



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:25 PM UTC

PDB ID : 1N1Z / pdb_00001n1z
Title : (+)-Bornyl Diphosphate Synthase: Complex with Mg and pyrophosphate
Authors : Whittington, D.A.; Wise, M.L.; Urbansky, M.; Coates, R.M.; Croteau, R.B.; Christianson, D.W.
Deposited on : 2002-10-21
Resolution : 2.30 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
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

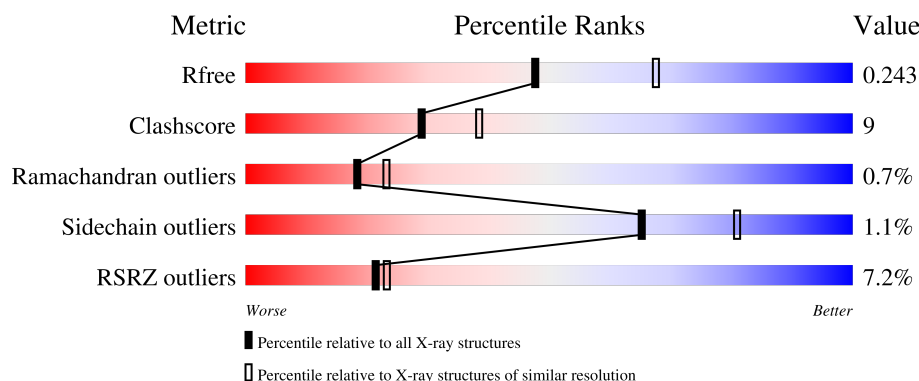
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

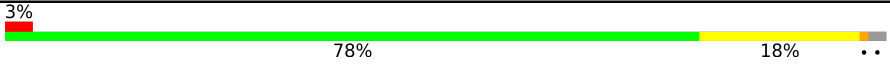
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 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	549	
1	B	549	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9041 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.

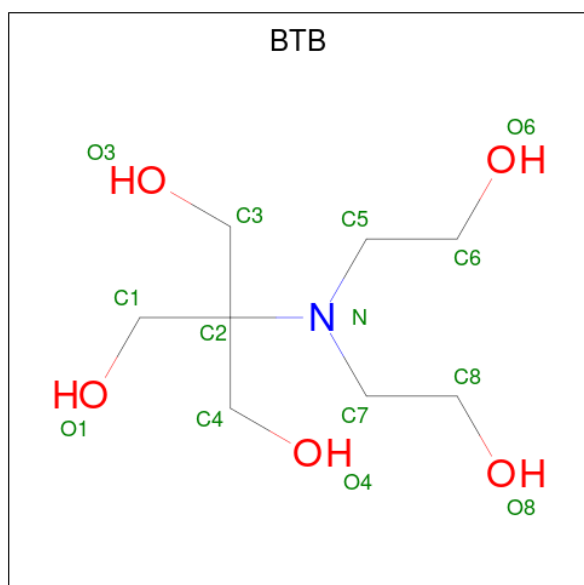
- Molecule 1 is a protein called (+)-bornyl diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4433	2874	736	805	18			
1	B	517	Total	C	N	O	S	0	0	0
			4266	2766	703	779	18			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

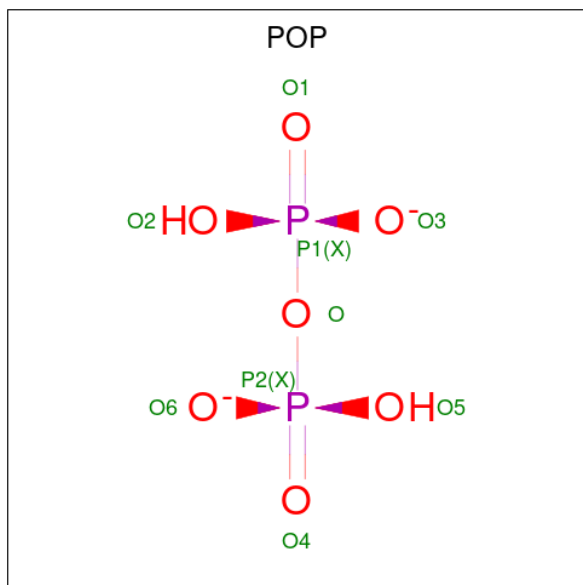
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mg	0	0
			3	3		
2	B	3	Total	Mg	0	0
			3	3		

