



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 10:50 PM UTC

PDB ID : 4XC7 / pdb_00004xc7
Title : Isobutyryl-CoA mutase fused with bound butyryl-CoA and without cobalamin or GDP (apo-IcmF)
Authors : Jost, M.; Drennan, C.L.
Deposited on : 2014-12-17
Resolution : 3.45 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

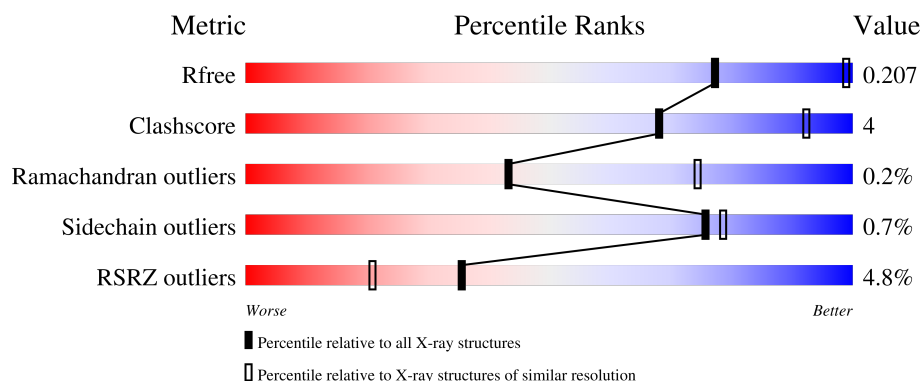
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	1113	6% 85% 9% 5%
1	B	1113	3% 86% 10% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16179 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 Isobutyryl-CoA mutase fused.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1053	Total	C	N	O	S	0	0	0
			7951	4974	1413	1528	36			
1	B	1063	Total	C	N	O	S	0	0	0
			8128	5075	1455	1562	36			

There are 40 discrepancies between the modelled and reference sequences:

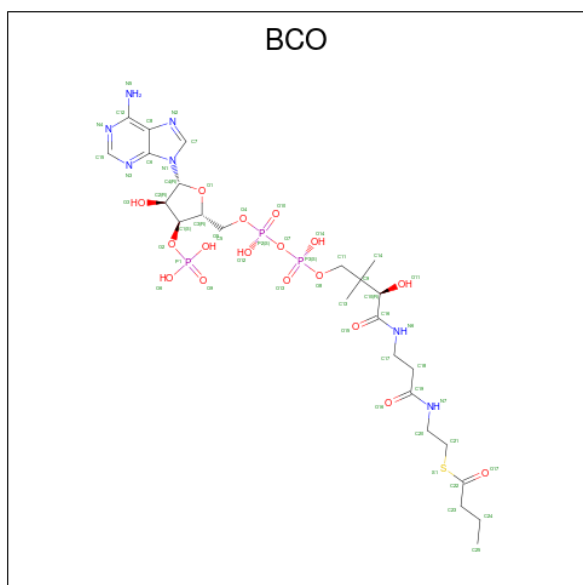
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q1LRY0
A	-18	GLY	-	expression tag	UNP Q1LRY0
A	-17	SER	-	expression tag	UNP Q1LRY0
A	-16	SER	-	expression tag	UNP Q1LRY0
A	-15	HIS	-	expression tag	UNP Q1LRY0
A	-14	HIS	-	expression tag	UNP Q1LRY0
A	-13	HIS	-	expression tag	UNP Q1LRY0
A	-12	HIS	-	expression tag	UNP Q1LRY0
A	-11	HIS	-	expression tag	UNP Q1LRY0
A	-10	HIS	-	expression tag	UNP Q1LRY0
A	-9	SER	-	expression tag	UNP Q1LRY0
A	-8	SER	-	expression tag	UNP Q1LRY0
A	-7	GLY	-	expression tag	UNP Q1LRY0
A	-6	LEU	-	expression tag	UNP Q1LRY0
A	-5	VAL	-	expression tag	UNP Q1LRY0
A	-4	PRO	-	expression tag	UNP Q1LRY0
A	-3	ARG	-	expression tag	UNP Q1LRY0
A	-2	GLY	-	expression tag	UNP Q1LRY0
A	-1	SER	-	expression tag	UNP Q1LRY0
A	0	HIS	-	expression tag	UNP Q1LRY0
B	-19	MET	-	initiating methionine	UNP Q1LRY0
B	-18	GLY	-	expression tag	UNP Q1LRY0
B	-17	SER	-	expression tag	UNP Q1LRY0
B	-16	SER	-	expression tag	UNP Q1LRY0
B	-15	HIS	-	expression tag	UNP Q1LRY0

