



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:19 PM UTC

PDB ID : 6A0R / pdb_00006a0r
Title : Homoserine dehydrogenase from *Thermus thermophilus* HB8 unliganded form
Authors : Akai, S.; Ikushiro, H.; Sawai, T.; Yano, T.; Kamiya, N.; Miyahara, I.
Deposited on : 2018-06-06
Resolution : 1.83 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 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

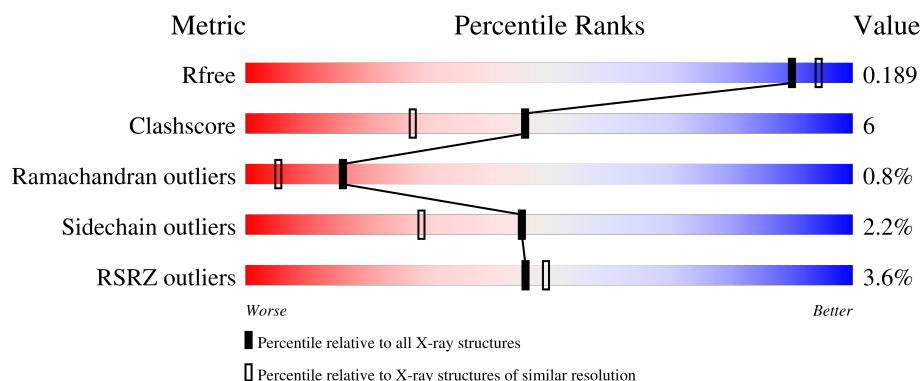
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	332	2% 78% 20% .
1	B	332	5% 75% 23% ..

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	FMT	B	411	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6155 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.

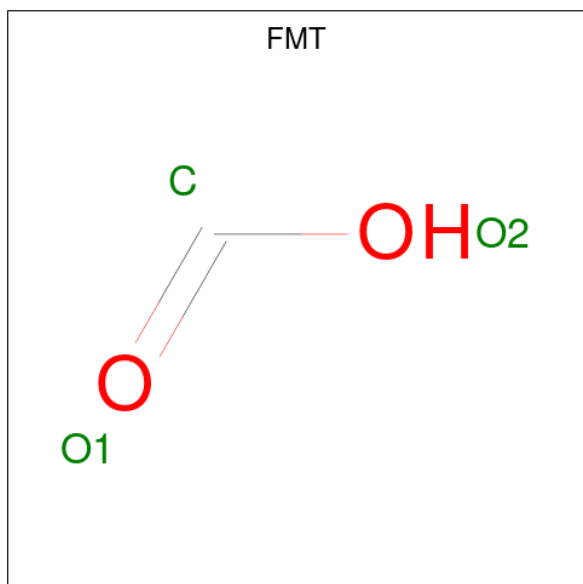
- Molecule 1 is a protein called Homoserine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	331	Total	C	N	O	S	0	15	0
			2609	1668	461	476	4			
1	A	332	Total	C	N	O	S	0	17	0
			2644	1687	469	484	4			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

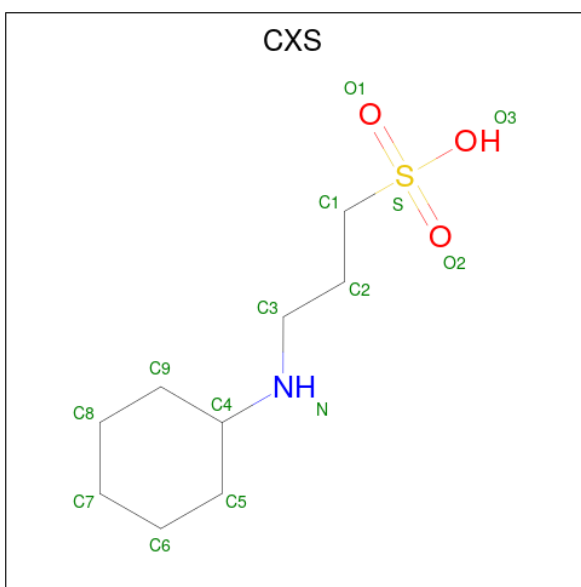
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



