Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:35 am BST

PDB ID	:	5H7J
Title	:	Crystal structure of Elongation factor 2
Authors	:	Tanzawa, T.; Kato, K.; Uchiumi, T.; Yao, M.
Deposited on	:	2016-11-18
Resolution	:	2.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

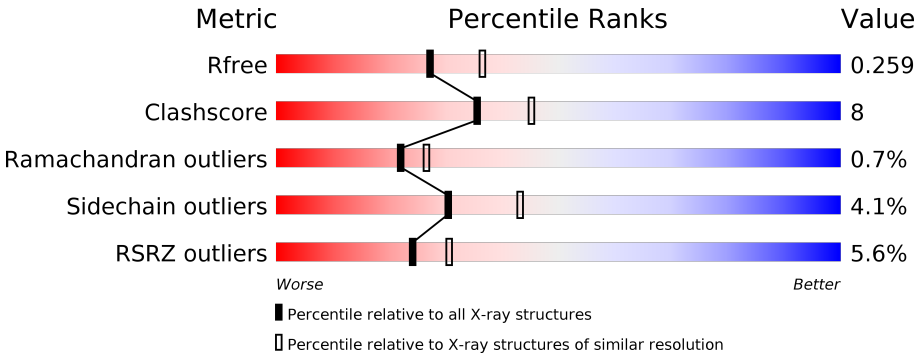
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	743	8% 73% 16% 8%
1	B	743	2% 77% 15% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11116 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.

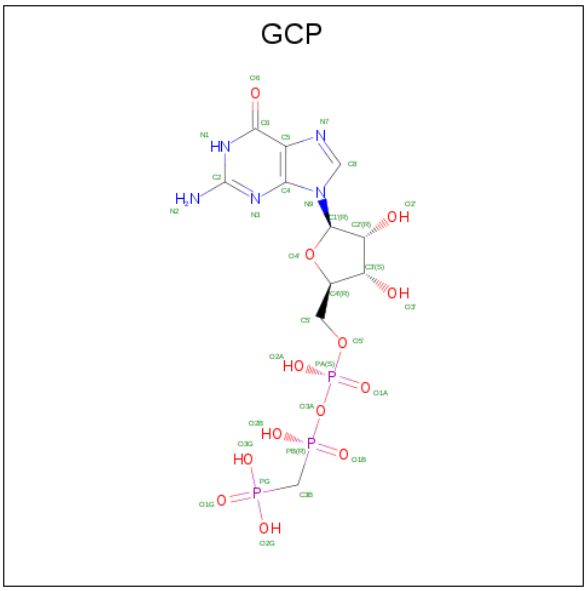
- Molecule 1 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5419	3444	951	991	33			
1	B	692	Total	C	N	O	S	0	0	0
			5460	3467	957	1002	34			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP O59521
A	2	VAL	-	expression tag	UNP O59521
A	3	GLU	-	expression tag	UNP O59521
A	736	LEU	-	expression tag	UNP O59521
A	737	GLU	-	expression tag	UNP O59521
A	738	HIS	-	expression tag	UNP O59521
A	739	HIS	-	expression tag	UNP O59521
A	740	HIS	-	expression tag	UNP O59521
A	741	HIS	-	expression tag	UNP O59521
A	742	HIS	-	expression tag	UNP O59521
A	743	HIS	-	expression tag	UNP O59521
B	1	MET	-	expression tag	UNP O59521
B	2	VAL	-	expression tag	UNP O59521
B	3	GLU	-	expression tag	UNP O59521
B	736	LEU	-	expression tag	UNP O59521
B	737	GLU	-	expression tag	UNP O59521
B	738	HIS	-	expression tag	UNP O59521
B	739	HIS	-	expression tag	UNP O59521
B	740	HIS	-	expression tag	UNP O59521
B	741	HIS	-	expression tag	UNP O59521
B	742	HIS	-	expression tag	UNP O59521
B	743	HIS	-	expression tag	UNP O59521

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



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

- Molecule 3 is water.

