



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2025 – 01:58 AM EDT

PDB ID : 2CTZ
Title : Crystal structure of o-acetyl homoserine sulphydrylase from *Thermus thermophilus* HB8
Authors : Imagawa, T.; Kousumi, Y.; Tsuge, H.; Utsunomiya, H.; Ebihara, A.; Nakagawa, N.; Yokoyama, S.; Kuramitsu, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-05-24
Resolution : 2.60 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

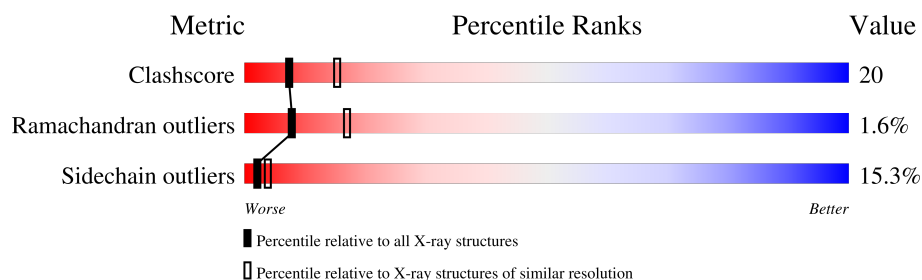
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	421	
1	B	421	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	A	600	-	-	X	-
2	PLP	B	600	-	-	X	-

2 Entry composition [i](#)

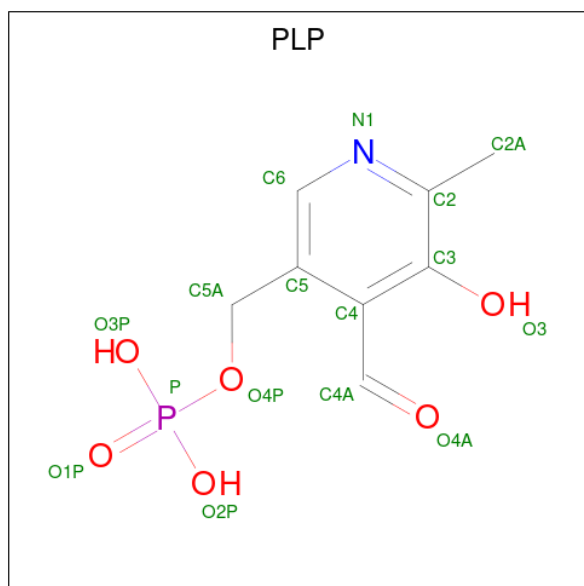
There are 3 unique types of molecules in this entry. The entry contains 6726 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 O-acetyl-L-homoserine sulfhydrylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3261	2089	575	592	5			
1	B	421	Total	C	N	O	S	0	0	0
			3261	2089	575	592	5			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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.

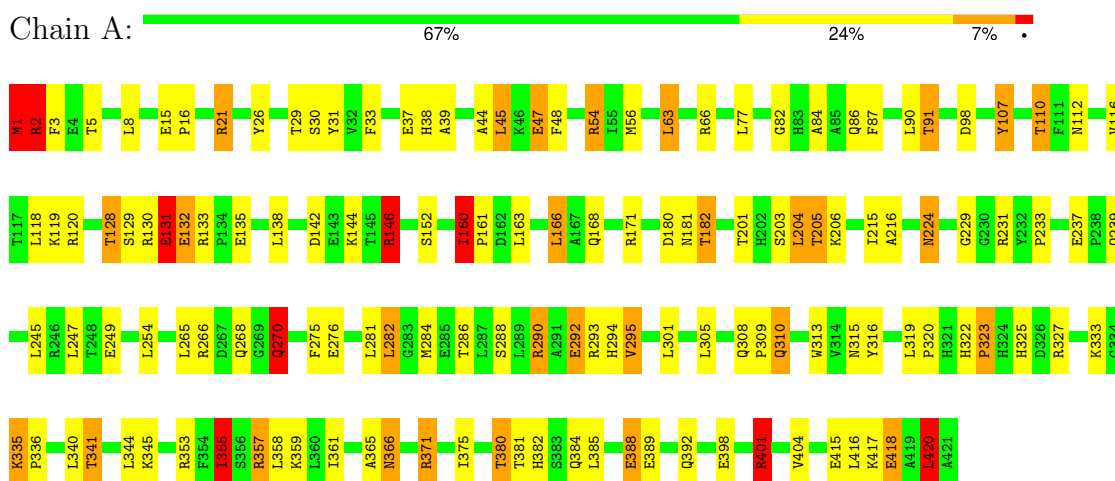
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total 83	O 83	0	0
3	B	91	Total 91	O 91	0	0

