



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:48 PM UTC

PDB ID : 8A0C / pdb_00008a0c
Title : Capsular polysaccharide synthesis multienzyme in complex with CMP
Authors : Cifuentes, J.O.; Schulze, J.; Bethe, A.; Di Domenico, V.; Litschko, C.; Budde, I.; Eidenberger, L.; Thiesler, H.; Ramon-Roth, I.; Berger, M.; Claus, H.; D'Angelo, C.; Marina, A.; Gerardy-Schahn, R.; Schubert, M.; Guerin, M.E.; Fiebig, T.
Deposited on : 2022-05-27
Resolution : 2.90 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](#) ①) 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

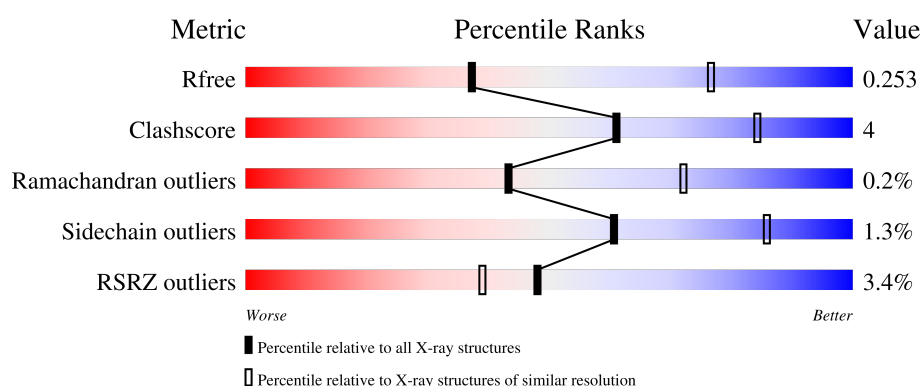
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	1173	2% 84% 10% 5%
1	B	1173	4% 84% 10% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36797 atoms, of which 17912 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.

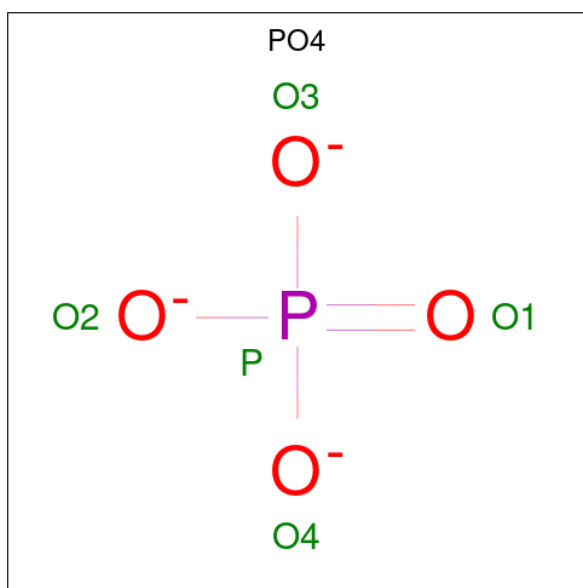
- Molecule 1 is a protein called Bcs3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1116	Total	C	H	N	O	S	0	0	0
			18195	5944	8982	1525	1716	28			
1	B	1113	Total	C	H	N	O	S	0	0	0
			18004	5887	8876	1513	1700	28			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q2ERG0
A	-1	PRO	-	expression tag	UNP Q2ERG0
A	0	VAL	-	expression tag	UNP Q2ERG0
A	1	ASP	-	expression tag	UNP Q2ERG0
A	1163	LEU	-	expression tag	UNP Q2ERG0
A	1164	GLU	-	expression tag	UNP Q2ERG0
A	1165	HIS	-	expression tag	UNP Q2ERG0
A	1166	HIS	-	expression tag	UNP Q2ERG0
A	1167	HIS	-	expression tag	UNP Q2ERG0
A	1168	HIS	-	expression tag	UNP Q2ERG0
A	1169	HIS	-	expression tag	UNP Q2ERG0
A	1170	HIS	-	expression tag	UNP Q2ERG0
B	-2	GLY	-	expression tag	UNP Q2ERG0
B	-1	PRO	-	expression tag	UNP Q2ERG0
B	0	VAL	-	expression tag	UNP Q2ERG0
B	1	ASP	-	expression tag	UNP Q2ERG0
B	1163	LEU	-	expression tag	UNP Q2ERG0
B	1164	GLU	-	expression tag	UNP Q2ERG0
B	1165	HIS	-	expression tag	UNP Q2ERG0
B	1166	HIS	-	expression tag	UNP Q2ERG0
B	1167	HIS	-	expression tag	UNP Q2ERG0
B	1168	HIS	-	expression tag	UNP Q2ERG0
B	1169	HIS	-	expression tag	UNP Q2ERG0
B	1170	HIS	-	expression tag	UNP Q2ERG0

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).