- Molecule 3 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			9	7	2		
4	B	1	Total	O	P	0	0
			9	7	2		

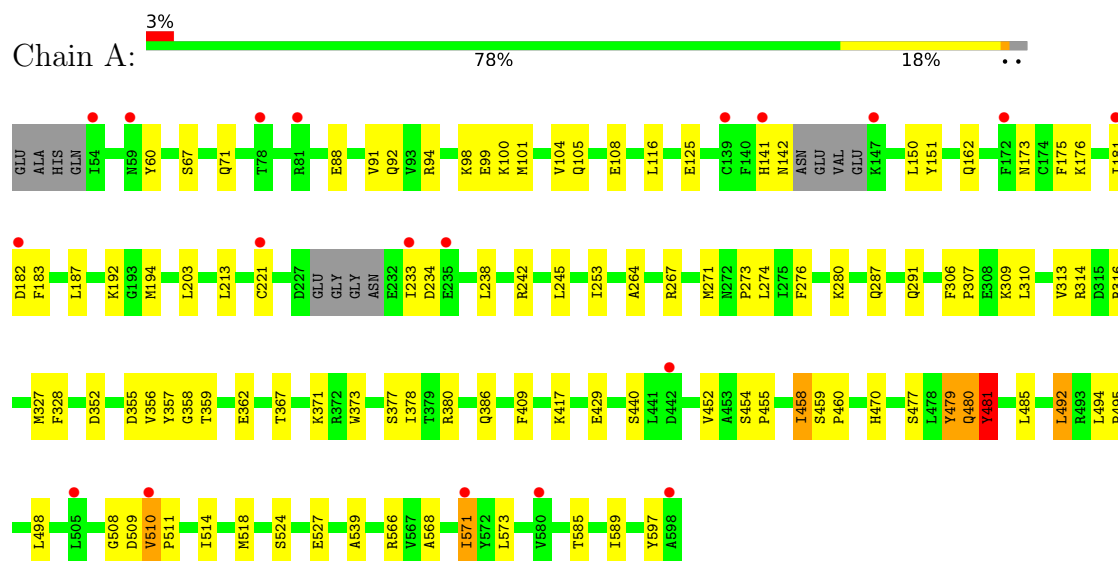
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	151	Total	O	0	0
			151	151		
5	B	139	Total	O	0	0
			139	139		

