



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 11:20 PM BST

PDB ID : 6A0R  
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.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

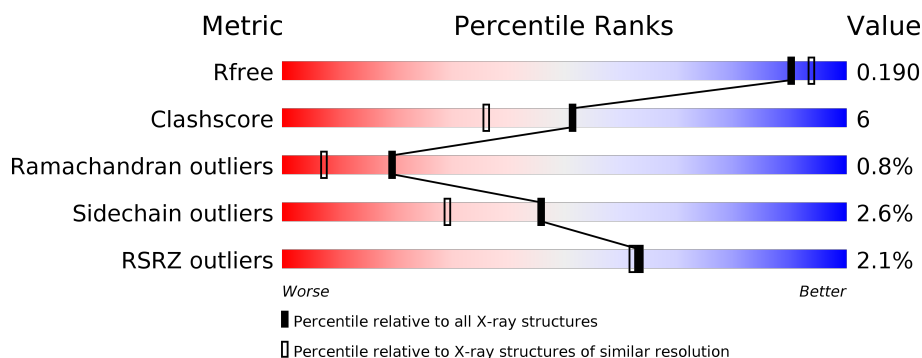
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 1%; height: 10px; background-color: red;"></div> <div style="width: 86%; height: 10px; background-color: green;"></div> <div style="width: 11%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: orange;"></div> </div> </div> <div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 3%; height: 10px; background-color: red;"></div> <div style="width: 82%; height: 10px; background-color: green;"></div> <div style="width: 15%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: orange;"></div> </div> </div> </div> </div>
1	B	332	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 1%; height: 10px; background-color: red;"></div> <div style="width: 86%; height: 10px; background-color: green;"></div> <div style="width: 11%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: orange;"></div> </div> </div> <div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 3%; height: 10px; background-color: red;"></div> <div style="width: 82%; height: 10px; background-color: green;"></div> <div style="width: 15%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: orange;"></div> </div> </div> </div> </div>

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.

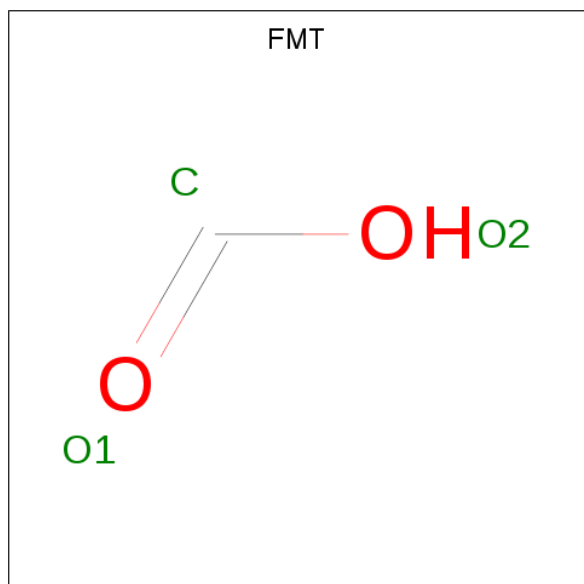
- Molecule 1 is a protein called Homoserine dehydrogenase.

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 (three-letter code: NA) (formula: Na).

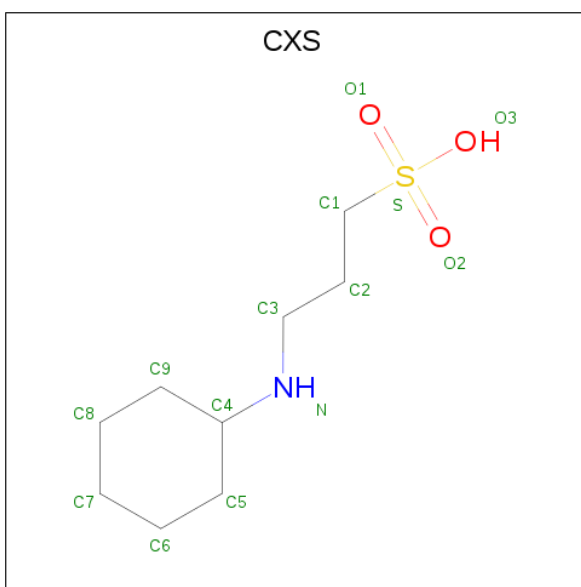
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



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 (three-letter code: CXS) (formula: C<sub>9</sub>H<sub>19</sub>NO<sub>3</sub>S).



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 (three-letter code: 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 (three-letter code: UNL) (formula: ).