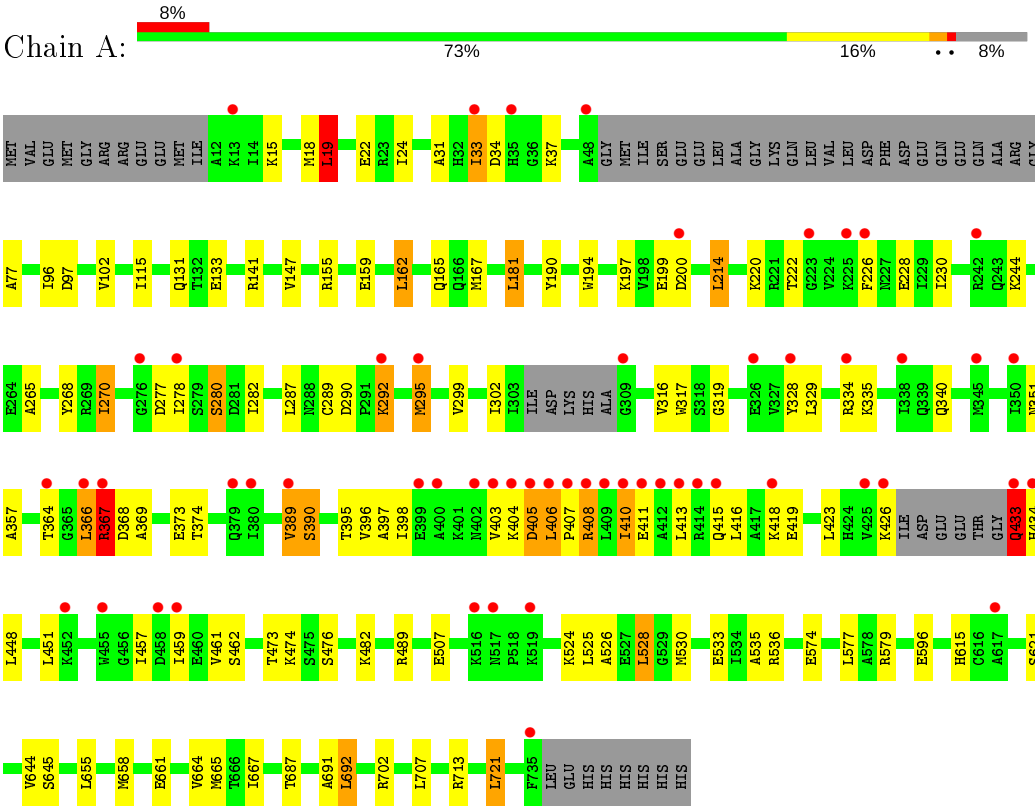
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total	O	0	0
			92	92		
3	B	113	Total	O	0	0
			113	113		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

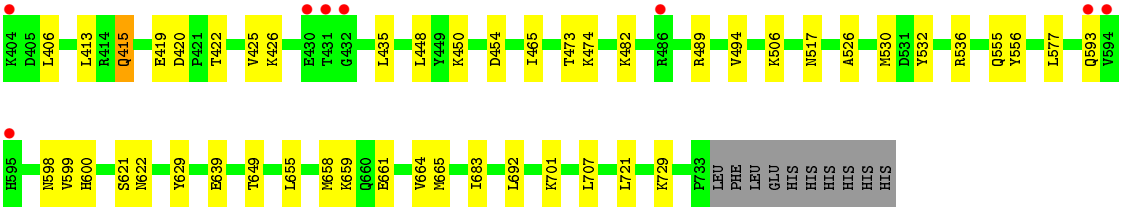
- Molecule 1: Elongation factor 2

Chain A:



- Molecule 1: Elongation factor 2

Chain B:


K404
D405
L406
L413
R414
Q415
E419
D420
P421
T422
V425
K426
E430
T431
G432
L435
L448
Y449
K450
D454
I465
T473
K474
K482
R486
R489
V494
K506
N517
A526
M530
D531
Y532
R536
Q555
Y556
L577
Q593
V594
B596
N598
V599
H600
S621
N622
Y629
E639
T649
L655
M658
K659
Q660
E661
V664
M665
I683
L692
K701
L707
L721
K729
P733
LEU
PHE
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.22Å 116.13Å 189.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.59 – 2.30 46.29 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.59-2.30) 99.2 (46.29-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.215 , 0.257 0.218 , 0.259	Depositor DCC
R_{free} test set	4130 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11116	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.47	0/5519	0.66	6/7462 (0.1%)
1	B	0.47	0/5560	0.62	1/7519 (0.0%)
All	All	0.47	0/11079	0.64	7/14981 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	241	LEU	CA-CB-CG	6.79	130.91	115.30
1	A	692	LEU	CA-CB-CG	6.27	129.72	115.30
1	A	435	LEU	CA-CB-CG	6.02	129.14	115.30
1	A	19	LEU	CA-CB-CG	5.64	128.27	115.30
1	A	367	ARG	CA-CB-CG	5.51	125.53	113.40
1	A	292	LYS	CB-CG-CD	5.44	125.75	111.60
1	A	292	LYS	CA-CB-CG	5.07	124.54	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	433	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5419	0	5544	105	0
1	B	5460	0	5587	72	0
2	B	32	0	14	4	0
3	A	92	0	0	8	0
3	B	113	0	0	6	0
All	All	11116	0	11145	178	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 8.

