



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:06 PM UTC

PDB ID : 1N23 / pdb_00001n23
Title : (+)-Bornyl diphosphate synthase: Complex with Mg, pyrophosphate, and (1R,4S)-2-azabornane
Authors : Whittington, D.A.; Wise, M.L.; Urbansky, M.; Coates, R.M.; Croteau, R.B.; Christianson, D.W.
Deposited on : 2002-10-21
Resolution : 2.40 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

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

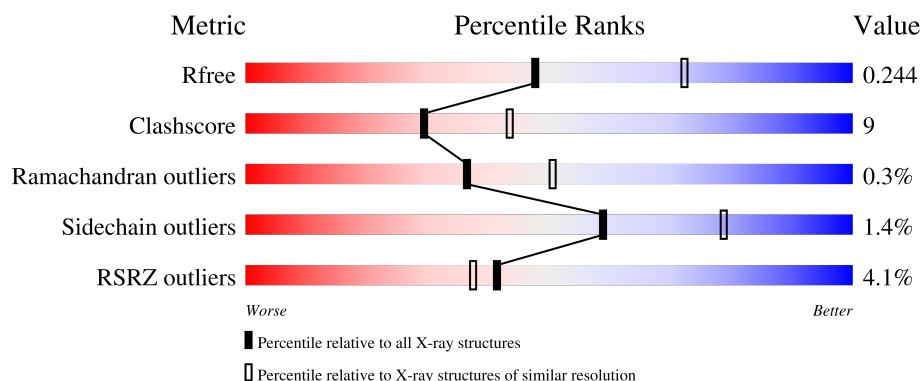
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

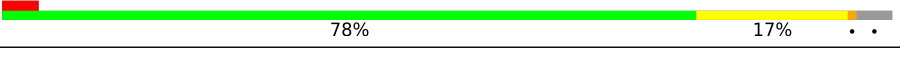
The reported resolution of this entry is 2.40 Å.

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	 4% 77% 19% ..
1	B	549	 4% 78% 17% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9008 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.

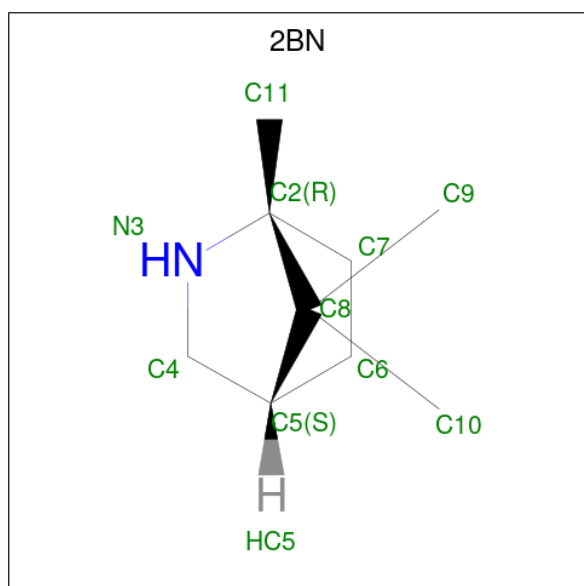
- Molecule 1 is a protein called (+)-bornyl diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	0	0
			4398	2852	728	800	18			
1	B	527	Total	C	N	O	S	0	0	0
			4344	2817	716	794	17			

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

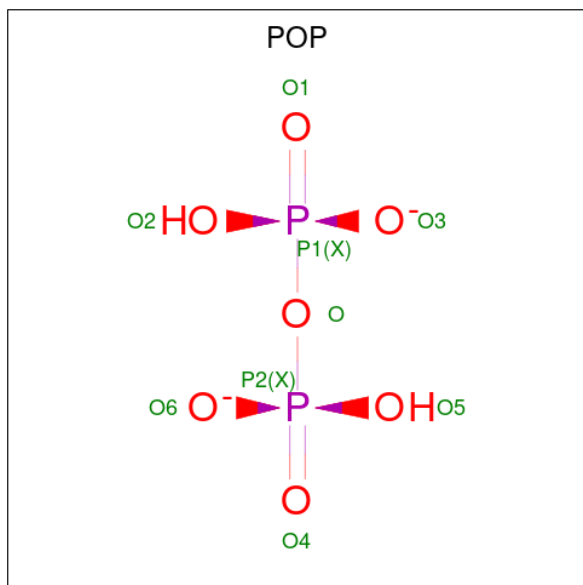
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mg	0	0
			3	3		
2	B	3	Total	Mg	0	0
			3	3		

