



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2017 – 07:02 AM EDT

PDB ID : 4XC8
Title : Isobutyryl-CoA mutase fused with bound butyryl-CoA, GDP, and Mg and without cobalamin (apo-IcmF/GDP)
Authors : Jost, M.; Drennan, C.L.
Deposited on : unknown
Resolution : 3.25 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

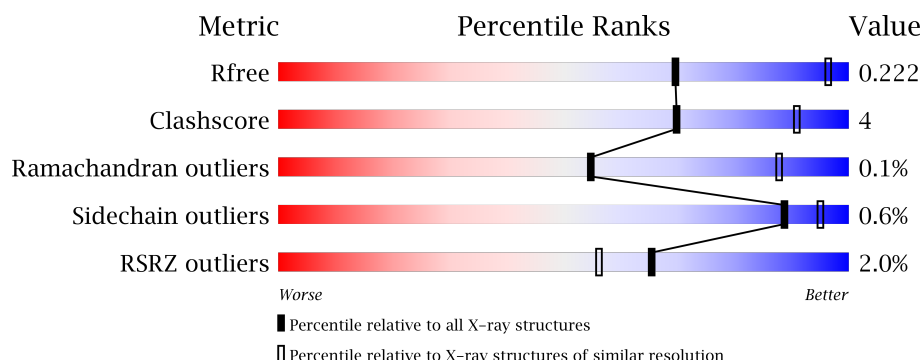
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	100719	1852 (3.32-3.20)
Clashscore	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)
RSRZ outliers	101464	1861 (3.32-3.20)

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. 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	<div> <div>4%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
1	B	1113	<div> <div>84%</div> <div>11%</div> <div>5%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16245 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	1058	Total	C	N	O	S	0	0	0
			7995	5004	1418	1537	36			
1	B	1060	Total	C	N	O	S	0	0	0
			8098	5058	1446	1558	36			

There are 40 discrepancies between the modelled and reference sequences:

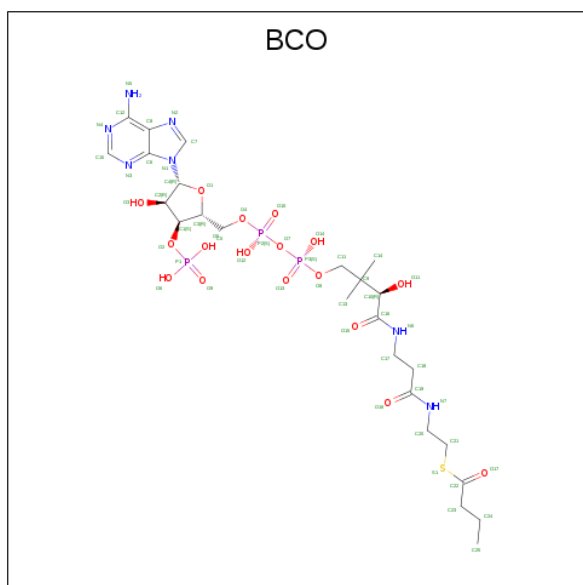
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q1LRY0
A	-18	GLY	-	expression tag	UNP Q1LRY0
A	-17	SER	-	expression tag	UNP Q1LRY0
A	-16	SER	-	expression tag	UNP Q1LRY0
A	-15	HIS	-	expression tag	UNP Q1LRY0
A	-14	HIS	-	expression tag	UNP Q1LRY0
A	-13	HIS	-	expression 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

Continued on next page...

Continued from previous page...

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 (three-letter code: 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
			39	16	5	15	3			

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	B	1	Total 28	C 10	N 5	O 11	P 2	0	0