3 Residue-property plots

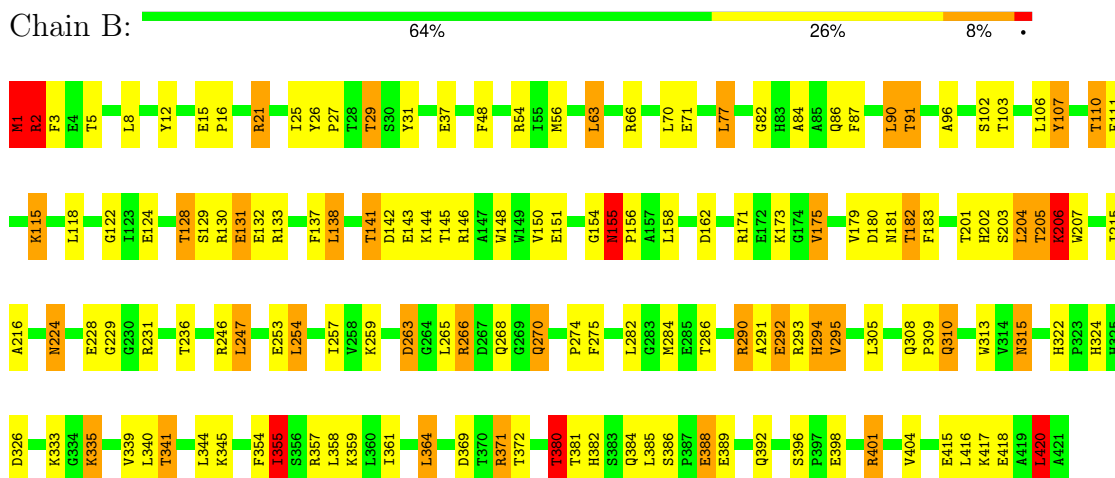
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: O-acetyl-L-homoserine sulphydrylase



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	149.09Å 149.09Å 219.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 2.60	Depositor
% Data completeness (in resolution range)	100.0 (19.88-2.60)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.187 , 0.217	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6726	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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: 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	1.36	14/3345 (0.4%)	1.29	24/4550 (0.5%)
1	B	1.37	18/3345 (0.5%)	1.31	29/4550 (0.6%)
All	All	1.36	32/6690 (0.5%)	1.30	53/9100 (0.6%)

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

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	GLU	CG-CD	8.96	1.65	1.51
1	A	345	LYS	CD-CE	8.88	1.73	1.51
1	B	345	LYS	CD-CE	8.28	1.72	1.51
1	B	107	TYR	CD2-CE2	7.54	1.50	1.39
1	B	26	TYR	CD2-CE2	7.49	1.50	1.39
1	A	107	TYR	CD2-CE2	7.45	1.50	1.39
1	A	292	GLU	CG-CD	7.19	1.62	1.51
1	B	143	GLU	CG-CD	7.12	1.62	1.51
1	B	292	GLU	CG-CD	6.93	1.62	1.51
1	A	26	TYR	CD2-CE2	6.53	1.49	1.39
1	A	275	PHE	CD2-CE2	6.02	1.51	1.39
1	A	3	PHE	CE1-CZ	5.95	1.48	1.37
1	A	355	ILE	CG1-CD1	5.88	1.91	1.50
1	B	12	TYR	CD1-CE1	5.82	1.48	1.39
1	B	355	ILE	CG1-CD1	5.70	1.89	1.50
1	B	37	GLU	CG-CD	5.64	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	GLU	CG-CD	5.59	1.60	1.51
1	A	3	PHE	CG-CD1	5.55	1.47	1.38
1	B	107	TYR	CG-CD2	5.53	1.46	1.39
1	A	131	GLU	CD-OE2	5.52	1.31	1.25
1	B	12	TYR	CD2-CE2	5.52	1.47	1.39
1	B	107	TYR	CD1-CE1	5.44	1.47	1.39
1	B	326	ASP	CB-CG	5.43	1.63	1.51
1	A	276	GLU	CD-OE1	5.37	1.31	1.25
1	B	359	LYS	CD-CE	5.35	1.64	1.51
1	A	107	TYR	CG-CD2	5.30	1.46	1.39
1	B	275	PHE	CD2-CE2	5.25	1.49	1.39
1	B	107	TYR	CE1-CZ	5.13	1.45	1.38
1	B	292	GLU	CD-OE1	5.03	1.31	1.25
1	A	290	ARG	CG-CD	5.02	1.64	1.51
1	B	124	GLU	CG-CD	5.02	1.59	1.51
1	B	175	VAL	CB-CG2	-5.02	1.42	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	371	ARG	NE-CZ-NH2	-19.18	110.71	120.30
1	A	290	ARG	NE-CZ-NH2	-17.66	111.47	120.30
1	B	290	ARG	NE-CZ-NH2	-16.14	112.23	120.30
1	A	371	ARG	NE-CZ-NH1	15.91	128.25	120.30
1	B	371	ARG	NE-CZ-NH1	15.17	127.88	120.30
1	A	371	ARG	NE-CZ-NH2	-14.30	113.15	120.30
1	A	290	ARG	NE-CZ-NH1	13.40	127.00	120.30
1	B	290	ARG	NE-CZ-NH1	13.12	126.86	120.30
1	A	146	ARG	NE-CZ-NH2	-11.09	114.75	120.30
1	A	146	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	A	1	MET	CG-SD-CE	8.96	114.53	100.20
1	B	1	MET	CG-SD-CE	7.68	112.49	100.20
1	B	2	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	A	284	MET	CA-CB-CG	7.15	125.46	113.30
1	A	231	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	66	ARG	NE-CZ-NH2	6.85	123.72	120.30
1	B	266	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	B	231	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	B	371	ARG	CG-CD-NE	-6.48	98.18	111.80
1	B	130	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	B	2	ARG	NE-CZ-NH1	-6.39	117.11	120.30
1	B	355	ILE	CG1-CB-CG2	6.32	125.30	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	ARG	CD-NE-CZ	6.19	132.27	123.60
1	B	364	LEU	CA-CB-CG	6.14	129.42	115.30
1	A	355	ILE	CG1-CB-CG2	6.13	124.89	111.40
1	B	263	ASP	CB-CG-OD1	5.96	123.66	118.30
1	B	90	LEU	CB-CG-CD1	5.93	121.08	111.00
1	B	204	LEU	CB-CG-CD1	5.90	121.03	111.00
1	B	344	LEU	CB-CG-CD2	-5.88	101.00	111.00
1	B	56	MET	CG-SD-CE	-5.87	90.80	100.20
1	B	162	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	B	66	ARG	NE-CZ-NH2	5.67	123.13	120.30
1	A	371	ARG	CD-NE-CZ	5.57	131.40	123.60
1	A	357	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	344	LEU	CB-CG-CD2	-5.45	101.74	111.00
1	A	66	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	B	371	ARG	CD-NE-CZ	5.36	131.10	123.60
1	A	401	ARG	CG-CD-NE	5.35	123.04	111.80
1	A	420	LEU	CA-CB-CG	5.34	127.58	115.30
1	B	420	LEU	CA-CB-CG	5.33	127.56	115.30
1	B	155	ASN	N-CA-CB	5.29	120.13	110.60
1	A	146	ARG	CG-CD-NE	-5.26	100.75	111.80
1	B	315	ASN	O-C-N	-5.26	114.28	122.70
1	A	56	MET	CG-SD-CE	-5.21	91.86	100.20
1	B	29	THR	N-CA-CB	-5.21	100.41	110.30
1	A	204	LEU	CB-CG-CD1	5.20	119.84	111.00
1	B	77	LEU	CB-CG-CD2	5.20	119.83	111.00
1	A	160	ILE	CB-CA-C	5.12	121.85	111.60
1	A	2	ARG	NE-CZ-NH2	5.11	122.85	120.30
1	B	231	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	335	LYS	CD-CE-NZ	-5.08	100.02	111.70
1	B	290	ARG	CD-NE-CZ	5.07	130.70	123.60
1	A	270	GLN	CB-CA-C	-5.01	100.38	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	154	GLY	Peptide

