WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2024 – 07:11 PM EST

PDB ID	:	1N22
Title	:	(+)-Bornyl Diphosphate Synthase: Complex with Mg, pyrophosphate, and (4 R)-7-aza-7,8-dihydrolimonene
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:

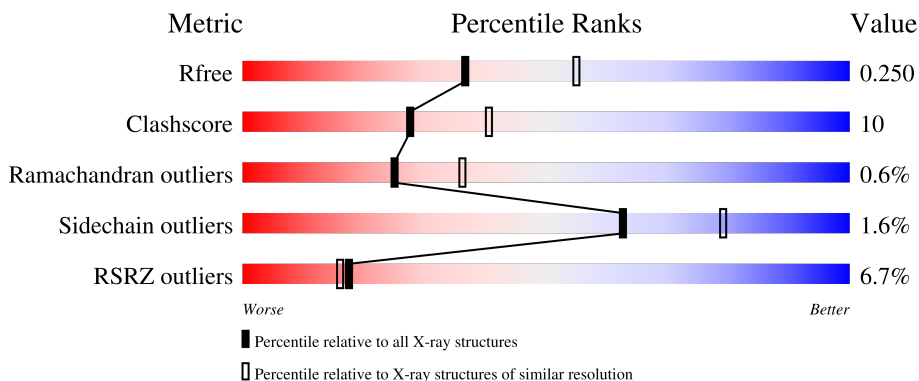|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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:
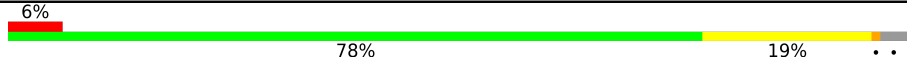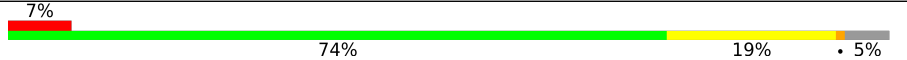*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	Percentile Ranks	Value
Rfree		0.250
Clashscore		10
Ramachandran outliers		0.6%
Sidechain outliers		1.6%
RSRZ outliers		6.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures
▌ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	6% / 78% / 19% / · ·
1	B	549	7% / 74% / 19% / · 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8934 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	534	Total	C	N	O	S	0	0	0
			4408	2859	731	801	17			
1	B	522	Total	C	N	O	S	0	0	0
			4311	2797	709	787	18			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mg	0	0
			3	3		
2	B	4	Total	Mg	0	0
			4	4		

- Molecule 3 is (1R)-DIMETHYL-(4-METHYL-CYCLOHEX-3-ENYL)-AMINE (three-letter code: 7A8) (formula: $C_9H_{17}N$).
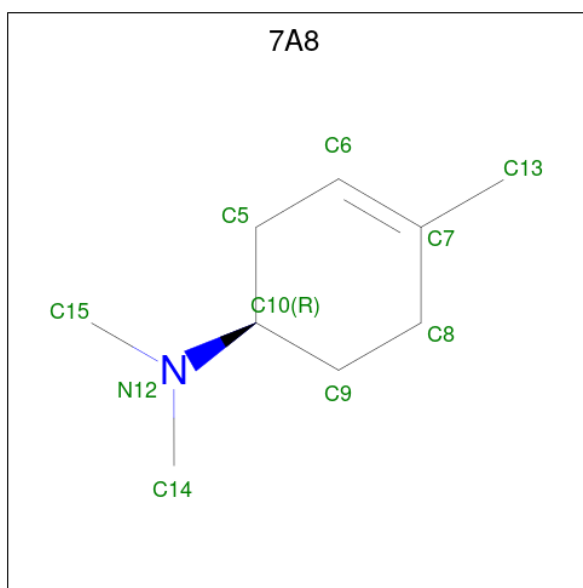
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 10	C 9	N 1	0	0
3	B	1	Total 10	C 9	N 1	0	0

