



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:42 AM UTC

PDB ID : 1GKM / pdb_00001gkm
Title : HISTIDINE AMMONIA-LYASE (HAL) FROM PSEUDOMONAS PUTIDA
INHIBITED WITH L-CYSTEINE
Authors : Baedeker, M.; Schulz, G.E.
Deposited on : 2001-08-16
Resolution : 1.00 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

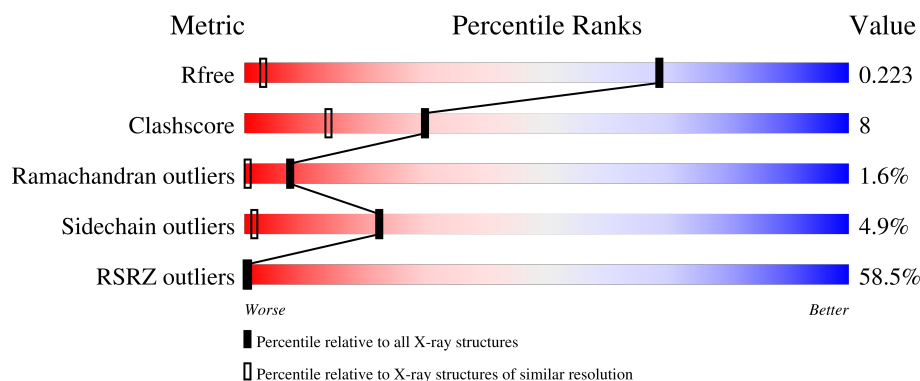
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.00 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	1358 (1.04-0.96)
Clashscore	190562	1411 (1.04-0.96)
Ramachandran outliers	187476	1347 (1.04-0.96)
Sidechain outliers	187428	1348 (1.04-0.96)
RSRZ outliers	180081	1355 (1.04-0.96)

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	B	507	

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	CYS	B	601	X	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4360 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.

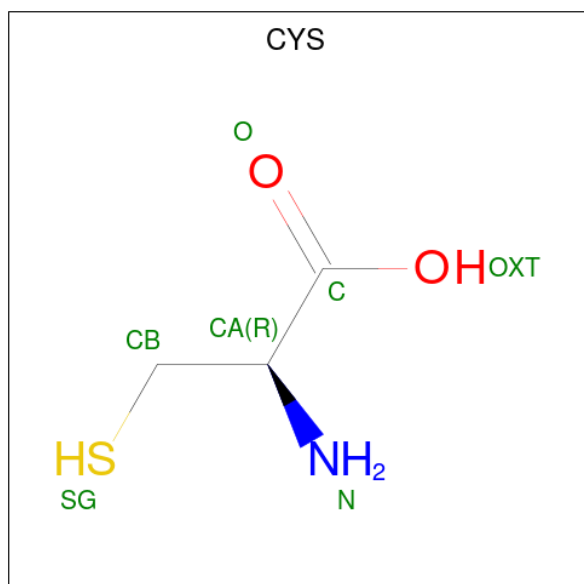
- Molecule 1 is a protein called Histidine ammonia-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	507	3797	2376	674	729	18	0	12	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ALA	deletion	UNP P21310
B	?	-	SER	deletion	UNP P21310
B	142	ZRF	GLY	conflict	UNP P21310
B	271	ALA	CYS	conflict	UNP P21310

- Molecule 2 is CYSTEINE (CCD ID: CYS) (formula: C₃H₇NO₂S).



