



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 02:53 am BST

PDB ID : 1V8Z
Title : X-ray crystal structure of the Tryptophan Synthase b2 Subunit from Hyperthermophile, *Pyrococcus furiosus*
Authors : Hioki, Y.; Ogasahara, K.; Lee, S.J.; Ma, J.; Ishida, M.; Yamagata, Y.; Matsuura, Y.; Ota, M.; Kuramitsu, S.; Yutani, K.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2004-01-15
Resolution : 2.21 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 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

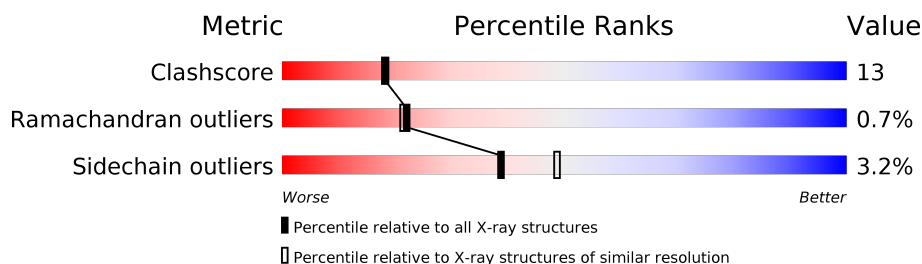
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	388	
1	B	388	
1	C	388	
1	D	388	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12245 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 Tryptophan synthase beta chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			2981	1904	513	552	12			
1	B	387	Total	C	N	O	S	0	0	0
			2989	1908	515	554	12			
1	C	387	Total	C	N	O	S	0	0	0
			2989	1908	515	554	12			
1	D	385	Total	C	N	O	S	0	0	0
			2972	1898	511	551	12			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 4 is water.

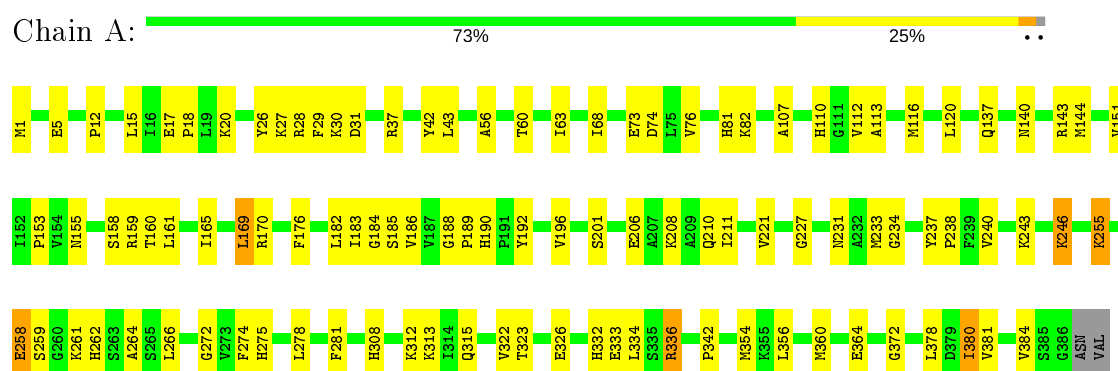
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	89	Total	O	0	0
			89	89		
4	C	61	Total	O	0	0
			61	61		
4	D	46	Total	O	0	0
			46	46		

3 Residue-property plots

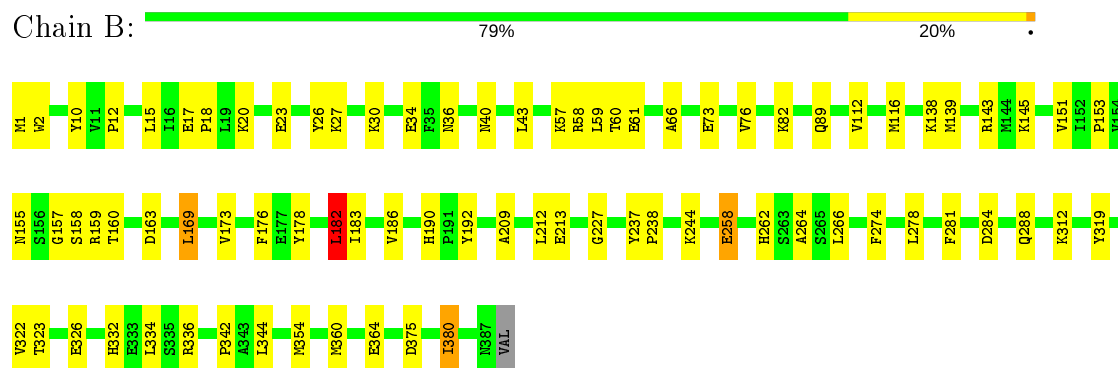
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

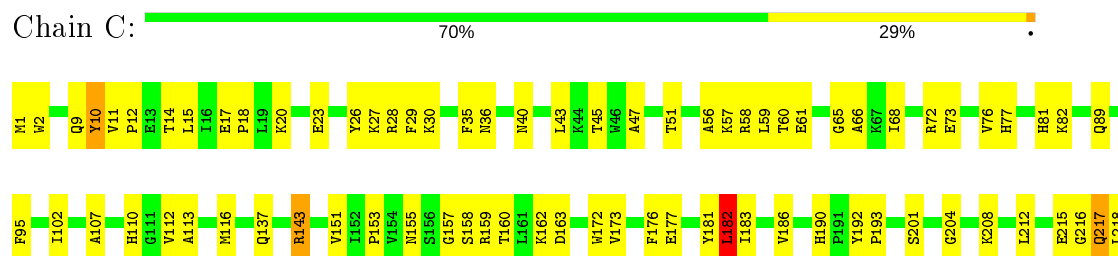
• Molecule 1: Tryptophan synthase beta chain 1

