B:324:TYR:O	1:B:371:ALA:HA	2.20	0.41
1:A:209:ALA:HB2	1:A:243:LEU:HD12	2.02	0.41
1:A:540:ASN:OD1	1:A:580:LEU:HB2	2.21	0.41
1:B:209:ALA:O	1:B:241:CYS:HB3	2.20	0.41
1:B:220:ILE:HD11	1:B:240:ARG:CZ	2.50	0.41
1:B:244:HIS:O	1:B:248:ASN:HB2	2.20	0.41
1:B:301:ASP:O	1:B:305:GLY:N	2.54	0.41
1:B:707:VAL:O	1:B:711:ARG:HG3	2.21	0.41
1:A:78:SER:HB3	1:A:89:LEU:HD11	2.02	0.41
1:A:224:GLU:HG2	1:A:228:TYR:CE2	2.55	0.41
1:B:708:MET:HE1	1:B:718:LEU:C	2.46	0.41
1:A:12:THR:O	1:A:15:MET:HG3	2.21	0.41
1:A:620:LEU:HB2	1:A:698:ILE:HD13	2.02	0.41
1:B:202:GLY:HA2	1:B:208:TRP:CZ3	2.55	0.41
1:B:28:ALA:HB3	1:B:34:LYS:HG3	2.03	0.40
1:B:622:GLU:HB3	1:B:698:ILE:HG22	2.02	0.40
1:A:212:VAL:HB	1:A:213:PRO:HD3	2.03	0.40
1:A:527:LYS:O	1:A:531:LYS:HG2	2.21	0.40
1:B:30:ILE:HA	2:B:801:GCP:O3G	2.21	0.40
1:B:625:GLN:CG	1:B:671:LEU:HD12	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:HG12	1:A:164[A]:MET:SD	2.62	0.40
1:A:529:GLU:HB3	1:A:543:ILE:HD13	2.02	0.40
1:B:551:TYR:O	1:B:554:GLU:HG2	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	718/753 (95%)	696 (97%)	21 (3%)	1 (0%)	48	50
1	B	716/753 (95%)	702 (98%)	14 (2%)	0	100	100
All	All	1434/1506 (95%)	1398 (98%)	35 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	576/631 (91%)	566 (98%)	10 (2%)	53	62
1	B	566/631 (90%)	556 (98%)	10 (2%)	51	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1142/1262 (90%)	1122 (98%)	20 (2%)	51 60

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	39	ASP
1	A	47	MET
1	A	332	ASN
1	A	333	ARG
1	A	350	ARG
1	A	351	ILE
1	A	385	HIS
1	A	433	LEU
1	A	643	ILE
1	B	16	ASP
1	B	201	PHE
1	B	318	GLU
1	B	332	ASN
1	B	345	ARG
1	B	351	ILE
1	B	385	HIS
1	B	408	GLU
1	B	636	MET
1	B	680	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	HIS
1	A	385	HIS
1	A	431	HIS
1	A	670	GLN
1	B	207	ASN
1	B	336	GLN
1	B	399	HIS
1	B	504	ASN
1	B	595	ASN
1	B	630	HIS