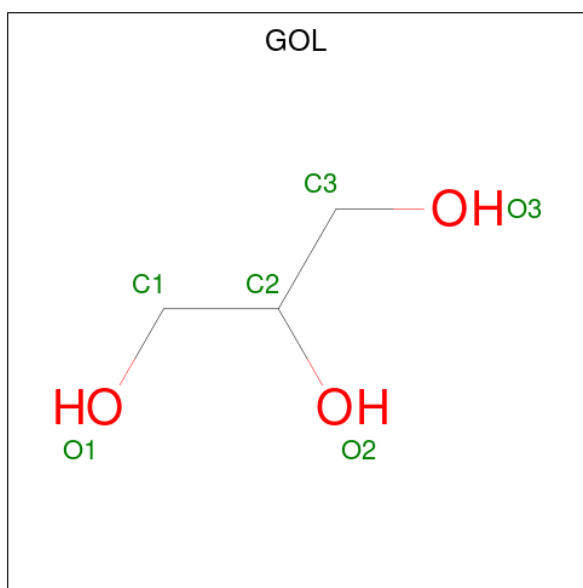
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	B	1	7	3	1	2	1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

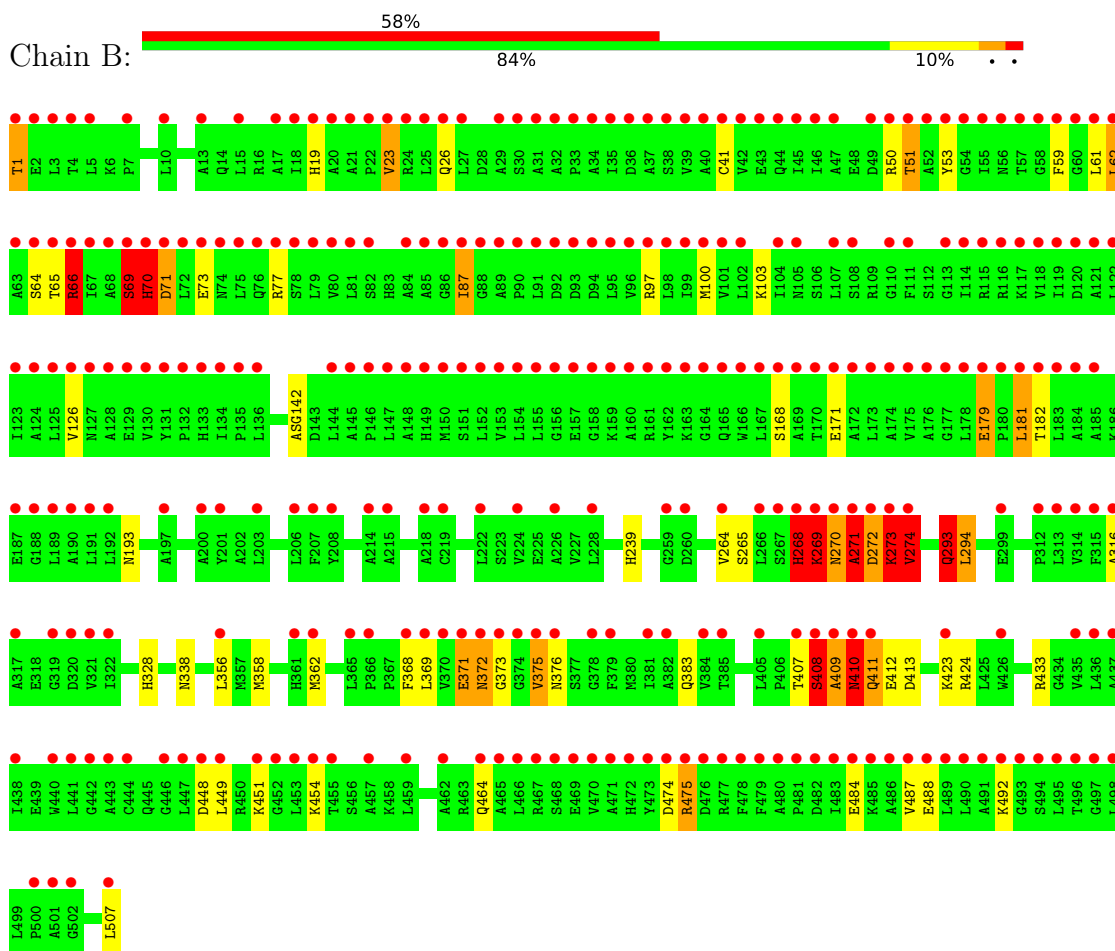
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	545	Total 545	O 545	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 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: Histidine ammonia-lyase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	79.27Å 116.79Å 129.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.00 40.00 – 1.01	Depositor EDS
% Data completeness (in resolution range)	96.0 (40.00-1.00) 95.8 (40.00-1.01)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.01Å)	Xtriage
Refinement program	SHELX	Depositor
R, R_{free}	0.119 , 0.135 0.227 , 0.223	Depositor DCC
R_{free} test set	15248 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	6.9	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 68.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4360	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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: SO4, GOL, ZRF

