



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2024 – 08:07 PM EST

PDB ID : 1N1B  
Title : Crystal Structure of (+)-Bornyl Diphosphate Synthase from Sage  
Authors : Whittington, D.A.; Wise, M.L.; Urbansky, M.; Coates, R.M.; Croteau, R.B.;  
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Deposited on : 2002-10-17  
Resolution : 2.00 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

<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>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

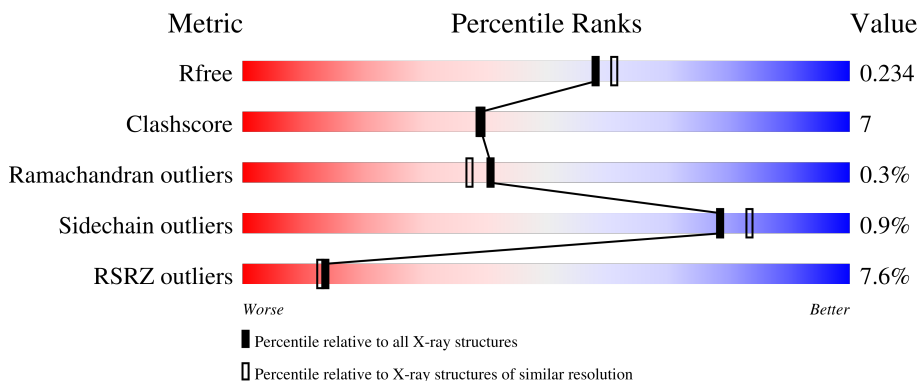
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

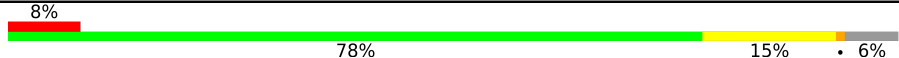
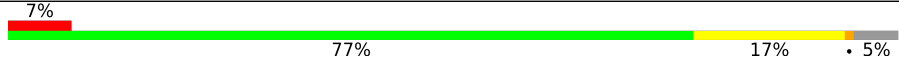
The reported resolution of this entry is 2.00 Å.

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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	549	
1	B	549	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9156 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 (+)-bornyl diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	516	4265	2768	702	777	18	0	0	0
1	B	519	4290	2783	706	782	19	0	1	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Hg	0	0
			5	5		
3	B	6	Total	Hg	0	0
			6	6		

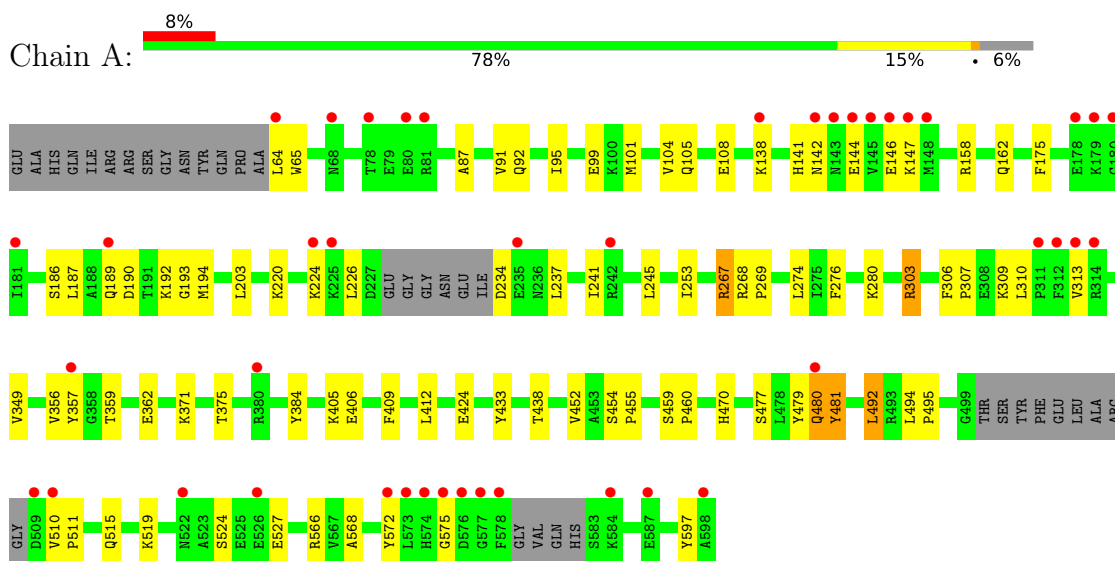
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	277	Total	O	0	0
			277	277		
4	B	311	Total	O	0	0
			311	311		