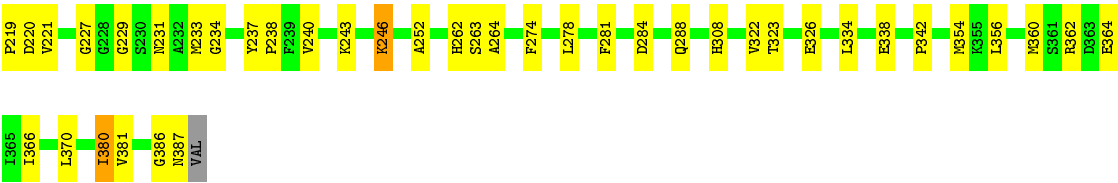


• Molecule 1: Tryptophan synthase beta chain 1

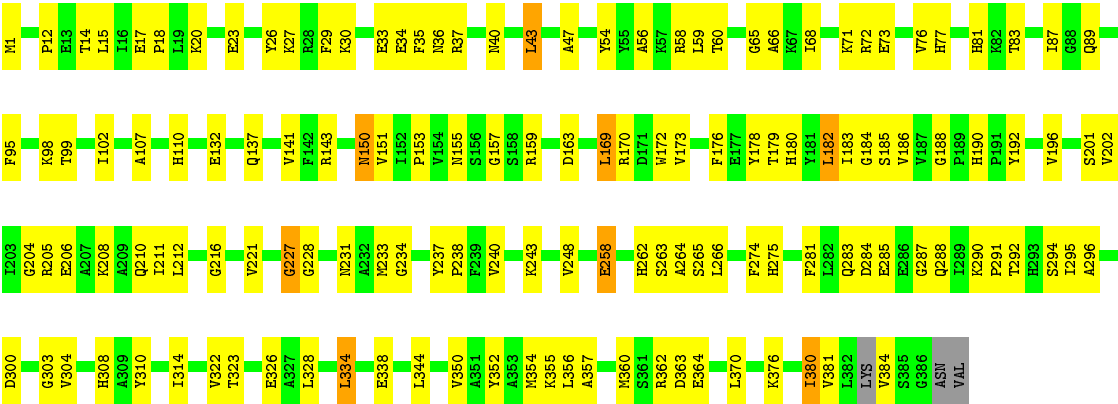


• Molecule 1: Tryptophan synthase beta chain 1





• Molecule 1: Tryptophan synthase beta chain 1



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.83 Å 110.53 Å 160.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.30 – 2.21	Depositor
% Data completeness (in resolution range)	98.3 (67.30-2.21)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.208 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12245	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

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: NA, 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	0.34	0/3042	0.62	1/4104 (0.0%)
1	B	0.35	0/3050	0.62	2/4115 (0.0%)
1	C	0.33	0/3050	0.61	2/4115 (0.0%)
1	D	0.33	0/3032	0.61	1/4090 (0.0%)
All	All	0.34	0/12174	0.62	6/16424 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	LEU	CA-CB-CG	5.87	128.80	115.30
1	C	182	LEU	CA-CB-CG	5.48	127.90	115.30
1	D	227	GLY	N-CA-C	-5.29	99.86	113.10
1	B	227	GLY	N-CA-C	-5.22	100.05	113.10
1	C	227	GLY	N-CA-C	-5.20	100.11	113.10
1	A	227	GLY	N-CA-C	-5.14	100.24	113.10

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	2981	0	3002	75	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2989	0	3008	58	0
1	C	2989	0	3008	81	0
1	D	2972	0	2988	114	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	15	0	7	0	0
3	B	15	0	7	1	0
3	C	15	0	6	0	0
3	D	15	0	7	0	0
4	A	55	0	0	2	0
4	B	89	0	0	4	0
4	C	61	0	0	5	0
4	D	46	0	0	11	0
All	All	12245	0	12033	321	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 13.