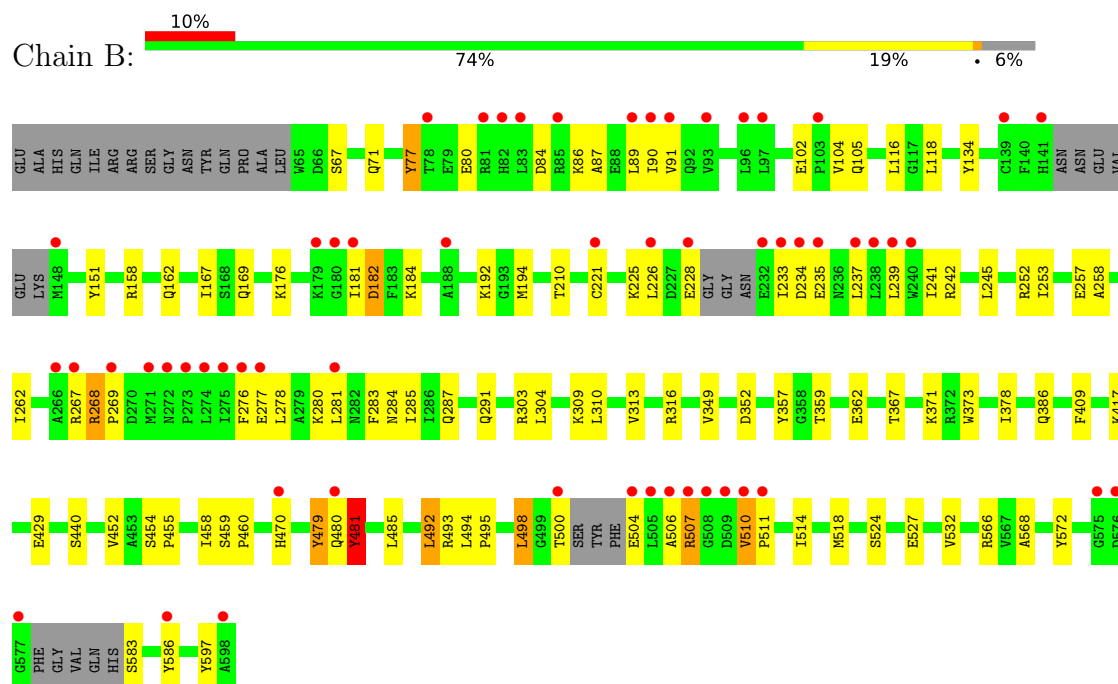
3 Residue-property plots [i](#)

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



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.21Å 117.75Å 120.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.44 – 2.30 29.44 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.44-2.30) 99.7 (29.44-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.25 (at 2.26Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.244 0.213 , 0.243	Depositor DCC
R_{free} test set	3269 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9041	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, POP, BTB

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	0.40	0/4552	0.87	10/6167 (0.2%)
1	B	0.39	0/4377	0.86	10/5928 (0.2%)
All	All	0.39	0/8929	0.86	20/12095 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	480	GLN	N-CA-C	-13.09	97.30	113.01
1	A	480	GLN	N-CA-C	-12.79	96.94	112.54
1	A	357	TYR	N-CA-C	10.18	123.82	111.40
1	B	479	TYR	N-CA-C	7.29	122.00	113.18
1	A	440	SER	N-CA-C	-7.19	100.84	110.55
1	B	458	ILE	N-CA-C	6.99	117.10	110.53
1	A	316	ARG	N-CA-C	6.62	118.38	110.44
1	A	458	ILE	N-CA-C	6.40	116.55	110.53
1	A	358	GLY	N-CA-C	6.32	120.29	112.14
1	A	479	TYR	N-CA-C	6.30	120.83	113.20
1	B	316	ARG	N-CA-C	6.29	117.99	110.44
1	B	357	TYR	N-CA-C	6.14	121.16	113.43
1	B	116	LEU	N-CA-C	-5.95	105.33	113.30
1	B	493	ARG	N-CA-C	5.88	117.36	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	440	SER	N-CA-C	-5.83	103.24	110.41
1	B	268	ARG	CA-C-N	5.65	126.91	119.84
1	B	268	ARG	C-N-CA	5.65	126.91	119.84
1	A	116	LEU	N-CA-C	-5.57	105.84	113.30
1	A	571	ILE	N-CA-C	5.46	115.60	110.30
1	A	481	TYR	N-CA-C	-5.08	99.98	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	481	TYR	Sidechain

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	4433	0	4321	69	0
1	B	4266	0	4157	81	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	14	0	19	0	0
3	B	14	0	19	0	0
4	A	9	0	0	0	0
4	B	9	0	0	0	0
5	A	151	0	0	2	0
5	B	139	0	0	3	0
All	All	9041	0	8516	150	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 9.

