



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:10 PM GMT

PDB ID : 4WXB
Title : Crystal Structure of Serine Hydroxymethyltransferase from *Streptococcus thermophilus*
Authors : Hernandez, K.; Zelen, I.; Petrillo, G.; Uson, I.; Wandtke, C.; Bujons, J.; Joglar, J.; Parella, T.; Clapes, P.
Deposited on : 2014-11-13
Resolution : 2.05 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

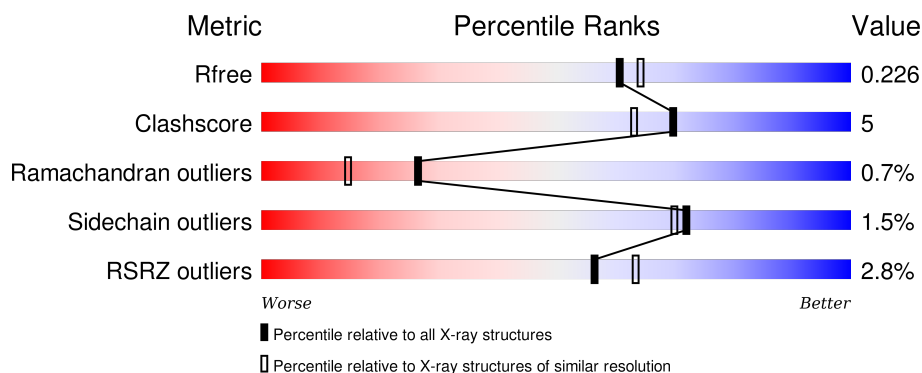
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	428	<div> <div>3%</div> <div>83% 11% . .</div> </div>
1	B	428	<div> <div>2%</div> <div>83% 10% . 7%</div> </div>
1	C	428	<div> <div>%</div> <div>86% 7% . 7%</div> </div>
1	D	428	<div> <div>5%</div> <div>83% 11% . .</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
2	CIT	A	501	-	-	-	X
2	CIT	D	501	-	-	-	X
3	CAC	B	502	-	-	-	X
3	CAC	C	502	-	-	-	X
3	CAC	D	502	-	-	-	X
4	GOL	C	504	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13047 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 Serine hydroxymethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3124	1979	536	600	9			
1	B	400	Total	C	N	O	S	0	0	0
			3061	1942	522	588	9			
1	C	400	Total	C	N	O	S	0	0	0
			3061	1942	522	588	9			
1	D	410	Total	C	N	O	S	0	0	0
			3124	1979	536	600	9			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q5M0B4
A	-16	ARG	-	expression tag	UNP Q5M0B4
A	-15	GLY	-	expression tag	UNP Q5M0B4
A	-14	SER	-	expression tag	UNP Q5M0B4
A	-13	HIS	-	expression tag	UNP Q5M0B4
A	-12	HIS	-	expression tag	UNP Q5M0B4
A	-11	HIS	-	expression tag	UNP Q5M0B4
A	-10	HIS	-	expression tag	UNP Q5M0B4
A	-9	HIS	-	expression tag	UNP Q5M0B4
A	-8	HIS	-	expression tag	UNP Q5M0B4
A	-7	GLY	-	expression tag	UNP Q5M0B4
A	-6	SER	-	expression tag	UNP Q5M0B4
B	-17	MET	-	initiating methionine	UNP Q5M0B4
B	-16	ARG	-	expression tag	UNP Q5M0B4
B	-15	GLY	-	expression tag	UNP Q5M0B4
B	-14	SER	-	expression tag	UNP Q5M0B4
B	-13	HIS	-	expression tag	UNP Q5M0B4
B	-12	HIS	-	expression tag	UNP Q5M0B4
B	-11	HIS	-	expression tag	UNP Q5M0B4
B	-10	HIS	-	expression tag	UNP Q5M0B4
B	-9	HIS	-	expression tag	UNP Q5M0B4

