



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:37 AM UTC

PDB ID : 3H98 / pdb_00003h98
Title : Crystal structure of HCV NS5b 1b with (1,1-dioxo-2H-[1,2,4]benzothiadiazin-3-yl) azolo[1,5-a]pyrimidine derivative
Authors : Wang, G.; Lei, H.; Wang, X.; Das, D.; Mackinnon, C.; Montalbetti, C.A.G.; Mears, R.; Gai, X.; Bailey, S.; Ruhmund, D.; Hooi, L.; Misialek, S.; Rajagopalan, R.; Cheng, R.K.Y.; Barker, J.L.; Felicetti, B.; Stoycheva, A.; Buckman, B.; Kossen, K.; Seiwert, S.; Beigelmana, L.
Deposited on : 2009-04-30
Resolution : 1.90 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)

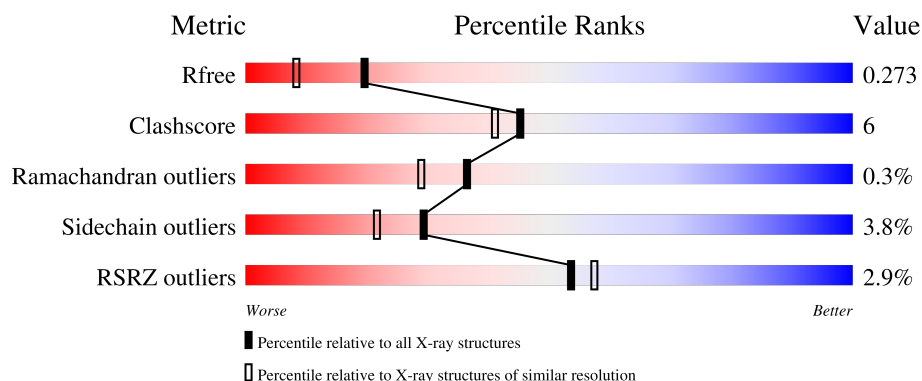
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	576	
1	B	576	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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
3	GOL	A	572	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9544 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.

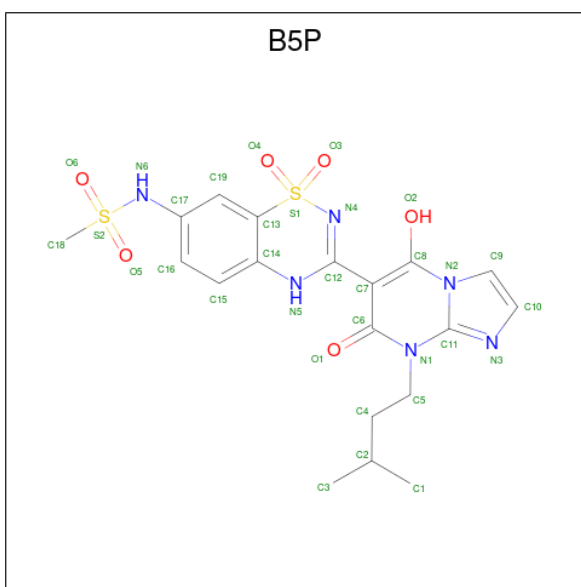
- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	8	0
			4292	2709	754	795	34			
1	B	559	Total	C	N	O	S	0	6	0
			4340	2740	761	805	34			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP P26663
A	-4	HIS	-	expression tag	UNP P26663
A	-3	HIS	-	expression tag	UNP P26663
A	-2	HIS	-	expression tag	UNP P26663
A	-1	HIS	-	expression tag	UNP P26663
A	0	HIS	-	expression tag	UNP P26663
A	1	HIS	-	expression tag	UNP P26663
B	-5	MET	-	expression tag	UNP P26663
B	-4	HIS	-	expression tag	UNP P26663
B	-3	HIS	-	expression tag	UNP P26663
B	-2	HIS	-	expression tag	UNP P26663
B	-1	HIS	-	expression tag	UNP P26663
B	0	HIS	-	expression tag	UNP P26663
B	1	HIS	-	expression tag	UNP P26663

- Molecule 2 is N-{3-[5-hydroxy-8-(3-methylbutyl)-7-oxo-7,8-dihydroimidazo[1,2-a]pyrimidin-6-yl]-1,1-dioxido-4H-1,2,4-benzothiadiazin-7-yl}methanesulfonamide (CCD ID: B5P) (formula: C₁₉H₂₂N₆O₆S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			33	19	6	6	2		
2	B	1	Total	C	N	O	S	0	0
			33	19	6	6	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