All (150) 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:225:LYS:HG3	1:B:233:ILE:HD11	1.38	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:PHE:CZ	1:A:280:LYS:HE3	2.01	0.95
1:B:226:LEU:HD11	1:B:242:ARG:HG2	1.54	0.90
1:A:280:LYS:HE2	1:A:597:TYR:CE2	2.08	0.88
1:B:313:VAL:HG23	1:B:352:ASP:HB2	1.59	0.84
1:B:492:LEU:HD13	1:B:568:ALA:HB2	1.60	0.83
1:A:492:LEU:HD13	1:A:568:ALA:HB2	1.60	0.83
1:B:225:LYS:HG3	1:B:233:ILE:CD1	2.11	0.81
1:B:500:THR:HB	1:B:504:GLU:CD	2.08	0.78
1:A:280:LYS:HE2	1:A:597:TYR:HE2	1.49	0.77
1:A:409:PHE:HB2	1:A:470:HIS:CE1	2.19	0.77
1:B:313:VAL:HG21	1:B:349:VAL:HA	1.68	0.75
1:B:583:SER:HB2	1:B:586:TYR:CD1	2.23	0.73
1:B:409:PHE:HB2	1:B:470:HIS:CE1	2.24	0.72
1:A:409:PHE:HB2	1:A:470:HIS:HE1	1.57	0.69
1:A:585:THR:HG22	1:A:589:ILE:HG13	1.72	0.69
1:A:494:LEU:HB2	1:A:495:PRO:HD3	1.74	0.69
1:B:87:ALA:O	1:B:91:VAL:HG23	1.92	0.69
1:B:479:TYR:C	1:B:481:TYR:N	2.42	0.67
1:B:494:LEU:HB2	1:B:495:PRO:HD3	1.75	0.67
1:B:479:TYR:C	1:B:481:TYR:H	1.94	0.66
1:B:158:ARG:O	1:B:162:GLN:HG3	1.97	0.65
1:A:355:ASP:OD1	1:A:356:VAL:HG23	1.98	0.64
1:B:313:VAL:CG2	1:B:349:VAL:HA	2.28	0.63
1:A:359:THR:OG1	1:A:362:GLU:HG3	1.99	0.62
1:B:80:GLU:HG2	1:B:84:ASP:OD2	1.99	0.62
1:B:239:LEU:HD12	1:B:267:ARG:NH2	2.15	0.62
1:B:239:LEU:HD12	1:B:267:ARG:HH22	1.66	0.61
1:B:429:GLU:O	1:B:510:VAL:HG23	2.01	0.60
1:A:98:LYS:HE3	1:A:125:GLU:HG2	1.83	0.60
1:B:409:PHE:HB2	1:B:470:HIS:HE1	1.66	0.60
1:A:104:VAL:O	1:A:108:GLU:HG3	2.00	0.59
1:A:479:TYR:C	1:A:481:TYR:N	2.53	0.58
1:B:181:ILE:O	1:B:181:ILE:HG22	2.02	0.58
1:B:225:LYS:CG	1:B:233:ILE:HD11	2.22	0.58
1:A:373:TRP:HB2	5:A:911:HOH:O	2.03	0.58
1:B:181:ILE:O	1:B:182:ASP:HB2	2.04	0.56
1:A:101:MET:HG2	1:A:105:GLN:HB2	1.86	0.56
1:A:492:LEU:HD12	1:A:492:LEU:O	2.06	0.56
1:B:276:PHE:CZ	1:B:280:LYS:HD2	2.41	0.56
1:B:583:SER:HB2	1:B:586:TYR:HD1	1.69	0.56
1:B:417:LYS:HE3	1:B:479:TYR:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:LYS:HE3	1:B:233:ILE:HD11	1.87	0.55
1:B:239:LEU:CD1	1:B:267:ARG:HH22	2.20	0.55
1:B:310:LEU:O	1:B:313:VAL:HG12	2.07	0.55
1:B:524:SER:OG	1:B:527:GLU:HG3	2.07	0.54
1:B:237:LEU:O	1:B:241:ILE:HG13	2.07	0.54
1:A:454:SER:HB2	1:A:455:PRO:HD3	1.89	0.54
1:A:514:ILE:HG22	1:A:518:MET:HE2	1.90	0.54
1:A:310:LEU:O	1:A:313:VAL:HG22	2.08	0.53
1:A:162:GLN:HG3	1:A:203:LEU:HD21	1.91	0.53
1:A:417:LYS:HE3	1:A:479:TYR:HB3	1.91	0.53
