



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:44 PM GMT

PDB ID : 1LT7
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
<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

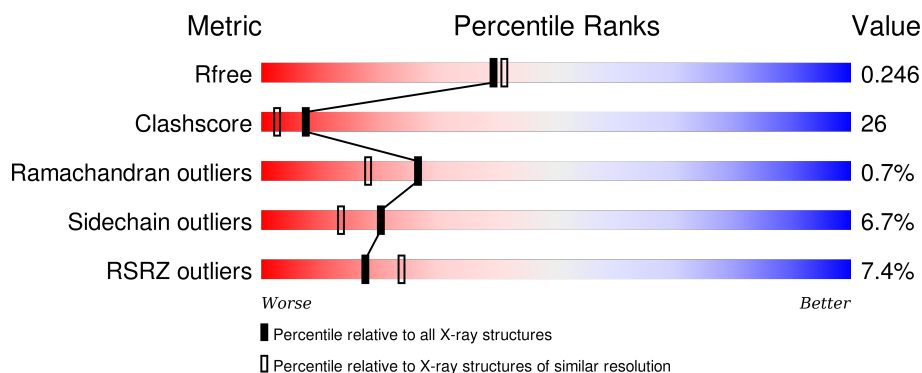
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (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 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	406	<div> <div>6%</div> <div> <div></div> <div>48%</div> <div>25%</div> <div>•</div> <div>25%</div> </div> </div>
1	B	406	<div> <div>5%</div> <div> <div></div> <div>47%</div> <div>26%</div> <div>•</div> <div>22%</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	CIT	A	601	-	-	X	-
3	CIT	B	602	-	-	-	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 BETAIN-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	UNP Q93088
A	104	ALA	CYS	ENGINEERED	UNP Q93088
A	131	ALA	CYS	ENGINEERED	UNP Q93088
A	186	ALA	CYS	ENGINEERED	UNP Q93088
A	201	ALA	CYS	ENGINEERED	UNP Q93088
A	239	GLN	ARG	SEE REMARK 999	UNP Q93088
A	256	ALA	CYS	ENGINEERED	UNP Q93088
B	2	ALA	PRO	ENGINEERED	UNP Q93088
B	104	ALA	CYS	ENGINEERED	UNP Q93088
B	131	ALA	CYS	ENGINEERED	UNP Q93088
B	186	ALA	CYS	ENGINEERED	UNP Q93088
B	201	ALA	CYS	ENGINEERED	UNP Q93088
B	239	GLN	ARG	SEE REMARK 999	UNP Q93088
B	256	ALA	CYS	ENGINEERED	UNP Q93088

- Molecule 2 is SAMARIUM (III) ION (three-letter code: SM) (formula: Sm).

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

- Molecule 3 is CITRIC ACID (three-letter code: 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		

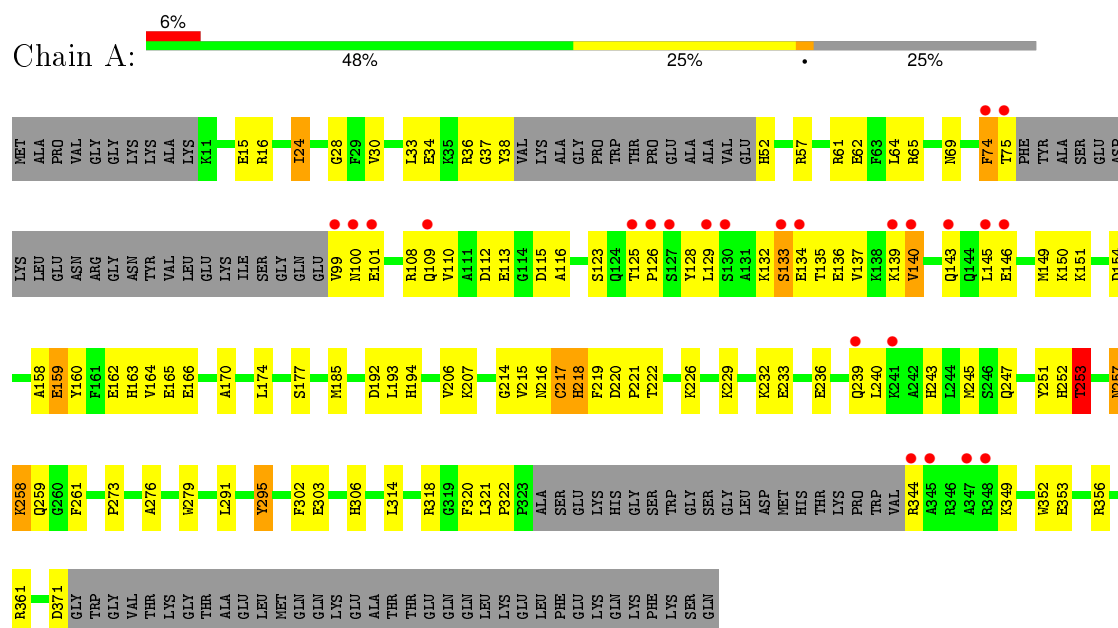
- Molecule 4 is water.