- Molecule 3 is (1R,4S)-2-AZABORNANE (CCD ID: 2BN) (formula: C₉H₁₇N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			10	9	1		
3	B	1	Total	C	N	0	0
			10	9	1		

- 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		

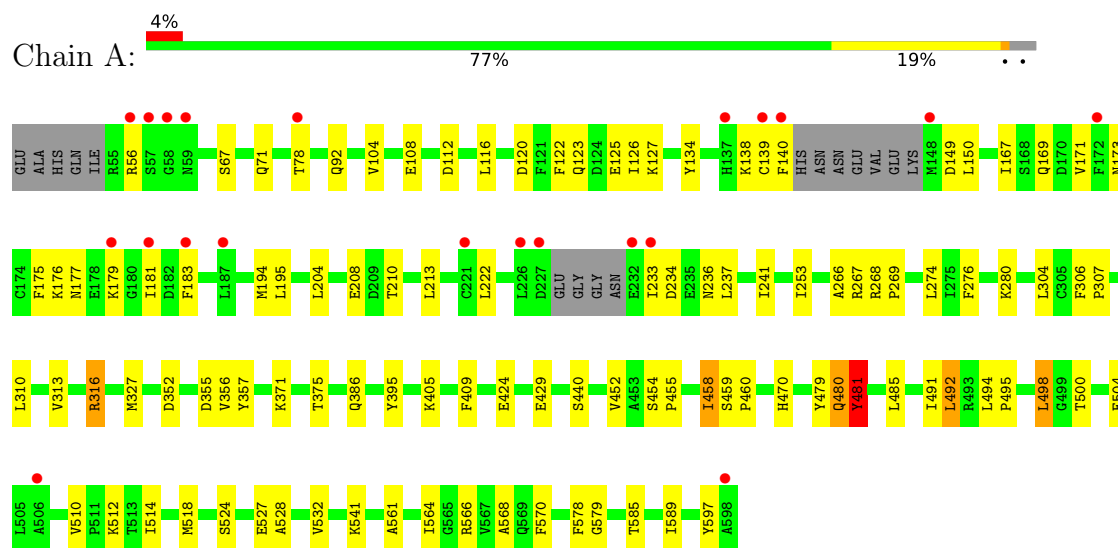
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	101	Total	O	0	0
			101	101		
5	B	121	Total	O	0	0
			121	121		

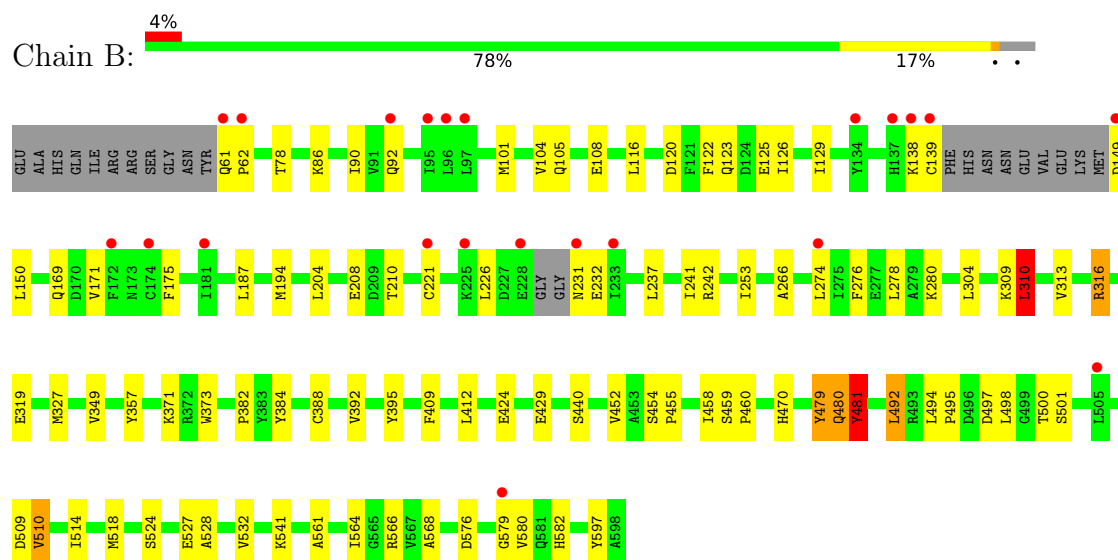
3 Residue-property plots [i](#)

