



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 06:47 PM BST

PDB ID : 5B87
Title : Crystal structure of a Cysteine Desulfurase from *Thermococcus onnurineus* NA1 in complex with alanine at 2.3 Angstrom resolution
Authors : Ho, T.-H.; Kang, L.-W.
Deposited on : 2016-06-13
Resolution : 2.28 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) : 1.13
EDS : 2.14.4.dev1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

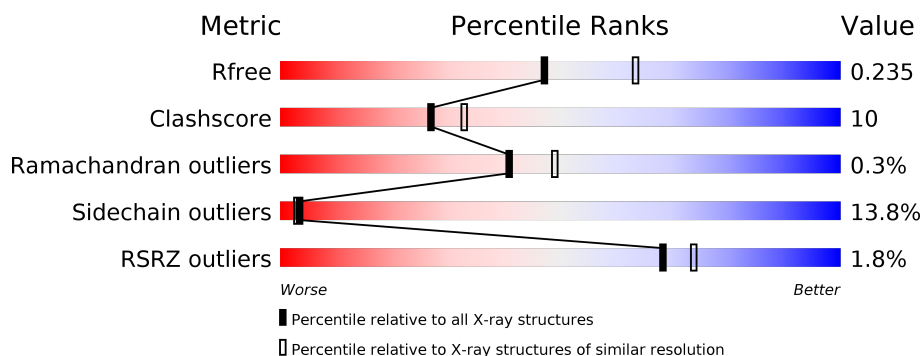
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	419	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>22%</div> <div>5%</div> <div>5%</div> </div> </div>
1	B	419	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>.</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6397 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 Cysteine desulfurase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3088	1967	535	577	9			
1	B	401	Total	C	N	O	S	0	0	0
			3130	1995	542	582	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP B6YT87
A	-18	HIS	-	expression tag	UNP B6YT87
A	-17	HIS	-	expression tag	UNP B6YT87
A	-16	HIS	-	expression tag	UNP B6YT87
A	-15	HIS	-	expression tag	UNP B6YT87
A	-14	HIS	-	expression tag	UNP B6YT87
A	-13	HIS	-	expression tag	UNP B6YT87
A	-12	SER	-	expression tag	UNP B6YT87
A	-11	SER	-	expression tag	UNP B6YT87
A	-10	GLU	-	expression tag	UNP B6YT87
A	-9	ASN	-	expression tag	UNP B6YT87
A	-8	LEU	-	expression tag	UNP B6YT87
A	-7	TYR	-	expression tag	UNP B6YT87
A	-6	PHE	-	expression tag	UNP B6YT87
A	-5	GLN	-	expression tag	UNP B6YT87
A	-4	GLY	-	expression tag	UNP B6YT87
A	-3	HIS	-	expression tag	UNP B6YT87
A	-2	MET	-	expression tag	UNP B6YT87
A	-1	ALA	-	expression tag	UNP B6YT87
A	0	SER	-	expression tag	UNP B6YT87
B	-19	MET	-	expression tag	UNP B6YT87
B	-18	HIS	-	expression tag	UNP B6YT87
B	-17	HIS	-	expression tag	UNP B6YT87
B	-16	HIS	-	expression tag	UNP B6YT87
B	-15	HIS	-	expression tag	UNP B6YT87