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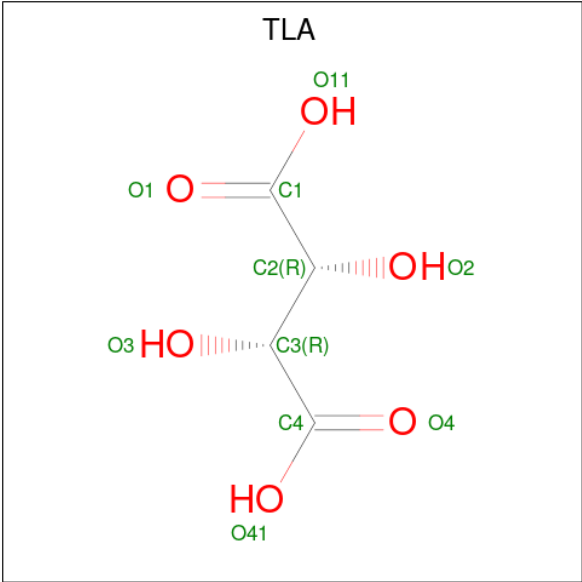
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q1LRY0
B	-13	HIS	-	expression tag	UNP Q1LRY0
B	-12	HIS	-	expression tag	UNP Q1LRY0
B	-11	HIS	-	expression tag	UNP Q1LRY0
B	-10	HIS	-	expression tag	UNP Q1LRY0
B	-9	SER	-	expression tag	UNP Q1LRY0
B	-8	SER	-	expression tag	UNP Q1LRY0
B	-7	GLY	-	expression tag	UNP Q1LRY0
B	-6	LEU	-	expression tag	UNP Q1LRY0
B	-5	VAL	-	expression tag	UNP Q1LRY0
B	-4	PRO	-	expression tag	UNP Q1LRY0
B	-3	ARG	-	expression tag	UNP Q1LRY0
B	-2	GLY	-	expression tag	UNP Q1LRY0
B	-1	SER	-	expression tag	UNP Q1LRY0
B	0	HIS	-	expression tag	UNP Q1LRY0

- Molecule 2 is Butyryl Coenzyme A (CCD ID: BCO) (formula: $C_{25}H_{42}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		
2	B	1	Total	C	N	O	P		0	0
			27	10	5	10	2			

- Molecule 3 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: $C_4H_6O_6$).

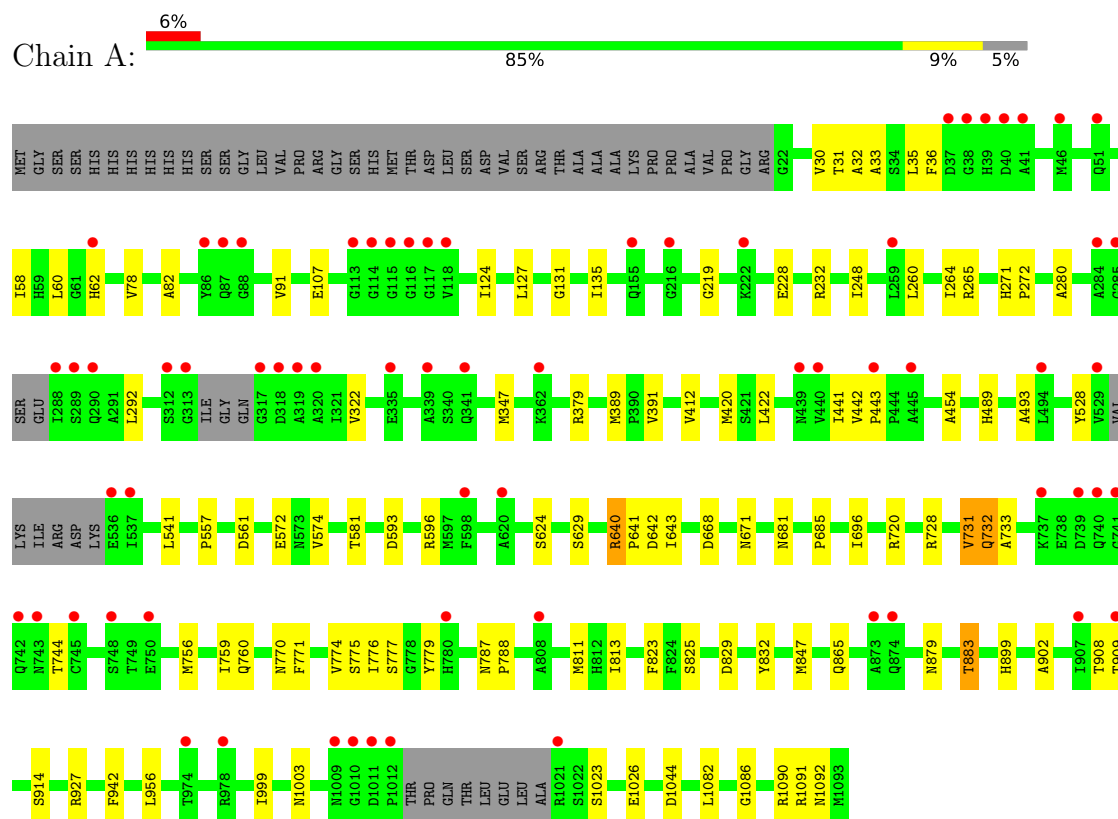


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		

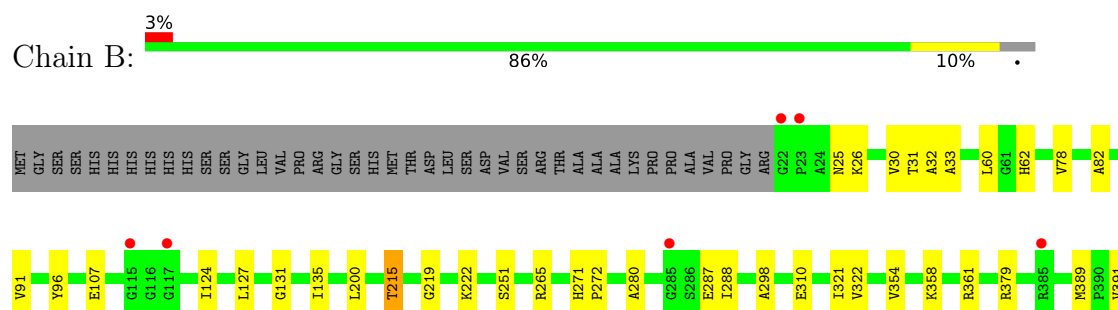
3 Residue-property plots [i](#)