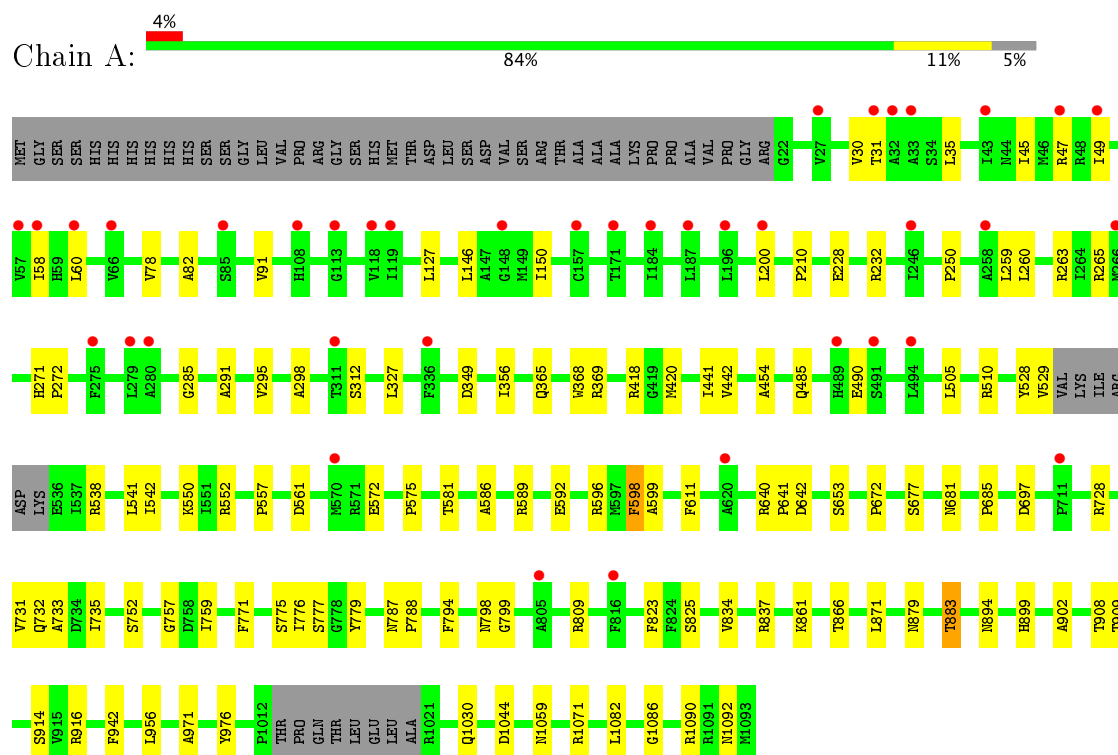
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

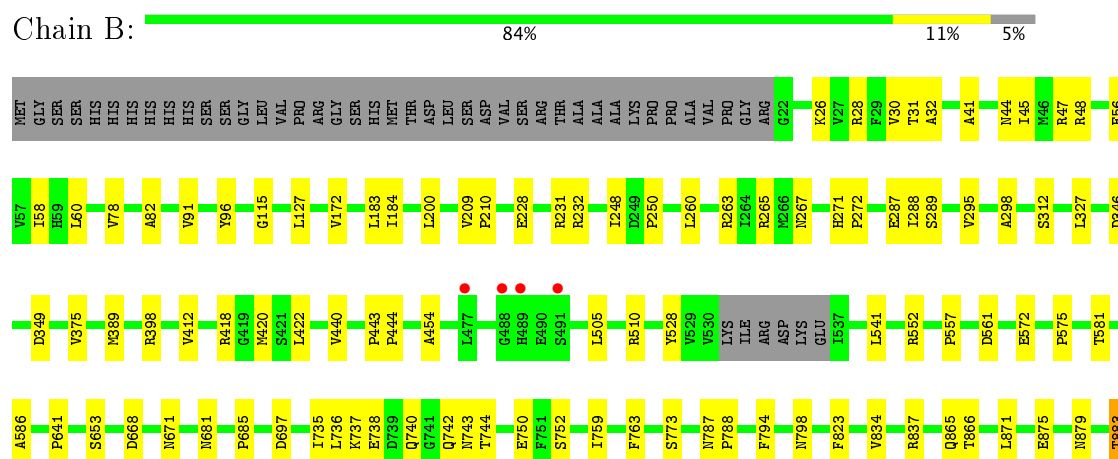
3 Residue-property plots

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: Isobutryl-CoA mutase fused