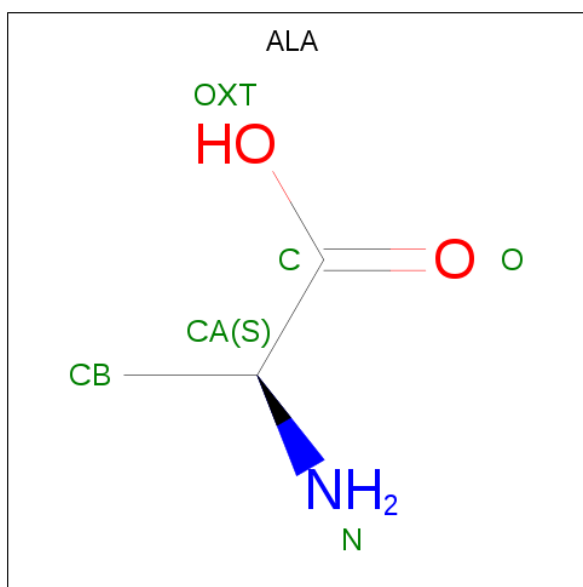
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP B6YT87
B	-13	HIS	-	expression tag	UNP B6YT87
B	-12	SER	-	expression tag	UNP B6YT87
B	-11	SER	-	expression tag	UNP B6YT87
B	-10	GLU	-	expression tag	UNP B6YT87
B	-9	ASN	-	expression tag	UNP B6YT87
B	-8	LEU	-	expression tag	UNP B6YT87
B	-7	TYR	-	expression tag	UNP B6YT87
B	-6	PHE	-	expression tag	UNP B6YT87
B	-5	GLN	-	expression tag	UNP B6YT87
B	-4	GLY	-	expression tag	UNP B6YT87
B	-3	HIS	-	expression tag	UNP B6YT87
B	-2	MET	-	expression tag	UNP B6YT87
B	-1	ALA	-	expression tag	UNP B6YT87
B	0	SER	-	expression tag	UNP B6YT87

- PLP
-
- The diagram shows the chemical structure of Pyridoxal phosphate (PLP). It consists of a pyridine ring with a phosphate group at the 3-position and an aldehyde group at the 4-position. The pyridine ring is labeled with N1 (nitrogen), C2, C3, C4, C5, and C6. The phosphate group is labeled with P (phosphorus), O1P, O2P, O3P, and O4P. The aldehyde group is labeled with C4A (aldehyde carbon) and O4A (aldehyde oxygen). The hydroxyl group at the 3-position is labeled with O3 (oxygen) and C3A (carbon). The hydroxyl group at the 4-position is labeled with O3 (oxygen) and C4A (carbon).

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

- WORLDWIDE
PDB
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	3	1	2		
3	B	1	Total	C	N	O	0	0
			6	3	1	2		

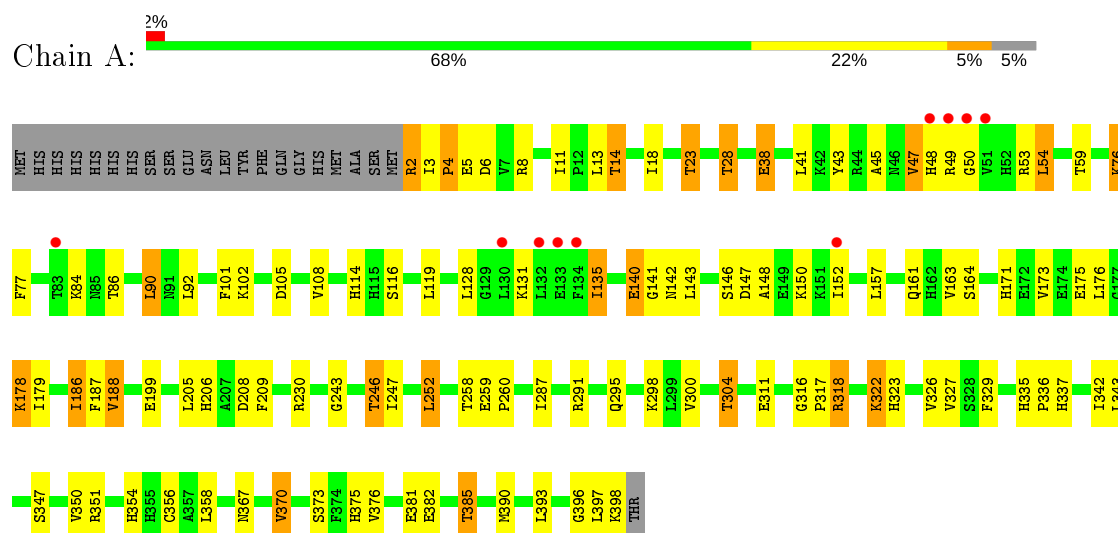
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O	0	0
			68	68		
4	B	69	Total	O	0	0
			69	69		

