



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2022 – 10:09 AM JST

PDB ID : 7XJT
Title : Catabolic ornithine carbamoyltransferases (OTCs) from *Psychrobacter* sp.
PAMC 21119
Authors : Do, H.; Lee, J.H.
Deposited on : 2022-04-18
Resolution : 2.60 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.30
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) : 2.30

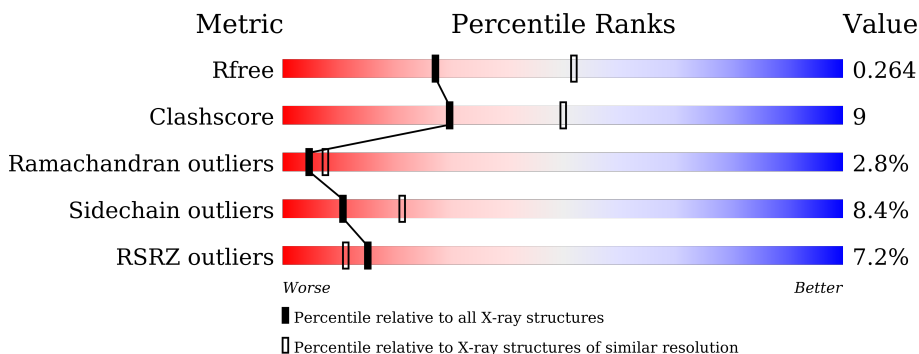
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	336	
1	B	336	
1	C	336	
1	D	336	

2 Entry composition [i](#)

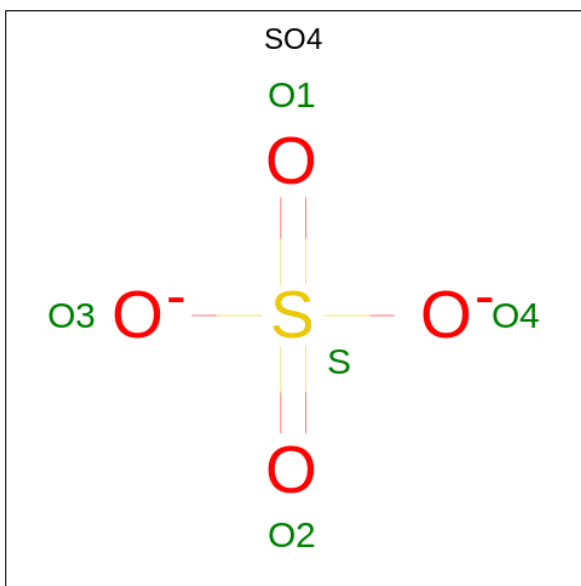
There are 3 unique types of molecules in this entry. The entry contains 10433 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ornithine carbamoyltransferases.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	329	Total 2607	C 1642	N 446	O 499	S 20	0	0	0
1	B	330	Total 2615	C 1646	N 448	O 501	S 20	0	0	0
1	C	328	Total 2596	C 1636	N 442	O 498	S 20	0	0	0
1	D	325	Total 2565	C 1617	N 438	O 490	S 20	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	Total 5	O 4	S 1	0	0

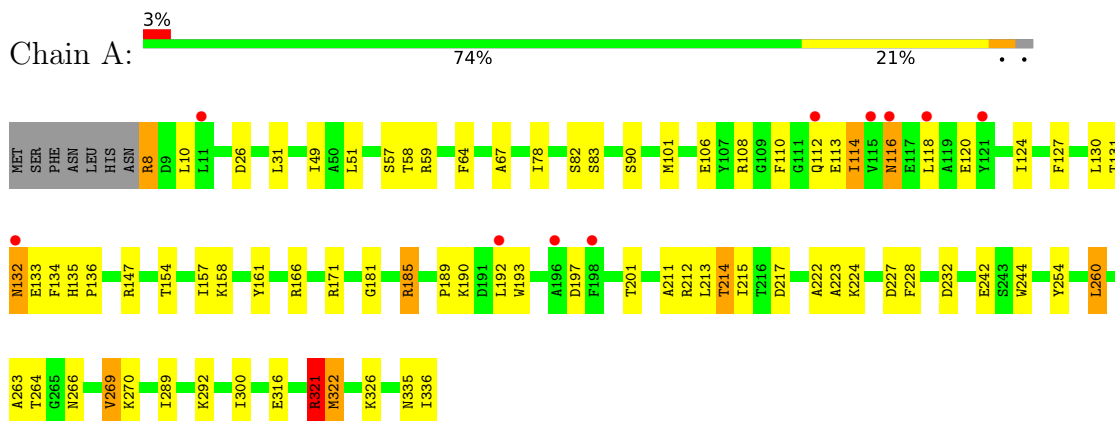
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	7	Total O 7 7	0	0
3	B	20	Total O 20 20	0	0
3	C	6	Total O 6 6	0	0
3	D	12	Total O 12 12	0	0