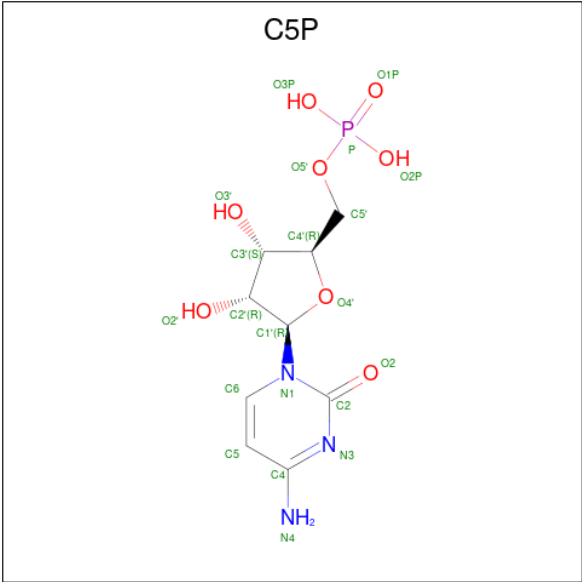


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			12	3	6	3		
3	A	1	Total	C	H	O	0	0
			13	3	7	3		
3	A	1	Total	C	H	O	0	0
			12	3	6	3		
3	B	1	Total	C	H	O	0	0
			13	3	7	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is CYTIDINE-5'-MONOPHOSPHATE (CCD ID: C5P) (formula: C₉H₁₄N₃O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	B	1	Total	C	H	N	O	P	0	0
			33	9	12	3	8	1		

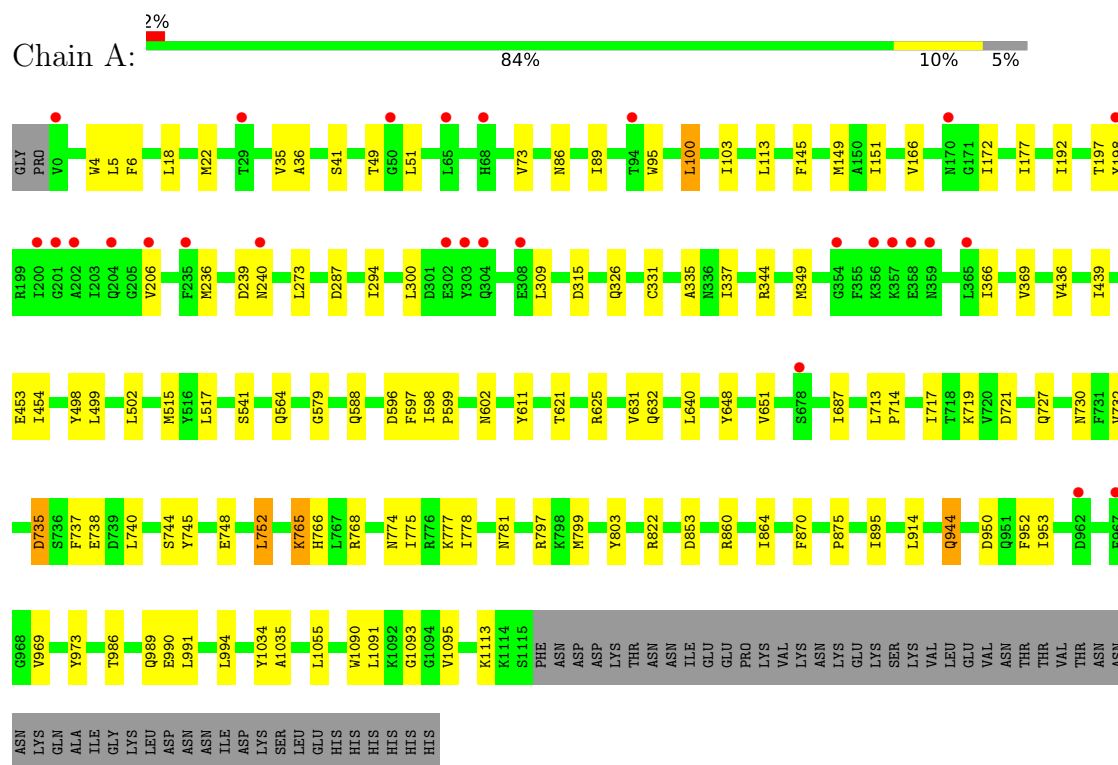
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	244	Total	O	0	0
			244	244		
6	B	196	Total	O	0	0
			196	196		

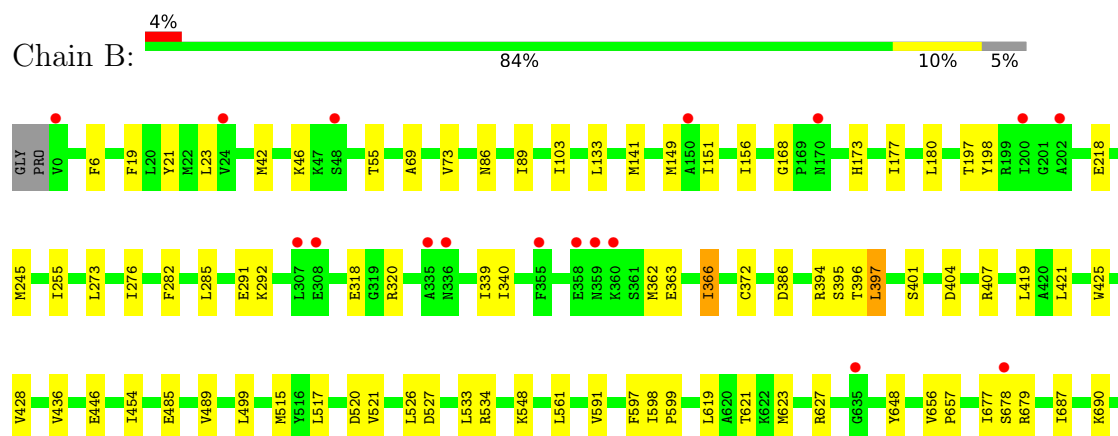
3 Residue-property plots [i](#)