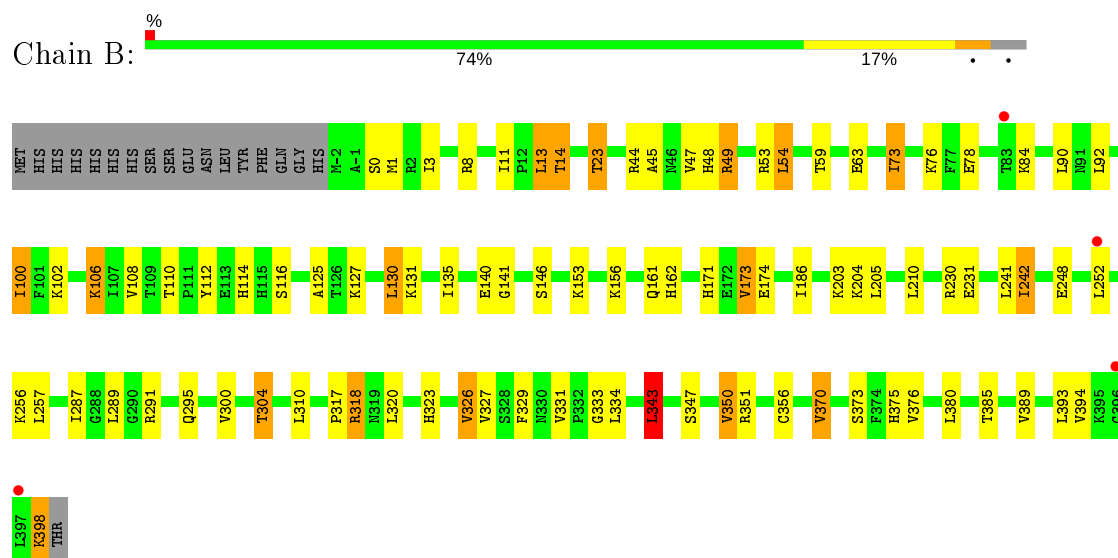
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cysteine desulfurase



• Molecule 1: Cysteine desulfurase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.28 Å 93.81 Å 145.53 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 – 2.28 49.40 – 2.28	Depositor EDS
% Data completeness (in resolution range)	95.9 (49.40-2.28) 95.9 (49.40-2.28)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.50 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.183 , 0.232 0.194 , 0.235	Depositor DCC
R_{free} test set	2040 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6397	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSS, 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	1.03	0/3147	0.97	2/4257 (0.0%)
1	B	1.01	1/3189 (0.0%)	0.99	5/4308 (0.1%)
All	All	1.02	1/6336 (0.0%)	0.98	7/8565 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	GLU	CG-CD	5.14	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	318	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	B	393	LEU	CA-CB-CG	6.81	130.95	115.30
1	B	343	LEU	CA-CB-CG	5.88	128.81	115.30
1	A	318	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	140	GLU	N-CA-C	5.27	125.23	111.00
1	B	230	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	331	VAL	C-N-CD	5.03	138.96	128.40

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	3088	0	3067	90	0
1	B	3130	0	3140	42	0
2	A	15	0	7	1	0
2	B	15	0	7	1	0
3	A	6	0	4	1	0
3	B	6	0	4	1	0
4	A	68	0	0	6	0
4	B	69	0	0	0	0
All	All	6397	0	6229	127	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 10.