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).
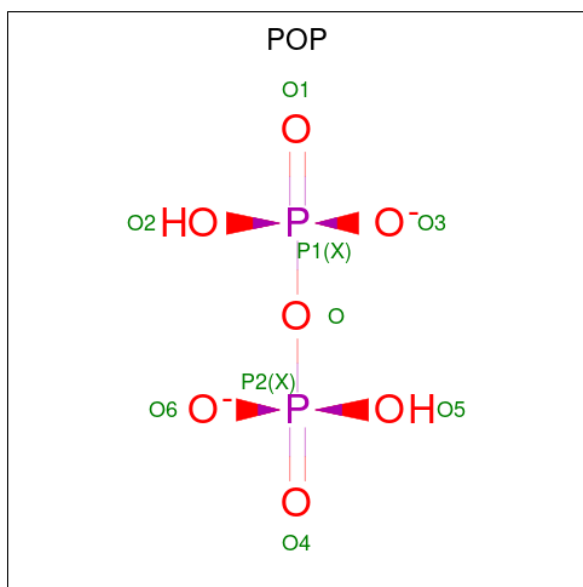
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 9	O 7	P 2	0	0
4	B	1	Total 9	O 7	P 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total 87	O 87	0	0
5	B	83	Total 83	O 83	0	0

3 Residue-property plots ⓘ

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

Chain A:

• Molecule 1: (+)-bornyl diphosphate synthase

Chain B:
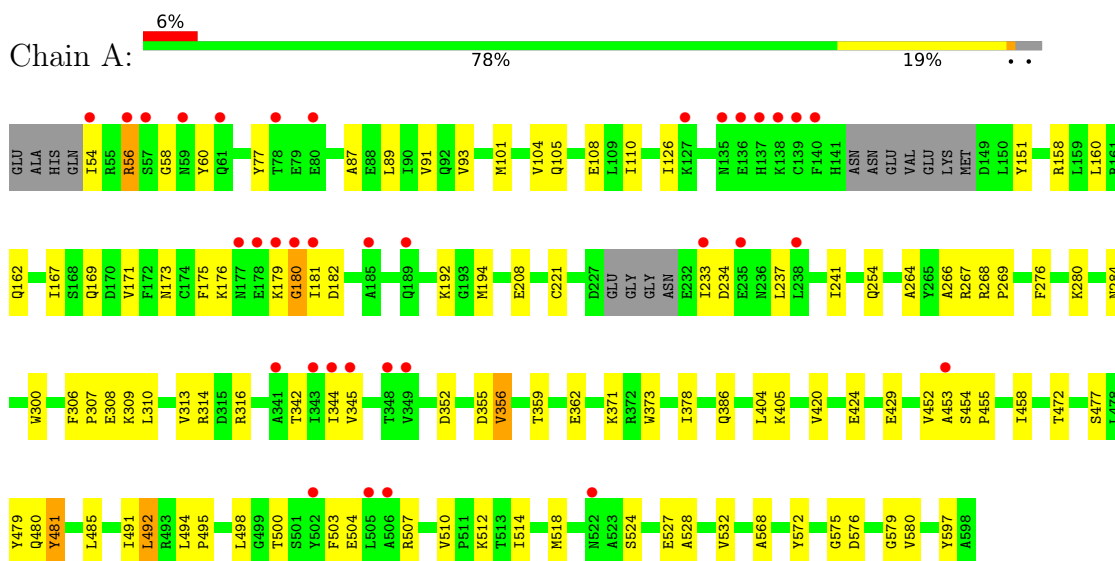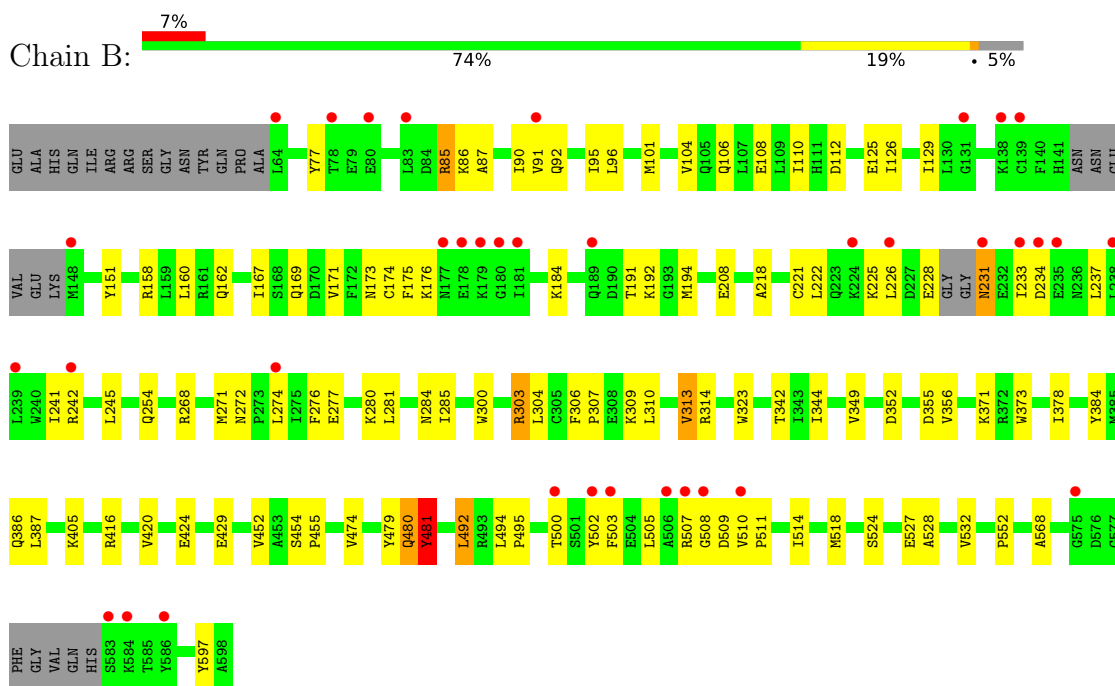
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.67Å 117.99Å 120.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.14 – 2.40 29.14 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.14-2.40) 99.2 (29.14-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.66 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.258 0.216 , 0.250	Depositor DCC
R_{free} test set	2862 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	43.7	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8934	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 7A8, POP, MG