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

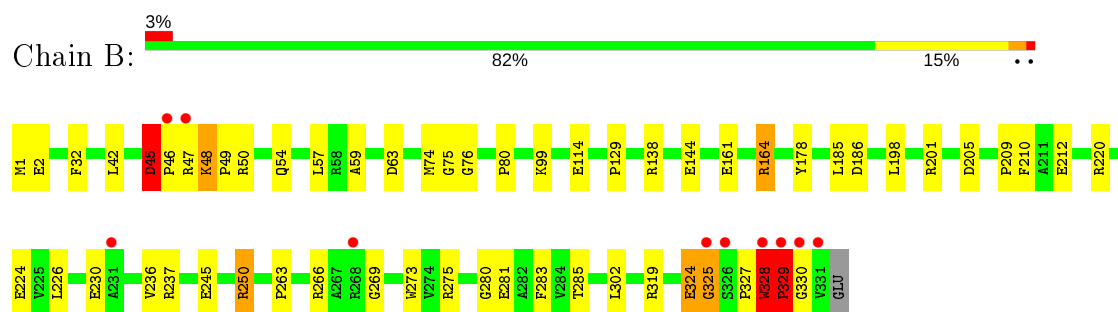
- Molecule 7 is water.

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

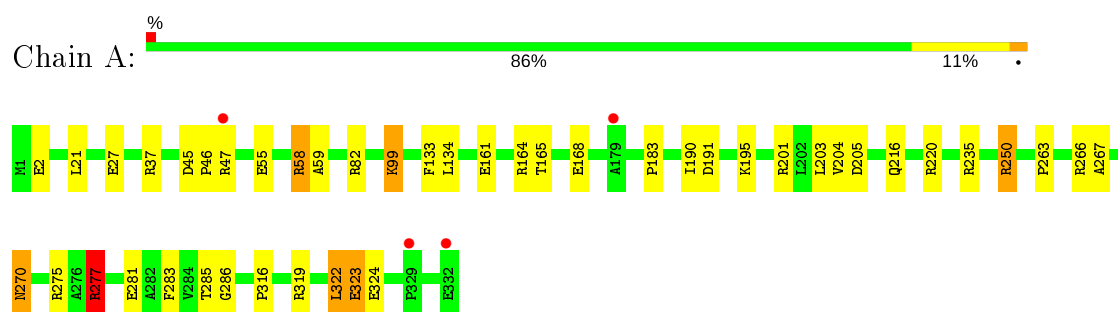
### 3 Residue-property plots [i](#)

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: 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, $\alpha$ , $\beta$ , $\gamma$	119.20Å 119.20Å 144.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.83 19.87 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.83) 99.9 (19.87-1.83)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.27 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.148 , 0.177 0.160 , 0.190	Depositor DCC
$R_{free}$ test set	5231 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 61.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FMT, CXS, UNL, 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	1.36	5/2703 (0.2%)	1.26	16/3674 (0.4%)
1	B	1.48	14/2674 (0.5%)	1.32	21/3637 (0.6%)
All	All	1.42	19/5377 (0.4%)	1.29	37/7311 (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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	GLU	CD-OE1	8.15	1.34	1.25
1	B	114	GLU	CD-OE1	-7.90	1.17	1.25
1	B	2	GLU	CB-CG	-7.11	1.38	1.52
1	A	190	ILE	N-CA	-6.84	1.32	1.46
1	B	212	GLU	CD-OE1	6.74	1.33	1.25
1	B	75	GLY	N-CA	6.50	1.55	1.46
1	B	161	GLU	CD-OE2	-6.44	1.18	1.25
1	B	144	GLU	CB-CG	-6.03	1.40	1.52
1	B	178	TYR	CG-CD1	5.97	1.47	1.39
1	B	2	GLU	CD-OE1	-5.91	1.19	1.25
1	B	224	GLU	CG-CD	5.86	1.60	1.51
1	B	144	GLU	CD-OE2	-5.78	1.19	1.25
1	B	80	PRO	CA-C	-5.75	1.41	1.52
1	A	270	ASN	CB-CG	5.56	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	GLU	CD-OE2	-5.42	1.19	1.25
1	B	76	GLY	CA-C	-5.35	1.43	1.51
1	B	266	ARG	CD-NE	5.24	1.55	1.46
1	B	280	GLY	N-CA	-5.15	1.38	1.46
1	A	286	GLY	CA-C	5.01	1.59	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	ASP	CB-CG-OD1	9.86	127.18	118.30
1	A	250	ARG	NE-CZ-NH2	8.59	124.59	120.30
1	A	277[A]	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	A	277[B]	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	B	237	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	B	186	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	B	328	TRP	N-CA-C	6.42	128.33	111.00
1	A	82	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	47	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	58	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	37	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	235	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	B	138	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	B	74	MET	C-N-CA	-5.99	109.71	122.30
1	B	210	PHE	CB-CG-CD1	5.98	124.99	120.80
1	B	138	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	191	ASP	CB-CG-OD1	-5.96	112.94	118.30
1	B	45	ASP	CB-CG-OD1	5.86	123.57	118.30
1	B	266	ARG	CG-CD-NE	5.83	124.03	111.80
1	B	269[A]	GLY	N-CA-C	-5.81	98.57	113.10
1	B	269[B]	GLY	N-CA-C	-5.81	98.57	113.10
1	A	134	LEU	CB-CG-CD2	5.67	120.65	111.00
1	B	1	MET	CG-SD-CE	5.66	109.25	100.20
1	A	250	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	B	50	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	B	57	LEU	CB-CG-CD1	5.56	120.45	111.00
1	A	277[A]	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	277[B]	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	198	LEU	CB-CG-CD2	5.53	120.40	111.00
1	A	58	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	266	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	B	42	LEU	CB-CG-CD1	-5.33	101.93	111.00
1	B	220	ARG	NE-CZ-NH1	5.28	122.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	LEU	CB-CG-CD2	5.26	119.94	111.00
1	A	322	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	220	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	164	ARG	CG-CD-NE	5.09	122.49	111.80

