



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:06 AM UTC

PDB ID : 5B87 / pdb_00005b87
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 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

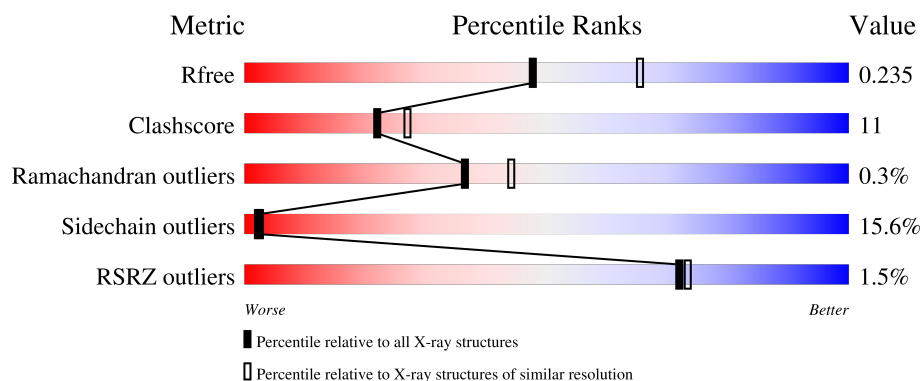
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (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 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 $\leq 5\%$. 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	
1	B	419	

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
3	ALA	B	401	-	X	-	-

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:

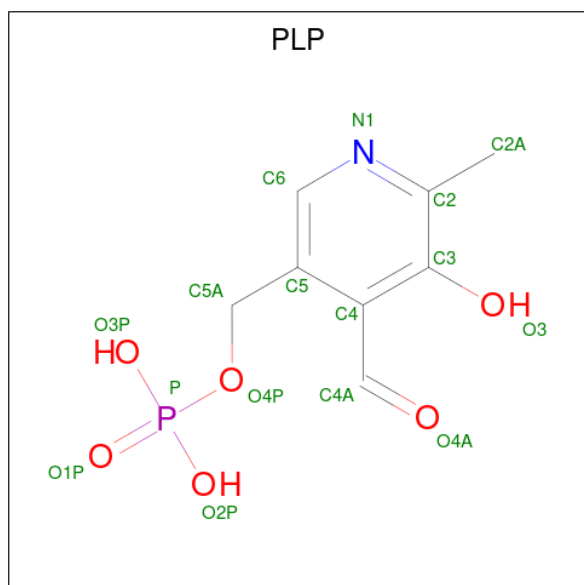
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP B6YT87
A	-18	HIS	-	expression tag	UNP B6YT87
A	-17	HIS	-	expression tag	UNP B6YT87
A	-16	HIS	-	expression tag	UNP B6YT87
A	-15	HIS	-	expression tag	UNP B6YT87
A	-14	HIS	-	expression tag	UNP B6YT87
A	-13	HIS	-	expression tag	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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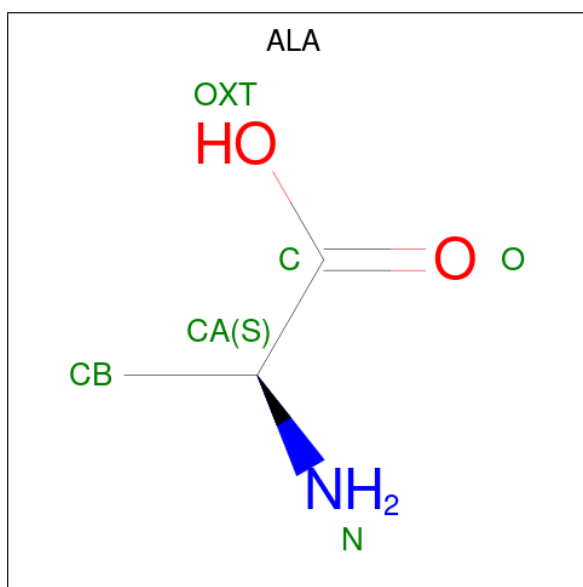
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP B6YT87
B	-13	HIS	-	expression tag	UNP B6YT87
B	-12	SER	-	expression tag	UNP B6YT87
B	-11	SER	-	expression tag	UNP B6YT87
B	-10	GLU	-	expression tag	UNP B6YT87
B	-9	ASN	-	expression tag	UNP B6YT87
B	-8	LEU	-	expression tag	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

- 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 ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$).