1:A:380:ARG:HH21	1:A:380:ARG:HG3	1.74	0.52
1:B:452:VAL:HG22	1:B:492:LEU:HG	1.90	0.52
1:A:150:LEU:HD21	1:A:194:MET:HE2	1.91	0.52
1:B:454:SER:HB2	1:B:455:PRO:HD3	1.91	0.52
1:A:524:SER:OG	1:A:527:GLU:HG3	2.09	0.52
1:A:429:GLU:O	1:A:510:VAL:HG23	2.10	0.52
1:A:233:ILE:HG22	1:A:234:ASP:N	2.25	0.52
1:B:118:LEU:HD22	1:B:278:LEU:HG	1.91	0.52
1:B:226:LEU:O	1:B:226:LEU:HD23	2.09	0.52
1:B:253:ILE:HD11	1:B:566:ARG:HB2	1.91	0.52
1:A:92:GLN:HB3	1:A:274:LEU:HD13	1.92	0.51
1:B:514:ILE:HG22	1:B:518:MET:HE2	1.91	0.51
1:A:176:LYS:HA	1:A:183:PHE:HA	1.93	0.51
1:A:480:GLN:O	1:A:481:TYR:HB2	2.11	0.51
1:B:313:VAL:HG23	1:B:352:ASP:CB	2.36	0.51
1:B:492:LEU:HD12	1:B:492:LEU:O	2.11	0.51
1:B:504:GLU:N	1:B:507:ARG:HH21	2.09	0.51
1:B:102:GLU:HB3	1:B:105:GLN:HG3	1.94	0.50
1:B:373:TRP:HB2	5:B:938:HOH:O	2.11	0.50
1:B:409:PHE:CB	1:B:470:HIS:CE1	2.93	0.50
1:A:141:HIS:O	1:A:142:ASN:C	2.55	0.50
1:A:452:VAL:HG22	1:A:492:LEU:HG	1.93	0.50
1:B:194:MET:HG3	1:B:221:CYS:SG	2.51	0.49
1:B:89:LEU:HD11	1:B:277:GLU:HG2	1.95	0.49
1:B:77:TYR:CD1	1:B:284:ASN:HB3	2.47	0.49
1:B:498:LEU:HD13	1:B:532:VAL:HG11	1.95	0.49
1:A:60:TYR:CD1	1:A:314:ARG:HG3	2.47	0.49
1:A:91:VAL:HA	1:A:94:ARG:HH12	1.76	0.49
1:B:303:ARG:NH2	5:B:1018:HOH:O	2.44	0.49
1:B:309:LYS:C	1:B:310:LEU:HD12	2.37	0.49
1:A:98:LYS:HE3	1:A:125:GLU:CG	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:ILE:HG12	1:B:386:GLN:HG2	1.95	0.48
1:A:182:ASP:HA	1:A:213:LEU:HD21	1.95	0.48
1:B:359:THR:OG1	1:B:362:GLU:HG3	2.14	0.47
1:B:258:ALA:O	1:B:262:ILE:HG13	2.15	0.47
1:A:479:TYR:C	1:A:481:TYR:H	2.11	0.47
1:B:583:SER:HB2	1:B:586:TYR:CE1	2.50	0.47
1:B:169:GLN:OE1	1:B:210:THR:HB	2.15	0.46
1:A:194:MET:HG3	1:A:221:CYS:SG	2.55	0.46
1:A:409:PHE:CB	1:A:470:HIS:CE1	2.95	0.46
1:A:458:ILE:HG21	1:A:485:LEU:HD22	1.98	0.46
1:B:118:LEU:HD13	1:B:278:LEU:HD23	1.97	0.46
1:B:233:ILE:HG22	1:B:234:ASP:N	2.29	0.46
1:B:452:VAL:CG2	1:B:492:LEU:HG	2.45	0.46
1:B:367:THR:O	1:B:371:LYS:HG3	2.16	0.46
1:A:352:ASP:O	1:A:356:VAL:HB	2.16	0.45
1:A:452:VAL:CG2	1:A:492:LEU:HG	2.46	0.45
1:B:281:LEU:O	1:B:285:ILE:HG13	2.17	0.45
1:A:287:GLN:O	1:A:291:GLN:HG3	2.16	0.45
1:B:409:PHE:CB	1:B:470:HIS:HE1	2.29	0.45
1:A:378:ILE:HG12	1:A:386:GLN:HG2	1.99	0.45
1:B:510:VAL:O	1:B:511:PRO:C	2.59	0.45
1:A:306:PHE:N	1:A:307:PRO:CD	2.80	0.44
1:B:498:LEU:HD23	1:B:572:TYR:CE2	2.53	0.44
1:B:409:PHE:CG	1:B:470:HIS:ND1	2.86	0.44