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, α , β , γ	100.99Å 118.18Å 120.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.36 – 2.40 29.36 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.36-2.40) 99.4 (29.36-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.06 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.244 0.207 , 0.244	Depositor DCC
R_{free} test set	2864 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9008	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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, 2BN, POP

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	0/4516	0.85	9/6119 (0.1%)
1	B	0.42	0/4460	0.87	10/6046 (0.2%)
All	All	0.41	0/8976	0.86	19/12165 (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	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	480	GLN	N-CA-C	-12.46	98.06	113.01
1	A	480	GLN	N-CA-C	-11.84	98.09	111.71
1	B	479	TYR	N-CA-C	8.18	123.07	113.18
1	B	357	TYR	N-CA-C	7.23	122.66	113.55
1	B	440	SER	N-CA-C	-7.14	100.91	110.55
1	A	357	TYR	N-CA-C	6.95	121.80	113.12
1	A	440	SER	N-CA-C	-6.47	101.82	110.55
1	A	116	LEU	N-CA-C	-6.36	104.78	113.30
1	B	116	LEU	N-CA-C	-6.24	104.94	113.30
1	A	78	THR	N-CA-C	-5.99	105.70	114.39
1	B	316	ARG	N-CA-C	5.93	117.56	110.44
1	A	316	ARG	N-CA-C	5.83	117.44	110.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	458	ILE	N-CA-C	5.71	115.89	110.53
1	B	310	LEU	CA-C-N	5.46	125.29	119.28
1	B	310	LEU	C-N-CA	5.46	125.29	119.28
1	B	580	VAL	N-CA-C	5.38	116.01	110.36
1	A	481	TYR	N-CA-C	-5.27	99.58	110.80
1	A	458	ILE	N-CA-C	5.25	115.92	110.82
1	A	386	GLN	N-CA-C	-5.12	105.69	111.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	395	TYR	Sidechain
1	B	395	TYR	Sidechain
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	4398	0	4284	81	0
1	B	4344	0	4229	69	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	10	0	17	0	0
3	B	10	0	17	0	0
4	A	9	0	0	0	0
4	B	9	0	0	0	0
5	A	101	0	0	1	0
5	B	121	0	0	4	0
All	All	9008	0	8547	149	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 (149) 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:429:GLU:HB3	1:A:510:VAL:HG21	1.20	1.17
1:B:429:GLU:HB3	1:B:510:VAL:HG21	1.43	0.98
1:B:492:LEU:HD13	1:B:568:ALA:HB2	1.52	0.91
1:B:313:VAL:HG11	1:B:349:VAL:HG22	1.56	0.86
1:A:492:LEU:HD13	1:A:568:ALA:HB2	1.61	0.82
1:B:316:ARG:NH1	1:B:579:GLY:HA2	1.94	0.82
1:A:316:ARG:NH1	1:A:579:GLY:HA2	1.95	0.82
1:B:226:LEU:HD11	1:B:242:ARG:HE	1.44	0.82
1:A:316:ARG:HH12	1:A:579:GLY:HA2	1.44	0.81
1:B:266:ALA:HB2	1:B:276:PHE:CE1	2.16	0.80
1:B:316:ARG:HH12	1:B:579:GLY:HA2	1.49	0.77
1:B:429:GLU:HB3	1:B:510:VAL:CG2	2.19	0.73
1:A:56:ARG:HH21	1:A:56:ARG:HG2	1.52	0.73
1:A:355:ASP:OD1	1:A:356:VAL:HG23	1.92	0.70
1:A:429:GLU:HB3	1:A:510:VAL:CG2	2.13	0.69
1:B:479:TYR:C	1:B:481:TYR:N	2.51	0.67
1:A:409:PHE:HB2	1:A:470:HIS:CE1	2.29	0.67
1:B:494:LEU:HB2	1:B:495:PRO:HD3	1.76	0.66
1:A:494:LEU:HB2	1:A:495:PRO:HD3	1.77	0.65
1:B:309:LYS:C	1:B:310:LEU:HD23	2.22	0.64
1:B:409:PHE:HB2	1:B:470:HIS:CE1	2.33	0.64