All (178) 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:457:ILE:HG22	1:A:459:ILE:HG13	1.61	0.82
1:A:426:LYS:NZ	1:A:433:GLN:HE22	1.77	0.81
1:A:596:GLU:OE2	3:A:801:HOH:O	1.98	0.81
1:A:426:LYS:HZ2	1:A:433:GLN:HE22	1.29	0.80
1:A:622:ASN:ND2	3:A:803:HOH:O	2.13	0.80
1:A:367:ARG:HD3	1:A:368:ASP:N	1.97	0.80
1:A:316:VAL:HG12	1:A:357:ALA:HA	1.64	0.79
1:A:473:THR:HG22	1:A:622:ASN:HB3	1.65	0.79
1:A:525:LEU:HD13	1:A:530:MET:HE1	1.70	0.74
1:B:134:THR:HG23	1:B:692:LEU:HD21	1.73	0.71
1:A:426:LYS:HB3	1:A:435:LEU:H	1.57	0.70
1:B:163:THR:HG23	1:B:166:GLN:H	1.55	0.70
1:B:517:ASN:ND2	3:B:901:HOH:O	2.19	0.70
1:A:31:ALA:HB3	1:A:37:LYS:HB2	1.72	0.69
1:A:405:ASP:N	1:A:405:ASP:OD1	2.18	0.69
1:A:507:GLU:OE1	3:A:802:HOH:O	2.11	0.68
1:B:280:SER:O	1:B:282:ILE:N	2.26	0.68
1:A:407:PRO:O	1:A:410:ILE:HG13	1.94	0.68
1:A:405:ASP:OD2	1:A:457:ILE:HG23	1.94	0.68
1:B:593:GLN:NE2	3:B:902:HOH:O	2.26	0.67
1:B:35:HIS:NE2	1:B:126:GLU:OE1	2.27	0.67
1:A:416:LEU:HD13	1:A:447:LYS:HG3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:801:GCP:O3G	2:B:801:GCP:O2B	2.13	0.66
1:B:517:ASN:OD1	1:B:517:ASN:N	2.29	0.65
1:A:702:ARG:HD2	3:A:805:HOH:O	1.96	0.65
1:A:426:LYS:HB3	1:A:434:HIS:HB3	1.80	0.63
1:A:433:GLN:HG3	1:A:434:HIS:HA	1.81	0.63
1:A:423:LEU:HD11	1:A:436:LEU:HD22	1.81	0.63
1:A:367:ARG:HD3	1:A:368:ASP:H	1.64	0.63
1:B:599:VAL:HG13	1:B:600:HIS:CD2	2.34	0.62
1:A:416:LEU:HD11	1:A:451:LEU:HD13	1.82	0.61
1:A:340:GLN:H	1:A:364:THR:HG22	1.65	0.61
1:B:331:ASN:HB3	1:B:386:LEU:HD13	1.82	0.61
1:B:365:GLY:O	1:B:367:ARG:N	2.34	0.60
1:A:482:LYS:HG2	1:A:489:ARG:HG2	1.84	0.60
1:A:713:ARG:HD3	3:A:806:HOH:O	2.02	0.59
1:A:367:ARG:CD	1:A:368:ASP:H	2.15	0.59
1:B:282:ILE:HD13	1:B:380:ILE:HG21	1.85	0.58
1:A:433:GLN:CG	1:A:434:HIS:HA	2.34	0.58
1:A:408:ARG:HD3	1:A:408:ARG:N	2.19	0.57
1:B:33:ILE:HG22	1:B:101:HIS:CG	2.40	0.57
1:A:407:PRO:C	1:A:408:ARG:HD3	2.25	0.57
1:A:635:ASN:HB3	1:A:692:LEU:HB3	1.87	0.56
1:B:311:VAL:N	3:B:907:HOH:O	2.37	0.56
1:A:141:ARG:NE	1:A:635:ASN:HD21	2.03	0.56
1:B:532:TYR:CE2	1:B:536:ARG:HD3	2.40	0.56
1:B:173:LYS:NZ	1:B:177:ASP:OD1	2.39	0.55
1:B:77:ALA:O	1:B:97:ASP:HB2	2.06	0.55
1:A:406:LEU:HD12	1:A:406:LEU:H	1.72	0.54
1:B:188:GLU:HA	1:B:191:LYS:HD2	1.88	0.54
1:A:290:ASP:O	1:A:319:GLY:N	2.24	0.54
1:A:141:ARG:CZ	1:A:635:ASN:HD21	2.21	0.53
1:A:644:VAL:HG11	1:A:667:ILE:HD11	1.90	0.53
1:A:474:LYS:O	1:A:621:SER:HB3	2.09	0.53
1:A:133:GLU:HG2	1:A:181:LEU:HD21	1.91	0.53
1:B:19:LEU:HD12	1:B:356:PRO:HG3	1.91	0.52
1:A:423:LEU:CD2	1:A:447:LYS:HG2	2.39	0.52
1:B:23:ARG:HD2	1:B:89:LYS:NZ	2.26	0.51
1:A:525:LEU:HD13	1:A:530:MET:CE	2.41	0.51
1:A:459:ILE:HG22	1:A:461:VAL:HG23	1.92	0.51
1:A:290:ASP:OD2	1:A:292:LYS:HG2	2.11	0.51
1:A:77:ALA:O	1:A:97:ASP:HB2	2.11	0.51
1:A:579:ARG:HD2	1:A:721:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:MET:SD	1:A:355:VAL:HG12	2.52	0.50
1:A:265:ALA:HA	1:A:268:TYR:CE2	2.47	0.50
1:A:408:ARG:HA	1:A:411:GLU:HB2	1.92	0.50
1:B:291:PRO:O	1:B:320:THR:OG1	2.30	0.50
1:B:184:ARG:NH1	1:B:639:GLU:OE2	2.29	0.50
1:B:622:ASN:ND2	3:B:913:HOH:O	2.45	0.49
1:A:687:THR:HG21	1:A:691:ALA:HB2	1.94	0.49
1:B:555:GLN:HB3	1:B:556:TYR:CD1	2.47	0.49
1:A:661:GLU:O	1:A:664:VAL:HG12	2.13	0.49
1:A:397:ALA:HB3	1:A:462:SER:HB3	1.93	0.49
1:A:406:LEU:O	1:A:410:ILE:HG23	2.12	0.49
1:A:416:LEU:HD11	1:A:451:LEU:CD1	2.43	0.49
1:B:133:GLU:HG2	1:B:181:LEU:HD21	1.95	0.49
1:A:334:ARG:HA	1:A:334:ARG:NE	2.27	0.49
1:B:163:THR:HG23	1:B:166:GLN:HB2	1.95	0.49
1:A:367:ARG:CD	1:A:368:ASP:N	2.73	0.49
1:A:533:GLU:OE2	1:A:536:ARG:NH1	2.45	0.48
1:B:34:ASP:O	1:B:152:LYS:NZ	2.31	0.48
1:A:22:GLU:HG3	1:A:263:ILE:HG21	1.93	0.48
1:A:389:VAL:O	1:A:390:SER:HB3	2.13	0.48
1:A:396:VAL:HG13	1:A:398:ILE:HD13	1.95	0.48
1:B:536:ARG:HH21	1:B:536:ARG:HG3	1.78	0.48
1:B:152:LYS:HG2	2:B:801:GCP:C6	2.44	0.48
1:A:141:ARG:NH1	1:A:635:ASN:HD21	2.12	0.48
1:B:295:MET:HB3	1:B:377:GLU:CD	2.35	0.47
1:B:389:VAL:HG13	1:B:422:THR:HG22	1.96	0.47
1:A:530:MET:HE3	1:A:535:ALA:HA	1.96	0.47
