



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 04:50 pm GMT

PDB ID : 1B8G  
Title : 1-AMINOCYCLOPROPANE-1-CARBOXYLATE SYNTHASE  
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Deposited on : 1999-01-31  
Resolution : 2.37 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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

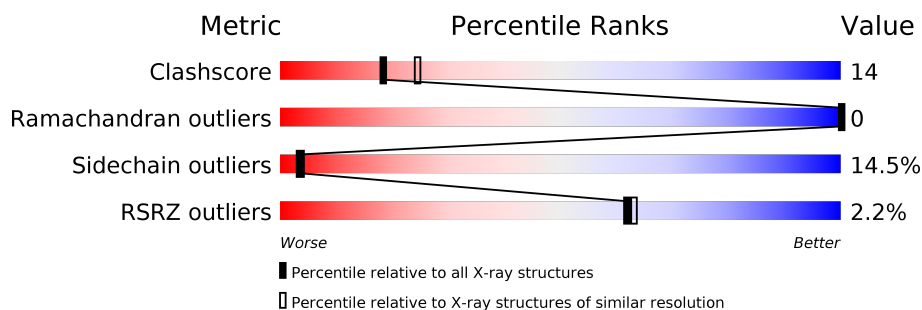
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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))
Clashscore	122126	5405 (2.40-2.36)
Ramachandran outliers	120053	5324 (2.40-2.36)
Sidechain outliers	120020	5326 (2.40-2.36)
RSRZ outliers	108989	4741 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	429	
1	B	429	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6905 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 PROTEIN (1-AMINOCYCLOPROPANE-1-CARBOXYLATE SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	1	0
			3333	2124	566	622	21			
1	B	425	Total	C	N	O	S	0	1	0
			3368	2145	571	631	21			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

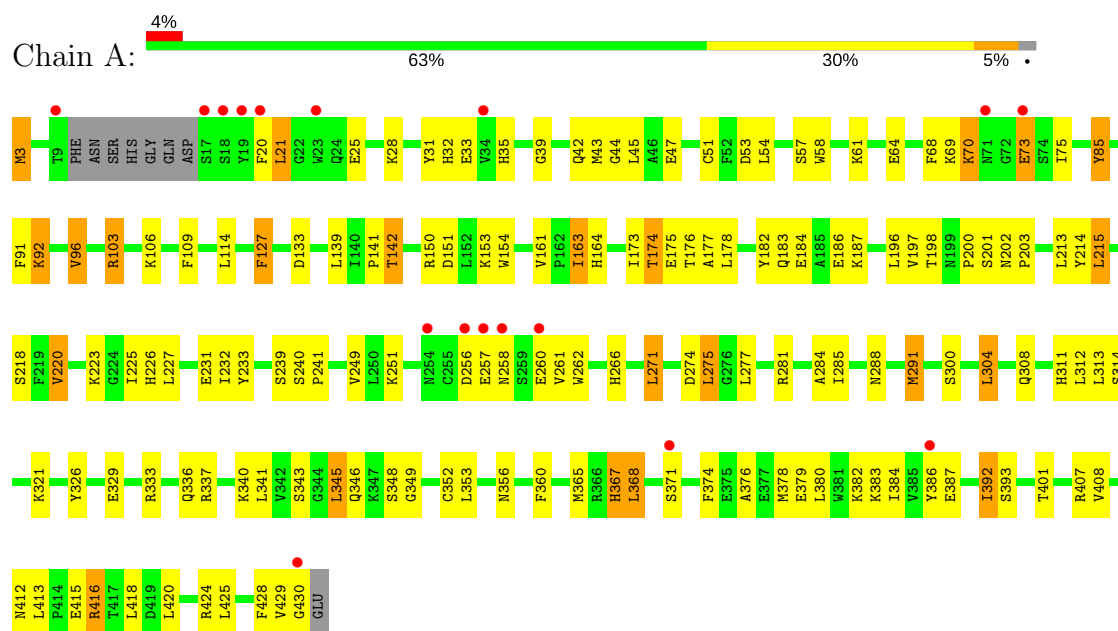
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total 55	O 55	0	0
3	B	119	Total 119	O 119	0	0

