



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:16 AM UTC

PDB ID : 7XJT / pdb_00007xjt
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	:	4-5-2 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

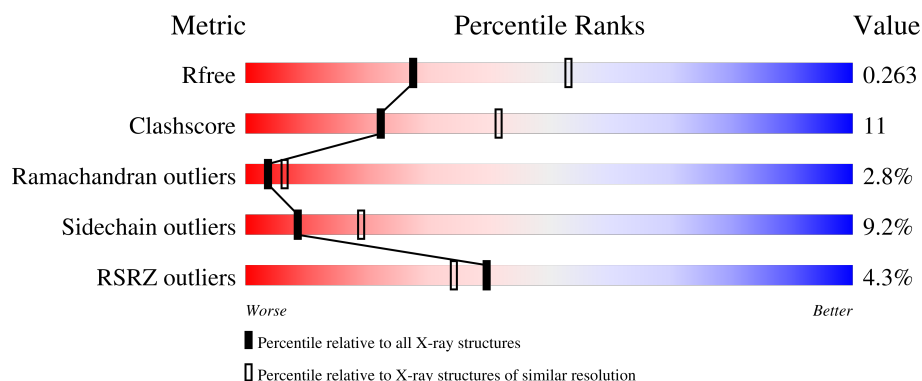
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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	2% 72% 23% ..
1	B	336	2% 80% 15% ..
1	C	336	6% 63% 30% ..
1	D	336	7% 60% 30% 6% .

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

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

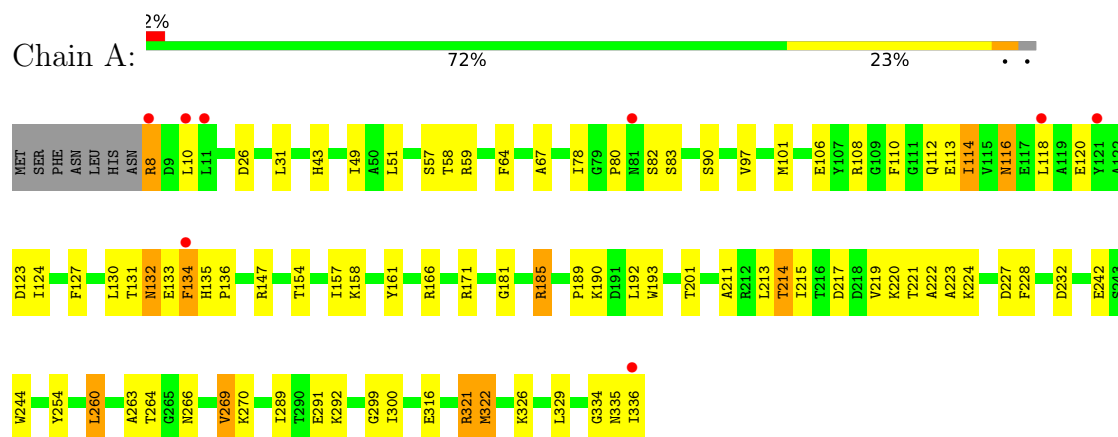
- Molecule 3 is water.

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

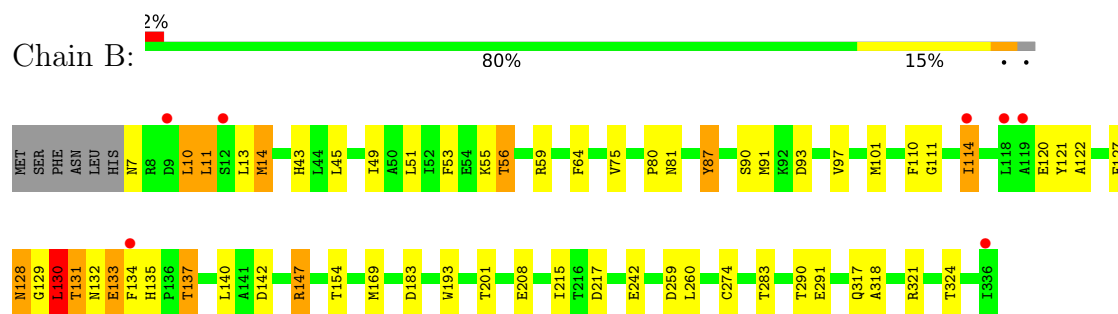
3 Residue-property plots [i](#)

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.

