



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:55 PM UTC

PDB ID : 2CTZ / pdb_00002ctz
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.

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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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

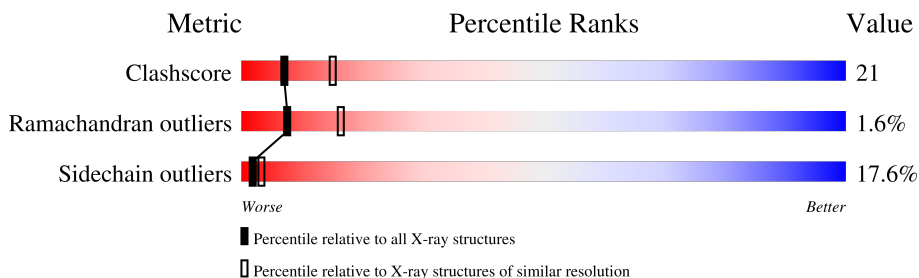
1 Overall quality at a glance

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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (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](#)

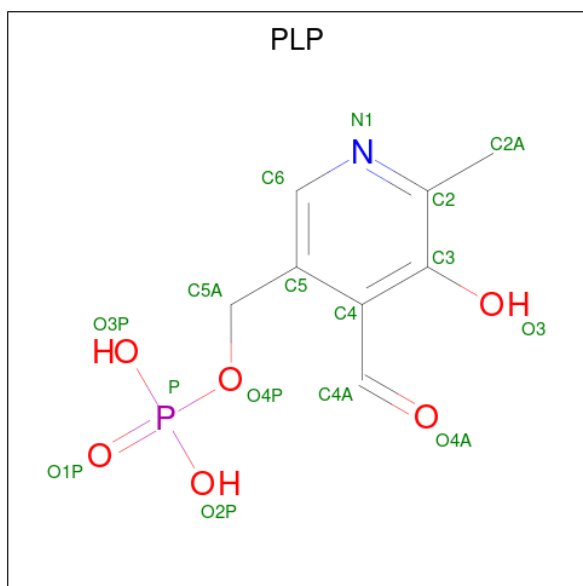
There are 3 unique types of molecules in this entry. The entry contains 6726 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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.

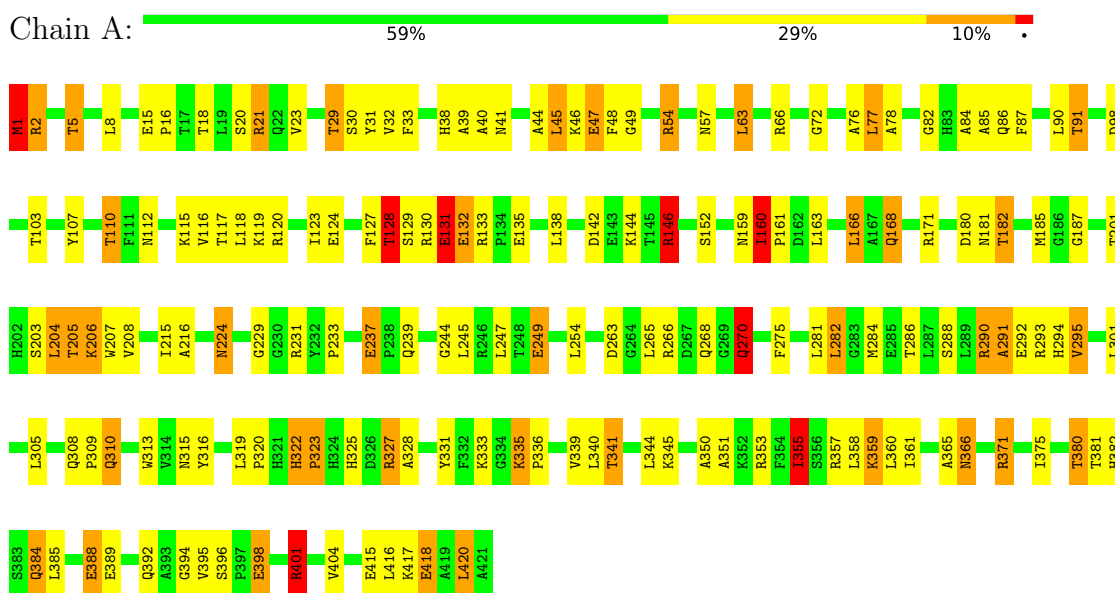
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total 83	O 83	0	0
3	B	91	Total 91	O 91	0	0