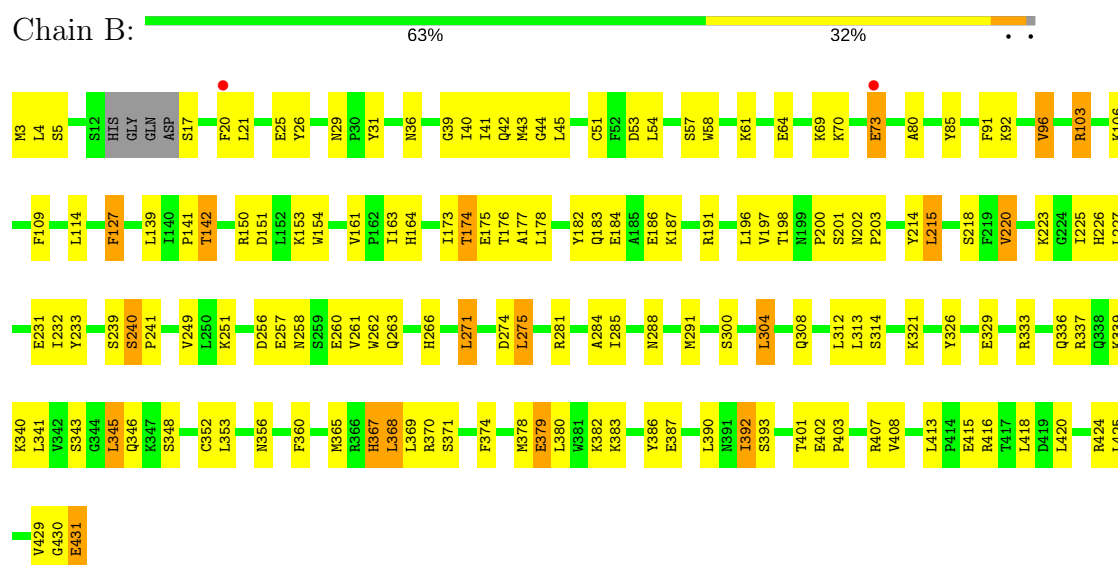
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: PROTEIN (1-AMINOCYCLOPROPANE-1-CARBOXYLATE SYNTHASE)



#### • Molecule 1: PROTEIN (1-AMINOCYCLOPROPANE-1-CARBOXYLATE SYNTHASE)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.63Å 69.06Å 123.24Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	19.70 – 2.37 19.69 – 2.37	Depositor EDS
% Data completeness (in resolution range)	93.6 (19.70-2.37) 93.4 (19.69-2.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	4.70	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.09 (at 2.38Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.179 , 0.242 0.185 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 59.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6905	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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: PLP

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	0.44	0/3413	0.66	2/4619 (0.0%)
1	B	0.47	0/3449	0.66	1/4666 (0.0%)
All	All	0.46	0/6862	0.66	3/9285 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ASN	N-CA-C	-6.06	94.64	111.00
1	B	202	ASN	N-CA-C	-5.55	96.02	111.00
1	A	163	ILE	N-CA-C	-5.03	97.41	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	3333	0	3281	104	0
1	B	3368	0	3308	102	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
3	A	55	0	0	2	0
3	B	119	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6905	0	6601	191	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 14.