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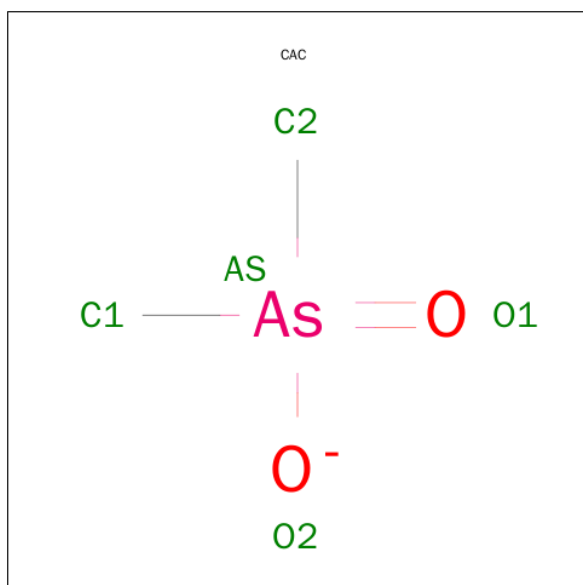
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP Q5M0B4
B	-7	GLY	-	expression tag	UNP Q5M0B4
B	-6	SER	-	expression tag	UNP Q5M0B4
C	-17	MET	-	initiating methionine	UNP Q5M0B4
C	-16	ARG	-	expression tag	UNP Q5M0B4
C	-15	GLY	-	expression tag	UNP Q5M0B4
C	-14	SER	-	expression tag	UNP Q5M0B4
C	-13	HIS	-	expression tag	UNP Q5M0B4
C	-12	HIS	-	expression tag	UNP Q5M0B4
C	-11	HIS	-	expression tag	UNP Q5M0B4
C	-10	HIS	-	expression tag	UNP Q5M0B4
C	-9	HIS	-	expression tag	UNP Q5M0B4
C	-8	HIS	-	expression tag	UNP Q5M0B4
C	-7	GLY	-	expression tag	UNP Q5M0B4
C	-6	SER	-	expression tag	UNP Q5M0B4
D	-17	MET	-	initiating methionine	UNP Q5M0B4
D	-16	ARG	-	expression tag	UNP Q5M0B4
D	-15	GLY	-	expression tag	UNP Q5M0B4
D	-14	SER	-	expression tag	UNP Q5M0B4
D	-13	HIS	-	expression tag	UNP Q5M0B4
D	-12	HIS	-	expression tag	UNP Q5M0B4
D	-11	HIS	-	expression tag	UNP Q5M0B4
D	-10	HIS	-	expression tag	UNP Q5M0B4
D	-9	HIS	-	expression tag	UNP Q5M0B4
D	-8	HIS	-	expression tag	UNP Q5M0B4
D	-7	GLY	-	expression tag	UNP Q5M0B4
D	-6	SER	-	expression tag	UNP Q5M0B4

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



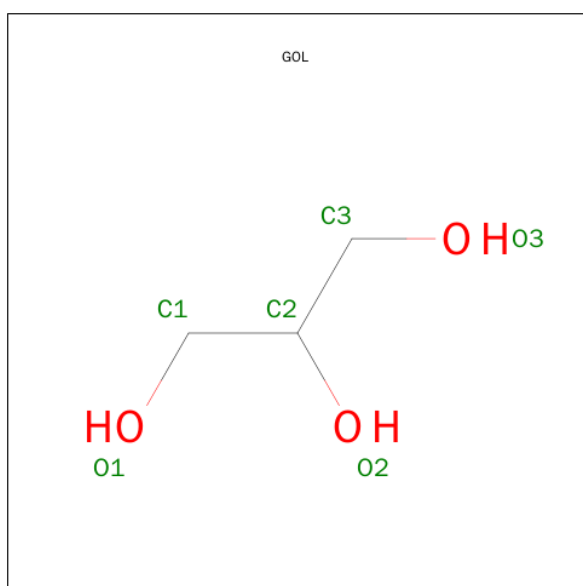
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: $\text{C}_2\text{H}_6\text{AsO}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	As	C	O	0	0
			5	1	2	2		
3	B	1	Total	As	C	O	0	0
			5	1	2	2		
3	C	1	Total	As	C	O	0	0
			5	1	2	2		
3	D	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		