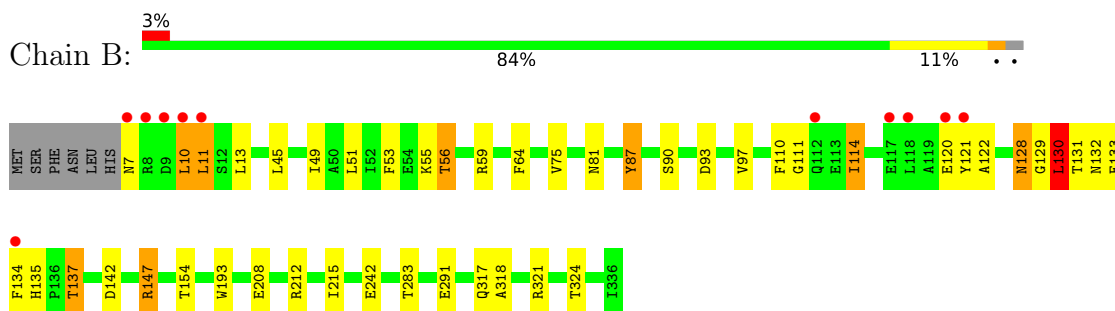
3 Residue-property plots [i](#)

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.

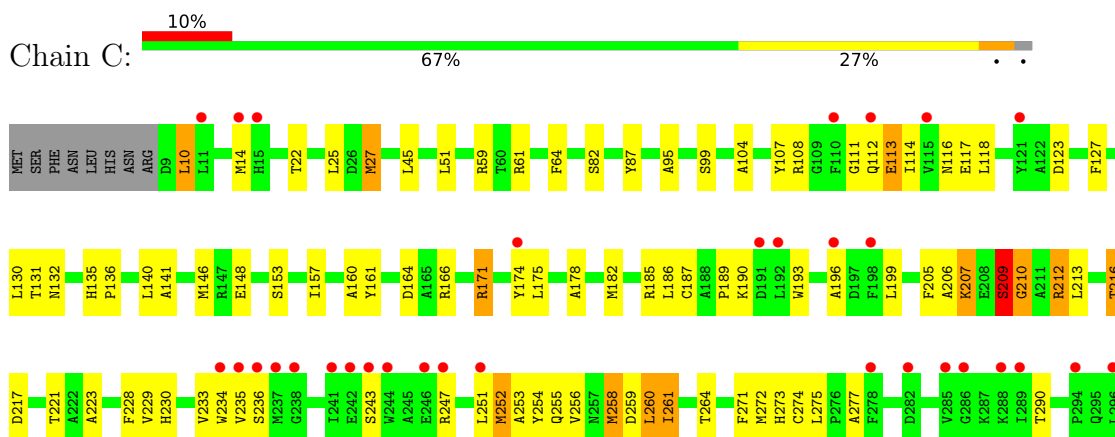
- Molecule 1: Ornithine carbamoyltransferases