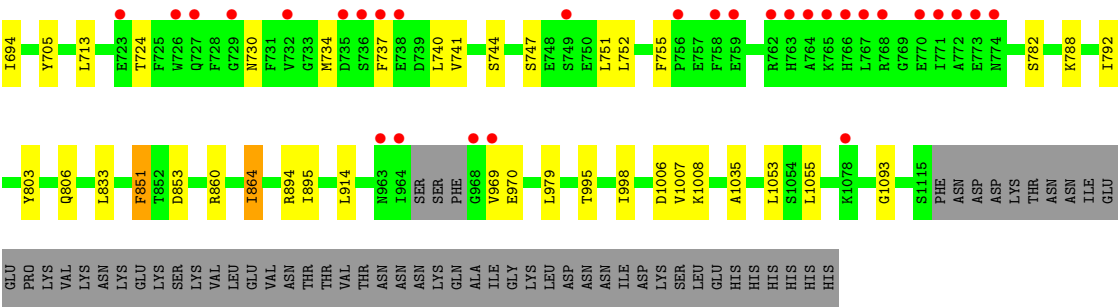
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Bcs3



• Molecule 1: Bcs3





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.97Å 164.78Å 302.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.40 – 2.90 57.40 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (57.40-2.90) 98.1 (57.40-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.197 , 0.256 0.194 , 0.253	Depositor DCC
R_{free} test set	1131 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	36797	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C5P, PO4, ZN, GOL

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	0.11	0/9446	0.27	0/12785
1	B	0.11	0/9355	0.27	0/12664
All	All	0.11	0/18801	0.27	0/25449

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	9213	8982	8997	74	0
1	B	9128	8876	8878	82	0
2	A	25	0	0	1	0
2	B	20	0	0	0	0
3	A	18	19	24	0	0
3	B	18	23	24	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	21	12	12	1	0
6	A	244	0	0	1	0
6	B	196	0	0	1	0
All	All	18885	17912	17935	154	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 4.