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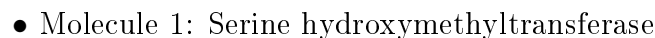
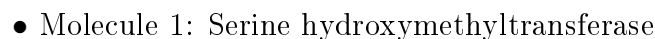
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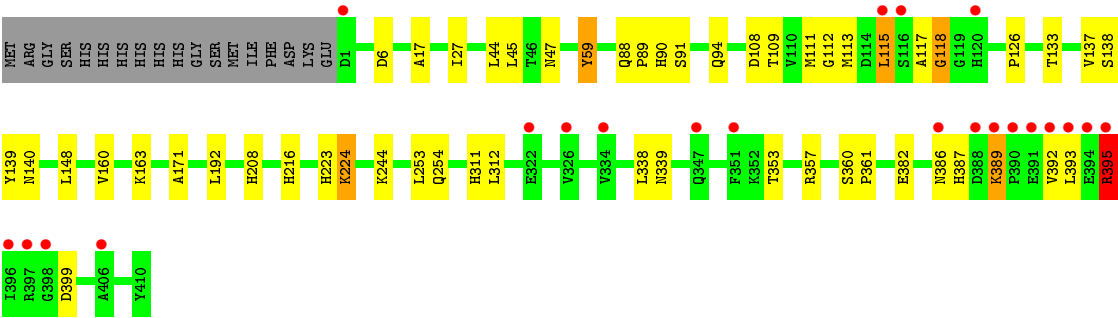
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	194	Total	O	0	0
			194	194		
6	B	135	Total	O	0	0
			135	135		
6	C	177	Total	O	0	0
			177	177		
6	D	72	Total	O	0	0
			72	72		

- Molecule 1: Serine hydroxymethyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	202.10Å 113.43Å 133.39Å 90.00° 93.85° 90.00°	Depositor
Resolution (Å)	66.54 – 2.05 66.54 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.7 (66.54-2.05) 99.7 (66.54-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.191 , 0.221 0.200 , 0.226	Depositor DCC
R_{free} test set	9372 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 187508 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13047	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CAC, GOL, CIT, 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	1.07	3/3187 (0.1%)	1.02	10/4327 (0.2%)
1	B	0.93	0/3121	0.97	11/4235 (0.3%)
1	C	1.04	1/3121 (0.0%)	1.02	9/4235 (0.2%)
1	D	0.82	1/3187 (0.0%)	0.89	4/4327 (0.1%)
All	All	0.97	5/12616 (0.0%)	0.98	34/17124 (0.2%)

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	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	59	TYR	CE1-CZ	6.72	1.47	1.38
1	A	410	TYR	CE1-CZ	6.04	1.46	1.38
1	A	191	TYR	CG-CD2	5.73	1.46	1.39
1	D	59	TYR	CE1-CZ	5.48	1.45	1.38
1	A	59	TYR	CE1-CZ	5.08	1.45	1.38