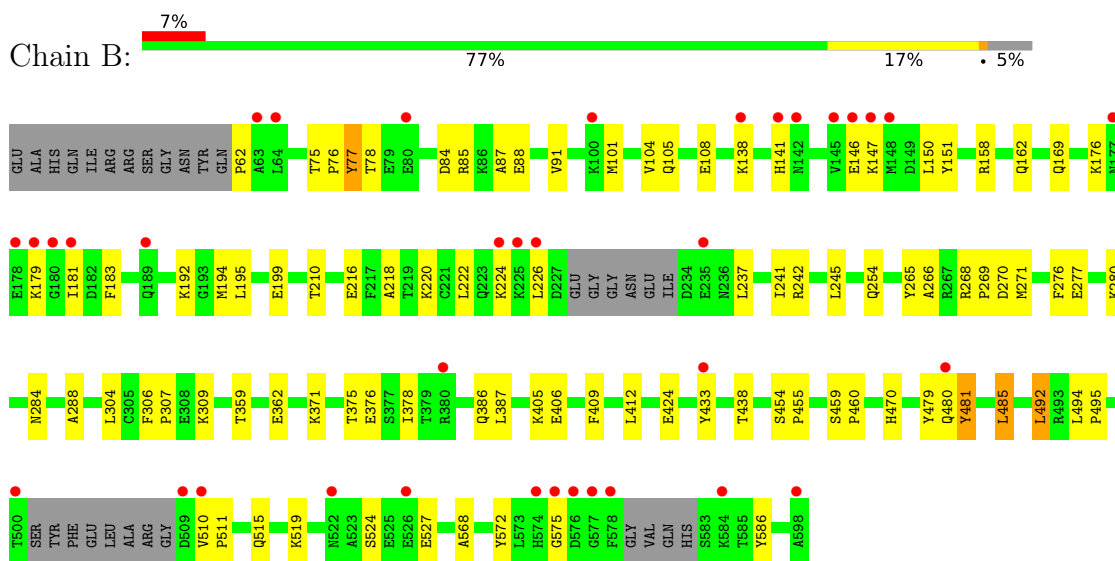
### 3 Residue-property plots [i](#)

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: (+)-bornyl diphosphate synthase



- Molecule 1: (+)-bornyl diphosphate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.06Å 116.77Å 120.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.83 – 2.00 19.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.9 (19.83-2.00) 96.1 (19.83-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.58 (at 2.01Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.203 , 0.234 0.203 , 0.234	Depositor DCC
$R_{free}$ test set	3756 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 56.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.009 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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, 0.333 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: MG, HG

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	0.33	0/4378	0.52	1/5931 (0.0%)
1	B	0.34	0/4404	0.53	1/5967 (0.0%)
All	All	0.34	0/8782	0.52	2/11898 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	GLN	N-CA-C	-5.56	96.00	111.00
1	B	480	GLN	N-CA-C	-5.51	96.12	111.00

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	4265	0	4152	64	0
1	B	4290	0	4174	63	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	6	0	0	0	0
4	A	277	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	311	0	0	1	0
All	All	9156	0	8326	125	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 7.