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		

- 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	67.28Å 93.81Å 145.53Å 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 2.29Å)	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 (4.79%)	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)	0.34 , 30.1	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

5.1 Standard geometry

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	1.45	14/3147 (0.4%)	1.31	30/4257 (0.7%)
1	B	1.39	13/3189 (0.4%)	1.26	21/4308 (0.5%)
All	All	1.42	27/6336 (0.4%)	1.28	51/8565 (0.6%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	GLY	C-O	-8.27	1.18	1.24
1	A	28	THR	C-O	-6.64	1.17	1.24
1	B	110	THR	C-N	6.45	1.38	1.33
1	B	53	ARG	C-O	-6.18	1.16	1.24
1	A	110	THR	C-N	6.12	1.38	1.33
1	A	326	VAL	C-O	-6.08	1.18	1.24
1	B	376	VAL	C-O	-5.99	1.16	1.24
1	A	25	THR	C-O	-5.73	1.16	1.23
1	A	259	GLU	C-N	5.69	1.38	1.33
1	A	169	VAL	C-O	-5.60	1.18	1.24
1	B	242	ILE	C-O	-5.57	1.18	1.24
1	B	217	GLY	C-O	-5.50	1.19	1.24
1	B	91	ASN	C-O	-5.49	1.17	1.24
1	A	260	PRO	C-O	-5.45	1.20	1.25
1	B	71	ASP	C-O	-5.38	1.17	1.24
1	B	73	ILE	C-O	-5.37	1.18	1.24
1	A	215	HIS	C-N	-5.34	1.26	1.33
1	A	328	SER	C-O	-5.26	1.17	1.23
1	B	25	THR	C-O	-5.23	1.17	1.24
1	B	72	PHE	C-O	-5.23	1.17	1.24
1	B	271	ILE	C-O	-5.23	1.18	1.24
1	A	371	ARG	C-O	-5.16	1.18	1.24
1	A	89	SER	C-O	-5.15	1.18	1.24
1	A	350	VAL	C-O	-5.12	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	90	LEU	C-O	-5.10	1.18	1.24
1	B	215	HIS	C-O	-5.01	1.17	1.24
1	A	374	PHE	C-O	-5.01	1.17	1.23