- Molecule 1: Ornithine carbamoyltransferases

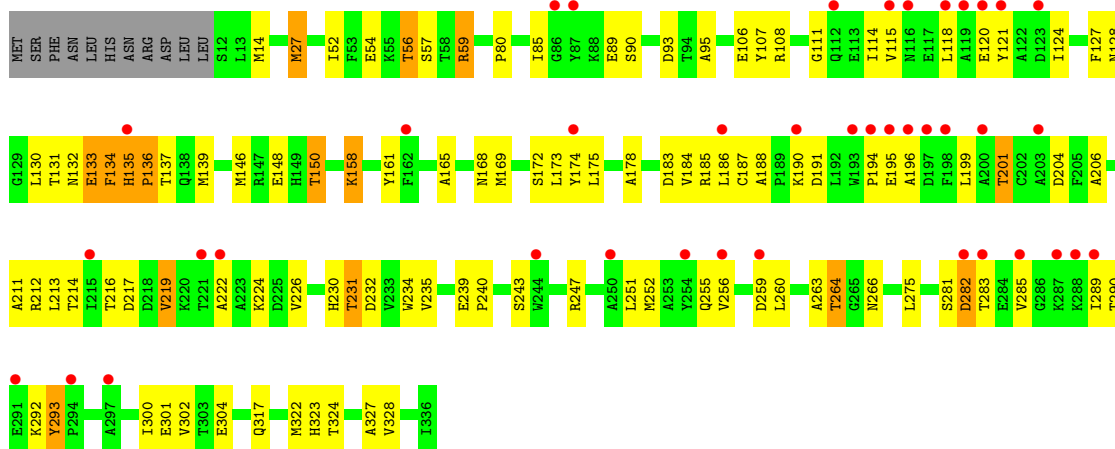


- Molecule 1: Ornithine carbamoyltransferases





● Molecule 1: Ornithine carbamoyltransferases



4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	130.06Å 130.06Å 329.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.53 – 2.60 46.48 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.53-2.60) 99.7 (46.48-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.201 , 0.264 0.203 , 0.264	Depositor DCC
R_{free} test set	3460 reflections (5.42%)	wwPDB-VP
Wilson B-factor (Å ²)	66.0	Xtrriage
Anisotropy	0.040	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.007 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.008 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.006 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$ 0.003 for $-h,2/3^*h+1/3^*k+1/3^*l,4/3^*h+8/3^*k-1/3^*l$ 0.002 for $1/3^*h+2/3^*k-1/3^*l,-k,-8/3^*h-4/3^*k-1/3^*l$ 0.008 for $-1/3^*h-2/3^*k+1/3^*l,-2/3^*h-1/3^*k-1/3^*l,4/3^*h-4/3^*k-1/3^*l$ 0.023 for $-h-k,k,-l$	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10433	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.78	0/2659	0.98	1/3591 (0.0%)
1	B	0.74	0/2667	0.91	0/3602
1	C	0.76	0/2648	0.92	0/3577
1	D	0.76	0/2617	0.90	0/3535
All	All	0.76	0/10591	0.93	1/14305 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2607	0	2552	48	0
1	B	2615	0	2558	25	0
1	C	2596	0	2539	66	0
1	D	2565	0	2505	57	0
2	A	5	0	0	0	0
3	A	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	0	1	0
3	C	6	0	0	1	0
3	D	12	0	0	1	0
All	All	10433	0	10154	192	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 9.