1:A:367:ARG:CG	1:A:368:ASP:H	2.28	0.47
1:B:32:HIS:CE1	1:B:33:ILE:HG12	2.50	0.47
1:A:155:ARG:NH1	1:A:159:GLU:OE2	2.48	0.46
1:A:295:MET:CE	1:A:316:VAL:HG13	2.45	0.46
1:A:33:ILE:O	1:A:34:ASP:HB2	2.15	0.46
1:A:645:SER:OG	3:A:804:HOH:O	2.18	0.46
1:B:213:ALA:O	1:B:250:VAL:HG21	2.15	0.46
1:B:31:ALA:HB3	1:B:37:LYS:HB2	1.96	0.46
1:B:598:ASN:ND2	3:B:904:HOH:O	2.48	0.46
1:A:15:LYS:O	1:A:19:LEU:HD13	2.15	0.46
1:A:398:ILE:HG13	1:A:461:VAL:HG22	1.96	0.46
1:B:19:LEU:O	1:B:21:PRO:HD3	2.16	0.46
1:A:295:MET:HE1	1:A:316:VAL:HG13	1.98	0.46
1:A:15:LYS:HA	1:A:18:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:LYS:HD2	1:B:506:LYS:HA	1.68	0.46
1:A:226:PHE:O	1:A:230:ILE:HG13	2.16	0.45
1:A:96:ILE:HD12	1:A:115:ILE:HG22	1.97	0.45
1:B:381:GLU:HG3	1:B:382:PRO:HD2	1.98	0.45
1:A:524:LYS:O	1:A:528:LEU:HD22	2.15	0.45
1:B:659:LYS:O	1:B:665:MET:HE3	2.17	0.45
1:A:270:ILE:HD11	1:A:317:TRP:CE3	2.51	0.45
1:A:658:MET:HG2	1:A:665:MET:HE2	1.98	0.45
1:A:426:LYS:HZ3	1:A:433:GLN:HE22	1.61	0.45
1:A:33:ILE:HG12	1:A:131:GLN:OE1	2.17	0.45
1:A:404:LYS:HG2	1:A:405:ASP:N	2.32	0.44
1:B:324:GLY:N	1:B:338:ILE:O	2.49	0.44
1:A:398:ILE:O	1:A:433:GLN:HA	2.17	0.44
1:B:138:GLN:HG3	1:B:141:ARG:NH1	2.33	0.44
1:B:532:TYR:CZ	1:B:536:ARG:HD3	2.52	0.44
1:B:18:MET:HE2	1:B:18:MET:HB3	1.74	0.44
1:B:413:LEU:HB3	1:B:425:VAL:HG21	2.00	0.44
1:A:190:TYR:HB3	1:A:194:TRP:CG	2.52	0.44
1:A:220:LYS:HE2	1:A:220:LYS:HB2	1.79	0.44
1:A:329:LEU:HD13	1:A:369:ALA:HB2	2.00	0.44
1:A:413:LEU:HA	1:A:413:LEU:HD23	1.70	0.44
1:B:137:ARG:NH2	1:B:692:LEU:HD23	2.32	0.44
1:B:297:MET:HG2	1:B:375:VAL:HB	2.00	0.44
1:B:661:GLU:O	1:B:664:VAL:HG12	2.18	0.44
1:A:278:ILE:HD11	1:A:287:LEU:HD13	2.00	0.43
1:B:152:LYS:HE2	2:B:801:GCP:C4	2.48	0.43
1:B:526:ALA:HA	1:B:530:MET:O	2.18	0.43
1:A:373:GLU:HG3	1:A:374:THR:N	2.32	0.43
1:A:282:ILE:HA	1:A:282:ILE:HD12	1.77	0.43
1:B:329:LEU:HD11	1:B:366:LEU:HG	2.01	0.43
1:B:137:ARG:HG3	1:B:185:TYR:CG	2.53	0.43
1:B:450:LYS:O	1:B:454:ASP:HB2	2.18	0.43
1:A:395:THR:HA	1:A:436:LEU:O	2.18	0.43
1:B:474:LYS:O	1:B:621:SER:HB3	2.19	0.43
1:A:457:ILE:CG2	1:A:459:ILE:HG13	2.41	0.43
1:B:415:GLN:O	1:B:419:GLU:HG3	2.19	0.43
1:A:418:LYS:HB3	1:A:419:GLU:HG3	2.01	0.43
1:A:411:GLU:O	1:A:415:GLN:HB2	2.19	0.42
1:B:163:THR:HG22	1:B:166:GLN:OE1	2.19	0.42
1:B:482:LYS:NZ	1:B:489:ARG:HE	2.17	0.42
1:B:426:LYS:HE3	1:B:435:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:SER:HB3	1:A:621:SER:OG	2.20	0.42
1:A:574:GLU:O	1:A:615:HIS:CE1	2.72	0.42
1:B:659:LYS:C	1:B:665:MET:HE3	2.40	0.42
1:A:526:ALA:HA	1:A:530:MET:O	2.18	0.42
1:A:436:LEU:HA	1:A:436:LEU:HD23	1.83	0.42
1:B:101:HIS:N	3:B:918:HOH:O	2.51	0.42
1:B:629:TYR:CZ	1:B:701:LYS:HD2	2.55	0.42
1:A:102:VAL:HG22	3:A:867:HOH:O	2.19	0.42
1:A:162:LEU:HB3	1:A:167:MET:HG3	2.01	0.42
1:B:170:ARG:HB2	1:B:170:ARG:HE	1.54	0.42
1:B:21:PRO:O	1:B:262:PRO:HD2	2.20	0.42
1:A:197:LYS:HE3	1:A:200:ASP:CG	2.41	0.41
1:A:228:GLU:OE1	1:A:244:LYS:NZ	2.52	0.41
1:B:465:ILE:O	1:B:465:ILE:HG13	2.20	0.41
1:A:258:HIS:ND1	3:A:809:HOH:O	2.36	0.41
1:B:658:MET:HG3	1:B:665:MET:HE2	2.03	0.41
1:B:34:ASP:HA	2:B:801:GCP:H5'2	2.02	0.41
1:A:214:LEU:HD13	1:A:214:LEU:HA	1.93	0.41
1:A:299:VAL:HG11	1:A:302:ILE:HD11	2.02	0.41
1:B:270:ILE:HD13	1:B:270:ILE:HA	1.92	0.41
1:B:683:ILE:HA	1:B:683:ILE:HD12	1.87	0.41
1:B:96:ILE:HD13	1:B:115:ILE:HG22	2.02	0.41
1:A:263:ILE:HA	1:A:289:CYS:HB2	2.02	0.41
1:B:33:ILE:HG22	1:B:101:HIS:CD2	2.56	0.41
1:A:24:ILE:HB	1:A:262:PRO:CD	2.51	0.41
1:A:277:ASP:HB3	1:A:280:SER:HB3	2.01	0.40
1:A:366:LEU:HD13	1:A:366:LEU:HA	1.93	0.40
1:A:328:TYR:CD1	1:A:335:LYS:HG2	2.56	0.40
1:A:18:MET:HE2	1:A:18:MET:HB3	1.77	0.40
1:B:189:GLU:HG2	1:B:190:TYR:CD2	2.56	0.40
1:B:355:VAL:HG11	1:B:361:VAL:HG12	2.04	0.40
1:B:729:LYS:HB3	1:B:729:LYS:HE3	1.80	0.40
1:B:265:ALA:HA	1:B:268:TYR:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	678/743 (91%)	657 (97%)	17 (2%)	4 (1%)	25	31
1	B	686/743 (92%)	664 (97%)	17 (2%)	5 (1%)	22	26
All	All	1364/1486 (92%)	1321 (97%)	34 (2%)	9 (1%)	22	26