1:A:233:ILE:HG22	1:A:234:ASP:H	1.82	0.44
1:B:429:GLU:O	1:B:510:VAL:CG2	2.65	0.43
1:A:571:ILE:C	1:A:573:LEU:H	2.27	0.43
1:A:459:SER:OG	1:A:460:PRO:HD3	2.18	0.43
1:B:89:LEU:CD1	1:B:277:GLU:HG2	2.48	0.43
1:B:252:ARG:NH1	1:B:257:GLU:OE2	2.44	0.43
1:A:271:MET:HE3	1:A:273:PRO:HA	2.00	0.43
1:B:86:LYS:O	1:B:90:ILE:HG13	2.19	0.43
1:A:245:LEU:HD23	1:A:245:LEU:HA	1.92	0.42
1:A:238:LEU:CD2	1:A:242:ARG:HH12	2.32	0.42
1:A:355:ASP:HB2	1:A:509:ASP:OD1	2.19	0.42
1:A:173:ASN:C	1:A:175:PHE:H	2.27	0.42
1:B:226:LEU:C	1:B:228:GLU:H	2.26	0.42
1:B:176:LYS:O	1:B:184:LYS:HE3	2.20	0.42
1:A:264:ALA:HA	1:A:267:ARG:CZ	2.50	0.42
1:B:280:LYS:HG2	1:B:597:TYR:CD2	2.55	0.42
1:A:175:PHE:HB3	1:A:187:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:TYR:HD2	1:A:481:TYR:HA	1.68	0.42
1:B:104:VAL:HG13	1:B:105:GLN:N	2.34	0.42
1:B:151:TYR:CD1	1:B:192:LYS:HG2	2.55	0.42
1:B:233:ILE:HG22	1:B:234:ASP:H	1.85	0.42
1:B:287:GLN:O	1:B:291:GLN:HG3	2.19	0.42
1:A:151:TYR:CD1	1:A:192:LYS:HG2	2.54	0.42
1:B:268:ARG:HA	1:B:269:PRO:HD3	1.92	0.42
1:A:477:SER:O	1:A:480:GLN:HG2	2.20	0.41
1:A:253:ILE:HD11	1:A:566:ARG:HB2	2.01	0.41
1:B:283:PHE:CD2	1:B:597:TYR:HB2	2.55	0.41
1:A:194:MET:HE2	1:A:194:MET:HA	2.01	0.41
1:A:67:SER:O	1:A:71:GLN:HG3	2.21	0.41
1:A:327:MET:HE2	1:A:328:PHE:CE1	2.56	0.41
1:A:88:GLU:O	1:A:91:VAL:HB	2.20	0.41
1:B:459:SER:OG	1:B:460:PRO:HD3	2.21	0.41
1:A:367:THR:O	1:A:371:LYS:HG3	2.20	0.41
1:A:539:ALA:HA	5:A:964:HOH:O	2.20	0.41
1:A:309:LYS:C	1:A:310:LEU:HD12	2.46	0.41
1:B:134:TYR:HE1	1:B:167:ILE:CD1	2.33	0.41
1:B:245:LEU:HD23	1:B:245:LEU:HA	1.94	0.41
1:B:67:SER:HB2	5:B:988:HOH:O	2.20	0.41
1:A:99:GLU:O	1:A:100:LYS:C	2.63	0.40
1:A:377:SER:HB2	1:A:380:ARG:NH1	2.36	0.40
1:A:181:ILE:HG13	1:A:182:ASP:OD1	2.20	0.40
1:A:510:VAL:O	1:A:511:PRO:C	2.65	0.40
1:B:514:ILE:O	1:B:518:MET:HG3	2.21	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	531/549 (97%)	515 (97%)	14 (3%)	2 (0%)	30	38
1	B	507/549 (92%)	480 (95%)	22 (4%)	5 (1%)	12	15
All	All	1038/1098 (94%)	995 (96%)	36 (4%)	7 (1%)	18	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	481	TYR
1	B	481	TYR
1	B	506	ALA
1	B	507	ARG
1	B	77	TYR
1	B	182	ASP
1	A	508	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	471/480 (98%)	468 (99%)	3 (1%)	78	89
1	B	454/480 (95%)	447 (98%)	7 (2%)	57	75
All	All	925/960 (96%)	915 (99%)	10 (1%)	65	81