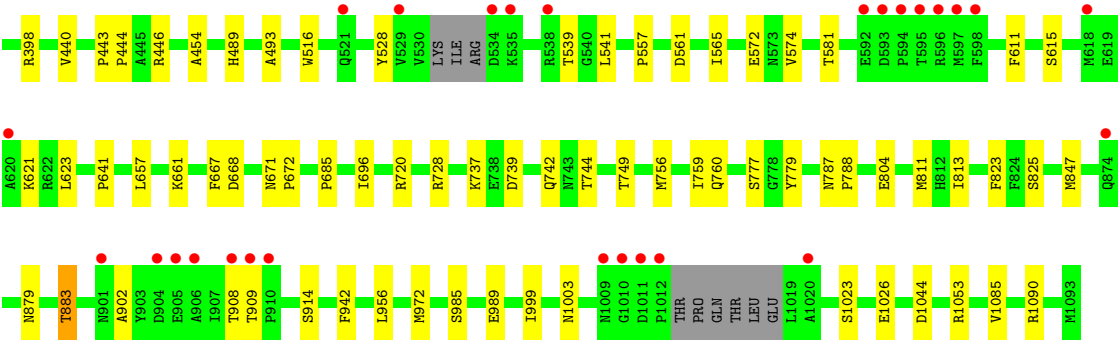
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Isobutyryl-CoA mutase fused





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	318.18Å 318.18Å 344.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	91.85 – 3.45 91.85 – 3.45	Depositor EDS
% Data completeness (in resolution range)	95.7 (91.85-3.45) 95.7 (91.85-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1760)	Depositor
R, R_{free}	0.186 , 0.203 0.192 , 0.207	Depositor DCC
R_{free} test set	4218 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	92.7	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 82.7	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	16179	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.28	0/8091	0.70	2/10968 (0.0%)
1	B	0.28	0/8270	0.69	1/11199 (0.0%)
All	All	0.28	0/16361	0.70	3/22167 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	VAL	CB-CA-C	-5.88	108.12	114.35
1	A	640	ARG	CA-C-N	5.54	125.63	119.32
1	A	640	ARG	C-N-CA	5.54	125.63	119.32

There are no chirality outliers.

There are no planarity outliers.