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	GLU	N-CA-C	9.42	125.23	112.90
1	B	247	ILE	N-CA-C	9.16	123.27	108.99
1	A	247	ILE	N-CA-C	8.62	121.20	108.96
1	B	113	GLU	N-CA-C	8.52	121.32	110.24
1	A	374	PHE	N-CA-C	8.42	122.69	109.81
1	A	49	ARG	N-CA-C	8.14	121.77	108.26
1	A	208	ASP	N-CA-C	-7.67	103.53	113.12
1	A	3	ILE	C-N-CD	7.49	137.08	120.60
1	A	248	GLU	N-CA-C	-7.35	103.16	112.93
1	A	5	GLU	N-CA-C	7.26	119.19	111.28
1	A	155	ALA	N-CA-C	7.13	120.56	110.23
1	B	3	ILE	C-N-CD	7.08	136.18	120.60
1	B	53	ARG	N-CA-C	6.83	118.72	111.28
1	A	113	GLU	N-CA-C	6.74	120.00	110.23
1	A	53	ARG	N-CA-C	6.65	118.53	111.28
1	A	259	GLU	CA-C-N	-6.56	114.87	119.66
1	A	259	GLU	C-N-CA	-6.56	114.87	119.66
1	A	181	LYS	N-CA-C	-6.32	104.01	111.03
1	B	114	HIS	N-CA-C	-6.30	102.21	110.53
1	A	385	THR	CB-CA-C	6.25	121.48	110.85
1	B	208	ASP	N-CA-C	-6.12	105.47	113.12
1	A	114	HIS	N-CA-C	-6.12	101.87	110.50
1	B	242	ILE	N-CA-C	6.10	117.48	108.45
1	B	18	ILE	N-CA-C	-6.06	98.40	107.37
1	A	354	HIS	N-CA-C	5.91	120.49	113.28
1	B	248	GLU	N-CA-C	-5.88	105.77	113.12
1	A	173	VAL	N-CA-C	5.83	117.27	110.62
1	A	200	VAL	CB-CA-C	5.71	116.92	110.41
1	B	110	THR	CA-C-N	-5.58	114.52	121.00
1	B	110	THR	C-N-CA	-5.58	114.52	121.00
1	B	374	PHE	N-CA-C	5.56	118.31	109.81
1	B	73	ILE	N-CA-CB	-5.54	106.11	112.21
1	A	110	THR	CA-C-N	-5.51	114.61	121.00
1	A	110	THR	C-N-CA	-5.51	114.61	121.00
1	A	327	VAL	CB-CA-C	5.50	118.14	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	LYS	N-CA-C	5.44	117.96	108.76
1	B	119	LEU	CA-C-N	-5.44	113.02	119.05
1	B	119	LEU	C-N-CA	-5.44	113.02	119.05
1	B	254	GLY	N-CA-C	5.42	118.44	110.80
1	A	259	GLU	N-CA-C	5.40	117.59	110.36
1	B	50	GLY	N-CA-C	-5.37	105.75	111.93
1	A	220	GLY	CA-C-N	-5.35	115.25	120.98
1	A	220	GLY	C-N-CA	-5.35	115.25	120.98
1	A	27	LEU	N-CA-C	-5.34	101.83	110.32
1	B	49	ARG	N-CA-C	5.30	122.10	110.80
1	A	73	ILE	N-CA-C	5.30	117.28	111.77
1	A	342	ILE	N-CA-CB	5.28	118.50	110.58
1	A	146	SER	N-CA-C	-5.28	105.61	111.36
1	B	23	THR	N-CA-CB	5.22	118.90	110.40
1	A	18	ILE	N-CA-C	-5.21	99.75	107.51
1	B	162	HIS	N-CA-C	-5.14	105.13	111.40

There are no chirality outliers.

There are no planarity outliers.

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	3088	0	3067	94	0
1	B	3130	0	3140	45	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	134	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 11.

All (134) 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:A:28:THR:CG2	1:B:44:ARG:HE	1.93	0.81
1:B:375:HIS:CD2	1:B:376:VAL:H	1.98	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:390:MET:HA	1:A:390:MET:HE2	1.70	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:343:LEU:HD11	1:B:390:MET:HE3	1.74	0.69
1:B:23:THR:HG23	1:B:373:SER:CB	2.23	0.69
1:A:252:LEU:HD22	1:A:252:LEU:N	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:HH11	1:B:49:ARG:HG3	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
1:B:390:MET:HA	1:B:390:MET:HE2	1.76	0.65
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:49:ARG:HG3	1:B:49:ARG:NH1	2.12	0.63
1:B:106:LYS:HD3	1:B:108:VAL:HG12	1.80	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
1:A:76:LYS:O	1:A:77:PHE:C	2.43	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:343:LEU:CD1	1:A:390:MET:HE3	2.33	0.59
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:119:LEU:HB3	1:B:242:ILE:HG23	1.86	0.58
1:A:147:ASP:HA	1:A:150:LYS:HE3	1.85	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:B:78:GLU:H	1:B:78:GLU:CD	2.12	0.58
2:A:400:PLP:HO3	3:A:401:ALA:N	2.01	0.57
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: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:343:LEU:CD1	1:B:390:MET:HE3	2.38	0.53
1:B:174:GLU:HG3	1:B:204:LYS:O	2.09	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:23:THR:CG2	1:A:373:SER:HB3	2.40	0.52
1:A:101:PHE:HB2	1:A:128:LEU:HD23	1.90	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
1:A:252:LEU:N	1:A:252:LEU:CD2	2.72	0.51
1:A:53:ARG:NH2	1:B:347:SER:OG	2.44	0.51
1:A:396:GLY:C	1:A:398:LYS:H	2.18	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:247:ILE:HD12	1:A:247:ILE:C	2.37	0.50
1:A:258:THR:OG1	1:A:259:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:343:LEU:HD11	1:A:390:MET:HE3	1.95	0.47
1:B:343:LEU:HD23	1:B:350:VAL:HG11	1.97	0.47
1:A:23:THR:CG2	1:A:373:SER:HB2	2.45	0.47
1:A:28:THR:HG23	1:B:44:ARG:HE	1.76	0.47
1:A:157:LEU:HD12	1:A:186:ILE:CD1	2.37	0.47
1:A:252:LEU:CD2	1:A:252:LEU:H	2.26	0.47
1:A:343:LEU:HD13	1:A:390:MET:HE3	1.95	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: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: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: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:38:GLU:CG	1:A:43:TYR:HE1	2.28	0.43
1:A:102:LYS:HD3	1:A:102:LYS:HA	1.73	0.43
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:HA	1:B:295:GLN:HE21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:357:ALA:C	1:A:359:PRO:HD2	2.46	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