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 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	SO4	B	805	-	4,4,4	0.25	0	6,6,6	0.09	0
2	GCP	B	801	3	32,34,34	1.25	4 (12%)	49,54,54	1.73	11 (22%)
5	SO4	A	807	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	B	807	-	4,4,4	0.24	0	6,6,6	0.13	0
2	GCP	A	801	3	32,34,34	1.32	5 (15%)	49,54,54	1.74	8 (16%)
5	SO4	B	806	-	4,4,4	0.28	0	6,6,6	0.14	0
5	SO4	A	805	-	4,4,4	0.23	0	6,6,6	0.14	0
5	SO4	A	804	-	4,4,4	0.28	0	6,6,6	0.21	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
2	GCP	B	801	3	-	1/19/38/38	0/3/3/3
2	GCP	A	801	3	-	0/19/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	GCP	PG-O2G	3.09	1.61	1.55
2	A	801	GCP	PG-O3G	3.04	1.61	1.55
2	A	801	GCP	C5-C4	2.99	1.46	1.38
2	B	801	GCP	C5-C4	2.89	1.46	1.38
2	B	801	GCP	PG-O3G	2.79	1.61	1.55
2	B	801	GCP	C4-N9	-2.21	1.32	1.38
2	A	801	GCP	C4-N9	-2.07	1.32	1.38
2	B	801	GCP	PG-O2G	2.04	1.59	1.55
2	A	801	GCP	C6-N1	-2.02	1.35	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	GCP	C5-C4-N3	-5.13	120.23	128.39
2	B	801	GCP	C5-C4-N3	-4.95	120.51	128.39
2	A	801	GCP	C2-N3-C4	4.69	120.38	112.30
2	B	801	GCP	C2-N3-C4	4.22	119.57	112.30
2	A	801	GCP	C6-C5-N7	4.15	137.84	130.29
2	B	801	GCP	C6-C5-N7	3.66	136.95	130.29
2	A	801	GCP	N9-C4-N3	3.53	133.02	125.95
2	B	801	GCP	N9-C4-N3	3.26	132.47	125.95
2	B	801	GCP	C4-C5-N7	-2.95	105.99	110.67
2	A	801	GCP	C4-C5-N7	-2.85	106.15	110.67
2	B	801	GCP	O2G-PG-C3B	2.76	113.10	106.40
2	B	801	GCP	O2A-PA-O3A	2.76	114.73	107.27
2	A	801	GCP	O2A-PA-O3A	2.74	114.67	107.27
2	B	801	GCP	PB-O3A-PA	-2.40	124.55	132.37
2	B	801	GCP	O6-C6-C5	-2.23	120.64	126.53
2	B	801	GCP	N2-C2-N3	-2.19	115.39	119.67
2	A	801	GCP	O6-C6-C5	-2.09	121.01	126.53
2	A	801	GCP	C8-N7-C5	2.09	107.98	104.26
2	B	801	GCP	C8-N7-C5	2.01	107.84	104.26

There are no chirality outliers.

All (1) torsion outliers are listed below:

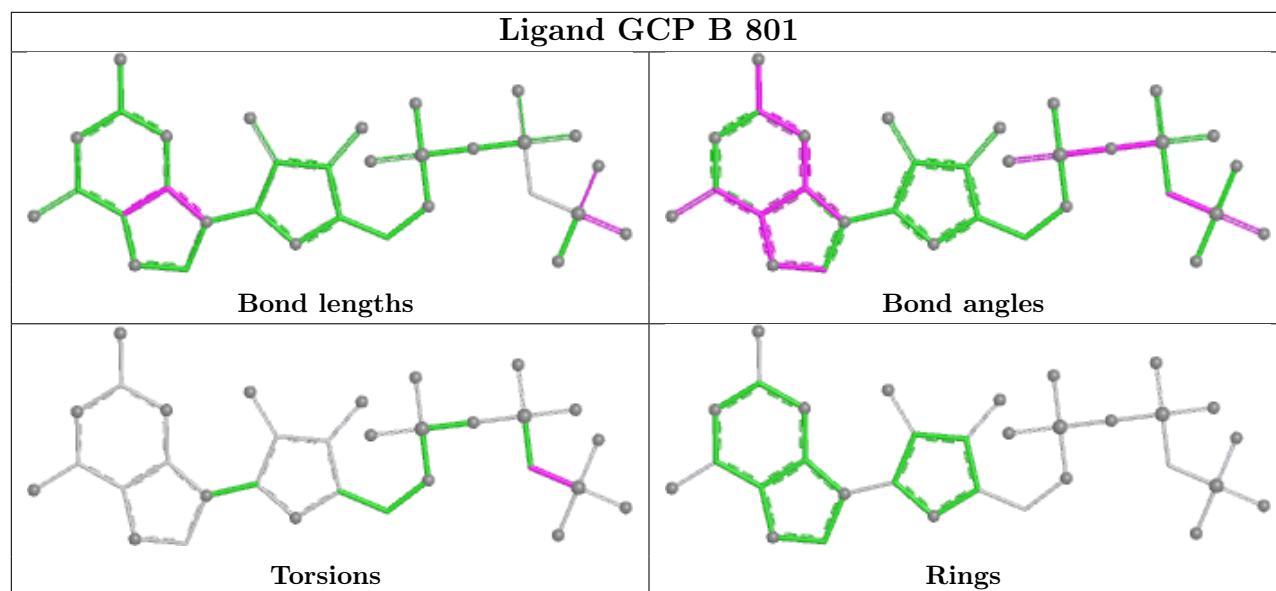
Mol	Chain	Res	Type	Atoms
2	B	801	GCP	PB-C3B-PG-O1G