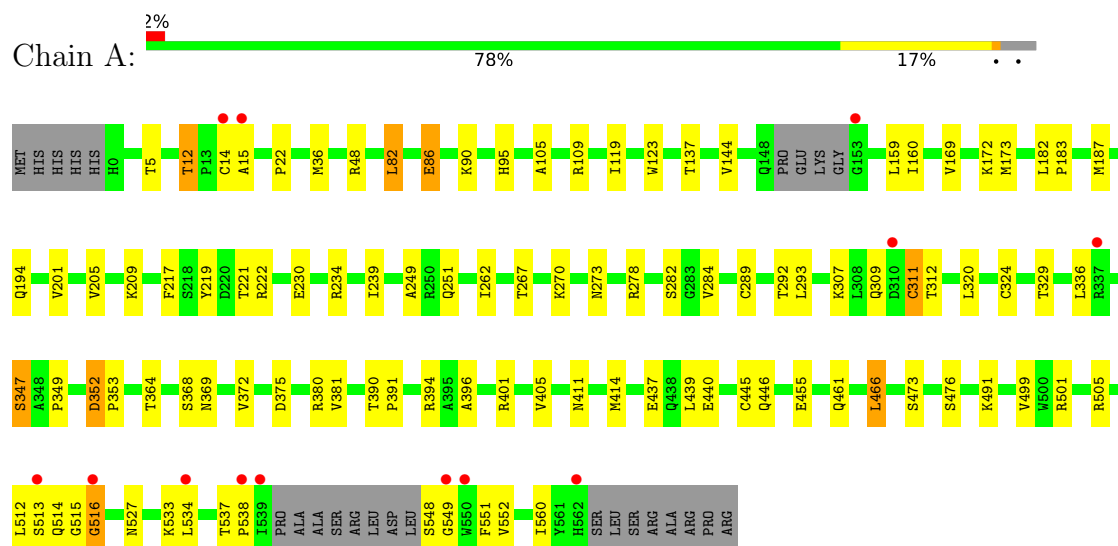
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	424	Total 424	O 424	0	0
4	B	410	Total 410	O 410	0	0

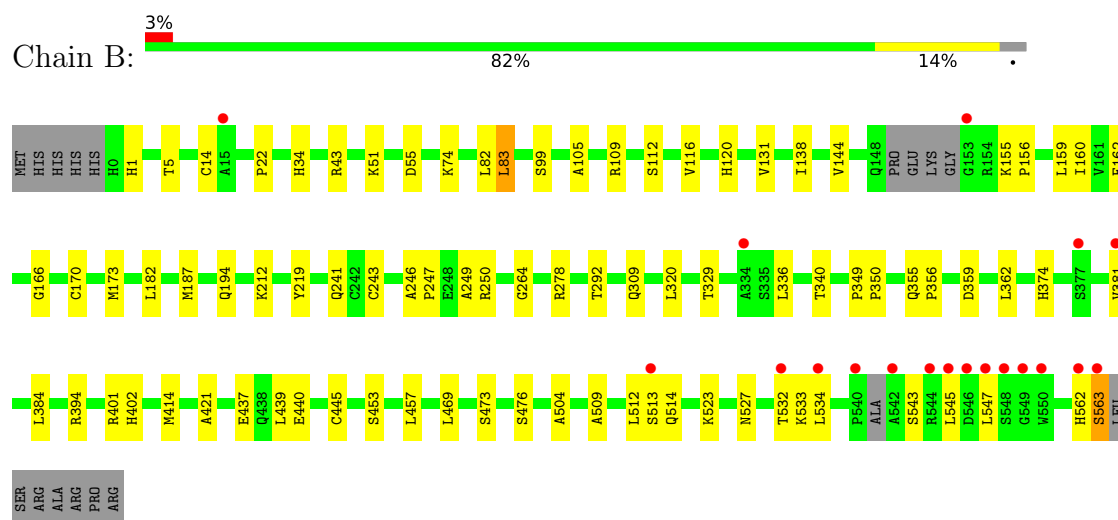
3 Residue-property plots

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: RNA-directed RNA polymerase



• Molecule 1: RNA-directed RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.93Å 106.20Å 126.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.99 – 1.90 37.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.99-1.90) 98.9 (37.99-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.208 , 0.274 0.206 , 0.273	Depositor DCC
R_{free} test set	4546 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9544	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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 49.94 % 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 6.9408e-05. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, B5P