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

Mol	Chain	Res	Type
1	A	492	LEU
1	A	498	LEU
1	A	510	VAL
1	B	71	GLN
1	B	235	GLU
1	B	304	LEU
1	B	485	LEU
1	B	492	LEU
1	B	498	LEU

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Mol	Chain	Res	Type
1	B	510	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	106	GLN
1	A	173	ASN
1	A	223	GLN
1	A	236	ASN
1	A	254	GLN
1	A	407	HIS
1	A	531	HIS
1	B	82	HIS
1	B	137	HIS
1	B	141	HIS
1	B	173	ASN
1	B	236	ASN
1	B	254	GLN
1	B	282	ASN
1	B	407	HIS
1	B	531	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 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	$\# Z > 2$
4	POP	B	902	2	6,8,8	1.83	2 (33%)	12,13,13	1.13	1 (8%)
4	POP	A	901	2	6,8,8	1.99	2 (33%)	12,13,13	1.21	1 (8%)
3	BTB	A	800	-	13,13,13	2.43	4 (30%)	7,16,16	0.91	0
3	BTB	B	801	-	13,13,13	2.35	4 (30%)	7,16,16	1.03	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
4	POP	B	902	2	-	0/6/6/6	-
4	POP	A	901	2	-	0/6/6/6	-
3	BTB	A	800	-	-	5/21/21/21	-
3	BTB	B	801	-	-	4/21/21/21	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	BTB	C1-C2	5.99	1.60	1.53
3	A	800	BTB	C4-C2	5.83	1.60	1.53
3	A	800	BTB	C1-C2	4.61	1.58	1.53
3	B	801	BTB	C3-C2	3.82	1.57	1.53
3	B	801	BTB	C4-C2	3.56	1.57	1.53
3	A	800	BTB	C3-C2	3.45	1.57	1.53
4	A	901	POP	P2-O4	3.24	1.60	1.50
4	B	902	POP	P2-O4	2.85	1.59	1.50
4	A	901	POP	P1-O1	2.83	1.59	1.50
4	B	902	POP	P1-O1	2.83	1.59	1.50
3	A	800	BTB	C2-N	2.51	1.53	1.48
3	B	801	BTB	C2-N	2.44	1.53	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	POP	O3-P1-O	2.80	114.03	104.64
4	B	902	POP	O3-P1-O	2.40	112.69	104.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	800	BTB	C1-C2-C4-O4
3	B	801	BTB	O1-C1-C2-C3
3	B	801	BTB	O1-C1-C2-C4
3	B	801	BTB	O1-C1-C2-N
3	A	800	BTB	N-C5-C6-O6
3	B	801	BTB	N-C5-C6-O6
3	A	800	BTB	N-C7-C8-O8
3	A	800	BTB	N-C2-C4-O4
3	A	800	BTB	C3-C2-C4-O4

