



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:20 PM UTC

PDB ID : 1LT7 / pdb_00001lt7
Title : Oxidized Homo sapiens betaine-homocysteine S-methyltransferase in complex with four Sm(III) ions
Authors : Evans, J.C.; Huddler, D.P.; Jiracek, J.; Castro, C.; Millian, N.S.; Garrow, T.A.; Ludwig, M.L.
Deposited on : 2002-05-20
Resolution : 2.15 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

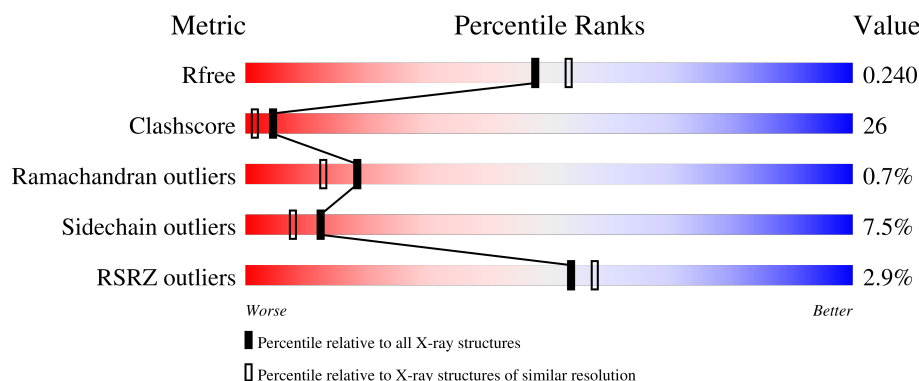
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

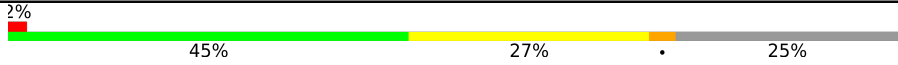
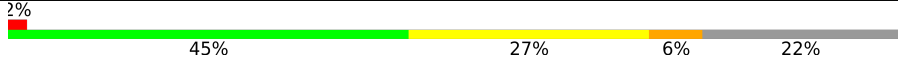
The reported resolution of this entry is 2.15 Å.

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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	406	
1	B	406	

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	CIT	A	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5146 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 BETAINE-HOMOCYSTEINE METHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2368	1511	414	434	9			
1	B	315	Total	C	N	O	S	0	0	0
			2450	1565	428	447	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	PRO	engineered mutation	UNP Q93088
A	104	ALA	CYS	engineered mutation	UNP Q93088
A	131	ALA	CYS	engineered mutation	UNP Q93088
A	186	ALA	CYS	engineered mutation	UNP Q93088
A	201	ALA	CYS	engineered mutation	UNP Q93088
A	239	GLN	ARG	SEE REMARK 999	UNP Q93088
A	256	ALA	CYS	engineered mutation	UNP Q93088
B	2	ALA	PRO	engineered mutation	UNP Q93088
B	104	ALA	CYS	engineered mutation	UNP Q93088
B	131	ALA	CYS	engineered mutation	UNP Q93088
B	186	ALA	CYS	engineered mutation	UNP Q93088
B	201	ALA	CYS	engineered mutation	UNP Q93088
B	239	GLN	ARG	SEE REMARK 999	UNP Q93088
B	256	ALA	CYS	engineered mutation	UNP Q93088

- Molecule 2 is SAMARIUM (III) ION (CCD ID: SM) (formula: Sm).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Sm	0	0
			2	2		
2	B	2	Total	Sm	0	0
			2	2		

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	150	Total	O	0	0
			150	150		
4	B	148	Total	O	0	0
			148	148		

E350	Y351	K352	E353	A358	S359	G360	R361	P362	Y363	S366	K367	S368	K369	P370	D371	GLY	TRP	GLY	GLY	VAL	THR	THR	LYS	LYS	GLY	THR	ALA	ALA	GLU	LEU	MET	GLN	GLN	LYS	GLU	ALA	ALA	THR	THR	GLU	GLN	GLN	LYS	LEU	GLU	LEU	GLU	PHE	LYS	LYS	GLN	LYS	PHE	LYS	SER	GLN
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.99Å 90.08Å 89.08Å 90.00° 122.10° 90.00°	Depositor
Resolution (Å)	9.99 – 2.15 9.99 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.3 (9.99-2.15) 95.2 (9.99-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.15Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.249 0.198 , 0.240	Depositor DCC
R_{free} test set	7403 reflections (9.50%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.50 , 85.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5146	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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: CIT, SM