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	7951	0	7616	61	0
1	B	8128	0	7885	59	0
2	A	53	0	40	1	0
2	B	27	0	13	0	0
3	A	10	0	4	1	0
3	B	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16179	0	15562	115	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 (115) 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:1053:ARG:HG2	1:B:1085:VAL:HB	1.72	0.72
1:B:760:GLN:HG3	1:B:811:MET:HE1	1.74	0.70
1:A:732:GLN:HA	1:A:775:SER:HB3	1.75	0.68
1:A:420:MET:HE2	1:A:422:LEU:HD21	1.80	0.63
1:A:248:ILE:HD11	1:A:292:LEU:HD13	1.80	0.63
1:A:561:ASP:HB2	1:B:561:ASP:HB2	1.82	0.62
1:A:777:SER:HA	1:A:823:PHE:HB3	1.80	0.62
1:A:728:ARG:NH2	2:A:1101:BCO:O14	2.33	0.61
1:A:731:VAL:HG12	1:A:771:PHE:HE1	1.67	0.60
1:B:615:SER:O	1:B:621:LYS:NZ	2.35	0.60
1:B:454:ALA:HA	1:B:956:LEU:HD22	1.84	0.59
1:A:30:VAL:HG23	1:A:78:VAL:HG11	1.86	0.57
1:A:696:ILE:HD13	1:A:720:ARG:HG3	1.87	0.57
1:B:30:VAL:HG23	1:B:78:VAL:HG11	1.87	0.57
1:A:31:THR:HG22	1:A:82:ALA:HB3	1.88	0.56
1:B:696:ILE:HD13	1:B:720:ARG:HG3	1.87	0.56
1:B:879:ASN:O	1:B:883:THR:OG1	2.25	0.55
1:B:742:GLN:HB3	1:B:744:THR:OG1	2.07	0.54
1:A:260:LEU:HD21	1:A:280:ALA:HB2	1.90	0.54
1:B:31:THR:HG22	1:B:82:ALA:HB3	1.89	0.53
1:A:908:THR:OG1	1:A:909:THR:N	2.42	0.53
1:B:685:PRO:HB3	1:B:759:ILE:HD11	1.91	0.52
1:A:454:ALA:HA	1:A:956:LEU:HD22	1.92	0.52
1:A:787:ASN:HB2	1:A:788:PRO:HD2	1.93	0.51
1:A:685:PRO:HB3	1:A:759:ILE:HD11	1.92	0.51
1:A:58:ILE:HG13	1:A:260:LEU:HD12	1.92	0.51
1:B:999:ILE:N	1:B:1003:ASN:OD1	2.42	0.51
1:A:572:GLU:HG2	1:A:581:THR:HG21	1.94	0.50
1:A:36:PHE:HE2	1:A:643:ILE:HG23	1.77	0.50
1:B:787:ASN:HB2	1:B:788:PRO:HD2	1.92	0.50
1:A:1082:LEU:O	1:A:1086:GLY:N	2.44	0.49
1:B:572:GLU:HG2	1:B:581:THR:HG21	1.93	0.49
1:A:999:ILE:N	1:A:1003:ASN:OD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ALA:HB3	1:B:62:HIS:HA	1.94	0.48
1:A:33:ALA:HB3	1:A:62:HIS:HA	1.94	0.48
1:A:35:LEU:HD22	1:A:642:ASP:HB3	1.95	0.48
1:B:777:SER:HA	1:B:823:PHE:HB3	1.96	0.47
1:B:26:LYS:HD3	1:B:26:LYS:HA	1.82	0.47
1:A:942:PHE:CZ	1:B:557:PRO:HB3	2.49	0.47
1:B:908:THR:OG1	1:B:909:THR:N	2.47	0.47
1:A:902:ALA:HB1	1:A:914:SER:OG	2.14	0.47
1:A:1023:SER:HB3	1:A:1026:GLU:HG3	1.96	0.47
1:B:215:THR:HB	1:B:321:ILE:HG21	1.96	0.47
1:B:672:PRO:O	1:B:728:ARG:NH2	2.45	0.47
1:B:737:LYS:HD3	1:B:777:SER:HB3	1.97	0.46
1:B:1023:SER:HB3	1:B:1026:GLU:HG3	1.97	0.46
1:A:813:ILE:HD11	1:A:847:MET:HE1	1.98	0.46
1:A:322:VAL:HG22	1:A:347:MET:HE1	1.98	0.45
1:A:760:GLN:HG3	1:A:811:MET:HE1	1.99	0.45
1:A:557:PRO:HB3	1:B:942:PHE:CZ	2.52	0.45
1:A:36:PHE:HB3	1:A:629:SER:HB2	1.99	0.45
1:A:228:GLU:OE1	1:A:232:ARG:NH2	2.50	0.45
1:A:264:ILE:HG12	1:A:1091:ARG:HB2	1.98	0.45
1:A:412:VAL:HG13	1:A:422:LEU:HD13	1.99	0.45
1:B:446:ARG:NH2	1:B:804:GLU:OE2	2.50	0.44
1:B:32:ALA:HB2	1:B:60:LEU:HB2	1.99	0.44
1:B:379:ARG:HD2	1:B:389:MET:HE1	1.99	0.44
1:B:739:ASP:HB3	1:B:972:MET:HE3	2.00	0.44
1:A:681:ASN:HA	1:A:733:ALA:HA	1.98	0.43
1:A:879:ASN:O	1:A:883:THR:OG1	2.30	0.43
1:A:640:ARG:NH2	1:A:642:ASP:OD2	2.51	0.43
1:B:611:PHE:CD1	1:B:623:LEU:HD22	2.53	0.43
1:B:287:GLU:HG2	1:B:288:ILE:HG23	2.01	0.43
1:A:379:ARG:HD2	1:A:389:MET:HE1	2.00	0.43
1:B:398:ARG:NH1	1:B:440:VAL:HA	2.34	0.43
1:B:96:TYR:HB2	1:B:641:PRO:HB2	2.00	0.43
1:B:358:LYS:O	1:B:361:ARG:HG2	2.19	0.43
1:B:443:PRO:HA	1:B:444:PRO:HD3	1.85	0.43
1:A:32:ALA:HB2	1:A:60:LEU:HB2	2.00	0.42
1:A:596:ARG:HG2	1:A:624:SER:HB2	2.00	0.42
1:A:528:TYR:HB2	1:A:541:LEU:HD21	2.02	0.42
1:B:902:ALA:HB1	1:B:914:SER:OG	2.19	0.42
1:A:1044:ASP:OD1	1:A:1044:ASP:N	2.53	0.42
1:B:749:THR:HG21	1:B:972:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:779:TYR:CD1	1:B:825:SER:HB2	2.55	0.42
1:A:489:HIS:CE1	1:B:493:ALA:HB1	2.55	0.41
1:A:668:ASP:HB3	1:A:671:ASN:HB2	2.02	0.41
1:B:265:ARG:HE	1:B:1090:ARG:HD3	1.83	0.41
1:B:107:GLU:H	1:B:107:GLU:CD	2.27	0.41
1:B:219:GLY:O	1:B:358:LYS:NZ	2.46	0.41
1:A:728:ARG:HG2	1:A:770:ASN:HB3	2.02	0.41
1:B:528:TYR:HB2	1:B:541:LEU:HD21	2.01	0.41
1:B:813:ILE:HD11	1:B:847:MET:HE1	2.01	0.41
1:A:441:ILE:HG22	1:A:442:VAL:HG23	2.03	0.41
1:A:593:ASP:OD1	1:A:927:ARG:NH2	2.53	0.41
1:A:779:TYR:CD1	1:A:825:SER:HB2	2.56	0.41
1:B:222:LYS:HD2	1:B:310:GLU:HB2	2.02	0.41
1:B:985:SER:O	1:B:989:GLU:HG2	2.20	0.41
1:B:1044:ASP:N	1:B:1044:ASP:OD1	2.53	0.41
1:B:251:SER:HB3	1:B:280:ALA:HB1	2.02	0.41
1:B:271:HIS:CG	1:B:272:PRO:HD2	2.56	0.41
1:B:668:ASP:HB3	1:B:671:ASN:HB2	2.03	0.41
1:A:265:ARG:NH1	1:A:1092:ASN:OD1	2.53	0.41
1:A:219:GLY:HA2	3:A:1102:TLA:O2	2.21	0.41
1:A:829:ASP:HB2	1:A:832:TYR:CE2	2.56	0.41
1:B:516:TRP:CE2	1:B:565:ILE:HD12	2.56	0.41
1:A:91:VAL:HA	1:A:127:LEU:HD11	2.03	0.41
1:A:107:GLU:H	1:A:107:GLU:CD	2.27	0.41
1:A:493:ALA:HB1	1:B:489:HIS:CD2	2.55	0.41
1:A:640:ARG:HA	1:A:641:PRO:HD3	1.93	0.41
1:B:200:LEU:HD11	1:B:298:ALA:HA	2.01	0.41
1:B:354:VAL:HB	1:B:391:VAL:HG22	2.03	0.41
1:B:528:TYR:HB3	1:B:539:THR:HB	2.03	0.41
1:A:927:ARG:HA	1:A:927:ARG:HD3	1.82	0.41
1:B:446:ARG:HH11	1:B:446:ARG:HA	1.86	0.41
1:B:124:ILE:HG23	1:B:135:ILE:HB	2.02	0.40
1:A:265:ARG:O	1:A:1090:ARG:NH2	2.51	0.40
1:B:611:PHE:HB3	1:B:667:PHE:CZ	2.57	0.40
1:A:124:ILE:HG23	1:A:135:ILE:HB	2.03	0.40
1:A:389:MET:C	1:A:391:VAL:H	2.29	0.40
1:A:442:VAL:HA	1:A:443:PRO:HD2	1.93	0.40
1:B:91:VAL:HA	1:B:127:LEU:HD11	2.03	0.40
1:A:865:GLN:HG3	1:A:899:HIS:HD2	1.86	0.40
1:A:271:HIS:CG	1:A:272:PRO:HD2	2.56	0.40
1:B:657:LEU:HG	1:B:661:LYS:HE3	2.04	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	1043/1113 (94%)	997 (96%)	43 (4%)	3 (0%)	36	67
1	B	1057/1113 (95%)	1013 (96%)	43 (4%)	1 (0%)	48	79
All	All	2100/2226 (94%)	2010 (96%)	86 (4%)	4 (0%)	43	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	776	ILE
1	A	732	GLN
1	A	131	GLY
1	B	131	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	795/906 (88%)	789 (99%)	6 (1%)	73	77
1	B	830/906 (92%)	825 (99%)	5 (1%)	78	80
All	All	1625/1812 (90%)	1614 (99%)	11 (1%)	76	78