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	1.36	8/4417 (0.2%)	1.21	13/5997 (0.2%)
1	B	1.34	9/4459 (0.2%)	1.18	7/6055 (0.1%)
All	All	1.35	17/8876 (0.2%)	1.19	20/12052 (0.2%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	MET	SD-CE	-7.26	1.61	1.79
1	B	504	ALA	CA-CB	7.08	1.64	1.53
1	B	160	ILE	CA-CB	6.30	1.61	1.54
1	B	509	ALA	N-CA	6.10	1.53	1.46
1	A	284	VAL	CA-CB	6.06	1.64	1.54
1	B	166	GLY	N-CA	5.82	1.53	1.45
1	B	421	ALA	CA-CB	5.62	1.62	1.53
1	A	396	ALA	CA-CB	5.60	1.62	1.53
1	B	246	ALA	CA-C	5.54	1.59	1.53
1	A	499	VAL	CA-C	5.46	1.59	1.52
1	A	14	CYS	N-CA	5.38	1.52	1.46
1	B	116	VAL	CA-CB	5.32	1.60	1.54
1	B	162	PHE	C-O	5.28	1.29	1.24
1	A	369	ASN	C-O	5.25	1.30	1.23
1	A	349	PRO	CA-C	5.24	1.55	1.52
1	A	251	GLN	C-O	-5.04	1.18	1.24
1	B	99	SER	CA-C	5.00	1.59	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	PRO	O-C-N	6.86	124.37	121.15
1	A	12	THR	CA-C-N	6.65	126.61	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	THR	C-N-CA	6.65	126.61	120.03
1	B	264	GLY	CA-C-N	6.51	126.27	119.76
1	B	264	GLY	C-N-CA	6.51	126.27	119.76
1	A	455	GLU	CA-C-N	6.47	126.23	119.05
1	A	455	GLU	C-N-CA	6.47	126.23	119.05
1	B	131	VAL	N-CA-C	5.87	117.05	112.12
1	A	466	LEU	N-CA-C	5.74	119.46	112.23
1	A	352	ASP	CA-C-N	-5.62	114.59	120.38
1	A	352	ASP	C-N-CA	-5.62	114.59	120.38
1	A	123	TRP	N-CA-C	-5.61	105.08	111.14
1	A	552	VAL	N-CA-C	-5.54	106.80	111.56
1	A	312	THR	N-CA-C	-5.40	99.63	108.76
1	A	411	ASN	N-CA-C	5.39	117.16	111.28
1	B	155	LYS	CA-C-N	-5.33	115.09	120.31
1	B	155	LYS	C-N-CA	-5.33	115.09	120.31
1	A	15	ALA	N-CA-C	-5.23	99.67	110.80
1	B	349	PRO	O-C-N	5.18	123.58	121.15
1	B	34	HIS	N-CA-C	5.00	117.47	111.71

