



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:17 PM GMT

PDB ID : 5CJW  
Title : Isobutyryl-CoA mutase fused with bound adenosylcobalamin, GDP, Mg (holo-IcmF/GDP), and substrate pivalyl-coenzyme A  
Authors : Jost, M.; Drennan, C.L.  
Deposited on : 2015-07-15  
Resolution : 3.40 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20026982

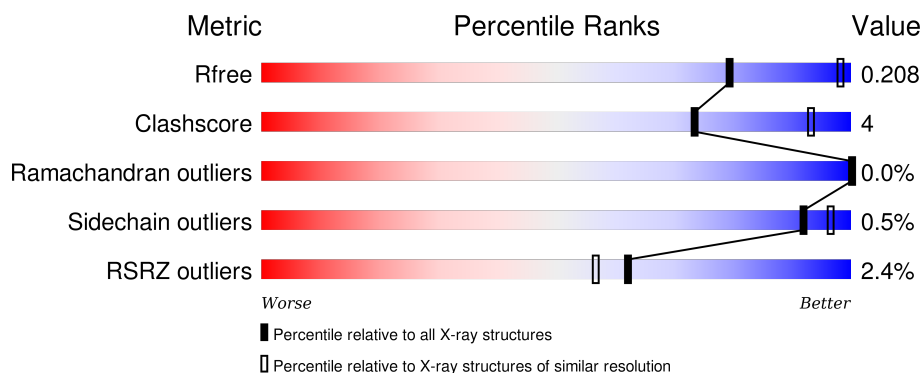
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>85%</div> <div>10%</div> <div>.</div> </div>
1	B	1113	<div> <div>%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard 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	5AD	A	1102[A]	-	-	-	X
3	5AD	A	1102[B]	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16502 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	1063	Total	C	N	O	S	0	0	0
			8098	5060	1453	1548	37			
1	B	1060	Total	C	N	O	S	0	0	0
			8045	5022	1447	1539	37			

There are 40 discrepancies between the modelled and reference sequences:

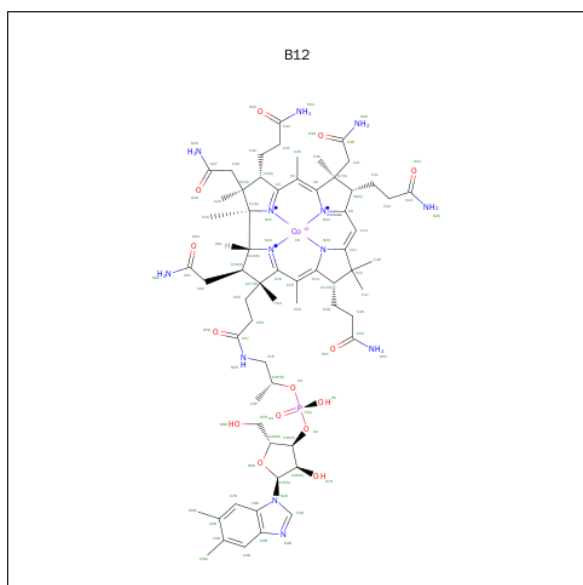
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q1LRY0
A	-18	GLY	-	expression tag	UNP Q1LRY0
A	-17	SER	-	expression tag	UNP Q1LRY0
A	-16	SER	-	expression tag	UNP Q1LRY0
A	-15	HIS	-	expression tag	UNP Q1LRY0
A	-14	HIS	-	expression tag	UNP Q1LRY0
A	-13	HIS	-	expression 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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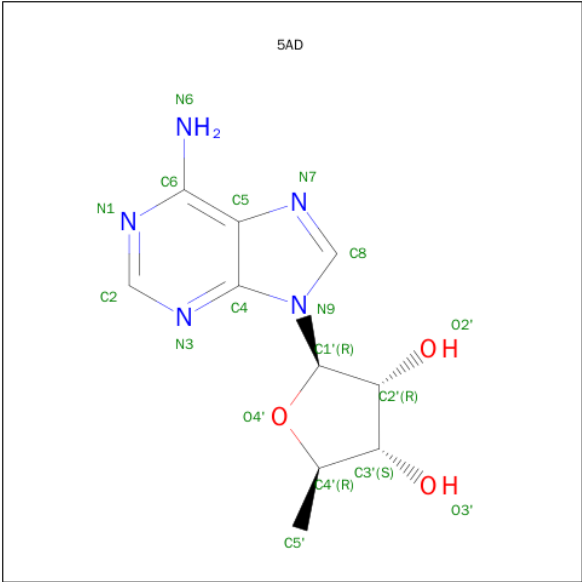
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q1LRY0
B	-13	HIS	-	expression tag	UNP Q1LRY0
B	-12	HIS	-	expression tag	UNP Q1LRY0
B	-11	HIS	-	expression tag	UNP Q1LRY0
B	-10	HIS	-	expression tag	UNP Q1LRY0
B	-9	SER	-	expression tag	UNP Q1LRY0
B	-8	SER	-	expression tag	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 COBALAMIN (three-letter code: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ).