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	3261	0	3249	119	0
1	B	3261	0	3249	141	0
2	A	15	0	7	9	0
2	B	15	0	7	8	0
3	A	83	0	0	10	0
3	B	91	0	0	13	0
All	All	6726	0	6512	261	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 20.

All (261) 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:B:355:ILE:CD1	1:B:355:ILE:CG1	1.89	1.50
1:B:206:LYS:HZ2	2:B:600:PLP:C4A	1.25	1.49
1:A:355:ILE:CD1	1:A:355:ILE:CG1	1.91	1.49
1:A:206:LYS:HZ1	2:A:600:PLP:C4A	1.32	1.38
1:A:315:ASN:HB3	1:A:341:THR:HG22	1.20	1.13
1:A:380:THR:CG2	1:A:381:THR:H	1.65	1.08
1:B:388:GLU:HB3	3:B:691:HOH:O	1.53	1.07
1:B:155:ASN:HB3	1:B:156:PRO:HD3	1.34	1.06
1:B:315:ASN:HB3	1:B:341:THR:HG22	1.29	1.05
1:A:380:THR:HG22	1:A:381:THR:H	1.21	1.04
1:B:380:THR:CG2	1:B:381:THR:H	1.70	1.03
1:B:401:ARG:HG2	1:B:401:ARG:HH11	1.24	1.02
1:B:310:GLN:H	1:B:310:GLN:HE21	1.04	1.00
1:B:292:GLU:HG2	3:B:688:HOH:O	1.61	1.00
1:B:206:LYS:HZ1	2:B:600:PLP:C4A	1.75	0.95
1:A:310:GLN:H	1:A:310:GLN:HE21	1.04	0.95
1:A:206:LYS:HZ2	2:A:600:PLP:C4A	1.70	0.95
1:A:315:ASN:HB3	1:A:341:THR:CG2	2.02	0.90
1:B:380:THR:HG22	1:B:381:THR:H	1.35	0.90
1:A:128:THR:HG21	1:A:132:GLU:HA	1.53	0.89
1:B:357:ARG:NH1	1:B:418:GLU:O	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:THR:HG21	1:B:132:GLU:HA	1.54	0.88
1:A:401:ARG:HG2	1:A:401:ARG:HH11	1.37	0.86
1:A:310:GLN:HE21	1:A:310:GLN:N	1.74	0.85
1:A:128:THR:CG2	1:A:132:GLU:HA	2.07	0.85
1:A:160:ILE:HD13	1:A:160:ILE:C	1.95	0.84
1:A:380:THR:CG2	1:A:381:THR:N	2.37	0.84
1:B:341:THR:HG21	3:B:634:HOH:O	1.78	0.84
1:B:137:PHE:O	1:B:141:THR:HG22	1.78	0.83
1:A:341:THR:HG21	3:A:639:HOH:O	1.79	0.83
1:A:160:ILE:HD12	1:A:327:ARG:HB3	1.60	0.83
1:A:308:GLN:HG3	3:A:631:HOH:O	1.79	0.83
1:B:128:THR:HG22	1:B:129:SER:O	1.79	0.82
1:B:381:THR:HG22	1:B:382:HIS:ND1	1.96	0.81
1:B:131:GLU:OE2	1:B:133:ARG:NH1	2.13	0.80
1:B:155:ASN:HB3	1:B:156:PRO:CD	2.11	0.80
1:B:310:GLN:H	1:B:310:GLN:NE2	1.78	0.79
1:B:380:THR:CG2	1:B:381:THR:N	2.44	0.79
1:A:295:VAL:HG11	1:A:335:LYS:HG2	1.65	0.78
1:A:180:ASP:OD1	1:A:182:THR:HG23	1.83	0.78
1:B:180:ASP:OD1	1:B:182:THR:HG23	1.82	0.78
1:A:309:PRO:HG2	1:A:310:GLN:HE22	1.46	0.77
1:A:128:THR:HG22	1:A:129:SER:O	1.83	0.77
1:A:224:ASN:C	1:A:224:ASN:HD22	1.85	0.77
1:B:128:THR:CG2	1:B:132:GLU:HA	2.14	0.76
1:B:401:ARG:HH11	1:B:401:ARG:CG	1.97	0.76
1:B:309:PRO:HG2	1:B:310:GLN:HE22	1.49	0.75
1:A:86:GLN:NE2	2:A:600:PLP:H6	2.03	0.74
1:B:310:GLN:HE21	1:B:310:GLN:N	1.83	0.74
1:B:315:ASN:HB3	1:B:341:THR:CG2	2.12	0.74
2:B:600:PLP:C4A	2:B:600:PLP:O4P	2.36	0.73
1:A:380:THR:HG22	1:A:381:THR:N	2.01	0.73
1:B:380:THR:HG23	1:B:381:THR:H	1.53	0.72
1:A:171:ARG:HH22	1:A:224:ASN:ND2	1.86	0.71
1:A:15:GLU:OE1	1:B:15:GLU:OE1	2.07	0.71
1:A:91:THR:HG21	1:A:268:GLN:OE1	1.90	0.70
1:A:205:THR:HB	1:A:215:ILE:HA	1.73	0.70
1:B:63:LEU:HD23	1:B:284:MET:HE1	1.72	0.70
1:A:388:GLU:HB3	3:A:651:HOH:O	1.92	0.69
1:A:87:PHE:O	1:A:91:THR:HB	1.92	0.69
1:A:292:GLU:HG2	3:A:674:HOH:O	1.90	0.69