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	339	GLN
1	B	366	LEU
1	A	33	ILE
1	B	280	SER
1	B	281	ASP
1	A	390	SER
1	B	420	ASP
1	A	280	SER
1	A	403	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	589/638 (92%)	563 (96%)	26 (4%)	28	39
1	B	594/638 (93%)	571 (96%)	23 (4%)	32	46
All	All	1183/1276 (93%)	1134 (96%)	49 (4%)	30	43

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	147	VAL
1	A	162	LEU
1	A	165	GLN
1	A	181	LEU
1	A	199	GLU
1	A	214	LEU
1	A	222	THR
1	A	270	ILE
1	A	295	MET
1	A	351	ASN
1	A	366	LEU
1	A	367	ARG
1	A	389	VAL
1	A	405	ASP
1	A	406	LEU
1	A	408	ARG
1	A	410	ILE
1	A	433	GLN
1	A	435	LEU
1	A	448	LEU
1	A	528	LEU
1	A	577	LEU
1	A	655	LEU
1	A	707	LEU
1	A	721	LEU
1	B	19	LEU
1	B	22	GLU
1	B	23	ARG
1	B	147	VAL
1	B	160	LEU
1	B	161	LYS
1	B	163	THR
1	B	232	LEU
1	B	241	LEU
1	B	295	MET
1	B	329	LEU
1	B	349	ARG
1	B	388	TYR
1	B	406	LEU
1	B	415	GLN
1	B	448	LEU