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, 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	537/549 (97%)	0.19	19 (3%)	47	49	21, 39, 70, 93	0
1	B	517/549 (94%)	0.47	57 (11%)	10	11	18, 40, 81, 97	0
All	All	1054/1098 (95%)	0.33	76 (7%)	21	23	18, 39, 78, 97	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	506	ALA	8.4
1	B	500	THR	5.9
1	B	274	LEU	5.8
1	B	508	GLY	5.7
1	B	510	VAL	5.3
1	B	577	GLY	4.6
1	B	504	GLU	4.4
1	B	234	ASP	4.1
1	B	507	ARG	3.9
1	A	598	ALA	3.9
1	B	90	ILE	3.9
1	B	505	LEU	3.7
1	B	148	MET	3.7
1	A	54	ILE	3.4
1	B	91	VAL	3.3
1	A	141	HIS	3.2
1	B	586	TYR	3.2
1	B	179	LYS	3.2
1	B	576	ASP	3.2
1	A	221	CYS	3.2
1	B	275	ILE	3.2
1	B	233	ILE	3.1
1	B	81	ARG	3.0
1	B	509	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	228	GLU	3.0
1	A	571	ILE	3.0
1	B	226	LEU	2.9
1	B	239	LEU	2.9
1	B	180	GLY	2.9
1	B	139	CYS	2.9
1	B	221	CYS	2.8
1	A	147	LYS	2.8
1	B	237	LEU	2.8
1	B	575	GLY	2.7
1	B	232	GLU	2.7
1	B	511	PRO	2.7
1	B	269	PRO	2.7
1	B	89	LEU	2.7
1	B	272	ASN	2.6
1	A	233	ILE	2.6
1	B	181	ILE	2.6
1	B	240	TRP	2.6
1	B	273	PRO	2.6
1	B	480	GLN	2.6
1	B	82	HIS	2.6
1	B	598	ALA	2.5
1	B	276	PHE	2.4
1	B	141	HIS	2.4
1	A	81	ARG	2.4
1	A	235	GLU	2.4
1	B	235	GLU	2.4
1	A	181	ILE	2.4
1	B	96	LEU	2.4
1	A	78	THR	2.4
1	A	510	VAL	2.4
1	B	281	LEU	2.4
1	B	188	ALA	2.3
1	B	78	THR	2.3
1	B	267	ARG	2.3
1	B	97	LEU	2.3
1	B	266	ALA	2.2
1	B	85	ARG	2.2
1	A	580	VAL	2.1
1	B	238	LEU	2.1
1	B	271	MET	2.1
1	B	93	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	505	LEU	2.1
1	B	277	GLU	2.1
1	B	103	PRO	2.1
1	A	172	PHE	2.1
1	A	139	CYS	2.1
1	A	442	ASP	2.1
1	B	470	HIS	2.1
1	A	59	ASN	2.0
1	A	182	ASP	2.0
1	B	83	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 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	BTB	A	800	14/14	0.87	0.14	29,39,45,45	0
3	BTB	B	801	14/14	0.87	0.16	43,49,52,55	0
2	MG	A	702	1/1	0.98	0.04	40,40,40,40	0
2	MG	B	706	1/1	0.98	0.04	29,29,29,29	0
2	MG	B	705	1/1	0.99	0.02	24,24,24,24	0
4	POP	A	901	9/9	0.99	0.04	27,31,34,35	0
4	POP	B	902	9/9	0.99	0.04	23,25,29,30	0
2	MG	A	701	1/1	1.00	0.02	31,31,31,31	0
2	MG	A	703	1/1	1.00	0.03	29,29,29,29	0
2	MG	B	704	1/1	1.00	0.01	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.