1:A:310:GLN:H	1:A:310:GLN:NE2	1.85	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:NH1	1:A:418:GLU:O	2.26	0.69
1:B:270:GLN:H	1:B:270:GLN:HE21	1.41	0.69
1:B:205:THR:HB	1:B:215:ILE:HA	1.73	0.69
1:A:295:VAL:CG1	1:A:335:LYS:HG2	2.23	0.68
1:A:380:THR:HG23	1:A:381:THR:H	1.56	0.68
1:A:270:GLN:H	1:A:270:GLN:HE21	1.42	0.68
1:B:385:LEU:HB3	1:B:389:GLU:HG3	1.76	0.68
1:B:203:SER:OG	1:B:205:THR:HG23	1.94	0.68
1:B:106:LEU:C	1:B:155:ASN:HB2	2.15	0.67
1:A:86:GLN:HE22	2:A:600:PLP:H6	1.60	0.67
1:A:286:THR:OG1	1:A:290:ARG:HD3	1.94	0.66
1:B:381:THR:HG22	1:B:382:HIS:CE1	2.31	0.66
1:A:310:GLN:N	1:A:310:GLN:NE2	2.42	0.65
1:A:294:HIS:HD2	1:A:404:VAL:O	1.79	0.65
1:B:286:THR:OG1	1:B:290:ARG:HD3	1.96	0.65
1:A:131:GLU:OE1	1:A:133:ARG:NH1	2.30	0.65
1:B:247:LEU:HD23	1:B:259:LYS:HB2	1.77	0.65
1:B:86:GLN:NE2	2:B:600:PLP:H6	2.11	0.65
1:B:386:SER:OG	1:B:389:GLU:HG2	1.96	0.65
1:A:180:ASP:OD1	1:A:182:THR:CG2	2.45	0.64
1:A:401:ARG:HH11	1:A:401:ARG:CG	2.10	0.64
1:B:141:THR:HB	1:B:145:THR:HG21	1.79	0.64
1:B:87:PHE:O	1:B:91:THR:HB	1.98	0.64
1:B:71:GLU:OE2	1:B:202:HIS:HE1	1.81	0.64
1:B:111:PHE:CZ	1:B:115:LYS:HD3	2.32	0.64
1:B:155:ASN:CB	1:B:156:PRO:HD3	2.20	0.64
1:B:310:GLN:NE2	1:B:310:GLN:N	2.43	0.64
1:A:107:TYR:HD2	1:A:110:THR:HG22	1.62	0.63
1:B:63:LEU:HD23	1:B:284:MET:CE	2.26	0.63
1:A:84:ALA:HB1	1:A:270:GLN:HG2	1.79	0.63
1:A:224:ASN:C	1:A:224:ASN:ND2	2.51	0.63
1:B:224:ASN:C	1:B:224:ASN:HD22	2.02	0.63
1:B:309:PRO:HG2	1:B:310:GLN:NE2	2.14	0.63
1:B:274:PRO:HD2	3:B:652:HOH:O	1.97	0.62
1:B:207:TRP:O	1:B:290:ARG:NH2	2.28	0.62
1:A:171:ARG:HH22	1:A:224:ASN:HD21	1.46	0.62
1:A:309:PRO:HG2	1:A:310:GLN:NE2	2.14	0.61
1:A:110:THR:HG21	3:A:661:HOH:O	1.99	0.61
1:B:110:THR:HG21	3:B:651:HOH:O	2.00	0.61
2:A:600:PLP:C4A	2:A:600:PLP:O4P	2.49	0.60
1:A:389:GLU:O	1:A:392:GLN:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:O	1:B:2:ARG:HB2	2.01	0.60
1:B:137:PHE:O	1:B:141:THR:CG2	2.50	0.60
1:A:381:THR:HG22	1:A:382:HIS:ND1	2.16	0.59
1:B:293:ARG:HD2	3:B:638:HOH:O	2.02	0.59
1:B:84:ALA:HB1	1:B:270:GLN:HG2	1.83	0.59
1:B:21:ARG:O	1:B:21:ARG:HD3	2.03	0.59
1:A:380:THR:HG23	1:A:381:THR:N	2.12	0.58
1:A:313:TRP:HZ3	1:A:341:THR:HG23	1.67	0.58
1:B:358:LEU:HD22	1:B:361:ILE:HB	1.86	0.58
1:A:21:ARG:O	1:A:21:ARG:HD3	2.04	0.57
1:A:293:ARG:HD2	3:A:621:HOH:O	2.03	0.57
1:B:180:ASP:OD1	1:B:182:THR:CG2	2.51	0.57
1:A:98:ASP:CG	1:A:146:ARG:HH11	2.08	0.57
1:B:294:HIS:HD2	1:B:404:VAL:O	1.87	0.57
1:B:86:GLN:HE22	2:B:600:PLP:H6	1.69	0.57
1:B:155:ASN:CB	1:B:156:PRO:CD	2.78	0.56
1:B:380:THR:HG23	1:B:381:THR:N	2.15	0.56
1:B:401:ARG:HG2	1:B:401:ARG:NH1	2.07	0.56
1:A:270:GLN:H	1:A:270:GLN:NE2	2.04	0.56
1:B:310:GLN:HG2	1:B:420:LEU:HG	1.88	0.56
1:A:31:TYR:N	1:A:31:TYR:CD2	2.74	0.56
1:B:274:PRO:CD	3:B:652:HOH:O	2.54	0.55
1:A:205:THR:CG2	2:A:600:PLP:O1P	2.53	0.55
1:B:205:THR:CG2	2:B:600:PLP:O1P	2.54	0.55
1:A:385:LEU:HB3	1:A:389:GLU:HG3	1.87	0.55
1:B:308:GLN:HG3	3:B:613:HOH:O	2.05	0.55