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	0.36	0/4527	0.54	0/6135
1	B	0.37	0/4425	0.55	1/5995 (0.0%)
All	All	0.36	0/8952	0.54	1/12130 (0.0%)

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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	480	GLN	N-CA-C	-5.07	97.31	111.00

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	4408	0	4293	89	0
1	B	4311	0	4198	85	0
2	A	3	0	0	0	0
2	B	4	0	0	0	0
3	A	10	0	17	2	0
3	B	10	0	17	2	0
4	A	9	0	0	0	0
4	B	9	0	0	0	0
5	A	87	0	0	4	0
5	B	83	0	0	3	0
All	All	8934	0	8525	173	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 10.

All (173) 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	1.32	1.10
1:A:169:GLN:HE22	1:A:208:GLU:HA	1.16	1.09
1:B:429:GLU:HB3	1:B:510:VAL:HG21	1.39	1.03
1:A:169:GLN:NE2	1:A:208:GLU:HA	1.72	1.02
1:B:169:GLN:HE22	1:B:208:GLU:HA	1.21	1.01
1:B:169:GLN:NE2	1:B:208:GLU:HA	1.75	1.00
1:A:169:GLN:HE22	1:A:208:GLU:CA	1.78	0.94
1:B:169:GLN:HE22	1:B:208:GLU:CA	1.81	0.92
1:B:169:GLN:NE2	1:B:208:GLU:CA	2.38	0.86
1:A:169:GLN:NE2	1:A:208:GLU:CA	2.36	0.85
1:A:492:LEU:HD13	1:A:568:ALA:HB2	1.58	0.83
1:A:352:ASP:O	1:A:356:VAL:HG13	1.81	0.81
1:A:276:PHE:CZ	1:A:280:LYS:HE3	2.17	0.79
1:B:344:ILE:HG23	3:B:802:7A8:H82	1.66	0.78
1:A:169:GLN:NE2	1:A:208:GLU:CB	2.55	0.70
1:B:492:LEU:HD13	1:B:568:ALA:HB2	1.74	0.70
1:A:179:LYS:O	1:A:181:ILE:HG13	1.91	0.70
1:B:310:LEU:HD22	1:B:384:TYR:HB2	1.74	0.69
1:B:218:ALA:O	1:B:222:LEU:HB2	1.93	0.69
1:B:169:GLN:NE2	1:B:208:GLU:CB	2.55	0.69
1:A:56:ARG:HH21	1:A:56:ARG:HG2	1.57	0.68
1:A:494:LEU:HB2	1:A:495:PRO:HD3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:MET:HG2	1:A:105:GLN:HB2	1.79	0.64
1:B:226:LEU:HD11	1:B:242:ARG:HG2	1.80	0.63
1:B:160:LEU:HD13	1:B:167:ILE:HD11	1.80	0.63
1:A:373:TRP:HB2	5:A:904:HOH:O	1.98	0.62
1:B:492:LEU:HD21	3:B:802:7A8:H132	1.80	0.62
1:B:494:LEU:HB2	1:B:495:PRO:HD3	1.80	0.62
1:A:160:LEU:HD13	1:A:167:ILE:HD11	1.80	0.62
1:B:169:GLN:HE21	1:B:208:GLU:CB	2.13	0.61
1:A:276:PHE:CE2	1:A:280:LYS:HE3	2.35	0.61
1:A:280:LYS:HG2	1:A:597:TYR:CD2	2.36	0.60
1:A:479:TYR:C	1:A:481:TYR:N	2.54	0.60