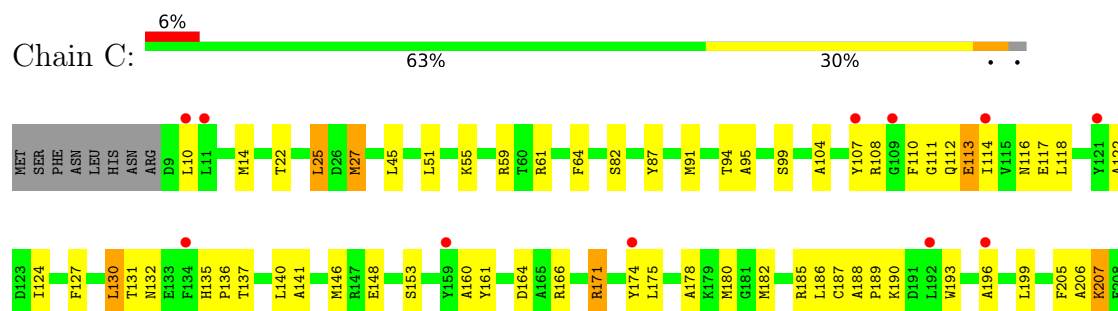
• Molecule 1: Ornithine carbamoyltransferases

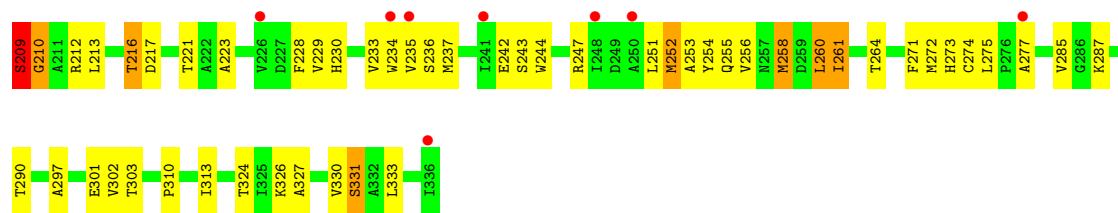


• Molecule 1: Ornithine carbamoyltransferases

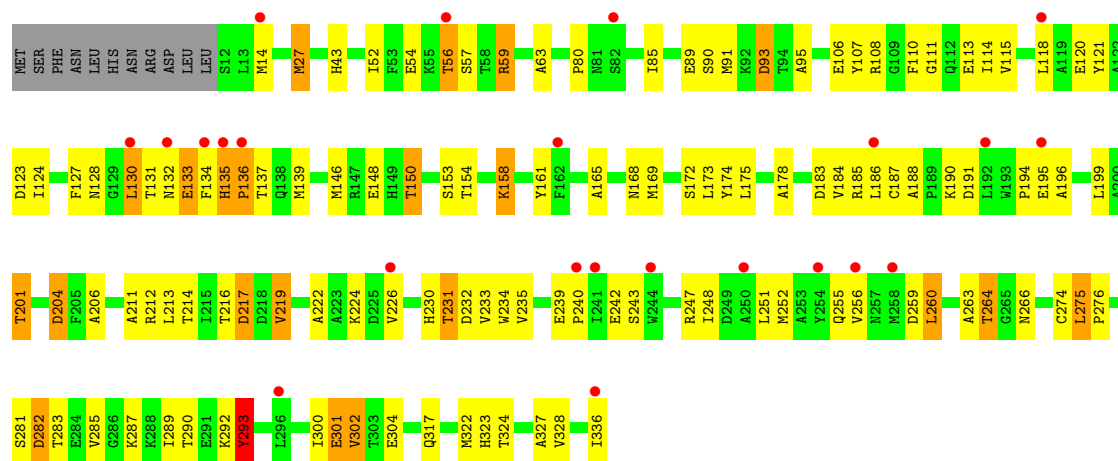


• Molecule 1: Ornithine carbamoyltransferases





● Molecule 1: Ornithine carbamoyltransferases



4 Data and refinement statistics

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 46.53 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.53-2.60) 99.7 (46.53-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.201 , 0.264 0.203 , 0.263	Depositor DCC
R_{free} test set	3460 reflections (5.40%)	wwPDB-VP
Wilson B-factor (Å ²)	66.0	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
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 $-h-k,k,-l$	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10433	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage'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	1.15	4/2659 (0.2%)	1.57	8/3591 (0.2%)
1	B	1.11	1/2667 (0.0%)	1.51	9/3602 (0.2%)
1	C	1.14	0/2648	1.52	4/3577 (0.1%)
1	D	1.13	1/2617 (0.0%)	1.57	9/3535 (0.3%)
All	All	1.13	6/10591 (0.1%)	1.54	30/14305 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	VAL	C-O	5.58	1.30	1.24
1	A	329	LEU	C-O	-5.49	1.17	1.24
1	D	43	HIS	CE1-NE2	5.47	1.38	1.32
1	A	43	HIS	CE1-NE2	5.38	1.38	1.32
1	B	43	HIS	CE1-NE2	5.14	1.37	1.32
1	A	334	GLY	C-O	5.03	1.30	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	PRO	CA-C-N	8.29	132.49	120.38