All (127) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:HG12	1:A:48:HIS:H	1.33	0.92
1:A:28:THR:HG22	4:A:521:HOH:O	1.70	0.92
1:A:140:GLU:O	1:A:316:GLY:HA2	1.70	0.92
1:A:178:LYS:HE2	1:A:206:HIS:HE1	1.36	0.90
1:A:157:LEU:HD12	1:A:186:ILE:HD11	1.55	0.86
1:A:304:THR:CG2	4:A:568:HOH:O	2.27	0.83
1:B:375:HIS:CD2	1:B:376:VAL:H	1.98	0.81
1:A:28:THR:CG2	1:B:44:ARG:HE	1.93	0.81
1:A:2:ARG:HB3	1:A:6:ASP:OD2	1.82	0.79
1:A:47:VAL:HG12	1:A:48:HIS:N	1.98	0.78
1:B:73:ILE:HD11	1:B:210:LEU:HD22	1.68	0.75
1:B:333:GLY:HA2	1:B:398:LYS:HE2	1.69	0.74
1:B:375:HIS:HD2	1:B:376:VAL:H	1.33	0.74
1:A:38:GLU:HG2	4:A:505:HOH:O	1.88	0.72
1:A:178:LYS:HE2	1:A:206:HIS:CE1	2.24	0.71
1:A:23:THR:HG23	1:A:373:SER:CB	2.21	0.69
1:B:23:THR:HG23	1:B:373:SER:CB	2.23	0.69
1:A:252:LEU:N	1:A:252:LEU:HD22	2.08	0.69
1:A:38:GLU:HG3	1:A:43:TYR:HE1	1.57	0.69
1:A:178:LYS:CE	1:A:206:HIS:HE1	2.05	0.67
1:A:300:VAL:O	1:A:304:THR:HB	1.94	0.67
1:A:23:THR:CG2	1:A:373:SER:CB	2.72	0.67
1:B:49:ARG:HG3	1:B:49:ARG:HH11	1.59	0.67
1:A:157:LEU:CD1	1:A:186:ILE:HD11	2.24	0.67
1:A:142:ASN:OD1	1:A:322:LYS:CE	2.44	0.66
1:A:375:HIS:CD2	1:A:376:VAL:H	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:HIS:HD2	1:A:116:SER:H	1.45	0.64
1:B:300:VAL:O	1:B:304:THR:HB	1.97	0.64
1:B:106:LYS:HD3	1:B:108:VAL:HG12	1.80	0.63
1:B:49:ARG:HG3	1:B:49:ARG:NH1	2.12	0.63
1:B:161:GLN:HE21	1:B:171:HIS:HE1	1.48	0.62
1:B:317:PRO:O	1:B:323:HIS:HD2	1.84	0.61
1:B:112:TYR:CZ	1:B:141:GLY:HA2	2.36	0.61
1:A:135:ILE:HD12	1:A:148:ALA:HB2	1.82	0.60
1:A:2:ARG:HD3	1:A:291:ARG:NH2	2.16	0.60
1:B:333:GLY:CA	1:B:398:LYS:HE2	2.32	0.60
1:A:114:HIS:CD2	1:A:116:SER:H	2.19	0.60
2:A:400:PLP:HO3	3:A:401:ALA:N	1.99	0.60
1:B:3:ILE:HD12	1:B:291:ARG:CZ	2.31	0.60
1:B:23:THR:HG23	1:B:373:SER:HB3	1.84	0.60
2:B:400:PLP:HO3	3:B:401:ALA:N	2.01	0.59
1:B:140:GLU:OE2	1:B:318:ARG:HG2	2.03	0.58
1:A:147:ASP:HA	1:A:150:LYS:HE3	1.85	0.58
1:A:119:LEU:HB3	1:B:242:ILE:HG23	1.86	0.58
1:A:317:PRO:O	1:A:323:HIS:HD2	1.87	0.58
1:A:142:ASN:OD1	1:A:322:LYS:HE3	2.03	0.58
1:A:351:ARG:HG2	4:A:555:HOH:O	2.02	0.58
1:A:187:PHE:N	1:A:208:ASP:OD2	2.25	0.57
1:B:161:GLN:HE21	1:B:171:HIS:CE1	2.23	0.56
1:A:38:GLU:HG3	1:A:43:TYR:CE1	2.38	0.56
1:A:76:LYS:O	1:A:77:PHE:C	2.43	0.55
1:A:11:ILE:O	1:A:14:THR:HB	2.07	0.54
1:A:375:HIS:HD2	1:A:376:VAL:H	1.53	0.54
1:A:47:VAL:CG1	1:A:48:HIS:N	2.71	0.54
1:B:100:ILE:HG22	1:B:100:ILE:O	2.08	0.53
1:A:208:ASP:OD1	1:A:230:ARG:NH1	2.42	0.53
1:B:174:GLU:HG3	1:B:204:LYS:O	2.09	0.53
1:B:78:GLU:H	1:B:78:GLU:CD	2.12	0.53
1:A:135:ILE:HG12	1:A:143:LEU:HD22	1.89	0.53
1:A:347:SER:OG	1:B:53:ARG:NH2	2.41	0.52
1:A:335:HIS:HE1	1:A:337:HIS:CD2	2.27	0.52
1:A:135:ILE:CG1	1:A:143:LEU:HD22	2.40	0.52
1:A:135:ILE:CD1	1:A:148:ALA:HB2	2.39	0.52
1:A:101:PHE:HB2	1:A:128:LEU:HD23	1.90	0.52
1:A:23:THR:CG2	1:A:373:SER:HB3	2.40	0.52
1:A:3:ILE:HD11	1:A:287:ILE:HG23	1.91	0.51
1:A:329:PHE:CZ	1:A:370:VAL:HG22	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LEU:CD2	1:A:252:LEU:N	2.72	0.51