1:A:169:GLN:HE21	1:A:208:GLU:CB	2.15	0.60
1:A:429:GLU:CB	1:A:510:VAL:HG21	2.21	0.60
1:B:87:ALA:O	1:B:91:VAL:HG23	2.02	0.60
1:A:498:LEU:HD11	1:A:532:VAL:HG11	1.84	0.59
1:B:169:GLN:NE2	1:B:208:GLU:HB3	2.18	0.58
1:A:89:LEU:O	1:A:93:VAL:HG23	2.04	0.58
1:A:104:VAL:O	1:A:108:GLU:HG3	2.04	0.58
1:A:355:ASP:OD1	1:A:356:VAL:HG12	2.04	0.58
1:B:507:ARG:O	1:B:507:ARG:HG2	2.04	0.58
1:A:310:LEU:O	1:A:313:VAL:HG22	2.04	0.57
1:A:498:LEU:CD1	1:A:532:VAL:HG11	2.34	0.57
1:B:96:LEU:HD13	1:B:272:ASN:ND2	2.19	0.57
1:B:104:VAL:O	1:B:108:GLU:HG3	2.04	0.57
1:A:181:ILE:HG22	1:A:182:ASP:OD1	2.04	0.57
1:B:237:LEU:O	1:B:241:ILE:HG13	2.05	0.57
1:A:169:GLN:NE2	1:A:208:GLU:HB3	2.20	0.56
1:B:479:TYR:C	1:B:481:TYR:N	2.50	0.56
1:A:280:LYS:HE2	1:A:597:TYR:CE2	2.40	0.56
1:B:280:LYS:HG2	1:B:597:TYR:CD2	2.40	0.56
1:B:454:SER:HB2	1:B:455:PRO:HD3	1.87	0.56
1:A:280:LYS:HE2	1:A:597:TYR:HE2	1.69	0.56
1:A:454:SER:HB2	1:A:455:PRO:HD3	1.87	0.55
1:A:371:LYS:HD3	1:A:424:GLU:OE2	2.06	0.55
1:B:313:VAL:HG11	1:B:349:VAL:HG22	1.87	0.55
1:B:352:ASP:O	1:B:356:VAL:HB	2.07	0.54
1:B:371:LYS:HD3	1:B:424:GLU:OE2	2.06	0.54
1:B:373:TRP:HB2	5:B:959:HOH:O	2.06	0.54
1:B:500:THR:HG21	1:B:505:LEU:HD11	1.90	0.54
1:A:237:LEU:O	1:A:241:ILE:HG13	2.07	0.54
1:B:524:SER:OG	1:B:527:GLU:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:LEU:HD11	1:B:274:LEU:HD12	1.90	0.53
1:A:504:GLU:OE1	1:A:512:LYS:HE3	2.08	0.53
1:A:344:ILE:HG23	3:A:801:7A8:H82	1.89	0.53
1:A:56:ARG:HB2	1:A:356:VAL:O	2.10	0.52
1:A:524:SER:OG	1:A:527:GLU:HG3	2.09	0.52
1:B:514:ILE:O	1:B:518:MET:HG3	2.10	0.52
1:A:492:LEU:HD12	1:A:492:LEU:O	2.10	0.52
1:A:500:THR:O	1:A:504:GLU:HG3	2.10	0.52
1:B:101:MET:CE	1:B:106:GLN:HG2	2.40	0.51
1:A:158:ARG:O	1:A:162:GLN:HG3	2.11	0.51
1:B:313:VAL:HG21	1:B:349:VAL:HG13	1.92	0.51
1:B:313:VAL:CG1	1:B:349:VAL:HG22	2.41	0.51
1:A:359:THR:OG1	1:A:362:GLU:HG3	2.11	0.51
1:B:226:LEU:HD22	1:B:245:LEU:HD12	1.94	0.51
1:B:510:VAL:O	1:B:511:PRO:C	2.47	0.50
1:B:233:ILE:HG22	1:B:234:ASP:N	2.27	0.50
1:A:514:ILE:O	1:A:518:MET:HG3	2.12	0.50
1:B:158:ARG:O	1:B:162:GLN:HG3	2.11	0.50