All (321) 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:C:12:PRO:HD2	1:C:15:LEU:HD12	1.41	1.02
1:D:98:LYS:HB3	4:D:432:HOH:O	1.59	0.99
1:B:27:LYS:HA	1:B:27:LYS:HE2	1.50	0.93
1:C:262:HIS:HD2	1:C:264:ALA:H	1.17	0.93
1:B:262:HIS:HD2	1:B:264:ALA:H	1.18	0.90
1:D:155:ASN:HA	1:D:159:ARG:HG2	1.54	0.88
1:B:155:ASN:HA	1:B:159:ARG:HG2	1.57	0.86
1:C:155:ASN:HA	1:C:159:ARG:HG2	1.58	0.85
1:A:262:HIS:HD2	1:A:264:ALA:H	1.21	0.84
1:D:17:GLU:HG3	1:D:20:LYS:NZ	1.93	0.84
1:C:17:GLU:HG3	1:C:20:LYS:NZ	1.92	0.83
1:A:155:ASN:HA	1:A:159:ARG:HG2	1.59	0.82
1:D:262:HIS:HD2	1:D:264:ALA:H	1.25	0.82
1:D:27:LYS:HA	1:D:27:LYS:HE2	1.62	0.80
1:D:290:LYS:HG3	1:D:291:PRO:HD2	1.62	0.80
1:B:237:TYR:HB3	1:B:238:PRO:HD3	1.64	0.79
1:A:27:LYS:HE2	1:A:27:LYS:HA	1.66	0.78
1:B:59:LEU:HD11	1:B:354:MET:HE3	1.66	0.78
1:B:344:LEU:HD11	1:B:380:ILE:HD11	1.66	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LYS:HA	1:C:27:LYS:HE2	1.66	0.77
1:A:246:LYS:HB2	1:A:246:LYS:NZ	2.00	0.76
1:D:263:SER:OG	4:D:446:HOH:O	2.02	0.75
1:C:73:GLU:O	1:C:76:VAL:HG12	1.87	0.75
1:D:73:GLU:O	1:D:76:VAL:HG12	1.86	0.75
1:D:237:TYR:HB3	1:D:238:PRO:HD3	1.71	0.73
1:A:60:THR:CG2	1:A:68:ILE:H	2.02	0.73
1:C:113:ALA:HA	1:C:116:MET:CE	2.18	0.73
1:B:380:ILE:HG23	4:B:426:HOH:O	1.90	0.72
1:B:73:GLU:O	1:B:76:VAL:HG12	1.89	0.72
1:A:258:GLU:H	1:A:258:GLU:CD	1.93	0.72
1:D:292:THR:HG21	1:D:300:ASP:O	1.91	0.71
1:D:258:GLU:H	1:D:258:GLU:CD	1.94	0.71
1:A:73:GLU:O	1:A:76:VAL:HG12	1.90	0.71
1:D:12:PRO:HD2	1:D:15:LEU:HD12	1.70	0.70
1:C:113:ALA:HA	1:C:116:MET:HE3	1.71	0.70
1:C:237:TYR:HB3	1:C:238:PRO:HD3	1.73	0.69
1:B:17:GLU:HG3	1:B:20:LYS:NZ	2.08	0.68
1:C:17:GLU:HG3	1:C:20:LYS:HZ3	1.57	0.68
1:C:58:ARG:HB2	1:C:338:GLU:OE2	1.93	0.68
1:D:60:THR:CG2	1:D:68:ILE:H	2.07	0.68
1:A:12:PRO:HD2	1:A:15:LEU:HD12	1.75	0.68
1:A:113:ALA:HA	1:A:116:MET:CE	2.24	0.68
1:A:56:ALA:O	1:A:60:THR:HG23	1.93	0.68
1:A:107:ALA:O	1:A:137:GLN:HG3	1.92	0.68
1:B:169:LEU:O	1:B:173:VAL:HG23	1.95	0.67
1:D:17:GLU:O	1:D:20:LYS:HG2	1.94	0.67
1:C:56:ALA:O	1:C:60:THR:HG23	1.95	0.67
1:A:113:ALA:HA	1:A:116:MET:HE2	1.76	0.66
1:A:1:MET:HA	1:A:190:HIS:CD2	2.30	0.66
1:D:291:PRO:HA	4:D:433:HOH:O	1.97	0.65
1:B:258:GLU:CD	1:B:258:GLU:H	1.99	0.64
1:A:380:ILE:HG23	4:A:428:HOH:O	1.97	0.64
1:A:274:PHE:HB3	1:A:281:PHE:CE2	2.31	0.64
1:D:274:PHE:HB3	1:D:281:PHE:CE2	2.32	0.64
1:D:58:ARG:HG3	4:D:410:HOH:O	1.97	0.64
1:B:158:SER:OG	1:B:160:THR:HG22	1.98	0.63
1:A:262:HIS:CD2	1:A:264:ALA:H	2.11	0.63
1:B:332:HIS:O	1:B:336:ARG:HG2	1.98	0.63
1:D:137:GLN:O	1:D:141:VAL:HG23	1.98	0.63
1:C:112:VAL:O	1:C:116:MET:HG3	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:THR:OG1	1:C:326:GLU:HG3	1.98	0.62
1:C:2:TRP:HH2	1:C:10:TYR:HH	1.47	0.61
1:B:58:ARG:HG3	4:B:442:HOH:O	2.00	0.60
1:B:26:TYR:O	1:B:30:LYS:HB2	2.02	0.60
1:B:1:MET:HA	1:B:190:HIS:CD2	2.36	0.60
1:D:47:ALA:HA	1:D:77:HIS:HB3	1.83	0.60
1:B:284:ASP:OD2	1:B:288:GLN:HB2	2.01	0.60
1:B:2:TRP:HH2	1:B:10:TYR:HH	1.49	0.60
1:A:60:THR:HG22	1:A:68:ILE:H	1.65	0.59
1:D:295:ILE:HD13	1:D:328:LEU:HD13	1.83	0.59
1:C:17:GLU:O	1:C:20:LYS:HG2	2.02	0.59
1:D:233:MET:HG2	1:D:308:HIS:NE2	2.17	0.59
1:C:60:THR:HG22	1:C:68:ILE:H	1.67	0.59
1:D:221:VAL:HG11	1:D:356:LEU:HD21	1.83	0.59
1:D:380:ILE:C	1:D:380:ILE:HD12	2.23	0.59
1:A:18:PRO:HG3	1:A:176:PHE:CD2	2.38	0.59
1:B:312:LYS:NZ	4:B:480:HOH:O	2.35	0.59
1:D:26:TYR:O	1:D:30:LYS:HB2	2.03	0.58
1:D:266:LEU:HG	1:D:304:VAL:HG11	1.86	0.58
1:A:60:THR:HG21	1:A:68:ILE:H	1.67	0.58
1:C:59:LEU:HD11	1:C:354:MET:HE3	1.86	0.58