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	B	1.09	8/3899 (0.2%)	1.42	50/5284 (0.9%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411	GLN	C-O	9.60	1.35	1.24
1	B	507	LEU	C-OXT	9.38	1.42	1.23
1	B	271	ALA	N-CA	9.28	1.58	1.46
1	B	273	LYS	CA-C	6.18	1.61	1.52
1	B	19	HIS	ND1-CE1	5.69	1.38	1.32
1	B	274	VAL	N-CA	5.57	1.54	1.46
1	B	423	LYS	CA-CB	5.38	1.61	1.53
1	B	97	ARG	CZ-NH2	-5.24	1.26	1.33

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	411	GLN	CA-C-O	10.45	131.50	120.42
1	B	293	GLN	OE1-CD-NE2	-9.59	113.01	122.60
1	B	87	ILE	CG1-CB-CG2	-9.25	82.95	110.70
1	B	411	GLN	N-CA-CB	-8.91	96.97	110.16
1	B	411	GLN	N-CA-C	8.72	120.87	111.36
1	B	69	SER	CA-C-O	7.87	131.76	120.51
1	B	66	ARG	CD-NE-CZ	7.84	135.37	124.40
1	B	268	HIS	CG-CD2-NE2	7.82	115.02	107.20
1	B	87	ILE	CA-CB-CG2	7.48	123.22	110.50
1	B	372	ASN	CA-CB-CG	7.48	120.08	112.60
1	B	368	PHE	CA-CB-CG	-7.47	106.33	113.80
1	B	239	HIS	CA-CB-CG	-7.46	106.34	113.80
1	B	274	VAL	CB-CA-C	-7.41	101.36	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	HIS	ND1-CG-CD2	-7.30	98.80	106.10
1	B	53	TYR	CB-CG-CD2	7.23	131.64	120.80
1	B	294	LEU	CB-CA-C	7.21	124.52	110.67
1	B	97	ARG	NE-CZ-NH2	-6.85	113.04	119.20
1	B	274	VAL	CA-C-N	6.80	134.53	121.54
1	B	274	VAL	C-N-CA	6.80	134.53	121.54
1	B	371	GLU	O-C-N	-6.79	115.11	122.85
1	B	372	ASN	CB-CA-C	-6.72	103.21	111.82
1	B	1	THR	CA-CB-OG1	6.53	119.39	109.60
1	B	293	GLN	CG-CD-NE2	6.49	126.13	116.40
1	B	77	ARG	NH1-CZ-NH2	6.33	127.53	119.30
1	B	87	ILE	CB-CG1-CD1	-6.20	100.77	113.80
1	B	70	HIS	N-CA-CB	-6.19	100.03	110.49
1	B	376	ASN	OD1-CG-ND2	-5.97	116.63	122.60
1	B	423	LYS	CB-CG-CD	5.93	124.94	111.30
1	B	59	PHE	CA-CB-CG	-5.87	107.93	113.80
1	B	77	ARG	NE-CZ-NH1	-5.81	115.69	121.50
1	B	70	HIS	CA-C-O	5.71	128.67	120.51
1	B	66	ARG	CA-C-N	-5.69	112.81	120.95
1	B	66	ARG	C-N-CA	-5.69	112.81	120.95
1	B	268	HIS	CA-C-O	5.68	126.18	119.48
1	B	71	ASP	CA-CB-CG	-5.64	106.96	112.60
1	B	411	GLN	CB-CG-CD	5.63	122.17	112.60
1	B	103	LYS	CB-CG-CD	5.61	124.20	111.30
1	B	410	ASN	CA-C-N	-5.61	112.33	120.29
1	B	410	ASN	C-N-CA	-5.61	112.33	120.29
1	B	69	SER	CA-C-N	5.38	131.82	121.54
1	B	69	SER	C-N-CA	5.38	131.82	121.54
1	B	50	ARG	CA-C-N	-5.37	115.42	122.99
1	B	50	ARG	C-N-CA	-5.37	115.42	122.99
1	B	407	THR	CA-CB-OG1	5.35	117.63	109.60
1	B	193	ASN	CA-CB-CG	5.24	117.84	112.60
1	B	407	THR	OG1-CB-CG2	-5.18	98.94	109.30
1	B	328	HIS	ND1-CE1-NE2	5.15	113.55	108.40
1	B	271	ALA	N-CA-CB	5.13	119.16	110.49
1	B	61	LEU	O-C-N	5.03	127.45	122.12
1	B	179	GLU	CB-CG-CD	-5.02	104.07	112.60