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	4292	0	4268	57	0
1	B	4340	0	4315	43	0
2	A	33	0	21	2	0
2	B	33	0	21	3	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0
4	A	424	0	0	10	0
4	B	410	0	0	10	0
All	All	9544	0	8641	103	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 (103) 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:187:MET:HE2	1:A:293:LEU:HD23	1.27	1.15
1:B:170:CYS:HA	1:B:173:MET:HE3	1.35	1.09
1:B:355:GLN:HB3	4:B:878:HOH:O	1.59	1.01
1:A:187:MET:HE2	1:A:293:LEU:CD2	1.93	0.98
1:B:170:CYS:HA	1:B:173:MET:CE	2.02	0.90
1:A:90:LYS:HE2	1:A:109:ARG:O	1.76	0.86
1:A:311:CYS:HB3	1:A:324:CYS:HB3	1.59	0.85
1:A:466:LEU:O	4:A:950:HOH:O	2.05	0.75
1:A:221:THR:O	4:A:768:HOH:O	2.06	0.73
1:B:194:GLN:O	4:B:764:HOH:O	2.07	0.72
1:A:5:THR:HG23	1:A:278:ARG:HH12	1.55	0.71
1:A:187:MET:CE	1:A:293:LEU:HD23	2.16	0.71
1:A:194:GLN:O	4:A:816:HOH:O	2.08	0.70
1:B:138:ILE:HD11	1:B:159:LEU:HD13	1.72	0.70
1:A:445:CYS:HB2	4:A:781:HOH:O	1.91	0.70
1:B:120:HIS:HE1	4:B:740:HOH:O	1.75	0.70
1:B:445:CYS:HB2	4:B:819:HOH:O	1.92	0.69
1:A:182:LEU:HD23	1:A:182:LEU:C	2.19	0.68
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.80	0.64
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.79	0.63
1:A:501:ARG:HD3	4:A:910:HOH:O	1.99	0.63
1:B:241:GLN:OE1	1:B:250:ARG:HG3	2.00	0.61
1:B:512:LEU:O	1:B:514:GLN:N	2.33	0.61
1:B:414:MET:HG3	2:B:571:B5P:C10	2.32	0.60
1:B:402:HIS:HB3	4:B:725:HOH:O	2.00	0.59
1:A:36[B]:MET:HE1	1:A:491:LYS:HG2	1.84	0.58
1:A:414:MET:HG3	2:A:571:B5P:C10	2.34	0.58
1:B:512:LEU:C	1:B:514:GLN:H	2.11	0.58
1:A:278:ARG:NH2	4:A:814:HOH:O	2.37	0.58
1:A:466:LEU:HD22	1:A:551:PHE:HE2	1.69	0.57
1:B:182:LEU:HD12	1:B:243:CYS:SG	2.44	0.57
1:B:439:LEU:HB3	1:B:457:LEU:HG	1.85	0.57
1:B:336:LEU:HD12	1:B:356:PRO:HD3	1.86	0.57
1:B:384:LEU:HD23	2:B:571:B5P:H21	1.86	0.56
1:B:523:LYS:HE3	1:B:534:LEU:HD13	1.87	0.56
1:B:5:THR:HG23	1:B:278:ARG:HH12	1.71	0.56
1:B:512:LEU:O	4:B:845:HOH:O	2.18	0.55
1:A:405:VAL:HG21	1:A:446:GLN:HE21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374[B]:HIS:HD2	1:B:476:SER:HB2	1.72	0.55
1:A:187:MET:HE1	1:A:292:THR:HG22	1.87	0.55
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.88	0.54
1:A:187:MET:SD	1:A:292:THR:HG22	2.48	0.54
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.91	0.53
1:B:340:THR:CG2	1:B:350:PRO:HG3	2.38	0.53
1:A:364:THR:HA	1:A:368:SER:O	2.09	0.52
1:B:105:ALA:O	1:B:109:ARG:HG3	2.10	0.52
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.92	0.52
1:A:512:LEU:C	1:A:514:GLN:H	2.17	0.52
1:B:51:LYS:HE2	1:B:156:PRO:HG3	1.92	0.51
1:B:359:ASP:HB3	1:B:362:LEU:HD12	1.92	0.50