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

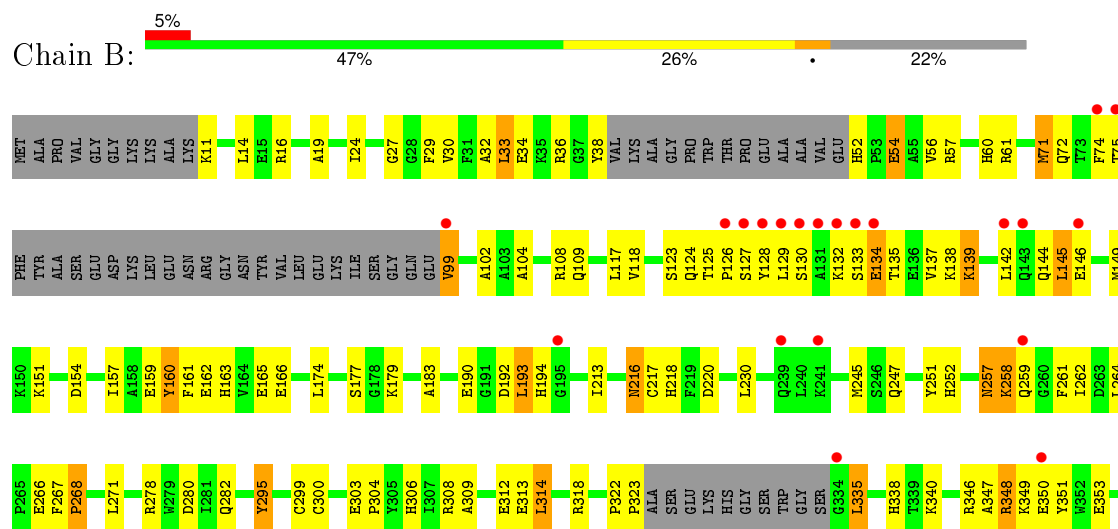
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: BETAINE-HOMOCYSTEINE METHYLTRANSFERASE



• Molecule 1: BETAINE-HOMOCYSTEINE METHYLTRANSFERASE



A358	S359	G360	R361	P362	Y363	S366	M367	S368	K369	P370	D371	GLY	THR	GLY	GLY	VAL	THR	THR	LYS	GLY	THR	ALA	GLU	LEU	MET	GLN	GLN	LYS	GLU	ALA	THR	THR	GLU	GLN	GLN	LEU	LYS	GLU	LEU	PHE	GLU	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	109.99 Å 90.08 Å 89.08 Å 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) 98.7 (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 2.15 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.249 0.204 , 0.246	Depositor DCC
R_{free} test set	3871 reflections (10.98%)	DCC
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.52 , 95.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 77937 reflections	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, 0.375 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: SM, CIT

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	0.70	0/2421	0.80	3/3274 (0.1%)
1	B	0.66	1/2507 (0.0%)	0.77	3/3392 (0.1%)
All	All	0.68	1/4928 (0.0%)	0.78	6/6666 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	358	ALA	CA-CB	5.06	1.63	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	CYS	N-CA-C	6.01	127.24	111.00
1	B	217	CYS	N-CA-C	5.81	126.69	111.00
1	A	253	THR	N-CA-CB	-5.38	100.08	110.30
1	B	361	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	A	158	ALA	N-CA-C	-5.19	96.99	111.00
1	B	361	ARG	NE-CZ-NH1	-5.00	117.80	120.30

