



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:02 PM UTC

PDB ID : 5B7U / pdb_00005b7u
Title : Apo Structure of Cysteine Desulfurase from Thermococcus onnurineus NA1 at 1.89Å
Authors : Ho, T.-H.; Kang, L.-W.
Deposited on : 2016-06-09
Resolution : 1.90 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

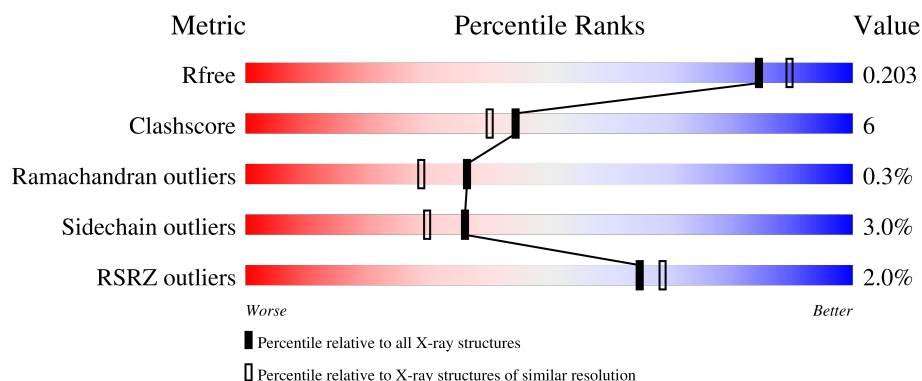
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	2% 72% 22% • •
1	B	419	2% 72% 21% • 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6556 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	402	Total	C	N	O	P	S	0	0	0
			3150	2005	545	588	1	11			
1	B	400	Total	C	N	O	P	S	0	0	0
			3136	1997	541	586	1	11			

There are 40 discrepancies between the modelled and reference sequences:

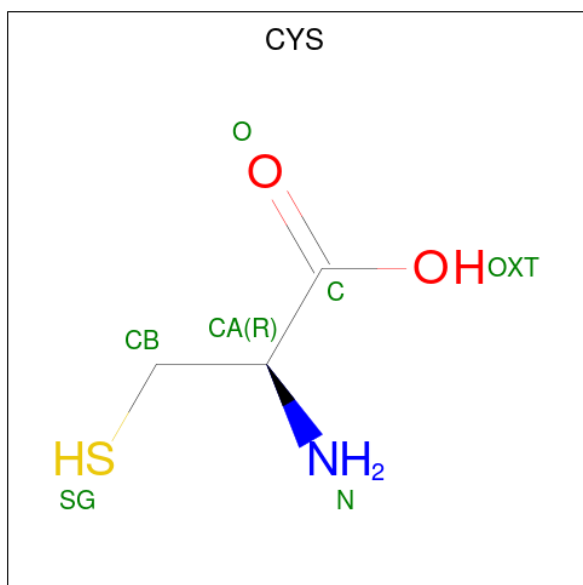
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP B6YT87
A	-18	HIS	-	expression tag	UNP B6YT87
A	-17	HIS	-	expression tag	UNP B6YT87
A	-16	HIS	-	expression tag	UNP B6YT87
A	-15	HIS	-	expression tag	UNP B6YT87
A	-14	HIS	-	expression tag	UNP B6YT87
A	-13	HIS	-	expression tag	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 CYSTEINE (CCD ID: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