All (154) 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:527:ASP:OD2	1:B:534:ARG:NH2	2.19	0.75
1:A:4:TRP:CZ3	1:A:22:MET:HE1	2.23	0.74
1:B:86:ASN:OD1	1:B:89:ILE:N	2.21	0.73
1:A:287:ASP:HA	1:A:349:MET:HE1	1.73	0.71
1:A:799:MET:HG3	1:A:895:ILE:HD12	1.72	0.70
1:A:651:VAL:HG12	1:A:914:LEU:HD21	1.75	0.67
1:B:737:PHE:HZ	1:B:752:LEU:HD11	1.59	0.66
1:B:362:MET:O	1:B:366:ILE:HD12	1.96	0.66
1:A:853:ASP:O	1:A:860:ARG:NH1	2.30	0.65
1:A:166:VAL:HG13	1:A:172:ILE:HD13	1.79	0.64
1:A:145:PHE:HB3	1:A:149:MET:HE2	1.79	0.64
1:B:1006:ASP:OD1	1:B:1007:VAL:N	2.30	0.64
1:B:853:ASP:O	1:B:860:ARG:NH1	2.30	0.64
1:A:86:ASN:OD1	1:A:89:ILE:N	2.32	0.63
1:A:177:ILE:HD12	1:A:177:ILE:H	1.64	0.62
1:B:318:GLU:HG2	1:B:340:ILE:HD12	1.81	0.62
1:B:788:LYS:O	1:B:792:ILE:HD12	2.00	0.61
1:B:42:MET:HE2	1:B:46:LYS:HE3	1.83	0.61
1:B:515:MET:HE3	1:B:517:LEU:HG	1.82	0.60
1:B:291:GLU:HB3	1:B:339:ILE:HG23	1.83	0.60
1:B:526:LEU:HD22	1:B:533:LEU:HD13	1.82	0.60
1:A:192:ILE:HG12	1:A:273:LEU:HD23	1.82	0.60
1:A:315:ASP:O	1:A:344:ARG:NH2	2.34	0.60
1:B:396:THR:HG21	1:B:401:SER:CB	2.32	0.60
1:A:22:MET:HE2	1:A:366:ILE:HG12	1.83	0.59
1:B:724:THR:HG23	1:B:730:ASN:OD1	2.03	0.58
1:A:22:MET:HE2	1:A:366:ILE:CD1	2.33	0.57
1:A:611:TYR:CD2	1:B:419:LEU:HD21	2.39	0.57
1:B:42:MET:HE3	1:B:55:THR:HA	1.87	0.57
1:B:141:MET:HA	1:B:141:MET:HE2	1.86	0.57
1:A:18:LEU:HG	1:A:22:MET:HE3	1.87	0.56
1:A:1091:LEU:HD12	1:A:1095:VAL:HB	1.87	0.56
1:B:197:THR:HG23	5:B:1207:C5P:O3P	2.07	0.55
1:A:100:LEU:CD1	1:A:309:LEU:HD13	2.37	0.54
1:B:245:MET:HA	1:B:245:MET:HE2	1.88	0.54
1:B:969:VAL:HG22	1:B:970:GLU:H	1.73	0.54
1:A:864:ILE:HD11	1:A:870:PHE:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:LYS:HE2	1:B:694:ILE:HD11	1.89	0.54
1:B:741:VAL:HG12	1:B:751:LEU:HD23	1.87	0.54
1:B:397:LEU:HD22	1:B:597:PHE:CE1	2.43	0.54
1:B:687:ILE:HD11	1:B:914:LEU:HD22	1.90	0.54
1:A:273:LEU:HD21	1:A:294:ILE:HD12	1.90	0.53
1:B:177:ILE:H	1:B:177:ILE:HD12	1.74	0.53
1:B:19:PHE:CZ	1:B:23:LEU:HD11	2.45	0.53
1:B:168:GLY:O	1:B:173:HIS:NE2	2.41	0.52
1:B:282:PHE:HA	1:B:285:LEU:HD12	1.91	0.52
1:A:436:VAL:HG12	1:A:454:ILE:CG2	2.39	0.52
1:A:331:CYS:SG	1:A:337:ILE:HD11	2.49	0.52
1:B:395:SER:O	1:B:621:THR:HG21	2.10	0.51
1:B:69:ALA:O	1:B:86:ASN:ND2	2.43	0.51
1:B:619:LEU:HG	1:B:623:MET:HE3	1.92	0.51
1:A:765:LYS:O	1:A:766:HIS:ND1	2.44	0.51
1:B:397:LEU:HD22	1:B:597:PHE:CD1	2.45	0.51
1:A:439:ILE:HG23	1:B:851:PHE:O	2.10	0.51
1:A:986:THR:N	1:A:990:GLU:OE1	2.42	0.50
1:B:151:ILE:HD12	1:B:156:ILE:CD1	2.41	0.50
1:A:989:GLN:OE1	1:A:989:GLN:N	2.41	0.50
1:B:851:PHE:CD1	1:B:851:PHE:N	2.79	0.50
1:B:42:MET:HE2	1:B:46:LYS:CE	2.41	0.50
1:B:436:VAL:HG12	1:B:454:ILE:CG2	2.42	0.50
1:A:515:MET:HE3	1:A:517:LEU:CD1	2.42	0.50
1:B:803:TYR:HB2	1:B:895:ILE:HG21	1.92	0.50
1:A:717:ILE:HD13	1:A:797:ARG:NE	2.27	0.49
1:B:499:LEU:C	1:B:499:LEU:HD23	2.36	0.49
1:B:446:GLU:OE1	1:B:446:GLU:N	2.41	0.49
1:B:396:THR:HG22	1:B:397:LEU:N	2.26	0.49
1:B:436:VAL:HG12	1:B:454:ILE:HG21	1.95	0.49
1:B:520:ASP:OD1	1:B:521:VAL:N	2.46	0.48
1:A:22:MET:HE2	1:A:366:ILE:CG1	2.43	0.48
1:A:596:ASP:OD1	1:A:597:PHE:N	2.47	0.48
1:B:734:MET:CE	1:B:740:LEU:HD13	2.43	0.48
1:B:1053:LEU:HD23	1:B:1055:LEU:HD23	1.96	0.48
1:A:273:LEU:HD21	1:A:294:ILE:CD1	2.44	0.48
1:B:320:ARG:NH2	6:B:1311:HOH:O	2.46	0.48
1:B:995:THR:HG23	1:B:998:ILE:HD13	1.95	0.48
1:B:741:VAL:HG12	1:B:751:LEU:CD2	2.43	0.47
1:A:1055:LEU:HD11	1:A:1113:LYS:HE2	1.95	0.47
1:B:755:PHE:HE1	1:B:782:SER:HG	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:PHE:CE2	1:B:73:VAL:HG21	2.49	0.47