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	B	3797	0	3836	65	0
2	B	7	0	3	0	0
3	B	5	0	0	0	0
4	B	6	0	8	0	0
5	B	545	0	0	12	0
All	All	4360	0	3847	65	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 8.

All (65) 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:274:VAL:HG22	1:B:274:VAL:O	1.80	0.81
1:B:268:HIS:ND1	1:B:271:ALA:HB2	1.98	0.78
1:B:1:THR:OG1	1:B:23:VAL:HG23	1.89	0.72
1:B:265:SER:HA	1:B:268:HIS:CD2	2.25	0.72
1:B:265:SER:HA	1:B:268:HIS:NE2	2.05	0.71
1:B:51:THR:HG22	1:B:66:ARG:HH21	1.57	0.70
1:B:362:MET:HG3	5:B:1025:HOH:O	1.92	0.68
1:B:375:VAL:HG13	5:B:711:HOH:O	1.92	0.68
1:B:269:LYS:C	1:B:271:ALA:H	2.02	0.66
1:B:168:SER:OG	1:B:171:GLU:HG3	1.95	0.66
1:B:268:HIS:ND1	1:B:271:ALA:CB	2.59	0.65
1:B:408:SER:OG	1:B:412[B]:GLU:OE1	2.13	0.65
1:B:268:HIS:CG	1:B:271:ALA:HB2	2.34	0.62
1:B:269:LYS:C	1:B:271:ALA:N	2.59	0.60
1:B:411:GLN:HG3	5:B:750:HOH:O	2.02	0.60
1:B:433[B]:ARG:HE	1:B:487:VAL:HG13	1.66	0.60
1:B:62:LEU:HD12	1:B:65:THR:HG21	1.84	0.60
1:B:268:HIS:C	1:B:269:LYS:HG2	2.27	0.60
1:B:51:THR:HG22	1:B:66:ARG:HE	1.68	0.59
1:B:51:THR:CG2	1:B:66:ARG:HH21	2.15	0.59
1:B:488:GLU:OE2	1:B:492:LYS:HE3	2.03	0.59
1:B:274:VAL:CG2	5:B:1073:HOH:O	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:VAL:HG21	5:B:1073:HOH:O	2.04	0.57
1:B:484:GLU:HB3	5:B:1066:HOH:O	2.05	0.55
1:B:268:HIS:CE1	1:B:271:ALA:HB3	2.42	0.54
1:B:69:SER:HG	1:B:70:HIS:CD2	2.24	0.54
1:B:464:GLN:NE2	5:B:709:HOH:O	2.39	0.54
1:B:1:THR:HG23	5:B:888:HOH:O	2.08	0.54
1:B:293:GLN:HE21	1:B:338:ASN:HB3	1.73	0.54
1:B:41[B]:CYS:SG	1:B:316:ALA:HA	2.48	0.53
1:B:373:GLY:HA3	5:B:811:HOH:O	2.09	0.53
1:B:268:HIS:C	1:B:268:HIS:HD1	2.18	0.51
1:B:269:LYS:O	1:B:271:ALA:N	2.44	0.50
1:B:179:GLU:O	1:B:181:LEU:HD23	2.11	0.50
1:B:371:GLU:O	1:B:372:ASN:HB2	2.12	0.49
1:B:474:ASP:OD1	1:B:475:ARG:HG2	2.13	0.49
1:B:409:ALA:O	1:B:411:GLN:N	2.46	0.48
1:B:268:HIS:ND1	1:B:268:HIS:C	2.72	0.48
1:B:408:SER:HG	1:B:412[B]:GLU:CD	2.20	0.48