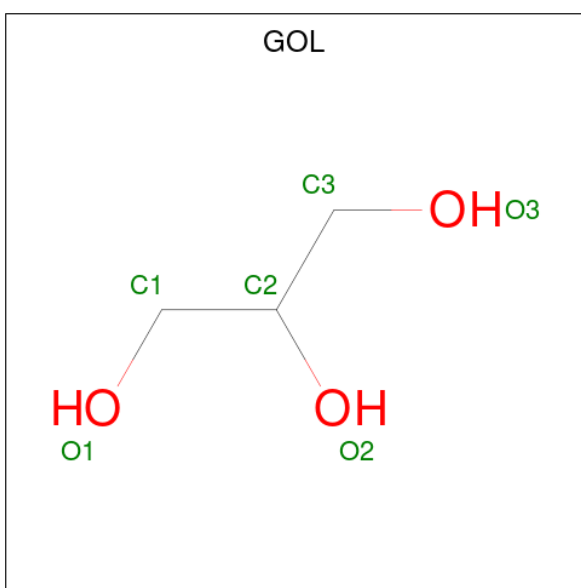
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 6 2 4	0	1
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0

- Molecule 4 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (CCD ID: CXS) (formula: $C_9H_{19}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
4	B	1	Total	C	N	O	S	0	1
			14	9	1	3	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	1
			12	6	6		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	11	2		

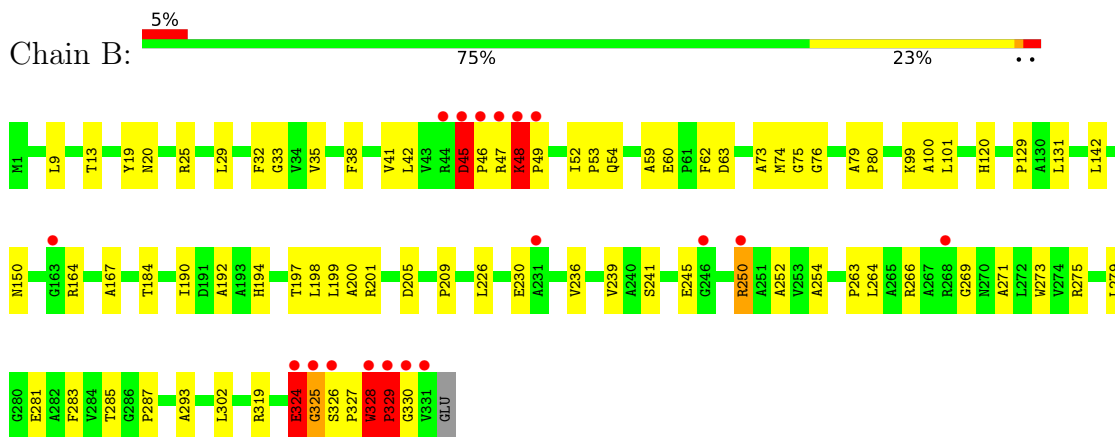
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	379	Total	O	0	31
			393	393		
7	A	380	Total	O	0	25
			394	394		