- Molecule 3 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		

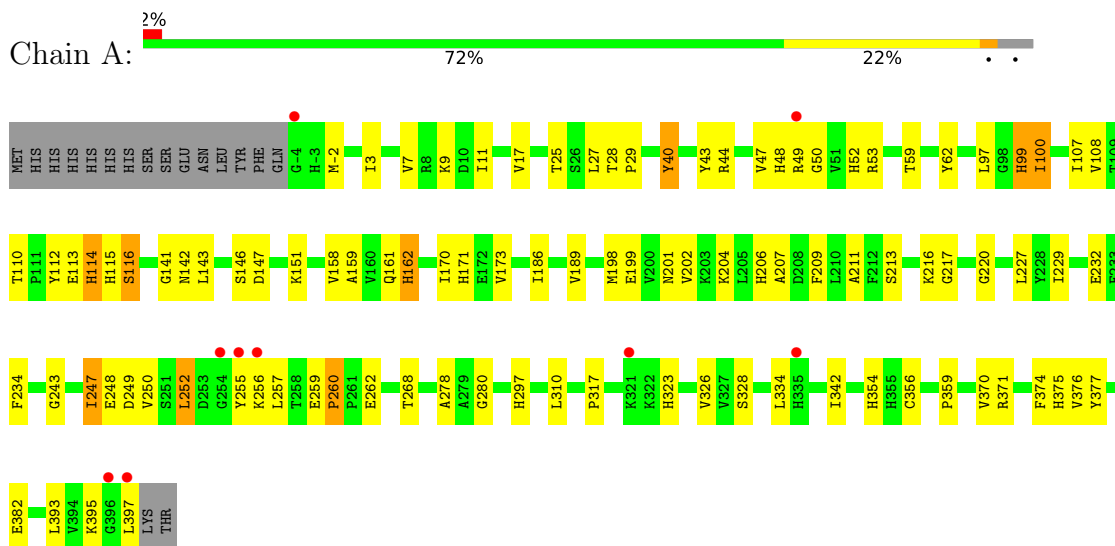
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	159	Total	O	0	0
			159	159		
4	B	100	Total	O	0	0
			100	100		

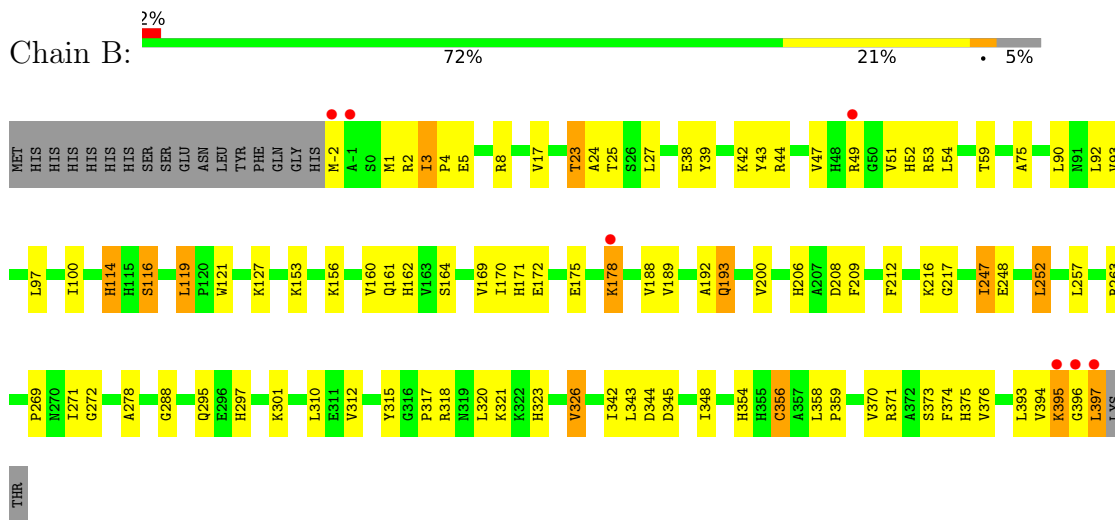
3 Residue-property plots [i](#)

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	78.49Å 62.79Å 171.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.18 – 1.90 46.18 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.18-1.90) 97.1 (46.18-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.23 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.166 , 0.203 0.172 , 0.203	Depositor DCC
R_{free} test set	3326 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6556	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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, IPA, LLP

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	1.69	49/3185 (1.5%)	1.19	21/4303 (0.5%)
1	B	1.63	45/3170 (1.4%)	1.19	18/4283 (0.4%)
All	All	1.66	94/6355 (1.5%)	1.19	39/8586 (0.5%)