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
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	23	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	2	0
7	B	393	0	0	6	0
All	All	6155	0	5388	60	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 (60) 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:CE3	1:B:328:TRP:HA	2.30	0.66
1:B:327:PRO:O	1:B:328:TRP:HB2	1.94	0.65
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:HH11	1:A:164[B]:ARG:HG2	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: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: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:B:230:GLU:C	1:B:230:GLU:OE1	2.51	0.49
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:B:45:ASP:OD1	1:B:45:ASP:C	2.53	0.46
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:CA	1:B:328:TRP:CE3	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:PRO:HB3	1:A:283[B]:PHE:CZ	2.51	0.45
1:B:46:PRO:HG3	1:B:59:ALA:HB2	1.98	0.45
1:B:328:TRP:HE3	1:B:329:PRO:HD2	1.78	0.45
1:A:21[A]:LEU:O	1:A:21[A]:LEU:HD12	2.17	0.45
1:A:203:LEU:HB3	1:A:204:VAL:HG13	1.99	0.45
1:B:226:LEU:HD22	1:B:236:VAL:HB	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
1:B:48:LYS:HG2	1:B:49:PRO:HD2	2.00	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:HE3	1:B:328:TRP:HA	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%)	25	12
1	B	344/332 (104%)	328 (95%)	12 (4%)	4 (1%)	13	3
All	All	691/664 (104%)	660 (96%)	25 (4%)	6 (1%)	19	6

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%)	250 (96%)	11 (4%)	30	12
1	B	258/248 (104%)	253 (98%)	5 (2%)	57	42
All	All	519/496 (105%)	503 (97%)	16 (3%)	46	23

All (16) 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	250	ARG
1	A	277[A]	ARG
1	A	277[B]	ARG
1	A	319	ARG
1	A	322	LEU
1	A	323	GLU

Some 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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 1 is unknown and 2 are monoatomic - 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
4	CXS	B	412	-	14,14,14	2.63	2 (14%)	18,18,18	1.97	5 (27%)
3	FMT	A	404	-	0,2,2	0.00	-	0,1,1	0.00	-
4	CXS	B	413[A]	-	14,14,14	2.71	2 (14%)	18,18,18	2.69	10 (55%)
3	FMT	B	405	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	A	409	-	5,5,5	1.33	1 (20%)	5,5,5	1.65	2 (40%)
3	FMT	A	403	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	407	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	409[B]	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	411	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	409[A]	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	410	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	408	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	B	414[A]	-	5,5,5	0.52	0	5,5,5	1.89	1 (20%)
3	FMT	B	406	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	B	414[B]	-	5,5,5	0.83	0	5,5,5	1.34	1 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FMT	B	403	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	404	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	407	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	402	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	405	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	406	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	408	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	402	-	0,2,2	0.00	-	0,1,1	0.00	-

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	413[A]	CXS	C1-S	-7.33	1.67	1.77
4	B	412	CXS	O1-S	7.18	1.66	1.45
4	B	413[A]	CXS	O2-S	6.31	1.63	1.45
4	B	412	CXS	C1-S	-6.21	1.68	1.77
5	A	409	GOL	O2-C2	2.54	1.51	1.43