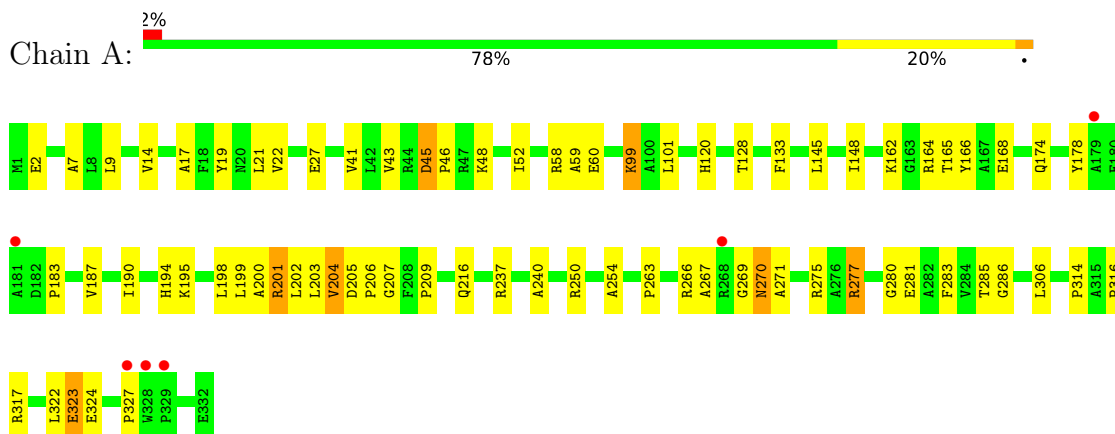
3 Residue-property plots

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: Homoserine dehydrogenase



- Molecule 1: Homoserine dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.20Å 119.20Å 144.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.83 20.00 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.83) 99.8 (20.00-1.83)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.27 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.148 , 0.177 (Not available) , 0.189	Depositor DCC
R_{free} test set	5231 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6155	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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: GOL, UNL, CXS, FMT, NA

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	1.79	42/2703 (1.6%)	1.42	12/3674 (0.3%)
1	B	1.92	48/2674 (1.8%)	1.53	24/3637 (0.7%)
All	All	1.86	90/5377 (1.7%)	1.48	36/7311 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
All	All	0	6