All (192) 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:C:290:THR:HG22	1:C:297:ALA:HA	1.61	0.82
1:A:189:PRO:HD3	1:A:254:TYR:CE1	2.16	0.81
1:A:108:ARG:HD2	1:A:132:ASN:HB2	1.65	0.78
1:A:108:ARG:HD2	1:A:132:ASN:CB	2.15	0.76
1:A:260:LEU:HD12	1:A:260:LEU:O	1.85	0.76
1:A:110:PHE:O	1:A:114:ILE:HD11	1.87	0.75
1:A:223:ALA:O	1:A:264:THR:HA	1.89	0.72
1:A:322:MET:HE3	1:A:326:LYS:HE3	1.72	0.70
1:A:31:LEU:HD13	1:A:326:LYS:HG2	1.74	0.70
1:C:174:TYR:CZ	1:C:213:LEU:HD22	2.27	0.69
1:C:234:TRP:CH2	1:C:301:GLU:HA	2.26	0.69
1:C:117:GLU:HA	3:C:402:HOH:O	1.93	0.67
1:D:239:GLU:HB3	1:D:240:PRO:HD2	1.77	0.67
1:D:216:THR:HG21	3:D:402:HOH:O	1.95	0.67
1:C:166:ARG:O	1:C:171:ARG:HD3	1.93	0.66
1:B:147:ARG:HD2	1:B:154:THR:OG1	1.96	0.66
1:D:322:MET:HE3	1:D:323:HIS:CE1	2.31	0.66
1:C:261:ILE:O	1:C:264:THR:OG1	2.08	0.64
1:A:181:GLY:HA2	1:A:211:ALA:HB2	1.79	0.64
1:B:56:THR:HB	1:C:82:SER:O	1.97	0.64
1:A:189:PRO:HD3	1:A:254:TYR:CZ	2.32	0.64
1:B:133:GLU:O	1:B:135:HIS:N	2.32	0.63
1:C:174:TYR:CD1	1:C:186:LEU:HD12	2.33	0.63
1:D:322:MET:CE	1:D:323:HIS:CE1	2.82	0.62
1:A:133:GLU:O	1:A:135:HIS:N	2.32	0.62
1:C:258:MET:HA	1:C:261:ILE:HD13	1.82	0.62
1:C:273:HIS:CD2	1:C:277:ALA:HB2	2.34	0.62
1:A:321:ARG:CG	1:A:321:ARG:HH11	2.13	0.61
1:D:165:ALA:HB1	1:D:186:LEU:HD13	1.81	0.61
1:C:174:TYR:CE2	1:C:213:LEU:HD22	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ALA:HB1	1:C:118:LEU:HD13	1.82	0.61
1:C:10:LEU:O	1:C:10:LEU:HG	2.00	0.60
1:C:313:ILE:O	1:C:313:ILE:HG13	1.99	0.60
1:C:209:SER:OG	1:C:210:GLY:N	2.36	0.59
1:A:228:PHE:CE1	1:A:270:LYS:HB2	2.38	0.58
1:A:26:ASP:OD1	1:A:147:ARG:NH2	2.37	0.58
1:D:256:VAL:HA	1:D:260:LEU:HD23	1.85	0.58
1:A:322:MET:CE	1:A:326:LYS:HE3	2.34	0.58
1:A:166:ARG:O	1:A:171:ARG:HD3	2.04	0.57
1:D:174:TYR:HA	1:D:184:VAL:HG21	1.86	0.57
1:B:51:LEU:HD21	1:B:64:PHE:CD1	2.39	0.57
1:C:230:HIS:HA	1:C:272:MET:O	2.05	0.57
1:C:274:CYS:O	1:C:275:LEU:HB2	2.05	0.57
1:C:166:ARG:O	1:C:171:ARG:CD	2.53	0.56
1:B:137:THR:CG2	1:B:321:ARG:HE	2.19	0.56
1:D:174:TYR:OH	1:D:213:LEU:HB3	2.06	0.56
1:D:194:PRO:HD2	1:D:199:LEU:HD11	1.88	0.56
1:D:134:PHE:HE1	1:D:169:MET:HG2	1.70	0.56
1:D:247:ARG:NH1	1:D:251:LEU:HD11	2.22	0.55
1:C:290:THR:CG2	1:C:297:ALA:HA	2.35	0.55
1:B:142:ASP:OD1	1:B:317:GLN:NE2	2.40	0.54
1:D:185:ARG:HA	1:D:214:THR:O	2.07	0.54
1:D:90:SER:HB3	1:D:93:ASP:OD1	2.07	0.54
1:C:164:ASP:OD2	1:C:247:ARG:NH2	2.41	0.54
1:D:264:THR:C	1:D:266:ASN:H	2.12	0.53
1:D:132:ASN:O	1:D:134:PHE:N	2.42	0.53
1:D:133:GLU:HA	1:D:136:PRO:HD2	1.91	0.53
1:C:104:ALA:HB2	1:C:333:LEU:HD21	1.90	0.53
1:A:185:ARG:HD3	1:A:222:ALA:O	2.08	0.53
1:D:115:VAL:HG11	1:D:128:ASN:HA	1.91	0.53
1:D:139:MET:SD	1:D:172:SER:HB3	2.49	0.53
1:B:49:ILE:O	1:B:75:VAL:HA	2.10	0.52
1:D:259:ASP:O	1:D:263:ALA:N	2.42	0.52
1:C:174:TYR:CD1	1:C:186:LEU:CD1	2.93	0.52
1:D:216:THR:HG21	1:D:222:ALA:HB2	1.90	0.52