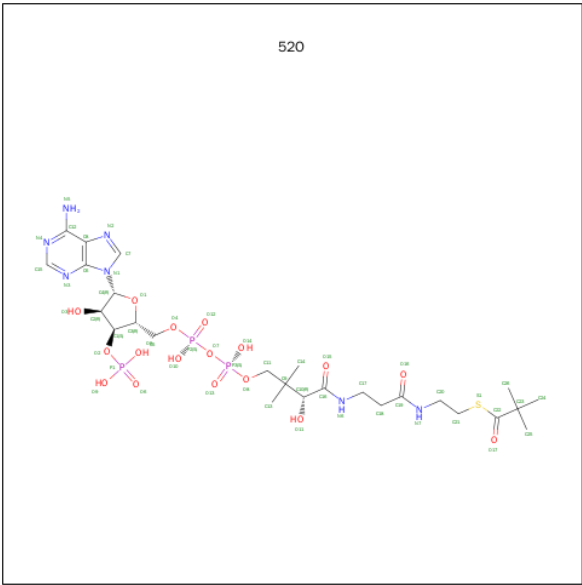
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 3 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula:  $C_{10}H_{13}N_5O_3$ ).

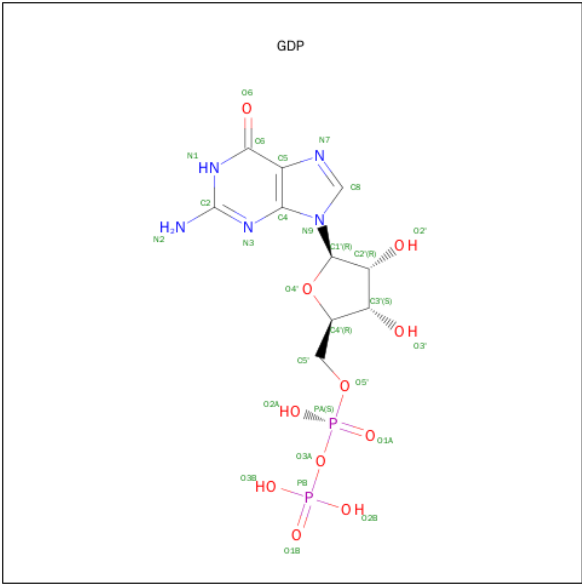


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			36	20	10	6		

- Molecule 4 is pivalyl-coenzyme A (three-letter code: 52O) (formula: C<sub>26</sub>H<sub>44</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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

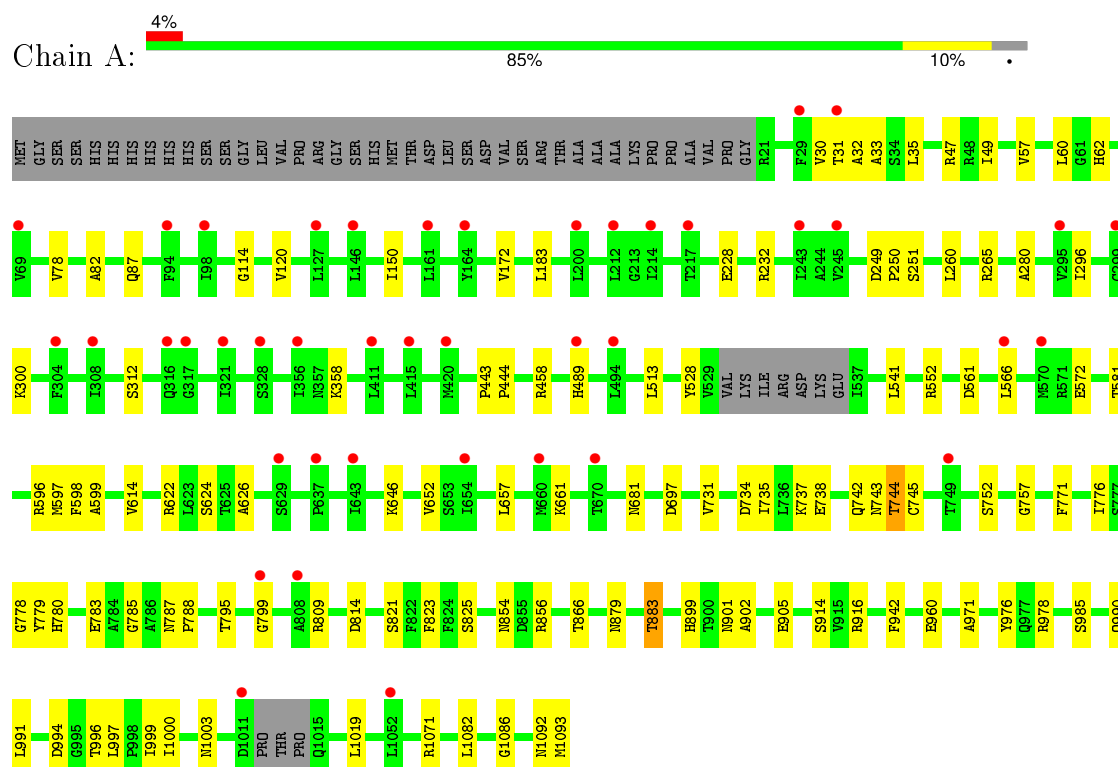
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