All (191) 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:32:HIS:HD2	1:A:35:HIS:CD2	1.67	1.11
1:A:367:HIS:CE1	1:A:368:LEU:HD13	1.98	0.98
1:B:174:THR:HG22	1:B:177:ALA:H	1.35	0.92
1:A:32:HIS:CD2	1:A:35:HIS:CD2	2.58	0.91
1:A:32:HIS:CD2	1:A:35:HIS:NE2	2.38	0.91
1:A:174:THR:HG22	1:A:177:ALA:H	1.41	0.85
1:B:392:ILE:HD11	1:B:408:VAL:HB	1.62	0.82
1:A:32:HIS:HD2	1:A:35:HIS:NE2	1.74	0.81
1:A:392:ILE:HD11	1:A:408:VAL:HB	1.63	0.80
1:B:43:MET:HB2	1:B:392:ILE:HD12	1.65	0.78
1:A:43:MET:HB2	1:A:392:ILE:HD12	1.67	0.76
1:A:367:HIS:ND1	1:A:368:LEU:HD13	1.99	0.76
1:A:308:GLN:OE1	1:B:308:GLN:OE1	2.06	0.74
1:B:379:GLU:HG3	3:B:605:HOH:O	1.86	0.74
1:A:198:THR:HG22	1:A:201:SER:HA	1.69	0.73
1:B:142:THR:CG2	3:B:571:HOH:O	2.37	0.73
1:B:198:THR:HG22	1:B:201:SER:HA	1.68	0.72
1:B:378:MET:O	1:B:382:LYS:HG3	1.90	0.71
1:B:263:GLN:HG3	3:B:585:HOH:O	1.91	0.70
1:A:378:MET:O	1:A:382:LYS:HG3	1.90	0.70
1:A:341:LEU:HD21	1:A:408:VAL:HG22	1.75	0.69
1:B:21:LEU:HD21	1:B:386:TYR:OH	1.93	0.68
1:A:33:GLU:OE2	1:A:416:ARG:NH1	2.26	0.68
1:A:425:LEU:O	1:A:429:VAL:HG23	1.95	0.66
1:B:425:LEU:O	1:B:429:VAL:HG23	1.94	0.66
1:A:329:GLU:OE2	1:A:333:ARG:HD2	1.96	0.65
1:B:300:SER:O	1:B:304:LEU:HD13	1.96	0.65
1:B:70:LYS:O	1:B:73:GLU:HB2	1.95	0.65
1:A:300:SER:O	1:A:304:LEU:HD13	1.98	0.64
1:B:341:LEU:HD21	1:B:408:VAL:HG22	1.79	0.64
1:B:329:GLU:OE2	1:B:333:ARG:HD2	1.97	0.63
1:A:308:GLN:OE1	1:B:308:GLN:HG2	1.99	0.63
1:B:103:ARG:NH2	3:B:560:HOH:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:HIS:CE1	1:B:368:LEU:HD13	2.34	0.62
1:B:53:ASP:OD1	1:B:333:ARG:NH2	2.33	0.61
1:B:26:TYR:HD1	1:B:40:ILE:HG22	1.65	0.60
1:A:21:LEU:HD11	1:A:386:TYR:OH	2.01	0.60
1:A:214:TYR:HE1	1:A:249:VAL:HG13	1.67	0.59
1:A:53:ASP:OD1	1:A:333:ARG:NH2	2.35	0.59
1:A:70:LYS:HD2	1:A:311:HIS:HE1	1.68	0.59
1:A:214:TYR:CE1	1:A:249:VAL:HG13	2.38	0.59
1:B:43:MET:HB2	1:B:392:ILE:CD1	2.33	0.58
1:A:31:TYR:HA	1:A:39:GLY:HA3	1.84	0.57
1:A:43:MET:HB2	1:A:392:ILE:CD1	2.35	0.57
1:A:173:ILE:HG22	1:A:215:LEU:HD21	1.87	0.57
1:B:73:GLU:OE1	1:B:73:GLU:HA	2.03	0.56
1:B:142:THR:HG22	3:B:571:HOH:O	2.03	0.56
1:B:17:SER:HB3	1:B:20:PHE:CE2	2.41	0.56
1:B:262:TRP:CZ3	1:B:288:ASN:HB3	2.40	0.56
1:A:127:PHE:CZ	1:A:266:HIS:HB3	2.41	0.56
1:B:142:THR:HG21	1:B:164:HIS:HD2	1.71	0.55
1:A:340:LYS:HE2	1:A:415:GLU:HB3	1.88	0.55
1:A:96:VAL:HG22	1:A:109:PHE:HB2	1.88	0.55
1:A:114:LEU:HD11	1:A:284:ALA:HB1	1.88	0.55
1:B:127:PHE:CE2	1:B:285:ILE:HG23	2.42	0.54
1:A:3:MET:HE2	1:B:191:ARG:HH22	1.72	0.54
1:A:142:THR:HG21	1:A:164:HIS:HD2	1.72	0.54
1:A:262:TRP:CZ3	1:A:288:ASN:HB3	2.42	0.54
1:B:64:GLU:CD	1:B:64:GLU:H	2.11	0.54
1:A:198:THR:HG22	1:A:200:PRO:O	2.07	0.54
1:B:198:THR:HG22	1:B:200:PRO:O	2.08	0.54
1:B:214:TYR:CE1	1:B:249:VAL:HG13	2.43	0.54
1:A:240:SER:HA	1:A:241:PRO:C	2.28	0.54
1:B:178:LEU:HD12	1:B:215:LEU:HD11	1.88	0.53
1:A:281:ARG:HD2	1:B:304:LEU:CB	2.38	0.53
1:A:239:SER:O	1:A:356:ASN:HB2	2.07	0.53