1:A:203:SER:OG	1:A:205:THR:HG23	2.06	0.55
1:B:173:LYS:O	1:B:173:LYS:HG3	2.05	0.55
1:A:107:TYR:HD1	3:A:677:HOH:O	1.89	0.55
1:B:389:GLU:O	1:B:392:GLN:HB3	2.07	0.55
1:A:381:THR:HG21	3:A:667:HOH:O	2.05	0.55
1:B:107:TYR:OH	3:B:687:HOH:O	2.02	0.54
1:B:128:THR:HG21	1:B:132:GLU:CA	2.32	0.54
1:B:381:THR:CG2	1:B:382:HIS:CE1	2.90	0.54
1:A:1:MET:O	1:A:1:MET:CE	2.56	0.54
1:B:313:TRP:CZ3	1:B:341:THR:HG23	2.43	0.53
1:A:313:TRP:CZ3	1:A:341:THR:HG23	2.43	0.53
1:B:91:THR:HG21	1:B:268:GLN:OE1	2.09	0.53
1:B:133:ARG:HD2	3:B:658:HOH:O	2.08	0.53
1:B:361:ILE:HG23	1:B:372:THR:HG22	1.90	0.53
1:B:107:TYR:HD2	1:B:110:THR:HG22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:TRP:HZ3	1:B:341:THR:HG23	1.75	0.52
1:B:205:THR:HG21	2:B:600:PLP:O1P	2.08	0.52
1:B:224:ASN:C	1:B:224:ASN:ND2	2.62	0.52
1:A:358:LEU:HD22	1:A:361:ILE:HB	1.92	0.52
1:B:270:GLN:H	1:B:270:GLN:NE2	2.06	0.52
1:B:128:THR:CG2	1:B:129:SER:O	2.56	0.51
1:A:44:ALA:O	1:A:45:LEU:HB2	2.11	0.51
1:B:21:ARG:O	1:B:21:ARG:CD	2.58	0.51
1:B:202:HIS:CD2	3:B:643:HOH:O	2.64	0.51
1:B:107:TYR:HB2	3:B:685:HOH:O	2.11	0.51
1:B:202:HIS:HD2	3:B:643:HOH:O	1.94	0.51
1:B:401:ARG:CG	1:B:401:ARG:NH1	2.69	0.50
1:A:142:ASP:C	1:A:142:ASP:OD1	2.49	0.50
1:A:130:ARG:HD3	3:A:635:HOH:O	2.10	0.50
1:B:171:ARG:HH22	1:B:224:ASN:ND2	2.09	0.50
1:B:381:THR:CG2	1:B:382:HIS:ND1	2.73	0.50
1:B:205:THR:HG22	1:B:216:ALA:O	2.12	0.50
1:A:205:THR:HG22	1:A:216:ALA:H	1.77	0.49
1:A:381:THR:HG22	1:A:382:HIS:CE1	2.47	0.49
1:B:71:GLU:OE2	1:B:202:HIS:CE1	2.63	0.49
1:B:182:THR:CG2	1:B:203:SER:H	2.25	0.49
1:B:82:GLY:HA3	2:B:600:PLP:H5A2	1.95	0.49
1:A:353:ARG:O	1:A:357:ARG:HG3	2.12	0.49
1:B:228:GLU:HA	1:B:228:GLU:OE1	2.12	0.49
1:A:206:LYS:HZ3	2:A:600:PLP:C4A	2.10	0.49
1:A:398:GLU:OE1	1:A:398:GLU:N	2.41	0.48
1:B:340:LEU:HD12	1:B:340:LEU:C	2.34	0.48
1:B:398:GLU:OE1	1:B:398:GLU:N	2.44	0.48
1:B:102:SER:OG	1:B:103:THR:O	2.31	0.48
1:A:21:ARG:HD3	1:A:21:ARG:HA	1.58	0.48
1:A:82:GLY:HA3	2:A:600:PLP:H5A2	1.96	0.47
1:B:380:THR:HG22	1:B:381:THR:N	2.15	0.47
1:A:310:GLN:HG2	1:A:420:LEU:HG	1.95	0.47
1:A:233:PRO:O	1:A:237:GLU:HG3	2.14	0.47
1:A:320:PRO:HA	1:A:325:HIS:CD2	2.48	0.47
1:A:365:ALA:O	1:A:366:ASN:HB2	2.14	0.47
1:B:181:ASN:O	1:B:182:THR:C	2.53	0.47
1:B:205:THR:HG22	1:B:216:ALA:H	1.80	0.47
1:A:21:ARG:HD3	1:A:21:ARG:C	2.22	0.46
1:A:54:ARG:HE	1:A:54:ARG:HB2	1.49	0.46
1:A:340:LEU:C	1:A:340:LEU:HD12	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:PHE:CZ	1:B:70:LEU:HD22	2.50	0.46
1:A:239:GLN:HB2	1:A:245:LEU:O	2.15	0.46
1:A:181:ASN:O	1:A:182:THR:C	2.53	0.46
1:B:141:THR:HG21	1:B:148:TRP:CZ2	2.50	0.46
1:B:257:ILE:HD12	1:B:257:ILE:HA	1.79	0.46
1:A:205:THR:HG21	2:A:600:PLP:O1P	2.16	0.46
1:B:236:THR:O	1:B:246:ARG:HG2	2.16	0.46
1:B:295:VAL:HG11	1:B:335:LYS:HG2	1.98	0.46
1:A:63:LEU:HD23	1:A:63:LEU:O	2.16	0.46
1:B:259:LYS:HE2	1:B:263:ASP:OD2	2.16	0.45
1:B:203:SER:HG	1:B:205:THR:HG23	1.78	0.45
1:B:96:ALA:HA	1:B:122:GLY:O	2.16	0.45