- Molecule 1: Isobutryl-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	316.51Å 316.51Å 342.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.16 – 3.25 99.16 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (99.16-3.25) 99.3 (99.16-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1760)	Depositor
R, R_{free}	0.205 , 0.222 0.205 , 0.222	Depositor DCC
R_{free} test set	5143 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	84.0	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16245	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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: GDP, MG, 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	0.21	0/8137	0.40	3/11034 (0.0%)
1	B	0.21	0/8239	0.40	3/11158 (0.0%)
All	All	0.21	0/16376	0.40	6/22192 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	552	ARG	NE-CZ-NH2	-11.21	114.70	120.30
1	A	552	ARG	NE-CZ-NH1	-11.05	114.77	120.30
1	B	552	ARG	NE-CZ-NH1	11.05	125.83	120.30
1	A	552	ARG	NE-CZ-NH2	10.85	125.72	120.30
1	A	552	ARG	CD-NE-CZ	5.49	131.28	123.60
1	B	552	ARG	CD-NE-CZ	5.47	131.26	123.60

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	7995	0	7674	68	0
1	B	8098	0	7861	70	0
2	A	53	0	40	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	39	0	23	0	0
3	A	28	0	12	2	0
3	B	28	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	16245	0	15622	133	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 (133) 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:1092:ASN:OD1	3:A:1102:GDP:O3'	2.08	0.70
1:A:916:ARG:NH1	1:B:875:GLU:OE1	2.23	0.69
1:B:412:VAL:HG13	1:B:422:LEU:HD11	1.77	0.66
1:A:908:THR:OG1	1:A:909:THR:N	2.29	0.64
1:A:265:ARG:NH2	3:A:1102:GDP:O2A	2.34	0.60
1:A:735:ILE:HG13	1:A:752:SER:HB3	1.84	0.60
1:A:1082:LEU:O	1:A:1086:GLY:N	2.34	0.60
1:B:454:ALA:HA	1:B:956:LEU:HD22	1.84	0.60
1:B:265:ARG:NH2	3:B:1102:GDP:O2A	2.35	0.59
1:B:902:ALA:HB3	1:B:905:GLU:HG3	1.84	0.59
1:A:250:PRO:HD3	1:A:312:SER:HB2	1.85	0.59
1:B:735:ILE:HG13	1:B:752:SER:HB3	1.84	0.59
1:A:47:ARG:HH11	1:A:259:LEU:HD11	1.68	0.59
1:A:365:GLN:HG3	1:A:369:ARG:HH22	1.69	0.58
1:A:31:THR:HG22	1:A:82:ALA:HB3	1.86	0.57
1:A:91:VAL:HA	1:A:127:LEU:HD11	1.86	0.57
1:B:250:PRO:HD3	1:B:312:SER:HB2	1.87	0.57
1:B:91:VAL:HA	1:B:127:LEU:HD11	1.87	0.57
1:B:31:THR:HG22	1:B:82:ALA:HB3	1.86	0.56
1:A:640:ARG:NH1	1:A:642:ASP:OD2	2.39	0.55
1:A:529:VAL:HG12	1:A:538:ARG:HG2	1.87	0.55
1:A:35:LEU:HD22	1:A:642:ASP:HB3	1.88	0.55
1:B:685:PRO:HB3	1:B:759:ILE:HD11	1.89	0.55
1:A:356:ILE:HD12	1:A:368:TRP:HA	1.89	0.54