1:A:92:LYS:HG2	1:A:114:LEU:HD23	1.91	0.53
1:A:308:GLN:HG2	1:B:308:GLN:OE1	2.09	0.53
1:B:182:TYR:CE1	1:B:223:LYS:HG2	2.44	0.52
1:B:31:TYR:HA	1:B:39:GLY:HA3	1.90	0.52
1:A:178:LEU:HD12	1:A:215:LEU:HD11	1.92	0.52
1:B:114:LEU:HD11	1:B:284:ALA:HB1	1.90	0.52
1:B:214:TYR:HE1	1:B:249:VAL:HG13	1.74	0.52
1:A:64:GLU:CD	1:A:64:GLU:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:THR:HG23	1:B:176:THR:H	1.73	0.52
1:A:345:LEU:HD23	1:A:352:CYS:SG	2.49	0.52
1:A:226:HIS:HD2	1:A:266:HIS:NE2	2.08	0.51
1:A:85[B]:TYR:HD1	1:A:304:LEU:HD21	1.75	0.51
1:B:240:SER:HA	1:B:241:PRO:C	2.30	0.51
1:A:174:THR:CG2	1:A:176:THR:H	2.23	0.51
1:B:239:SER:O	1:B:356:ASN:HB2	2.11	0.51
1:B:174:THR:HG22	1:B:177:ALA:N	2.16	0.51
1:A:220:VAL:HG22	1:A:225:ILE:HG13	1.92	0.51
1:A:341:LEU:HD21	1:A:408:VAL:CG2	2.41	0.50
1:A:383:LYS:HG2	1:A:387:GLU:OE2	2.11	0.50
1:B:340:LYS:HE2	1:B:415:GLU:HB3	1.94	0.50
1:B:96:VAL:HG22	1:B:109:PHE:HB2	1.93	0.50
1:B:127:PHE:CZ	1:B:266:HIS:HB3	2.45	0.50
1:B:174:THR:CG2	1:B:176:THR:H	2.25	0.49
1:A:127:PHE:CE2	1:A:285:ILE:HG23	2.47	0.49
1:A:349:GLY:HA2	3:A:534:HOH:O	2.12	0.49
1:A:257:GLU:H	1:A:257:GLU:CD	2.16	0.49
1:A:68:PHE:CZ	1:A:308:GLN:HG3	2.48	0.49
1:A:3:MET:CE	1:B:191:ARG:HH22	2.26	0.49
1:B:226:HIS:HD2	1:B:266:HIS:NE2	2.11	0.49
1:A:281:ARG:HD2	1:B:304:LEU:HB2	1.94	0.49
1:B:220:VAL:HG22	1:B:225:ILE:HG13	1.94	0.48
1:A:174:THR:HG23	1:A:176:THR:H	1.79	0.48
1:A:226:HIS:CD2	1:A:266:HIS:NE2	2.82	0.47
1:B:173:ILE:HG22	1:B:215:LEU:HD21	1.95	0.47
1:B:345:LEU:HD23	1:B:352:CYS:SG	2.54	0.47
1:A:304:LEU:HB2	1:B:281:ARG:HD2	1.96	0.47
1:A:174:THR:HG22	1:A:177:ALA:N	2.20	0.47
1:A:174:THR:CG2	1:A:176:THR:HB	2.44	0.47
1:B:365:MET:HE2	1:B:368:LEU:HD23	1.96	0.47
1:A:256:ASP:OD1	1:A:258:ASN:HB2	2.15	0.47
1:B:383:LYS:HG2	1:B:387:GLU:OE2	2.14	0.47
1:B:275:LEU:HD12	1:B:326:TYR:CE1	2.49	0.47
1:B:53:ASP:CG	1:B:333:ARG:HH22	2.18	0.47
1:A:174:THR:HG22	1:A:176:THR:N	2.30	0.46
1:A:53:ASP:CG	1:A:333:ARG:HH22	2.18	0.46
1:B:226:HIS:CD2	1:B:266:HIS:NE2	2.84	0.46
1:B:29:ASN:OD1	1:B:36:ASN:ND2	2.43	0.46
1:B:150:ARG:NH1	1:B:151:ASP:OD1	2.49	0.46
1:A:374:PHE:O	1:A:378:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:LEU:HB3	1:B:371:SER:O	2.16	0.46
1:A:428:PHE:C	1:A:430:GLY:N	2.69	0.46
1:A:25:GLU:HA	1:A:25:GLU:OE1	2.16	0.46
1:A:127:PHE:HZ	1:A:266:HIS:HB3	1.79	0.46
1:A:367:HIS:CE1	1:A:368:LEU:CD1	2.86	0.46
1:A:271:LEU:HD23	1:A:313:LEU:HD13	1.97	0.46
1:B:25:GLU:HG3	1:B:386:TYR:CE1	2.51	0.46
1:A:203:PRO:HB3	1:A:407:ARG:HD3	1.99	0.45
1:A:291:MET:HB3	1:B:4:LEU:HD11	1.98	0.45
1:A:275:LEU:HD12	1:A:326:TYR:CE1	2.52	0.45
1:B:341:LEU:HD21	1:B:408:VAL:CG2	2.46	0.45
1:B:92:LYS:HG2	1:B:114:LEU:HD23	1.97	0.45
1:A:182:TYR:CE1	1:A:223:LYS:HG2	2.51	0.45
1:A:139:LEU:HD23	1:A:161:VAL:HB	1.99	0.45
1:B:430:GLY:C	1:B:431:GLU:HG2	2.36	0.45
1:A:371:SER:HB2	1:A:376:ALA:HB2	1.99	0.45
1:B:288:ASN:HB2	3:B:587:HOH:O	2.17	0.45