1:A:266:ALA:HB2	1:A:276:PHE:CE1	2.47	0.50
1:A:503:PHE:CD2	1:A:580:VAL:HG11	2.46	0.50
1:A:56:ARG:HG2	1:A:56:ARG:NH2	2.25	0.49
1:A:233:ILE:HG22	1:A:234:ASP:N	2.27	0.49
1:A:194:MET:HG3	1:A:221:CYS:SG	2.53	0.49
1:B:169:GLN:HE22	1:B:208:GLU:C	2.16	0.49
1:B:429:GLU:CB	1:B:510:VAL:HG21	2.28	0.49
1:A:87:ALA:O	1:A:91:VAL:HG23	2.13	0.48
1:B:309:LYS:C	1:B:310:LEU:HD23	2.33	0.48
1:A:309:LYS:C	1:A:310:LEU:HD12	2.34	0.48
1:B:85:ARG:NE	1:B:277:GLU:OE2	2.46	0.48
1:A:344:ILE:HG23	3:A:801:7A8:C8	2.43	0.47
1:B:85:ARG:NH1	1:B:281:LEU:HD22	2.29	0.47
1:B:474:VAL:HG13	1:B:552:PRO:HB2	1.95	0.47
1:B:480:GLN:O	1:B:481:TYR:HB2	2.14	0.47
1:A:169:GLN:HE21	1:A:208:GLU:HG2	1.79	0.47
1:A:480:GLN:O	1:A:481:TYR:HB2	2.14	0.47
1:A:472:THR:HG23	5:A:962:HOH:O	2.14	0.47
1:B:355:ASP:HB2	1:B:509:ASP:OD1	2.15	0.47
1:A:306:PHE:N	1:A:307:PRO:CD	2.78	0.47
1:A:458:ILE:HG21	1:A:485:LEU:HD22	1.97	0.47
1:B:173:ASN:C	1:B:175:PHE:H	2.18	0.47
1:B:452:VAL:HG22	1:B:492:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLN:HE22	1:A:208:GLU:C	2.17	0.46
1:A:429:GLU:O	1:A:510:VAL:HG22	2.15	0.46
1:A:452:VAL:HG22	1:A:492:LEU:HG	1.97	0.46
1:A:110:ILE:HD13	1:A:126:ILE:HG23	1.96	0.46
1:A:54:ILE:HG22	1:A:54:ILE:O	2.15	0.46
1:B:110:ILE:HD13	1:B:126:ILE:HG23	1.97	0.46
1:B:194:MET:HG3	1:B:221:CYS:SG	2.56	0.46
1:B:303:ARG:NH2	5:B:917:HOH:O	2.31	0.46
1:A:60:TYR:CD1	1:A:314:ARG:HG3	2.51	0.46
1:A:452:VAL:CG2	1:A:492:LEU:HG	2.47	0.45
1:B:112:ASP:OD1	1:B:268:ARG:NH1	2.47	0.45
1:B:528:ALA:O	1:B:532:VAL:HG23	2.17	0.45
1:A:316:ARG:HE	1:A:579:GLY:HA2	1.82	0.45
1:B:452:VAL:CG2	1:B:492:LEU:HG	2.47	0.45
1:B:479:TYR:C	1:B:481:TYR:H	2.08	0.45
1:B:276:PHE:CZ	1:B:280:LYS:HD2	2.52	0.45
1:A:404:LEU:HG	1:B:387:LEU:HD13	1.98	0.45
1:B:125:GLU:O	1:B:129:ILE:HG13	2.17	0.45
1:B:151:TYR:CD1	1:B:192:LYS:HG2	2.52	0.45
1:B:492:LEU:HD12	1:B:492:LEU:O	2.16	0.45
1:A:169:GLN:HE21	1:A:208:GLU:CG	2.30	0.44
1:B:85:ARG:NH2	1:B:277:GLU:OE2	2.51	0.44
1:A:342:THR:O	1:A:345:VAL:HG12	2.17	0.44
1:B:169:GLN:HE21	1:B:208:GLU:HB3	1.81	0.43
1:B:191:THR:OG1	1:B:225:LYS:HD3	2.18	0.43