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	0.84	1/2421 (0.0%)	1.11	12/3274 (0.4%)
1	B	0.79	1/2507 (0.0%)	1.11	16/3392 (0.5%)
All	All	0.81	2/4928 (0.0%)	1.11	28/6666 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	MET	SD-CE	-6.84	1.62	1.79
1	B	358	ALA	CA-CB	6.15	1.63	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	CYS	N-CA-C	11.38	126.69	113.38
1	A	100	ASN	N-CA-C	-8.05	102.46	111.07
1	A	217	CYS	N-CA-C	7.72	127.24	110.80
1	B	126	PRO	N-CA-C	-7.18	104.58	114.27
1	B	135	THR	N-CA-C	-7.10	103.62	111.36
1	A	250	ALA	N-CA-C	-6.75	104.80	113.16
1	B	74	PHE	N-CA-C	6.61	118.99	109.14
1	A	158	ALA	N-CA-C	-6.53	96.99	108.23
1	A	132	LYS	N-CA-C	-6.10	106.16	113.97
1	B	129	LEU	N-CA-C	-6.07	105.13	112.54
1	B	269	PHE	N-CA-C	5.97	120.58	112.88
1	B	125	THR	CA-C-N	-5.80	113.78	120.04
1	B	125	THR	C-N-CA	-5.80	113.78	120.04
1	A	131	ALA	N-CA-C	5.79	119.09	111.28
1	A	253	THR	N-CA-CB	-5.78	100.08	110.37
1	B	174	LEU	N-CA-C	5.69	117.48	111.28
1	B	250	ALA	N-CA-C	-5.68	106.20	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	PHE	N-CA-C	5.61	119.82	112.92
1	A	275	VAL	N-CA-C	5.55	116.57	109.30
1	B	197	PRO	CA-C-N	5.53	125.62	119.32
1	B	197	PRO	C-N-CA	5.53	125.62	119.32
1	A	346	ARG	N-CA-C	-5.53	106.12	112.92
1	A	142	LEU	N-CA-C	-5.49	104.53	111.11
1	B	310	ILE	CB-CA-C	-5.26	105.04	112.14
1	B	100	ASN	N-CA-C	-5.20	105.78	111.82
1	B	249	LEU	N-CA-C	-5.17	103.71	110.53
1	B	216	ASN	N-CA-C	5.14	115.95	108.14
1	A	351	TYR	N-CA-C	-5.12	105.61	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2368	0	2350	125	0
1	B	2450	0	2432	128	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	13	0	4	10	0
3	B	13	0	4	0	0
4	A	150	0	0	30	0
4	B	148	0	0	27	0
All	All	5146	0	4790	250	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 26.