1:A:53:ARG:NH2	1:B:347:SER:OG	2.44	0.51
1:A:247:ILE:HD12	1:A:247:ILE:O	2.11	0.51
1:A:140:GLU:O	1:A:316:GLY:CA	2.51	0.50
1:A:23:THR:HG22	1:A:373:SER:HB2	1.92	0.50
1:A:2:ARG:N	4:A:502:HOH:O	2.45	0.50
1:B:114:HIS:HD2	1:B:116:SER:H	1.60	0.50
1:A:258:THR:OG1	1:A:259:GLU:N	2.45	0.49
1:A:23:THR:HG23	1:A:373:SER:OG	2.11	0.49
1:B:3:ILE:HD11	1:B:287:ILE:HG23	1.93	0.49
1:A:186:ILE:O	1:A:186:ILE:HG13	2.12	0.49
1:A:354:HIS:HD2	1:A:356:CSS:N	2.11	0.49
1:B:323:HIS:HE1	1:B:326:VAL:O	1.96	0.49
1:A:41:LEU:O	1:B:13:LEU:HD22	2.13	0.48
1:A:243:GLY:O	1:A:246:THR:HB	2.13	0.48
1:A:135:ILE:HD11	1:A:143:LEU:HB3	1.94	0.48
1:A:8:ARG:HB3	1:A:14:THR:HG21	1.95	0.47
1:B:343:LEU:HD23	1:B:350:VAL:HG11	1.97	0.47
1:A:157:LEU:HD12	1:A:186:ILE:CD1	2.37	0.47
1:A:23:THR:CG2	1:A:373:SER:HB2	2.45	0.47
1:A:252:LEU:CD2	1:A:252:LEU:H	2.26	0.47
1:A:28:THR:HG23	1:B:44:ARG:HE	1.76	0.47
1:B:23:THR:CG2	1:B:373:SER:CB	2.92	0.47
1:A:45:ALA:HB2	1:A:54:LEU:HB3	1.97	0.46
1:A:161:GLN:HE21	1:A:171:HIS:HE1	1.63	0.46
1:A:178:LYS:CE	1:A:206:HIS:CE1	2.93	0.46
1:A:396:GLY:C	1:A:398:LYS:H	2.18	0.46
1:B:45:ALA:HB2	1:B:54:LEU:HB3	1.97	0.46
1:A:18:ILE:HG12	1:A:382:GLU:HG2	1.98	0.45
1:A:323:HIS:HE1	1:A:326:VAL:O	1.98	0.45
1:A:247:ILE:HD12	1:A:247:ILE:C	2.37	0.45
1:A:173:VAL:HG23	1:A:205:LEU:HG	1.99	0.45
1:B:49:ARG:HH11	1:B:49:ARG:CG	2.24	0.45
1:B:329:PHE:CZ	1:B:370:VAL:HG22	2.52	0.45
1:A:390:MET:CE	1:A:390:MET:HA	2.47	0.45
1:A:335:HIS:CE1	1:A:337:HIS:CD2	3.05	0.44
1:A:2:ARG:CD	1:A:291:ARG:HH22	2.31	0.44
1:A:47:VAL:HG13	1:A:59:THR:HG23	2.00	0.44
1:B:76:LYS:NZ	1:B:231:GLU:OE2	2.51	0.43
1:A:102:LYS:HD3	1:A:102:LYS:HA	1.73	0.43
1:A:38:GLU:CG	1:A:43:TYR:HE1	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ARG:HG2	1:A:50:GLY:N	2.33	0.43
1:A:171:HIS:HD2	4:A:513:HOH:O	2.01	0.42
1:B:49:ARG:HG2	1:B:59:THR:HG21	2.02	0.42
1:A:3:ILE:HA	1:A:4:PRO:HA	1.59	0.42
1:B:162:HIS:HA	1:B:173:VAL:HG11	2.01	0.42
1:A:336:PRO:HB3	1:A:370:VAL:HG12	2.02	0.42
1:B:295:GLN:HE21	1:B:295:GLN:HA	1.85	0.42
1:A:142:ASN:OD1	1:A:322:LYS:HE2	2.20	0.42
1:A:161:GLN:NE2	1:A:164:SER:HB2	2.35	0.42
1:A:140:GLU:N	1:A:141:GLY:HA2	2.35	0.42
1:A:152:ILE:HG21	1:A:179:ILE:HG22	2.01	0.41
1:A:28:THR:HG21	1:B:44:ARG:HE	1.82	0.41
1:A:381:GLU:O	1:A:385:THR:CG2	2.69	0.41
1:A:86:THR:HG22	1:A:90:LEU:HD22	2.03	0.41
1:B:8:ARG:HB3	1:B:14:THR:HG21	2.02	0.41
1:A:188:VAL:HB	1:A:209:PHE:HB2	2.03	0.40
1:A:295:GLN:HE22	1:A:298:LYS:NZ	2.20	0.40
1:B:11:ILE:O	1:B:14:THR:HB	2.22	0.40
1:B:125:ALA:HA	1:B:130:LEU:HB2	2.02	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	394/419 (94%)	384 (98%)	9 (2%)	1 (0%)	41	49
1	B	398/419 (95%)	387 (97%)	10 (2%)	1 (0%)	41	49
All	All	792/838 (94%)	771 (97%)	19 (2%)	2 (0%)	41	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	VAL
1	B	47	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	326/350 (93%)	284 (87%)	42 (13%)	4	4
1	B	333/350 (95%)	284 (85%)	49 (15%)	3	2
All	All	659/700 (94%)	568 (86%)	91 (14%)	3	3