1:A:58:TRP:HA	1:A:61:LYS:HE2	1.98	0.45
1:A:308:GLN:OE1	1:B:308:GLN:CG	2.64	0.44
1:B:370:ARG:NH2	3:B:608:HOH:O	2.48	0.44
1:A:274:ASP:OD1	1:A:275:LEU:N	2.49	0.44
1:B:25:GLU:HA	1:B:25:GLU:OE1	2.17	0.44
1:A:277:LEU:HD23	1:B:80:ALA:HB1	1.99	0.44
1:A:103:ARG:NH1	1:A:231:GLU:OE1	2.50	0.44
1:B:103:ARG:NH1	1:B:231:GLU:OE1	2.51	0.44
1:B:141:PRO:HA	1:B:163:ILE:HB	2.00	0.44
1:B:271:LEU:HD23	1:B:313:LEU:HD13	2.00	0.44
1:A:91:PHE:HA	1:A:314:SER:HB2	2.00	0.43
1:B:58:TRP:HA	1:B:61:LYS:HE2	1.99	0.43
1:A:51:CYS:HB3	1:A:54:LEU:HD12	2.01	0.43
1:A:150:ARG:NH1	1:A:151:ASP:OD1	2.50	0.43
1:B:196:LEU:HD23	1:B:197:VAL:N	2.32	0.43
1:B:232:ILE:HG23	1:B:233:TYR:CD2	2.53	0.43
1:B:257:GLU:H	1:B:257:GLU:CD	2.21	0.43
1:A:85[B]:TYR:CD1	1:A:304:LEU:HD21	2.52	0.43
1:A:343:SER:O	1:A:346:GLN:HG2	2.18	0.43
1:A:133:ASP:OD1	1:B:5:SER:HB2	2.19	0.43
1:A:196:LEU:HD23	1:A:197:VAL:N	2.33	0.43
1:B:174:THR:CG2	1:B:176:THR:HB	2.48	0.43
1:A:304:LEU:CB	1:B:281:ARG:HD2	2.48	0.43
1:B:256:ASP:OD1	1:B:258:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:TRP:CH2	1:B:288:ASN:HB3	2.53	0.43
1:A:365:MET:HE1	1:A:384:ILE:HD11	2.00	0.42
1:B:139:LEU:HD23	1:B:161:VAL:HB	2.01	0.42
1:A:232:ILE:HG23	1:A:233:TYR:CD2	2.55	0.42
1:B:274:ASP:OD1	1:B:275:LEU:N	2.51	0.42
1:B:44:GLY:HA2	3:B:529:HOH:O	2.19	0.42
1:A:75:ILE:HD11	1:A:311:HIS:CE1	2.55	0.42
1:A:141:PRO:HA	1:A:163:ILE:HB	2.02	0.42
1:B:127:PHE:HZ	1:B:266:HIS:HB3	1.85	0.42
1:A:150:ARG:HD3	1:A:154:TRP:CE3	2.55	0.42
1:A:44:GLY:HA2	3:A:506:HOH:O	2.19	0.42
1:A:262:TRP:CH2	1:A:288:ASN:HB3	2.55	0.42
1:B:374:PHE:O	1:B:378:MET:HG2	2.20	0.41
1:B:41:ILE:HB	1:B:390:LEU:HD23	2.02	0.41
1:B:196:LEU:HD23	1:B:196:LEU:C	2.41	0.41
1:B:163:ILE:HD13	1:B:178:LEU:HD23	2.01	0.41
1:B:203:PRO:HB3	1:B:407:ARG:HD3	2.02	0.41
1:B:127:PHE:CZ	1:B:285:ILE:HG23	2.55	0.41
1:B:91:PHE:HA	1:B:314:SER:HB2	2.02	0.41
1:B:402:GLU:HA	1:B:403:PRO:HD3	1.89	0.41
1:A:281:ARG:HD2	1:B:304:LEU:HB3	2.01	0.41
1:A:163:ILE:HD13	1:A:178:LEU:HD23	2.03	0.41
1:A:142:THR:HG21	1:A:401:THR:HG23	2.02	0.41
1:B:174:THR:HG22	1:B:176:THR:N	2.36	0.41
1:A:73:GLU:H	1:A:73:GLU:HG2	1.70	0.41
1:B:142:THR:HG21	1:B:401:THR:HG23	2.03	0.41
1:A:428:PHE:C	1:A:430:GLY:H	2.23	0.40
1:A:47:GLU:HG3	1:A:412:ASN:HB3	2.04	0.40
1:B:150:ARG:HD3	1:B:154:TRP:CE3	2.56	0.40
1:A:365:MET:CE	1:A:384:ILE:HD11	2.51	0.40
1:A:213:LEU:HD13	1:A:249:VAL:HG21	2.03	0.40
1:A:425:LEU:HA	1:A:425:LEU:HD12	1.82	0.40
1:A:308:GLN:CG	1:B:308:GLN:OE1	2.69	0.40
1:B:343:SER:O	1:B:346:GLN:HG2	2.21	0.40
1:B:51:CYS:HB3	1:B:54:LEU:HD12	2.02	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	418/429 (97%)	399 (96%)	19 (4%)	0	100	100
1	B	422/429 (98%)	399 (94%)	23 (6%)	0	100	100
All	All	840/858 (98%)	798 (95%)	42 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	365/371 (98%)	310 (85%)	55 (15%)	3	3
1	B	369/371 (100%)	316 (86%)	53 (14%)	3	4
All	All	734/742 (99%)	626 (85%)	108 (15%)	3	3