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	C	149	ASP	CB-CG-OD1	8.29	125.76	118.30
1	B	182	ARG	NE-CZ-NH1	8.23	124.41	120.30
1	B	227	ARG	NE-CZ-NH2	-8.16	116.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	6	ASP	CB-CG-OD2	-7.68	111.38	118.30
1	A	161	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	B	227	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	C	75	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	D	395	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	57	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	C	75	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	C	226	LEU	CB-CG-CD2	-5.98	100.84	111.00
1	B	75	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	C	182	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	180	LYS	CG-CD-CE	-5.62	95.04	111.90
1	B	75	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	366	ARG	CB-CA-C	-5.55	99.30	110.40
1	A	6	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	161	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	A	380	MET	CG-SD-CE	5.43	108.89	100.20
1	B	238	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	238	ASP	CB-CG-OD1	5.42	123.17	118.30
1	D	6	ASP	CB-CG-OD1	5.36	123.12	118.30
1	C	238	ASP	CB-CG-OD1	5.33	123.10	118.30
1	C	101	MET	CA-CB-CG	5.27	122.27	113.30
1	C	151	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	D	108	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	374	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	65	ILE	CG1-CB-CG2	-5.11	100.16	111.40
1	A	378	GLU	CB-CA-C	-5.08	100.24	110.40
1	A	115	LEU	CA-CB-CG	5.04	126.88	115.30
1	B	161	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	374	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	B	238	ASP	CB-CG-OD1	-5.00	113.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ALA	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	3124	0	3105	34	0
1	B	3061	0	3049	29	0
1	C	3061	0	3049	16	0
1	D	3124	0	3105	42	0
2	A	13	0	5	1	0
2	B	13	0	5	2	0
2	C	13	0	5	0	0
2	D	13	0	5	0	0
3	A	5	0	0	0	0
3	B	5	0	0	2	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	194	0	0	1	0
6	B	135	0	0	0	0
6	C	177	0	0	2	0
6	D	72	0	0	6	0
All	All	13047	0	12360	112	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 5.