1:A:731:VAL:HG12	1:A:771:PHE:HE1	1.71	0.54
1:B:1053:ARG:HG2	1:B:1085:VAL:HB	1.90	0.54
1:A:30:VAL:HG23	1:A:78:VAL:HG11	1.90	0.54
1:B:572:GLU:HG2	1:B:581:THR:HG21	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:PRO:HB3	1:A:759:ILE:HD11	1.91	0.53
1:A:879:ASN:O	1:A:883:THR:OG1	2.28	0.52
1:B:742:GLN:HB3	1:B:744:THR:OG1	2.09	0.52
1:A:572:GLU:HG2	1:A:581:THR:HG21	1.92	0.52
1:B:200:LEU:HD11	1:B:298:ALA:HA	1.91	0.52
1:B:30:VAL:HG23	1:B:78:VAL:HG11	1.90	0.52
1:A:732:GLN:HA	1:A:775:SER:HB3	1.92	0.51
1:A:672:PRO:O	1:A:728:ARG:NH2	2.41	0.51
1:B:794:PHE:O	1:B:798:ASN:ND2	2.43	0.51
1:B:879:ASN:O	1:B:883:THR:OG1	2.28	0.51
1:A:454:ALA:HA	1:A:956:LEU:HD22	1.93	0.50
1:B:96:TYR:HB2	1:B:641:PRO:HB2	1.93	0.50
1:B:231:ARG:NH1	1:B:1084:GLU:HA	2.26	0.50
1:B:971:ALA:HB1	1:B:976:TYR:HB3	1.94	0.49
1:A:561:ASP:HB2	1:B:561:ASP:HB2	1.94	0.49
1:A:916:ARG:NH2	1:B:1005:PHE:O	2.46	0.49
1:B:228:GLU:OE1	1:B:232:ARG:NH1	2.46	0.49
1:B:248:ILE:HD13	1:B:289:SER:H	1.77	0.49
1:A:794:PHE:O	1:A:798:ASN:ND2	2.45	0.49
1:A:787:ASN:HB2	1:A:788:PRO:HD2	1.95	0.48
1:A:861:LYS:NZ	2:A:1101:BCO:O6	2.39	0.48
1:A:228:GLU:OE1	1:A:232:ARG:NH1	2.46	0.48
1:B:787:ASN:HB2	1:B:788:PRO:HD2	1.95	0.47
1:A:776:ILE:HD13	1:A:799:GLY:HA2	1.96	0.47
1:A:942:PHE:CZ	1:B:557:PRO:HB3	2.50	0.47
1:A:971:ALA:HB1	1:A:976:TYR:HB3	1.95	0.47
1:A:779:TYR:CD2	1:A:825:SER:HB2	2.50	0.47
1:A:485:GLN:HA	1:A:490:GLU:HG2	1.98	0.46
1:A:542:ILE:HD13	1:A:550:LYS:HD3	1.97	0.46
1:A:598:PHE:HB2	1:A:899:HIS:NE2	2.31	0.46
1:B:740:GLN:NE2	1:B:798:ASN:OD1	2.46	0.45
1:A:640:ARG:HA	1:A:641:PRO:HD3	1.86	0.45
1:A:777:SER:HA	1:A:823:PHE:HB3	1.98	0.45
1:A:599:ALA:HB3	1:A:611:PHE:CE1	2.52	0.44
1:B:267:ASN:ND2	1:B:1089:TYR:O	2.50	0.44
1:B:287:GLU:HG2	1:B:288:ILE:HG23	1.98	0.44
1:A:589:ARG:NE	1:A:592:GLU:HB2	2.33	0.44
1:B:1056:VAL:HB	1:B:1085:VAL:HG21	2.00	0.44
1:A:598:PHE:H	1:A:899:HIS:CD2	2.36	0.44
1:B:528:TYR:HB2	1:B:541:LEU:HD21	1.99	0.44
1:A:697:ASP:OD1	1:A:1071:ARG:NH1	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:HIS:CG	1:B:272:PRO:HD2	2.53	0.44
1:B:60:LEU:HD21	1:B:263:ARG:HD3	1.99	0.44
1:A:441:ILE:HG22	1:A:442:VAL:HG23	2.00	0.43
1:B:443:PRO:HA	1:B:444:PRO:HD3	1.85	0.43
1:B:26:LYS:HD2	1:B:26:LYS:HA	1.62	0.43
1:A:528:TYR:HB2	1:A:541:LEU:HD21	1.99	0.43
1:B:653:SER:O	1:B:1030:GLN:NE2	2.51	0.43
1:A:681:ASN:HA	1:A:733:ALA:HA	2.00	0.43
1:B:209:VAL:HA	1:B:210:PRO:HD3	1.87	0.43
1:A:871:LEU:HD22	1:A:879:ASN:HB3	2.01	0.43
1:A:210:PRO:HG2	1:A:420:MET:HB2	2.01	0.43
1:A:866:THR:HG21	1:A:883:THR:HG22	2.01	0.43
