



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 06:37 AM GMT

PDB ID : 1CX9
Title : CRYSTAL STRUCTURE OF THE COMPLEX OF BACTERIAL TRYPTOPHAN SYNTHASE WITH THE TRANSITION STATE ANALOGUE INHIBITOR 4-(2-AMINOPHENYLTHIO)-BUTYLPHOSPHONICACID
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Deposited on : 1999-08-29
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

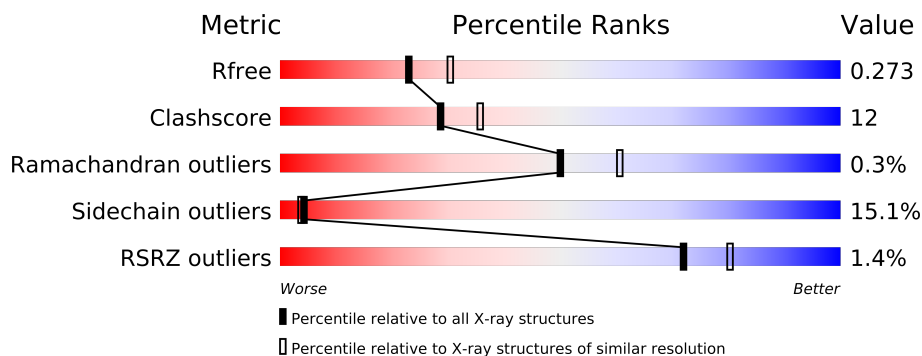
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	268	
2	B	397	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5115 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TRYPTOPHAN SYNTHASE (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			1992	1264	348	373	7			

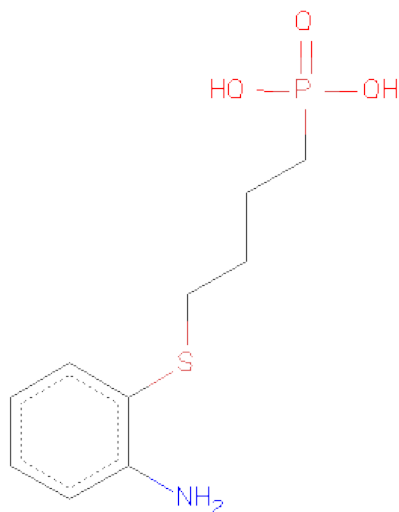
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	387	Total	C	N	O	S	0	0	0
			2934	1843	516	556	19			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

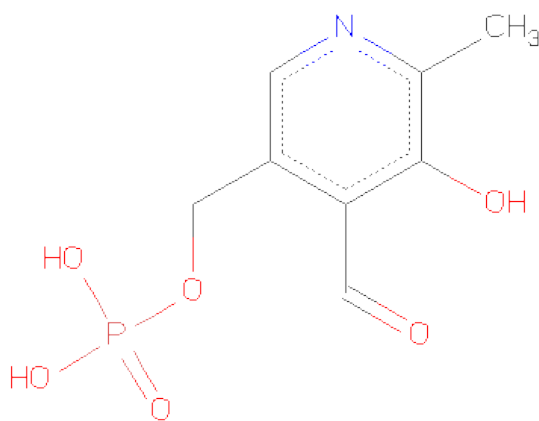
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is 4-(2-AMINOPHENYLTHIO)-BUTYLPHOSPHONICACID (three-letter code: NHP) (formula: C₁₀H₁₆NO₃PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	A	1	16	10	1	3	1	1	0	0

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 6 is water.