All (112) 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:D:192:LEU:H	1:D:216:HIS:HD2	1.10	0.97
1:B:192:LEU:H	1:B:216:HIS:HD2	1.21	0.86
1:A:117:ALA:HB2	1:A:140:ASN:OD1	1.77	0.85
1:D:192:LEU:H	1:D:216:HIS:CD2	1.94	0.83
1:A:192:LEU:H	1:A:216:HIS:HD2	1.27	0.80
1:D:113:MET:HE3	6:D:669:HOH:O	1.82	0.78
1:A:90:HIS:H	1:A:254:GLN:HE22	1.30	0.77
1:C:293:ASP:O	1:C:297:GLN:HG2	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:HIS:H	1:C:254:GLN:HE22	1.34	0.73
1:B:44:LEU:HD21	1:D:17:ALA:HB2	1.74	0.69
1:D:395:ARG:NH1	1:D:399:ASP:OD2	2.25	0.69
1:B:192:LEU:H	1:B:216:HIS:CD2	2.08	0.68
1:A:118:GLY:O	1:A:169:ALA:HB1	1.94	0.67
1:A:192:LEU:H	1:A:216:HIS:CD2	2.11	0.66
1:D:90:HIS:H	1:D:254:GLN:HE22	1.47	0.63
1:B:44:LEU:HD21	1:D:17:ALA:CB	2.29	0.63
1:B:44:LEU:HD12	1:B:45:LEU:HD12	1.81	0.62
1:D:208:HIS:O	6:D:601:HOH:O	2.16	0.61
1:B:311:HIS:H	1:B:311:HIS:CD2	2.21	0.58
1:A:16:GLU:HG2	1:C:45:LEU:HD22	1.86	0.58
1:B:198:HIS:NE2	3:B:502:CAC:O1	2.32	0.57
1:C:325:LYS:HE2	1:C:329:ASN:HD21	1.70	0.56
1:D:111:MET:HA	1:D:137:VAL:O	2.04	0.56
1:D:88:GLN:N	1:D:89:PRO:CD	2.69	0.55
1:C:311:HIS:H	1:C:311:HIS:CD2	2.25	0.55
1:D:382:GLU:OE2	1:D:395:ARG:NH2	2.39	0.55
1:B:129:PHE:HB3	1:D:253:LEU:HA	1.89	0.54
1:A:311:HIS:H	1:A:311:HIS:CD2	2.25	0.54
1:C:349:SER:HB3	1:C:352:LYS:HD2	1.90	0.54
1:B:33:VAL:H	1:D:47:ASN:HD21	1.57	0.52
1:A:115:LEU:HD13	1:A:115:LEU:O	2.10	0.52
1:A:312:LEU:C	1:A:312:LEU:HD12	2.30	0.52
1:B:205:SER:OG	1:B:207:HIS:HD2	1.92	0.51
1:B:389:LYS:O	1:B:392:VAL:HG12	2.11	0.51
1:B:370:GLU:O	1:B:374:ARG:HG3	2.10	0.51
1:A:111:MET:HA	1:A:137:VAL:O	2.11	0.51
1:D:109:THR:HG21	1:D:160:VAL:HG13	1.93	0.51
1:A:59:TYR:OH	3:C:502:CAC:O1	2.25	0.50
1:A:117:ALA:HB1	1:A:141:VAL:HG13	1.92	0.50
1:D:113:MET:HE2	1:D:148:LEU:HD21	1.93	0.50
2:B:501:CIT:O3	1:D:90:HIS:HE1	1.94	0.50
1:D:311:HIS:NE2	1:D:312:LEU:HD23	2.26	0.50
1:A:90:HIS:H	1:A:254:GLN:NE2	2.06	0.49
1:A:118:GLY:HA2	1:A:171:ALA:HB3	1.95	0.49
1:D:115:LEU:HD23	6:D:660:HOH:O	2.13	0.48
1:D:117:ALA:HB2	1:D:140:ASN:OD1	2.14	0.48
1:D:360:SER:N	1:D:361:PRO:CD	2.77	0.48
1:D:91:SER:OG	1:D:94:GLN:HG2	2.14	0.48
1:D:112:GLY:O	1:D:138:SER:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:MET:CE	1:D:148:LEU:HD21	2.45	0.47
1:A:374:ARG:O	1:A:378:GLU:HG2	2.15	0.47
1:B:91:SER:OG	1:B:94:GLN:HG2	2.15	0.47
1:D:339:ASN:HD21	1:D:357:ARG:HH21	1.63	0.47
1:C:90:HIS:H	1:C:254:GLN:NE2	2.05	0.47
1:D:27:ILE:HG13	1:D:338:LEU:HA	1.97	0.46
2:B:501:CIT:O2	2:B:501:CIT:O7	2.28	0.46
1:D:89:PRO:HA	1:D:254:GLN:HE22	1.80	0.46
1:B:318:THR:HA	1:B:321:VAL:O	2.15	0.46
1:D:90:HIS:HD2	6:D:627:HOH:O	1.98	0.46