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	4	PRO
1	A	5	GLU
1	A	13	LEU
1	A	14	THR
1	A	23	THR
1	A	28	THR
1	A	38	GLU
1	A	54	LEU
1	A	76	LYS
1	A	84	LYS
1	A	90	LEU
1	A	92	LEU
1	A	105	ASP
1	A	108	VAL
1	A	131	LYS
1	A	135	ILE
1	A	146	SER
1	A	163	VAL
1	A	175	GLU
1	A	176	LEU
1	A	178	LYS

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Mol	Chain	Res	Type
1	A	186	ILE
1	A	188	VAL
1	A	199	GLU
1	A	246	THR
1	A	252	LEU
1	A	260	PRO
1	A	304	THR
1	A	311	GLU
1	A	318	ARG
1	A	322	LYS
1	A	327	VAL
1	A	342	ILE
1	A	343	LEU
1	A	350	VAL
1	A	358	LEU
1	A	367	ASN
1	A	370	VAL
1	A	385	THR
1	A	393	LEU
1	A	397	LEU
1	B	0	SER
1	B	1	MET
1	B	13	LEU
1	B	14	THR
1	B	23	THR
1	B	48	HIS
1	B	49	ARG
1	B	54	LEU
1	B	73	ILE
1	B	84	LYS
1	B	90	LEU
1	B	92	LEU
1	B	100	ILE
1	B	102	LYS
1	B	106	LYS
1	B	110	THR
1	B	127	LYS
1	B	130	LEU
1	B	131	LYS
1	B	135	ILE
1	B	146	SER
1	B	153	LYS

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Mol	Chain	Res	Type
1	B	156	LYS
1	B	173	VAL
1	B	186	ILE
1	B	203	LYS
1	B	205	LEU
1	B	241	LEU
1	B	242	ILE
1	B	248	GLU
1	B	252	LEU
1	B	256	LYS
1	B	257	LEU
1	B	289	LEU
1	B	304	THR
1	B	310	LEU
1	B	320	LEU
1	B	326	VAL
1	B	327	VAL
1	B	334	LEU
1	B	343	LEU
1	B	350	VAL
1	B	351	ARG
1	B	370	VAL
1	B	380	LEU
1	B	385	THR
1	B	389	VAL
1	B	394	VAL
1	B	398	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	171	HIS
1	A	206	HIS
1	A	295	GLN
1	A	297	HIS
1	A	323	HIS
1	A	354	HIS
1	A	375	HIS
1	B	114	HIS
1	B	142	ASN
1	B	171	HIS