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	ILE	N-CA	-11.35	1.32	1.46
1	B	100	ALA	CA-C	-9.14	1.41	1.52
1	B	9	LEU	CA-C	-8.63	1.41	1.52
1	B	75	GLY	N-CA	8.28	1.55	1.45
1	A	194	HIS	CA-C	7.76	1.62	1.52
1	B	35	VAL	CA-CB	7.72	1.60	1.54
1	B	241	SER	CA-C	-7.61	1.43	1.52
1	B	80	PRO	CA-C	-7.41	1.41	1.52
1	B	190	ILE	N-CA	-6.84	1.38	1.46
1	A	240	ALA	N-CA	-6.82	1.37	1.46
1	A	41	VAL	CA-CB	-6.80	1.45	1.54
1	A	101	LEU	N-CA	-6.79	1.38	1.46
1	A	200	ALA	CA-C	-6.71	1.44	1.52
1	B	279	LEU	CA-C	-6.67	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	271	ALA	CA-C	-6.66	1.44	1.52
1	B	76	GLY	CA-C	-6.60	1.43	1.52
1	B	41	VAL	CA-CB	-6.58	1.45	1.53
1	B	266	ARG	CD-NE	6.50	1.55	1.46
1	A	45	ASP	C-O	-6.44	1.16	1.24
1	A	207	GLY	CA-C	-6.27	1.45	1.51
1	A	250	ARG	CA-C	6.22	1.60	1.52
1	A	166	TYR	CA-C	-6.16	1.44	1.52
1	A	19	TYR	C-O	6.16	1.31	1.24
1	B	328	TRP	CA-C	6.12	1.60	1.52
1	B	53	PRO	N-CA	6.11	1.54	1.47
1	B	194	HIS	CA-C	6.11	1.60	1.52
1	B	131	LEU	N-CA	-6.07	1.39	1.46
1	B	192	ALA	N-CA	6.04	1.53	1.46
1	A	199	LEU	N-CA	6.04	1.53	1.46
1	A	9	LEU	CA-C	-6.00	1.45	1.52
1	B	73	ALA	CA-C	5.99	1.59	1.53
1	A	306	LEU	CB-CG	-5.96	1.41	1.53
1	B	38	PHE	CA-CB	-5.86	1.44	1.53
1	A	48	LYS	CA-C	5.85	1.60	1.53
1	A	206	PRO	CA-CB	-5.82	1.44	1.53
1	A	22	VAL	CA-CB	-5.80	1.48	1.54
1	B	29	LEU	N-CA	-5.79	1.39	1.46
1	A	314	PRO	CA-C	5.77	1.59	1.52
1	A	194	HIS	N-CA	-5.73	1.39	1.46
1	B	239	VAL	CA-C	-5.72	1.45	1.52
1	A	174	GLN	C-O	-5.69	1.17	1.24
1	A	201	ARG	N-CA	-5.69	1.39	1.46
1	A	7	ALA	CA-CB	-5.68	1.45	1.53
1	B	184	THR	CA-C	5.66	1.60	1.52
1	A	280	GLY	N-CA	-5.63	1.39	1.45
1	B	62	PHE	CA-C	-5.57	1.45	1.52
1	B	329	PRO	CA-C	5.57	1.60	1.52
1	A	286	GLY	CA-C	5.57	1.59	1.51
1	A	43	VAL	C-O	-5.53	1.17	1.23
1	B	19	TYR	N-CA	5.52	1.52	1.46
1	B	25	ARG	CA-C	-5.52	1.45	1.52
1	B	199	LEU	N-CA	5.51	1.52	1.46
1	A	209	PRO	CA-C	-5.51	1.44	1.52
1	B	197	THR	CA-CB	5.50	1.61	1.53
1	B	150	ASN	N-CA	5.48	1.52	1.46
1	A	270	ASN	N-CA	-5.46	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	ALA	N-CA	5.46	1.52	1.45
1	A	19	TYR	N-CA	5.44	1.52	1.46
1	B	142	LEU	CA-CB	5.43	1.61	1.53
1	A	60	GLU	N-CA	-5.42	1.39	1.45
1	A	327	PRO	C-O	5.41	1.30	1.24
1	B	190	ILE	CA-CB	5.36	1.61	1.54
1	A	317	ARG	CA-C	-5.35	1.46	1.52
1	A	162	LYS	N-CA	-5.34	1.39	1.46
1	B	42	LEU	N-CA	5.33	1.53	1.46
1	A	52	ILE	N-CA	-5.32	1.40	1.46