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	GLY	C-O	8.16	1.29	1.23
1	A	189	VAL	C-O	-7.87	1.15	1.24
1	B	358	LEU	C-O	-7.70	1.17	1.24
1	A	107	ILE	C-O	-7.69	1.16	1.24
1	B	54	LEU	C-O	-7.56	1.15	1.24
1	A	17	VAL	C-O	-7.41	1.15	1.23
1	B	24	ALA	C-O	-7.03	1.15	1.24
1	B	209	PHE	C-O	-7.01	1.15	1.23
1	A	209	PHE	C-O	-6.96	1.15	1.23
1	B	189	VAL	C-O	-6.89	1.16	1.24
1	B	121	TRP	C-O	-6.86	1.16	1.24
1	A	7	VAL	C-O	-6.83	1.16	1.24
1	A	43	TYR	C-O	-6.65	1.18	1.24
1	B	43	TYR	C-O	-6.65	1.16	1.24
1	B	44	ARG	C-O	-6.63	1.16	1.24
1	B	271	ILE	C-O	-6.59	1.16	1.24
1	A	201	ASN	C-O	-6.50	1.16	1.24
1	A	29	PRO	C-O	-6.50	1.16	1.23
1	A	44	ARG	C-O	-6.46	1.16	1.24
1	A	278	ALA	C-O	-6.31	1.16	1.24
1	A	159	ALA	C-O	-6.28	1.17	1.24
1	B	348	ILE	N-CA	-6.24	1.38	1.46
1	B	38	GLU	C-O	-6.23	1.16	1.24
1	B	326	VAL	C-O	-6.13	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	VAL	C-O	-6.12	1.17	1.24
1	B	192	ALA	C-O	-6.09	1.17	1.24
1	A	262	GLU	C-O	-6.04	1.16	1.24
1	A	377	TYR	C-O	-6.02	1.16	1.24
1	B	17	VAL	C-O	-5.92	1.17	1.23
1	A	213	SER	C-O	-5.91	1.16	1.24
1	A	-2	MET	C-O	-5.85	1.16	1.23
1	B	344	ASP	C-O	-5.84	1.17	1.24
1	B	318	ARG	C-O	-5.76	1.16	1.24
1	B	263	ARG	C-O	-5.75	1.17	1.24
1	B	92	LEU	C-O	-5.71	1.17	1.24
1	B	160	VAL	C-O	-5.71	1.18	1.23
1	B	315	TYR	C-O	-5.69	1.16	1.23
1	B	75	ALA	C-O	-5.67	1.16	1.23
1	A	229	ILE	C-O	-5.66	1.17	1.24
1	B	52	HIS	C-O	-5.64	1.16	1.23
1	A	52	HIS	C-O	-5.61	1.16	1.23
1	A	247	ILE	C-O	-5.61	1.17	1.23
1	B	321	LYS	C-O	-5.58	1.16	1.24
1	B	39	TYR	C-O	-5.58	1.17	1.24
1	B	371	ARG	C-O	-5.58	1.17	1.23
1	A	99	HIS	C-O	-5.56	1.16	1.24
1	B	212	PHE	C-O	-5.56	1.16	1.23
1	A	259	GLU	C-N	5.55	1.40	1.33
1	A	280	GLY	C-O	-5.55	1.17	1.23
1	A	211	ALA	C-O	-5.54	1.16	1.23
1	A	147	ASP	C-O	-5.52	1.17	1.24
1	A	158	VAL	C-O	-5.46	1.18	1.24
1	A	199	GLU	C-O	-5.46	1.17	1.23
1	A	207	ALA	C-O	-5.43	1.17	1.23
1	B	394	VAL	C-O	-5.42	1.17	1.24
1	A	110	THR	C-O	-5.42	1.17	1.23
1	A	62	TYR	C-O	-5.39	1.18	1.24
1	B	343	LEU	C-O	-5.38	1.17	1.24
1	A	143	LEU	C-O	-5.37	1.17	1.23
1	A	142	ASN	C-O	-5.34	1.17	1.24
1	A	170	ILE	C-O	-5.34	1.18	1.24
1	B	116	SER	C-O	-5.34	1.17	1.24
1	B	51	VAL	C-O	-5.32	1.18	1.24
1	A	28	THR	C-O	-5.30	1.18	1.24
1	A	100	ILE	C-O	-5.29	1.17	1.24
1	A	186	ILE	C-O	-5.28	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	LYS	C-O	-5.28	1.17	1.24
1	B	272	GLY	C-O	5.27	1.30	1.23
1	A	162	HIS	C-O	-5.27	1.17	1.24
1	B	278	ALA	C-O	5.26	1.30	1.24
1	B	193	GLN	C-O	-5.23	1.17	1.24
1	B	269	PRO	C-O	-5.21	1.17	1.23
1	A	113	GLU	C-O	-5.21	1.17	1.23
1	A	382	GLU	N-CA	-5.20	1.40	1.46
1	B	301	LYS	C-O	-5.18	1.18	1.24
1	B	27	LEU	C-O	-5.17	1.17	1.23
1	B	188	VAL	C-O	-5.16	1.18	1.24
1	A	115	HIS	C-O	-5.15	1.18	1.24
1	A	268	THR	C-O	-5.15	1.17	1.24
1	B	162	HIS	C-O	-5.14	1.18	1.24
1	A	198	MET	C-O	-5.13	1.18	1.23
1	A	11	ILE	C-O	-5.12	1.18	1.24
1	B	156	LYS	N-CA	-5.12	1.39	1.46
1	B	93	VAL	C-O	5.09	1.29	1.24
1	A	227	LEU	C-O	-5.07	1.18	1.24
1	B	172	GLU	C-O	-5.06	1.17	1.23
1	A	146	SER	C-O	-5.05	1.18	1.24
1	B	170	ILE	C-O	-5.05	1.18	1.24
1	A	9	LYS	C-O	-5.05	1.17	1.24
1	B	119	LEU	C-O	-5.04	1.19	1.24
1	B	90	LEU	C-O	-5.04	1.18	1.24
1	A	151	LYS	C-O	-5.03	1.18	1.24
1	B	200	VAL	C-O	-5.01	1.18	1.24
1	A	40	TYR	C-O	-5.00	1.18	1.24