1:B:226:LEU:HD11	1:B:242:ARG:NE	2.32	0.43
1:B:176:LYS:O	1:B:184:LYS:HE3	2.17	0.43
1:A:268:ARG:HA	1:A:269:PRO:HD3	1.87	0.43
1:B:96:LEU:CD1	1:B:272:ASN:ND2	2.81	0.43
1:A:151:TYR:CD1	1:A:192:LYS:HG2	2.53	0.43
1:B:306:PHE:N	1:B:307:PRO:CD	2.81	0.43
1:B:77:TYR:CD1	1:B:284:ASN:HB3	2.54	0.42
1:B:300:TRP:CH2	1:B:342:THR:HG23	2.55	0.42
1:A:500:THR:HG22	1:A:576:ASP:CG	2.40	0.42
1:B:314:ARG:HD3	1:B:502:TYR:HB3	2.02	0.42
1:A:264:ALA:HA	1:A:267:ARG:CZ	2.50	0.42
1:A:477:SER:O	1:A:480:GLN:HG2	2.19	0.42
1:A:77:TYR:CD1	1:A:284:ASN:HB3	2.55	0.42
1:A:300:TRP:CH2	1:A:342:THR:HG23	2.54	0.42
1:A:491:ILE:O	1:A:495:PRO:CD	2.68	0.42
1:A:510:VAL:HG23	5:A:935:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:VAL:HG12	1:A:171:VAL:O	2.20	0.41
1:A:420:VAL:O	1:A:424:GLU:HG3	2.19	0.41
1:B:416:ARG:O	1:B:420:VAL:HG23	2.20	0.41
1:A:481:TYR:HD2	1:A:481:TYR:HA	1.69	0.41
1:A:58:GLY:HA2	1:A:507:ARG:HG2	2.03	0.41
1:A:528:ALA:O	1:A:532:VAL:HG23	2.20	0.41
1:B:306:PHE:HB2	5:B:956:HOH:O	2.21	0.41
1:B:309:LYS:O	1:B:310:LEU:HD23	2.21	0.41
1:B:92:GLN:O	1:B:95:ILE:N	2.47	0.41
1:B:169:GLN:HE21	1:B:208:GLU:HG2	1.86	0.41
1:B:169:GLN:HE21	1:B:208:GLU:CG	2.33	0.41
1:B:171:VAL:O	1:B:171:VAL:HG12	2.21	0.41
1:B:226:LEU:HD11	1:B:242:ARG:CG	2.50	0.41
1:B:378:ILE:HG12	1:B:386:GLN:HG2	2.03	0.41
1:B:228:GLU:O	1:B:231:ASN:N	2.53	0.41
1:A:173:ASN:C	1:A:175:PHE:H	2.24	0.41
1:A:378:ILE:HG12	1:A:386:GLN:HG2	2.03	0.41
1:A:481:TYR:HB2	5:A:941:HOH:O	2.20	0.41
1:B:281:LEU:O	1:B:285:ILE:HG13	2.21	0.41
1:A:176:LYS:HB3	1:A:180:GLY:HA2	2.03	0.40
1:A:308:GLU:OE2	1:A:309:LYS:HE2	2.22	0.40
1:A:491:ILE:O	1:A:495:PRO:HD2	2.21	0.40
1:A:479:TYR:C	1:A:481:TYR:H	2.12	0.40
1:A:572:TYR:HA	1:A:575:GLY:O	2.20	0.40
1:B:86:LYS:O	1:B:90:ILE:HG13	2.21	0.40
1:B:420:VAL:O	1:B:424:GLU:HG3	2.22	0.40
1:A:452:VAL:O	1:A:453:ALA:HB3	2.22	0.40
1:B:112:ASP:CG	1:B:268:ARG:HH12	2.24	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	528/549 (96%)	498 (94%)	28 (5%)	2 (0%)	34	48
1	B	514/549 (94%)	481 (94%)	29 (6%)	4 (1%)	19	29
All	All	1042/1098 (95%)	979 (94%)	57 (6%)	6 (1%)	25	36