1:D:350:VAL:O	1:D:354:MET:HG3	2.04	0.58
1:D:56:ALA:O	1:D:60:THR:HG23	2.04	0.58
1:A:322:VAL:HG13	1:A:326:GLU:HB2	1.86	0.58
1:C:380:ILE:HG13	1:C:381:VAL:N	2.19	0.58
1:A:246:LYS:HZ2	1:A:246:LYS:HB2	1.68	0.57
1:C:60:THR:CG2	1:C:68:ILE:H	2.17	0.57
1:D:60:THR:HG22	1:D:68:ILE:H	1.69	0.57
1:C:360:MET:SD	1:C:366:ILE:HD11	2.43	0.57
1:D:107:ALA:O	1:D:137:GLN:HG3	2.04	0.57
1:D:344:LEU:HD11	1:D:380:ILE:HD11	1.86	0.57
1:C:1:MET:HA	1:C:190:HIS:CD2	2.39	0.57
1:C:233:MET:HG2	1:C:308:HIS:NE2	2.20	0.57
1:D:227:GLY:HA2	4:D:445:HOH:O	2.02	0.57
1:A:158:SER:OG	1:A:160:THR:HG22	2.05	0.56
1:B:59:LEU:HD11	1:B:354:MET:CE	2.36	0.56
1:D:323:THR:OG1	1:D:326:GLU:HG3	2.06	0.56
1:B:27:LYS:HA	1:B:27:LYS:CE	2.30	0.56
1:A:81:HIS:CE1	1:A:231:ASN:HB3	2.41	0.56
1:C:151:VAL:O	1:C:153:PRO:HD3	2.05	0.56
1:A:380:ILE:O	1:A:384:VAL:HG23	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:TRP:HH2	1:C:10:TYR:OH	1.89	0.56
1:D:284:ASP:OD2	1:D:288:GLN:HB2	2.05	0.55
1:B:322:VAL:HG13	1:B:326:GLU:HB2	1.88	0.55
1:B:89:GLN:CD	1:B:182:LEU:HD13	2.27	0.55
1:B:57:LYS:O	1:B:61:GLU:HG3	2.06	0.55
1:D:58:ARG:HB2	1:D:338:GLU:OE2	2.07	0.55
1:B:344:LEU:CD1	1:B:380:ILE:HD11	2.37	0.55
1:C:82:LYS:HD3	1:C:110:HIS:HA	1.89	0.55
1:C:183:ILE:HD12	1:C:192:TYR:CD2	2.41	0.55
1:C:204:GLY:HA3	1:C:238:PRO:HG2	1.89	0.54
1:A:18:PRO:HG3	1:A:176:PHE:CG	2.41	0.54
1:A:332:HIS:O	1:A:336:ARG:HG2	2.07	0.54
1:A:82:LYS:HD3	1:A:110:HIS:HA	1.89	0.54
1:B:145:LYS:NZ	1:D:363:ASP:CG	2.61	0.54
1:D:322:VAL:CG1	1:D:326:GLU:HB2	2.36	0.54
1:D:185:SER:O	1:D:196:VAL:HG21	2.07	0.54
1:D:290:LYS:CG	1:D:291:PRO:HD2	2.35	0.54
1:D:17:GLU:HG3	1:D:20:LYS:HZ1	1.73	0.54
1:A:274:PHE:HB3	1:A:281:PHE:CZ	2.42	0.54
1:A:322:VAL:CG1	1:A:326:GLU:HB2	2.38	0.54
1:A:333:GLU:OE1	1:A:336:ARG:NH1	2.41	0.54
1:C:35:PHE:HA	1:C:95:PHE:CZ	2.43	0.53
1:C:322:VAL:HG13	1:C:326:GLU:HB2	1.90	0.53
1:C:284:ASP:OD2	1:C:288:GLN:HB2	2.09	0.53
1:A:160:THR:OG1	1:A:161:LEU:N	2.41	0.53
1:A:17:GLU:HB3	1:A:18:PRO:HD3	1.91	0.53
1:C:158:SER:OG	1:C:160:THR:HG22	2.07	0.53
1:C:9:GLN:O	1:C:11:VAL:N	2.42	0.53
1:C:183:ILE:HD12	1:C:192:TYR:CG	2.44	0.53
1:C:220:ASP:O	1:C:246:LYS:HB2	2.08	0.53
1:D:1:MET:HA	1:D:190:HIS:CD2	2.44	0.53
1:D:322:VAL:HG13	1:D:326:GLU:HB2	1.90	0.53
1:D:59:LEU:HD11	1:D:354:MET:CE	2.38	0.53
1:D:14:THR:HB	1:D:173:VAL:HG13	1.90	0.53
1:D:17:GLU:HG3	1:D:20:LYS:HZ3	1.71	0.53
1:A:246:LYS:HD3	4:A:446:HOH:O	2.07	0.53
1:D:99:THR:HG22	4:D:423:HOH:O	2.08	0.53
1:B:17:GLU:O	1:B:20:LYS:HG2	2.08	0.53
1:C:59:LEU:HD11	1:C:354:MET:CE	2.39	0.53
1:C:262:HIS:CD2	1:C:264:ALA:H	2.09	0.52
1:D:23:GLU:O	1:D:27:LYS:HG2	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:THR:HG23	1:B:66:ALA:O	2.09	0.52
1:C:274:PHE:HB3	1:C:281:PHE:CE2	2.45	0.52
1:D:237:TYR:HA	1:D:240:VAL:HG23	1.92	0.52
1:A:272:GLY:O	1:A:278:LEU:HD12	2.10	0.52
1:D:157:GLY:HA3	1:D:163:ASP:OD1	2.10	0.52
1:D:180:HIS:N	4:D:432:HOH:O	2.43	0.51
1:D:132:GLU:CD	1:D:159:ARG:HH12	2.14	0.51
1:C:113:ALA:HA	1:C:116:MET:HE2	1.90	0.51
1:D:295:ILE:CD1	1:D:328:LEU:HD13	2.39	0.51
1:A:151:VAL:O	1:A:153:PRO:HD3	2.10	0.51
1:D:262:HIS:CD2	1:D:264:ALA:H	2.16	0.51
1:A:221:VAL:HG11	1:A:356:LEU:HD21	1.93	0.51
1:D:23:GLU:OE1	1:D:190:HIS:HE1	1.94	0.51
1:A:237:TYR:HA	1:A:240:VAL:HG23	1.93	0.50
1:A:63:ILE:HD11	1:A:354:MET:HE3	1.93	0.50
1:C:81:HIS:CE1	1:C:231:ASN:HB3	2.46	0.50
1:D:150:ASN:HD22	1:D:151:VAL:N	2.10	0.50
1:B:262:HIS:CD2	1:B:264:ALA:H	2.10	0.50
1:A:237:TYR:HB3	1:A:238:PRO:HD3	1.93	0.50
1:B:244:LYS:HB2	4:B:478:HOH:O	2.11	0.50
1:B:2:TRP:HH2	1:B:10:TYR:OH	1.93	0.50