All (125) 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:138:LYS:HA	1:A:141:HIS:CE1	2.20	0.76
1:A:303:ARG:HH11	1:A:303:ARG:HB3	1.50	0.76
1:B:492:LEU:HD13	1:B:568:ALA:HB2	1.70	0.74
1:A:492:LEU:HD13	1:A:568:ALA:HB2	1.71	0.72
1:B:276:PHE:CZ	1:B:280:LYS:HD2	2.25	0.72
1:A:276:PHE:CZ	1:A:280:LYS:HD2	2.25	0.71
1:A:479:TYR:C	1:A:481:TYR:N	2.45	0.69
1:A:310:LEU:O	1:A:313:VAL:HG12	1.96	0.65
1:A:494:LEU:HB2	1:A:495:PRO:HD3	1.78	0.65
1:B:479:TYR:C	1:B:481:TYR:N	2.45	0.64
1:B:479:TYR:C	1:B:481:TYR:H	1.95	0.63
1:B:146:GLU:HG3	1:B:147:LYS:H	1.64	0.62
1:A:146:GLU:HG3	1:A:147:LYS:H	1.65	0.61
1:B:494:LEU:HB2	1:B:495:PRO:HD3	1.80	0.61
1:A:313:VAL:HG21	1:A:349:VAL:HG13	1.80	0.61
1:A:101:MET:HG2	1:A:105:GLN:HB2	1.82	0.61
1:A:64:LEU:HG	1:A:65:TRP:H	1.64	0.61
1:B:62:PRO:HG3	1:B:586:TYR:CD2	2.36	0.60
1:A:267:ARG:HH11	1:A:267:ARG:HG2	1.67	0.59
1:B:378:ILE:HG12	1:B:386:GLN:HG2	1.84	0.58
1:A:158:ARG:O	1:A:162:GLN:HG3	2.04	0.58
1:B:138:LYS:HA	1:B:141:HIS:CE1	2.39	0.58
1:B:158:ARG:O	1:B:162:GLN:HG3	2.04	0.58
1:B:359:THR:OG1	1:B:362:GLU:HG3	2.04	0.57
1:A:280:LYS:HE3	1:A:597:TYR:CD2	2.39	0.57
1:B:306:PHE:HB2	1:B:307:PRO:HD3	1.87	0.57
1:A:313:VAL:HG21	1:A:349:VAL:HG22	1.86	0.57
1:B:524:SER:OG	1:B:527:GLU:HG3	2.05	0.57
1:B:218:ALA:O	1:B:222:LEU:HD13	2.05	0.56
1:B:309:LYS:HG3	1:B:387:LEU:HD23	1.87	0.56
1:A:175:PHE:HB3	1:A:187:LEU:HD11	1.88	0.56
1:A:303:ARG:HB3	1:A:303:ARG:NH1	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:LEU:HD22	1:B:245:LEU:HD12	1.87	0.55
1:B:179:LYS:HB3	1:B:181:ILE:HD13	1.87	0.55
1:B:265:TYR:CE2	1:B:271:MET:HG2	2.41	0.55
1:B:409:PHE:HB2	1:B:470:HIS:CD2	2.42	0.55
1:B:309:LYS:HG3	1:B:387:LEU:CD2	2.36	0.55
1:B:181:ILE:HD12	1:B:181:ILE:N	2.22	0.55
1:B:237:LEU:O	1:B:241:ILE:HG13	2.07	0.55
1:A:524:SER:OG	1:A:527:GLU:HG3	2.07	0.54
1:B:101:MET:HG2	1:B:105:GLN:HB2	1.89	0.54
1:A:237:LEU:O	1:A:241:ILE:HG13	2.08	0.53
1:A:479:TYR:C	1:A:481:TYR:H	2.01	0.52