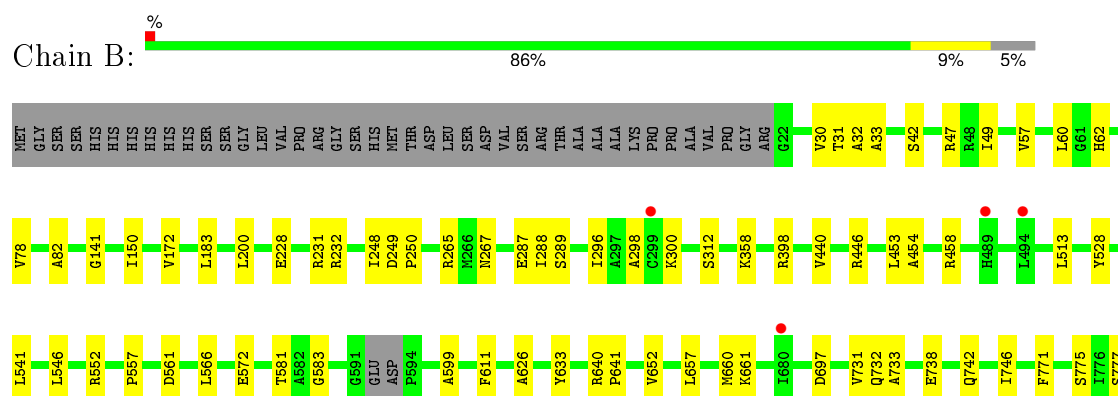
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

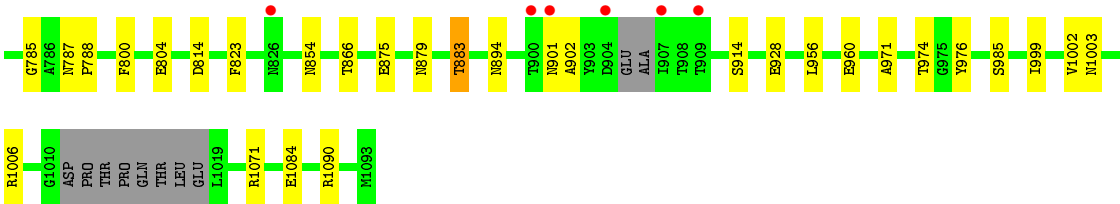
- Molecule 1: Isobutyryl-CoA mutase fused



- 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, $\alpha$ , $\beta$ , $\gamma$	317.52Å 317.52Å 343.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 3.40 127.62 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (100.00-3.40) 99.3 (127.62-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.183 , 0.200 0.191 , 0.208	Depositor DCC
$R_{free}$ test set	4549 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	104.9	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 77.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 90203 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16502	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GDP, MG, 52O, B12, 5AD

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	0/8240	0.39	2/11165 (0.0%)
1	B	0.22	0/8183	0.39	3/11083 (0.0%)
All	All	0.21	0/16423	0.39	5/22248 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	552	ARG	NE-CZ-NH2	-10.35	115.12	120.30
1	A	552	ARG	NE-CZ-NH1	10.05	125.33	120.30
1	B	552	ARG	NE-CZ-NH2	8.98	124.79	120.30
1	B	552	ARG	NE-CZ-NH1	-8.41	116.09	120.30
1	B	552	ARG	CD-NE-CZ	5.08	130.71	123.60