1:A:183:ILE:HD12	1:A:192:TYR:CG	2.47	0.50
1:C:102:ILE:HG13	1:C:181:TYR:HA	1.93	0.50
1:B:209:ALA:O	1:B:213:GLU:HG3	2.12	0.50
1:D:183:ILE:HD12	1:D:192:TYR:CG	2.47	0.50
1:D:360:MET:HB3	1:D:364:GLU:OE2	2.12	0.50
1:D:60:THR:HG21	1:D:68:ILE:H	1.74	0.50
1:A:259:SER:HB3	1:C:28:ARG:HH12	1.77	0.49
1:C:57:LYS:O	1:C:61:GLU:HG3	2.12	0.49
1:C:360:MET:HB3	1:C:364:GLU:OE2	2.11	0.49
1:C:65:GLY:O	1:C:362:ARG:HA	2.11	0.49
1:A:165:ILE:O	1:A:169:LEU:HD22	2.12	0.49
1:D:188:GLY:HA2	1:D:275:HIS:O	2.12	0.49
1:B:34:GLU:OE1	1:B:34:GLU:HA	2.11	0.49
1:D:334:LEU:HD22	1:D:338:GLU:HB2	1.93	0.49
4:C:434:HOH:O	1:D:143:ARG:HD3	2.11	0.49
1:D:208:LYS:O	1:D:211:ILE:HG22	2.12	0.49
1:D:151:VAL:O	1:D:153:PRO:HD3	2.13	0.49
1:B:274:PHE:HB3	1:B:281:PHE:CE2	2.48	0.49
1:D:66:ALA:HB1	1:D:364:GLU:O	2.12	0.49
1:A:31:ASP:OD1	1:A:31:ASP:N	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:HIS:NE2	1:C:231:ASN:HB3	2.27	0.49
1:D:212:LEU:O	1:D:216:GLY:HA2	2.13	0.49
1:D:204:GLY:HA3	1:D:238:PRO:HG2	1.93	0.48
1:D:380:ILE:O	1:D:384:VAL:HG23	2.13	0.48
1:A:266:LEU:HD22	1:A:312:LYS:HD2	1.95	0.48
1:D:183:ILE:HD12	1:D:192:TYR:CD2	2.48	0.48
1:D:380:ILE:HG23	4:D:431:HOH:O	2.14	0.48
1:A:81:HIS:NE2	1:A:231:ASN:HB3	2.28	0.48
1:D:380:ILE:HG13	1:D:381:VAL:N	2.28	0.48
1:A:255:LYS:HB2	1:A:261:LYS:HB2	1.96	0.48
1:B:18:PRO:HB3	1:B:176:PHE:CG	2.49	0.48
1:B:17:GLU:HB3	1:B:18:PRO:CD	2.44	0.48
1:B:237:TYR:HB3	1:B:238:PRO:CD	2.41	0.47
1:D:35:PHE:HA	1:D:95:PHE:CZ	2.50	0.47
1:D:59:LEU:HD11	1:D:354:MET:HE3	1.96	0.47
1:D:23:GLU:CD	1:D:190:HIS:HE1	2.17	0.47
1:A:221:VAL:HG13	1:A:246:LYS:HG2	1.97	0.47
1:D:71:LYS:HD2	4:D:441:HOH:O	2.14	0.47
1:B:278:LEU:C	1:B:278:LEU:HD23	2.35	0.47
1:C:23:GLU:O	1:C:27:LYS:HG2	2.15	0.47
1:D:248:VAL:HG11	1:D:352:TYR:CE1	2.50	0.47
1:B:17:GLU:HG3	1:B:20:LYS:HZ3	1.77	0.47
1:C:172:TRP:O	1:C:176:PHE:HB3	2.15	0.47
1:C:380:ILE:HG23	4:C:406:HOH:O	2.14	0.47
1:D:15:LEU:O	1:D:18:PRO:HG2	2.15	0.47
1:C:14:THR:HB	1:C:173:VAL:HG13	1.97	0.46
1:C:158:SER:OG	1:C:162:LYS:HE2	2.15	0.46
1:C:201:SER:HA	1:C:234:GLY:O	2.15	0.46
1:C:47:ALA:HA	1:C:77:HIS:HB3	1.98	0.46
1:A:112:VAL:O	1:A:116:MET:HG3	2.16	0.46
1:C:26:TYR:O	1:C:30:LYS:HB2	2.16	0.46
1:A:42:TYR:CD2	1:A:120:LEU:HD21	2.51	0.46
1:B:82:LYS:NZ	3:B:400:PLP:O3	2.49	0.46
1:D:201:SER:HA	1:D:234:GLY:O	2.16	0.46
1:B:360:MET:HB3	1:B:364:GLU:OE2	2.16	0.46
1:C:89:GLN:CD	1:C:182:LEU:HD13	2.36	0.46
1:D:110:HIS:CE1	1:D:184:GLY:HA2	2.50	0.46
1:A:110:HIS:CE1	1:A:184:GLY:HA2	2.51	0.46
1:C:107:ALA:O	1:C:137:GLN:HG3	2.15	0.46
1:C:10:TYR:CE2	1:C:278:LEU:HB2	2.50	0.46
1:D:310:TYR:CE2	1:D:314:ILE:HD13	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LYS:C	1:A:315:GLN:H	2.19	0.45
1:B:12:PRO:HD2	1:B:15:LEU:HD12	1.97	0.45
1:A:81:HIS:CD2	1:A:231:ASN:HB3	2.51	0.45
1:B:183:ILE:HD12	1:B:192:TYR:CD2	2.52	0.45
1:A:113:ALA:HA	1:A:116:MET:HE3	1.96	0.45
1:A:380:ILE:HG13	1:A:381:VAL:N	2.32	0.45
1:D:17:GLU:N	1:D:18:PRO:HD2	2.32	0.45
1:B:151:VAL:O	1:B:153:PRO:HD3	2.17	0.45
1:B:274:PHE:HB3	1:B:281:PHE:CZ	2.52	0.45
1:C:81:HIS:CD2	1:C:231:ASN:HB3	2.51	0.45
1:C:157:GLY:HA3	1:C:163:ASP:OD1	2.17	0.45
1:D:169:LEU:O	1:D:173:VAL:HG23	2.17	0.45
1:A:60:THR:HG22	1:A:68:ILE:N	2.31	0.45
1:C:27:LYS:CE	1:C:27:LYS:HA	2.40	0.45
1:C:237:TYR:HA	1:C:240:VAL:HG23	1.98	0.45
1:C:212:LEU:O	1:C:216:GLY:HA2	2.17	0.44
1:B:266:LEU:HD13	1:B:319:TYR:CG	2.53	0.44
1:A:378:LEU:HB3	1:B:139:MET:CE	2.47	0.44
1:D:376:LYS:HE2	4:D:413:HOH:O	2.17	0.44
1:D:27:LYS:HA	1:D:27:LYS:CE	2.41	0.44
1:C:221:VAL:HG11	1:C:356:LEU:HD21	1.99	0.44