1:A:220:LYS:O	1:A:224:LYS:HG3	2.08	0.52
1:B:376:GLU:HG3	4:B:1135:HOH:O	2.09	0.52
1:A:142:ASN:HB3	1:A:144:GLU:HG3	1.92	0.51
1:A:104:VAL:O	1:A:108:GLU:HG3	2.09	0.51
1:A:357:TYR:HD2	1:A:384:TYR:CZ	2.29	0.50
1:B:459:SER:OG	1:B:460:PRO:HD3	2.12	0.50
1:A:64:LEU:HG	1:A:65:TRP:N	2.27	0.50
1:B:85:ARG:NH2	1:B:277:GLU:HG2	2.28	0.49
1:A:438:THR:HG21	1:A:519:LYS:HD3	1.94	0.49
1:B:104:VAL:O	1:B:108:GLU:HG3	2.13	0.48
1:B:276:PHE:CE1	1:B:280:LYS:HD2	2.47	0.48
1:B:77:TYR:CD1	1:B:284:ASN:HB3	2.49	0.48
1:B:438:THR:HG21	1:B:519:LYS:HD3	1.95	0.48
1:B:433:TYR:CD1	1:B:510:VAL:HG22	2.49	0.48
1:B:492:LEU:CD1	1:B:568:ALA:HB2	2.41	0.47
1:A:433:TYR:CD1	1:A:510:VAL:HG22	2.49	0.47
1:B:226:LEU:HD21	1:B:242:ARG:HG2	1.95	0.47
1:A:146:GLU:HG3	1:A:147:LYS:N	2.30	0.46
1:A:192:LYS:HG3	4:A:1147:HOH:O	2.15	0.46
1:A:253:ILE:HD11	1:A:566:ARG:HB2	1.97	0.46
1:A:492:LEU:HD12	1:A:492:LEU:O	2.16	0.46
1:B:85:ARG:NH2	1:B:277:GLU:CG	2.79	0.46
1:B:146:GLU:HG3	1:B:147:LYS:N	2.30	0.46
1:B:220:LYS:O	1:B:224:LYS:HG3	2.17	0.45
1:B:169:GLN:OE1	1:B:210:THR:HB	2.17	0.45
1:B:78:THR:HG23	1:B:288:ALA:HB1	1.97	0.45
1:A:375:THR:HB	1:B:412:LEU:HD23	1.98	0.45
1:A:405:LYS:NZ	1:A:406:GLU:HG2	2.32	0.45
1:B:176:LYS:HA	1:B:183:PHE:HA	1.99	0.45
1:A:371:LYS:HD3	1:A:424:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:LYS:NZ	1:B:406:GLU:HG2	2.32	0.45
1:B:194:MET:HB3	1:B:222:LEU:HD11	1.98	0.45
1:B:454:SER:HB2	1:B:455:PRO:HD3	1.98	0.44
1:A:515:GLN:H	1:A:515:GLN:CD	2.21	0.44
1:A:452:VAL:CG2	1:A:492:LEU:HG	2.47	0.44
1:A:459:SER:OG	1:A:460:PRO:HD3	2.17	0.44
1:B:276:PHE:CE2	1:B:280:LYS:HD2	2.53	0.44
1:B:151:TYR:CD1	1:B:192:LYS:HG2	2.53	0.44
1:A:280:LYS:HE3	1:A:597:TYR:CE2	2.53	0.43
1:B:515:GLN:CD	1:B:515:GLN:H	2.22	0.43
1:A:309:LYS:C	1:A:310:LEU:HD12	2.38	0.43
1:A:409:PHE:CG	1:A:470:HIS:CD2	3.07	0.43
1:A:481:TYR:HD2	1:A:481:TYR:HA	1.70	0.43
1:B:409:PHE:HB2	1:B:470:HIS:NE2	2.34	0.43