3 Residue-property plots

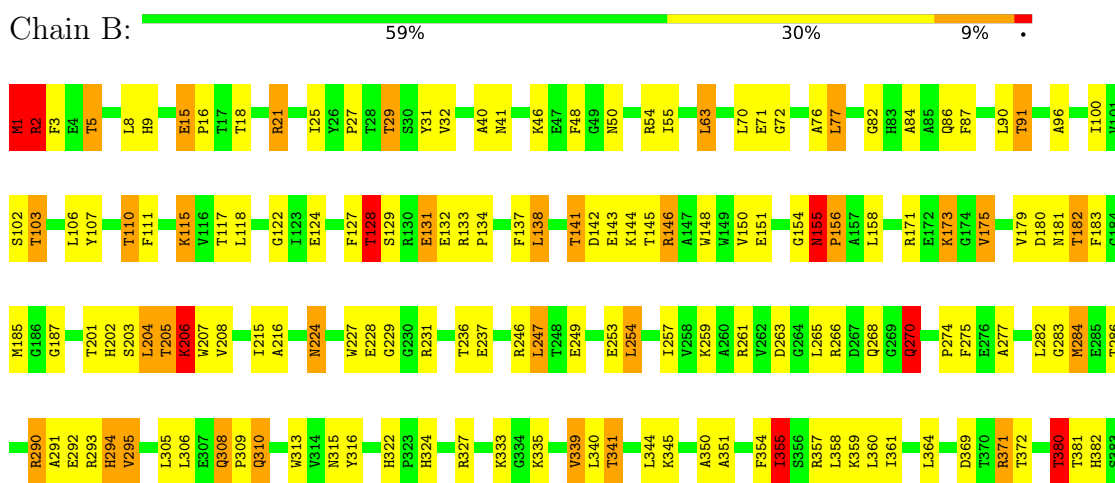
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



Q384	L385	S386	P387	E388	E389
Q392	V395	S396	P397	E398	
R401	L402	S403	V404		
E415	L416	K417	E418	A419	L420
				A421	

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

5.1 Standard geometry

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	1.60	21/3345 (0.6%)	1.55	57/4550 (1.3%)
1	B	1.63	24/3345 (0.7%)	1.54	44/4550 (1.0%)
All	All	1.61	45/6690 (0.7%)	1.54	101/9100 (1.1%)