1:A:208:LYS:O	1:A:211:ILE:HG22	2.18	0.43
1:D:72:ARG:N	4:D:441:HOH:O	2.51	0.43
1:C:17:GLU:HB3	1:C:18:PRO:CD	2.48	0.43
1:D:233:MET:HG2	1:D:308:HIS:HE2	1.82	0.43
1:D:43:LEU:HA	1:D:43:LEU:HD12	1.91	0.43
1:C:143:ARG:NH1	4:C:437:HOH:O	2.46	0.43
1:A:360:MET:HB3	1:A:364:GLU:OE2	2.18	0.43
1:C:36:ASN:O	1:C:40:ASN:ND2	2.51	0.43
1:D:206:GLU:O	1:D:210:GLN:HG3	2.17	0.43
1:D:326:GLU:OE2	1:D:355:LYS:NZ	2.41	0.43
1:D:172:TRP:O	1:D:176:PHE:HB3	2.19	0.43
1:A:140:ASN:O	1:A:144:MET:HG3	2.19	0.43
1:B:323:THR:OG1	1:B:326:GLU:HG3	2.18	0.43
1:C:192:TYR:HB2	1:C:193:PRO:HD3	2.01	0.43
1:C:28:ARG:HD3	4:C:451:HOH:O	2.17	0.43
1:D:132:GLU:HB2	1:D:159:ARG:O	2.18	0.43
1:C:386:GLY:O	1:C:387:ASN:HB2	2.18	0.42
1:D:283:GLN:OE1	1:D:287:GLY:HA2	2.20	0.42
1:A:5:GLU:O	1:A:278:LEU:HD23	2.19	0.42
1:B:23:GLU:OE1	1:B:190:HIS:HE1	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:HIS:CE1	1:D:231:ASN:HB3	2.54	0.42
1:C:218:LEU:HB3	1:C:219:PRO:HD2	2.01	0.42
1:D:29:PHE:CE1	1:D:95:PHE:HB3	2.55	0.42
1:A:201:SER:HA	1:A:234:GLY:O	2.19	0.42
1:D:178:TYR:N	1:D:178:TYR:CD1	2.86	0.42
1:C:370:LEU:HD12	1:C:370:LEU:HA	1.91	0.42
1:B:112:VAL:O	1:B:116:MET:HG3	2.20	0.42
1:D:34:GLU:O	1:D:37:ARG:N	2.52	0.42
1:B:145:LYS:HZ3	1:D:363:ASP:CG	2.21	0.42
1:D:89:GLN:CB	1:D:182:LEU:HD22	2.50	0.42
1:D:185:SER:OG	1:D:228:GLY:HA3	2.20	0.42
1:D:59:LEU:HD11	1:D:354:MET:HE2	2.02	0.42
1:D:73:GLU:HB2	1:D:370:LEU:O	2.19	0.42
1:A:233:MET:HG2	1:A:308:HIS:NE2	2.35	0.42
1:B:23:GLU:CD	1:B:190:HIS:HE1	2.23	0.42
1:A:74:ASP:HA	1:A:372:GLY:HA2	2.02	0.41
1:A:206:GLU:O	1:A:210:GLN:HG3	2.19	0.41
1:B:212:LEU:HD23	1:B:212:LEU:HA	1.92	0.41
1:A:26:TYR:O	1:A:30:LYS:N	2.46	0.41
1:C:18:PRO:HB3	1:C:176:PHE:CG	2.55	0.41
1:C:208:LYS:O	1:C:212:LEU:HG	2.21	0.41
1:C:51:THR:HB	1:C:72:ARG:O	2.20	0.41
1:D:265:SER:OG	1:D:303:GLY:HA2	2.20	0.41
1:A:29:PHE:O	1:A:30:LYS:C	2.58	0.41
1:A:185:SER:O	1:A:196:VAL:HG21	2.20	0.41
1:C:380:ILE:HG13	1:C:381:VAL:H	1.85	0.41
1:A:189:PRO:HD3	1:A:275:HIS:O	2.21	0.41
1:C:66:ALA:HB1	1:C:364:GLU:O	2.21	0.41
1:A:155:ASN:CA	1:A:159:ARG:HG2	2.42	0.41
1:C:28:ARG:HG3	1:C:29:PHE:N	2.36	0.41
1:D:15:LEU:CD2	1:D:173:VAL:HG22	2.51	0.41
1:A:15:LEU:O	1:A:18:PRO:HD2	2.21	0.41
1:B:36:ASN:O	1:B:40:ASN:ND2	2.53	0.41
1:C:229:GLY:HA2	4:C:401:HOH:O	2.21	0.41
1:C:252:ALA:HB3	1:C:263:SER:HB3	2.03	0.41
1:D:36:ASN:O	1:D:40:ASN:ND2	2.54	0.41
1:B:157:GLY:HA3	1:B:163:ASP:OD1	2.20	0.41
1:D:102:ILE:HG23	1:D:179:THR:CG2	2.51	0.41
1:D:202:VAL:HA	1:D:205:ARG:NH1	2.35	0.41
1:B:138:LYS:HD2	1:D:362:ARG:HH21	1.86	0.41
1:C:215:GLU:O	1:C:217:GLN:HG2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:GLU:CD	1:D:159:ARG:NH1	2.74	0.41
1:D:294:SER:C	1:D:296:ALA:N	2.73	0.41
1:D:89:GLN:HB2	1:D:182:LEU:HD22	2.03	0.41
1:A:5:GLU:OE1	1:A:5:GLU:N	2.52	0.41
1:D:65:GLY:HA3	1:D:357:ALA:O	2.20	0.41
1:D:380:ILE:C	1:D:380:ILE:CD1	2.88	0.41
1:A:188:GLY:HA2	1:A:275:HIS:O	2.21	0.40
1:D:83:THR:O	1:D:87:ILE:HG13	2.20	0.40
1:D:29:PHE:O	1:D:30:LYS:C	2.59	0.40
1:A:28:ARG:HG3	1:A:29:PHE:N	2.36	0.40
1:C:45:THR:O	1:D:54:TYR:HB2	2.22	0.40
1:B:178:TYR:CD1	1:B:178:TYR:N	2.89	0.40
1:A:323:THR:OG1	1:A:326:GLU:HG3	2.21	0.40
1:A:37:ARG:HH11	1:A:37:ARG:HG2	1.87	0.40
1:B:145:LYS:HZ1	1:D:363:ASP:HB2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	384/388 (99%)	362 (94%)	20 (5%)	2 (0%)	29	30
1	B	385/388 (99%)	365 (95%)	19 (5%)	1 (0%)	41	45
1	C	385/388 (99%)	364 (94%)	18 (5%)	3 (1%)	19	18
1	D	381/388 (98%)	353 (93%)	24 (6%)	4 (1%)	15	13
All	All	1535/1552 (99%)	1444 (94%)	81 (5%)	10 (1%)	22	21