1:B:327:LEU:HD21	1:B:418:ARG:NH2	2.34	0.43
1:B:398:ARG:NH2	1:B:440:VAL:HA	2.34	0.43
1:B:668:ASP:HB3	1:B:671:ASN:HB2	2.01	0.43
1:A:653:SER:O	1:A:1030:GLN:NE2	2.52	0.43
1:A:327:LEU:HD21	1:A:418:ARG:NH2	2.34	0.43
1:A:271:HIS:CG	1:A:272:PRO:HD2	2.54	0.42
1:A:45:ILE:O	1:A:49:ILE:HG12	2.18	0.42
1:A:834:VAL:HG12	1:A:837:ARG:HD3	2.01	0.42
1:B:697:ASP:OD1	1:B:1071:ARG:NH1	2.52	0.42
1:B:871:LEU:HD22	1:B:879:ASN:HB3	2.01	0.42
1:B:210:PRO:HG2	1:B:420:MET:HB2	2.01	0.42
1:B:738:GLU:O	1:B:743:ASN:N	2.51	0.42
1:B:866:THR:HG21	1:B:883:THR:HG22	2.01	0.42
1:A:1044:ASP:N	1:A:1044:ASP:OD1	2.53	0.42
1:A:757:GLY:HA3	1:A:809:ARG:NH1	2.35	0.42
1:B:763:PHE:CE2	1:B:773:SER:HB3	2.55	0.42
1:B:912:ALA:O	1:B:916:ARG:HG3	2.19	0.42
1:A:265:ARG:O	1:A:1090:ARG:NH1	2.53	0.42
1:A:902:ALA:HB1	1:A:914:SER:OG	2.20	0.42
1:B:902:ALA:HB1	1:B:914:SER:OG	2.19	0.42
1:B:28:ARG:HG2	1:B:56:GLU:HB2	2.02	0.42
1:B:736:LEU:HB3	1:B:798:ASN:OD1	2.20	0.42
1:A:58:ILE:HG13	1:A:260:LEU:HD12	2.02	0.41
1:B:44:ASN:HA	1:B:47:ARG:HG2	2.01	0.41
1:A:1059:ASN:O	1:A:1059:ASN:ND2	2.54	0.41
1:A:200:LEU:HD11	1:A:298:ALA:HA	2.02	0.41
1:B:834:VAL:HG12	1:B:837:ARG:HD3	2.02	0.41
1:B:184:ILE:HG23	1:B:295:VAL:HG22	2.01	0.41
1:A:575:PRO:O	1:A:586:ALA:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:681:ASN:HD21	1:B:737:LYS:HE2	1.85	0.41
1:B:41:ALA:O	1:B:45:ILE:HG12	2.21	0.41
1:B:32:ALA:HB2	1:B:60:LEU:HB2	2.02	0.41
1:B:823:PHE:HZ	1:B:865:GLN:HE21	1.69	0.41
1:B:912:ALA:O	1:B:915:VAL:HG12	2.21	0.41
1:A:291:ALA:O	1:A:295:VAL:HG23	2.20	0.41
1:A:505:LEU:O	1:A:510:ARG:NH1	2.54	0.41
1:B:1044:ASP:N	1:B:1044:ASP:OD1	2.54	0.41
1:B:267:ASN:HD21	1:B:1090:ARG:HA	1.85	0.41
1:B:505:LEU:O	1:B:510:ARG:NH1	2.54	0.41
1:B:172:VAL:HG21	1:B:183:LEU:HD22	2.03	0.41
1:B:398:ARG:HD3	1:B:750:GLU:OE2	2.20	0.41
1:A:598:PHE:HD1	1:A:598:PHE:HA	1.72	0.41
1:B:999:ILE:N	1:B:1003:ASN:OD1	2.52	0.41
1:B:58:ILE:HG13	1:B:260:LEU:HD12	2.03	0.41
1:A:60:LEU:HD21	1:A:263:ARG:HD3	2.03	0.40
1:B:575:PRO:O	1:B:586:ALA:HA	2.20	0.40
1:A:557:PRO:HB3	1:B:942:PHE:CZ	2.56	0.40
1:B:375:VAL:HG12	1:B:389:MET:HE2	2.03	0.40
1:A:146:LEU:O	1:A:150:ILE:HG12	2.22	0.40
1:A:596:ARG:HD3	1:A:677:SER:HB3	2.02	0.40
1:B:44:ASN:O	1:B:48:ARG:HG3	2.21	0.40
1:B:902:ALA:HA	1:B:918:ALA:HB2	2.03	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	1052/1113 (94%)	1001 (95%)	50 (5%)	1 (0%)	55 88
1	B	1054/1113 (95%)	1015 (96%)	38 (4%)	1 (0%)	55 88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2106/2226 (95%)	2016 (96%)	88 (4%)	2 (0%)	55 88