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 (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	ILE	CG1-CD1	10.07	1.91	1.51
1	B	355	ILE	CG1-CD1	9.75	1.89	1.51
1	B	155	ASN	CA-C	-8.85	1.41	1.52
1	B	208	VAL	CA-CB	-8.59	1.44	1.54
1	B	284	MET	SD-CE	-8.56	1.58	1.79
1	A	284	MET	SD-CE	-7.54	1.60	1.79
1	B	2	ARG	N-CA	7.01	1.55	1.46
1	A	345	LYS	CD-CE	7.00	1.73	1.52
1	A	77	LEU	C-O	6.95	1.31	1.23
1	A	160	ILE	CA-CB	6.94	1.62	1.54
1	B	5	THR	CA-CB	6.58	1.64	1.53
1	B	345	LYS	CD-CE	6.50	1.72	1.52
1	B	77	LEU	C-O	6.40	1.31	1.23
1	A	398	GLU	CA-C	6.24	1.61	1.52
1	A	18	THR	CA-CB	6.14	1.62	1.54
1	A	208	VAL	CA-CB	-6.13	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	395	VAL	CA-CB	6.11	1.61	1.53
1	A	5	THR	CA-CB	6.03	1.63	1.53
1	B	100	ILE	CA-CB	6.03	1.65	1.55
1	B	395	VAL	CA-CB	5.90	1.61	1.53
1	B	9	HIS	C-O	-5.80	1.18	1.24
1	B	156	PRO	N-CA	5.66	1.54	1.47
1	A	231	ARG	CA-C	5.60	1.60	1.52
1	B	270	GLN	CA-C	5.59	1.60	1.52
1	B	339	VAL	CA-CB	-5.55	1.47	1.54
1	B	40	ALA	N-CA	5.51	1.52	1.46
1	A	85	ALA	CA-C	5.45	1.59	1.52
1	A	131	GLU	CG-CD	5.34	1.65	1.52
1	A	168	GLN	N-CA	5.29	1.52	1.46
1	A	339	VAL	CA-CB	-5.27	1.48	1.54
1	A	40	ALA	N-CA	5.27	1.52	1.46
1	A	290	ARG	CD-NE	-5.26	1.38	1.46
1	B	231	ARG	CA-C	5.18	1.59	1.52
1	B	277	ALA	C-O	5.17	1.30	1.24
1	A	76	ALA	CA-CB	-5.17	1.44	1.53
1	B	1	MET	CA-C	5.17	1.63	1.52
1	B	350	ALA	CA-C	5.13	1.59	1.52
1	A	350	ALA	CA-C	5.12	1.59	1.52
1	B	380	THR	CA-CB	5.10	1.62	1.53
1	B	18	THR	CA-CB	5.07	1.61	1.54
1	A	291	ALA	CA-CB	-5.05	1.45	1.53
1	B	351	ALA	N-CA	-5.02	1.40	1.46
1	A	263	ASP	N-CA	-5.02	1.41	1.46
1	B	76	ALA	CA-CB	-5.01	1.44	1.53
1	B	402	LEU	CA-CB	-5.00	1.46	1.53