1:B:187:MET:SD	1:B:292:THR:HG22	2.52	0.50
1:A:533:LYS:N	1:A:533:LYS:HD2	2.27	0.49
1:A:90:LYS:CE	1:A:109:ARG:O	2.57	0.49
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.95	0.49
3:B:572:GOL:H12	4:B:958:HOH:O	2.12	0.49
1:A:12:THR:HG21	1:A:270:LYS:HD2	1.95	0.48
1:B:527:ASN:ND2	1:B:533:LYS:HG3	2.28	0.48
1:A:537:THR:HB	1:A:538:PRO:CD	2.42	0.48
1:B:1:HIS:N	1:B:55:ASP:OD1	2.28	0.47
1:A:160:ILE:HA	1:A:282:SER:OG	2.14	0.47
1:A:48:ARG:HG2	1:A:159:LEU:HG	1.96	0.47
1:A:201:VAL:O	1:A:205:VAL:HG23	2.14	0.47
1:A:527:ASN:ND2	1:A:533:LYS:HG3	2.29	0.47
1:B:340:THR:HG21	1:B:350:PRO:HG3	1.97	0.47
1:A:230:GLU:HB2	4:A:914:HOH:O	2.14	0.46
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.98	0.46
1:A:187:MET:CE	1:A:292:THR:HG22	2.46	0.46
1:B:22:PRO:HG2	1:B:401:ARG:HG3	1.98	0.46
1:A:273:ASN:ND2	4:A:841:HOH:O	2.40	0.45
1:B:453:SER:H	1:B:563:SER:CB	2.28	0.45
1:B:182:LEU:C	1:B:182:LEU:HD23	2.42	0.45
1:A:105:ALA:O	1:A:109:ARG:HG3	2.17	0.45
1:A:86:GLU:H	1:A:86:GLU:CD	2.24	0.45
1:B:278:ARG:NH2	4:B:832:HOH:O	2.49	0.45
1:A:234:ARG:HG2	1:A:262:ILE:HD11	1.98	0.45
1:A:182:LEU:HD23	1:A:182:LEU:O	2.16	0.44
1:A:549:GLY:N	4:A:793:HOH:O	2.50	0.44
1:B:545:LEU:HB3	1:B:547:LEU:CD2	2.47	0.44
1:A:36[A]:MET:HE3	1:A:36[A]:MET:HB3	1.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:THR:HB	1:A:391:PRO:HD3	1.99	0.43
1:A:182:LEU:HD11	1:A:239:ILE:HG22	2.00	0.43
1:A:515:GLY:O	1:A:516:GLY:C	2.61	0.43
1:A:380:ARG:HD3	4:B:820:HOH:O	2.17	0.43
1:A:144:VAL:HB	1:A:394:ARG:HG2	2.00	0.43
1:B:512:LEU:C	1:B:514:GLN:N	2.74	0.43
1:B:336:LEU:HA	1:B:336:LEU:HD23	1.72	0.42
2:B:571:B5P:H11	2:B:571:B5P:H25	1.82	0.42
1:A:352:ASP:O	1:A:353:PRO:C	2.60	0.42
1:A:217:PHE:CE1	1:A:336:LEU:HD21	2.55	0.42
1:B:469:LEU:HD23	1:B:469:LEU:HA	1.83	0.42
1:A:22:PRO:HG2	1:A:401:ARG:HG3	2.02	0.42
1:A:182:LEU:C	1:A:182:LEU:CD2	2.91	0.42
1:B:83:LEU:HB2	1:B:173:MET:HA	2.02	0.42
1:A:137:THR:HA	1:A:267:THR:O	2.19	0.41
2:A:571:B5P:O1	2:A:571:B5P:N5	2.44	0.41
1:A:375:ASP:OD1	1:A:375:ASP:C	2.62	0.41
1:B:170:CYS:SG	1:B:173:MET:HE1	2.61	0.41
1:A:183:PRO:HG3	1:A:289:CYS:SG	2.60	0.41
1:A:505:ARG:HH11	1:A:505:ARG:HG2	1.85	0.41
1:A:95:HIS:HE1	4:A:968:HOH:O	2.04	0.40
1:B:187:MET:HE1	1:B:292:THR:HG22	2.02	0.40
1:B:43:ARG:NH2	4:B:587:HOH:O	2.41	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	553/576 (96%)	535 (97%)	16 (3%)	2 (0%)	30 22
1	B	559/576 (97%)	543 (97%)	15 (3%)	1 (0%)	43 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1112/1152 (96%)	1078 (97%)	31 (3%)	3 (0%)	36 29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	513	SER
1	A	513	SER
1	A	516	GLY