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	GLU	N-CA-C	8.20	121.25	111.33
1	A	374	PHE	N-CA-C	7.84	121.66	110.14
1	A	260	PRO	C-N-CD	7.10	136.21	120.60
1	B	247	ILE	N-CA-C	6.74	119.50	108.99
1	B	3	ILE	C-N-CD	6.57	135.05	120.60
1	B	374	PHE	N-CA-C	6.51	119.78	109.81
1	B	248	GLU	N-CA-C	-6.49	105.38	113.55
1	B	189	VAL	N-CA-C	6.43	117.12	108.11
1	A	53	ARG	N-CA-C	6.38	119.04	111.33
1	A	27	LEU	N-CA-C	-6.28	102.07	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	ILE	CB-CA-C	-6.25	103.68	110.37
1	A	114	HIS	N-CA-C	-6.13	101.85	110.50
1	B	27	LEU	N-CA-C	-6.00	102.45	110.55
1	A	116	SER	N-CA-C	5.90	118.50	111.71
1	B	53	ARG	N-CA-C	5.87	118.46	111.71
1	A	268	THR	CA-C-N	-5.82	114.62	120.21
1	A	268	THR	C-N-CA	-5.82	114.62	120.21
1	A	52	HIS	N-CA-C	5.75	118.98	110.48
1	A	247	ILE	N-CA-C	5.72	117.91	108.99
1	B	370	VAL	N-CA-C	-5.66	100.27	108.87
1	A	202	VAL	N-CA-C	5.50	116.23	110.62
1	A	50	GLY	N-CA-C	-5.37	105.08	111.36
1	B	396	GLY	N-CA-C	-5.33	100.54	113.18
1	B	114	HIS	N-CA-C	-5.33	102.98	110.50
1	B	312	VAL	CA-C-N	-5.33	114.47	119.85
1	B	312	VAL	C-N-CA	-5.33	114.47	119.85
1	B	320	LEU	N-CA-C	5.32	119.25	112.87
1	B	247	ILE	CB-CA-C	-5.22	103.39	110.90
1	A	220	GLY	CA-C-N	-5.20	115.37	120.52
1	A	220	GLY	C-N-CA	-5.20	115.37	120.52
1	A	370	VAL	N-CA-C	-5.19	100.98	108.71
1	B	42	LYS	N-CA-C	5.17	120.46	114.04
1	A	28	THR	O-C-N	5.11	125.94	121.39
1	B	208	ASP	N-CA-C	-5.11	107.18	113.41
1	A	28	THR	CA-C-N	-5.07	114.73	119.85
1	A	28	THR	C-N-CA	-5.07	114.73	119.85
1	A	110	THR	CA-C-N	-5.01	114.89	120.45
1	A	110	THR	C-N-CA	-5.01	114.89	120.45
1	B	8	ARG	N-CA-C	5.01	117.39	111.33

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	3150	0	3142	40	0
1	B	3136	0	3132	40	0
2	A	7	0	4	2	0
3	A	4	0	8	1	0
4	A	159	0	0	5	1
4	B	100	0	0	2	0
All	All	6556	0	6286	76	1

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 6.