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ILE	CB-CA-C	10.68	121.85	110.53
1	B	371	ARG	NE-CZ-NH2	-9.44	110.71	119.20
1	A	237	GLU	CA-C-N	-9.02	110.74	119.85
1	A	237	GLU	C-N-CA	-9.02	110.74	119.85
1	A	290	ARG	NE-CZ-NH2	-8.59	111.47	119.20
1	B	360	LEU	N-CA-C	7.81	119.57	111.14
1	B	290	ARG	NE-CZ-NH2	-7.74	112.23	119.20
1	B	127	PHE	N-CA-C	7.59	121.11	108.73
1	B	355	ILE	N-CA-CB	7.21	120.35	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	THR	CA-C-N	-7.04	112.91	120.94
1	A	103	THR	C-N-CA	-7.04	112.91	120.94
1	A	396	SER	CB-CA-C	6.99	118.73	108.87
1	B	29	THR	N-CA-CB	-6.88	100.41	110.53
1	A	127	PHE	N-CA-C	6.81	119.83	108.73
1	A	371	ARG	NE-CZ-NH1	6.75	128.25	121.50
1	B	396	SER	CB-CA-C	6.73	118.04	108.68
1	A	371	ARG	NE-CZ-NH2	-6.72	113.15	119.20
1	B	371	ARG	NE-CZ-NH1	6.38	127.88	121.50
1	A	5	THR	CB-CA-C	6.34	120.02	109.56
1	B	55	ILE	CB-CA-C	-6.29	103.40	111.20
1	B	371	ARG	CG-CD-NE	-6.28	98.18	112.00
1	A	115	LYS	N-CA-C	6.26	119.08	111.82
1	A	249	GLU	N-CA-C	6.22	117.86	111.14
1	A	1	MET	CG-SD-CE	6.20	114.53	100.90
1	A	204	LEU	N-CA-C	-6.14	105.05	112.54
1	A	18	THR	N-CA-C	-6.11	106.42	114.31
1	A	331	TYR	N-CA-C	6.10	119.92	112.23
1	A	355	ILE	N-CA-CB	6.06	121.01	110.65
1	B	316	TYR	N-CA-C	6.01	117.23	109.72
1	A	23	VAL	CB-CA-C	-5.97	105.39	110.94
1	A	284	MET	N-CA-C	-5.96	104.86	111.71
1	A	394	GLY	N-CA-C	-5.92	106.55	115.32
1	B	283	GLY	N-CA-C	-5.89	105.03	113.86
1	A	351	ALA	N-CA-C	-5.84	104.84	111.14
1	B	72	GLY	N-CA-C	-5.83	106.11	115.08
1	B	41	ASN	N-CA-C	5.78	117.58	111.28
1	B	146	ARG	CB-CA-C	5.76	118.69	109.02
1	B	18	THR	N-CA-C	-5.74	106.91	114.31
1	B	204	LEU	N-CA-C	-5.70	105.58	112.54
1	A	284	MET	CA-CB-CG	5.68	125.46	114.10
1	B	103	THR	CA-C-N	-5.67	114.42	121.00
1	B	103	THR	C-N-CA	-5.67	114.42	121.00
1	A	384	GLN	CB-CA-C	5.66	118.57	109.07
1	B	261	ARG	N-CA-C	5.66	117.31	111.03
1	A	290	ARG	CD-NE-CZ	5.62	132.27	124.40
1	B	290	ARG	N-CA-C	-5.60	104.80	111.69
1	A	20	SER	N-CA-C	5.59	118.58	110.42
1	A	29	THR	N-CA-CB	-5.58	102.33	110.53
1	A	159	ASN	CA-C-N	-5.52	117.96	123.04
1	A	159	ASN	C-N-CA	-5.52	117.96	123.04
1	B	173	LYS	N-CA-C	5.52	119.27	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	GLY	N-CA-C	-5.51	107.50	115.27
1	A	290	ARG	NE-CZ-NH1	5.50	127.00	121.50
1	A	29	THR	N-CA-C	-5.49	106.74	113.50
1	B	155	ASN	N-CA-CB	5.48	120.13	110.37
1	A	360	LEU	N-CA-C	5.47	116.92	111.07
1	A	187	GLY	N-CA-C	-5.45	107.83	114.92
1	A	290	ARG	N-CA-C	-5.45	104.99	111.69
1	A	124	GLU	CA-C-N	-5.40	116.10	123.12
1	A	124	GLU	C-N-CA	-5.40	116.10	123.12
1	A	275	PHE	N-CA-CB	5.38	118.03	110.12
1	A	128	THR	N-CA-CB	-5.37	101.41	110.49
1	B	290	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	B	155	ASN	O-C-N	5.35	127.47	121.32
1	A	146	ARG	CB-CA-C	5.33	118.02	109.07
1	A	244	GLY	N-CA-C	5.32	122.54	114.61
1	A	72	GLY	N-CA-C	-5.30	106.91	115.08
1	B	2	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	B	5	THR	CB-CA-C	5.29	118.28	109.56
1	A	123	ILE	N-CA-C	-5.27	100.06	107.75
1	A	57	ASN	CA-C-N	-5.27	114.24	119.56
1	A	57	ASN	C-N-CA	-5.27	114.24	119.56
1	B	1	MET	CG-SD-CE	5.27	112.49	100.90
1	A	160	ILE	CA-CB-CG2	5.23	119.40	110.50
1	A	49	GLY	N-CA-C	5.23	120.42	114.67
1	A	322	HIS	CA-C-N	5.23	126.37	119.84
1	A	322	HIS	C-N-CA	5.23	126.37	119.84
1	B	404	VAL	CB-CA-C	-5.22	104.37	111.15
1	A	41	ASN	N-CA-C	5.20	117.63	111.33
1	B	124	GLU	CA-C-N	-5.20	116.24	122.90
1	B	124	GLU	C-N-CA	-5.20	116.24	122.90
1	B	351	ALA	N-CA-C	-5.17	105.56	111.14
1	B	237	GLU	CA-C-N	-5.15	114.64	119.85
1	B	237	GLU	C-N-CA	-5.15	114.64	119.85
1	B	249	GLU	N-CA-C	5.15	118.02	111.69
1	B	227	TRP	CA-C-N	5.14	127.17	120.28
1	B	227	TRP	C-N-CA	5.14	127.17	120.28
1	B	275	PHE	N-CA-CB	5.13	117.67	110.12
1	A	78	ALA	CA-C-N	-5.13	114.27	122.53
1	A	78	ALA	C-N-CA	-5.13	114.27	122.53
1	A	146	ARG	CG-CD-NE	-5.11	100.75	112.00
1	A	328	ALA	N-CA-C	-5.10	105.72	111.28
1	B	128	THR	N-CA-CB	-5.08	101.90	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	VAL	CB-CA-C	-5.06	103.96	110.84
1	B	46	LYS	CA-C-N	-5.06	111.88	121.54
1	B	46	LYS	C-N-CA	-5.06	111.88	121.54
1	A	46	LYS	N-CA-C	5.05	117.68	111.82
1	A	270	GLN	CB-CA-C	-5.05	100.38	110.42
1	B	50	ASN	N-CA-C	5.04	119.56	113.41
1	A	66	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	A	401	ARG	CG-CD-NE	5.02	123.04	112.00