1:A:189:PRO:HG2	1:A:192:LEU:HD12	1.92	0.52
1:D:127:PHE:CG	1:D:130:LEU:HD22	2.45	0.51
1:A:108:ARG:HD2	1:A:132:ASN:HB3	1.91	0.51
1:C:251:LEU:O	1:C:253:ALA:N	2.43	0.51
1:A:131:THR:O	1:A:133:GLU:N	2.43	0.51
1:B:135:HIS:CD2	1:B:137:THR:HB	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:ARG:NH2	1:D:131:THR:O	2.44	0.51
1:C:135:HIS:CD2	1:C:136:PRO:HD2	2.46	0.51
1:D:54:GLU:O	1:D:80:PRO:HB3	2.10	0.51
1:C:161:TYR:HA	1:C:230:HIS:O	2.10	0.51
1:A:135:HIS:CG	1:A:136:PRO:HD2	2.46	0.51
1:A:127:PHE:HB3	1:A:130:LEU:HB2	1.92	0.50
1:A:67:ALA:HB1	1:A:326:LYS:HB2	1.92	0.50
1:A:213:LEU:C	1:A:214:THR:HG22	2.32	0.50
1:A:8:ARG:HB2	1:A:112:GLN:OE1	2.11	0.50
1:C:27:MET:HG2	1:C:327:ALA:HB1	1.93	0.50
1:C:256:VAL:O	1:C:302:VAL:HA	2.12	0.50
1:C:14:MET:HG2	1:C:175:LEU:HD21	1.92	0.50
1:D:161:TYR:CE1	1:D:231:THR:HA	2.46	0.50
1:D:322:MET:HE1	1:D:323:HIS:CE1	2.47	0.49
1:D:195:GLU:N	1:D:195:GLU:OE1	2.45	0.49
1:A:116:ASN:O	1:A:120:GLU:OE1	2.31	0.49
1:B:87:TYR:O	1:D:283:THR:HB	2.13	0.48
1:C:95:ALA:HB1	1:C:118:LEU:HD22	1.95	0.48
1:C:205:PHE:C	1:C:207:LYS:H	2.16	0.48
1:D:95:ALA:HB1	1:D:118:LEU:HD22	1.94	0.48
1:D:130:LEU:HD21	1:D:328:VAL:HG11	1.96	0.48
1:B:130:LEU:HD12	1:B:135:HIS:CE1	2.48	0.48
1:C:146:MET:HG2	1:C:228:PHE:CD1	2.49	0.48
1:C:189:PRO:HD3	1:C:254:TYR:CE1	2.48	0.48
1:D:134:PHE:CE1	1:D:169:MET:HG2	2.47	0.48
1:D:146:MET:O	1:D:150:THR:OG1	2.28	0.48
1:C:216:THR:OG1	1:C:217:ASP:N	2.45	0.48
1:C:223:ALA:O	1:C:264:THR:HA	2.14	0.48
1:C:251:LEU:O	1:C:254:TYR:N	2.44	0.48
1:B:10:LEU:HD12	1:B:10:LEU:O	2.13	0.47
1:B:130:LEU:HD12	1:B:135:HIS:NE2	2.29	0.47
1:C:326:LYS:O	1:C:330:VAL:HG23	2.15	0.47
1:C:216:THR:HG21	1:C:221:THR:HG23	1.95	0.47
1:A:154:THR:O	1:A:157:ILE:HG13	2.15	0.47
1:A:64:PHE:HE2	1:A:130:LEU:HD23	1.80	0.47
1:A:190:LYS:HE2	1:A:217:ASP:OD2	2.15	0.47
1:D:158:LYS:HB2	1:D:226:VAL:HA	1.96	0.46
1:B:135:HIS:HD2	1:B:137:THR:H	1.63	0.46
1:D:234:TRP:CD1	1:D:235:VAL:N	2.84	0.46
1:D:234:TRP:CG	1:D:251:LEU:HD13	2.50	0.46
1:D:187:CYS:SG	1:D:219:VAL:HA	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ARG:HH11	1:A:321:ARG:HG3	1.80	0.46
1:A:113:GLU:HG2	1:A:114:ILE:N	2.31	0.45
1:A:130:LEU:HD12	1:A:135:HIS:CE1	2.50	0.45
1:B:53:PHE:HZ	1:B:131:THR:HG21	1.81	0.45
1:C:108:ARG:HD2	1:C:131:THR:O	2.17	0.45
1:C:190:LYS:HA	1:C:193:TRP:NE1	2.31	0.45
1:C:251:LEU:C	1:C:253:ALA:H	2.19	0.45
1:C:45:LEU:HD12	1:C:45:LEU:HA	1.84	0.45
1:D:292:LYS:HB2	1:D:293:TYR:CD1	2.52	0.45
1:A:106:GLU:HG2	1:A:127:PHE:HB2	1.99	0.45
1:C:196:ALA:HA	1:C:199:LEU:HD12	1.98	0.45
1:A:266:ASN:OD1	1:A:266:ASN:C	2.53	0.45
1:B:7:ASN:O	1:B:11:LEU:HD23	2.17	0.44
1:C:140:LEU:O	1:C:141:ALA:C	2.56	0.44
1:D:206:ALA:CB	1:D:211:ALA:HB3	2.47	0.44
1:C:327:ALA:O	1:C:331:SER:OG	2.35	0.44
1:B:283:THR:HB	1:C:87:TYR:O	2.17	0.44
1:C:187:CYS:HA	1:C:216:THR:O	2.18	0.44
1:A:133:GLU:C	1:A:135:HIS:N	2.71	0.43
1:A:322:MET:HE3	1:A:326:LYS:CE	2.47	0.43