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Mol	Chain	Res	Type
1	B	206	HIS
1	B	295	GLN
1	B	323	HIS
1	B	375	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSS	B	356	1	4,6,7	1.37	1 (25%)	1,6,8	0.80	0
1	CSS	A	356	1	4,6,7	1.05	0	1,6,8	0.28	0

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
1	CSS	B	356	1	-	0/1/5/7	-
1	CSS	A	356	1	-	0/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	356	CSS	CB-SG	-2.18	1.74	1.81

There are no bond angle outliers.

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
1	A	356	CSS	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	B	400	1,3	15,15,16	1.69	1 (6%)	20,22,23	1.62	2 (10%)
3	ALA	B	401	2	2,5,5	0.88	0	2,6,6	1.52	0
3	ALA	A	401	2	2,5,5	0.56	0	2,6,6	1.25	0
2	PLP	A	400	1,3	15,15,16	1.98	5 (33%)	20,22,23	2.14	9 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	B	400	1,3	-	0/6/6/8	0/1/1/1
3	ALA	B	401	2	-	0/0/4/4	-
3	ALA	A	401	2	-	0/0/4/4	-
2	PLP	A	400	1,3	-	0/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	PLP	C5-C4	-5.63	1.34	1.40
2	A	400	PLP	C4A-C4	4.29	1.60	1.51
2	A	400	PLP	C3-C2	3.45	1.44	1.40
2	A	400	PLP	O3-C3	3.12	1.44	1.37
2	A	400	PLP	P-O2P	-2.30	1.46	1.54
2	A	400	PLP	C3-C4	-2.09	1.35	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	PLP	C4A-C4-C5	4.55	125.62	120.94
2	A	400	PLP	O3-C3-C2	4.24	126.73	117.49
2	A	400	PLP	C4A-C4-C5	3.51	124.55	120.94
2	A	400	PLP	O3P-P-O4P	3.49	116.02	106.73
2	A	400	PLP	C3-C2-N1	2.75	124.32	120.77
2	A	400	PLP	C4A-C4-C3	-2.71	115.90	120.50
2	A	400	PLP	C2A-C2-N1	-2.60	112.59	117.67
2	A	400	PLP	O3P-P-O2P	-2.26	99.00	107.64
2	A	400	PLP	C4-C3-C2	-2.14	116.91	120.07
2	A	400	PLP	C6-C5-C4	2.10	119.81	118.16
2	B	400	PLP	O3-C3-C2	2.05	121.95	117.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	PLP	1	0
3	B	401	ALA	1	0
3	A	401	ALA	1	0
2	A	400	PLP	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	396/419 (94%)	-0.07	10 (2%) 57 63	25, 41, 67, 108	0
1	B	400/419 (95%)	-0.15	4 (1%) 82 86	23, 39, 63, 101	0
All	All	796/838 (94%)	-0.11	14 (1%) 68 74	23, 40, 66, 108	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252	LEU	4.2
1	A	49	ARG	3.5
1	B	83	THR	3.5
1	A	51	VAL	3.2
1	B	396	GLY	2.6
1	A	134	PHE	2.6
1	A	132	LEU	2.5
1	A	48	HIS	2.5
1	A	50	GLY	2.5
1	A	130	LEU	2.5
1	A	152	ILE	2.5
1	A	83	THR	2.4
1	B	397	LEU	2.1
1	A	133	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CSS	B	356	7/8	0.88	0.11	36,46,54,55	0
1	CSS	A	356	7/8	0.94	0.09	35,35,40,40	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ALA	B	401	6/6	0.90	0.14	51,56,58,63	0
3	ALA	A	401	6/6	0.95	0.10	39,47,49,52	0
2	PLP	B	400	15/16	0.98	0.15	24,30,37,44	0
2	PLP	A	400	15/16	0.98	0.13	24,29,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.