1:A:186:SER:O	1:A:189:GLN:HG2	2.19	0.43
1:A:268:ARG:HA	1:A:269:PRO:HD3	1.90	0.43
1:A:306:PHE:HB2	1:A:307:PRO:HD3	2.01	0.42
1:B:266:ALA:HB2	1:B:276:PHE:CE1	2.54	0.42
1:B:485:LEU:HD23	1:B:485:LEU:N	2.34	0.42
1:A:454:SER:HB2	1:A:455:PRO:HD3	2.00	0.42
1:A:92:GLN:HB3	1:A:274:LEU:HD13	2.01	0.42
1:A:480:GLN:O	1:A:481:TYR:HB2	2.19	0.42
1:A:572:TYR:HA	1:A:575:GLY:O	2.20	0.42
1:A:158:ARG:HG3	1:A:203:LEU:HD11	2.01	0.42
1:B:481:TYR:HD2	1:B:481:TYR:HA	1.80	0.42
1:A:510:VAL:HA	1:A:511:PRO:HD3	1.88	0.42
1:B:75:THR:HA	1:B:76:PRO:HD3	1.88	0.42
1:A:87:ALA:O	1:A:91:VAL:HG23	2.19	0.42
1:B:268:ARG:HA	1:B:269:PRO:HD3	1.93	0.41
1:A:95:ILE:O	1:A:99:GLU:HG3	2.20	0.41
1:B:510:VAL:HA	1:B:511:PRO:HD3	1.90	0.41
1:A:280:LYS:HE3	1:A:597:TYR:HD2	1.81	0.41
1:B:84:ASP:O	1:B:88:GLU:HG3	2.21	0.41
1:A:359:THR:OG1	1:A:362:GLU:HG3	2.20	0.41
1:B:268:ARG:HB3	1:B:270:ASP:OD1	2.20	0.41
1:A:313:VAL:CG2	1:A:349:VAL:HG22	2.49	0.41
1:A:492:LEU:CD1	1:A:568:ALA:HB2	2.45	0.41
1:A:190:ASP:OD2	1:A:193:GLY:HA3	2.21	0.41
1:B:150:LEU:HD21	1:B:194:MET:HE2	2.03	0.41
1:A:190:ASP:O	1:A:194:MET:HG2	2.20	0.41
1:A:226:LEU:HD22	1:A:245:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASP:HB3	1:A:237:LEU:HB3	2.03	0.41
1:A:452:VAL:HG22	1:A:492:LEU:HG	2.03	0.41
1:A:477:SER:O	1:A:480:GLN:HG2	2.20	0.41
1:B:216:GLU:O	1:B:220:LYS:HG3	2.21	0.41
1:B:371:LYS:HD3	1:B:424:GLU:OE2	2.20	0.41
1:A:412:LEU:HD23	1:B:375:THR:HB	2.03	0.41
1:B:87:ALA:O	1:B:91:VAL:HG23	2.20	0.41
1:B:245:LEU:HD23	1:B:245:LEU:HA	1.90	0.41
1:A:276:PHE:CE2	1:A:280:LYS:HD2	2.56	0.40
1:B:195:LEU:O	1:B:199:GLU:HG2	2.21	0.40
1:B:572:TYR:HA	1:B:575:GLY:O	2.22	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	508/549 (92%)	495 (97%)	12 (2%)	1 (0%)	47	44
1	B	512/549 (93%)	499 (98%)	11 (2%)	2 (0%)	34	30
All	All	1020/1098 (93%)	994 (98%)	23 (2%)	3 (0%)	41	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	481	TYR
1	B	77	TYR
1	B	481	TYR