All (250) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:NH2	3:A:601:CIT:H21	1.34	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:SER:HB3	4:B:673:HOH:O	1.33	1.28
1:B:368:SER:HB2	4:B:664:HOH:O	1.50	1.07
1:A:356:ARG:NH2	3:A:601:CIT:C2	2.19	1.05
1:A:215:VAL:HB	4:A:748:HOH:O	1.67	0.94
1:B:271:LEU:HG	4:B:662:HOH:O	1.67	0.94
1:A:218:HIS:HD2	4:A:670:HOH:O	1.52	0.93
1:A:132:LYS:HB3	1:A:136:GLU:HG2	1.49	0.93
1:B:348:ARG:HD3	1:B:350:GLU:HB2	1.49	0.93
1:A:356:ARG:HH22	3:A:601:CIT:H21	1.31	0.92
1:A:303:GLU:H	1:A:306:HIS:HD2	1.18	0.91
1:A:64:LEU:HB3	4:A:740:HOH:O	1.74	0.88
1:A:75:THR:HA	4:A:729:HOH:O	1.74	0.87
1:B:126:PRO:O	1:B:129:LEU:HG	1.75	0.87
1:B:303:GLU:H	1:B:306:HIS:HD2	1.17	0.86
1:B:33:LEU:HD22	1:B:38:TYR:HB2	1.57	0.85
1:B:75:THR:HA	1:B:144:GLN:HE21	1.42	0.84
1:A:24:ILE:H	1:A:69:ASN:HD22	1.20	0.84
1:B:267:PHE:HA	1:B:271:LEU:HD21	1.59	0.83
1:A:61:ARG:HA	4:A:740:HOH:O	1.79	0.83
1:B:127:SER:HB2	1:B:132:LYS:HE3	1.58	0.83
1:A:258:LYS:H	1:A:258:LYS:HZ3	1.25	0.82
1:A:356:ARG:CZ	3:A:601:CIT:H21	2.10	0.80
1:B:308:ARG:HG3	4:B:695:HOH:O	1.83	0.79
1:B:322:PRO:O	1:B:323:PRO:O	2.00	0.79
1:B:145:LEU:HD13	1:B:149:MET:HE2	1.65	0.78
1:A:16:ARG:NH1	4:A:747:HOH:O	2.16	0.77
1:A:243:HIS:HD2	4:A:689:HOH:O	1.67	0.76
1:A:257:ASN:C	1:A:257:ASN:HD22	1.94	0.75
1:A:125:THR:HG22	1:A:166:GLU:OE2	1.87	0.75
1:B:303:GLU:H	1:B:306:HIS:CD2	2.05	0.74
1:B:338:HIS:HD2	1:B:340:LYS:H	1.33	0.74
1:B:132:LYS:HA	4:B:749:HOH:O	1.87	0.74
1:A:361:ARG:HD2	4:B:731:HOH:O	1.89	0.73
1:A:24:ILE:H	1:A:69:ASN:ND2	1.85	0.73
1:A:99:VAL:HG13	1:A:100:ASN:N	2.04	0.73
1:B:264:LEU:HD22	4:B:664:HOH:O	1.88	0.72
1:A:252:HIS:HD2	1:B:360:GLY:O	1.73	0.72
1:A:163:HIS:HB3	4:A:713:HOH:O	1.88	0.72
1:A:258:LYS:H	1:A:258:LYS:NZ	1.88	0.71
1:B:157:ILE:HG22	1:B:159:GLU:HG2	1.72	0.71
1:A:140:VAL:O	1:A:143:GLN:HB3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:THR:HG23	4:A:721:HOH:O	1.90	0.70
4:A:751:HOH:O	1:B:361:ARG:HD2	1.90	0.70
1:B:190:GLU:OE1	1:B:258:LYS:HB3	1.92	0.70
1:A:132:LYS:CB	1:A:136:GLU:HG2	2.21	0.70
1:A:69:ASN:HD21	1:A:318:ARG:HH12	1.39	0.70
1:B:264:LEU:HB3	4:B:738:HOH:O	1.91	0.70
1:A:356:ARG:HH22	3:A:601:CIT:C6	2.04	0.70
1:B:99:VAL:HG23	1:B:102:ALA:H	1.56	0.70
1:A:356:ARG:NH2	3:A:601:CIT:O5	2.21	0.69
1:A:165:GLU:HB3	4:A:713:HOH:O	1.92	0.69
4:A:690:HOH:O	1:B:371:ASP:HA	1.92	0.69
1:B:157:ILE:CG2	1:B:159:GLU:HG2	2.22	0.69
1:A:356:ARG:HH22	3:A:601:CIT:C2	1.94	0.69
1:A:52:HIS:N	4:A:663:HOH:O	2.27	0.68
1:A:303:GLU:H	1:A:306:HIS:CD2	2.07	0.67
1:A:69:ASN:HD21	1:A:318:ARG:NH1	1.93	0.66
1:B:108:ARG:HG3	4:B:709:HOH:O	1.95	0.66
1:B:125:THR:HG22	1:B:166:GLU:OE1	1.95	0.66
1:B:308:ARG:HD3	1:B:312:GLU:CD	2.21	0.66
1:A:101:GLU:HG2	1:A:150:LYS:HZ1	1.61	0.65
1:B:133:SER:O	1:B:134:GLU:HB2	1.95	0.65