1:C:251:LEU:C	1:C:253:ALA:N	2.72	0.43
1:D:196:ALA:HA	1:D:199:LEU:HD12	1.99	0.43
1:A:193:TRP:CG	1:A:215:ILE:HD11	2.53	0.43
1:A:335:ASN:O	1:A:336:ILE:HB	2.18	0.43
1:B:193:TRP:CG	1:B:215:ILE:HD11	2.53	0.43
1:C:210:GLY:O	1:C:212:ARG:NH2	2.48	0.43
1:C:256:VAL:HA	1:C:260:LEU:HD23	2.00	0.43
1:D:106:GLU:OE2	1:D:130:LEU:N	2.52	0.43
1:D:231:THR:OG1	1:D:232:ASP:O	2.36	0.43
1:B:110:PHE:O	1:B:114:ILE:HD11	2.18	0.43
1:C:127:PHE:CG	1:C:130:LEU:HD22	2.54	0.43
1:D:173:LEU:HD21	1:D:230:HIS:CD2	2.54	0.43
1:D:188:ALA:O	1:D:217:ASP:HB3	2.19	0.43
1:C:22:THR:O	1:C:25:LEU:N	2.51	0.43
1:C:271:PHE:CZ	1:C:273:HIS:HB2	2.53	0.43
1:D:136:PRO:HG2	1:D:137:THR:H	1.83	0.43
1:A:260:LEU:HD12	1:A:260:LEU:C	2.40	0.42
1:B:97:VAL:HG11	1:D:59:ARG:HG2	2.02	0.42
1:C:135:HIS:CD2	1:C:136:PRO:CD	3.03	0.42
1:A:51:LEU:HD12	1:A:51:LEU:HA	1.80	0.42
1:C:51:LEU:HD13	1:C:64:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:LEU:O	1:C:178:ALA:HB3	2.19	0.42
1:D:168:ASN:OD1	1:D:168:ASN:N	2.52	0.42
1:C:160:ALA:HA	1:C:185:ARG:O	2.19	0.42
1:D:158:LYS:HA	1:D:183:ASP:HB3	2.01	0.42
1:D:175:LEU:O	1:D:178:ALA:HB3	2.19	0.42
1:C:111:GLY:C	1:C:113:GLU:H	2.23	0.42
1:A:49:ILE:HG21	1:A:64:PHE:HE1	1.84	0.42
1:A:57:SER:HB2	1:A:108:ARG:NH2	2.35	0.42
1:B:90:SER:O	1:B:93:ASP:HB2	2.19	0.42
1:C:107:TYR:HE2	1:C:118:LEU:HD23	1.85	0.42
1:D:234:TRP:CD1	1:D:235:VAL:HG13	2.55	0.42
1:D:281:SER:OG	1:D:290:THR:HG21	2.19	0.42
1:B:133:GLU:O	1:B:135:HIS:HB2	2.19	0.41
1:D:285:VAL:HG12	1:D:289:ILE:HD12	2.01	0.41
1:B:128:ASN:HA	3:B:401:HOH:O	2.19	0.41
1:D:52:ILE:O	1:D:107:TYR:HA	2.21	0.41
1:D:201:THR:O	1:D:204:ASP:HB2	2.20	0.41
1:B:318:ALA:O	1:B:321:ARG:HB3	2.21	0.41
1:D:235:VAL:O	1:D:235:VAL:HG23	2.21	0.41
1:C:146:MET:SD	1:C:230:HIS:HE1	2.44	0.41
1:C:189:PRO:O	1:C:193:TRP:CD1	2.73	0.41
1:D:27:MET:HG2	1:D:327:ALA:HB1	2.02	0.41
1:D:206:ALA:HA	1:D:211:ALA:HB3	2.03	0.41
1:B:129:GLY:C	1:B:131:THR:H	2.24	0.41
1:C:10:LEU:O	1:C:10:LEU:CG	2.66	0.41
1:A:78:ILE:CG2	1:A:83:SER:HB3	2.51	0.41
1:A:158:LYS:O	1:A:227:ASP:N	2.50	0.41
1:A:244:TRP:CZ3	1:A:289:ILE:HG12	2.56	0.41
1:D:293:TYR:CD1	1:D:293:TYR:N	2.88	0.41
1:C:107:TYR:HE2	1:C:118:LEU:CD2	2.34	0.40
1:A:228:PHE:CD1	1:A:270:LYS:HB2	2.55	0.40
1:B:45:LEU:HD12	1:B:45:LEU:HA	1.88	0.40
1:C:273:HIS:CD2	1:C:277:ALA:CB	3.02	0.40
1:D:301:GLU:HG2	1:D:302:VAL:HG12	2.03	0.40
1:A:161:TYR:OH	1:A:232:ASP:HB3	2.21	0.40
1:A:269:VAL:O	1:A:270:LYS:HD3	2.22	0.40
1:C:61:ARG:O	1:C:64:PHE:N	2.55	0.40
1:C:157:ILE:HB	1:C:182:MET:HE3	2.03	0.40
1:C:205:PHE:O	1:C:207:LYS:N	2.54	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	327/336 (97%)	297 (91%)	23 (7%)	7 (2%)	7	13
1	B	328/336 (98%)	292 (89%)	27 (8%)	9 (3%)	5	8
1	C	326/336 (97%)	283 (87%)	35 (11%)	8 (2%)	5	9
1	D	323/336 (96%)	278 (86%)	33 (10%)	12 (4%)	3	4
All	All	1304/1344 (97%)	1150 (88%)	118 (9%)	36 (3%)	5	7