1:A:104:VAL:O	1:A:108:GLU:HG3	1.97	0.64
1:A:429:GLU:CB	1:A:510:VAL:HG21	2.12	0.63
1:B:92:GLN:HB3	1:B:274:LEU:HD21	1.81	0.63
1:A:179:LYS:HD3	1:A:181:ILE:HD11	1.81	0.63
1:B:104:VAL:O	1:B:108:GLU:HG3	2.00	0.62
1:A:452:VAL:HG22	1:A:492:LEU:HG	1.82	0.62
1:B:452:VAL:HG22	1:B:492:LEU:HG	1.81	0.61
1:A:452:VAL:CG2	1:A:492:LEU:HG	2.30	0.61
1:B:313:VAL:CG1	1:B:349:VAL:HG22	2.32	0.59
1:B:492:LEU:HD13	1:B:568:ALA:CB	2.30	0.58
1:B:524:SER:OG	1:B:527:GLU:HG3	2.04	0.58
1:B:92:GLN:CB	1:B:274:LEU:HD21	2.33	0.58
1:A:176:LYS:HA	1:A:183:PHE:HA	1.85	0.58
1:B:231:ASN:CG	1:B:232:GLU:H	2.11	0.58
1:B:169:GLN:OE1	1:B:210:THR:HB	2.04	0.57
1:A:504:GLU:OE1	1:A:512:LYS:HE3	2.03	0.57
1:A:169:GLN:OE1	1:A:210:THR:HB	2.05	0.57
1:B:120:ASP:HA	1:B:123:GLN:HE21	1.70	0.57
1:A:524:SER:OG	1:A:527:GLU:HG3	2.04	0.57
1:B:479:TYR:C	1:B:481:TYR:H	2.05	0.57
1:A:179:LYS:HD3	1:A:181:ILE:CD1	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:THR:O	1:A:504:GLU:HG3	2.06	0.56
1:B:276:PHE:CZ	1:B:280:LYS:HD2	2.40	0.56
1:B:514:ILE:HB	5:B:1005:HOH:O	2.06	0.56
1:B:452:VAL:CG2	1:B:492:LEU:HG	2.35	0.56
1:A:236:ASN:OD1	1:A:267:ARG:HD2	2.05	0.55
1:A:120:ASP:HA	1:A:123:GLN:HE21	1.71	0.55
1:A:480:GLN:O	1:A:481:TYR:HB2	2.06	0.55
1:B:101:MET:HG2	1:B:105:GLN:HB2	1.88	0.55
1:A:514:ILE:HG22	1:A:518:MET:HE2	1.88	0.54
1:B:310:LEU:HD22	1:B:384:TYR:HB2	1.88	0.54
1:A:181:ILE:O	1:A:213:LEU:HD21	2.08	0.54
1:B:528:ALA:O	1:B:532:VAL:HG23	2.06	0.54
1:A:276:PHE:CZ	1:A:280:LYS:HD2	2.42	0.54
1:A:280:LYS:HG2	1:A:597:TYR:CD2	2.43	0.54
1:A:585:THR:HG22	1:A:589:ILE:HG13	1.89	0.54
1:B:382:PRO:HD3	5:B:909:HOH:O	2.08	0.53
1:A:56:ARG:HG2	1:A:56:ARG:NH2	2.22	0.53
1:A:139:CYS:O	1:A:171:VAL:HG13	2.09	0.53
1:B:373:TRP:HB2	5:B:926:HOH:O	2.10	0.52
1:B:514:ILE:HG22	1:B:518:MET:HE2	1.89	0.52
1:A:454:SER:HB2	1:A:455:PRO:HD3	1.91	0.52
1:A:528:ALA:O	1:A:532:VAL:HG23	2.10	0.52
1:B:122:PHE:O	1:B:126:ILE:HG13	2.11	0.51
1:B:253:ILE:HD11	1:B:566:ARG:HB2	1.91	0.51
1:A:112:ASP:CG	1:A:268:ARG:HH12	2.18	0.51
1:B:280:LYS:HG2	1:B:597:TYR:CD2	2.46	0.51
1:B:237:LEU:O	1:B:241:ILE:HG13	2.11	0.51
1:A:122:PHE:O	1:A:126:ILE:HG13	2.11	0.50
1:A:253:ILE:HD11	1:A:566:ARG:HB2	1.92	0.50
1:B:492:LEU:HD12	1:B:492:LEU:O	2.10	0.50
1:B:194:MET:HG3	1:B:221:CYS:SG	2.50	0.50
1:A:479:TYR:C	1:A:481:TYR:N	2.58	0.50
1:B:497:ASP:O	1:B:501:SER:HB3	2.12	0.50
1:A:237:LEU:O	1:A:241:ILE:HG13	2.12	0.50
1:A:375:THR:HB	1:B:412:LEU:HD23	1.94	0.49
1:B:86:LYS:O	1:B:90:ILE:HG12	2.12	0.49
1:A:316:ARG:HH12	1:A:579:GLY:CA	2.20	0.49
1:A:92:GLN:HB3	1:A:274:LEU:HD13	1.94	0.49
1:A:280:LYS:HE3	1:A:597:TYR:HD2	1.78	0.48
1:A:204:LEU:HG	1:A:541:LYS:HG3	1.95	0.48
1:A:266:ALA:HB2	1:A:276:PHE:CE1	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:LEU:HD12	1:A:492:LEU:O	2.14	0.47
1:A:429:GLU:O	1:A:510:VAL:HG22	2.14	0.47
1:A:173:ASN:C	1:A:175:PHE:H	2.22	0.47
1:A:459:SER:OG	1:A:460:PRO:HD3	2.15	0.47
1:B:454:SER:HB2	1:B:455:PRO:HD3	1.96	0.46
1:B:150:LEU:HD21	1:B:194:MET:HE2	1.98	0.46
1:A:492:LEU:HD13	1:A:568:ALA:CB	2.40	0.46