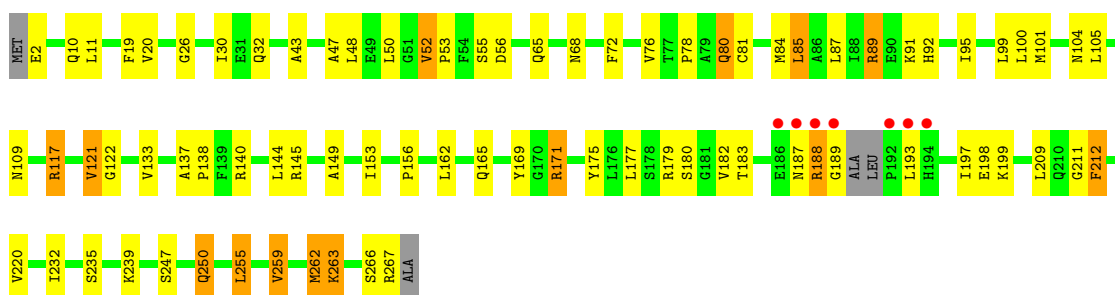
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	52	Total 52	O 52	0	0
6	B	105	Total 105	O 105	0	0

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 errors 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.

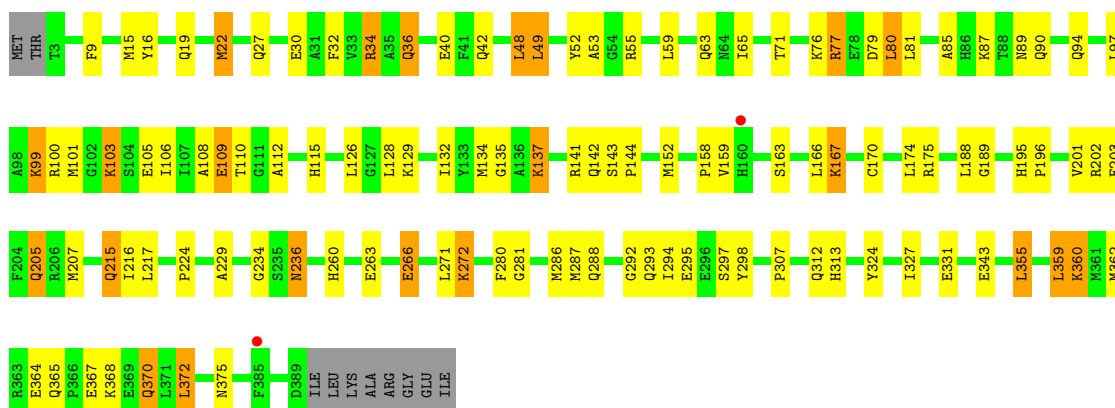
• Molecule 1: TRYPTOPHAN SYNTHASE (ALPHA CHAIN)

Chain A: 



• Molecule 2: TRYPTOPHAN SYNTHASE (BETA CHAIN)

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.65Å 59.34Å 67.30Å 90.00° 94.50° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 42.67 – 2.27	Depositor EDS
% Data completeness (in resolution range)	91.9 (30.00-2.30) 89.4 (42.67-2.27)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.27Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.210 , 0.276 0.210 , 0.273	Depositor DCC
R_{free} test set	2971 reflections (10.03%)	DCC
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 20.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 30288 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5115	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, NHP, 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	0/2031	0.73	0/2757
2	B	0.47	0/2992	0.80	0/4042
All	All	0.46	0/5023	0.77	0/6799