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Mol	Chain	Res	Type
1	B	473	THR
1	B	494	VAL
1	B	577	LEU
1	B	649	THR
1	B	655	LEU
1	B	707	LEU
1	B	721	LEU

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

Mol	Chain	Res	Type
1	A	32	HIS
1	A	76	ASN
1	A	433	GLN
1	A	635	ASN
1	B	288	ASN
1	B	433	GLN
1	B	600	HIS
1	B	622	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 carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is 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	GCP	B	801	-	26,34,34	2.86	8 (30%)	31,54,54	1.61	3 (9%)

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	-	-	6/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	GCP	C4-N9	-11.58	1.32	1.47
2	B	801	GCP	PG-O1G	5.41	1.61	1.50
2	B	801	GCP	PG-O3G	2.98	1.61	1.54
2	B	801	GCP	C8-N9	-2.77	1.36	1.45
2	B	801	GCP	PG-O2G	-2.54	1.49	1.54
2	B	801	GCP	PB-O2B	2.30	1.61	1.56
2	B	801	GCP	C2-N1	-2.25	1.35	1.44
2	B	801	GCP	C5-C6	-2.17	1.49	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	GCP	PA-O3A-PB	-6.12	113.14	132.56
2	B	801	GCP	O4'-C1'-N9	3.43	114.14	109.04
2	B	801	GCP	C4-C5-N7	3.40	106.97	102.46

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	GCP	PG-C3B-PB-O1B
2	B	801	GCP	PG-C3B-PB-O3A
2	B	801	GCP	C2'-C1'-N9-C4