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	574	VAL
1	A	731	VAL
1	A	744	THR
1	A	756	MET
1	A	774	VAL
1	A	883	THR
1	B	25	ASN
1	B	215	THR
1	B	574	VAL
1	B	756	MET
1	B	883	THR

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

Mol	Chain	Res	Type
1	A	481	HIS
1	A	760	GLN
1	A	819	ASN
1	A	865	GLN
1	A	899	HIS
1	B	400	ASN
1	B	481	HIS
1	B	760	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	$\# Z > 2$
3	TLA	A	1102	-	9,9,9	1.17	0	12,12,12	1.05	1 (8%)
2	BCO	A	1101	-	53,55,55	2.03	12 (22%)	75,81,81	2.00	19 (25%)
2	BCO	B	1101	-	29,29,55	1.91	6 (20%)	44,45,81	1.95	11 (25%)
3	TLA	B	1102	-	9,9,9	1.29	0	12,12,12	1.04	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	TLA	A	1102	-	-	4/12/12/12	-
2	BCO	A	1101	-	-	18/54/70/70	0/3/3/3
2	BCO	B	1101	-	-	3/15/31/70	0/3/3/3
3	TLA	B	1102	-	-	3/12/12/12	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	BCO	C19-N7	5.70	1.46	1.33
2	A	1101	BCO	C16-N6	5.52	1.46	1.33
2	A	1101	BCO	C12-N5	5.34	1.47	1.34
2	B	1101	BCO	C12-N5	5.33	1.47	1.34
2	A	1101	BCO	C2-C1	-5.07	1.41	1.53
2	B	1101	BCO	C2-C1	-4.92	1.42	1.53
2	A	1101	BCO	C23-C22	4.18	1.55	1.50
2	B	1101	BCO	P2-O10	4.11	1.63	1.50
2	A	1101	BCO	P2-O7	3.42	1.63	1.59
2	A	1101	BCO	O17-C22	3.20	1.26	1.21
2	A	1101	BCO	C22-S1	2.96	1.83	1.76
2	A	1101	BCO	C2-C4	-2.92	1.44	1.53
2	B	1101	BCO	C2-C4	-2.83	1.44	1.53
2	B	1101	BCO	O1-C3	-2.33	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	BCO	O1-C3	-2.33	1.39	1.45
2	A	1101	BCO	P3-O7	-2.26	1.57	1.59
2	B	1101	BCO	C1-C3	-2.12	1.47	1.52
2	A	1101	BCO	C1-C3	-2.03	1.47	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	BCO	C23-C22-S1	5.76	120.27	113.40
2	A	1101	BCO	C8-C6-N3	-5.68	118.89	126.72
2	B	1101	BCO	C8-C6-N3	-5.63	118.97	126.72
2	B	1101	BCO	N4-C15-N3	-5.33	120.52	128.58
2	A	1101	BCO	N4-C15-N3	-5.22	120.69	128.58
2	B	1101	BCO	N3-C6-N1	4.54	134.89	127.17
2	A	1101	BCO	N3-C6-N1	4.54	134.88	127.17
2	A	1101	BCO	O8-C11-C9	4.27	117.41	110.55
2	A	1101	BCO	O17-C22-C23	-3.85	119.53	123.98
2	A	1101	BCO	C15-N3-C6	3.76	121.02	111.83
2	B	1101	BCO	C15-N3-C6	3.76	121.02	111.83
2	A	1101	BCO	C18-C17-N6	3.76	119.99	112.00
2	A	1101	BCO	N1-C7-N2	-3.43	109.07	113.94
2	B	1101	BCO	N1-C7-N2	-3.36	109.17	113.94
2	B	1101	BCO	C1-C2-C4	3.04	106.58	99.89
2	A	1101	BCO	C6-N1-C7	3.04	108.93	105.74
2	A	1101	BCO	C17-C18-C19	3.02	117.43	112.39
2	A	1101	BCO	C21-C20-N7	2.99	118.66	112.41
2	B	1101	BCO	C6-N1-C7	2.97	108.85	105.74
2	A	1101	BCO	C8-N2-C7	2.82	107.88	103.45
2	A	1101	BCO	C21-S1-C22	2.81	110.15	101.84
2	B	1101	BCO	C8-N2-C7	2.76	107.80	103.45
2	A	1101	BCO	O4-C5-C3	2.62	117.90	108.99
2	B	1101	BCO	O4-C5-C3	2.48	117.44	108.99
2	A	1101	BCO	C6-C8-N2	-2.34	107.90	110.58
2	A	1101	BCO	C1-C2-C4	2.26	104.87	99.89
2	B	1101	BCO	C6-C8-N2	-2.22	108.04	110.58
2	A	1101	BCO	O17-C22-S1	-2.18	119.91	122.68
3	A	1102	TLA	O41-C4-C3	2.08	119.10	113.31
2	A	1101	BCO	C24-C23-C22	2.08	117.74	112.63
2	B	1101	BCO	C15-N4-C12	2.03	122.07	118.73