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	298	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1992	0	1995	55	0
2	B	2934	0	2902	73	0
3	B	1	0	0	0	0
4	A	16	0	14	4	0
5	B	15	0	7	0	0
6	A	52	0	0	2	0
6	B	105	0	0	7	0
All	All	5115	0	4918	123	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (123) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:89:ARG:HD2	1:A:122:GLY:HA3	1.53	0.90
1:A:182:VAL:HG11	2:B:175:ARG:HG2	1.56	0.84
2:B:135:GLY:HA2	2:B:159:VAL:HG22	1.64	0.80
1:A:133:VAL:H	2:B:19:GLN:HE22	1.29	0.79
1:A:183:THR:HB	4:A:270:NHP:H101	1.66	0.77
1:A:89:ARG:HG3	1:A:89:ARG:HH21	1.51	0.76
2:B:202:ARG:HH21	2:B:312:GLN:HE22	1.32	0.76
2:B:202:ARG:HD3	2:B:312:GLN:HE22	1.51	0.75
2:B:77:ARG:HG2	2:B:80:LEU:HD22	1.68	0.74
2:B:142:GLN:HG3	6:B:1071:HOH:O	1.90	0.70
2:B:112:ALA:O	2:B:142:GLN:HG2	1.93	0.69
2:B:89:ASN:HD22	2:B:205:GLN:NE2	1.91	0.69
2:B:202:ARG:HH21	2:B:312:GLN:NE2	1.90	0.69
2:B:108:ALA:HB3	2:B:132:ILE:HG12	1.72	0.69
2:B:327:ILE:HG23	2:B:331:GLU:HB3	1.75	0.68
2:B:89:ASN:HB2	2:B:205:GLN:HE22	1.60	0.67
2:B:87:LYS:HG2	6:B:1046:HOH:O	1.95	0.66
1:A:255:LEU:O	1:A:259:VAL:HG13	1.97	0.65
2:B:99:LYS:NZ	2:B:126:LEU:HB3	2.10	0.65
1:A:211:GLY:O	1:A:212:PHE:HB2	1.95	0.64
2:B:134:MET:O	2:B:158:PRO:HA	2.00	0.62
2:B:77:ARG:HG3	2:B:79:ASP:OD2	2.00	0.61
1:A:179:ARG:HG3	1:A:189:GLY:HA2	1.80	0.61
2:B:216:ILE:HG21	2:B:224:PRO:HD3	1.83	0.61
1:A:212:PHE:HA	4:A:270:NHP:O3	2.01	0.60
1:A:85:LEU:HB3	1:A:121:VAL:CG1	2.32	0.60
1:A:183:THR:HG22	1:A:212:PHE:CE2	2.38	0.59
1:A:53:PRO:HA	1:A:68:ASN:HD22	1.67	0.59
2:B:288:GLN:HE21	2:B:292:GLY:HA2	1.67	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:109:GLU:O	2:B:115:HIS:HD2	1.87	0.58
2:B:59:LEU:HD22	2:B:215:GLN:HB3	1.85	0.58
2:B:89:ASN:HD22	2:B:205:GLN:HE22	1.51	0.57
1:A:43:ALA:HB3	1:A:259:VAL:HG22	1.85	0.57
2:B:137:LYS:O	2:B:141:ARG:HB2	2.04	0.57
2:B:106:ILE:HD13	2:B:128:LEU:HD13	1.86	0.57
1:A:55:SER:HB3	2:B:293:GLN:HG3	1.86	0.56
2:B:106:ILE:CD1	2:B:128:LEU:HD13	2.37	0.55