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	LYS
1	C	10	TYR
1	C	243	LYS
1	D	243	LYS
1	D	33	GLU
1	D	285	GLU
1	B	186	VAL
1	C	186	VAL
1	D	186	VAL
1	A	186	VAL

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	306/308 (99%)	293 (96%)	13 (4%)	30	36
1	B	307/308 (100%)	298 (97%)	9 (3%)	42	53
1	C	307/308 (100%)	298 (97%)	9 (3%)	42	53
1	D	305/308 (99%)	297 (97%)	8 (3%)	46	57
All	All	1225/1232 (99%)	1186 (97%)	39 (3%)	39	49

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	43	LEU
1	A	143	ARG
1	A	169	LEU
1	A	170	ARG
1	A	182	LEU
1	A	246	LYS
1	A	255	LYS
1	A	258	GLU
1	A	334	LEU
1	A	336	ARG
1	A	342	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	380	ILE
1	B	43	LEU
1	B	143	ARG
1	B	169	LEU
1	B	182	LEU
1	B	258	GLU
1	B	334	LEU
1	B	342	PRO
1	B	375	ASP
1	B	380	ILE
1	C	43	LEU
1	C	143	ARG
1	C	177	GLU
1	C	182	LEU
1	C	217	GLN
1	C	246	LYS
1	C	334	LEU
1	C	342	PRO
1	C	380	ILE
1	D	43	LEU
1	D	150	ASN
1	D	169	LEU
1	D	170	ARG
1	D	182	LEU
1	D	258	GLU
1	D	334	LEU
1	D	380	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	36	ASN
1	A	40	ASN
1	A	150	ASN
1	A	166	ASN
1	A	190	HIS
1	A	217	GLN
1	A	241	ASN
1	A	262	HIS
1	A	267	ASN
1	B	9	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	40	ASN
1	B	150	ASN
1	B	190	HIS
1	B	217	GLN
1	B	241	ASN
1	B	262	HIS
1	C	9	GLN
1	C	150	ASN
1	C	190	HIS
1	C	217	GLN
1	C	241	ASN
1	C	262	HIS
1	C	267	ASN
1	C	270	GLN
1	D	9	GLN
1	D	40	ASN
1	D	150	ASN
1	D	190	HIS
1	D	217	GLN
1	D	241	ASN
1	D	262	HIS
1	D	267	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 3 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	PLP	D	400	1	15,15,16	1.52	4 (26%)	20,22,23	1.80	4 (20%)
3	PLP	C	400	1	15,15,16	1.61	4 (26%)	20,22,23	1.79	3 (15%)
3	PLP	B	400	1	15,15,16	1.57	6 (40%)	20,22,23	2.00	4 (20%)
3	PLP	A	400	1	15,15,16	1.45	3 (20%)	20,22,23	1.94	4 (20%)