1	A	178	TYR	CA-C	5.32	1.59	1.52
1	A	237	ARG	CA-C	-5.32	1.46	1.52
1	B	33	GLY	CA-C	5.30	1.58	1.51
1	B	241	SER	N-CA	5.30	1.52	1.46
1	B	13	THR	N-CA	-5.25	1.40	1.46
1	A	271	ALA	CA-C	-5.23	1.46	1.52
1	B	266	ARG	NE-CZ	5.18	1.38	1.33
1	B	101	LEU	N-CA	-5.16	1.40	1.46
1	A	187	VAL	CA-CB	5.14	1.60	1.54
1	B	100	ALA	N-CA	5.13	1.52	1.46
1	B	198	LEU	CA-C	5.12	1.59	1.52
1	A	17	ALA	C-O	5.12	1.29	1.24
1	B	63	ASP	C-O	-5.10	1.17	1.23
1	A	148	ILE	CA-CB	-5.09	1.47	1.53
1	A	14	VAL	N-CA	5.09	1.52	1.46
1	B	252	ALA	CA-C	-5.08	1.46	1.52
1	B	20	ASN	N-CA	-5.06	1.40	1.46
1	B	254	ALA	CA-C	-5.04	1.46	1.52
1	B	264	LEU	CA-CB	-5.03	1.45	1.53
1	B	79	ALA	CA-CB	-5.02	1.47	1.53
1	B	287	PRO	N-CA	5.01	1.53	1.47
1	B	25	ARG	N-CA	5.00	1.51	1.46
1	B	190	ILE	C-O	5.00	1.30	1.24
1	A	128	THR	C-N	5.00	1.39	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	TRP	N-CA-C	8.38	128.33	109.81
1	B	269[A]	GLY	N-CA-C	-8.13	98.57	112.06
1	B	269[B]	GLY	N-CA-C	-8.13	98.57	112.06
1	A	45	ASP	CA-C-N	7.80	127.52	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ASP	C-N-CA	7.80	127.52	119.56
1	B	74	MET	CA-C-N	-7.36	109.71	121.05
1	B	74	MET	C-N-CA	-7.36	109.71	121.05
1	A	254	ALA	N-CA-C	7.35	114.84	108.22
1	B	324	GLU	N-CA-C	-7.04	104.95	113.97
1	B	167	ALA	N-CA-C	6.84	118.73	111.28
1	A	204	VAL	N-CA-C	6.83	120.19	113.71
1	A	120	HIS	N-CA-C	6.72	119.00	110.61
1	A	270	ASN	CA-CB-CG	-6.66	105.94	112.60
1	B	194	HIS	O-C-N	6.64	128.91	122.07
1	B	293	ALA	O-C-N	-6.05	115.25	122.15
1	A	250	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	B	48	LYS	CA-C-N	-5.91	113.67	119.76
1	B	48	LYS	C-N-CA	-5.91	113.67	119.76
1	B	200	ALA	N-CA-C	5.82	117.63	111.28
1	B	326	SER	CA-C-N	-5.75	112.66	119.84
1	B	326	SER	C-N-CA	-5.75	112.66	119.84
1	B	45	ASP	CA-C-N	-5.69	113.89	120.04
1	B	45	ASP	C-N-CA	-5.69	113.89	120.04
1	B	60	GLU	N-CA-C	5.58	118.64	110.10
1	B	266	ARG	CG-CD-NE	5.47	124.03	112.00
1	A	269[A]	GLY	N-CA-C	-5.44	103.18	112.64
1	A	269[B]	GLY	N-CA-C	-5.44	103.18	112.64
1	B	52	ILE	CA-C-N	-5.41	114.14	119.93
1	B	52	ILE	C-N-CA	-5.41	114.14	119.93
1	B	269[A]	GLY	O-C-N	5.40	128.29	123.59
1	B	269[B]	GLY	O-C-N	5.40	128.29	123.59
1	A	202	LEU	N-CA-C	-5.24	105.65	111.36
1	B	101	LEU	CA-C-O	5.24	126.50	120.90
1	A	194	HIS	O-C-N	5.14	127.36	122.07
1	A	198	LEU	O-C-N	5.10	127.97	122.15
1	B	120	HIS	N-CA-C	5.08	116.41	110.41