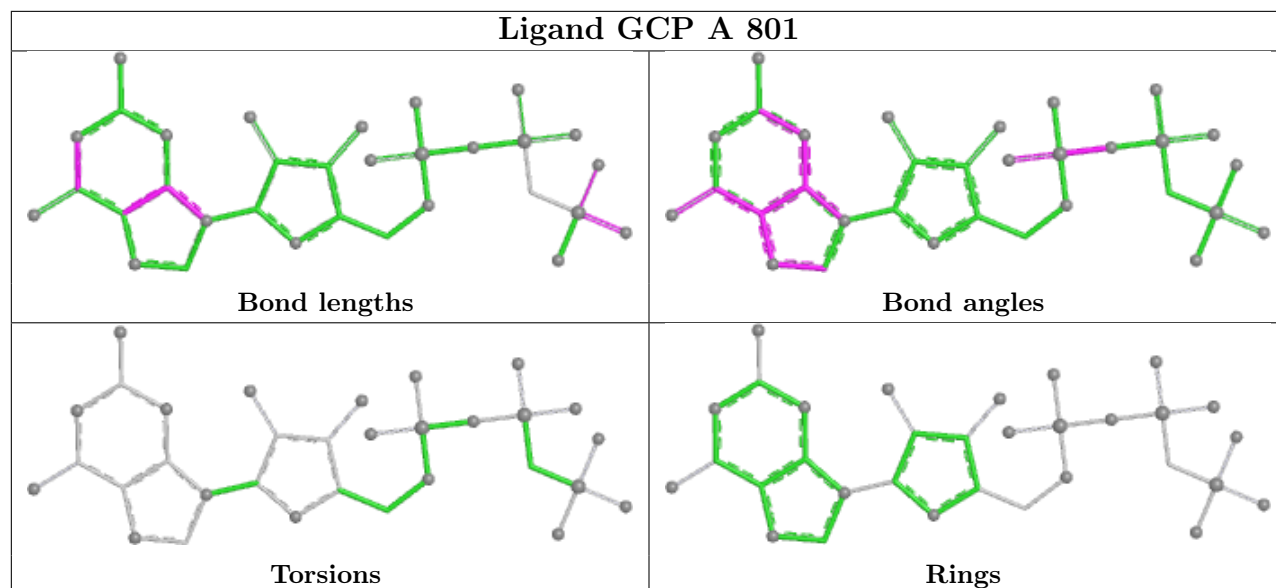
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	GCP	2	0
2	A	801	GCP	1	0
5	B	806	SO4	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.





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	715/753 (94%)	0.62	53 (7%) 20 22	19, 45, 75, 98	8 (1%)
1	B	715/753 (94%)	0.41	34 (4%) 35 38	13, 39, 67, 101	5 (0%)
All	All	1430/1506 (94%)	0.52	87 (6%) 27 29	13, 42, 72, 101	13 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222[A]	PHE	5.5
1	A	345	ARG	4.8
1	B	7	MET	4.1
1	A	447[A]	ARG	4.1
1	B	57	LEU	3.9
1	A	713	ARG	3.7
1	B	346	ILE	3.5
1	B	728	SER	3.4
1	A	303	HIS	3.4
1	B	428	THR	3.4
1	B	8	VAL	3.4
1	B	345	ARG	3.2
1	A	643	ILE	3.2
1	B	454	VAL	3.1
1	A	304	ALA	3.1
1	A	307	VAL	3.1
1	B	181	GLY	3.0
1	B	302	PRO	3.0
1	B	429	GLY	3.0
1	B	386	VAL	2.9
1	A	433	LEU	2.9
1	A	340	PHE	2.9
1	B	385	HIS	2.9
1	A	301	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	658	ASP	2.8
1	A	302	PRO	2.8
1	B	727	ILE	2.8
1	A	385	HIS	2.7
1	B	384	ARG	2.7
1	A	12	THR	2.7
1	B	636	MET	2.7
1	B	549	ILE	2.7
1	A	370	THR	2.7
1	A	279	GLY	2.7
1	A	346	ILE	2.6
1	A	19	GLU	2.6
1	B	400	MET	2.6
1	A	339	LEU	2.6
1	A	514	VAL	2.6
1	A	728	SER	2.6
1	B	339	LEU	2.6
1	A	387	SER	2.5
1	A	57	LEU	2.5
1	A	420	LEU	2.5
1	A	378	VAL	2.5
1	A	627	VAL	2.4
1	A	384	ARG	2.4
1	A	425	ASN	2.4
1	A	15	MET	2.4
1	A	10	ARG	2.4
1	B	49	SER	2.4
1	B	18	PRO	2.4
1	A	454	VAL	2.3
1	B	303	HIS	2.3
1	A	288	ASN	2.3
1	A	49	SER	2.3
1	A	589	LEU	2.3
1	A	9	GLU	2.3
1	B	222	PHE	2.3
1	A	285	VAL	2.3
1	B	659	THR	2.3
1	A	274	LYS	2.3
1	A	718	LEU	2.2
1	A	507	ILE	2.2
1	B	304	ALA	2.2
1	B	430	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	518	ASP	2.2
1	A	305	GLY	2.2
1	A	515	GLU	2.2
1	A	426	GLN	2.2
1	A	355	ASN	2.2
1	B	643	ILE	2.1
1	A	429	GLY	2.1
1	B	426	GLN	2.1
1	B	185	ASP	2.1
1	A	8	VAL	2.1
1	B	279	GLY	2.1
1	A	14	LEU	2.1
1	B	589	LEU	2.1
1	B	633	GLN	2.1
1	A	549	ILE	2.1
1	A	389	PRO	2.0
1	A	275	GLY	2.0
1	A	159	LEU	2.0
1	B	450	ARG	2.0
1	A	158	LYS	2.0
1	A	682	THR	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 oligosaccharides 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.