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	PHE
1	A	224	LYS
1	A	269	VAL
1	B	87	TYR
1	B	128	ASN
1	B	132	ASN
1	B	134	PHE
1	D	133	GLU
1	D	135	HIS
1	A	132	ASN
1	A	263	ALA
1	C	206	ALA
1	C	209	SER
1	C	252	MET
1	D	111	GLY
1	D	121	TYR
1	B	122	ALA
1	D	136	PRO
1	D	219	VAL
1	D	224	LYS
1	B	120	GLU
1	B	121	TYR

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Mol	Chain	Res	Type
1	D	56	THR
1	D	57	SER
1	D	275	LEU
1	B	111	GLY
1	B	130	LEU
1	C	210	GLY
1	C	243	SER
1	A	242	GLU
1	C	112	GLN
1	D	282	ASP
1	D	300	ILE
1	C	233	VAL
1	C	310	PRO
1	A	300	ILE

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	278/285 (98%)	257 (92%)	21 (8%)	13	26
1	B	279/285 (98%)	263 (94%)	16 (6%)	20	41
1	C	277/285 (97%)	249 (90%)	28 (10%)	7	14
1	D	272/285 (95%)	244 (90%)	28 (10%)	7	13
All	All	1106/1140 (97%)	1013 (92%)	93 (8%)	11	21

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	10	LEU
1	A	58	THR
1	A	59	ARG
1	A	82	SER
1	A	90	SER
1	A	101	MET

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Mol	Chain	Res	Type
1	A	114	ILE
1	A	116	ASN
1	A	118	LEU
1	A	124	ILE
1	A	185	ARG
1	A	197	ASP
1	A	201	THR
1	A	212	ARG
1	A	214	THR
1	A	260	LEU
1	A	292	LYS
1	A	316	GLU
1	A	321	ARG
1	A	322	MET
1	B	10	LEU
1	B	11	LEU
1	B	13	LEU
1	B	55	LYS
1	B	56	THR
1	B	59	ARG
1	B	81	ASN
1	B	114	ILE
1	B	130	LEU
1	B	137	THR
1	B	147	ARG
1	B	208	GLU
1	B	212	ARG
1	B	242	GLU
1	B	291	GLU
1	B	324	THR
1	C	10	LEU
1	C	27	MET
1	C	59	ARG
1	C	99	SER
1	C	113	GLU
1	C	114	ILE
1	C	116	ASN
1	C	123	ASP
1	C	132	ASN
1	C	148	GLU
1	C	153	SER
1	C	171	ARG

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Mol	Chain	Res	Type
1	C	207	LYS
1	C	209	SER
1	C	212	ARG
1	C	216	THR
1	C	229	VAL
1	C	235	VAL
1	C	236	SER
1	C	252	MET
1	C	255	GLN
1	C	258	MET
1	C	259	ASP
1	C	260	LEU
1	C	261	ILE
1	C	303	THR
1	C	324	THR
1	C	331	SER
1	D	14	MET
1	D	27	MET
1	D	56	THR
1	D	59	ARG
1	D	85	ILE
1	D	89	GLU
1	D	114	ILE
1	D	120	GLU
1	D	124	ILE
1	D	134	PHE
1	D	135	HIS
1	D	148	GLU
1	D	150	THR
1	D	158	LYS
1	D	190	LYS
1	D	191	ASP
1	D	201	THR
1	D	212	ARG
1	D	231	THR
1	D	243	SER
1	D	252	MET
1	D	255	GLN
1	D	264	THR
1	D	282	ASP
1	D	293	TYR
1	D	304	GLU