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	GLY
1	B	508	GLY
1	A	481	TYR
1	B	481	TYR
1	B	174	CYS
1	B	271	MET

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	468/480 (98%)	463 (99%)	5 (1%)	73	87
1	B	459/480 (96%)	449 (98%)	10 (2%)	52	71
All	All	927/960 (97%)	912 (98%)	15 (2%)	62	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ARG
1	A	254	GLN
1	A	356	VAL
1	A	405	LYS
1	A	492	LEU
1	B	85	ARG
1	B	231	ASN
1	B	254	GLN
1	B	303	ARG
1	B	304	LEU

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Mol	Chain	Res	Type
1	B	313	VAL
1	B	323	TRP
1	B	405	LYS
1	B	492	LEU
1	B	503	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	A	254	GLN
1	A	531	HIS
1	B	169	GLN
1	B	231	ASN
1	B	254	GLN
1	B	531	HIS
1	B	574	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 7 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	A	901	2	6,8,8	1.86	2 (33%)	13,13,13	1.06	1 (7%)
3	7A8	A	801	-	9,10,10	2.33	4 (44%)	12,13,13	2.35	5 (41%)
4	POP	B	902	2	6,8,8	1.95	2 (33%)	13,13,13	1.05	1 (7%)
3	7A8	B	802	-	9,10,10	2.38	5 (55%)	12,13,13	2.29	4 (33%)

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	A	901	2	-	0/6/6/6	-
3	7A8	A	801	-	-	0/4/14/14	0/1/1/1
4	POP	B	902	2	-	0/6/6/6	-
3	7A8	B	802	-	-	1/4/14/14	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	7A8	C5-C10	4.31	1.60	1.52
3	A	801	7A8	C5-C10	4.17	1.59	1.52
3	A	801	7A8	C5-C6	3.19	1.57	1.50
4	B	902	POP	P2-O4	3.07	1.60	1.50
3	B	802	7A8	C5-C6	3.05	1.56	1.50
4	A	901	POP	P2-O4	3.02	1.60	1.50
3	B	802	7A8	C9-C8	2.96	1.59	1.52
4	B	902	POP	P1-O1	2.80	1.59	1.50
3	A	801	7A8	C9-C8	2.71	1.59	1.52
4	A	901	POP	P1-O1	2.57	1.58	1.50
3	A	801	7A8	C9-C10	2.20	1.58	1.52
3	B	802	7A8	C9-C10	2.14	1.57	1.52
3	B	802	7A8	C15-N12	-2.05	1.39	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	7A8	C14-N12-C10	5.87	122.49	112.39
3	B	802	7A8	C14-N12-C10	5.76	122.30	112.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	802	7A8	C15-N12-C14	-2.38	103.34	110.38
4	A	901	POP	O3-P1-O	2.34	112.49	104.64
3	A	801	7A8	C15-N12-C14	-2.29	103.63	110.38
3	B	802	7A8	C15-N12-C10	2.25	116.25	112.39
4	B	902	POP	O3-P1-O	2.24	112.14	104.64
3	A	801	7A8	C15-N12-C10	2.12	116.03	112.39
3	B	802	7A8	C5-C6-C7	-2.11	115.61	124.21
3	A	801	7A8	C5-C6-C7	-2.01	116.04	124.21
3	A	801	7A8	C9-C10-C5	2.00	112.21	109.44