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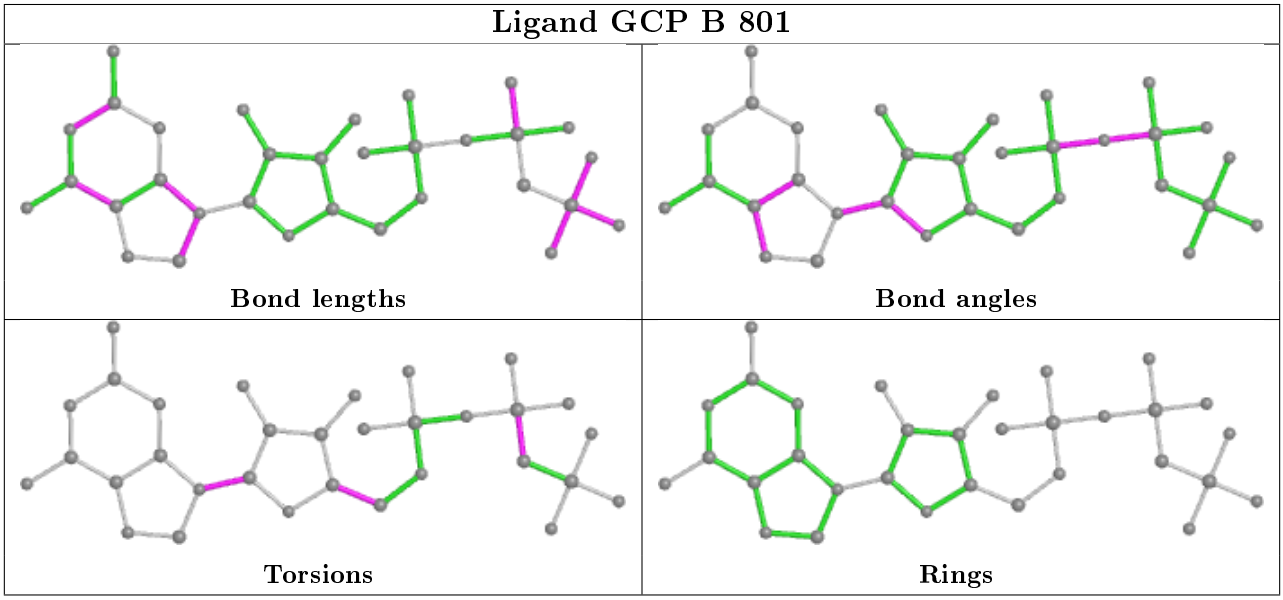
Mol	Chain	Res	Type	Atoms
2	B	801	GCP	O4'-C4'-C5'-O5'
2	B	801	GCP	C3'-C4'-C5'-O5'
2	B	801	GCP	PG-C3B-PB-O2B

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	GCP	4	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.



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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	686/743 (92%)	0.60	59 (8%)	10	14	32, 60, 97, 115	0
1	B	692/743 (93%)	0.33	18 (2%)	56	63	26, 55, 85, 108	0
All	All	1378/1486 (92%)	0.46	77 (5%)	24	30	26, 57, 93, 115	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	408	ARG	5.9
1	A	413	LEU	5.7
1	A	403	VAL	5.5
1	B	388	TYR	5.4
1	A	405	ASP	5.1
1	A	412	ALA	5.0
1	A	434	HIS	4.9
1	A	407	PRO	4.8
1	A	328	TYR	4.3
1	A	415	GLN	4.2
1	A	402	ASN	4.0
1	A	345	MET	3.9
1	B	593	GLN	3.8
1	A	223	GLY	3.8
1	A	410	ILE	3.6
1	A	425	VAL	3.6
1	A	354	ALA	3.4
1	B	594	VAL	3.4
1	A	458	ASP	3.4
1	A	292	LYS	3.3
1	B	430	GLU	3.3
1	A	400	ALA	3.3
1	A	735	PHE	3.3
1	A	414	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	242	ARG	3.2
1	A	364	THR	3.2
1	A	516	LYS	3.1
1	A	379	GLN	3.1
1	A	433	GLN	3.1
1	A	278	ILE	3.1
1	A	426	LYS	3.0
1	A	406	LEU	3.0
1	A	13	LYS	3.0
1	A	309	GLY	2.9
1	A	404	LYS	2.9
1	B	369	ALA	2.9
1	A	48	ALA	2.8
1	A	380	ILE	2.7
1	B	404	LYS	2.7
1	A	435	LEU	2.7
1	A	326	GLU	2.7
1	A	334	ARG	2.6
1	B	350	ILE	2.6
1	A	366	LEU	2.5
1	B	431	THR	2.5
1	B	486	ARG	2.4
1	B	386	LEU	2.4
1	A	200	ASP	2.4
1	A	459	ILE	2.4
1	B	595	HIS	2.4
1	B	432	GLY	2.4
1	B	385	ALA	2.3
1	A	411	GLU	2.3
1	A	455	TRP	2.3
1	B	304	ILE	2.3
1	A	276	GLY	2.3
1	A	226	PHE	2.3
1	B	352	MET	2.3
1	B	339	GLN	2.3
1	A	409	LEU	2.2
1	A	225	LYS	2.2
1	A	517	ASN	2.2
1	A	295	MET	2.2
1	A	452	LYS	2.2
1	A	33	ILE	2.2
1	A	617	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	418	LYS	2.1
1	A	389	VAL	2.1
1	A	350	ILE	2.1
1	A	399	GLU	2.1
1	A	623	PRO	2.1
1	B	28	GLY	2.1
1	B	89	LYS	2.0
1	A	35	HIS	2.0
1	A	338	ILE	2.0
1	A	367	ARG	2.0
1	A	519	LYS	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 carbohydrates in this entry.