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	20	PHE
1	A	21	LEU
1	A	28	LYS
1	A	42	GLN
1	A	45	LEU
1	A	57	SER
1	A	69	LYS

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Mol	Chain	Res	Type
1	A	70	LYS
1	A	73	GLU
1	A	85[A]	TYR
1	A	85[B]	TYR
1	A	92	LYS
1	A	96	VAL
1	A	103	ARG
1	A	106	LYS
1	A	127	PHE
1	A	142	THR
1	A	153	LYS
1	A	174	THR
1	A	175	GLU
1	A	183	GLN
1	A	184	GLU
1	A	186	GLU
1	A	187	LYS
1	A	215	LEU
1	A	218	SER
1	A	220	VAL
1	A	227	LEU
1	A	251	LYS
1	A	260	GLU
1	A	261	VAL
1	A	271	LEU
1	A	275	LEU
1	A	291	MET
1	A	304	LEU
1	A	312	LEU
1	A	321	LYS
1	A	336	GLN
1	A	337	ARG
1	A	345	LEU
1	A	348	SER
1	A	353	LEU
1	A	360	PHE
1	A	367	HIS
1	A	368	LEU
1	A	379	GLU
1	A	380	LEU
1	A	392	ILE
1	A	393	SER

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Mol	Chain	Res	Type
1	A	413	LEU
1	A	416	ARG
1	A	418	LEU
1	A	420	LEU
1	A	424	ARG
1	B	3	MET
1	B	42	GLN
1	B	45	LEU
1	B	57	SER
1	B	69	LYS
1	B	73	GLU
1	B	85[A]	TYR
1	B	85[B]	TYR
1	B	96	VAL
1	B	103	ARG
1	B	106	LYS
1	B	127	PHE
1	B	142	THR
1	B	153	LYS
1	B	174	THR
1	B	175	GLU
1	B	183	GLN
1	B	184	GLU
1	B	186	GLU
1	B	187	LYS
1	B	215	LEU
1	B	218	SER
1	B	220	VAL
1	B	227	LEU
1	B	240	SER
1	B	251	LYS
1	B	260	GLU
1	B	261	VAL
1	B	271	LEU
1	B	275	LEU
1	B	291	MET
1	B	304	LEU
1	B	312	LEU
1	B	321	LYS
1	B	336	GLN
1	B	337	ARG
1	B	339	LYS