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	115	GLY
1	A	285	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	802/906 (88%)	798 (100%)	4 (0%)	91 95
1	B	828/906 (91%)	822 (99%)	6 (1%)	87 94
All	All	1630/1812 (90%)	1620 (99%)	10 (1%)	89 95

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	349	ASP
1	A	598	PHE
1	A	883	THR
1	A	894	ASN
1	B	346	ASP
1	B	349	ASP
1	B	883	THR
1	B	894	ASN
1	B	974	THR
1	B	1059	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	865	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	894	ASN
1	A	1030	GLN
1	B	439	ASN
1	B	894	ASN
1	B	1030	GLN
1	B	1059	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 ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
2	BCO	A	1101	-	48,55,55	2.09	11 (22%)	55,81,81	2.25	13 (23%)
3	GDP	A	1102	4	25,30,30	2.53	9 (36%)	26,47,47	1.60	6 (23%)
2	BCO	B	1101	-	35,41,55	1.68	4 (11%)	40,64,81	1.92	4 (10%)
3	GDP	B	1102	-	25,30,30	2.51	8 (32%)	26,47,47	1.70	7 (26%)

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	BCO	A	1101	-	-	0/50/70/70	0/3/3/3
3	GDP	A	1102	4	-	0/12/32/32	0/3/3/3
2	BCO	B	1101	-	-	0/30/52/70	0/3/3/3
3	GDP	B	1102	-	-	0/12/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	BCO	C2-C4	-5.93	1.44	1.53
2	A	1101	BCO	C2-C4	-5.75	1.44	1.53
2	A	1101	BCO	C2-C1	-5.04	1.41	1.53
2	B	1101	BCO	C2-C1	-4.82	1.42	1.53
3	A	1102	GDP	C2-N1	-3.92	1.28	1.35
3	B	1102	GDP	C2-N1	-3.81	1.28	1.35
3	A	1102	GDP	O5'-C5'	-3.81	1.29	1.44
3	B	1102	GDP	O5'-C5'	-3.72	1.30	1.44
3	A	1102	GDP	C5-C4	-3.20	1.33	1.40
3	A	1102	GDP	C2'-C1'	-3.16	1.48	1.53
3	B	1102	GDP	C5-C4	-3.13	1.33	1.40
3	B	1102	GDP	C2'-C1'	-2.92	1.49	1.53
3	B	1102	GDP	C2'-C3'	-2.89	1.45	1.53
3	A	1102	GDP	C2'-C3'	-2.74	1.46	1.53
3	A	1102	GDP	PA-O2A	-2.43	1.42	1.55
3	B	1102	GDP	PA-O2A	-2.40	1.43	1.55
3	A	1102	GDP	PB-O3A	-2.37	1.56	1.60
2	A	1101	BCO	O1-C3	-2.32	1.39	1.45
2	B	1101	BCO	O1-C3	-2.32	1.39	1.45
2	A	1101	BCO	C1-C3	-2.14	1.46	1.52
2	A	1101	BCO	P1-O2	-2.03	1.56	1.59
2	A	1101	BCO	O17-C22	3.25	1.26	1.21
2	A	1101	BCO	C22-S1	3.27	1.83	1.76
2	A	1101	BCO	C12-N5	3.35	1.47	1.34
2	B	1101	BCO	C12-N5	3.36	1.47	1.34
2	A	1101	BCO	C23-C22	3.71	1.55	1.50
3	A	1102	GDP	O6-C6	4.94	1.37	1.24
3	B	1102	GDP	O6-C6	5.04	1.37	1.24
2	A	1101	BCO	C19-N7	5.78	1.47	1.33
2	A	1101	BCO	C16-N6	6.29	1.46	1.33
3	A	1102	GDP	C2-N2	6.96	1.48	1.34
3	B	1102	GDP	C2-N2	6.97	1.48	1.34