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Mol	Chain	Res	Type
1	D	317	GLN
1	D	324	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	132	ASN
1	B	135	HIS
1	C	230	HIS
1	D	279	HIS
1	D	323	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	SO4	A	401	-	4,4,4	0.37	0	6,6,6	0.40	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	329/336 (97%)	0.00	10 (3%) 50 43	36, 67, 124, 176	0
1	B	330/336 (98%)	-0.04	11 (3%) 46 39	41, 64, 139, 191	0
1	C	328/336 (97%)	0.40	33 (10%) 7 4	47, 92, 149, 182	0
1	D	325/336 (96%)	0.53	40 (12%) 4 2	49, 92, 153, 177	0
All	All	1312/1344 (97%)	0.22	94 (7%) 15 11	36, 77, 148, 191	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	118	LEU	8.6
1	D	115	VAL	6.5
1	B	8	ARG	5.1
1	D	289	ILE	5.1
1	B	121	TYR	5.0
1	C	294	PRO	5.0
1	D	118	LEU	4.8
1	C	244	TRP	4.8
1	C	234	TRP	4.7
1	D	294	PRO	4.4
1	B	9	ASP	4.1
1	C	235	VAL	3.9
1	D	112	GLN	3.7
1	C	192	LEU	3.7
1	A	115	VAL	3.6
1	C	241	ILE	3.5
1	D	254	TYR	3.5
1	A	11	LEU	3.4
1	A	118	LEU	3.4
1	D	297	ALA	3.4
1	A	116	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	186	LEU	3.3
1	D	195	GLU	3.3
1	C	278	PHE	3.3
1	C	251	LEU	3.2
1	D	174	TYR	3.1
1	C	247	ARG	3.1
1	C	286	GLY	3.1
1	C	110	PHE	3.1
1	C	296	LEU	3.1
1	B	7	ASN	3.1
1	D	256	VAL	3.1
1	D	162	PHE	3.0
1	D	287	LYS	3.0
1	C	121	TYR	3.0
1	D	87	TYR	3.0
1	B	10	LEU	3.0
1	C	297	ALA	3.0
1	B	117	GLU	3.0
1	C	174	TYR	2.9
1	C	196	ALA	2.9
1	C	11	LEU	2.8
1	C	238	GLY	2.8
1	D	215	ILE	2.8
1	D	282	ASP	2.8
1	D	198	PHE	2.8
1	D	190	LYS	2.8
1	B	120	GLU	2.7
1	D	200	ALA	2.7
1	D	244	TRP	2.7
1	C	288	LYS	2.7
1	D	196	ALA	2.7
1	D	259	ASP	2.7
1	D	222	ALA	2.7
1	D	285	VAL	2.7
1	D	121	TYR	2.7
1	C	237	MET	2.6
1	D	197	ASP	2.6
1	D	283	THR	2.6
1	C	242	GLU	2.5
1	D	291	GLU	2.5
1	C	289	ILE	2.5
1	D	250	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	282	ASP	2.5
1	D	221	THR	2.5
1	D	120	GLU	2.4
1	A	196	ALA	2.4
1	A	121	TYR	2.4
1	D	193	TRP	2.4
1	C	198	PHE	2.4
1	D	119	ALA	2.4
1	D	116	ASN	2.3
1	D	194	PRO	2.3
1	A	132	ASN	2.3
1	C	15	HIS	2.3
1	C	115	VAL	2.2
1	C	112	GLN	2.2
1	C	243	SER	2.2
1	B	134	PHE	2.2
1	B	112	GLN	2.2
1	A	198	PHE	2.2
1	C	14	MET	2.2
1	D	288	LYS	2.1
1	B	11	LEU	2.1
1	A	112	GLN	2.1
1	C	236	SER	2.1
1	C	285	VAL	2.1
1	D	123	ASP	2.1
1	A	192	LEU	2.1
1	C	246	GLU	2.1
1	D	135	HIS	2.1
1	C	191	ASP	2.0
1	D	203	ALA	2.0
1	D	86	GLY	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 monosaccharides 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(Å ²)	Q<0.9
2	SO4	A	401	5/5	0.97	0.18	57,62,75,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.