All (76) 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:40:TYR:HH	2:A:401:CYS:N	1.75	0.84
1:A:161:GLN:HE21	1:A:171:HIS:HE1	1.25	0.83
1:B:114:HIS:HD2	1:B:116:SER:H	1.27	0.83
1:B:161:GLN:HE21	1:B:171:HIS:HE1	1.22	0.82
1:A:114:HIS:HD2	1:A:116:SER:H	1.30	0.80
1:A:371:ARG:HH22	3:A:402:IPA:H31	1.49	0.76
1:A:375:HIS:CD2	1:A:376:VAL:H	2.04	0.76
1:A:249:ASP:O	1:A:256:LYS:N	2.19	0.75
1:B:375:HIS:CD2	1:B:376:VAL:H	2.04	0.74
1:A:375:HIS:HD2	1:A:376:VAL:H	1.35	0.73
1:B:375:HIS:HD2	1:B:376:VAL:H	1.39	0.70
1:A:255:TYR:CD1	1:B:119:LEU:HG	2.27	0.69
1:A:252:LEU:HD13	1:B:359:PRO:HB3	1.74	0.69
1:B:161:GLN:HE21	1:B:171:HIS:CE1	2.09	0.68
1:B:23:THR:HG23	1:B:373:SER:CB	2.25	0.65
1:A:114:HIS:CD2	1:A:116:SER:H	2.12	0.64
1:A:161:GLN:HE21	1:A:171:HIS:CE1	2.11	0.64
1:B:178:LYS:HG3	1:B:206:HIS:CE1	2.32	0.64
1:A:317:PRO:O	1:A:323:HIS:HD2	1.81	0.64
1:B:49:ARG:HG2	1:B:59:THR:HG21	1.81	0.62
1:B:247:ILE:C	1:B:247:ILE:HD12	2.24	0.62
1:A:323:HIS:HE1	1:A:326:VAL:O	1.84	0.61
1:A:217:GLY:O	1:A:375:HIS:HE1	1.83	0.61
1:B:23:THR:CG2	1:B:373:SER:CB	2.80	0.60
1:A:112:TYR:CZ	1:A:141:GLY:HA2	2.38	0.59
1:B:317:PRO:O	1:B:323:HIS:HD2	1.86	0.58
1:A:359:PRO:HB3	1:B:252:LEU:HD13	1.85	0.58
1:A:247:ILE:C	1:A:247:ILE:HD12	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:LYS:O	1:B:397:LEU:N	2.36	0.57
1:B:323:HIS:HE1	1:B:326:VAL:O	1.87	0.56
1:B:114:HIS:CD2	1:B:116:SER:H	2.14	0.56
1:B:354:HIS:HD2	1:B:356:CSS:N	2.04	0.55
1:B:247:ILE:HD12	1:B:247:ILE:O	2.08	0.54
1:B:23:THR:HG23	1:B:373:SER:OG	2.08	0.53
1:A:114:HIS:HD2	1:A:116:SER:N	2.04	0.52
1:A:255:TYR:HE2	1:A:257:LEU:HD13	1.74	0.52
1:B:161:GLN:HE22	1:B:164:SER:HB2	1.75	0.52
1:B:161:GLN:NE2	1:B:164:SER:HB2	2.24	0.52
1:B:175:GLU:HA	1:B:178:LYS:HE3	1.92	0.51
1:B:217:GLY:O	1:B:375:HIS:HE1	1.93	0.51
1:B:97:LEU:O	1:B:100:ILE:HG12	2.11	0.51
1:A:354:HIS:HD2	1:A:356:CSS:N	2.08	0.51
1:A:342:ILE:HD13	1:A:393:LEU:CD2	2.42	0.50
1:A:206:HIS:HE1	4:A:647:HOH:O	1.95	0.50
1:B:171:HIS:HD2	4:B:438:HOH:O	1.95	0.50
1:A:250:VAL:HG22	1:A:255:TYR:HB2	1.94	0.49
1:B:395:LYS:C	1:B:397:LEU:N	2.70	0.49
1:B:23:THR:HB	1:B:193:GLN:NE2	2.28	0.49
1:A:255:TYR:CE2	1:A:257:LEU:HD13	2.48	0.48
1:A:250:VAL:HA	1:A:255:TYR:HA	1.95	0.48
1:A:171:HIS:HD2	4:A:574:HOH:O	1.95	0.48
1:A:395:LYS:C	1:A:397:LEU:H	2.22	0.48
1:B:23:THR:HG21	1:B:326:VAL:HG22	1.96	0.47
1:A:234:PHE:CD2	1:A:260:PRO:HG2	2.50	0.47
1:A:342:ILE:HD13	1:A:393:LEU:HD23	1.96	0.46
1:A:97:LEU:O	1:A:100:ILE:HG12	2.16	0.46
1:A:323:HIS:CE1	1:A:326:VAL:O	2.68	0.46
1:B:23:THR:CG2	1:B:373:SER:HB2	2.46	0.46
1:A:49:ARG:HG2	1:A:59:THR:HG21	1.98	0.46
1:B:23:THR:HG22	1:B:373:SER:HB2	1.96	0.45
1:B:3:ILE:HA	1:B:4:PRO:HA	1.75	0.45
1:A:40:TYR:OH	2:A:401:CYS:N	2.45	0.43
1:A:99:HIS:HD2	4:A:563:HOH:O	2.02	0.43
1:B:342:ILE:O	1:B:345:ASP:HB2	2.18	0.42
1:A:247:ILE:HD12	1:A:247:ILE:O	2.18	0.42
1:A:48:HIS:CE1	4:A:556:HOH:O	2.72	0.42
1:A:248:GLU:N	1:A:256:LYS:O	2.36	0.42
1:B:-2:MET:HE2	1:B:288:GLY:HA3	2.02	0.42
1:A:297:HIS:HD2	4:A:589:HOH:O	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ILE:C	1:B:247:ILE:CD1	2.90	0.41
1:B:295:GLN:HE21	1:B:295:GLN:HA	1.85	0.41
1:B:323:HIS:CE1	1:B:326:VAL:O	2.72	0.41
1:A:162:HIS:HA	1:A:173:VAL:HG21	2.03	0.41
1:B:164:SER:HB3	1:B:169:VAL:HG12	2.03	0.41
1:B:297:HIS:HD2	4:B:439:HOH:O	2.03	0.41
1:A:255:TYR:CG	1:B:119:LEU:HG	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:604:HOH:O	4:A:616:HOH:O[3_655]	1.77	0.43