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Mol	Chain	Res	Type
1	B	345	LEU
1	B	348	SER
1	B	353	LEU
1	B	360	PHE
1	B	367	HIS
1	B	368	LEU
1	B	379	GLU
1	B	380	LEU
1	B	392	ILE
1	B	393	SER
1	B	413	LEU
1	B	416	ARG
1	B	418	LEU
1	B	420	LEU
1	B	424	ARG
1	B	431	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	35	HIS
1	A	164	HIS
1	A	172	GLN
1	A	226	HIS
1	A	311	HIS
1	A	346	GLN
1	B	24	GLN
1	B	35	HIS
1	B	164	HIS
1	B	172	GLN
1	B	226	HIS
1	B	311	HIS
1	B	346	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PLP	A	500	1	15,15,16	1.20	2 (13%)	20,22,23	1.51	6 (30%)
2	PLP	B	500	1	15,15,16	1.01	1 (6%)	20,22,23	1.48	5 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	500	1	-	0/6/6/8	0/1/1/1
2	PLP	B	500	1	-	0/6/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	PLP	C5-C4	2.12	1.43	1.40
2	B	500	PLP	C5-C4	2.20	1.43	1.40
2	A	500	PLP	C3-C2	2.98	1.42	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	PLP	C3-C2-N1	-2.31	117.72	120.75
2	B	500	PLP	C4A-C4-C3	-2.30	116.54	120.53
2	A	500	PLP	C3-C2-N1	-2.28	117.75	120.75
2	A	500	PLP	C4A-C4-C3	-2.26	116.61	120.53
2	A	500	PLP	O3P-P-O1P	2.01	118.46	110.60
2	A	500	PLP	C6-N1-C2	2.03	123.10	119.19
2	B	500	PLP	O3P-P-O1P	2.06	118.62	110.60
2	B	500	PLP	C6-N1-C2	2.12	123.27	119.19
2	A	500	PLP	C2A-C2-C3	2.26	123.65	120.96
2	A	500	PLP	C4A-C4-C5	3.63	124.51	120.85
2	B	500	PLP	C4A-C4-C5	3.70	124.58	120.85

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	421/429 (98%)	-0.06	17 (4%) 38 41	13, 31, 67, 97	0
1	B	425/429 (99%)	-0.38	2 (0%) 90 91	11, 23, 51, 84	0
All	All	846/858 (98%)	-0.22	19 (2%) 62 63	11, 27, 60, 97	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	ASN	5.2
1	B	20	PHE	4.2
1	A	20	PHE	4.1
1	A	18	SER	3.4
1	B	73	GLU	3.3
1	A	17	SER	3.2
1	A	19	TYR	3.1
1	A	254	ASN	3.1
1	A	34	VAL	2.7
1	A	73	GLU	2.6
1	A	71	ASN	2.6
1	A	260	GLU	2.5
1	A	9	THR	2.5
1	A	256	ASP	2.4
1	A	23	TRP	2.4
1	A	430	GLY	2.4
1	A	257	GLU	2.3
1	A	386	TYR	2.3
1	A	371	SER	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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( $\text{\AA}^2$ )	Q<0.9
2	PLP	A	500	15/16	0.98	0.09	20,25,31,34	0
2	PLP	B	500	15/16	0.99	0.07	14,18,22,22	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.