1:B:87:ILE:HA	1:B:87:ILE:HD13	1.56	0.48
1:B:264:VAL:HG12	5:B:786:HOH:O	2.14	0.48
1:B:26:GLN:HB3	5:B:877:HOH:O	2.14	0.47
1:B:70:HIS:CD2	1:B:70:HIS:H	2.18	0.47
1:B:410:ASN:O	1:B:413:ASP:HB3	2.14	0.46
1:B:449:LEU:HA	1:B:451:LYS:HE3	1.98	0.46
1:B:475:ARG:NH2	5:B:715:HOH:O	2.49	0.45
1:B:71:ASP:OD1	1:B:71:ASP:N	2.47	0.44
1:B:358:MET:HG3	1:B:383:GLN:OE1	2.17	0.44
1:B:408:SER:OG	1:B:412[B]:GLU:CD	2.61	0.43
1:B:448:ASP:O	1:B:451:LYS:HD3	2.18	0.43
1:B:270:ASN:O	1:B:271:ALA:C	2.61	0.43
1:B:100[B]:MET:HE3	1:B:126:VAL:HG22	2.01	0.42
1:B:356:LEU:CD1	1:B:362:MET:HB3	2.49	0.42
1:B:408:SER:O	1:B:409:ALA:C	2.61	0.42
1:B:73:GLU:OE1	1:B:182:THR:HG21	2.20	0.42
1:B:264:VAL:HG23	1:B:454:LYS:O	2.20	0.42
1:B:271:ALA:O	1:B:273:LYS:N	2.53	0.42
1:B:51:THR:HG22	1:B:66:ARG:NH2	2.30	0.41
1:B:87:ILE:HG23	1:B:87:ILE:HD12	0.83	0.41
1:B:181:LEU:HD23	1:B:181:LEU:N	2.34	0.41
1:B:265:SER:O	1:B:268:HIS:CE1	2.73	0.41
1:B:293:GLN:HE21	1:B:338:ASN:CB	2.32	0.41
1:B:69:SER:OG	1:B:70:HIS:NE2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:MET:HE1	1:B:369:LEU:HD12	2.02	0.41
1:B:410:ASN:ND2	1:B:410:ASN:N	2.69	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	B	514/507 (101%)	496 (96%)	10 (2%)	8 (2%)	7 0

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	271	ALA
1	B	272	ASP
1	B	410	ASN
1	B	270	ASN
1	B	273	LYS
1	B	408	SER
1	B	409	ALA
1	B	269	LYS

5.3.2 Protein sidechains [i](#)

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	B	399/387 (103%)	380 (95%)	19 (5%)	23 2

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

Mol	Chain	Res	Type
1	B	23	VAL
1	B	51	THR
1	B	62	LEU
1	B	64	SER
1	B	66	ARG
1	B	69	SER
1	B	70	HIS
1	B	181	LEU
1	B	268	HIS
1	B	269	LYS
1	B	272	ASP
1	B	273	LYS
1	B	274	VAL
1	B	293	GLN
1	B	294	LEU
1	B	375	VAL
1	B	408	SER
1	B	424	ARG
1	B	475	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	193	ASN
1	B	464	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	ZRF	B	142	2,1	12,14,15	1.67	2 (16%)	16,19,21	1.86	3 (18%)