1:A:206:VAL:HB	1:A:236:MET:HE3	1.96	0.47
1:B:151:ILE:HD12	1:B:156:ILE:HD11	1.95	0.47
1:B:197:THR:HG22	1:B:198:TYR:N	2.30	0.47
1:B:273:LEU:HD12	1:B:292:LYS:O	2.15	0.47
1:B:421:LEU:CD1	1:B:428:VAL:HG11	2.45	0.47
1:B:180:LEU:HD12	1:B:180:LEU:N	2.30	0.47
1:B:276:ILE:HD13	1:B:282:PHE:CD1	2.50	0.47
1:A:803:TYR:HB2	1:A:895:ILE:HG21	1.97	0.47
1:A:499:LEU:HD23	1:A:499:LEU:C	2.40	0.46
1:A:300:LEU:HD23	1:A:300:LEU:O	2.15	0.46
1:A:498:TYR:CE2	1:A:502:LEU:HD11	2.50	0.46
1:A:822:ARG:N	2:A:1201:PO4:O2	2.46	0.46
1:A:719:LYS:NZ	1:A:721:ASP:OD1	2.45	0.46
1:A:737:PHE:HZ	1:A:752:LEU:HD21	1.81	0.46
1:A:744:SER:O	1:A:745:TYR:HB2	2.15	0.46
1:A:598:ILE:HB	1:A:599:PRO:CD	2.46	0.46
1:B:713:LEU:HD21	1:B:792:ILE:HG22	1.97	0.46
1:B:404:ASP:OD1	1:B:407:ARG:NH1	2.43	0.46
1:A:632:GLN:HB3	1:A:1090:TRP:CE2	2.52	0.45
1:A:239:ASP:OD1	1:A:240:ASN:N	2.50	0.45
1:A:687:ILE:HD11	1:A:914:LEU:HD22	1.99	0.45
1:A:4:TRP:CH2	1:A:369:VAL:HG11	2.52	0.44
1:B:656:VAL:HB	1:B:657:PRO:HD3	1.99	0.44
1:B:677:ILE:HG22	1:B:678:SER:N	2.32	0.44
1:A:515:MET:HE3	1:A:517:LEU:HG	2.00	0.44
1:A:735:ASP:OD1	1:A:768:ARG:NH1	2.50	0.44
1:B:103:ILE:CD1	1:B:149:MET:HE3	2.47	0.44
1:B:741:VAL:O	1:B:744:SER:OG	2.34	0.44
1:A:6:PHE:CE2	1:A:73:VAL:HG21	2.52	0.44
1:B:678:SER:HB2	1:B:705:TYR:HA	2.00	0.44
1:A:149:MET:CE	1:A:151:ILE:HD13	2.47	0.44
1:B:979:LEU:HD12	1:B:1008:LYS:HE3	1.99	0.44
1:A:36:ALA:HB1	1:A:41:SER:HB2	1.99	0.43
1:A:86:ASN:OD1	1:A:86:ASN:C	2.61	0.43
1:A:331:CYS:O	1:A:335:ALA:HB3	2.18	0.43
1:B:394:ARG:HB2	1:B:396:THR:O	2.18	0.43
1:B:598:ILE:HB	1:B:599:PRO:CD	2.48	0.43
1:B:864:ILE:O	1:B:864:ILE:HG13	2.18	0.43
1:A:453:GLU:OE2	1:A:541:SER:OG	2.34	0.43
1:A:713:LEU:HB3	1:A:714:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:GLN:O	1:A:732:VAL:HG21	2.18	0.43
1:A:149:MET:HE3	1:A:151:ILE:HD13	2.00	0.43
1:A:944:GLN:HG3	1:A:953:ILE:HD11	2.01	0.43
1:A:991:LEU:HA	1:A:994:LEU:HD23	2.01	0.42
1:B:218:GLU:HB2	1:B:255:ILE:HD12	2.01	0.42
1:B:485:GLU:O	1:B:489:VAL:HG23	2.19	0.42
1:B:737:PHE:CZ	1:B:752:LEU:HD11	2.48	0.42
1:A:49:THR:CB	1:A:51:LEU:HD12	2.49	0.42
1:A:631:VAL:HG21	1:A:1034:TYR:CE2	2.55	0.42
1:A:719:LYS:NZ	6:A:1316:HOH:O	2.47	0.42
1:A:740:LEU:HD11	1:A:775:ILE:HG21	2.02	0.42
1:B:86:ASN:OD1	1:B:86:ASN:C	2.62	0.42
1:B:1035:ALA:N	1:B:1093:GLY:O	2.53	0.42
1:B:339:ILE:H	1:B:339:ILE:HD12	1.85	0.42
1:B:734:MET:HE3	1:B:740:LEU:HB2	2.01	0.42
1:A:49:THR:HB	1:A:51:LEU:HD12	2.02	0.42
1:B:133:LEU:HD22	1:B:133:LEU:N	2.34	0.42
1:B:21:TYR:OH	1:B:363:GLU:OE2	2.37	0.41
1:B:421:LEU:HD11	1:B:425:TRP:HZ3	1.85	0.41
1:A:436:VAL:HG12	1:A:454:ILE:HG21	2.02	0.41
1:B:747:SER:O	1:B:751:LEU:N	2.52	0.41
1:A:4:TRP:CE3	1:A:22:MET:HE1	2.54	0.41
1:A:598:ILE:HB	1:A:599:PRO:HD2	2.02	0.41
1:A:621:THR:O	1:A:625:ARG:HG2	2.21	0.41
1:A:950:ASP:OD1	1:A:952:PHE:N	2.50	0.41
1:B:386:ASP:OD1	1:B:548:LYS:NZ	2.52	0.41
1:B:598:ILE:HG23	1:B:627:ARG:NH2	2.36	0.41
1:A:777:LYS:O	1:A:781:ASN:ND2	2.46	0.41
1:A:875:PRO:HG3	1:A:973:TYR:CD1	2.57	0.41
1:B:969:VAL:HG22	1:B:970:GLU:N	2.36	0.40
1:A:5:LEU:HD23	1:A:35:VAL:CG2	2.51	0.40
1:A:774:ASN:O	1:A:778:ILE:HG12	2.21	0.40
1:A:1035:ALA:N	1:A:1093:GLY:O	2.54	0.40
1:B:197:THR:HG22	1:B:198:TYR:H	1.87	0.40
1:A:197:THR:HG22	1:A:198:TYR:H	1.86	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	1114/1173 (95%)	1062 (95%)	49 (4%)	3 (0%)	36	65
1	B	1109/1173 (94%)	1056 (95%)	51 (5%)	2 (0%)	43	72
All	All	2223/2346 (95%)	2118 (95%)	100 (4%)	5 (0%)	43	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	648	TYR
1	B	648	TYR
1	B	679	ARG
1	A	95	TRP
1	A	579	GLY