1:B:303:GLU:N	1:B:306:HIS:HD2	1.92	0.65
1:A:125:THR:HG23	1:A:128:TYR:H	1.62	0.64
1:B:32:ALA:O	1:B:36:ARG:HG3	1.96	0.64
1:A:135:THR:O	1:A:139:LYS:HG2	1.98	0.64
1:A:33:LEU:HG	1:A:38:TYR:HB2	1.81	0.63
1:A:194:HIS:NE2	4:A:718:HOH:O	2.29	0.63
1:A:101:GLU:CG	1:A:151:LYS:HE2	2.28	0.63
1:B:338:HIS:CD2	1:B:340:LYS:H	2.17	0.63
1:A:123:SER:HA	1:A:159:GLU:O	2.00	0.62
1:B:370:PRO:O	1:B:371:ASP:HB2	1.98	0.62
1:A:259:GLN:HG2	4:A:701:HOH:O	2.00	0.61
1:A:149:MET:HE1	1:A:177:SER:HA	1.82	0.61
1:A:164:VAL:HG22	1:A:185:MET:HE2	1.82	0.61
1:A:349:LYS:HE2	1:A:353:GLU:OE1	2.00	0.61
1:B:133:SER:HA	1:B:137:VAL:HG23	1.82	0.60
1:A:101:GLU:HG3	1:A:151:LYS:HE2	1.83	0.60
1:B:74:PHE:HA	4:B:735:HOH:O	2.00	0.60
1:A:229:LYS:O	1:A:233:GLU:HG3	2.01	0.60
1:A:30:VAL:HG23	4:A:648:HOH:O	2.01	0.60
1:A:30:VAL:O	1:A:34:GLU:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ALA:O	1:A:174:LEU:HG	2.02	0.60
1:B:264:LEU:CB	4:B:738:HOH:O	2.50	0.60
1:A:216:ASN:ND2	1:A:217:CYS:SG	2.76	0.59
1:B:163:HIS:CE1	1:B:193:LEU:HD23	2.38	0.59
1:B:133:SER:O	1:B:134:GLU:CB	2.51	0.58
1:B:245:MET:CB	1:B:295:TYR:HB3	2.33	0.58
1:B:257:ASN:C	1:B:257:ASN:HD22	2.11	0.58
1:B:216:ASN:C	1:B:216:ASN:HD22	2.10	0.58
1:B:282:GLN:CD	4:B:723:HOH:O	2.47	0.58
1:B:145:LEU:HD13	1:B:149:MET:CE	2.34	0.58
1:B:123:SER:HB2	1:B:160:TYR:HB3	1.86	0.58
1:B:348:ARG:HE	1:B:348:ARG:CA	2.17	0.58
1:A:99:VAL:HG13	1:A:100:ASN:H	1.68	0.57
1:B:165:GLU:H	1:B:165:GLU:CD	2.12	0.57
1:B:266:GLU:O	1:B:271:LEU:HD22	2.04	0.57
1:B:124:GLN:NE2	1:B:162:GLU:H	2.02	0.57
1:B:57:ARG:NE	1:B:109:GLN:OE1	2.36	0.56
1:A:371:ASP:O	4:A:668:HOH:O	2.18	0.56
1:A:253:THR:HG23	1:A:253:THR:O	2.05	0.56
1:B:278:ARG:NH1	1:B:308:ARG:NH2	2.53	0.56
1:A:99:VAL:CG1	1:A:100:ASN:N	2.68	0.56
1:B:75:THR:HA	1:B:144:GLN:NE2	2.15	0.56
1:A:252:HIS:CD2	1:B:360:GLY:O	2.58	0.56
1:A:149:MET:CE	1:A:177:SER:HA	2.36	0.56
1:B:72:GLN:NE2	1:B:159:GLU:OE2	2.39	0.56
1:A:75:THR:HG23	1:A:100:ASN:OD1	2.07	0.55
1:B:129:LEU:HD12	4:B:690:HOH:O	2.06	0.55
1:B:252:HIS:HE1	1:B:280:ASP:OD2	1.88	0.55
1:B:30:VAL:HG12	1:B:34:GLU:OE2	2.06	0.55
1:A:162:GLU:O	1:A:192:ASP:HB2	2.07	0.54
1:A:257:ASN:ND2	1:A:259:GLN:H	2.05	0.54
1:B:314:LEU:O	1:B:318:ARG:HG3	2.08	0.54
1:B:308:ARG:C	1:B:308:ARG:HD2	2.33	0.54
1:B:216:ASN:C	1:B:216:ASN:ND2	2.65	0.54
1:B:257:ASN:ND2	1:B:259:GLN:H	2.06	0.53
1:B:134:GLU:HA	4:B:679:HOH:O	2.07	0.53
1:A:101:GLU:CB	1:A:151:LYS:HE2	2.38	0.53
1:A:219:PHE:HA	1:A:253:THR:HG21	1.91	0.53
1:B:135:THR:HG23	1:B:139:LYS:NZ	2.23	0.53
1:A:36:ARG:HH22	1:A:62:GLU:CD	2.17	0.53
1:A:99:VAL:CG1	1:A:100:ASN:H	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ASN:HB2	1:A:258:LYS:HZ3	1.73	0.52
1:B:60:HIS:HD1	1:B:71:MET:HG3	1.74	0.52
1:B:60:HIS:ND1	1:B:71:MET:HG3	2.24	0.52