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	398/419 (95%)	391 (98%)	6 (2%)	1 (0%)	36	29
1	B	396/419 (94%)	389 (98%)	6 (2%)	1 (0%)	36	29
All	All	794/838 (95%)	780 (98%)	12 (2%)	2 (0%)	36	29

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	332/349 (95%)	326 (98%)	6 (2%)	51	50
1	B	331/349 (95%)	318 (96%)	13 (4%)	28	21
All	All	663/698 (95%)	644 (97%)	19 (3%)	36	31

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	THR
1	A	232	GLU
1	A	252	LEU
1	A	310	LEU
1	A	328	SER
1	A	334	LEU
1	B	1	MET
1	B	2	ARG
1	B	23	THR
1	B	25	THR
1	B	127	LYS
1	B	153	LYS
1	B	178	LYS
1	B	252	LEU
1	B	257	LEU
1	B	310	LEU
1	B	393	LEU
1	B	395	LYS
1	B	397	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
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	193	GLN
1	A	206	HIS
1	A	295	GLN
1	A	297	HIS
1	A	323	HIS
1	A	330	ASN
1	A	354	HIS
1	A	367	ASN
1	A	375	HIS
1	B	15	ASN
1	B	114	HIS
1	B	161	GLN
1	B	171	HIS
1	B	206	HIS
1	B	295	GLN
1	B	297	HIS
1	B	323	HIS
1	B	330	ASN
1	B	346	HIS
1	B	354	HIS
1	B	367	ASN
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 ⓘ