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	471/491 (96%)	451 (96%)	20 (4%)	26 19
1	B	475/491 (97%)	459 (97%)	16 (3%)	32 25
All	All	946/982 (96%)	910 (96%)	36 (4%)	29 21

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LEU
1	A	86	GLU
1	A	209	LYS
1	A	222	ARG
1	A	307	LYS
1	A	309	GLN
1	A	311	CYS
1	A	329	THR
1	A	347[A]	SER
1	A	347[B]	SER
1	A	372	VAL
1	A	381	VAL
1	A	437	GLU
1	A	439	LEU
1	A	440	GLU

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Mol	Chain	Res	Type
1	A	461	GLN
1	A	473	SER
1	A	476	SER
1	A	534	LEU
1	A	548	SER
1	B	14	CYS
1	B	74	LYS
1	B	83	LEU
1	B	112	SER
1	B	212	LYS
1	B	247	PRO
1	B	309	GLN
1	B	329	THR
1	B	381	VAL
1	B	437	GLU
1	B	440	GLU
1	B	473	SER
1	B	532	THR
1	B	543	SER
1	B	562	HIS
1	B	563	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	527	ASN
1	B	120	HIS
1	B	406	ASN
1	B	483	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	B5P	B	571	-	34,36,36	2.69	11 (32%)	45,56,56	2.57	20 (44%)
2	B5P	A	571	-	34,36,36	2.53	11 (32%)	45,56,56	2.26	17 (37%)
3	GOL	B	572	-	5,5,5	0.55	0	5,5,5	0.85	0
3	GOL	A	572	-	5,5,5	0.39	0	5,5,5	1.68	2 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B5P	B	571	-	-	0/10/29/29	0/4/4/4
2	B5P	A	571	-	-	0/10/29/29	0/4/4/4
3	GOL	B	572	-	-	2/4/4/4	-
3	GOL	A	572	-	-	4/4/4/4	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	571	B5P	C13-S1	-10.40	1.63	1.74
2	B	571	B5P	C13-S1	-9.58	1.64	1.74
2	B	571	B5P	C14-C13	5.58	1.49	1.40
2	B	571	B5P	C11-N3	4.57	1.36	1.30
2	A	571	B5P	C17-N6	-4.52	1.36	1.43
2	B	571	B5P	C17-N6	-4.38	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	571	B5P	C14-C13	3.36	1.46	1.40
2	B	571	B5P	C14-N5	-3.30	1.34	1.39
2	A	571	B5P	C12-N4	3.07	1.34	1.30
2	B	571	B5P	O1-C6	3.03	1.29	1.23
2	B	571	B5P	C9-N2	-3.02	1.34	1.39
2	A	571	B5P	C9-N2	-3.01	1.34	1.39
2	A	571	B5P	O4-S1	2.98	1.47	1.44
2	B	571	B5P	C18-S2	-2.95	1.68	1.75
2	A	571	B5P	C11-N2	-2.73	1.32	1.37
2	A	571	B5P	C18-S2	-2.61	1.69	1.75
2	B	571	B5P	C12-N4	2.44	1.33	1.30
2	A	571	B5P	C11-N3	2.27	1.33	1.30
2	B	571	B5P	C15-C14	2.26	1.43	1.39
2	B	571	B5P	C7-C6	2.22	1.49	1.44
2	A	571	B5P	C14-N5	-2.06	1.36	1.39
2	A	571	B5P	S2-N6	-2.03	1.60	1.63

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	571	B5P	O4-S1-N4	-5.79	101.44	108.95
2	B	571	B5P	O3-S1-O4	-5.25	109.55	115.90
2	B	571	B5P	O4-S1-C13	5.02	113.31	108.82
2	A	571	B5P	C13-S1-N4	4.95	112.27	105.10
2	B	571	B5P	O3-S1-C13	4.92	113.22	108.82
2	B	571	B5P	C19-C13-C14	-4.64	116.22	120.85
2	A	571	B5P	N2-C11-N3	-4.62	108.90	113.69
2	B	571	B5P	N2-C11-N3	-4.53	108.99	113.69
2	B	571	B5P	O5-S2-O6	-4.36	113.03	118.87
2	A	571	B5P	O3-S1-N4	4.29	114.53	108.95
2	B	571	B5P	C19-C13-S1	4.22	125.77	120.33
2	A	571	B5P	O4-S1-N4	-3.96	103.81	108.95
2	B	571	B5P	C11-N2-C8	-3.52	118.12	122.99
2	A	571	B5P	O2-C8-C7	-3.52	119.43	125.74
2	A	571	B5P	C10-N3-C11	3.48	107.63	103.27
2	A	571	B5P	C18-S2-N6	3.39	110.39	106.56
2	B	571	B5P	C16-C17-C19	3.38	123.74	119.66
2	B	571	B5P	C15-C14-C13	3.14	122.21	117.81
2	A	571	B5P	O3-S1-O4	-3.05	112.20	115.90
2	B	571	B5P	C13-C14-N5	-2.98	118.93	121.00
2	B	571	B5P	O2-C8-C7	-2.88	120.57	125.74
2	A	571	B5P	O1-C6-C7	-2.81	119.16	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	571	B5P	C19-C13-S1	2.76	123.89	120.33
2	A	571	B5P	O3-S1-C13	-2.70	106.40	108.82
2	A	571	B5P	C9-N2-C11	2.56	109.09	105.99
3	A	572	GOL	O1-C1-C2	-2.56	98.86	110.38
3	A	572	GOL	O2-C2-C1	-2.55	98.60	109.18
2	B	571	B5P	C9-N2-C11	2.54	109.06	105.99
2	A	571	B5P	O5-S2-C18	2.54	112.27	108.26
2	A	571	B5P	C11-N2-C8	-2.52	119.52	122.99
2	B	571	B5P	C13-S1-N4	2.51	108.74	105.10
2	A	571	B5P	C16-C17-N6	-2.41	114.94	120.02
2	B	571	B5P	C14-N5-C12	2.39	128.92	123.58
2	B	571	B5P	O5-S2-N6	2.34	111.78	107.10
2	B	571	B5P	C10-N3-C11	2.19	106.02	103.27
2	A	571	B5P	C9-C10-N3	-2.18	107.88	110.74
2	B	571	B5P	C16-C17-N6	-2.14	115.51	120.02
2	B	571	B5P	C18-S2-N6	2.11	108.94	106.56
2	A	571	B5P	C13-C14-N5	-2.02	119.59	121.00