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	BCO	C11-O8-P3-O7
2	A	1101	BCO	C11-O8-P3-O13
2	A	1101	BCO	O11-C10-C9-C11
2	A	1101	BCO	N7-C20-C21-S1
2	A	1101	BCO	C20-C21-S1-C22
2	B	1101	BCO	C1-C3-C5-O4
2	B	1101	BCO	O1-C3-C5-O4
3	A	1102	TLA	C1-C2-C3-O3
3	A	1102	TLA	C1-C2-C3-C4
3	A	1102	TLA	O2-C2-C3-O3
3	A	1102	TLA	O2-C2-C3-C4
2	A	1101	BCO	C1-C3-C5-O4
3	B	1102	TLA	O1-C1-C2-O2
3	B	1102	TLA	O11-C1-C2-O2
2	A	1101	BCO	O1-C3-C5-O4
2	A	1101	BCO	C2-C1-O2-P1
2	A	1101	BCO	C3-C1-O2-P1
2	A	1101	BCO	P2-O7-P3-O8
2	A	1101	BCO	P2-O7-P3-O13
2	A	1101	BCO	C16-C10-C9-C11
2	A	1101	BCO	C11-O8-P3-O14
2	A	1101	BCO	O11-C10-C9-C14
2	A	1101	BCO	C1-O2-P1-O9
2	A	1101	BCO	O11-C10-C9-C13
2	A	1101	BCO	C1-O2-P1-O5
2	B	1101	BCO	C1-O2-P1-O6
3	B	1102	TLA	C2-C3-C4-O4
2	A	1101	BCO	C17-C18-C19-N7