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	ARG	Mainchain
1	A	270	ASN	Sidechain
1	B	324	GLU	Peptide
1	B	325	GLY	Peptide
1	B	328	TRP	Peptide

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Mol	Chain	Res	Type	Group
1	B	329	PRO	Peptide

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	2644	0	2668	26	0
1	B	2609	0	2641	36	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	21	0	7	0	0
3	B	33	0	12	4	0
4	B	28	0	36	0	0
5	A	6	0	8	1	0
5	B	12	0	16	1	0
6	B	13	0	0	0	0
7	A	394	0	0	3	0
7	B	393	0	0	6	0
All	All	6155	0	5388	63	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 6.

All (63) 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:275[B]:ARG:HG2	1:B:281[B]:GLU:HG2	1.23	1.16
1:B:250[A]:ARG:HD2	7:B:514[A]:HOH:O	1.49	1.11
1:A:275[B]:ARG:HG2	1:A:281[B]:GLU:HG2	1.56	0.85
1:B:275[B]:ARG:HG2	1:B:281[B]:GLU:CG	2.12	0.77
1:B:275[B]:ARG:CG	1:B:281[B]:GLU:HG2	2.10	0.73
1:B:283[A]:PHE:CE2	1:B:285[A]:THR:CG2	2.77	0.68
1:B:45:ASP:OD1	1:B:47:ARG:N	2.28	0.67
1:A:58:ARG:HA	5:A:409:GOL:H2	1.78	0.66
1:B:328:TRP:HA	1:B:328:TRP:CE3	2.30	0.66
1:B:327:PRO:O	1:B:328:TRP:HB2	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:PHE:CE1	1:A:316:PRO:HG3	2.32	0.64
1:B:328:TRP:HE3	1:B:329:PRO:CD	2.11	0.64
1:A:164[B]:ARG:HG2	1:A:164[B]:ARG:HH11	1.62	0.63
1:A:165:THR:OG1	1:A:168:GLU:HG3	1.99	0.62
1:B:283[A]:PHE:CE2	1:B:285[A]:THR:HG23	2.35	0.61
1:A:27[B]:GLU:HA	1:A:27[B]:GLU:OE1	1.99	0.61
1:B:46:PRO:O	1:B:54:GLN:NE2	2.32	0.60
1:A:283[A]:PHE:CE2	1:A:285[A]:THR:CG2	2.84	0.60
1:B:263:PRO:HB3	1:B:283[B]:PHE:CZ	2.38	0.59
1:B:283[A]:PHE:CZ	1:B:285[A]:THR:CG2	2.85	0.58
1:A:164[B]:ARG:HG2	1:A:164[B]:ARG:NH1	2.18	0.57
1:A:277[A]:ARG:HH11	1:A:277[A]:ARG:HG3	1.69	0.57
1:A:323:GLU:HG3	1:A:324[B]:GLU:O	2.04	0.56
1:A:283[A]:PHE:CZ	1:A:285[A]:THR:CG2	2.89	0.55
1:A:283[A]:PHE:CE2	1:A:285[A]:THR:HG23	2.42	0.54
1:B:230:GLU:OE1	1:B:230:GLU:C	2.51	0.54
1:B:319[A]:ARG:HD2	7:A:636:HOH:O	2.08	0.54
1:B:324:GLU:HB3	7:B:661:HOH:O	2.06	0.54
1:A:46:PRO:HG3	1:A:59:ALA:HB2	1.91	0.53
3:B:411:FMT:H	7:B:530:HOH:O	2.08	0.52
1:B:45:ASP:OD1	1:B:45:ASP:C	2.53	0.51
1:B:263:PRO:HB3	1:B:283[B]:PHE:CE2	2.46	0.51
1:B:328:TRP:CE3	1:B:329:PRO:HD2	2.46	0.50
1:B:327:PRO:O	1:B:328:TRP:CB	2.59	0.50
1:B:164:ARG:HD3	7:B:739[B]:HOH:O	2.12	0.49
3:B:411:FMT:C	7:B:530:HOH:O	2.60	0.49
1:A:99:LYS:NZ	7:A:508:HOH:O	2.45	0.48
1:A:281[B]:GLU:HG3	7:A:744[B]:HOH:O	2.14	0.48
1:A:99:LYS:HE2	1:A:195:LYS:HE3	1.97	0.47
1:A:99:LYS:HE2	1:A:195:LYS:CE	2.46	0.46
1:B:245:GLU:HB3	1:B:250[B]:ARG:HE	1.79	0.46
1:B:328:TRP:CE3	1:B:328:TRP:CA	2.99	0.46
1:B:46:PRO:HG3	1:B:59:ALA:HB2	1.98	0.45
1:A:263:PRO:HB3	1:A:283[B]:PHE:CZ	2.51	0.45
1:B:328:TRP:HE3	1:B:329:PRO:HD2	1.78	0.45
1:A:21[A]:LEU:HD12	1:A:21[A]:LEU:O	2.17	0.45
1:B:226:LEU:HD22	1:B:236:VAL:HB	1.99	0.45
1:A:203:LEU:HB3	1:A:204:VAL:HG13	1.99	0.45
1:B:129:PRO:HG2	1:A:133:PHE:CD1	2.53	0.44
1:B:283[A]:PHE:CZ	1:B:285[A]:THR:HG22	2.52	0.43
1:B:273:TRP:CH2	1:B:275[B]:ARG:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:C	1:A:145:LEU:HD23	2.44	0.42
1:B:48:LYS:HG2	1:B:49:PRO:HD2	2.00	0.42
1:A:21[B]:LEU:C	1:A:21[B]:LEU:HD13	2.45	0.42
1:A:201:ARG:HA	1:A:205:ASP:O	2.19	0.42
1:A:45:ASP:HA	1:A:46:PRO:HD2	1.96	0.41
1:B:209:PRO:HA	3:B:411:FMT:H	2.02	0.41
1:B:209:PRO:HA	3:B:411:FMT:C	2.51	0.41
1:A:99:LYS:H	1:A:99:LYS:HD2	1.85	0.40
1:B:201:ARG:HA	1:B:205:ASP:O	2.21	0.40
5:B:414[B]:GOL:H2	7:B:598:HOH:O	2.22	0.40
1:B:328:TRP:HA	1:B:328:TRP:HE3	1.83	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	347/332 (104%)	332 (96%)	13 (4%)	2 (1%)	21	9
1	B	344/332 (104%)	328 (95%)	12 (4%)	4 (1%)	10	3
All	All	691/664 (104%)	660 (96%)	25 (4%)	6 (1%)	16	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	325	GLY
1	B	328	TRP
1	B	329	PRO
1	B	330	GLY
1	A	267[A]	ALA
1	A	267[B]	ALA

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	261/248 (105%)	252 (97%)	9 (3%)	32	15
1	B	258/248 (104%)	253 (98%)	5 (2%)	50	34
All	All	519/496 (105%)	505 (97%)	14 (3%)	45	22

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	45	ASP
1	B	48	LYS
1	B	99	LYS
1	B	250[A]	ARG
1	B	250[B]	ARG
1	A	2	GLU
1	A	99	LYS
1	A	183	PRO
1	A	216[A]	GLN
1	A	216[B]	GLN
1	A	277[A]	ARG
1	A	277[B]	ARG
1	A	322	LEU
1	A	323	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 2 are monoatomic and 1 is unknown - leaving 23 for Mogul analysis.