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	572	GOL	O1-C1-C2-C3
3	A	572	GOL	C1-C2-C3-O3
3	B	572	GOL	C1-C2-C3-O3
3	A	572	GOL	O1-C1-C2-O2
3	A	572	GOL	O2-C2-C3-O3
3	B	572	GOL	O2-C2-C3-O3

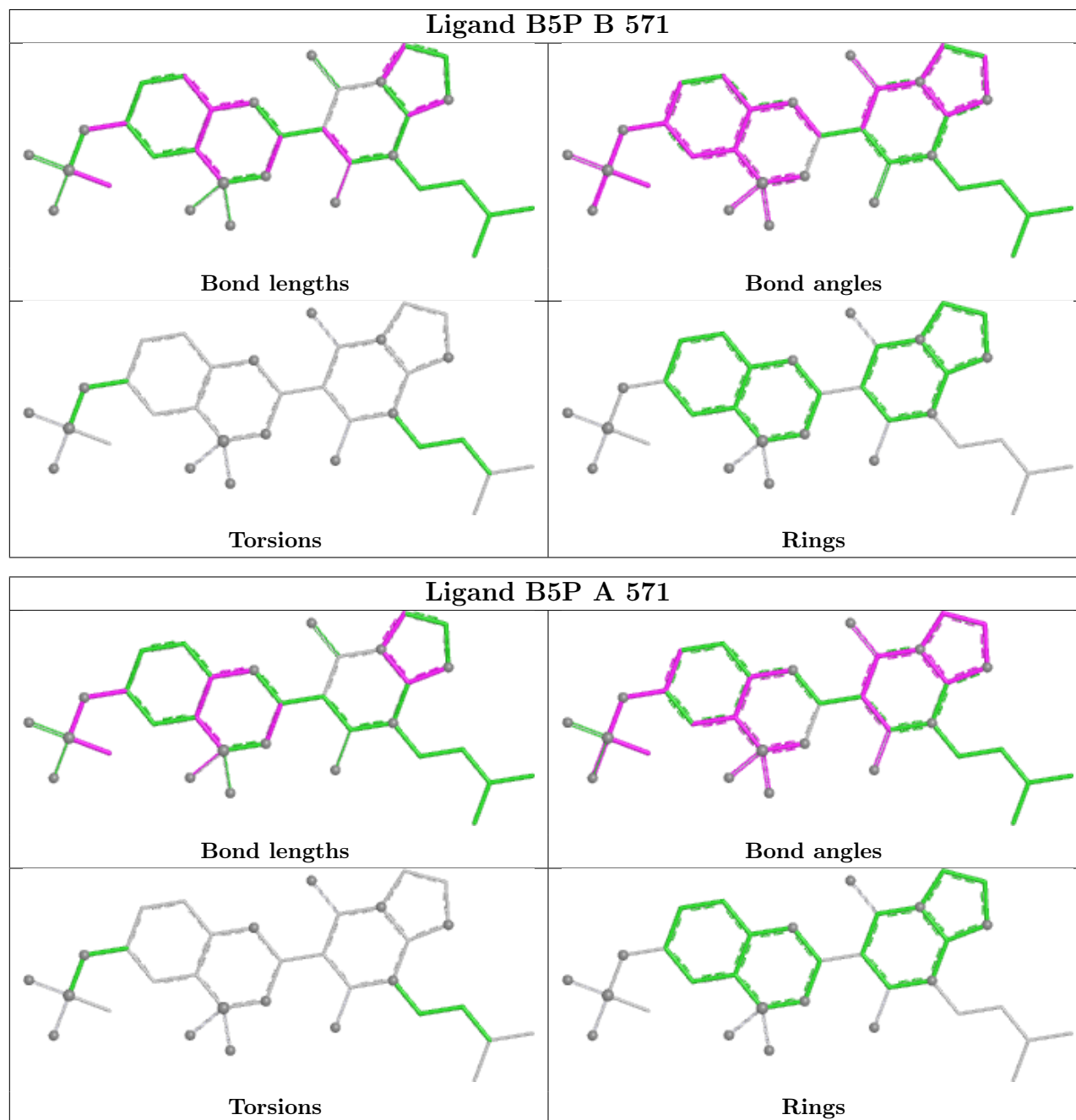
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	571	B5P	3	0
2	A	571	B5P	2	0
3	B	572	GOL	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 ⓘ