1:B:218:HIS:CD2	4:B:671:HOH:O	2.62	0.52
1:B:127:SER:HA	1:B:130:SER:OG	2.09	0.52
1:B:216:ASN:CB	1:B:247:GLN:HB2	2.39	0.52
1:B:218:HIS:HD2	4:B:671:HOH:O	1.92	0.52
1:A:356:ARG:NH2	3:A:601:CIT:C1	2.73	0.52
1:A:303:GLU:N	1:A:306:HIS:HD2	1.99	0.52
1:A:253:THR:O	1:A:253:THR:CG2	2.58	0.51
1:B:164:VAL:HG22	1:B:185:MET:HE2	1.92	0.51
1:A:74:PHE:CD1	1:A:74:PHE:N	2.78	0.51
1:A:24:ILE:HG13	1:A:318:ARG:NH1	2.26	0.51
1:A:126:PRO:O	1:A:129:LEU:HG	2.11	0.51
1:A:28:GLY:N	4:A:677:HOH:O	2.24	0.50
1:A:116:ALA:N	4:A:747:HOH:O	2.43	0.50
1:B:128:TYR:HA	1:B:133:SER:OG	2.10	0.50
1:B:11:LYS:HG2	1:B:16:ARG:HG3	1.94	0.50
1:B:216:ASN:HB2	1:B:247:GLN:HB2	1.93	0.50
1:B:108:ARG:NE	4:B:709:HOH:O	2.39	0.50
1:A:57:ARG:HD2	4:A:716:HOH:O	2.10	0.49
1:B:57:ARG:NH1	1:B:109:GLN:OE1	2.45	0.49
1:B:348:ARG:HD2	4:B:708:HOH:O	2.12	0.49
1:A:216:ASN:HB2	1:A:247:GLN:HB2	1.92	0.49
1:B:123:SER:HA	1:B:159:GLU:O	2.12	0.49
1:A:37:GLY:O	4:A:727:HOH:O	2.20	0.49
1:B:348:ARG:HE	1:B:348:ARG:HA	1.76	0.49
1:A:232:LYS:O	1:A:236:GLU:HG3	2.13	0.48
1:A:28:GLY:HA3	1:A:302:PHE:O	2.13	0.48
1:B:220:ASP:HB3	1:B:251:TYR:O	2.12	0.48
1:A:245:MET:HB3	1:A:295:TYR:HB3	1.94	0.48
1:A:108:ARG:NH1	1:A:154:ASP:OD1	2.39	0.47
1:A:273:PRO:HB3	4:B:731:HOH:O	2.13	0.47
3:A:601:CIT:H42	1:B:363:TYR:CD1	2.48	0.47
1:B:348:ARG:HE	1:B:349:LYS:N	2.12	0.47
1:B:135:THR:HG23	1:B:139:LYS:HZ1	1.79	0.47
1:B:19:ALA:HB3	4:B:703:HOH:O	2.13	0.47
1:B:33:LEU:HD11	1:B:56:VAL:HG22	1.97	0.47
1:A:70:VAL:O	1:A:71:MET:HE2	2.15	0.47
1:B:194:HIS:CE1	4:B:693:HOH:O	2.67	0.47
1:B:108:ARG:NH1	1:B:154:ASP:OD2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ARG:HB2	4:B:747:HOH:O	2.14	0.46
1:A:115:ASP:C	4:A:747:HOH:O	2.58	0.46
1:B:104:ALA:HB3	1:B:151:LYS:HD3	1.96	0.46
1:B:245:MET:HB3	1:B:295:TYR:HB3	1.97	0.46
1:B:52:HIS:HB3	1:B:54:GLU:OE1	2.16	0.46
1:B:266:GLU:N	4:B:738:HOH:O	2.46	0.46
1:A:52:HIS:CD2	4:A:694:HOH:O	2.69	0.46
1:A:133:SER:C	1:A:134:GLU:HG3	2.40	0.46
1:A:160:TYR:HA	4:A:702:HOH:O	2.16	0.46
1:B:161:PHE:HE2	1:B:166:GLU:HG2	1.81	0.46
1:B:313:GLU:HG3	1:B:314:LEU:HD13	1.98	0.46
1:A:273:PRO:HB2	1:B:359:SER:HA	1.98	0.46
1:A:320:PHE:HD2	1:A:321:LEU:O	1.99	0.46
1:B:348:ARG:NE	1:B:349:LYS:N	2.64	0.46
1:A:206:VAL:HG21	1:A:240:LEU:HD13	1.98	0.45
1:A:239:GLN:HE21	1:A:239:GLN:HA	1.81	0.45
1:A:37:GLY:HA3	4:A:727:HOH:O	2.16	0.45
1:A:214:GLY:HA3	1:A:245:MET:O	2.17	0.45
1:B:134:GLU:H	1:B:137:VAL:HG23	1.81	0.45
1:A:110:VAL:HA	1:A:113:GLU:HG3	1.98	0.45
1:B:179:LYS:HD2	4:B:706:HOH:O	2.16	0.45
1:A:276:ALA:O	1:A:306:HIS:HE1	1.98	0.45
1:B:346:ARG:HG2	1:B:351:TYR:CE1	2.52	0.45
1:B:109:GLN:NE2	4:B:705:HOH:O	2.50	0.45
1:B:108:ARG:HA	1:B:118:VAL:HG21	1.99	0.45
1:B:127:SER:O	1:B:130:SER:HB2	2.15	0.45
1:B:145:LEU:HD22	1:B:149:MET:HG3	1.99	0.44
1:B:145:LEU:HD21	1:B:177:SER:HB3	1.99	0.44