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	998/1063 (94%)	982 (98%)	16 (2%)	55	83
1	B	979/1063 (92%)	969 (99%)	10 (1%)	68	89
All	All	1977/2126 (93%)	1951 (99%)	26 (1%)	61	86

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU

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Mol	Chain	Res	Type
1	A	103	ILE
1	A	113	LEU
1	A	326	GLN
1	A	564	GLN
1	A	588	GLN
1	A	602	ASN
1	A	640	LEU
1	A	730	ASN
1	A	735	ASP
1	A	738	GLU
1	A	748	GLU
1	A	752	LEU
1	A	765	LYS
1	A	944	GLN
1	A	969	VAL
1	B	366	ILE
1	B	372	CYS
1	B	397	LEU
1	B	561	LEU
1	B	591	VAL
1	B	806	GLN
1	B	833	LEU
1	B	851	PHE
1	B	864	ILE
1	B	894	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	144	HIS
1	A	164	ASN
1	A	223	HIS
1	A	334	ASN
1	A	493	GLN
1	A	547	GLN
1	A	632	GLN
1	A	786	HIS
1	A	1037	ASN
1	A	1081	ASN
1	B	68	HIS
1	B	124	ASN

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Mol	Chain	Res	Type
1	B	187	GLN
1	B	448	GLN
1	B	1102	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 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\# Z > 2$
3	GOL	A	1207	-	5,5,5	0.96	0	5,5,5	1.03	0
2	PO4	B	1204	-	4,4,4	0.98	0	6,6,6	0.45	0
2	PO4	A	1202	-	4,4,4	0.96	0	6,6,6	0.45	0
3	GOL	A	1206	-	5,5,5	0.87	0	5,5,5	1.08	0
3	GOL	B	1206	-	5,5,5	0.87	0	5,5,5	1.04	0
2	PO4	A	1203	4	4,4,4	0.93	0	6,6,6	0.50	0
5	C5P	B	1207	-	22,22,22	2.91	8 (36%)	32,33,33	0.70	0
2	PO4	B	1203	4	4,4,4	0.95	0	6,6,6	0.45	0
2	PO4	A	1201	-	4,4,4	0.97	0	6,6,6	0.47	0
2	PO4	B	1202	-	4,4,4	0.95	0	6,6,6	0.46	0
3	GOL	B	1201	-	5,5,5	0.92	0	5,5,5	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	A	1205	-	4,4,4	0.96	0	6,6,6	0.46	0
2	PO4	B	1205	-	4,4,4	0.95	0	6,6,6	0.46	0
2	PO4	A	1204	-	4,4,4	0.95	0	6,6,6	0.45	0
3	GOL	B	1209	-	5,5,5	0.89	0	5,5,5	1.14	1 (20%)
3	GOL	A	1208	-	5,5,5	0.87	0	5,5,5	1.01	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	GOL	A	1207	-	-	0/4/4/4	-
3	GOL	B	1206	-	-	0/4/4/4	-
3	GOL	A	1206	-	-	2/4/4/4	-
5	C5P	B	1207	-	-	0/10/26/26	0/2/2/2
3	GOL	B	1201	-	-	0/4/4/4	-
3	GOL	B	1209	-	-	0/4/4/4	-
3	GOL	A	1208	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1207	C5P	C2-N3	6.61	1.49	1.36
5	B	1207	C5P	C6-C5	6.17	1.49	1.35
5	B	1207	C5P	C4-N3	5.48	1.45	1.34
5	B	1207	C5P	C4-N4	5.09	1.46	1.33
5	B	1207	C5P	C2-N1	4.49	1.49	1.40
5	B	1207	C5P	C6-N1	3.29	1.45	1.38
5	B	1207	C5P	C5-C4	2.82	1.49	1.42
5	B	1207	C5P	O2-C2	-2.64	1.18	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1209	GOL	C3-C2-C1	-2.08	104.16	111.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