1:A:561:ALA:O	1:A:564:ILE:HG22	2.16	0.46
1:A:179:LYS:CE	1:A:181:ILE:HD11	2.46	0.46
1:A:316:ARG:NH1	1:A:578:PHE:O	2.49	0.46
1:A:138:LYS:C	1:A:140:PHE:H	2.23	0.45
1:A:491:ILE:O	1:A:495:PRO:CD	2.64	0.45
1:B:480:GLN:O	1:B:481:TYR:HB2	2.16	0.45
1:A:125:GLU:OE1	1:A:125:GLU:N	2.48	0.45
1:A:195:LEU:HA	1:A:222:LEU:HD11	1.99	0.45
1:B:319:GLU:OE2	1:B:582:HIS:HD2	1.99	0.45
1:B:561:ALA:O	1:B:564:ILE:HG22	2.16	0.45
1:B:204:LEU:HG	1:B:541:LYS:HG3	1.97	0.45
1:B:61:GLN:HA	1:B:62:PRO:HD3	1.80	0.45
1:B:175:PHE:HB3	1:B:187:LEU:HD11	1.98	0.45
1:A:498:LEU:HD13	1:A:532:VAL:HG11	2.00	0.44
1:A:371:LYS:HD3	1:A:424:GLU:OE2	2.17	0.44
1:B:138:LYS:HG3	1:B:139:CYS:H	1.81	0.44
1:B:226:LEU:HD21	1:B:242:ARG:HG2	1.99	0.44
1:A:150:LEU:HD21	1:A:194:MET:HE2	1.99	0.44
1:A:112:ASP:OD1	1:A:268:ARG:NH1	2.44	0.44
1:B:231:ASN:ND2	1:B:232:GLU:N	2.66	0.44
1:A:134:TYR:CE1	1:A:167:ILE:HD11	2.53	0.44
1:A:481:TYR:HD2	1:A:481:TYR:HA	1.60	0.44
1:B:125:GLU:OE1	1:B:125:GLU:N	2.48	0.44
1:B:409:PHE:CB	1:B:470:HIS:CE1	3.00	0.43
1:B:125:GLU:O	1:B:129:ILE:HG13	2.18	0.43
1:A:138:LYS:C	1:A:140:PHE:N	2.76	0.43
1:B:316:ARG:HH12	1:B:579:GLY:CA	2.25	0.43
1:B:481:TYR:HB2	5:B:979:HOH:O	2.19	0.43
1:A:409:PHE:HB2	1:A:470:HIS:HE1	1.82	0.43
1:A:134:TYR:CE1	1:A:167:ILE:CD1	3.02	0.43
1:A:171:VAL:O	1:A:171:VAL:HG12	2.19	0.43
1:A:233:ILE:HG22	1:A:234:ASP:N	2.34	0.42
1:B:459:SER:OG	1:B:460:PRO:HD3	2.19	0.42
1:B:171:VAL:O	1:B:171:VAL:HG12	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLN:O	1:A:127:LYS:HG3	2.19	0.42
1:A:169:GLN:NE2	1:A:208:GLU:HA	2.34	0.42
1:A:452:VAL:HG21	1:A:492:LEU:HG	2.02	0.42
1:A:179:LYS:CD	1:A:181:ILE:HD11	2.48	0.42
1:B:509:ASP:OD1	1:B:510:VAL:HG23	2.20	0.42
1:B:90:ILE:HD13	1:B:278:LEU:HD21	2.02	0.42
1:B:169:GLN:NE2	1:B:208:GLU:HA	2.35	0.42
1:B:388:CYS:O	1:B:392:VAL:HG23	2.20	0.42
1:B:231:ASN:CG	1:B:232:GLU:N	2.78	0.41
1:B:371:LYS:HD3	1:B:424:GLU:OE2	2.19	0.41
1:B:138:LYS:HG3	1:B:139:CYS:N	2.35	0.41
1:B:226:LEU:HD11	1:B:242:ARG:NE	2.24	0.41
1:A:169:GLN:HE22	1:A:208:GLU:HA	1.85	0.41
1:A:352:ASP:O	1:A:356:VAL:HB	2.20	0.41
1:B:409:PHE:CG	1:B:470:HIS:ND1	2.86	0.41
1:A:67:SER:O	1:A:71:GLN:HG3	2.21	0.41
1:A:268:ARG:HA	1:A:269:PRO:HD3	1.88	0.41
1:A:306:PHE:N	1:A:307:PRO:CD	2.84	0.41
1:A:458:ILE:HG21	1:A:485:LEU:HD22	2.02	0.41
1:A:134:TYR:HE1	1:A:167:ILE:CD1	2.34	0.41
1:A:310:LEU:O	1:A:313:VAL:HG22	2.22	0.40
1:A:570:PHE:HB2	5:A:946:HOH:O	2.20	0.40
1:B:500:THR:HG22	1:B:576:ASP:CG	2.46	0.40
1:A:405:LYS:C	1:A:405:LYS:HD2	2.47	0.40
1:A:280:LYS:HE3	1:A:597:TYR:CD2	2.57	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	527/549 (96%)	503 (95%)	22 (4%)	2 (0%)	30 43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	521/549 (95%)	501 (96%)	19 (4%)	1 (0%)	43	58
All	All	1048/1098 (95%)	1004 (96%)	41 (4%)	3 (0%)	36	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	481	TYR
1	A	177	ASN
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	467/480 (97%)	462 (99%)	5 (1%)	65	82
1	B	462/480 (96%)	454 (98%)	8 (2%)	53	74
All	All	929/960 (97%)	916 (99%)	13 (1%)	59	79