1:A:128:THR:HG21	1:A:132:GLU:CA	2.37	0.45
1:A:166:LEU:HD23	1:A:166:LEU:HA	1.84	0.45
1:A:322:HIS:HA	1:A:323:PRO:HD2	1.72	0.45
1:B:106:LEU:O	1:B:155:ASN:HB2	2.17	0.45
1:A:63:LEU:HD23	1:A:63:LEU:C	2.37	0.44
1:B:86:GLN:OE1	1:B:110:THR:HB	2.18	0.44
1:B:142:ASP:OD1	1:B:142:ASP:C	2.56	0.44
1:A:98:ASP:OD2	1:A:146:ARG:HD3	2.18	0.44
1:B:31:TYR:N	1:B:31:TYR:CD2	2.85	0.44
1:A:21:ARG:O	1:A:21:ARG:CD	2.65	0.44
1:A:38:HIS:ND1	1:A:47:GLU:OE2	2.48	0.44
1:B:21:ARG:CD	1:B:21:ARG:C	2.86	0.44
1:B:155:ASN:OD1	1:B:155:ASN:C	2.55	0.44
1:B:369:ASP:OD2	1:B:371:ARG:HD2	2.18	0.44
1:A:33:PHE:CG	1:A:39:ALA:HB2	2.53	0.44
1:B:128:THR:CG2	1:B:129:SER:N	2.81	0.44
1:A:160:ILE:HD13	1:A:160:ILE:O	2.17	0.43
1:B:21:ARG:HD3	1:B:21:ARG:C	2.22	0.43
1:B:182:THR:HG22	1:B:203:SER:H	1.82	0.43
1:B:183:PHE:CE1	1:B:339:VAL:HG21	2.52	0.43
1:B:322:HIS:HD1	1:B:324:HIS:H	1.65	0.43
1:A:319:LEU:HD23	1:A:319:LEU:HA	1.90	0.43
1:A:359:LYS:HB2	1:A:359:LYS:HE3	1.74	0.43
1:A:416:LEU:O	1:A:420:LEU:HB2	2.19	0.43
1:B:15:GLU:HA	1:B:16:PRO:HD3	1.80	0.43
1:B:290:ARG:O	1:B:291:ALA:C	2.57	0.43
1:A:131:GLU:CD	1:A:133:ARG:HH11	2.21	0.43
1:B:150:VAL:HG22	1:B:151:GLU:N	2.34	0.43
1:A:375:ILE:HD11	1:A:380:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:SER:O	1:A:292:GLU:HG3	2.19	0.43
1:A:142:ASP:OD1	1:A:144:LYS:N	2.33	0.43
1:B:107:TYR:HB3	1:B:110:THR:HG23	2.01	0.42
1:A:316:TYR:OH	1:A:336:PRO:HD2	2.19	0.42
1:B:25:ILE:O	1:B:27:PRO:HD3	2.18	0.42
1:B:150:VAL:HG22	1:B:151:GLU:H	1.84	0.42
1:A:205:THR:HG22	1:A:216:ALA:O	2.20	0.42
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.89	0.42
1:A:375:ILE:HD11	1:A:380:THR:CG2	2.49	0.42
1:B:150:VAL:O	1:B:179:VAL:HA	2.20	0.42
1:B:315:ASN:ND2	1:B:315:ASN:O	2.52	0.42
1:A:98:ASP:HB3	1:A:146:ARG:HD2	2.01	0.42
1:B:254:LEU:HD12	1:B:254:LEU:HA	1.78	0.42
1:B:308:GLN:HA	1:B:309:PRO:HD2	1.89	0.42
1:B:310:GLN:HG3	1:B:420:LEU:O	2.20	0.42
1:B:416:LEU:O	1:B:420:LEU:HB2	2.20	0.42
1:B:315:ASN:O	1:B:315:ASN:CG	2.58	0.42
1:A:30:SER:C	1:A:31:TYR:CD2	2.93	0.42
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.77	0.42
1:A:63:LEU:HA	1:A:281:LEU:HD21	2.02	0.41
1:A:132:GLU:OE1	1:A:161:PRO:HB3	2.19	0.41
1:B:21:ARG:HD3	1:B:21:ARG:HA	1.55	0.41
1:B:138:LEU:HD23	1:B:138:LEU:HA	1.92	0.41
1:A:15:GLU:HA	1:A:16:PRO:HD3	1.88	0.41
1:A:116:VAL:O	1:A:120:ARG:HG3	2.21	0.41
1:A:171:ARG:NH2	1:A:224:ASN:HD21	2.14	0.41
1:A:152:SER:OG	1:A:181:ASN:ND2	2.53	0.41
1:B:142:ASP:OD1	1:B:144:LYS:N	2.41	0.41
1:A:282:LEU:HA	1:A:282:LEU:HD12	1.67	0.41
1:A:294:HIS:HE1	3:A:619:HOH:O	2.04	0.41
1:B:107:TYR:HB3	1:B:110:THR:CG2	2.51	0.40
1:B:295:VAL:CG1	1:B:335:LYS:HG2	2.51	0.40
1:B:354:PHE:CD1	1:B:420:LEU:HD13	2.56	0.40
1:A:381:THR:CG2	1:A:382:HIS:CE1	3.04	0.40
1:B:106:LEU:O	1:B:155:ASN:CB	2.70	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	419/421 (100%)	390 (93%)	23 (6%)	6 (1%)	9	19
1	B	419/421 (100%)	388 (93%)	24 (6%)	7 (2%)	7	16
All	All	838/842 (100%)	778 (93%)	47 (6%)	13 (2%)	8	17