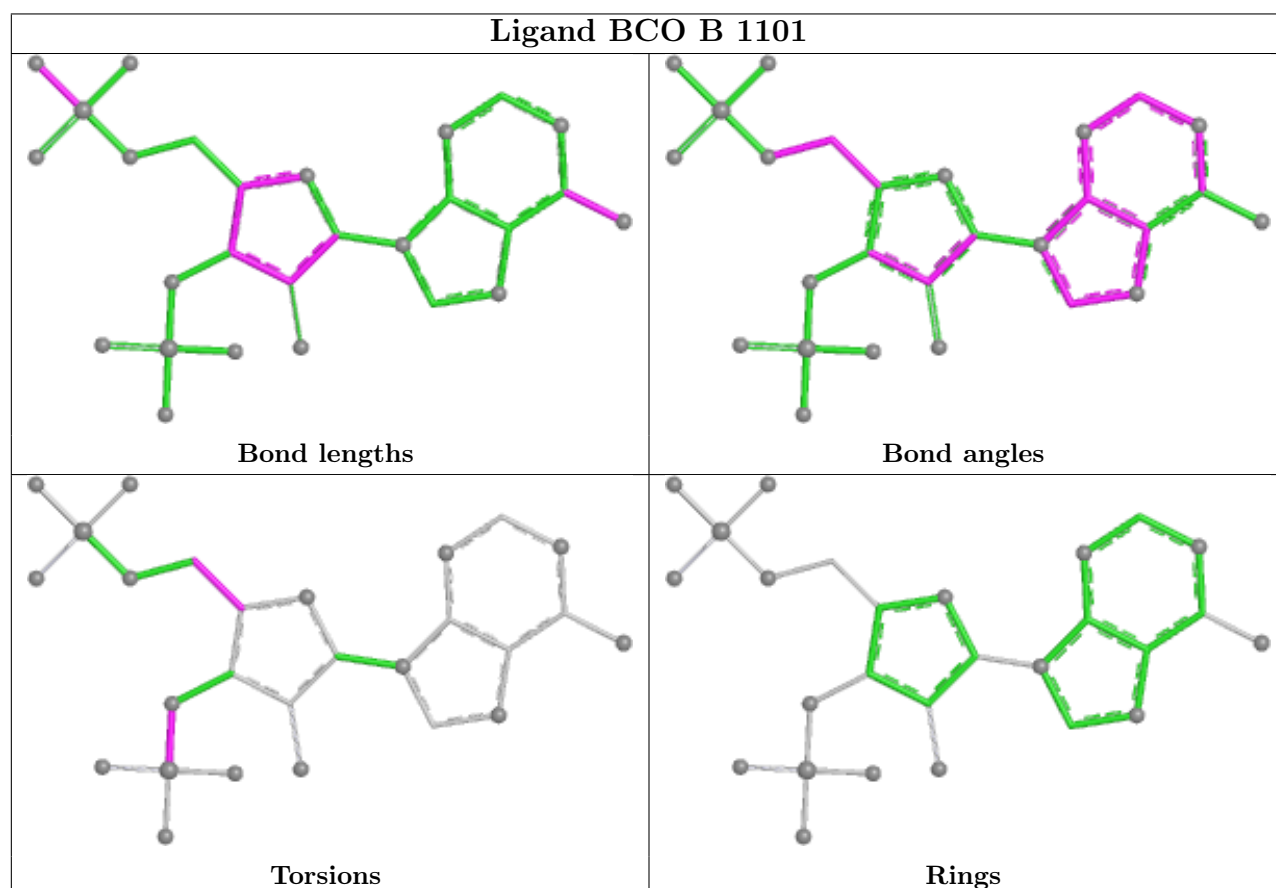
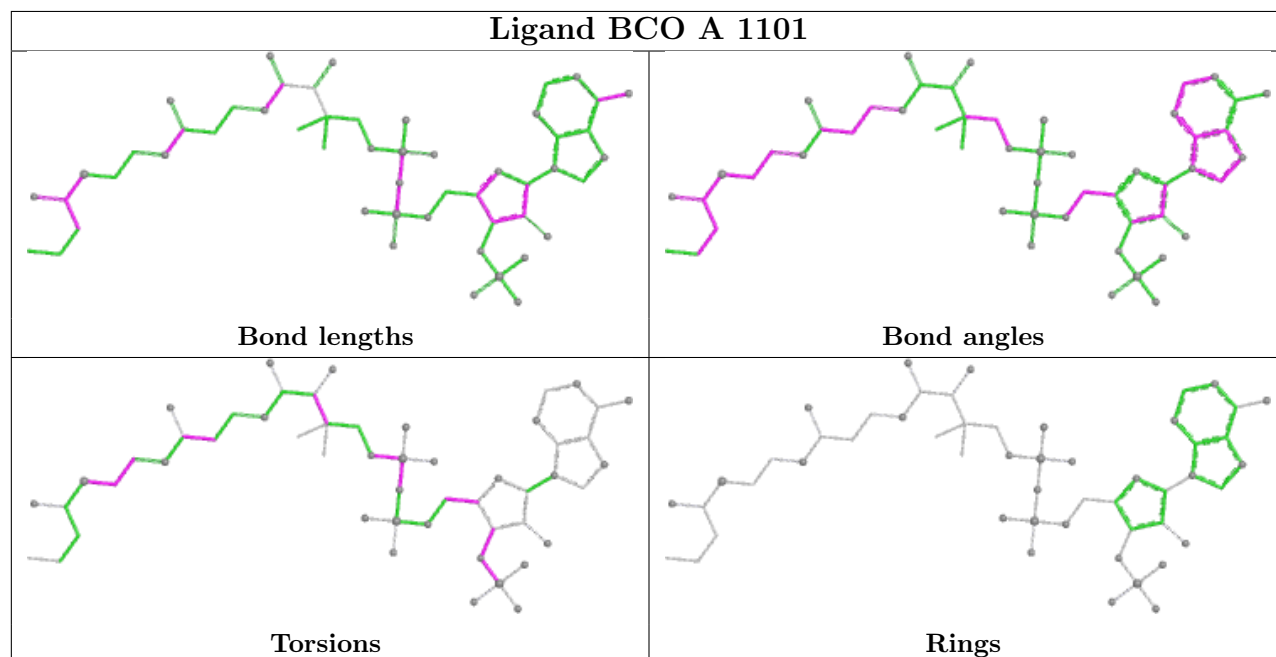
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	TLA	1	0
2	A	1101	BCO	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	1053/1113 (94%)	0.31	68 (6%)	25	17	72, 114, 169, 224	0
1	B	1063/1113 (95%)	-0.06	33 (3%)	51	31	56, 89, 156, 209	0
All	All	2116/2226 (95%)	0.13	101 (4%)	35	21	56, 102, 162, 224	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	HIS	7.8
1	B	285	GLY	6.7
1	B	905	GLU	6.4
1	A	289	SER	5.9
1	A	1012	PRO	5.9
1	B	23	PRO	5.5
1	A	313	GLY	5.0
1	A	290	GLN	5.0
1	A	115	GLY	5.0
1	A	116	GLY	4.9
1	A	40	ASP	4.9
1	A	740	GLN	4.8
1	B	117	GLY	4.7
1	A	536	GLU	4.5
1	A	439	ASN	4.4
1	A	808	ALA	4.3
1	A	86	TYR	4.3
1	B	906	ALA	4.2
1	A	750	GLU	4.2
1	A	114	GLY	4.1
1	A	41	ALA	4.0
1	A	743	ASN	4.0
1	A	1011	ASP	4.0
1	B	534	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	529	VAL	4.0
1	B	596	ARG	4.0
1	A	62	HIS	3.9
1	B	1012	PRO	3.9
1	A	978	ARG	3.8
1	A	741	GLY	3.8
1	A	780	HIS	3.7
1	A	494	LEU	3.7
1	A	285	GLY	3.7
1	B	594	PRO	3.5
1	B	598	PHE	3.4
1	A	907	ILE	3.4
1	A	38	GLY	3.4
1	A	739	ASP	3.3
1	A	288	ILE	3.2
1	A	537	ILE	3.2
1	A	312	SER	3.1
1	A	319	ALA	3.1
1	A	339	ALA	3.1
1	B	595	THR	3.1
1	B	593	ASP	3.1
1	A	88	GLY	3.0
1	A	51	GLN	3.0
1	B	1011	ASP	2.9
1	A	748	SER	2.9
1	A	874	GLN	2.9
1	A	873	ALA	2.9
1	B	1009	ASN	2.8
1	A	113	GLY	2.8
1	A	317	GLY	2.7
1	A	335	GLU	2.7
1	A	1010	GLY	2.7
1	A	1009	ASN	2.7
1	B	908	THR	2.6
1	A	118	VAL	2.6
1	B	521	GLN	2.6
1	A	216	GLY	2.6
1	A	284	ALA	2.6
1	A	620	ALA	2.6
1	B	1020	ALA	2.6
1	A	87	GLN	2.6
1	B	115	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	320	ALA	2.6
1	A	46	MET	2.5
1	A	443	PRO	2.5
1	A	742	GLN	2.5
1	B	910	PRO	2.5
1	A	1021	ARG	2.5
1	B	904	ASP	2.5
1	B	529	VAL	2.5
1	A	362	LYS	2.4
1	B	538	ARG	2.4
1	B	535	LYS	2.4
1	A	909	THR	2.4
1	B	22	GLY	2.4
1	B	1010	GLY	2.4
1	A	440	VAL	2.4
1	A	737	LYS	2.3
1	B	901	ASN	2.3
1	A	341	GLN	2.3
1	B	597	MET	2.3
1	B	618	MET	2.3
1	B	909	THR	2.2
1	A	222	LYS	2.2
1	A	318	ASP	2.2
1	B	620	ALA	2.1
1	B	385	ARG	2.1
1	A	117	GLY	2.1
1	B	592	GLU	2.1
1	A	259	LEU	2.1
1	A	445	ALA	2.1
1	B	874	GLN	2.1
1	A	745	CYS	2.1
1	A	598	PHE	2.1
1	A	37	ASP	2.1
1	A	155	GLN	2.0
1	A	974	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