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	8098	0	7834	72	0
1	B	8045	0	7756	54	0
2	A	91	0	88	14	0
2	B	91	0	88	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	36	0	26	4	0
4	A	54	0	41	7	0
4	B	27	0	12	0	0
5	A	28	0	12	2	0
5	B	28	0	12	2	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
All	All	16502	0	15869	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:87:GLN:HE22	2:A:1101:B12:H421	1.46	0.80
1:A:783:GLU:HB3	2:A:1101:B12:H532	1.68	0.76
1:B:454:ALA:HA	1:B:956:LEU:HD22	1.79	0.64
3:A:1102[A]:5AD:H5'1	4:A:1103:52O:H42	1.80	0.63
1:A:31:THR:HG22	1:A:82:ALA:HB3	1.82	0.61
1:A:905:GLU:O	2:A:1101:B12:N29	2.25	0.61
1:A:681:ASN:ND2	1:A:742:GLN:OE1	2.35	0.60
1:A:622:ARG:NH1	4:A:1103:52O:O13	2.21	0.59
1:A:734:ASP:HB3	1:A:737:LYS:HZ2	1.68	0.59
1:A:742:GLN:HE21	2:A:1101:B12:H411	1.67	0.58
1:A:990:GLN:O	1:A:994:ASP:HB2	2.04	0.58
1:B:31:THR:HG22	1:B:82:ALA:HB3	1.84	0.57
1:A:1082:LEU:O	1:A:1086:GLY:N	2.37	0.56
1:A:821:SER:OG	4:A:1103:52O:O11	2.19	0.56
1:A:856:ARG:NH1	4:A:1103:52O:O9	2.39	0.56
1:A:780:HIS:HA	2:A:1101:B12:H461	1.88	0.55
2:A:1101:B12:H261	3:A:1102[A]:5AD:H3'	1.89	0.55
1:A:35:LEU:HB3	1:A:646:LYS:HE3	1.89	0.55
1:A:33:ALA:HB3	1:A:62:HIS:HA	1.89	0.55
1:B:738:GLU:OE2	1:B:742:GLN:NE2	2.39	0.54
1:A:596:ARG:HG2	1:A:624:SER:HB2	1.89	0.54
1:B:1002:VAL:O	1:B:1006:ARG:NH1	2.36	0.54
1:A:561:ASP:HB2	1:B:561:ASP:HB2	1.90	0.54
1:B:33:ALA:HB3	1:B:62:HIS:HA	1.90	0.53
1:B:267:ASN:HD21	1:B:1090:ARG:HA	1.73	0.53
1:A:458:ARG:NH1	1:A:960:GLU:OE2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:942:PHE:CZ	1:B:557:PRO:HB3	2.44	0.53
1:B:583:GLY:HA3	1:B:894:ASN:HD22	1.74	0.53
1:B:30:VAL:HG23	1:B:78:VAL:HG11	1.90	0.53
1:A:30:VAL:HG23	1:A:78:VAL:HG11	1.91	0.53
1:A:528:TYR:HB2	1:A:541:LEU:HD21	1.90	0.52
1:B:528:TYR:HB2	1:B:541:LEU:HD21	1.90	0.52
1:B:513:LEU:HD21	1:B:566:LEU:HB2	1.91	0.52
1:A:513:LEU:HD21	1:A:566:LEU:HB2	1.91	0.51
1:A:785:GLY:HA3	1:A:985:SER:HB2	1.92	0.51
1:A:735:ILE:HG13	1:A:752:SER:HB3	1.92	0.51
1:A:991:LEU:HD22	1:A:996:THR:HB	1.92	0.51
1:A:32:ALA:HB2	1:A:60:LEU:HB2	1.94	0.50
1:B:228:GLU:OE1	1:B:232:ARG:NH1	2.45	0.50
1:A:228:GLU:OE1	1:A:232:ARG:NH1	2.45	0.49
1:B:785:GLY:HA3	1:B:985:SER:HB2	1.94	0.49
1:A:916:ARG:NH1	1:B:875:GLU:OE2	2.45	0.49
1:B:32:ALA:HB2	1:B:60:LEU:HB2	1.95	0.49
1:A:598:PHE:CE2	4:A:1103:52O:H40	2.48	0.49
1:B:787:ASN:HB2	1:B:788:PRO:HD2	1.95	0.49
1:B:777:SER:HA	1:B:823:PHE:HB3	1.95	0.49
1:A:787:ASN:HB2	1:A:788:PRO:HD2	1.94	0.49
1:A:62:HIS:CE1	1:A:743:ASN:HB3	2.47	0.48
1:B:296:ILE:O	1:B:300:LYS:HG3	2.13	0.48
1:A:814:ASP:CG	1:A:854:ASN:HD22	2.17	0.48
1:A:1000:ILE:N	1:B:928:GLU:OE2	2.36	0.48
1:B:814:ASP:CG	1:B:854:ASN:HD22	2.17	0.48
1:A:250:PRO:HD3	1:A:312:SER:HB2	1.96	0.48
1:B:572:GLU:HG2	1:B:581:THR:HG21	1.96	0.48
1:A:731:VAL:HG12	1:A:771:PHE:HE1	1.79	0.47
1:B:879:ASN:O	1:B:883:THR:OG1	2.29	0.47
1:A:697:ASP:OD1	1:A:1071:ARG:NH1	2.48	0.47
1:A:296:ILE:O	1:A:300:LYS:HG3	2.14	0.47
1:A:572:GLU:HG2	1:A:581:THR:HG21	1.97	0.47
1:A:779:TYR:OH	3:A:1102[B]:5AD:O3'	2.19	0.47
1:B:231:ARG:NH1	1:B:1084:GLU:HA	2.30	0.47
1:A:978:ARG:NE	1:A:1093:MET:OXT	2.46	0.47
1:B:697:ASP:OD1	1:B:1071:ARG:NH1	2.48	0.46
1:A:734:ASP:O	1:A:737:LYS:HG2	2.16	0.46