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	229	GLY
1	B	2	ARG
1	B	128	THR
1	B	229	GLY
1	A	128	THR
1	A	366	ASN
1	B	48	PHE
1	B	380	THR
1	A	48	PHE
1	B	155	ASN
1	B	206	LYS
1	A	323	PRO

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	333/333 (100%)	280 (84%)	53 (16%)	2	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	333/333 (100%)	284 (85%)	49 (15%)	2	4
All	All	666/666 (100%)	564 (85%)	102 (15%)	2	4

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	5	THR
1	A	8	LEU
1	A	21	ARG
1	A	29	THR
1	A	45	LEU
1	A	47	GLU
1	A	54	ARG
1	A	63	LEU
1	A	77	LEU
1	A	90	LEU
1	A	91	THR
1	A	110	THR
1	A	112	ASN
1	A	118	LEU
1	A	119	LYS
1	A	131	GLU
1	A	132	GLU
1	A	135	GLU
1	A	138	LEU
1	A	146	ARG
1	A	160	ILE
1	A	163	LEU
1	A	166	LEU
1	A	168	GLN
1	A	182	THR
1	A	201	THR
1	A	204	LEU
1	A	205	THR
1	A	224	ASN
1	A	247	LEU
1	A	249	GLU
1	A	265	LEU
1	A	266	ARG
1	A	270	GLN