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	FMT	B	407	-	2,2,2	0.52	0	1,1,1	1.23	0
5	GOL	A	409	-	5,5,5	1.38	1 (20%)	5,5,5	1.74	2 (40%)
3	FMT	A	407	-	2,2,2	0.47	0	1,1,1	0.83	0
3	FMT	A	405	-	2,2,2	0.60	0	1,1,1	0.51	0
3	FMT	A	408	-	2,2,2	0.49	0	1,1,1	1.54	0
3	FMT	B	404	-	2,2,2	0.53	0	1,1,1	0.28	0
5	GOL	B	414[A]	-	5,5,5	0.56	0	5,5,5	2.00	1 (20%)
3	FMT	A	402	-	2,2,2	0.72	0	1,1,1	0.05	0
4	CXS	B	412	-	14,14,14	2.71	2 (14%)	18,18,18	1.86	3 (16%)
3	FMT	B	408	-	2,2,2	0.14	0	1,1,1	1.57	0
3	FMT	A	404	-	2,2,2	0.25	0	1,1,1	1.03	0
3	FMT	B	403	-	2,2,2	0.78	0	1,1,1	0.29	0
3	FMT	A	403	-	2,2,2	0.67	0	1,1,1	0.86	0
3	FMT	B	405	-	2,2,2	0.21	0	1,1,1	0.80	0
3	FMT	B	409[B]	-	2,2,2	0.68	0	1,1,1	0.96	0
3	FMT	B	410	-	2,2,2	0.90	0	1,1,1	0.82	0
3	FMT	B	406	-	2,2,2	0.99	0	1,1,1	0.38	0
4	CXS	B	413[A]	-	14,14,14	2.77	2 (14%)	18,18,18	2.62	10 (55%)
3	FMT	B	402	-	2,2,2	0.77	0	1,1,1	0.63	0
3	FMT	A	406	-	2,2,2	0.78	0	1,1,1	1.01	0
3	FMT	B	411	-	2,2,2	1.05	0	1,1,1	0.59	0
3	FMT	B	409[A]	-	2,2,2	2.19	1 (50%)	1,1,1	0.41	0
5	GOL	B	414[B]	-	5,5,5	0.85	0	5,5,5	1.40	1 (20%)

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
5	GOL	A	409	-	-	1/4/4/4	-
5	GOL	B	414[A]	-	-	1/4/4/4	-
4	CXS	B	412	-	-	5/8/16/16	0/1/1/1
5	GOL	B	414[B]	-	-	2/4/4/4	-
4	CXS	B	413[A]	-	-	1/8/16/16	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	413[A]	CXS	C1-S	-7.49	1.67	1.77
4	B	412	CXS	O1-S	7.48	1.66	1.45
4	B	413[A]	CXS	O2-S	6.57	1.63	1.45
4	B	412	CXS	C1-S	-6.35	1.68	1.77
5	A	409	GOL	O2-C2	2.62	1.51	1.43
3	B	409[A]	FMT	O2-C	2.41	1.41	1.28

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	413[A]	CXS	C2-C1-S	-6.29	103.61	113.25
4	B	412	CXS	C3-N-C4	4.77	123.38	114.18
4	B	413[A]	CXS	C3-N-C4	4.28	122.42	114.18
5	B	414[A]	GOL	C3-C2-C1	-3.81	97.83	111.80
4	B	413[A]	CXS	C7-C8-C9	3.20	118.00	111.42
4	B	412	CXS	O2-S-C1	3.19	111.55	106.73
4	B	413[A]	CXS	O3-S-C1	3.08	112.04	106.00
4	B	413[A]	CXS	C6-C5-C4	2.97	116.42	111.09
5	A	409	GOL	O2-C2-C3	2.63	120.08	109.18
5	A	409	GOL	O3-C3-C2	2.59	122.04	110.38
4	B	413[A]	CXS	O2-S-C1	2.57	110.61	106.73
4	B	413[A]	CXS	O3-S-O2	-2.44	105.29	111.40
5	B	414[B]	GOL	O1-C1-C2	2.41	121.24	110.38
4	B	412	CXS	C8-C7-C6	-2.41	104.04	111.19
4	B	413[A]	CXS	C9-C4-C5	2.29	114.76	110.80
4	B	413[A]	CXS	C8-C7-C6	2.28	117.97	111.19
4	B	413[A]	CXS	C8-C9-C4	2.20	115.04	111.09