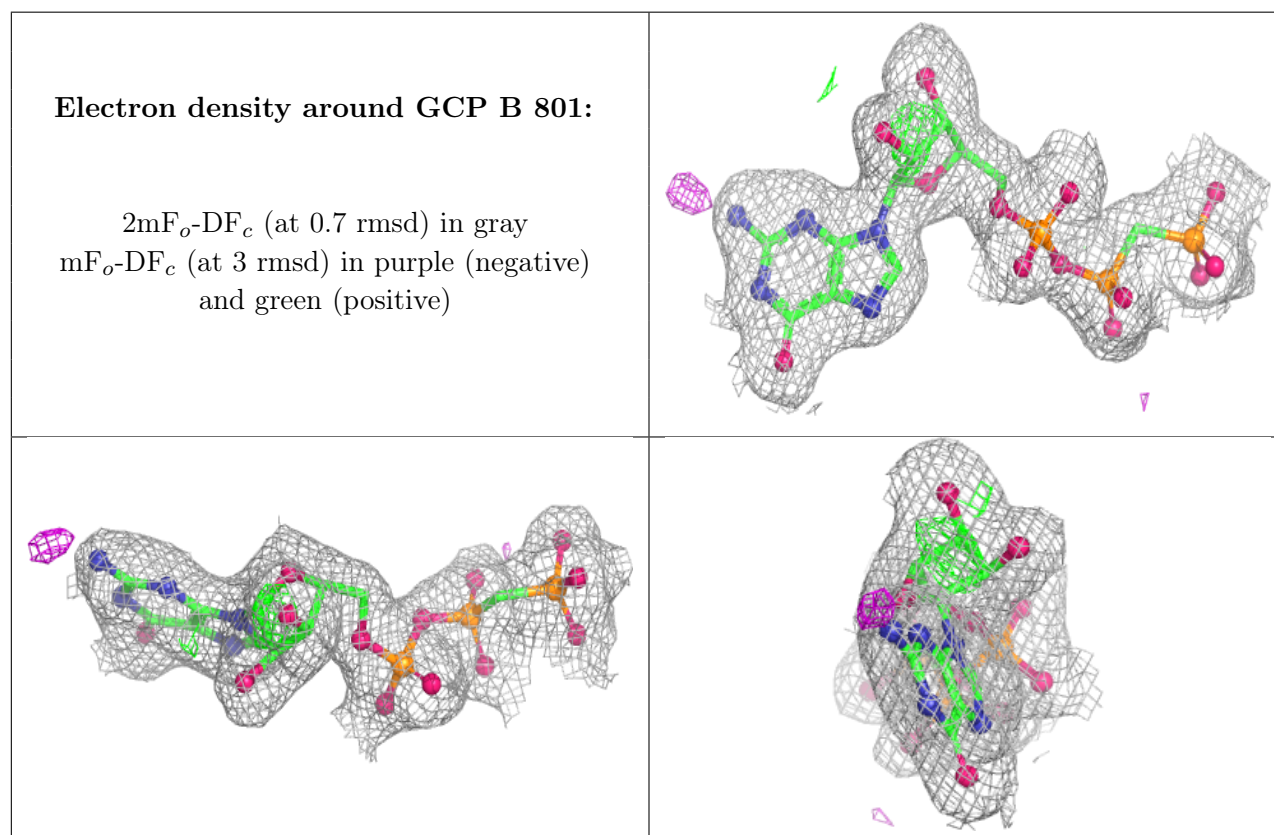
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	B	805	5/5	0.65	0.16	111,114,116,119	0
5	SO4	A	807	5/5	0.74	0.14	122,123,124,125	0