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	394/419 (94%)	384 (98%)	9 (2%)	1 (0%)	36	44
1	B	398/419 (95%)	387 (97%)	10 (2%)	1 (0%)	36	44
All	All	792/838 (94%)	771 (97%)	19 (2%)	2 (0%)	36	44

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%)	277 (85%)	49 (15%)	3	2
1	B	333/350 (95%)	279 (84%)	54 (16%)	2	2
All	All	659/700 (94%)	556 (84%)	103 (16%)	2	2

All (103) 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	25	THR
1	A	28	THR
1	A	33	VAL
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	128	LEU
1	A	131	LYS
1	A	135	ILE
1	A	146	SER
1	A	151	LYS
1	A	163	VAL
1	A	175	GLU
1	A	176	LEU
1	A	178	LYS
1	A	186	ILE

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Mol	Chain	Res	Type
1	A	188	VAL
1	A	199	GLU
1	A	200	VAL
1	A	204	LYS
1	A	246	THR
1	A	252	LEU
1	A	260	PRO
1	A	304	THR
1	A	311	GLU
1	A	322	LYS
1	A	326	VAL
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	389	VAL
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	33	VAL
1	B	48	HIS
1	B	49	ARG
1	B	54	LEU
1	B	73	ILE
1	B	78	GLU
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	108	VAL
1	B	110	THR
1	B	127	LYS

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Mol	Chain	Res	Type
1	B	130	LEU
1	B	131	LYS
1	B	135	ILE
1	B	153	LYS
1	B	156	LYS
1	B	163	VAL
1	B	173	VAL
1	B	186	ILE
1	B	188	VAL
1	B	200	VAL
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	370	VAL
1	B	380	LEU
1	B	385	THR
1	B	389	VAL
1	B	393	LEU
1	B	394	VAL
1	B	398	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	48	HIS
1	A	114	HIS
1	A	161	GLN

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Mol	Chain	Res	Type
1	A	171	HIS
1	A	206	HIS
1	A	295	GLN
1	A	297	HIS
1	A	323	HIS
1	A	335	HIS
1	A	354	HIS
1	A	375	HIS
1	B	91	ASN
1	B	114	HIS
1	B	142	ASN
1	B	171	HIS
1	B	206	HIS
1	B	295	GLN
1	B	323	HIS
1	B	355	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%)	2,6,8	0.67	0
1	CSS	A	356	1	4,6,7	1.07	0	2,6,8	1.79	1 (50%)

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	-2.15	1.74	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	CSS	CB-CA-C	2.52	117.64	110.80