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	ASP
1	A	304	LEU
1	A	327	MET
1	A	492	LEU
1	A	498	LEU
1	B	78	THR
1	B	149	ASP
1	B	304	LEU
1	B	310	LEU
1	B	327	MET
1	B	492	LEU
1	B	498	LEU
1	B	510	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	123	GLN
1	A	162	GLN
1	A	173	ASN
1	A	254	GLN
1	A	282	ASN
1	A	290	HIS
1	A	434	HIS
1	A	531	HIS
1	A	574	HIS
1	B	123	GLN
1	B	135	ASN
1	B	162	GLN
1	B	173	ASN
1	B	231	ASN
1	B	254	GLN
1	B	282	ASN
1	B	434	HIS
1	B	446	ASN
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
3	2BN	B	802	-	7,11,11	0.72	0	11,19,19	1.52	1 (9%)
3	2BN	A	801	-	7,11,11	0.82	0	11,19,19	1.56	2 (18%)
4	POP	A	901	2	6,8,8	1.98	2 (33%)	12,13,13	1.19	1 (8%)
4	POP	B	902	2	6,8,8	1.93	2 (33%)	12,13,13	1.23	1 (8%)

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	-
3	2BN	A	801	-	-	-	0/3/2/2
4	POP	A	901	2	-	0/6/6/6	-
3	2BN	B	802	-	-	-	0/3/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	POP	P2-O4	3.25	1.60	1.50
4	B	902	POP	P2-O4	2.95	1.59	1.50
4	B	902	POP	P1-O1	2.87	1.59	1.50
4	A	901	POP	P1-O1	2.75	1.59	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	2BN	C5-C4-N3	-3.52	102.41	106.65
3	A	801	2BN	C5-C4-N3	-3.41	102.54	106.65
4	B	902	POP	O3-P1-O	2.79	113.98	104.64
4	A	901	POP	O3-P1-O	2.56	113.23	104.64
3	A	801	2BN	C6-C5-C4	-2.42	103.72	107.47