6.4 Ligands (i)

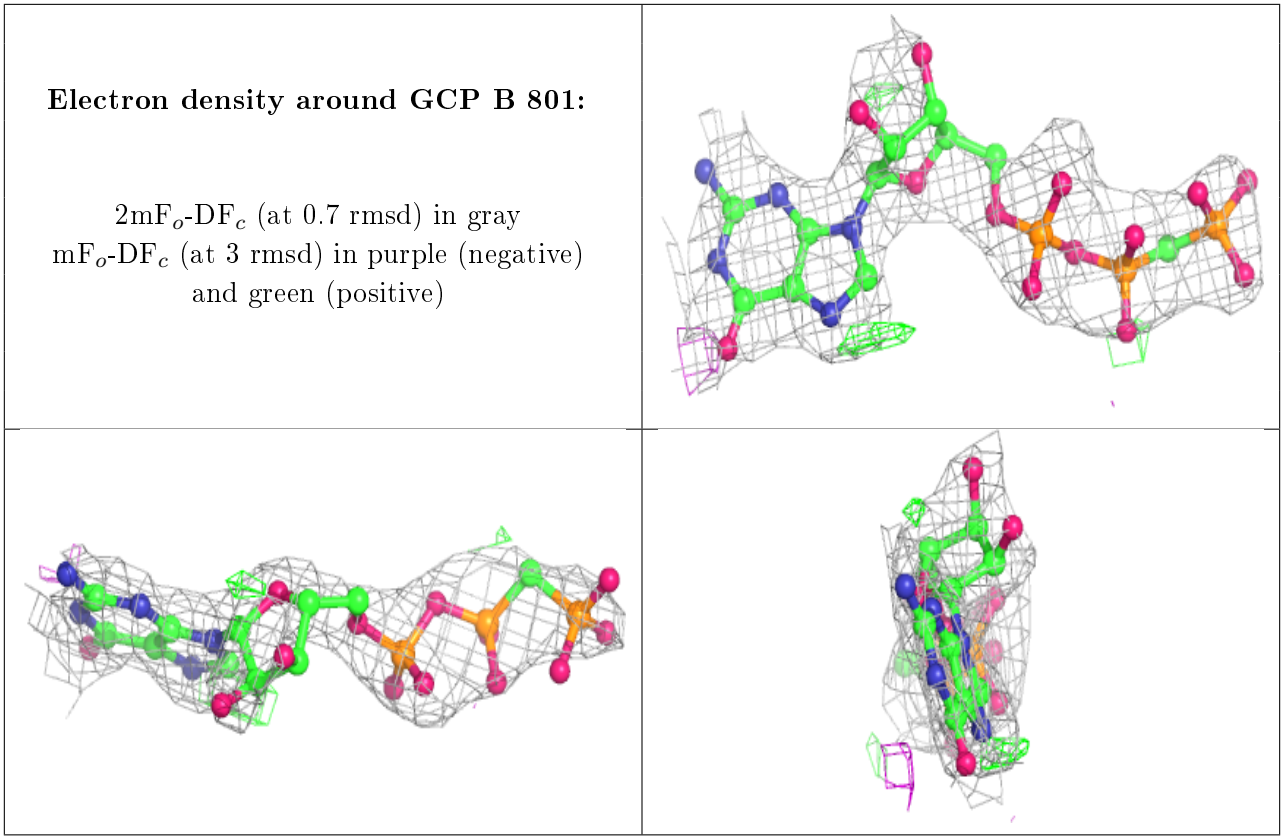
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GCP	B	801	32/32	0.84	0.21	51,69,87,88	32

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 GCP B 801:

$2mF_o$-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.