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	413[A]	CXS	C9-C4-N-C3
5	B	414[B]	GOL	O1-C1-C2-C3
5	A	409	GOL	O1-C1-C2-C3
4	B	412	CXS	C2-C1-S-O3
5	B	414[B]	GOL	O1-C1-C2-O2
4	B	412	CXS	C9-C4-N-C3
4	B	412	CXS	C2-C1-S-O1
4	B	412	CXS	C2-C1-S-O2
5	B	414[A]	GOL	O1-C1-C2-O2
4	B	412	CXS	C5-C4-N-C3

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	409	GOL	1	0
3	B	411	FMT	4	0
5	B	414[B]	GOL	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

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	A	332/332 (100%)	-0.25	6 (1%) 67 75	8, 23, 48, 91	17 (5%)
1	B	331/332 (99%)	-0.13	18 (5%) 31 34	8, 22, 56, 90	15 (4%)
All	All	663/664 (99%)	-0.19	24 (3%) 46 49	8, 22, 52, 91	32 (4%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	268[A]	ARG	17.4
1	A	268[A]	ARG	7.7
1	B	325	GLY	5.5
1	B	47	ARG	5.4
1	B	329	PRO	5.1
1	B	46	PRO	4.6
1	B	330	GLY	4.5
1	B	49	PRO	3.7
1	B	45	ASP	3.3
1	B	331	VAL	3.3
1	B	326	SER	3.3
1	B	328	TRP	3.2
1	A	328	TRP	3.1
1	A	179	ALA	3.1
1	A	327	PRO	2.7
1	B	250[A]	ARG	2.7
1	B	44	ARG	2.6
1	B	324	GLU	2.6
1	B	246	GLY	2.5
1	B	231	ALA	2.5
1	A	181	ALA	2.5
1	B	163	GLY	2.2
1	A	329	PRO	2.2
1	B	48	LYS	2.2

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
4	CXS	B	412	14/14	0.79	0.18	35,48,82,93	0
4	CXS	B	413[A]	14/14	0.84	0.25	36,46,62,63	14
3	FMT	A	407	3/3	0.86	0.15	51,51,56,57	3
3	FMT	A	408	3/3	0.86	0.16	37,37,39,44	0
5	GOL	A	409	6/6	0.86	0.14	43,48,58,59	0
3	FMT	B	407	3/3	0.87	0.15	36,36,38,46	0
5	GOL	B	414[B]	6/6	0.88	0.16	24,30,35,40	6
5	GOL	B	414[A]	6/6	0.88	0.16	27,29,32,36	6
3	FMT	B	409[B]	3/3	0.90	0.13	25,25,30,42	3
3	FMT	B	409[A]	3/3	0.90	0.13	22,22,25,37	3
3	FMT	A	406	3/3	0.93	0.16	35,35,49,58	0
3	FMT	B	410	3/3	0.94	0.14	37,37,49,49	0
3	FMT	B	405	3/3	0.95	0.10	31,31,32,47	0
3	FMT	B	406	3/3	0.95	0.08	35,35,45,47	0
3	FMT	A	403	3/3	0.95	0.12	31,31,33,38	0
3	FMT	A	404	3/3	0.95	0.07	29,29,33,40	0
3	FMT	B	402	3/3	0.95	0.11	23,23,26,27	0
3	FMT	B	404	3/3	0.95	0.09	29,29,34,40	0
6	UNL	B	415	13/-	0.95	0.07	22,26,34,38	0
3	FMT	A	405	3/3	0.96	0.13	26,26,35,44	0
3	FMT	A	402	3/3	0.96	0.09	25,25,25,27	0
3	FMT	B	411	3/3	0.97	0.18	28,28,32,51	0
3	FMT	B	408	3/3	0.97	0.06	27,27,28,39	0
2	NA	A	401	1/1	0.99	0.03	14,14,14,14	0
3	FMT	B	403	3/3	0.99	0.05	27,27,31,36	0
2	NA	B	401	1/1	1.00	0.02	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.