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 oligosaccharides 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
3	ALA	A	401	2	5,5,5	3.35	2 (40%)	6,6,6	1.56	2 (33%)
2	PLP	B	400	1,3	15,15,16	1.69	1 (6%)	21,22,23	1.66	4 (19%)
2	PLP	A	400	1,3	15,15,16	2.03	5 (33%)	21,22,23	2.13	8 (38%)
3	ALA	B	401	2	5,5,5	3.14	1 (20%)	6,6,6	1.72	2 (33%)

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	ALA	A	401	2	-	0/4/4/4	-
2	PLP	B	400	1,3	-	0/6/6/8	0/1/1/1
2	PLP	A	400	1,3	-	0/6/6/8	0/1/1/1
3	ALA	B	401	2	-	3/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ALA	OXT-C	-6.86	1.08	1.30
3	A	401	ALA	O-C	5.79	1.39	1.22
2	B	400	PLP	C5-C4	-5.56	1.34	1.40
2	A	400	PLP	C4A-C4	4.49	1.60	1.51
3	A	401	ALA	OXT-C	-4.33	1.16	1.30
2	A	400	PLP	C3-C2	3.26	1.44	1.41
2	A	400	PLP	O3-C3	3.19	1.44	1.36
2	A	400	PLP	P-O2P	-2.38	1.46	1.54
2	A	400	PLP	C3-C4	-2.29	1.35	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	PLP	C4A-C4-C5	4.54	125.62	120.94
2	A	400	PLP	O3-C3-C2	4.41	126.73	117.58
2	A	400	PLP	O3P-P-O4P	3.59	116.02	106.67
2	A	400	PLP	C4A-C4-C5	3.50	124.55	120.94
2	A	400	PLP	C4A-C4-C3	-2.77	115.90	120.52
2	A	400	PLP	C2A-C2-N1	-2.68	112.59	117.64
2	A	400	PLP	C3-C2-N1	2.66	124.32	120.96
3	B	401	ALA	C-CA-N	2.52	116.82	107.93
3	A	401	ALA	OXT-C-CA	2.48	122.32	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	ALA	OXT-C-O	-2.45	118.52	124.08
2	A	400	PLP	O3P-P-O2P	-2.35	99.00	107.80
2	B	400	PLP	C5A-C5-C4	-2.33	118.03	122.64
3	A	401	ALA	O-C-CA	-2.12	115.53	122.07
2	B	400	PLP	O3-C3-C2	2.11	121.95	117.58
2	A	400	PLP	C6-C5-C4	2.09	119.81	118.10
2	B	400	PLP	C5A-C5-C6	2.00	122.62	119.36

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	ALA	OXT-C-CA-CB
3	B	401	ALA	O-C-CA-CB
3	B	401	ALA	OXT-C-CA-N

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ALA	1	0
2	B	400	PLP	1	0
2	A	400	PLP	1	0
3	B	401	ALA	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 [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%)	0.15	6 (1%) 72 73	25, 41, 67, 108	0
1	B	400/419 (95%)	0.02	6 (1%) 72 73	23, 39, 63, 101	0
All	All	796/838 (94%)	0.08	12 (1%) 72 73	23, 40, 66, 108	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	397	LEU	6.0
1	A	48	HIS	3.9
1	B	48	HIS	3.9
1	A	252	LEU	3.8
1	A	398	LYS	3.1
1	B	-2	MET	3.0
1	B	398	LYS	2.9
1	A	49	ARG	2.1
1	A	186	ILE	2.1
1	A	135	ILE	2.1
1	B	73	ILE	2.1
1	B	357	ALA	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(Å ²)	Q<0.9
1	CSS	B	356	7/8	0.88	0.12	36,46,54,55	0
1	CSS	A	356	7/8	0.92	0.11	35,35,40,40	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	ALA	B	401	6/6	0.90	0.15	51,56,58,63	0
3	ALA	A	401	6/6	0.93	0.10	39,47,49,52	0
2	PLP	A	400	15/16	0.97	0.06	24,29,44,44	0
2	PLP	B	400	15/16	0.98	0.06	24,30,37,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.