1:A:55:GLY:O	1:A:56:LYS:HD2	2.16	0.46
1:D:113:MET:HE2	1:D:139:TYR:HE1	1.80	0.46
1:B:374:ARG:O	1:B:378:GLU:HG2	2.16	0.46
1:A:109:THR:HG21	1:A:160:VAL:HG13	1.98	0.45
1:D:115:LEU:HB2	6:D:660:HOH:O	2.16	0.45
1:A:99:VAL:HG22	1:A:217:VAL:HG11	1.98	0.45
1:D:126:PRO:O	1:D:133:THR:HG22	2.16	0.45
1:A:16:GLU:HG2	1:C:45:LEU:CD2	2.46	0.45
1:B:127:VAL:HG23	1:B:128:SER:N	2.32	0.45
1:C:132:LYS:NZ	1:C:132:LYS:HB3	2.31	0.45
1:A:137:VAL:HG11	1:A:160:VAL:HG21	1.99	0.45
1:A:253:LEU:HA	1:C:129:PHE:HB3	1.99	0.45
1:D:244:LYS:NZ	6:D:645:HOH:O	2.49	0.44
1:B:33:VAL:HG22	1:D:47:ASN:HD21	1.83	0.44
1:B:88:GLN:N	1:B:89:PRO:CD	2.81	0.44
1:D:386:ASN:CB	1:D:392:VAL:HG11	2.47	0.44
1:B:312:LEU:C	1:B:312:LEU:HD12	2.39	0.44
2:A:501:CIT:O7	2:A:501:CIT:O2	2.34	0.43
1:A:36:ALA:HB2	1:C:2:TYR:HB2	2.01	0.43
1:B:366:ARG:HG2	1:B:409:LEU:HD12	2.00	0.43
1:B:115:LEU:HD13	1:B:136:PHE:HB3	2.00	0.43
1:A:89:PRO:HA	1:A:254:GLN:HE22	1.84	0.42
1:C:89:PRO:HA	1:C:254:GLN:HE22	1.84	0.42
1:D:360:SER:N	1:D:361:PRO:HD3	2.33	0.42
1:B:16:GLU:HG2	1:D:45:LEU:HD12	2.01	0.42
1:A:311:HIS:CE1	1:A:312:LEU:HD23	2.54	0.42
1:B:44:LEU:HD12	1:B:45:LEU:N	2.34	0.42
1:A:118:GLY:O	1:A:170:SER:N	2.53	0.42
1:D:389:LYS:HB2	1:D:389:LYS:HE3	1.71	0.42
1:C:126:PRO:CD	6:C:733:HOH:O	2.67	0.42
1:D:223:HIS:O	1:D:224:LYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:HIS:HD2	1:C:251:PRO:O	2.02	0.42
1:A:88:GLN:N	1:A:89:PRO:CD	2.83	0.42
1:A:91:SER:OG	1:A:94:GLN:HG3	2.20	0.42
3:B:502:CAC:O2	1:D:59:TYR:OH	2.37	0.42
1:B:221:THR:HB	1:B:223:HIS:CE1	2.54	0.42
1:D:137:VAL:HG11	1:D:160:VAL:HG21	2.01	0.42
1:A:49:TYR:CE1	1:A:51:GLU:HG3	2.55	0.42
1:D:109:THR:HG21	1:D:160:VAL:CG1	2.50	0.41
1:B:360:SER:N	1:B:361:PRO:CD	2.83	0.41
1:C:339:ASN:ND2	6:C:659:HOH:O	2.51	0.41
1:A:382:GLU:OE2	1:A:395:ARG:NH2	2.54	0.41
1:D:118:GLY:HA2	1:D:171:ALA:HB3	2.01	0.41
1:A:11:ASN:ND2	6:A:760:HOH:O	2.53	0.41
1:A:102:SER:O	1:A:244:LYS:HE2	2.21	0.41
1:B:182:ARG:HD2	1:B:186:ASP:OD1	2.21	0.41
1:B:140:ASN:CG	1:B:141:VAL:H	2.24	0.41
1:B:44:LEU:CD1	1:B:45:LEU:HD12	2.49	0.41
1:A:295:PHE:HZ	1:A:380:MET:HE2	1.85	0.41
1:A:118:GLY:CA	1:A:171:ALA:HB3	2.51	0.40
1:B:389:LYS:HB2	1:B:392:VAL:CG1	2.52	0.40
1:D:387:HIS:O	1:D:393:LEU:HD11	2.21	0.40
1:C:379:TRP:CZ2	1:C:399:ASP:HB3	2.57	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	408/428 (95%)	388 (95%)	14 (3%)	6 (2%)	13	3
1	B	396/428 (92%)	384 (97%)	10 (2%)	2 (0%)	34	22
1	C	396/428 (92%)	384 (97%)	11 (3%)	1 (0%)	46	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	408/428 (95%)	389 (95%)	16 (4%)	3 (1%)	26	15
All	All	1608/1712 (94%)	1545 (96%)	51 (3%)	12 (1%)	26	15