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	ZRF	B	142	2,1	-	2/4/25/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	ZRF	CA2-C2	-3.98	1.44	1.48
1	B	142	ZRF	O1-CB2	-2.60	1.21	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	ZRF	C2-N3-C1	5.26	110.50	108.07
1	B	142	ZRF	O2-C2-CA2	3.14	133.03	131.02
1	B	142	ZRF	C2-CA2-N2	2.07	110.44	108.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	142	ZRF	N2-C1-CA1-CB
1	B	142	ZRF	N3-C1-CA1-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 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	B	601	3,1	5,6,6	2.50	3 (60%)	3,7,7	3.43	2 (66%)
4	GOL	B	603	-	5,5,5	0.91	0	5,5,5	0.64	0
3	SO4	B	602	2	4,4,4	0.49	0	6,6,6	0.78	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	B	601	3,1	1/1/2/2	6/6/6/6	-
4	GOL	B	603	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	CYS	CA-N	3.49	1.66	1.48
2	B	601	CYS	OXT-C	-3.33	1.20	1.30
2	B	601	CYS	CB-CA	-2.36	1.50	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	CYS	CB-CA-C	-4.90	105.01	109.89
2	B	601	CYS	OXT-C-O	-3.16	116.91	124.08

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	601	CYS	CA

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	CYS	O-C-CA-N
2	B	601	CYS	N-CA-CB-SG
2	B	601	CYS	C-CA-CB-SG
2	B	601	CYS	OXT-C-CA-N
2	B	601	CYS	O-C-CA-CB
2	B	601	CYS	OXT-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	B	506/507 (99%)	2.75	296 (58%) 0 0	3, 8, 40, 79	12 (2%)