1:B:458:ARG:NH1	1:B:960:GLU:OE2	2.43	0.46
1:B:657:LEU:HG	1:B:661:LYS:HE3	1.98	0.46
1:B:200:LEU:HD11	1:B:298:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:TYR:CD2	1:A:825:SER:HB2	2.51	0.45
2:B:1101:B12:H353	2:B:1101:B12:H311	1.98	0.45
1:A:757:GLY:HA3	1:A:809:ARG:NH2	2.31	0.45
2:B:1101:B12:H473	2:B:1101:B12:H481	1.77	0.45
2:B:1101:B12:H531	2:B:1101:B12:H552	1.98	0.45
1:A:172:VAL:HG21	1:A:183:LEU:HD22	1.97	0.45
1:B:172:VAL:HG21	1:B:183:LEU:HD22	1.98	0.45
1:B:731:VAL:O	1:B:733:ALA:N	2.50	0.45
1:A:776:ILE:HD13	1:A:799:GLY:HA2	1.98	0.45
1:A:999:ILE:N	1:A:1003:ASN:OD1	2.46	0.45
1:A:598:PHE:H	1:A:899:HIS:CE1	2.34	0.45
1:B:250:PRO:HD3	1:B:312:SER:HB2	1.98	0.45
1:B:971:ALA:HB1	1:B:976:TYR:HB3	1.99	0.45
1:A:657:LEU:HG	1:A:661:LYS:HE3	1.98	0.45
1:B:902:ALA:HB1	1:B:914:SER:OG	2.17	0.45
1:B:248:ILE:HD13	1:B:289:SER:H	1.82	0.45
1:A:823:PHE:CE2	4:A:1103:52O:H34	2.52	0.45
1:B:446:ARG:NH2	1:B:804:GLU:OE2	2.49	0.45
1:A:902:ALA:HB1	1:A:914:SER:OG	2.17	0.45
2:A:1101:B12:H261	3:A:1102[B]:5AD:H5'2	2.00	0.44
1:A:49:ILE:HB	1:A:150:ILE:HG13	1.99	0.44
1:A:742:GLN:HG3	2:A:1101:B12:H472	1.99	0.43
1:B:866:THR:O	1:B:901:ASN:ND2	2.49	0.43
1:A:443:PRO:HA	1:A:444:PRO:HD3	1.88	0.43
1:A:626:ALA:O	1:A:652:VAL:HG12	2.18	0.43
1:A:597:MET:HB2	1:A:614:VAL:HG11	2.01	0.43
1:A:971:ALA:HB1	1:A:976:TYR:HB3	2.00	0.43
1:A:598:PHE:HA	1:A:624:SER:HB3	2.00	0.43
1:A:879:ASN:O	1:A:883:THR:OG1	2.30	0.43
1:A:120:VAL:HG11	1:A:1019:LEU:HD11	2.00	0.43
1:A:265:ARG:NH1	5:A:1104:GDP:O1A	2.52	0.43
1:B:453:LEU:HD13	1:B:800:PHE:CD2	2.54	0.43
1:B:599:ALA:HB3	1:B:611:PHE:CE1	2.54	0.42
1:B:47:ARG:HB2	1:B:57:VAL:HG11	2.01	0.42
2:A:1101:B12:H362	2:A:1101:B12:H351	2.00	0.42
1:B:287:GLU:HG2	1:B:288:ILE:HG23	2.01	0.42
1:A:738:GLU:HB3	1:A:745:CYS:HB2	2.01	0.42
1:B:141:GLY:HA3	2:B:1101:B12:H5R2	2.02	0.42
1:A:866:THR:O	1:A:901:ASN:ND2	2.52	0.42
1:A:779:TYR:CE1	1:A:783:GLU:HG3	2.54	0.42
1:B:49:ILE:HB	1:B:150:ILE:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ARG:HB2	1:A:57:VAL:HG11	2.02	0.42
2:A:1101:B12:H252	2:A:1101:B12:H601	2.02	0.41
1:B:358:LYS:HG2	5:B:1103:GDP:C6	2.55	0.41
1:A:358:LYS:HG2	5:A:1104:GDP:C6	2.55	0.41
1:A:778:GLY:HA3	1:A:795:THR:OG1	2.21	0.41
1:B:626:ALA:O	1:B:652:VAL:HG12	2.20	0.41
1:B:265:ARG:NH1	5:B:1103:GDP:O2A	2.53	0.41
1:B:640:ARG:HA	1:B:641:PRO:HD3	1.91	0.41
1:B:999:ILE:N	1:B:1003:ASN:OD1	2.47	0.41
1:A:251:SER:HB2	1:A:280:ALA:HB1	2.03	0.41
1:A:114:GLY:HA3	2:A:1101:B12:C9B	2.50	0.41
1:A:681:ASN:HB2	1:A:744:THR:HB	2.02	0.41
2:A:1101:B12:H8	4:A:1103:52O:H36	2.03	0.41
2:B:1101:B12:H91	2:B:1101:B12:H262	1.88	0.41
1:B:660:MET:HE2	1:B:660:MET:HB2	1.93	0.41
1:B:732:GLN:HA	1:B:775:SER:HB3	2.03	0.41
2:A:1101:B12:H552	2:A:1101:B12:H531	2.03	0.40
1:B:42:SER:OG	2:B:1101:B12:N3B	2.46	0.40
1:A:735:ILE:HA	1:A:738:GLU:HG2	2.02	0.40
1:B:398:ARG:NH1	1:B:440:VAL:HA	2.36	0.40
1:B:633:TYR:HD2	1:B:746:ILE:HD13	1.86	0.40
1:A:997:LEU:HD22	1:B:546:LEU:HD11	2.04	0.40
1:B:731:VAL:HG23	1:B:771:PHE:CE1	2.57	0.40
1:A:599:ALA:O	1:A:626:ALA:N	2.46	0.40
2:A:1101:B12:H262	2:A:1101:B12:H91	1.93	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	1057/1113 (95%)	1009 (96%)	47 (4%)	1 (0%)	56	89