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	B	224	LYS
1	C	224	LYS
1	D	224	LYS
1	A	120	HIS
1	A	122	THR
1	A	224	LYS
1	A	116	SER
1	B	353	THR
1	A	118	GLY
1	D	118	GLY
1	D	353	THR

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	327/343 (95%)	323 (99%)	4 (1%)	78	76
1	B	322/343 (94%)	319 (99%)	3 (1%)	84	84
1	C	322/343 (94%)	315 (98%)	7 (2%)	60	53
1	D	327/343 (95%)	322 (98%)	5 (2%)	72	70
All	All	1298/1372 (95%)	1279 (98%)	19 (2%)	72	70

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

Mol	Chain	Res	Type
1	A	44	LEU
1	A	94	GLN

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Mol	Chain	Res	Type
1	A	115	LEU
1	A	121	LEU
1	B	44	LEU
1	B	93	SER
1	B	335	ASN
1	C	18	GLU
1	C	41	GLN
1	C	44	LEU
1	C	65	ILE
1	C	132	LYS
1	C	297	GLN
1	C	333	GLU
1	D	44	LEU
1	D	115	LEU
1	D	163	LYS
1	D	389	LYS
1	D	395	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	96	ASN
1	A	123	HIS
1	A	216	HIS
1	A	254	GLN
1	A	311	HIS
1	A	335	ASN
1	A	339	ASN
1	A	341	ASN
1	B	90	HIS
1	B	96	ASN
1	B	207	HIS
1	B	216	HIS
1	B	283	ASN
1	B	311	HIS
1	B	335	ASN
1	B	339	ASN
1	B	341	ASN
1	C	11	ASN
1	C	21	GLN
1	C	94	GLN