1:B:183:ALA:O	1:B:213:ILE:HA	2.17	0.44
1:A:109:GLN:O	1:A:112:ASP:HB2	2.18	0.44
1:A:35:LYS:HZ3	1:A:303:GLU:CD	2.25	0.44
1:A:163:HIS:CD2	1:A:193:LEU:HB2	2.53	0.44
1:B:267:PHE:HA	1:B:268:PRO:HA	1.79	0.44
1:A:218:HIS:ND1	4:A:680:HOH:O	2.34	0.44
1:B:308:ARG:NH1	1:B:309:ALA:HB2	2.32	0.44
1:B:162:GLU:O	1:B:192:ASP:HB2	2.18	0.44
1:B:262:ILE:HG13	4:B:657:HOH:O	2.17	0.44
1:A:36:ARG:HD2	4:A:619:HOH:O	2.17	0.44
1:A:125:THR:HG21	1:A:137:VAL:HG13	1.99	0.44
1:A:321:LEU:HB3	1:A:322:PRO:HD2	1.99	0.44
1:B:29:PHE:HZ	1:B:56:VAL:HG13	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ASN:HD21	1:B:259:GLN:HB2	1.83	0.43
1:B:266:GLU:OE2	1:B:368:SER:OG	2.34	0.43
1:A:57:ARG:HD3	1:A:61:ARG:NH2	2.34	0.43
1:A:220:ASP:HB2	1:A:221:PRO:CD	2.48	0.43
1:B:134:GLU:CG	1:B:135:THR:N	2.81	0.43
1:A:344:ARG:N	4:A:732:HOH:O	2.51	0.43
1:B:266:GLU:HB2	4:B:738:HOH:O	2.19	0.42
1:A:101:GLU:CG	1:A:150:LYS:HZ1	2.31	0.42
1:B:57:ARG:HD3	1:B:61:ARG:CZ	2.49	0.42
1:B:161:PHE:CE2	1:B:166:GLU:HG2	2.54	0.42
1:A:33:LEU:HD12	1:A:33:LEU:HA	1.73	0.42
1:A:129:LEU:C	1:A:131:ALA:H	2.27	0.42
1:A:175:ILE:C	1:A:177:SER:H	2.27	0.42
1:B:24:ILE:HD12	1:B:318:ARG:CZ	2.49	0.42
1:B:348:ARG:CD	1:B:350:GLU:HB2	2.36	0.42
1:A:175:ILE:C	1:A:177:SER:N	2.78	0.42
1:B:142:LEU:O	1:B:146:GLU:HG3	2.20	0.42
1:B:216:ASN:HB3	1:B:247:GLN:HB2	2.02	0.42
1:A:129:LEU:C	1:A:129:LEU:HD12	2.46	0.41
1:A:145:LEU:HD11	1:A:177:SER:HB3	2.01	0.41
1:A:146:GLU:O	1:A:149:MET:HB2	2.20	0.41
1:B:266:GLU:O	1:B:271:LEU:CD2	2.69	0.41
1:A:160:TYR:OH	1:A:218:HIS:HE1	2.04	0.41
1:A:220:ASP:HB3	1:A:251:TYR:O	2.20	0.41
1:A:279:TRP:CD2	1:A:352:TRP:HB3	2.56	0.41
1:A:65:ARG:HH21	1:A:65:ARG:HG3	1.85	0.41
1:A:218:HIS:CE1	4:A:680:HOH:O	2.74	0.41
1:B:138:LYS:O	1:B:142:LEU:HB2	2.20	0.41
1:A:143:GLN:O	1:A:146:GLU:HB2	2.20	0.41
1:A:164:VAL:HG23	1:A:192:ASP:OD1	2.20	0.41
1:A:57:ARG:NE	4:A:722:HOH:O	2.51	0.41
1:A:356:ARG:HH22	3:A:601:CIT:C3	2.33	0.41
1:B:146:GLU:O	1:B:147:VAL:C	2.62	0.41
1:B:130:SER:C	1:B:132:LYS:H	2.26	0.41
1:B:299:CYS:SG	1:B:300:CYS:N	2.94	0.41
1:B:130:SER:O	1:B:132:LYS:N	2.43	0.41
1:B:335:LEU:HB3	1:B:347:ALA:HB2	2.03	0.41
1:A:145:LEU:O	1:A:146:GLU:C	2.64	0.40
1:A:206:VAL:CG2	1:A:240:LEU:HD13	2.50	0.40
1:B:33:LEU:HD23	1:B:33:LEU:HA	1.85	0.40
1:B:127:SER:HA	1:B:130:SER:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:SER:HB2	1:A:160:TYR:HB3	2.02	0.40
1:A:206:VAL:HG23	1:A:207:LYS:N	2.36	0.40
1:B:349:LYS:O	1:B:353:GLU:HG3	2.22	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	297/406 (73%)	282 (95%)	14 (5%)	1 (0%)	36	34
1	B	307/406 (76%)	295 (96%)	9 (3%)	3 (1%)	12	8
All	All	604/812 (74%)	577 (96%)	23 (4%)	4 (1%)	18	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	SER
1	B	27	GLY
1	B	134	GLU
1	B	160	TYR