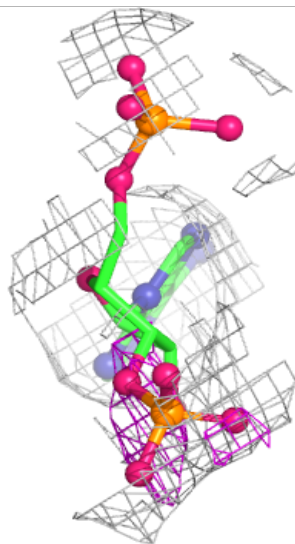
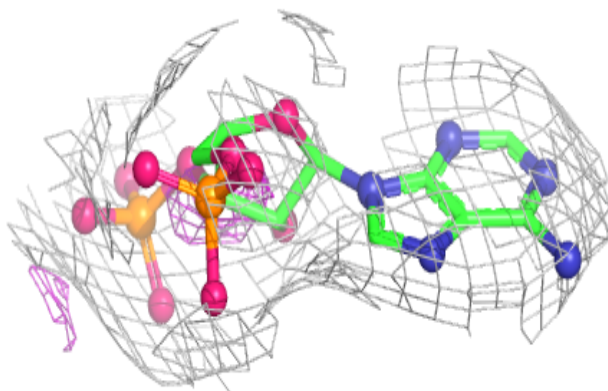
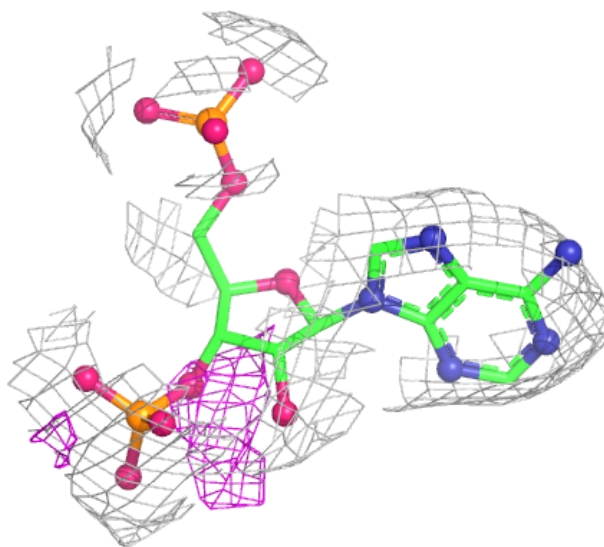
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	TLA	A	1102	10/10	0.71	0.11	135,140,141,142	0
2	BCO	B	1101	27/53	0.83	0.09	118,152,198,199	0
3	TLA	B	1102	10/10	0.88	0.11	93,98,100,102	0
2	BCO	A	1101	53/53	0.92	0.11	72,114,148,163	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.

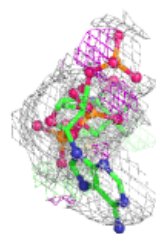
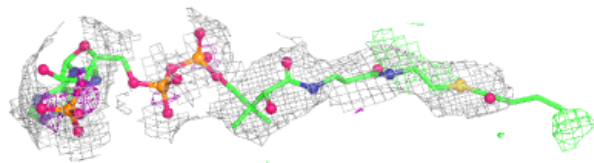
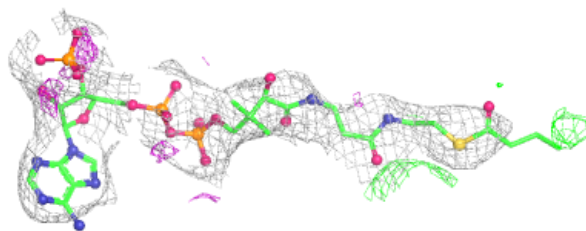
Electron density around BCO B 1101:

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



Electron density around BCO A 1101:

$2mF_o-DF_c$ (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.