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 [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	3261	0	3249	125	0
1	B	3261	0	3249	145	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	271	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 21.

All (271) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:63:LEU:HD23	1:B:284:MET:HE1	1.48	0.94
1:A:315:ASN:HB3	1:A:341:THR:CG2	2.02	0.90
1:A:160:ILE:HD13	1:A:160:ILE:C	1.95	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
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: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:A:224:ASN:C	1:A:224:ASN:HD22	1.85	0.82
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:TYR:OH	3:B:687:HOH:O	2.02	0.76
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:380:THR:CG2	1:A:381:THR:N	2.37	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:B:106:LEU:C	1:B:155:ASN:HB2	2.15	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: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
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:B:380:THR:CG2	1:B:381:THR:N	2.44	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:224:ASN:C	1:B:224:ASN:HD22	2.02	0.68
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:A:1:MET:HE2	1:A:1:MET:O	1.95	0.65
1:B:386:SER:OG	1:B:389:GLU:HG2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASP:OD1	1:A:182:THR:CG2	2.45	0.64
1:A:224:ASN:C	1:A:224:ASN:ND2	2.51	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:A:84:ALA:HB1	1:A:270:GLN:HG2	1.79	0.63
1:B:63:LEU:HD23	1:B:284:MET:CE	2.26	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:98:ASP:CG	1:A:146:ARG:HH11	2.08	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
1:B:1:MET:O	1:B:1:MET:HE2	2.01	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
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: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:224:ASN:C	1:B:224:ASN:ND2	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:380:THR:HG23	1:B:381:THR:N	2.15	0.55
1:A:142:ASP:C	1:A:142:ASP:OD1	2.49	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: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:B:340:LEU:HD12	1:B:340:LEU:C	2.34	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
1:A:185:MET:HE2	1:A:207:TRP:CD1	2.44	0.53
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: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:181:ASN:O	1:B:182:THR:C	2.53	0.52
1:B:128:THR:CG2	1:B:129:SER:O	2.56	0.51
1:A:21:ARG:HD3	1:A:21:ARG:C	2.22	0.51
1:A:44:ALA:O	1:A:45:LEU:HB2	2.11	0.51
1:A:340:LEU:C	1:A:340:LEU:HD12	2.35	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:63:LEU:HD23	1:A:63:LEU:C	2.37	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:155:ASN:OD1	1:B:155:ASN:C	2.55	0.48
1:B:21:ARG:CD	1:B:21:ARG:C	2.86	0.48
1:B:398:GLU:OE1	1:B:398:GLU:N	2.44	0.48
1:B:21:ARG:HD3	1:B:21:ARG:C	2.22	0.48
1:B:142:ASP:OD1	1:B:142:ASP:C	2.56	0.48
1:B:102:SER:OG	1:B:103:THR:O	2.31	0.48
1:B:290:ARG:O	1:B:291:ALA:C	2.57	0.48
1:A:131:GLU:CD	1:A:133:ARG:HH11	2.21	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:181:ASN:O	1:A:182:THR:C	2.53	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:205:THR:HG22	1:B:216:ALA:H	1.80	0.47
1:B:315:ASN:O	1:B:315:ASN:CG	2.58	0.47
1:A:30:SER:C	1:A:31:TYR:CD2	2.93	0.46
1:A:54:ARG:HE	1:A:54:ARG:HB2	1.49	0.46
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: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:A:160:ILE:C	1:A:160:ILE:CD1	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:LYS:HE2	1:B:263:ASP:OD2	2.16	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:86:GLN:OE1	1:B:110:THR:HB	2.18	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:369:ASP:OD2	1:B:371:ARG:HD2	2.18	0.44
1:A:21:ARG:C	1:A:21:ARG:CD	2.91	0.44
1:A:33:PHE:CG	1:A:39:ALA:HB2	2.53	0.44
1:B:106:LEU:O	1:B:155:ASN:HB2	2.17	0.44
1:A:160:ILE:HD13	1:A:160:ILE:O	2.17	0.43
1:B:63:LEU:CD2	1:B:284:MET:HE1	2.35	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: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
1:A:288:SER:O	1:A:292:GLU:HG3	2.19	0.43
1:B:128:THR:CG2	1:B:129:SER:N	2.81	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:B:185:MET:HE2	1:B:207:TRP:CD1	2.54	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:O	1:B:315:ASN:ND2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:306:LEU:C	1:B:308:GLN:H	2.28	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:290:ARG:O	1:A:291:ALA:C	2.64	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:A:63:LEU:C	1:A:63:LEU:CD2	2.94	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:B:133:ARG:O	1:B:134:PRO:C	2.61	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 [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	419/421 (100%)	390 (93%)	23 (6%)	6 (1%)	9	19
1	B	419/421 (100%)	388 (93%)	24 (6%)	7 (2%)	7	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	838/842 (100%)	778 (93%)	47 (6%)	13 (2%)	7	16