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	533/549 (97%)	0.11	21 (3%)	43 39	25, 44, 84, 101	0
1	B	527/549 (95%)	0.09	22 (4%)	40 36	21, 43, 85, 118	0
All	All	1060/1098 (96%)	0.10	43 (4%)	41 37	21, 44, 85, 118	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	SER	5.4
1	B	137	HIS	4.4
1	B	139	CYS	3.8
1	B	231	ASN	3.5
1	B	61	GLN	3.3
1	B	172	PHE	3.3
1	A	140	PHE	3.2
1	B	181	ILE	3.2
1	A	137	HIS	3.2
1	A	139	CYS	3.1
1	A	78	THR	3.1
1	A	148	MET	3.0
1	B	228	GLU	2.9
1	A	56	ARG	2.9
1	B	233	ILE	2.8
1	B	138	LYS	2.8
1	A	181	ILE	2.7
1	B	221	CYS	2.7
1	A	59	ASN	2.6
1	A	187	LEU	2.6
1	B	274	LEU	2.5
1	A	233	ILE	2.5
1	A	179	LYS	2.4
1	B	92	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	598	ALA	2.4
1	A	221	CYS	2.3
1	B	95	ILE	2.3
1	B	149	ASP	2.2
1	B	96	LEU	2.2
1	A	183	PHE	2.2
1	A	506	ALA	2.2
1	B	174	CYS	2.2
1	B	505	LEU	2.2
1	A	58	GLY	2.2
1	B	62	PRO	2.1
1	A	226	LEU	2.1
1	B	97	LEU	2.1
1	A	232	GLU	2.1
1	B	134	TYR	2.1
1	B	225	LYS	2.0
1	A	172	PHE	2.0
1	B	579	GLY	2.0
1	A	227	ASP	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	2BN	A	801	10/10	0.96	0.08	31,34,35,35	0
3	2BN	B	802	10/10	0.96	0.09	25,29,30,31	0
2	MG	A	701	1/1	0.98	0.03	39,39,39,39	0
4	POP	A	901	9/9	0.98	0.05	27,33,37,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	705	1/1	0.99	0.02	31,31,31,31	0
2	MG	B	706	1/1	0.99	0.02	29,29,29,29	0
2	MG	A	702	1/1	0.99	0.04	28,28,28,28	0
2	MG	A	703	1/1	0.99	0.03	31,31,31,31	0
2	MG	B	704	1/1	0.99	0.02	28,28,28,28	0
4	POP	B	902	9/9	0.99	0.04	27,30,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.