1:A:140:ARG:HD2	1:A:169:TYR:HB3	1.87	0.55
1:A:56:ASP:OD2	2:B:167:LYS:HD3	2.08	0.54
2:B:236:ASN:HD22	2:B:375:ASN:HD22	1.56	0.54
2:B:137:LYS:HE2	2:B:163:SER:O	2.08	0.54
1:A:26:GLY:HA3	1:A:76:VAL:HG21	1.90	0.54
1:A:76:VAL:HA	1:A:80:GLN:HE21	1.74	0.52
2:B:77:ARG:CG	2:B:80:LEU:HD22	2.39	0.52
1:A:149:ALA:HB1	1:A:171:ARG:HB3	1.91	0.52
1:A:104:ASN:HD21	2:B:288:GLN:NE2	2.07	0.52
1:A:78:PRO:HD3	6:B:1036:HOH:O	2.11	0.51
1:A:53:PRO:HA	1:A:68:ASN:ND2	2.26	0.50
2:B:297:SER:OG	2:B:307:PRO:HA	2.12	0.50
2:B:355:LEU:HD22	2:B:359:LEU:HD13	1.93	0.50
2:B:272:LYS:HD3	2:B:324:TYR:HB2	1.92	0.50
2:B:260:HIS:HD2	2:B:266:GLU:HG2	1.77	0.49
2:B:32:PHE:O	2:B:36:GLN:HB2	2.12	0.49
1:A:153:ILE:HD11	4:A:270:NHP:H6	1.94	0.49
1:A:43:ALA:CB	1:A:259:VAL:HG22	2.43	0.49
1:A:263:LYS:HE2	1:A:266:SER:OG	2.13	0.49
1:A:85:LEU:HB3	1:A:121:VAL:HG11	1.93	0.49
2:B:15:MET:SD	2:B:22:MET:HE1	2.53	0.49
1:A:89:ARG:HG3	1:A:89:ARG:NH2	2.20	0.49
2:B:370:GLN:HG2	6:B:1122:HOH:O	2.12	0.49
2:B:234:GLY:O	2:B:313:HIS:HE1	1.95	0.48
2:B:89:ASN:HB2	2:B:205:GLN:NE2	2.28	0.48
2:B:313:HIS:HD2	2:B:324:TYR:OH	1.96	0.48
1:A:117:ARG:NH2	6:A:1114:HOH:O	2.45	0.48
2:B:71:THR:CB	2:B:362:MET:HG3	2.44	0.47
2:B:16:TYR:O	2:B:281:GLY:HA2	2.13	0.47
2:B:49:LEU:O	2:B:53:ALA:HB3	2.15	0.47
1:A:177:LEU:HD21	6:B:1125:HOH:O	2.15	0.47
2:B:71:THR:OG1	2:B:362:MET:HG3	2.15	0.46
1:A:235:SER:O	1:A:239:LYS:HB2	2.14	0.46
1:A:89:ARG:NH1	1:A:95:ILE:O	2.48	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:110:THR:HG23	2:B:134:MET:HG3	1.98	0.46
1:A:91:LYS:HB3	1:A:92:HIS:CD2	2.51	0.46
2:B:195:HIS:HD2	6:B:1006:HOH:O	2.00	0.46
2:B:205:GLN:HA	2:B:205:GLN:NE2	2.31	0.45
2:B:48:LEU:O	2:B:52:TYR:HB3	2.16	0.45
1:A:89:ARG:NH2	1:A:92:HIS:O	2.49	0.45
2:B:109:GLU:HG3	2:B:170:CYS:SG	2.57	0.45
1:A:193:LEU:O	1:A:197:ILE:HG13	2.17	0.45
2:B:109:GLU:OE2	2:B:170:CYS:SG	2.72	0.45
1:A:20:VAL:HG22	1:A:47:ALA:HB3	1.99	0.45
1:A:175:TYR:OH	4:A:270:NHP:H72	2.17	0.45
2:B:76:LYS:HD2	2:B:76:LYS:HA	1.53	0.44