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1052/1113 (94%)	1016 (97%)	36 (3%)	0	100	100
All	All	2109/2226 (95%)	2025 (96%)	83 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	LEU

### 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	821/906 (91%)	816 (99%)	5 (1%)	90	96
1	B	810/906 (89%)	807 (100%)	3 (0%)	93	97
All	All	1631/1812 (90%)	1623 (100%)	8 (0%)	92	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	ASP
1	A	489	HIS
1	A	744	THR
1	A	883	THR
1	A	1092	ASN
1	B	249	ASP
1	B	883	THR
1	B	974	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	267	ASN
1	B	899	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	B12	A	1101	1,3	74,101,101	0.60	1 (1%)	114,166,166	1.36	14 (12%)
3	5AD	A	1102[A]	-	17,20,20	0.57	0	15,30,30	0.26	0
3	5AD	A	1102[B]	2	17,20,20	0.59	0	15,30,30	0.33	0
4	52O	A	1103	-	47,56,56	0.77	1 (2%)	59,85,85	0.70	1 (1%)
5	GDP	A	1104	6	24,30,30	2.50	9 (37%)	26,47,47	1.63	6 (23%)
2	B12	B	1101	1	74,101,101	0.55	1 (1%)	114,166,166	1.39	14 (12%)
4	52O	B	1102	-	25,29,56	0.90	1 (4%)	30,45,85	0.74	1 (3%)
5	GDP	B	1103	6	24,30,30	2.54	9 (37%)	26,47,47	1.64	6 (23%)