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	7A8	C5-C10-N12-C15

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	7A8	2	0
3	B	802	7A8	2	0

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	534/549 (97%)	0.16	35 (6%)	18	17	28, 47, 84, 112	0
1	B	522/549 (95%)	0.09	36 (6%)	16	15	23, 46, 90, 113	0
All	All	1056/1098 (96%)	0.13	71 (6%)	17	16	23, 47, 89, 113	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	ILE	5.7
1	B	274	LEU	5.5
1	A	139	CYS	5.1
1	A	137	HIS	4.8
1	B	139	CYS	4.7
1	B	181	ILE	4.4
1	A	138	LYS	4.3
1	B	231	ASN	4.2
1	A	233	ILE	4.2
1	A	140	PHE	4.2
1	B	583	SER	4.1
1	B	506	ALA	3.9
1	B	500	THR	3.9
1	B	239	LEU	3.9
1	B	233	ILE	3.9
1	B	235	GLU	3.8
1	B	238	LEU	3.8
1	A	179	LYS	3.7
1	B	180	GLY	3.6
1	B	226	LEU	3.6
1	A	57	SER	3.5
1	A	136	GLU	3.4
1	A	178	GLU	3.3
1	B	503	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	138	LYS	3.2
1	B	148	MET	3.1
1	A	59	ASN	3.1
1	B	575	GLY	3.1
1	B	83	LEU	3.1
1	B	586	TYR	3.0
1	A	185	ALA	3.0
1	B	584	LYS	3.0
1	B	502	TYR	2.9
1	B	510	VAL	2.8
1	B	507	ARG	2.8
1	A	502	TYR	2.8
1	A	61	GLN	2.7
1	A	181	ILE	2.7
1	A	344	ILE	2.6
1	A	343	ILE	2.6
1	B	64	LEU	2.6
1	B	177	ASN	2.6
1	A	235	GLU	2.6
1	B	80	GLU	2.6
1	A	80	GLU	2.6
1	B	224	LYS	2.6
1	B	91	VAL	2.6
1	A	177	ASN	2.5
1	A	345	VAL	2.5
1	A	453	ALA	2.5
1	A	78	THR	2.4
1	B	189	GLN	2.4
1	A	506	ALA	2.4
1	B	242	ARG	2.4
1	B	508	GLY	2.4
1	B	234	ASP	2.4
1	A	135	ASN	2.3
1	A	189	GLN	2.3
1	B	178	GLU	2.3
1	A	127	LYS	2.2
1	B	131	GLY	2.2
1	B	179	LYS	2.2
1	A	522	ASN	2.2
1	A	238	LEU	2.2
1	A	341	ALA	2.2
1	A	349	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	78	THR	2.1
1	A	348	THR	2.1
1	A	56	ARG	2.1
1	A	505	LEU	2.1
1	A	180	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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($Å^2$)	Q<0.9
2	MG	B	704	1/1	0.87	0.14	27,27,27,27	0
2	MG	B	707	1/1	0.87	0.16	43,43,43,43	0
3	7A8	A	801	10/10	0.89	0.49	52,52,53,53	0
3	7A8	B	802	10/10	0.90	0.32	47,49,50,51	0
2	MG	A	703	1/1	0.91	0.09	40,40,40,40	0
2	MG	B	705	1/1	0.94	0.11	32,32,32,32	0
2	MG	A	702	1/1	0.94	0.14	50,50,50,50	0
2	MG	A	701	1/1	0.97	0.10	38,38,38,38	0
2	MG	B	706	1/1	0.98	0.08	31,31,31,31	0
4	POP	A	901	9/9	0.98	0.14	36,40,42,43	0
4	POP	B	902	9/9	0.99	0.10	27,29,31,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.