All (296) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	VAL	18.4
1	B	271	ALA	13.1
1	B	61	LEU	10.4
1	B	270	ASN	9.5
1	B	175	VAL	9.3
1	B	62	LEU	9.1
1	B	268	HIS	8.9
1	B	68	ALA	8.8
1	B	130	VAL	8.3
1	B	409	ALA	8.1
1	B	272	ASP	8.1
1	B	375	VAL	7.9
1	B	67	ILE	7.7
1	B	167	LEU	7.5
1	B	181	LEU	7.5
1	B	178	LEU	7.4
1	B	65	THR	7.4
1	B	63	ALA	7.1
1	B	373	GLY	7.1
1	B	176	ALA	7.0
1	B	408	SER	6.8
1	B	269	LYS	6.8
1	B	172	ALA	6.8
1	B	170	THR	6.8
1	B	370	VAL	6.6
1	B	273	LYS	6.6
1	B	70	HIS	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	69	SER	6.4
1	B	162	TYR	6.4
1	B	60	GLY	6.4
1	B	374	GLY	6.3
1	B	131	TYR	6.2
1	B	166	TRP	6.2
1	B	173	LEU	6.2
1	B	153	VAL	6.1
1	B	470	VAL	6.1
1	B	118	VAL	6.0
1	B	123	ILE	6.0
1	B	168	SER	6.0
1	B	372	ASN	6.0
1	B	177	GLY	5.9
1	B	72	LEU	5.8
1	B	160	ALA	5.8
1	B	1	THR	5.8
1	B	87	ILE	5.7
1	B	126	VAL	5.7
1	B	174	ALA	5.7
1	B	59	PHE	5.7
1	B	164	GLY	5.7
1	B	71	ASP	5.6
1	B	169	ALA	5.6
1	B	489	LEU	5.5
1	B	410	ASN	5.5
1	B	128	ALA	5.5
1	B	152	LEU	5.5
1	B	23	VAL	5.4
1	B	368	PHE	5.4
1	B	182	THR	5.3
1	B	440	TRP	5.2
1	B	475	ARG	5.2
1	B	96	VAL	5.2
1	B	471	ALA	5.2
1	B	66	ARG	5.1
1	B	74	ASN	5.1
1	B	124	ALA	5.1
1	B	155	LEU	5.1
1	B	122	LEU	5.0
1	B	125	LEU	5.0
1	B	51	THR	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	81	LEU	5.0
1	B	154	LEU	5.0
1	B	64	SER	4.9
1	B	474	ASP	4.9
1	B	75	LEU	4.9
1	B	121	ALA	4.9
1	B	134	ILE	4.9
1	B	411	GLN	4.8
1	B	183	LEU	4.8
1	B	179	GLU	4.8
1	B	451	LYS	4.8
1	B	478	PHE	4.7
1	B	487	VAL	4.7
1	B	119	ILE	4.6
1	B	35	ILE	4.6
1	B	3	LEU	4.6
1	B	481	PRO	4.6
1	B	449	LEU	4.5
1	B	473	TYR	4.5
1	B	156	GLY	4.5
1	B	479	PHE	4.5
1	B	483	ILE	4.5
1	B	480	ALA	4.4
1	B	407	THR	4.4
1	B	25	LEU	4.4
1	B	493	GLY	4.4
1	B	22	PRO	4.3
1	B	21	ALA	4.3
1	B	165	GLN	4.3
1	B	20	ALA	4.2
1	B	80	VAL	4.2
1	B	466	LEU	4.2
1	B	27	LEU	4.2
1	B	132	PRO	4.1
1	B	32	ALA	4.1
1	B	171	GLU	4.1
1	B	486	ALA	4.1
1	B	314	VAL	4.1
1	B	444	CYS	4.1
1	B	79	LEU	4.0
1	B	507	LEU	4.0
1	B	40	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	185	ALA	4.0
1	B	53	TYR	4.0
1	B	42	VAL	3.9
1	B	104	ILE	3.9
1	B	85	ALA	3.9
1	B	184	ALA	3.9
1	B	148	ALA	3.9
1	B	190	ALA	3.9
1	B	191	LEU	3.9
1	B	39	VAL	3.9
1	B	465	ALA	3.8
1	B	114	ILE	3.8
1	B	490	LEU	3.8
1	B	371	GLU	3.8
1	B	163	LYS	3.7
1	B	18	ILE	3.7
1	B	491	ALA	3.7
1	B	498	LEU	3.7
1	B	120	ASP	3.7
1	B	101	VAL	3.7
1	B	264	VAL	3.7
1	B	91	LEU	3.7
1	B	57	THR	3.7
1	B	127	ASN	3.7
1	B	453	LEU	3.6
1	B	41[A]	CYS	3.6
1	B	58	GLY	3.6
1	B	452	GLY	3.6
1	B	468	SER	3.6
1	B	464	GLN	3.6
1	B	45	ILE	3.6
1	B	17	ALA	3.6
1	B	52	ALA	3.6
1	B	117	LYS	3.5
1	B	135	PRO	3.5
1	B	29	ALA	3.5
1	B	441	LEU	3.5
1	B	31	ALA	3.5
1	B	77	ARG	3.4
1	B	107	LEU	3.4
1	B	147	LEU	3.4
1	B	459	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	158	GLY	3.4