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	B12	A	1101	1,3	-	0/51/223/223	0/3/11/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5AD	A	1102[A]	-	-	0/0/20/20	0/3/3/3
3	5AD	A	1102[B]	2	-	0/0/20/20	0/3/3/3
4	52O	A	1103	-	-	0/53/73/73	0/3/3/3
5	GDP	A	1104	6	-	0/12/32/32	0/3/3/3
2	B12	B	1101	1	-	0/51/223/223	0/3/11/11
4	52O	B	1102	-	-	0/11/31/73	0/3/3/3
5	GDP	B	1103	6	-	0/12/32/32	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1104	GDP	O5'-C5'	-3.80	1.29	1.44
5	B	1103	GDP	O5'-C5'	-3.78	1.29	1.44
5	A	1104	GDP	C2-N1	-3.76	1.28	1.35
5	B	1103	GDP	C2-N1	-3.70	1.28	1.35
4	A	1103	52O	C23-C22	-3.57	1.50	1.53
5	B	1103	GDP	C5-C4	-3.21	1.33	1.40
5	A	1104	GDP	C5-C4	-3.21	1.33	1.40
5	B	1103	GDP	C2'-C1'	-3.14	1.48	1.53
5	A	1104	GDP	C2'-C1'	-3.02	1.48	1.53
5	B	1103	GDP	PA-O2A	-2.84	1.43	1.55
5	B	1103	GDP	C2'-C3'	-2.79	1.45	1.53
5	A	1104	GDP	C2'-C3'	-2.67	1.46	1.53
5	B	1103	GDP	PB-O3B	-2.38	1.46	1.54
5	A	1104	GDP	PB-O3B	-2.34	1.46	1.54
5	A	1104	GDP	PA-O1A	-2.28	1.43	1.51
2	B	1101	B12	C1P-C2P	2.21	1.57	1.51
2	A	1101	B12	C1P-C2P	2.32	1.57	1.51
4	B	1102	52O	P2-O12	2.89	1.59	1.50
5	A	1104	GDP	O6-C6	4.90	1.37	1.24
5	B	1103	GDP	O6-C6	4.95	1.37	1.24
5	A	1104	GDP	C2-N2	6.64	1.48	1.34
5	B	1103	GDP	C2-N2	6.69	1.48	1.34