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
3	PLP	D	400	1	-	0/6/6/8	0/1/1/1
3	PLP	C	400	1	-	0/6/6/8	0/1/1/1
3	PLP	B	400	1	-	0/6/6/8	0/1/1/1
3	PLP	A	400	1	-	0/6/6/8	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	400	PLP	C5-C4	2.71	1.43	1.40
3	D	400	PLP	C2-N1	2.69	1.38	1.33
3	C	400	PLP	C2-N1	2.68	1.38	1.33
3	B	400	PLP	C2-N1	2.49	1.38	1.33
3	A	400	PLP	C2-N1	2.47	1.38	1.33
3	A	400	PLP	C6-N1	2.44	1.39	1.34
3	B	400	PLP	C5-C4	2.42	1.43	1.40
3	C	400	PLP	C6-N1	2.34	1.39	1.34
3	B	400	PLP	P-O3P	-2.18	1.46	1.54
3	D	400	PLP	C5-C4	2.18	1.42	1.40
3	B	400	PLP	C4A-C4	2.14	1.56	1.51
3	B	400	PLP	C6-N1	2.12	1.38	1.34
3	A	400	PLP	P-O3P	-2.11	1.46	1.54
3	D	400	PLP	C6-N1	2.06	1.38	1.34
3	C	400	PLP	P-O3P	-2.06	1.46	1.54
3	B	400	PLP	C3-C2	-2.03	1.38	1.40
3	D	400	PLP	P-O3P	-2.03	1.47	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	400	PLP	O4P-C5A-C5	5.68	120.17	109.35
3	A	400	PLP	O4P-C5A-C5	4.97	118.83	109.35
3	C	400	PLP	O4P-C5A-C5	4.76	118.42	109.35
3	A	400	PLP	C2A-C2-C3	4.50	126.45	120.89
3	D	400	PLP	C2A-C2-C3	4.29	126.18	120.89
3	D	400	PLP	O4P-C5A-C5	4.22	117.40	109.35
3	B	400	PLP	C2A-C2-C3	4.02	125.85	120.89
3	C	400	PLP	C2A-C2-C3	3.91	125.72	120.89
3	A	400	PLP	C6-C5-C4	-2.43	116.25	118.16
3	D	400	PLP	C6-C5-C4	-2.31	116.34	118.16
3	B	400	PLP	C6-C5-C4	-2.24	116.40	118.16
3	C	400	PLP	C4-C3-C2	2.12	123.20	120.07
3	B	400	PLP	C4-C3-C2	2.05	123.11	120.07
3	A	400	PLP	C4-C3-C2	2.03	123.07	120.07
3	D	400	PLP	C4-C3-C2	2.02	123.06	120.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	400	PLP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.