4 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	1.00	0	2,6,8	1.44	1 (50%)
1	LLP	B	216	1	23,24,25	2.30	8 (34%)	25,32,34	1.74	5 (20%)
1	LLP	A	216	1	23,24,25	2.55	8 (34%)	25,32,34	1.71	5 (20%)
1	CSS	A	356	1	4,6,7	1.04	0	2,6,8	1.48	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	LLP	B	216	1	-	4/16/17/19	0/1/1/1
1	LLP	A	216	1	-	3/16/17/19	0/1/1/1
1	CSS	A	356	1	-	0/1/5/7	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	LLP	C3-C2	6.83	1.48	1.41
1	B	216	LLP	C3-C2	5.37	1.46	1.41
1	A	216	LLP	C4-C3	4.29	1.48	1.41
1	B	216	LLP	P-OP2	-4.28	1.38	1.54
1	A	216	LLP	P-OP3	-3.98	1.40	1.54
1	B	216	LLP	C4'-NZ	3.93	1.40	1.27
1	A	216	LLP	P-OP2	-3.72	1.41	1.54
1	A	216	LLP	C4'-NZ	3.68	1.39	1.27
1	B	216	LLP	C4-C3	3.56	1.47	1.41
1	A	216	LLP	P-OP1	-3.43	1.39	1.50
1	A	216	LLP	O3-C3	-3.37	1.29	1.36
1	B	216	LLP	C4-C5	3.03	1.46	1.42
1	B	216	LLP	P-OP1	-2.94	1.41	1.50
1	B	216	LLP	P-OP3	-2.88	1.44	1.54
1	B	216	LLP	O3-C3	-2.71	1.30	1.36
1	A	216	LLP	C4-C5	2.05	1.44	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	LLP	C4-C3-C2	-5.67	116.95	120.14
1	A	216	LLP	C4-C3-C2	-4.40	117.67	120.14
1	B	216	LLP	O3-C3-C2	3.27	124.37	117.58
1	B	216	LLP	C6-N1-C2	3.11	124.84	119.20
1	A	216	LLP	C6-N1-C2	3.07	124.77	119.20
1	A	216	LLP	OP4-C5'-C5	2.79	114.58	109.36
1	B	216	LLP	OP4-C5'-C5	2.41	113.87	109.36
1	B	216	LLP	C4-C4'-NZ	-2.19	113.91	124.04
1	A	216	LLP	C4-C4'-NZ	-2.15	114.10	124.04
1	A	216	LLP	OP3-P-OP2	2.07	115.56	107.80
1	B	356	CSS	CB-CA-C	2.03	116.33	110.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	216	LLP	O-C-CA-CB
1	B	216	LLP	O-C-CA-CB
1	A	216	LLP	C4-C4'-NZ-CE
1	B	216	LLP	C4-C4'-NZ-CE
1	A	216	LLP	C3-C4-C4'-NZ
1	B	216	LLP	CG-CD-CE-NZ
1	B	216	LLP	C3-C4-C4'-NZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	356	CSS	1	0
1	A	356	CSS	1	0

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	CYS	A	401	-	5,6,6	1.14	1 (20%)	3,7,7	2.35	2 (66%)
3	IPA	A	402	-	3,3,3	0.60	0	3,3,3	0.49	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
2	CYS	A	401	-	-	4/6/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	CYS	O-C	2.00	1.28	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	CYS	CB-CA-C	-3.08	106.83	109.89
2	A	401	CYS	CA-CB-SG	-2.66	108.71	114.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	CYS	O-C-CA-N
2	A	401	CYS	N-CA-CB-SG
2	A	401	CYS	C-CA-CB-SG
2	A	401	CYS	OXT-C-CA-N

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	CYS	2	0
3	A	402	IPA	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	400/419 (95%)	-0.09	9 (2%) 61 65	12, 20, 34, 63	0
1	B	398/419 (94%)	0.16	7 (1%) 67 71	12, 24, 41, 67	0
All	All	798/838 (95%)	0.04	16 (2%) 65 69	12, 22, 38, 67	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	397	LEU	7.0
1	B	397	LEU	7.0
1	A	256	LYS	5.3
1	A	255	TYR	5.1
1	B	396	GLY	4.2
1	B	-1	ALA	4.0
1	B	-2	MET	3.8
1	A	254	GLY	3.6
1	B	178	LYS	2.6
1	A	49	ARG	2.3
1	A	-4	GLY	2.3
1	A	321	LYS	2.2
1	A	396	GLY	2.2
1	A	335	HIS	2.2
1	B	395	LYS	2.1
1	B	49	ARG	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($\text{\AA}^2$)	Q<0.9
1	CSS	A	356	7/8	0.90	0.09	19,21,32,34	0
1	CSS	B	356	7/8	0.94	0.08	18,21,26,33	0
1	LLP	B	216	24/25	0.97	0.06	13,17,24,26	0
1	LLP	A	216	24/25	0.98	0.06	12,16,22,25	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
2	CYS	A	401	7/7	0.83	0.14	34,44,58,58	0
3	IPA	A	402	4/4	0.87	0.20	34,36,36,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.