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Mol	Chain	Res	Type
1	C	96	ASN
1	C	254	GLN
1	C	297	GLN
1	C	311	HIS
1	C	329	ASN
1	C	335	ASN
1	C	339	ASN
1	C	341	ASN
1	D	11	ASN
1	D	47	ASN
1	D	90	HIS
1	D	94	GLN
1	D	96	ASN
1	D	123	HIS
1	D	156	GLN
1	D	216	HIS
1	D	254	GLN
1	D	335	ASN
1	D	339	ASN
1	D	347	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	$\# Z > 2$
2	CIT	A	501	-	3,12,12	2.50	2 (66%)	3,17,17	3.55	2 (66%)
3	CAC	A	502	-	0,4,4	0.00	-	0,6,6	0.00	-
4	GOL	A	503	-	5,5,5	0.58	0	5,5,5	1.11	0
2	CIT	B	501	-	3,12,12	2.41	2 (66%)	3,17,17	3.19	2 (66%)
3	CAC	B	502	-	0,4,4	0.00	-	0,6,6	0.00	-
4	GOL	B	504	-	5,5,5	0.39	0	5,5,5	0.72	0
2	CIT	C	501	-	3,12,12	2.65	1 (33%)	3,17,17	3.13	3 (100%)
3	CAC	C	502	-	0,4,4	0.00	-	0,6,6	0.00	-
4	GOL	C	504	-	5,5,5	0.57	0	5,5,5	0.67	0
2	CIT	D	501	-	3,12,12	2.33	2 (66%)	3,17,17	3.04	2 (66%)
3	CAC	D	502	-	0,4,4	0.00	-	0,6,6	0.00	-
4	GOL	D	504	-	5,5,5	0.40	0	5,5,5	1.12	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	CIT	A	501	-	-	0/6/16/16	0/0/0/0
3	CAC	A	502	-	-	0/0/0/0	0/0/0/0
4	GOL	A	503	-	-	0/4/4/4	0/0/0/0
2	CIT	B	501	-	-	0/6/16/16	0/0/0/0
3	CAC	B	502	-	-	0/0/0/0	0/0/0/0
4	GOL	B	504	-	-	0/4/4/4	0/0/0/0
2	CIT	C	501	-	-	0/6/16/16	0/0/0/0
3	CAC	C	502	-	-	0/0/0/0	0/0/0/0
4	GOL	C	504	-	-	0/4/4/4	0/0/0/0
2	CIT	D	501	-	-	0/6/16/16	0/0/0/0
3	CAC	D	502	-	-	0/0/0/0	0/0/0/0
4	GOL	D	504	-	-	0/4/4/4	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	CIT	C4-C3	-4.50	1.47	1.54
2	A	501	CIT	C4-C3	-3.65	1.49	1.54
2	B	501	CIT	C4-C3	-3.54	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	CIT	C4-C3	-3.03	1.50	1.54
2	D	501	CIT	C2-C3	-2.26	1.51	1.54
2	B	501	CIT	C2-C3	-2.18	1.51	1.54
2	A	501	CIT	C2-C3	-2.12	1.51	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	CIT	C3-C2-C1	-4.79	107.30	114.96
2	C	501	CIT	C3-C2-C1	-4.51	107.75	114.96
2	A	501	CIT	C3-C2-C1	-4.45	107.85	114.96
2	D	501	CIT	C3-C2-C1	-4.25	108.17	114.96
2	A	501	CIT	C4-C3-C2	-4.06	100.09	109.81
2	B	501	CIT	C4-C3-C2	-2.75	103.23	109.81
2	D	501	CIT	C4-C3-C2	-2.66	103.45	109.81
2	C	501	CIT	C4-C3-C2	-2.04	104.92	109.81
2	C	501	CIT	C3-C4-C5	2.22	118.51	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	CIT	1	0
2	B	501	CIT	2	0
3	B	502	CAC	2	0
3	C	502	CAC	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	410/428 (95%)	-0.17	12 (2%) 55 62	21, 30, 53, 115	0
1	B	400/428 (93%)	-0.00	7 (1%) 71 76	21, 35, 63, 87	0
1	C	400/428 (93%)	-0.30	5 (1%) 79 83	19, 30, 55, 87	0
1	D	410/428 (95%)	0.08	22 (5%) 29 34	30, 45, 70, 111	1 (0%)
All	All	1620/1712 (94%)	-0.10	46 (2%) 56 63	19, 35, 64, 115	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	SER	5.9
1	A	117	ALA	5.3
1	D	116	SER	5.2
1	D	392	VAL	4.2
1	D	115	LEU	4.2
1	A	115	LEU	4.1
1	A	121	LEU	3.8
1	A	120	HIS	3.7
1	D	394	GLU	3.7
1	D	351	PHE	3.6
1	B	392	VAL	3.5
1	D	391	GLU	3.4
1	C	126	PRO	3.3
1	A	118	GLY	3.2
1	C	127	VAL	3.2
1	D	120	HIS	3.2
1	B	351	PHE	3.0
1	D	347	GLN	3.0
1	D	389	LYS	2.9
1	D	398	GLY	2.9
1	A	119	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	1	ASP	2.7
1	B	394	GLU	2.7
1	D	397	ARG	2.6
1	D	396	ILE	2.6
1	D	388	ASP	2.6
1	A	125	ALA	2.4
1	B	388	ASP	2.4
1	D	322	GLU	2.4
1	A	114	ASP	2.3
1	C	351	PHE	2.3
1	D	406	ALA	2.3
1	D	326	VAL	2.3
1	D	393	LEU	2.3
1	C	347	GLN	2.2
1	A	351	PHE	2.2
1	B	129	PHE	2.2
1	A	123	HIS	2.2
1	C	1	ASP	2.1
1	D	395	ARG	2.1
1	B	333	GLU	2.1
1	D	386	ASN	2.1
1	A	1	ASP	2.1
1	B	390	PRO	2.0
1	D	390	PRO	2.0
1	D	334	VAL	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	CAC	C	502	5/5	0.86	0.35	10.79	29,36,42,51	5
2	CIT	D	501	13/13	0.96	0.29	9.71	23,27,29,29	13
3	CAC	B	502	5/5	0.93	0.35	7.56	39,43,45,51	5
3	CAC	D	502	5/5	0.94	0.29	5.39	50,50,52,60	5
2	CIT	A	501	13/13	0.96	0.14	2.84	22,28,33,35	13
4	GOL	C	504	6/6	0.94	0.16	2.28	34,44,44,48	0
2	CIT	B	501	13/13	0.95	0.14	1.57	27,34,38,44	13
3	CAC	A	502	5/5	0.89	0.20	1.07	39,55,63,74	5
2	CIT	C	501	13/13	0.96	0.11	0.71	21,24,29,33	13
4	GOL	D	504	6/6	0.86	0.13	0.59	48,58,59,61	0
4	GOL	A	503	6/6	0.95	0.10	0.04	30,38,40,42	0
5	NA	C	503	1/1	0.86	0.10	-0.41	40,40,40,40	0
4	GOL	B	504	6/6	0.95	0.10	-0.68	36,40,44,44	0
5	NA	B	503	1/1	0.96	0.10	-1.10	41,41,41,41	0
5	NA	D	503	1/1	0.87	0.09	-1.54	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.