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(Å ²)	Q<0.9
1	A	551/576 (95%)	-0.02	13 (2%) 59 63	14, 23, 42, 55	8 (1%)
1	B	559/576 (97%)	0.08	19 (3%) 48 51	14, 25, 44, 74	6 (1%)
All	All	1110/1152 (96%)	0.03	32 (2%) 53 57	14, 24, 43, 74	14 (1%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	542	ALA	4.7
1	A	562	HIS	4.3
1	A	549	GLY	3.7
1	B	545	LEU	3.5
1	B	563	SER	3.5
1	B	534	LEU	3.3
1	A	534	LEU	3.2
1	A	550	TRP	3.2
1	B	547	LEU	3.2
1	B	153	GLY	3.1
1	A	15	ALA	3.0
1	B	548	SER	2.9
1	A	516	GLY	2.8
1	B	334	ALA	2.7
1	A	539	ILE	2.7
1	B	532	THR	2.6
1	B	549	GLY	2.5
1	B	540	PRO	2.5
1	A	310	ASP	2.3
1	B	377	SER	2.2
1	B	544	ARG	2.2
1	B	381	VAL	2.2
1	A	538	PRO	2.2
1	B	546	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	15	ALA	2.2
1	B	562	HIS	2.1
1	B	513	SER	2.1
1	A	153	GLY	2.1
1	A	14	CYS	2.0
1	B	550	TRP	2.0
1	A	513	SER	2.0
1	A	337	ARG	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](#)

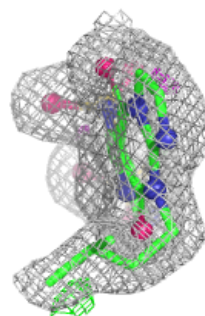
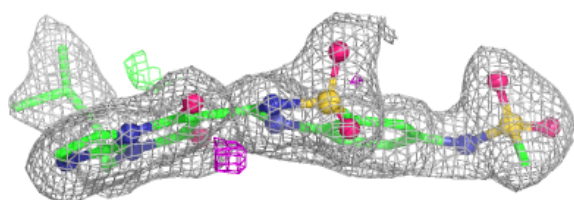
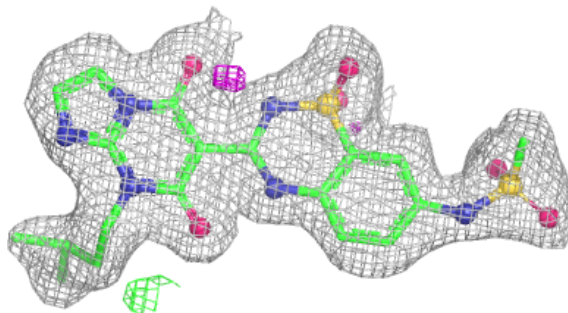
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	GOL	A	572	6/6	0.83	0.13	43,47,49,50	0
3	GOL	B	572	6/6	0.87	0.15	45,54,56,56	0
2	B5P	A	571	33/33	0.97	0.06	14,21,25,26	0
2	B5P	B	571	33/33	0.97	0.07	16,22,26,28	0

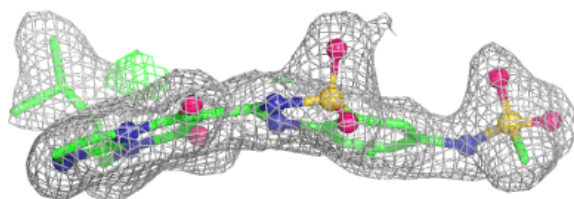
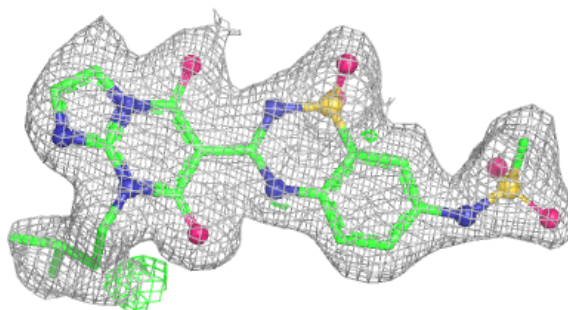
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around B5P A 571:

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

**Electron density around B5P B 571:**

$2mF_o-DF_c$ (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.