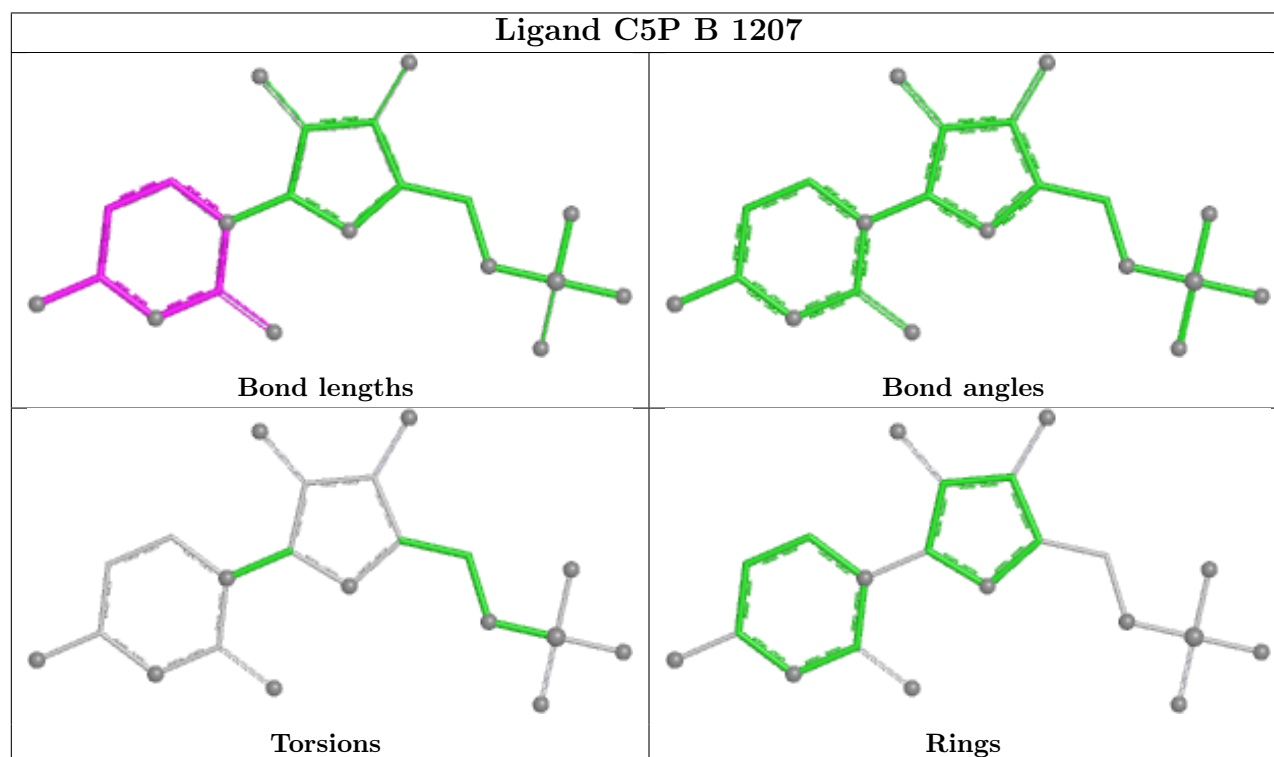
Mol	Chain	Res	Type	Atoms
3	A	1206	GOL	O1-C1-C2-C3
3	A	1206	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1207	C5P	1	0
2	A	1201	PO4	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	1116/1173 (95%)	0.15	28 (2%) 58 48	15, 41, 79, 106	0
1	B	1113/1173 (94%)	0.33	47 (4%) 40 32	21, 46, 87, 113	0
All	All	2229/2346 (95%)	0.24	75 (3%) 48 39	15, 44, 83, 113	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	304	GLN	5.0
1	A	302	GLU	4.8
1	B	738	GLU	4.7
1	B	360	LYS	4.6
1	B	763	HIS	4.5
1	B	770	GLU	4.2
1	B	736	SER	4.1
1	B	359	ASN	4.0
1	B	762	ARG	3.9
1	B	735	ASP	3.8
1	B	968	GLY	3.8
1	B	771	ILE	3.7
1	B	963	ASN	3.7
1	B	358	GLU	3.7
1	B	964	ILE	3.6
1	B	767	LEU	3.5
1	B	726	TRP	3.5
1	B	758	PHE	3.4
1	B	732	VAL	3.3
1	B	24	VAL	3.3
1	B	759	GLU	3.2
1	B	756	PRO	3.2
1	B	969	VAL	3.1
1	A	358	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	774	ASN	3.1
1	A	308	GLU	3.1
1	A	303	TYR	3.0
1	A	359	ASN	3.0
1	B	202	ALA	2.9
1	A	200	ILE	2.9
1	B	0	VAL	2.8
1	B	170	ASN	2.8
1	B	764	ALA	2.8
1	B	307	LEU	2.7
1	A	198	TYR	2.6
1	B	768	ARG	2.6
1	A	50	GLY	2.6
1	A	235	PHE	2.6
1	A	94	THR	2.5
1	A	204	GLN	2.5
1	B	765	LYS	2.5
1	B	355	PHE	2.5
1	B	727	GLN	2.5
1	B	336	ASN	2.5
1	B	773	GLU	2.4
1	A	678	SER	2.4
1	A	206	VAL	2.4
1	B	1078	LYS	2.4
1	A	356	LYS	2.3
1	B	635	GLY	2.3
1	A	29	THR	2.3
1	B	48	SER	2.3
1	B	678	SER	2.2
1	B	749	SER	2.2
1	B	308	GLU	2.2
1	A	967	PHE	2.2
1	A	202	ALA	2.2
1	A	365	LEU	2.2
1	A	201	GLY	2.2
1	A	962	ASP	2.2
1	A	65	LEU	2.2
1	B	335	ALA	2.2
1	A	240	ASN	2.1
1	B	766	HIS	2.1
1	A	0	VAL	2.1
1	B	737	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	772	ALA	2.1
1	B	200	ILE	2.1
1	A	354	GLY	2.1
1	B	723	GLU	2.1
1	A	170	ASN	2.1
1	B	729	GLY	2.1
1	A	357	LYS	2.0
1	A	68	HIS	2.0
1	B	150	ALA	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.