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	BCO	N3-C15-N4	-9.56	120.53	128.86
2	A	1101	BCO	N3-C15-N4	-9.42	120.66	128.86
2	A	1101	BCO	O17-C22-C23	-4.74	119.80	123.95
3	A	1102	GDP	N3-C2-N1	-3.78	121.93	127.46
3	B	1102	GDP	N3-C2-N1	-3.75	121.98	127.46
2	A	1101	BCO	O17-C22-S1	-2.94	119.75	122.84
3	B	1102	GDP	C5-C6-N1	-2.85	119.43	123.48
3	B	1102	GDP	C4'-O4'-C1'	-2.84	106.75	109.77
3	A	1102	GDP	C5-C6-N1	-2.59	119.79	123.48
3	B	1102	GDP	C6-C5-C4	-2.31	118.55	120.84
3	A	1102	GDP	C4'-O4'-C1'	-2.11	107.52	109.77
3	A	1102	GDP	C6-C5-C4	-2.11	118.75	120.84
3	B	1102	GDP	C4-C5-N7	-2.04	107.44	109.41
2	A	1101	BCO	C24-C23-C22	2.09	117.88	113.67
2	A	1101	BCO	C20-C21-S1	2.18	117.56	111.23
2	A	1101	BCO	O4-C5-C3	2.30	117.15	109.00
2	A	1101	BCO	C1-C2-C4	2.31	105.13	99.95
2	A	1101	BCO	C21-S1-C22	2.31	109.55	101.90
2	B	1101	BCO	C1-C2-C4	2.32	105.17	99.95
2	B	1101	BCO	O4-C5-C3	2.67	118.47	109.00
3	A	1102	GDP	C6-N1-C2	2.69	119.94	116.06
3	B	1102	GDP	C6-N1-C2	2.85	120.16	116.06
2	A	1101	BCO	C21-C20-N7	2.87	118.81	112.49
2	A	1101	BCO	C17-C18-C19	2.89	116.87	112.22
2	A	1101	BCO	C18-C17-N6	3.90	119.94	111.87
2	A	1101	BCO	O8-C11-C9	4.21	117.32	110.55
3	B	1102	GDP	C2-N3-C4	4.22	120.09	115.16
3	A	1102	GDP	C2-N3-C4	4.41	120.30	115.16
2	B	1101	BCO	O8-C11-C9	4.59	117.92	110.55
2	A	1101	BCO	C23-C22-S1	6.98	120.31	113.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	BCO	1	0
3	A	1102	GDP	2	0
3	B	1102	GDP	1	0

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	1058/1113 (95%)	0.50	39 (3%)	42 32	63, 102, 148, 200	0
1	B	1060/1113 (95%)	0.22	4 (0%)	92 90	53, 79, 129, 182	0
All	All	2118/2226 (95%)	0.36	43 (2%)	65 56	53, 91, 143, 200	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	620	ALA	5.7
1	A	494	LEU	5.4
1	A	280	ALA	3.5
1	B	489	HIS	3.5
1	A	570	MET	3.2
1	A	246	ILE	3.1
1	A	279	LEU	3.0
1	A	157	CYS	3.0
1	A	148	GLY	3.0
1	A	200	LEU	3.0
1	A	85	SER	2.9
1	A	57	VAL	2.7
1	A	119	ILE	2.7
1	A	805	ALA	2.6
1	B	488	GLY	2.6
1	A	32	ALA	2.6
1	A	108	HIS	2.6
1	A	43	ILE	2.5
1	A	184	ILE	2.5
1	A	491	SER	2.5
1	A	266	MET	2.5
1	A	187	LEU	2.5
1	A	816	PHE	2.4
1	A	258	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	477	LEU	2.4
1	A	113	GLY	2.4
1	A	49	ILE	2.4
1	A	171	THR	2.3
1	A	66	VAL	2.3
1	A	31	THR	2.2
1	A	118	VAL	2.2
1	A	47	ARG	2.2
1	A	711	PRO	2.2
1	B	491	SER	2.2
1	A	275	PHE	2.1
1	A	311	THR	2.1
1	A	33	ALA	2.1
1	A	336	PHE	2.1
1	A	58	ILE	2.1
1	A	196	LEU	2.1
1	A	489	HIS	2.1
1	A	27	VAL	2.1
1	A	60	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	GDP	B	1102	28/28	0.97	0.21	-0.75	52,59,74,76	0
2	BCO	B	1101	39/53	0.86	0.21	-0.78	108,139,221,267	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GDP	A	1102	28/28	0.95	0.19	-0.99	73,86,96,99	0
4	MG	B	1104	1/1	0.93	0.19	-1.04	61,61,61,61	0
2	BCO	A	1101	53/53	0.94	0.24	-1.07	65,105,132,135	0
4	MG	B	1103	1/1	0.96	0.12	-2.00	82,82,82,82	0
4	MG	A	1103	1/1	0.97	0.13	-2.65	77,77,77,77	0
4	MG	A	1104	1/1	0.89	0.10	-2.87	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.