2:B:195:HIS:CD2	2:B:196:PRO:HA	2.51	0.44
2:B:229:ALA:HB1	2:B:236:ASN:HD21	1.83	0.44
1:A:19:PHE:CE1	1:A:262:MET:HG2	2.53	0.44
2:B:27:GLN:HE22	2:B:103:LYS:NZ	2.16	0.44
2:B:167:LYS:NZ	2:B:294:ILE:O	2.50	0.44
2:B:34:ARG:HG2	2:B:100:ARG:HH11	1.83	0.44
2:B:9:PHE:CD2	2:B:312:GLN:HG3	2.53	0.43
2:B:81:LEU:HD23	2:B:85:ALA:O	2.17	0.43
1:A:30:ILE:HD11	1:A:80:GLN:HG2	1.99	0.43
2:B:135:GLY:CA	2:B:159:VAL:HG22	2.42	0.43
1:A:85:LEU:HB3	1:A:121:VAL:HG13	2.00	0.43
2:B:129:LYS:HE3	2:B:129:LYS:HB2	1.79	0.43
1:A:137:ALA:HB3	1:A:138:PRO:CD	2.48	0.43
2:B:143:SER:HB2	2:B:144:PRO:HD3	2.01	0.43
2:B:271:LEU:O	2:B:271:LEU:HD12	2.18	0.43
1:A:81:CYS:O	1:A:84:MET:HB2	2.19	0.43
1:A:19:PHE:CZ	1:A:262:MET:HG2	2.54	0.43
1:A:145:ARG:NH1	6:A:1057:HOH:O	2.51	0.43
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.54	0.42
1:A:43:ALA:HB3	1:A:259:VAL:CG2	2.49	0.42
1:A:188:ARG:HB3	1:A:189:GLY:H	1.67	0.42
2:B:263:GLU:CD	2:B:263:GLU:H	2.22	0.42
2:B:365:GLN:NE2	6:B:1016:HOH:O	2.53	0.42
1:A:20:VAL:O	1:A:232:ILE:HA	2.19	0.42
1:A:199:LYS:HA	1:A:199:LYS:HD2	1.79	0.42
2:B:201:VAL:O	2:B:205:GLN:HB2	2.20	0.42
1:A:100:LEU:HD13	1:A:100:LEU:C	2.40	0.41
1:A:52:VAL:HA	1:A:53:PRO:HD3	1.92	0.41
1:A:156:PRO:HD3	1:A:177:LEU:HB3	2.02	0.41
1:A:211:GLY:O	1:A:212:PHE:CB	2.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:87:LYS:HD3	2:B:115:HIS:HA	2.01	0.41
2:B:100:ARG:HG3	2:B:100:ARG:HH21	1.85	0.41
1:A:247:SER:HB2	1:A:250:GLN:HB2	2.03	0.41
2:B:360:LYS:O	2:B:364:GLU:HB2	2.20	0.41
1:A:2:GLU:O	1:A:2:GLU:HG2	2.21	0.41
2:B:71:THR:HG23	2:B:372:LEU:HD22	2.03	0.41
1:A:30:ILE:CD1	1:A:80:GLN:HG2	2.51	0.40
2:B:15:MET:HB3	2:B:22:MET:HE1	2.02	0.40
2:B:174:LEU:HD11	2:B:280:PHE:CE1	2.57	0.40
1:A:20:VAL:HG21	1:A:209:LEU:HD21	2.04	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	260/268 (97%)	247 (95%)	11 (4%)	2 (1%)	27	30
2	B	385/397 (97%)	372 (97%)	13 (3%)	0	100	100
All	All	645/665 (97%)	619 (96%)	24 (4%)	2 (0%)	50	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	PHE
1	A	188	ARG