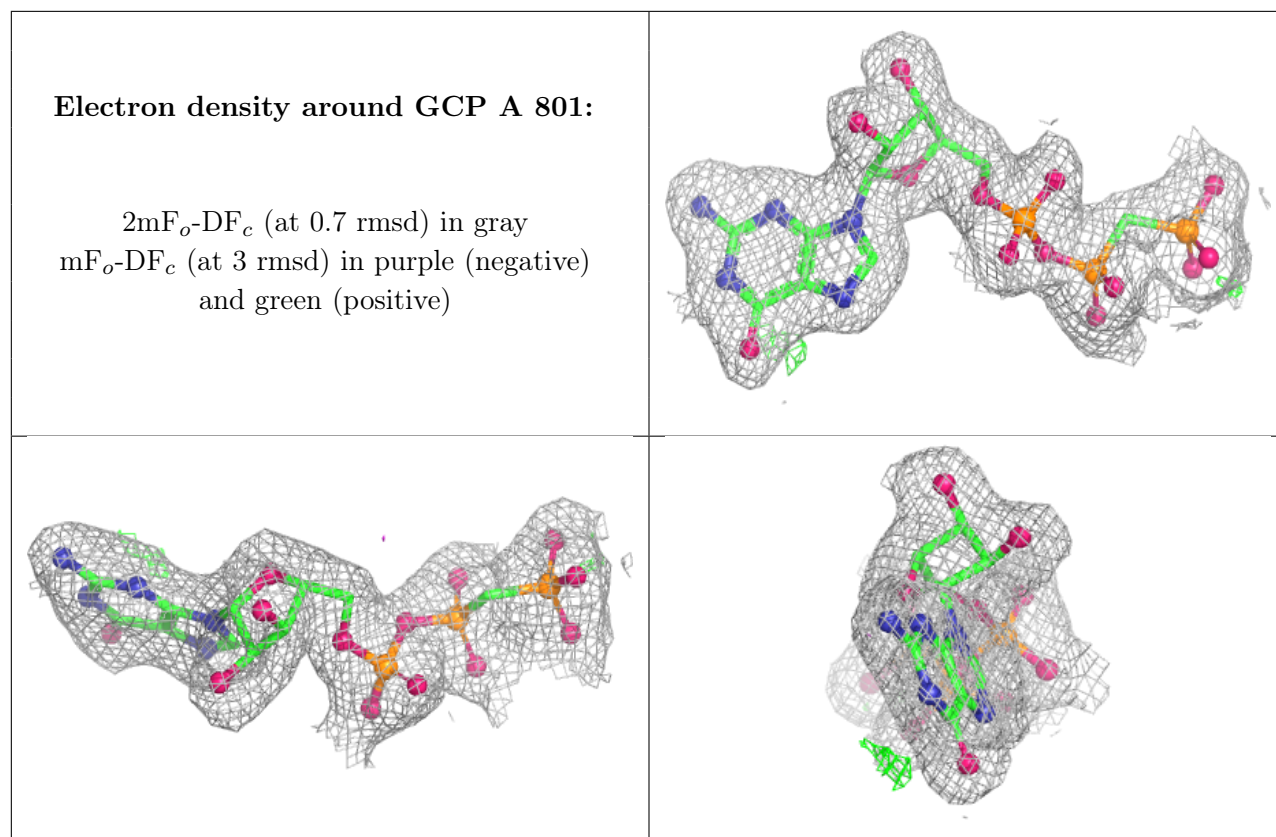
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	B	807	5/5	0.74	0.19	128,129,130,130	0
5	SO4	B	806	5/5	0.86	0.10	63,65,76,77	0
5	SO4	A	805	5/5	0.86	0.11	64,70,78,80	0
5	SO4	A	804	5/5	0.93	0.08	46,60,62,64	0
4	CL	A	803	1/1	0.95	0.16	66,66,66,66	0
4	CL	B	804	1/1	0.96	0.11	60,60,60,60	0
4	CL	A	806	1/1	0.97	0.06	49,49,49,49	0
2	GCP	B	801	32/32	0.97	0.06	24,31,38,40	0
4	CL	B	803	1/1	0.98	0.04	42,42,42,42	0
2	GCP	A	801	32/32	0.98	0.05	19,27,33,34	0
3	MG	A	802	1/1	0.99	0.05	26,26,26,26	0
3	MG	B	802	1/1	0.99	0.08	30,30,30,30	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.