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	121	0
1	B	2450	0	2432	126	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	31	0
4	B	148	0	0	28	0
All	All	5146	0	4790	244	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 (244) 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
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:HZ3	1:A:258:LYS:H	1.26	0.81
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:A:16:ARG:NH1	4:A:747:HOH:O	2.16	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:HIS:HD2	4:A:689:HOH:O	1.67	0.76
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:NZ	1:A:258:LYS:H	1.88	0.71
1:B:157:ILE:HG22	1:B:159:GLU:HG2	1.72	0.71
1:A:257:ASN:C	1:A:257:ASN:HD22	1.94	0.71
1:A:140:VAL:O	1:A:143:GLN:HB3	1.90	0.71
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:B:264:LEU:HB3	4:B:738:HOH:O	1.91	0.70
1:A:69:ASN:HD21	1:A:318:ARG:HH12	1.39	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: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:164:VAL:HG22	1:A:185:MET:HE2	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:308:ARG:HD3	1:B:312:GLU:CD	2.21	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
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:145:LEU:HD13	1:B:149:MET:CE	2.34	0.58
1:B:348:ARG:CA	1:B:348:ARG:HE	2.17	0.58
1:B:123:SER:HB2	1:B:160:TYR:HB3	1.86	0.58
1:A:99:VAL:HG13	1:A:100:ASN:H	1.68	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:B:278:ARG:NH1	1:B:308:ARG:NH2	2.53	0.56
1:A:253:THR:O	1:A:253:THR:HG23	2.05	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:B:72:GLN:NE2	1:B:159:GLU:OE2	2.39	0.56
1:A:149:MET:CE	1:A:177:SER:HA	2.36	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:A:149:MET:HE2	1:A:177:SER:HA	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:LEU:O	1:B:318:ARG:HG3	2.08	0.54
1:B:216:ASN:C	1:B:216:ASN:HD22	2.10	0.54
1:B:257:ASN:HD22	1:B:257:ASN:C	2.11	0.54
1:B:282:GLN:CD	4:B:723:HOH:O	2.47	0.53
1:B:257:ASN:ND2	1:B:259:GLN:H	2.06	0.53
1:A:257:ASN:HB2	1:A:258:LYS:HZ3	1.72	0.53
1:B:134:GLU:HA	4:B:679:HOH:O	2.07	0.53
1:B:340:LYS:NZ	4:B:734:HOH:O	2.41	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:99:VAL:CG1	1:A:100:ASN:H	2.22	0.53
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:B:145:LEU:HD13	1:B:149:MET:HE1	1.92	0.52
1:A:303:GLU:N	1:A:306:HIS:HD2	1.99	0.52
1:B:165:GLU:CD	1:B:165:GLU:H	2.12	0.52
1:A:218:HIS:ND1	4:A:680:HOH:O	2.34	0.51
1:A:253:THR:O	1:A:253:THR:CG2	2.58	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:348:ARG:HD2	4:B:708:HOH:O	2.12	0.49
1:B:57:ARG:NH1	1:B:109:GLN:OE1	2.45	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:216:ASN:ND2	1:B:216:ASN:C	2.65	0.49
1:B:348:ARG:HE	1:B:348:ARG:HA	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:308:ARG:C	1:B:308:ARG:HD2	2.33	0.48
1:A:36:ARG:HH22	1:A:62:GLU:CD	2.17	0.48
1:A:108:ARG:NH1	1:A:154:ASP:OD1	2.39	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:A:273:PRO:HB3	4:B:731:HOH:O	2.13	0.47
1:B:135:THR:HG23	1:B:139:LYS:HZ1	1.79	0.47
1:B:33:LEU:HD11	1:B:56:VAL:HG22	1.97	0.47
1:B:19:ALA:HB3	4:B:703:HOH:O	2.13	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
1:B:108:ARG:HB2	4:B:747:HOH:O	2.14	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:A:226:LYS:NZ	4:A:739:HOH:O	2.47	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:160:TYR:HA	4:A:702:HOH:O	2.16	0.46
1:A:52:HIS:CD2	4:A:694:HOH:O	2.69	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:HA	1:A:239:GLN:HE21	1.81	0.45
1:B:134:GLU:H	1:B:137:VAL:HG23	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:A:110:VAL:HA	1:A:113:GLU:HG3	1.98	0.45
1:A:150:LYS:HZ3	1:A:151:LYS:HD3	1.80	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:127:SER:O	1:B:130:SER:HB2	2.15	0.45
1:B:108:ARG:HA	1:B:118:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:125:THR:HG21	1:A:137:VAL:HG13	1.99	0.44
1:A:36:ARG:HD2	4:A:619:HOH:O	2.17	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
1:B:257:ASN:HD21	1:B:259:GLN:HB2	1.83	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:A:257:ASN:ND2	1:A:257:ASN:C	2.68	0.42
1:A:101:GLU:HG2	1:A:150:LYS:HZ1	1.84	0.42
1:B:266:GLU:HB2	4:B:738:HOH:O	2.19	0.42
1:A:115:ASP:C	4:A:747:HOH:O	2.58	0.42
1:B:161:PHE:CE2	1:B:166:GLU:HG2	2.54	0.42
1:B:57:ARG:HD3	1:B:61:ARG:CZ	2.49	0.42
1:A:33:LEU:HD12	1:A:33:LEU:HA	1.73	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: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:145:LEU:HD11	1:A:177:SER:HB3	2.01	0.41
1:B:266:GLU:O	1:B:271:LEU:CD2	2.69	0.41
1:A:146:GLU:O	1:A:149:MET:HB2	2.20	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: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:65:ARG:HG3	1:A:65:ARG:HH21	1.85	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:133:SER:C	1:A:134:GLU:HG3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:A:206:VAL:CG2	1:A:240:LEU:HD13	2.50	0.40
1:A:291:LEU:HG	1:A:291:LEU:O	2.21	0.40
1:B:145:LEU:HD13	1:B:149:MET:HE2	2.03	0.40
1:A:123:SER:HB2	1:A:160:TYR:HB3	2.02	0.40
1:B:349:LYS:O	1:B:353:GLU:HG3	2.22	0.40
1:A:206:VAL:HG23	1:A:207:LYS:N	2.36	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%)	46	42
1	B	307/406 (76%)	295 (96%)	9 (3%)	3 (1%)	19	11
All	All	604/812 (74%)	577 (96%)	23 (4%)	4 (1%)	26	18