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	206/208 (99%)	174 (84%)	32 (16%)	4	3
2	B	303/311 (97%)	258 (85%)	45 (15%)	4	4
All	All	509/519 (98%)	432 (85%)	77 (15%)	4	4

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	11	LEU
1	A	32	GLN
1	A	48	LEU
1	A	50	LEU
1	A	52	VAL
1	A	65	GLN
1	A	72	PHE
1	A	80	GLN
1	A	85	LEU
1	A	87	LEU
1	A	89	ARG
1	A	99	LEU
1	A	101	MET
1	A	105	LEU
1	A	109	ASN
1	A	117	ARG
1	A	121	VAL
1	A	144	LEU
1	A	162	LEU
1	A	165	GLN
1	A	171	ARG
1	A	180	SER
1	A	187	ASN
1	A	198	GLU
1	A	220	VAL
1	A	250	GLN
1	A	255	LEU
1	A	259	VAL
1	A	262	MET
1	A	263	LYS
1	A	267	ARG
2	B	22	MET
2	B	30	GLU
2	B	34	ARG

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Mol	Chain	Res	Type
2	B	36	GLN
2	B	40	GLU
2	B	42	GLN
2	B	48	LEU
2	B	49	LEU
2	B	55	ARG
2	B	63	GLN
2	B	65	ILE
2	B	77	ARG
2	B	80	LEU
2	B	90	GLN
2	B	94	GLN
2	B	97	LEU
2	B	99	LYS
2	B	101	MET
2	B	103	LYS
2	B	105	GLU
2	B	109	GLU
2	B	137	LYS
2	B	152	MET
2	B	166	LEU
2	B	167	LYS
2	B	188	LEU
2	B	203	GLU
2	B	205	GLN
2	B	207	MET
2	B	215	GLN
2	B	217	LEU
2	B	236	ASN
2	B	266	GLU
2	B	272	LYS
2	B	286	MET
2	B	287	MET
2	B	295	GLU
2	B	343	GLU
2	B	355	LEU
2	B	359	LEU
2	B	360	LYS
2	B	367	GLU
2	B	368	LYS
2	B	370	GLN
2	B	372	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	68	ASN
1	A	80	GLN
2	B	19	GLN
2	B	27	GLN
2	B	44	GLN
2	B	51	ASN
2	B	63	GLN
2	B	64	ASN
2	B	82	HIS
2	B	90	GLN
2	B	94	GLN
2	B	171	ASN
2	B	185	HIS
2	B	195	HIS
2	B	205	GLN
2	B	215	GLN
2	B	236	ASN
2	B	288	GLN
2	B	312	GLN
2	B	313	HIS
2	B	365	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	NHP	A	270	-	16,16,16	1.63	2 (12%)	21,21,21	1.78	5 (23%)
5	PLP	B	900	2	14,15,16	1.71	3 (21%)	20,22,23	3.50	9 (45%)

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	NHP	A	270	-	-	0/9/9/9	0/1/1/1
5	PLP	B	900	2	-	0/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	270	NHP	P1-C10	-5.23	1.73	1.79
5	B	900	PLP	C3-C2	-3.69	1.38	1.40
4	A	270	NHP	P1-O1	-2.77	1.49	1.54
5	B	900	PLP	P-O2P	-2.50	1.45	1.54
5	B	900	PLP	P-O3P	-2.03	1.47	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	900	PLP	P-O4P-C5A	7.88	149.65	121.22
5	B	900	PLP	O4P-P-O1P	7.60	128.98	106.71
5	B	900	PLP	O2P-P-O4P	-5.55	91.34	106.65
5	B	900	PLP	C3-C4-C5	-4.82	112.17	121.29
5	B	900	PLP	C4-C3-C2	4.71	125.08	119.67
5	B	900	PLP	C5A-C5-C6	-4.38	110.99	119.28
4	A	270	NHP	C7-S1-C2	4.15	112.54	102.89
4	A	270	NHP	O1-P1-O3	-3.52	103.18	112.56
4	A	270	NHP	O2-P1-C10	3.36	114.98	106.90
4	A	270	NHP	O2-P1-O3	-3.08	104.34	112.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	270	NHP	O1-P1-C10	2.79	113.62	106.90
5	B	900	PLP	O3P-P-O4P	-2.68	99.24	106.65
5	B	900	PLP	O4P-C5A-C5	-2.14	104.91	109.26
5	B	900	PLP	C5A-C5-C4	2.13	126.36	121.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	264/268 (98%)	-0.01	7 (2%)	52 62	7, 18, 46, 77	0
2	B	387/397 (97%)	-0.23	2 (0%)	88 94	3, 12, 30, 56	0
All	All	651/665 (97%)	-0.14	9 (1%)	72 80	3, 15, 36, 77	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	GLY	4.4
1	A	194	HIS	3.1
1	A	186	GLU	2.9
1	A	188	ARG	2.9
1	A	192	PRO	2.4
1	A	193	LEU	2.2
2	B	160	HIS	2.2
1	A	187	ASN	2.2
2	B	385	PHE	2.1

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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NA	B	1162	1/1	0.14	0.94	13,13,13,13	0
5	PLP	B	900	15/16	0.16	0.82	10,17,22,23	0
4	NHP	A	270	16/16	0.16	0.71	19,23,38,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.