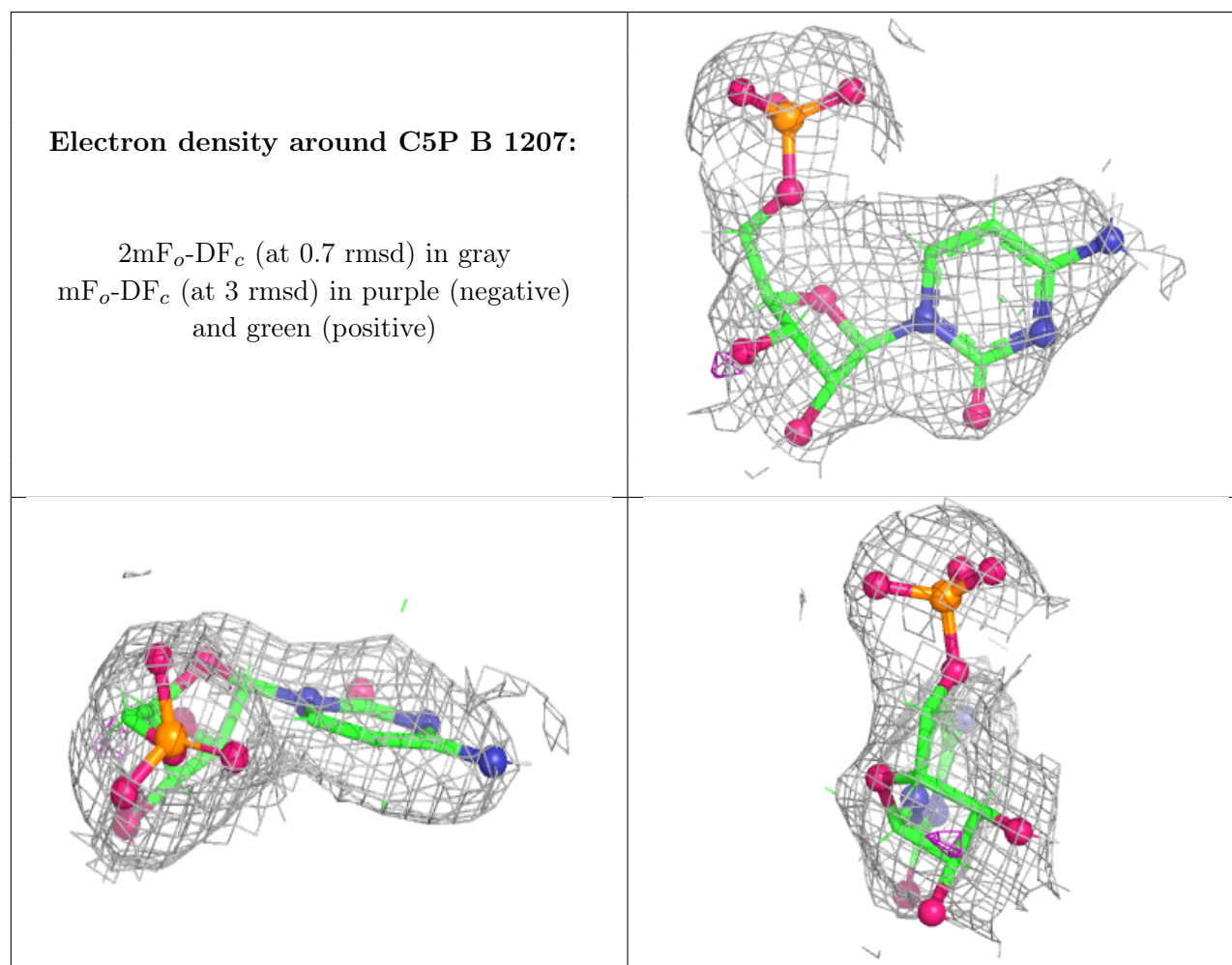
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	1206	6/6	0.79	0.19	56,68,76,81	0
2	PO4	A	1205	5/5	0.80	0.14	62,71,90,97	0
3	GOL	A	1208	6/6	0.82	0.17	35,53,64,64	0
2	PO4	B	1202	5/5	0.82	0.17	57,64,74,77	0
3	GOL	B	1209	6/6	0.84	0.15	40,50,60,61	0
2	PO4	A	1204	5/5	0.87	0.12	42,46,61,70	0
2	PO4	B	1205	5/5	0.88	0.12	50,57,61,68	0
3	GOL	A	1206	6/6	0.89	0.12	38,46,55,55	0
2	PO4	A	1202	5/5	0.90	0.12	55,56,65,69	0
3	GOL	B	1201	6/6	0.90	0.13	37,45,53,54	0
5	C5P	B	1207	21/21	0.90	0.13	46,59,73,76	0
3	GOL	A	1207	6/6	0.94	0.10	25,36,46,55	0
2	PO4	A	1203	5/5	0.96	0.07	24,29,31,36	0
2	PO4	A	1201	5/5	0.97	0.07	31,36,43,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	B	1204	5/5	0.97	0.09	28,39,47,47	0
4	ZN	A	1209	1/1	0.98	0.07	58,58,58,58	0
2	PO4	B	1203	5/5	0.98	0.05	28,29,36,40	0
4	ZN	B	1208	1/1	1.00	0.02	53,53,53,53	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 ⓘ

There are no such residues in this entry.