1	B	80	PRO	C-N-CA	8.29	132.49	120.38
1	B	140	LEU	N-CA-C	-6.37	104.42	111.36
1	B	131	THR	CA-C-N	6.08	133.16	121.54
1	B	131	THR	C-N-CA	6.08	133.16	121.54
1	D	123	ASP	CA-CB-CG	5.96	118.56	112.60
1	D	93	ASP	CA-CB-CG	5.86	118.46	112.60
1	C	25	LEU	CA-C-N	5.84	128.03	120.44
1	C	25	LEU	C-N-CA	5.84	128.03	120.44
1	A	299	GLY	CA-C-O	-5.79	118.14	122.37
1	A	80	PRO	CA-C-N	5.69	129.35	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	PRO	C-N-CA	5.69	129.35	120.82
1	A	123	ASP	CA-CB-CG	5.63	118.23	112.60
1	C	137	THR	N-CA-C	-5.60	105.08	111.07
1	D	336	ILE	CA-C-O	5.55	130.23	120.80
1	A	221	THR	CA-C-N	5.54	127.70	120.28
1	A	221	THR	C-N-CA	5.54	127.70	120.28
1	D	204	ASP	CA-C-N	5.31	127.39	120.28
1	D	204	ASP	C-N-CA	5.31	127.39	120.28
1	B	217	ASP	CA-CB-CG	5.29	117.89	112.60
1	D	217	ASP	CA-CB-CG	5.24	117.83	112.60
1	B	127	PHE	CB-CA-C	5.22	119.14	110.78
1	D	248	ILE	CA-C-N	5.21	127.57	120.54
1	D	248	ILE	C-N-CA	5.21	127.57	120.54
1	C	188	ALA	N-CA-C	5.12	112.83	108.22
1	B	259	ASP	CA-CB-CG	5.09	117.69	112.60
1	D	293	TYR	CB-CA-C	5.07	115.80	110.17
1	B	290	THR	CA-CB-OG1	-5.04	102.04	109.60
1	A	134	PHE	CA-C-N	5.02	129.70	121.57
1	A	134	PHE	C-N-CA	5.02	129.70	121.57

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	2607	0	2552	52	0
1	B	2615	0	2558	31	0
1	C	2596	0	2539	74	0
1	D	2565	0	2505	65	0
2	A	5	0	0	0	0
3	A	7	0	0	0	0
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	217	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 11.