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Mol	Chain	Res	Type
1	A	282	LEU
1	A	295	VAL
1	A	305	LEU
1	A	310	GLN
1	A	333	LYS
1	A	335	LYS
1	A	341	THR
1	A	355	ILE
1	A	371	ARG
1	A	380	THR
1	A	384	GLN
1	A	388	GLU
1	A	401	ARG
1	A	415	GLU
1	A	417	LYS
1	A	418	GLU
1	A	420	LEU
1	B	1	MET
1	B	2	ARG
1	B	5	THR
1	B	8	LEU
1	B	21	ARG
1	B	29	THR
1	B	54	ARG
1	B	63	LEU
1	B	77	LEU
1	B	90	LEU
1	B	91	THR
1	B	110	THR
1	B	115	LYS
1	B	118	LEU
1	B	131	GLU
1	B	138	LEU
1	B	141	THR
1	B	146	ARG
1	B	158	LEU
1	B	175	VAL
1	B	182	THR
1	B	201	THR
1	B	204	LEU
1	B	205	THR
1	B	206	LYS

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Mol	Chain	Res	Type
1	B	224	ASN
1	B	247	LEU
1	B	253	GLU
1	B	254	LEU
1	B	265	LEU
1	B	266	ARG
1	B	270	GLN
1	B	282	LEU
1	B	294	HIS
1	B	295	VAL
1	B	305	LEU
1	B	310	GLN
1	B	333	LYS
1	B	341	THR
1	B	355	ILE
1	B	364	LEU
1	B	380	THR
1	B	384	GLN
1	B	388	GLU
1	B	396	SER
1	B	401	ARG
1	B	415	GLU
1	B	417	LYS
1	B	420	LEU

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

Mol	Chain	Res	Type
1	A	41	ASN
1	A	99	ASN
1	A	181	ASN
1	A	224	ASN
1	A	270	GLN
1	A	294	HIS
1	A	310	GLN
1	A	315	ASN
1	A	325	HIS
1	A	384	GLN
1	B	41	ASN
1	B	99	ASN
1	B	181	ASN
1	B	202	HIS

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Mol	Chain	Res	Type
1	B	224	ASN
1	B	270	GLN
1	B	294	HIS
1	B	300	HIS
1	B	310	GLN
1	B	315	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	600	1	15,15,16	1.77	5 (33%)	21,22,23	1.74	5 (23%)
2	PLP	B	600	1	15,15,16	1.74	4 (26%)	21,22,23	1.80	8 (38%)

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	600	1	-	5/6/6/8	0/1/1/1
2	PLP	B	600	1	-	5/6/6/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	PLP	C6-N1	3.33	1.41	1.34
2	B	600	PLP	C3-C4	3.24	1.46	1.40
2	A	600	PLP	C2-N1	3.21	1.39	1.33
2	B	600	PLP	C5-C4	2.89	1.43	1.40
2	B	600	PLP	C6-N1	2.70	1.39	1.34
2	A	600	PLP	C5-C4	2.41	1.43	1.40
2	A	600	PLP	C3-C4	2.17	1.44	1.40
2	B	600	PLP	C2-N1	2.15	1.37	1.33
2	A	600	PLP	O3-C3	2.12	1.41	1.36

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	PLP	C3-C4-C5	3.55	122.85	118.59
2	A	600	PLP	C4A-C4-C5	-2.89	117.96	120.94
2	B	600	PLP	C4A-C4-C5	-2.86	117.99	120.94
2	B	600	PLP	O3P-P-O2P	2.85	118.51	107.80
2	A	600	PLP	O3P-P-O4P	2.83	114.05	106.67
2	B	600	PLP	C6-N1-C2	2.77	124.23	119.20
2	B	600	PLP	C2A-C2-C3	2.46	123.68	120.80
2	B	600	PLP	C3-C2-N1	-2.38	117.95	120.96
2	B	600	PLP	O3P-P-O4P	2.32	112.72	106.67
2	B	600	PLP	C3-C4-C5	2.28	121.33	118.59
2	A	600	PLP	C6-N1-C2	2.24	123.26	119.20
2	A	600	PLP	C3-C2-N1	-2.23	118.15	120.96
2	B	600	PLP	C5A-C5-C6	-2.10	115.94	119.36

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	PLP	C4-C5-C5A-O4P
2	A	600	PLP	C6-C5-C5A-O4P
2	A	600	PLP	C5A-O4P-P-O2P
2	A	600	PLP	C5A-O4P-P-O3P
2	B	600	PLP	C4-C5-C5A-O4P

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Mol	Chain	Res	Type	Atoms
2	B	600	PLP	C6-C5-C5A-O4P
2	B	600	PLP	C5A-O4P-P-O2P
2	B	600	PLP	C5A-O4P-P-O3P
2	A	600	PLP	C5A-O4P-P-O1P
2	B	600	PLP	C5A-O4P-P-O1P

There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	PLP	9	0
2	B	600	PLP	8	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.