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 ⓘ

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%)	230 (95%)	12 (5%)	30	25
1	B	251/323 (78%)	230 (92%)	21 (8%)	14	8
All	All	493/646 (76%)	460 (93%)	33 (7%)	20	13

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	24	ILE
1	A	74	PHE
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	174	LEU
1	B	193	LEU
1	B	216	ASN
1	B	230	LEU
1	B	257	ASN
1	B	258	LYS
1	B	261	PHE

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Mol	Chain	Res	Type
1	B	268	PRO
1	B	295	TYR
1	B	304	PRO
1	B	314	LEU
1	B	335	LEU
1	B	348	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	218	HIS
1	A	239	GLN
1	A	247	GLN
1	A	252	HIS
1	A	257	ASN
1	A	259	GLN
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	290	ASN
1	B	306	HIS
1	B	338	HIS
1	B	354	ASN

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 carbohydrates 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	3,12,12	3.21	1 (33%)	3,17,17	1.95	1 (33%)
3	CIT	B	602	-	3,12,12	2.23	1 (33%)	3,17,17	0.74	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
3	CIT	A	601	2	-	0/6/16/16	0/0/0/0
3	CIT	B	602	-	-	0/6/16/16	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	CIT	O7-C3	-5.42	1.34	1.43
3	B	602	CIT	O7-C3	-3.59	1.37	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	CIT	C3-C4-C5	2.77	119.39	114.96

There are no chirality outliers.

There are no torsion outliers.

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 [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	305/406 (75%)	0.19	24 (7%) 15 22	15, 35, 60, 76	0
1	B	315/406 (77%)	0.33	22 (6%) 19 26	15, 36, 55, 80	0
All	All	620/812 (76%)	0.26	46 (7%) 17 24	15, 36, 59, 80	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	SER	14.4
1	B	128	TYR	11.0
1	B	129	LEU	8.8
1	B	131	ALA	7.6
1	A	344	ARG	6.5
1	B	130	SER	6.5
1	A	146	GLU	5.1
1	B	75	THR	5.1
1	A	75	THR	4.9
1	A	129	LEU	4.8
1	B	143	GLN	4.7
1	A	130	SER	4.5
1	B	134	GLU	4.3
1	A	348	ARG	4.1
1	A	74	PHE	4.0
1	B	334	GLY	3.8
1	A	134	GLU	3.7
1	A	127	SER	3.4
1	B	350	GLU	3.4
1	A	133	SER	3.3
1	B	133	SER	3.1
1	B	241	LYS	3.1
1	A	139	LYS	3.0
1	A	125	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	345	ALA	2.8
1	B	371	ASP	2.8
1	A	239	GLN	2.7
1	A	109	GLN	2.4
1	B	146	GLU	2.4
1	B	74	PHE	2.4
1	B	132	LYS	2.3
1	A	126	PRO	2.3
1	A	143	GLN	2.3
1	B	99	VAL	2.3
1	B	259	GLN	2.2
1	A	140	VAL	2.2
1	B	195	GLY	2.2
1	A	347	ALA	2.1
1	A	145	LEU	2.1
1	A	101	GLU	2.1
1	A	241	LYS	2.1
1	B	126	PRO	2.1
1	A	100	ASN	2.1
1	A	99	VAL	2.1
1	B	142	LEU	2.0
1	B	239	GLN	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 carbohydrates 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. 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(\AA^2)	Q<0.9
3	CIT	B	602	13/13	0.87	0.14	2.32	30,33,35,37	13
3	CIT	A	601	13/13	0.84	0.18	1.81	24,27,32,34	13
2	SM	A	503	1/1	0.90	0.06	-	53,53,53,53	1
2	SM	B	502	1/1	0.94	0.07	-	46,46,46,46	1
2	SM	B	504	1/1	0.94	0.12	-	49,49,49,49	1
2	SM	A	501	1/1	0.95	0.06	-	35,35,35,35	1

6.5 Other polymers [i](#)

There are no such residues in this entry.