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	A	242/323 (75%)	228 (94%)	14 (6%)	18	14
1	B	251/323 (78%)	228 (91%)	23 (9%)	8	4
All	All	493/646 (76%)	456 (92%)	37 (8%)	12	8

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	24	ILE
1	A	36	ARG
1	A	74	PHE
1	A	122	VAL
1	A	140	VAL
1	A	159	GLU
1	A	218	HIS
1	A	253	THR
1	A	257	ASN
1	A	258	LYS
1	A	261	PHE
1	A	295	TYR
1	A	314	LEU
1	B	14	LEU
1	B	33	LEU
1	B	54	GLU
1	B	71	MET
1	B	99	VAL
1	B	117	LEU
1	B	139	LYS
1	B	145	LEU
1	B	165	GLU
1	B	174	LEU
1	B	193	LEU
1	B	213	ILE
1	B	215	VAL
1	B	216	ASN
1	B	230	LEU
1	B	257	ASN
1	B	258	LYS
1	B	268	PRO
1	B	295	TYR
1	B	304	PRO
1	B	314	LEU

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Mol	Chain	Res	Type
1	B	335	LEU
1	B	348	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	58	GLN
1	A	69	ASN
1	A	72	GLN
1	A	143	GLN
1	A	152	ASN
1	A	194	HIS
1	A	218	HIS
1	A	239	GLN
1	A	243	HIS
1	A	252	HIS
1	A	257	ASN
1	A	290	ASN
1	A	306	HIS
1	B	124	GLN
1	B	144	GLN
1	B	216	ASN
1	B	247	GLN
1	B	252	HIS
1	B	257	ASN
1	B	259	GLN
1	B	282	GLN
1	B	306	HIS
1	B	338	HIS