### 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	455/480 (95%)	451 (99%)	4 (1%)	78	83
1	B	458/480 (95%)	454 (99%)	4 (1%)	78	83
All	All	913/960 (95%)	905 (99%)	8 (1%)	78	83

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

Mol	Chain	Res	Type
1	A	267	ARG
1	A	303	ARG
1	A	356	VAL
1	A	492	LEU
1	B	254	GLN
1	B	304	LEU
1	B	485	LEU
1	B	492	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	123	GLN
1	A	142	ASN
1	A	254	GLN
1	A	470	HIS
1	B	141	HIS
1	B	142	ASN
1	B	163	HIS
1	B	254	GLN
1	B	470	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	516/549 (93%)	0.29	43 (8%) <b>11</b>   <b>10</b>	17, 33, 66, 77	0
1	B	519/549 (94%)	0.15	36 (6%) <b>16</b>   <b>16</b>	15, 30, 64, 76	0
All	All	1035/1098 (94%)	0.22	79 (7%) <b>13</b>   <b>13</b>	15, 32, 65, 77	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	575	GLY	7.9
1	B	576	ASP	6.6
1	A	509	ASP	6.5
1	A	576	ASP	6.3
1	B	148	MET	6.3
1	B	147	LYS	6.2
1	B	509	ASP	6.1
1	A	179	LYS	5.9
1	A	146	GLU	5.7
1	A	178	GLU	5.6
1	A	578	PHE	5.4
1	B	575	GLY	4.7
1	B	178	GLU	4.7
1	A	574	HIS	4.7
1	A	181	ILE	4.6
1	B	63	ALA	4.6
1	A	577	GLY	4.5
1	A	584	LYS	4.5
1	A	189	GLN	4.4
1	A	510	VAL	4.3
1	A	357	TYR	4.3
1	A	147	LYS	4.2
1	B	145	VAL	4.1
1	A	80	GLU	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	148	MET	4.0
1	A	522	ASN	4.0
1	A	313	VAL	4.0
1	A	138	LYS	4.0
1	B	146	GLU	3.9
1	B	180	GLY	3.9
1	B	138	LYS	3.9
1	B	142	ASN	3.9
1	B	574	HIS	3.9
1	B	225	LYS	3.8
1	A	81	ARG	3.8
1	A	224	LYS	3.8
1	A	180	GLY	3.7
1	B	189	GLN	3.6
1	A	64	LEU	3.5
1	B	80	GLU	3.5
1	B	100	LYS	3.4
1	A	242	ARG	3.4
1	A	142	ASN	3.3
1	A	225	LYS	3.2
1	B	510	VAL	3.1
1	A	78	THR	3.0
1	B	235	GLU	3.0
1	B	224	LYS	2.9
1	A	144	GLU	2.8
1	A	380	ARG	2.8
1	B	500	THR	2.8
1	B	64	LEU	2.8
1	A	598	ALA	2.7
1	B	522	ASN	2.7
1	B	141	HIS	2.6
1	B	598	ALA	2.6
1	B	480	GLN	2.5
1	A	145	VAL	2.5
1	A	312	PHE	2.5
1	A	587	GLU	2.5
1	B	433	TYR	2.5
1	B	181	ILE	2.5
1	B	179	LYS	2.5
1	A	311	PRO	2.4
1	B	226	LEU	2.4
1	A	573	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	380	ARG	2.3
1	B	584	LYS	2.3
1	B	526	GLU	2.2
1	A	314	ARG	2.2
1	B	177	ASN	2.2
1	A	526	GLU	2.2
1	B	578	PHE	2.1
1	A	572	TYR	2.1
1	B	577	GLY	2.1
1	A	143	ASN	2.1
1	A	68	ASN	2.1
1	A	480	GLN	2.1
1	A	235	GLU	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 monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	901	1/1	0.86	0.14	39,39,39,39	0
2	MG	A	902	1/1	0.88	0.16	53,53,53,53	0
3	HG	B	914	1/1	0.91	0.21	58,58,58,58	1
3	HG	B	909	1/1	0.92	0.17	34,34,34,34	1
3	HG	A	907	1/1	0.93	0.26	57,57,57,57	1
3	HG	A	908	1/1	0.93	0.10	52,52,52,52	1
3	HG	B	913	1/1	0.94	0.08	53,53,53,53	1
3	HG	A	906	1/1	0.95	0.10	59,59,59,59	1
3	HG	B	915	1/1	0.95	0.06	57,57,57,57	1
3	HG	A	903	1/1	0.97	0.12	33,33,33,33	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HG	A	904	1/1	0.99	0.14	23,23,23,23	1
3	HG	B	910	1/1	0.99	0.07	26,26,26,26	1
3	HG	B	911	1/1	0.99	0.05	24,24,24,24	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.