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1104	GDP	N3-C2-N1	-4.23	121.80	127.56
5	B	1103	GDP	N3-C2-N1	-4.18	121.87	127.56
2	B	1101	B12	C35-C5-C4	-4.00	112.30	117.81
2	A	1101	B12	C35-C5-C4	-3.69	112.73	117.81
2	A	1101	B12	C30-C3-C2	-3.57	111.97	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	B12	C2-C1-C19	-3.50	115.31	118.62
2	B	1101	B12	C9-C10-C11	-3.36	124.18	132.31
2	A	1101	B12	C9-C10-C11	-3.35	124.21	132.31
2	B	1101	B12	C30-C3-C2	-3.18	112.75	119.01
2	A	1101	B12	C13-C14-C15	-3.06	122.45	132.12
5	B	1103	GDP	C5-C6-N1	-3.03	119.56	123.52
2	A	1101	B12	C3-C4-C5	-2.99	122.67	132.12
2	B	1101	B12	C13-C14-C15	-2.99	122.67	132.12
5	A	1104	GDP	C5-C6-N1	-2.93	119.69	123.52
2	B	1101	B12	C3-C4-C5	-2.89	122.99	132.12
5	B	1103	GDP	C4'-O4'-C1'	-2.67	106.82	109.64
5	A	1104	GDP	C4'-O4'-C1'	-2.64	106.84	109.64
2	B	1101	B12	C2-C1-C19	-2.56	116.20	118.62
2	B	1101	B12	C25-C2-C3	-2.49	112.89	115.90
2	B	1101	B12	C55-C17-C18	-2.41	106.70	111.03
5	A	1104	GDP	C1'-N9-C4	-2.33	124.21	126.81
5	A	1104	GDP	C6-C5-C4	-2.27	118.26	120.86
2	A	1101	B12	C20-C1-C19	-2.27	107.11	109.36
5	B	1103	GDP	C1'-N9-C4	-2.23	124.32	126.81
5	B	1103	GDP	C6-C5-C4	-2.20	118.35	120.86
2	B	1101	B12	C16-C15-C14	-2.15	120.43	124.08
2	B	1101	B12	C20-C1-C19	-2.12	107.26	109.36
2	A	1101	B12	C16-C15-C14	-2.10	120.53	124.08
2	A	1101	B12	O3-P-O4	2.03	115.96	108.83
2	A	1101	B12	P-O2-C3R	2.12	126.35	120.10
2	B	1101	B12	P-O2-C3R	2.16	126.48	120.10
2	B	1101	B12	O3-P-O4	2.18	116.48	108.83
4	B	1102	52O	O7-P2-O4	2.24	113.25	106.72
2	A	1101	B12	C8-C7-C6	2.31	104.08	101.00
4	A	1103	52O	P1-O2-C1	2.43	127.78	121.56
2	A	1101	B12	C19-C1-N21	3.31	105.66	102.16
5	A	1104	GDP	C6-N1-C2	3.62	120.13	115.88
5	B	1103	GDP	C6-N1-C2	3.65	120.16	115.88
2	A	1101	B12	P-O3-C2P	4.90	127.86	120.94
2	A	1101	B12	C35-C5-C6	4.97	124.64	117.81
2	B	1101	B12	P-O3-C2P	5.35	128.48	120.94
2	B	1101	B12	C35-C5-C6	6.01	126.07	117.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	B12	14	0
3	A	1102[A]	5AD	2	0
3	A	1102[B]	5AD	2	0
4	A	1103	52O	7	0
5	A	1104	GDP	2	0
2	B	1101	B12	6	0
5	B	1103	GDP	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1063/1113 (95%)	0.47	42 (3%)	42 37	75, 108, 157, 214	0
1	B	1060/1113 (95%)	0.32	10 (0%)	85 81	71, 100, 157, 234	0
All	All	2123/2226 (95%)	0.40	52 (2%)	62 57	71, 104, 157, 234	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	420	MET	3.9
1	A	494	LEU	3.5
1	B	494	LEU	3.5
1	A	200	LEU	3.3
1	A	295	VAL	3.3
1	A	415	LEU	2.9
1	A	1011	ASP	2.8
1	A	98	ILE	2.8
1	A	94	PHE	2.7
1	A	146	LEU	2.7
1	A	316	GLN	2.7
1	B	680	ILE	2.6
1	A	127	LEU	2.6
1	A	808	ALA	2.6
1	B	826	ASN	2.5
1	A	660	MET	2.5
1	A	31	THR	2.5
1	A	321	ILE	2.5
1	B	909	THR	2.4
1	A	654	ILE	2.4
1	A	217	THR	2.4
1	A	299	CYS	2.4
1	A	489	HIS	2.4
1	B	299	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	214	ILE	2.4
1	A	749	THR	2.3
1	A	69	VAL	2.3
1	A	317	GLY	2.3
1	A	161	LEU	2.3
1	A	243	ILE	2.3
1	B	900	THR	2.3
1	A	356	ILE	2.2
1	A	629	SER	2.2
1	B	904	ASP	2.2
1	A	164	TYR	2.2
1	A	799	GLY	2.2
1	A	304	PHE	2.2
1	A	1052	LEU	2.2
1	B	901	ASN	2.2
1	A	411	LEU	2.2
1	A	328	SER	2.1
1	A	637	PRO	2.1
1	B	489	HIS	2.1
1	A	566	LEU	2.1
1	A	29	PHE	2.1
1	A	643	ILE	2.1
1	A	570	MET	2.1
1	A	212	LEU	2.0
1	A	670	THR	2.0
1	A	245	VAL	2.0
1	A	308	ILE	2.0
1	B	907	ILE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	5AD	A	1102[B]	18/18	0.91	0.81	8.37	170,174,177,179	18
3	5AD	A	1102[A]	18/18	0.91	0.81	7.85	171,173,177,178	18
2	B12	A	1101	91/91	0.96	0.35	0.64	65,83,104,110	0
2	B12	B	1101	91/91	0.92	0.30	0.31	106,130,151,162	0
6	MG	B	1104	1/1	0.99	0.23	-0.34	70,70,70,70	0
4	52O	A	1103	54/54	0.92	0.26	-0.61	75,113,160,165	0
5	GDP	B	1103	28/28	0.97	0.23	-0.68	72,81,92,133	0
6	MG	B	1105	1/1	0.96	0.22	-0.72	70,70,70,70	0
5	GDP	A	1104	28/28	0.97	0.17	-1.03	95,113,118,122	0
6	MG	A	1105	1/1	0.96	0.15	-1.12	78,78,78,78	0
4	52O	B	1102	27/54	0.81	0.18	-1.29	131,172,224,225	0
6	MG	A	1106	1/1	0.94	0.10	-2.18	107,107,107,107	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.