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	CIT	A	601	2	12,12,12	1.99	2 (16%)	17,17,17	1.49	5 (29%)
3	CIT	B	602	-	12,12,12	1.78	3 (25%)	17,17,17	1.19	4 (23%)

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
3	CIT	A	601	2	-	6/16/16/16	-
3	CIT	B	602	-	-	8/16/16/16	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	CIT	O7-C3	-4.73	1.34	1.43
3	B	602	CIT	O7-C3	-3.15	1.37	1.43
3	B	602	CIT	C3-C6	2.91	1.56	1.53
3	A	601	CIT	O4-C5	-2.39	1.22	1.30
3	B	602	CIT	C4-C3	2.30	1.56	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	CIT	O6-C6-C3	2.66	118.25	113.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	CIT	O6-C6-C3	2.55	118.03	113.14
3	A	601	CIT	O1-C1-C2	-2.42	116.09	122.95
3	A	601	CIT	O3-C5-C4	-2.41	116.12	122.95
3	B	602	CIT	O3-C5-C4	-2.25	116.58	122.95
3	A	601	CIT	O5-C6-C3	-2.15	117.93	122.09
3	B	602	CIT	O1-C1-C2	-2.05	117.15	122.95
3	B	602	CIT	O5-C6-C3	-2.03	118.16	122.09
3	A	601	CIT	C3-C4-C5	2.00	119.39	113.92

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	CIT	O7-C3-C6-O5
3	B	602	CIT	O7-C3-C6-O6
3	B	602	CIT	C2-C3-C6-O5
3	B	602	CIT	C2-C3-C6-O6
3	A	601	CIT	O1-C1-C2-C3
3	A	601	CIT	O2-C1-C2-C3
3	A	601	CIT	C3-C4-C5-O3
3	B	602	CIT	C4-C3-C6-O6
3	A	601	CIT	C3-C4-C5-O4
3	B	602	CIT	C4-C3-C6-O5
3	A	601	CIT	C2-C3-C6-O5
3	B	602	CIT	C3-C4-C5-O4
3	B	602	CIT	C3-C4-C5-O3
3	A	601	CIT	C2-C3-C6-O6

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	CIT	10	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	305/406 (75%)	-0.13	8 (2%) 57 61	15, 35, 60, 76	0
1	B	315/406 (77%)	-0.07	10 (3%) 50 54	15, 36, 55, 80	0
All	All	620/812 (76%)	-0.10	18 (2%) 53 57	15, 36, 59, 80	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	SER	7.1
1	B	129	LEU	5.7
1	B	128	TYR	4.8
1	B	131	ALA	4.4
1	B	75	THR	4.3
1	B	130	SER	4.0
1	B	134	GLU	3.6
1	B	133	SER	3.0
1	A	74	PHE	2.8
1	A	134	GLU	2.6
1	A	99	VAL	2.4
1	A	75	THR	2.4
1	A	133	SER	2.3
1	B	99	VAL	2.2
1	A	348	ARG	2.1
1	A	127	SER	2.1
1	B	126	PRO	2.1
1	A	146	GLU	2.0

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

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

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
3	CIT	B	602	13/13	0.81	0.10	30,33,35,37	13
3	CIT	A	601	13/13	0.83	0.11	24,27,32,34	13
2	SM	A	503	1/1	0.89	0.26	53,53,53,53	1
2	SM	B	504	1/1	0.92	0.21	49,49,49,49	1
2	SM	A	501	1/1	0.94	0.11	35,35,35,35	1
2	SM	B	502	1/1	0.96	0.18	46,46,46,46	1

6.5 Other polymers [i](#)

There are no such residues in this entry.