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%)	274 (82%)	59 (18%)	2	3
1	B	333/333 (100%)	275 (83%)	58 (17%)	2	3
All	All	666/666 (100%)	549 (82%)	117 (18%)	2	3

All (117) 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

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Mol	Chain	Res	Type
1	A	29	THR
1	A	32	VAL
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	117	THR
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	206	LYS
1	A	224	ASN
1	A	247	LEU
1	A	249	GLU
1	A	265	LEU
1	A	266	ARG
1	A	270	GLN
1	A	282	LEU
1	A	295	VAL
1	A	305	LEU
1	A	310	GLN
1	A	327	ARG
1	A	333	LYS
1	A	335	LYS
1	A	341	THR

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Mol	Chain	Res	Type
1	A	344	LEU
1	A	355	ILE
1	A	359	LYS
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	15	GLU
1	B	21	ARG
1	B	29	THR
1	B	32	VAL
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	117	THR
1	B	118	LEU
1	B	128	THR
1	B	131	GLU
1	B	138	LEU
1	B	141	THR
1	B	143	GLU
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	308	GLN
1	B	310	GLN
1	B	327	ARG
1	B	333	LYS
1	B	341	THR
1	B	344	LEU
1	B	355	ILE
1	B	359	LYS
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 (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	50	ASN
1	A	99	ASN
1	A	112	ASN
1	A	113	GLN
1	A	181	ASN
1	A	224	ASN
1	A	268	GLN
1	A	270	GLN
1	A	294	HIS

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Mol	Chain	Res	Type
1	A	300	HIS
1	A	310	GLN
1	A	315	ASN
1	A	325	HIS
1	A	366	ASN
1	A	384	GLN
1	B	41	ASN
1	B	99	ASN
1	B	112	ASN
1	B	181	ASN
1	B	202	HIS
1	B	224	ASN
1	B	268	GLN
1	B	270	GLN
1	B	294	HIS
1	B	300	HIS
1	B	310	GLN
1	B	315	ASN
1	B	325	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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.