1	B	46	ILE	3.4
1	B	90	PRO	3.4
1	B	34	ALA	3.4
1	B	462	ALA	3.4
1	B	5	LEU	3.4
1	B	457	ALA	3.4
1	B	2	GLU	3.4
1	B	488	GLU	3.4
1	B	84	ALA	3.3
1	B	93	ASP	3.3
1	B	192	LEU	3.3
1	B	378	GLY	3.3
1	B	426	TRP	3.3
1	B	56	ASN	3.3
1	B	47	ALA	3.3
1	B	55	ILE	3.2
1	B	133	HIS	3.2
1	B	33	PRO	3.2
1	B	180	PRO	3.2
1	B	26	GLN	3.2
1	B	365	LEU	3.2
1	B	73	GLU	3.2
1	B	151	SER	3.2
1	B	99	ILE	3.2
1	B	95	LEU	3.2
1	B	136	LEU	3.2
1	B	189	LEU	3.2
1	B	78	SER	3.2
1	B	447	LEU	3.1
1	B	157	GLU	3.1
1	B	37	ALA	3.1
1	B	437	ALA	3.1
1	B	501	ALA	3.1
1	B	379	PHE	3.1
1	B	102	LEU	3.1
1	B	129	GLU	3.0
1	B	188	GLY	3.0
1	B	472	HIS	3.0
1	B	381	ILE	3.0
1	B	438	ILE	3.0
1	B	89	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	382	ALA	3.0
1	B	369	LEU	3.0
1	B	361	HIS	3.0
1	B	485	LYS	3.0
1	B	317	ALA	3.0
1	B	322	ILE	2.9
1	B	159	LYS	2.9
1	B	321	VAL	2.9
1	B	98	LEU	2.9
1	B	92	ASP	2.9
1	B	82	SER	2.9
1	B	316	ALA	2.9
1	B	94	ASP	2.9
1	B	455	THR	2.8
1	B	146	PRO	2.8
1	B	315	PHE	2.8
1	B	36	ASP	2.8
1	B	320	ASP	2.8
1	B	111	PHE	2.8
1	B	207	PHE	2.8
1	B	299	GLU	2.7
1	B	366	PRO	2.7
1	B	482	ASP	2.7
1	B	15	LEU	2.7
1	B	376	ASN	2.7
1	B	161	ARG	2.7
1	B	145	ALA	2.7
1	B	49	ASP	2.7
1	B	448	ASP	2.7
1	B	385	THR	2.7
1	B	86	GLY	2.7
1	B	477	ARG	2.6
1	B	313	LEU	2.6
1	B	219	CYS	2.6
1	B	200	ALA	2.6
1	B	215	ALA	2.6
1	B	443	ALA	2.6
1	B	97	ARG	2.6
1	B	115	ARG	2.6
1	B	446	GLY	2.6
1	B	467	ARG	2.6
1	B	494[A]	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	150	MET	2.5
1	B	362	MET	2.5
1	B	222	LEU	2.5
1	B	224	VAL	2.5
1	B	50	ARG	2.5
1	B	267	SER	2.5
1	B	88	GLY	2.5
1	B	356	LEU	2.5
1	B	100[A]	MET	2.5
1	B	7	PRO	2.4
1	B	435	VAL	2.4
1	B	24	ARG	2.4
1	B	495	LEU	2.4
1	B	38	SER	2.4
1	B	469	GLU	2.4
1	B	476	ASP	2.4
1	B	43	GLU	2.4
1	B	228	LEU	2.4
1	B	19	HIS	2.4
1	B	116	ARG	2.4
1	B	201	TYR	2.4
1	B	208	TYR	2.4
1	B	218	ALA	2.4
1	B	4	THR	2.4
1	B	203	LEU	2.3
1	B	405	LEU	2.3
1	B	149	HIS	2.3
1	B	423	LYS	2.3
1	B	260	ASP	2.3
1	B	319	GLY	2.3
1	B	436	LEU	2.3
1	B	113	GLY	2.3
1	B	312	PRO	2.3
1	B	500	PRO	2.3
1	B	259	GLY	2.2
1	B	502	GLY	2.2
1	B	496	THR	2.2
1	B	105	ASN	2.2
1	B	30	SER	2.2
1	B	13	ALA	2.2
1	B	144	LEU	2.2
1	B	266	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	44	GLN	2.2
1	B	76	GLN	2.2
1	B	197	ALA	2.1
1	B	214	ALA	2.1
1	B	442	GLY	2.1
1	B	10	LEU	2.1
1	B	54	GLY	2.1
1	B	384	VAL	2.1
1	B	108	SER	2.1
1	B	110	GLY	2.1
1	B	454	LYS	2.1
1	B	492	LYS	2.1
1	B	484	GLU	2.1
1	B	226	ALA	2.1
1	B	206	LEU	2.0
1	B	187	GLU	2.0
1	B	497	GLY	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	ZRF	B	142	14/15	0.95	0.09	4,6,16,21	1

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	B	601	7/7	0.66	0.31	14,16,39,40	7
3	SO4	B	602	5/5	0.79	0.19	26,27,30,33	5
4	GOL	B	603	6/6	0.92	0.12	10,12,16,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.