All (19) 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	4.70	123.38	114.14
4	B	413[A]	CXS	C3-N-C4	4.22	122.42	114.14
4	B	413[A]	CXS	O3-S-C1	3.88	112.04	105.77
4	B	412	CXS	O2-S-C1	3.85	111.55	106.92
5	B	414[A]	GOL	C3-C2-C1	-3.57	97.83	111.70
4	B	413[A]	CXS	C7-C8-C9	3.23	118.00	111.42
4	B	413[A]	CXS	O2-S-C1	3.07	110.61	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	413[A]	CXS	C6-C5-C4	2.82	116.42	111.11
4	B	412	CXS	O1-S-C1	-2.61	103.77	106.92
5	A	409	GOL	O2-C2-C3	2.49	120.08	109.12
5	A	409	GOL	O3-C3-C2	2.47	122.04	110.20
4	B	413[A]	CXS	O3-S-O2	-2.45	105.29	111.27
4	B	412	CXS	C8-C7-C6	-2.32	104.04	111.18
5	B	414[B]	GOL	O1-C1-C2	2.30	121.24	110.20
4	B	413[A]	CXS	C9-C4-C5	2.27	114.76	110.82
4	B	413[A]	CXS	C8-C7-C6	2.21	117.97	111.18
4	B	413[A]	CXS	C8-C9-C4	2.09	115.04	111.11
4	B	412	CXS	O3-S-C1	2.09	109.14	105.77

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	332/332 (100%)	-0.53	4 (1%) 79 79	14, 23, 48, 91	0
1	B	331/332 (99%)	-0.51	10 (3%) 50 47	15, 23, 56, 90	0
All	All	663/664 (99%)	-0.52	14 (2%) 63 62	14, 23, 52, 91	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	330	GLY	4.4
1	B	47	ARG	3.9
1	B	325	GLY	3.7
1	A	332	GLU	3.6
1	B	46	PRO	2.9
1	B	329	PRO	2.8
1	A	329	PRO	2.8
1	A	47	ARG	2.4
1	A	179	ALA	2.3
1	B	326	SER	2.2
1	B	328	TRP	2.2
1	B	331	VAL	2.1
1	B	231	ALA	2.0
1	B	268[A]	ARG	2.0

### 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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	GOL	B	414[A]	6/6	0.78	0.19	27,29,32,36	6
5	GOL	B	414[B]	6/6	0.78	0.19	24,30,35,40	6
4	CXS	B	412	14/14	0.83	0.18	35,48,82,93	0
5	GOL	A	409	6/6	0.87	0.21	43,48,58,59	0
3	FMT	A	407	3/3	0.88	0.18	51,51,56,57	3
4	CXS	B	413[A]	14/14	0.89	0.22	36,46,62,63	14
3	FMT	B	409[B]	3/3	0.91	0.13	25,25,30,42	3
3	FMT	B	409[A]	3/3	0.91	0.13	22,22,25,37	3
3	FMT	A	408	3/3	0.94	0.22	37,37,39,44	0
3	FMT	B	407	3/3	0.95	0.15	36,36,38,46	0
6	UNL	B	415	13/-	0.95	0.08	22,26,34,38	0
3	FMT	B	410	3/3	0.95	0.18	37,37,49,49	0
3	FMT	B	406	3/3	0.96	0.11	35,35,45,47	0
3	FMT	A	406	3/3	0.96	0.23	35,35,49,58	0
3	FMT	B	402	3/3	0.96	0.08	23,23,26,27	0
3	FMT	A	403	3/3	0.97	0.14	31,31,33,38	0
3	FMT	B	408	3/3	0.98	0.05	27,27,28,39	0
3	FMT	B	411	3/3	0.98	0.19	28,28,32,51	0
3	FMT	A	404	3/3	0.98	0.06	29,29,33,40	0
3	FMT	A	405	3/3	0.98	0.09	26,26,35,44	0
3	FMT	B	405	3/3	0.98	0.12	31,31,32,47	0
3	FMT	B	404	3/3	0.98	0.07	29,29,34,40	0
3	FMT	A	402	3/3	0.98	0.08	25,25,25,27	0
2	NA	B	401	1/1	0.99	0.03	15,15,15,15	0
3	FMT	B	403	3/3	0.99	0.04	27,27,31,36	0
2	NA	A	401	1/1	1.00	0.04	14,14,14,14	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.