All (217) 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:O	1:A:260:LEU:HD12	1.85	0.76
1:A:110:PHE:O	1:A:114:ILE:HD11	1.87	0.75
1:C:22:THR:HG22	1:C:180:MET:HE1	1.70	0.74
1:A:322:MET:HE2	1:A:322:MET:C	2.14	0.73
1:A:223:ALA:O	1:A:264:THR:HA	1.89	0.72
1:A:322:MET:HE1	1:A:326:LYS:HE3	1.72	0.71
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:D:322:MET:HE1	1:D:323:HIS:CE1	2.27	0.69
1:C:237:MET:HE1	1:C:285:VAL:HG21	1.75	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:C:146:MET:CE	1:C:182:MET:HE1	2.25	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: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:A:322:MET:HE2	1:A:322:MET:O	1.98	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:HH11	1:A:321:ARG:CG	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
1:C:95:ALA:HB1	1:C:118:LEU:HD13	1.82	0.61
1:C:10:LEU:HG	1:C:10:LEU:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ILE:HG13	1:C:313:ILE:O	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:D:264:THR:C	1:D:266:ASN:H	2.12	0.57
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:A:67:ALA:HA	1:A:322:MET:HE3	1.87	0.57
1:C:230:HIS:HA	1:C:272:MET:O	2.05	0.57
1:C:166:ARG:O	1:C:171:ARG:CD	2.53	0.56
1:C:274:CYS:O	1:C:275:LEU:HB2	2.05	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:A:213:LEU:C	1:A:214:THR:HG22	2.32	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:D:91:MET:HE1	1:D:110:PHE:CD2	2.42	0.54
1:C:164:ASP:OD2	1:C:247:ARG:NH2	2.41	0.54
1:D:91:MET:HE1	1:D:110:PHE:CG	2.42	0.54
1:C:205:PHE:C	1:C:207:LYS:H	2.16	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:B:169:MET:HE2	1:B:274:CYS:HB3	1.91	0.53
1:C:104:ALA:HB2	1:C:333:LEU:HD21	1.90	0.53
1:B:14:MET:HE2	1:B:201:THR:HG21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:146:MET:O	1:D:150:THR:OG1	2.28	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
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: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:251:LEU:C	1:C:253:ALA:H	2.19	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:A:266:ASN:C	1:A:266:ASN:OD1	2.53	0.49
1:C:140:LEU:O	1:C:141:ALA:C	2.56	0.49
1:D:195:GLU:OE1	1:D:195:GLU:N	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: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:C:251:LEU:C	1:C:253:ALA:N	2.72	0.48
1:D:134:PHE:CE1	1:D:169:MET:HG2	2.47	0.48
1:C:91:MET:HE1	1:C:110:PHE:CD1	2.49	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:A:260:LEU:HD12	1:A:260:LEU:C	2.40	0.47
1:A:133:GLU:C	1:A:135:HIS:N	2.71	0.47
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:111:GLY:C	1:C:113:GLU:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:169:MET:HE2	1:D:274:CYS:HB3	1.95	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
1:A:321:ARG:HH11	1:A:321:ARG:HG3	1.80	0.46
1:B:91:MET:HE1	1:B:110:PHE:CD1	2.51	0.46
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:D:322:MET:HE3	1:D:323:HIS:CE1	2.52	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:B:101:MET:HE1	1:D:63:ALA:N	2.32	0.44
1:B:7:ASN:O	1:B:11:LEU:HD23	2.17	0.44
1:B:129:GLY:C	1:B:131:THR:H	2.24	0.44
1:D:206:ALA:CB	1:D:211:ALA:HB3	2.47	0.44
1:A:113:GLU:HG2	1:A:114:ILE:N	2.31	0.44
1:B:260:LEU:C	1:B:260:LEU:HD23	2.42	0.44
1:C:146:MET:HE2	1:C:182:MET:HE1	1.96	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:B:183:ASP:C	1:B:183:ASP:OD1	2.60	0.44
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:335:ASN:O	1:A:336:ILE:HB	2.18	0.43
1:C:242:GLU:C	1:C:244:TRP:H	2.27	0.43
1:C:271:PHE:CZ	1:C:273:HIS:HB2	2.53	0.43
1:D:91:MET:HE1	1:D:110:PHE:CD1	2.54	0.43
1:D:136:PRO:HG2	1:D:137:THR:H	1.83	0.43
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
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: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:D:322:MET:HE3	1:D:322:MET:HB3	1.91	0.42
1:C:107:TYR:HE2	1:C:118:LEU:HD23	1.85	0.42
1:C:301:GLU:CD	1:C:301:GLU:H	2.28	0.42
1:C:122:ALA:C	1:C:124:ILE:H	2.28	0.42
1:D:234:TRP:CD1	1:D:235:VAL:HG13	2.55	0.42
1:D:275:LEU:HA	1:D:276:PRO:C	2.45	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:A:67:ALA:CA	1:A:322:MET:HE3	2.49	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:C:205:PHE:C	1:C:207:LYS:N	2.77	0.41
1:D:153:SER:O	1:D:154:THR:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ALA:HA	1:D:211:ALA:HB3	2.03	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:A:213:LEU:C	1:A:214:THR:CG2	2.94	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: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%)	5	11
1	B	328/336 (98%)	292 (89%)	27 (8%)	9 (3%)	4	7
1	C	326/336 (97%)	283 (87%)	35 (11%)	8 (2%)	4	8
1	D	323/336 (96%)	278 (86%)	33 (10%)	12 (4%)	2	3
All	All	1304/1344 (97%)	1150 (88%)	118 (9%)	36 (3%)	4	6

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
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 ⓘ

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%)	256 (92%)	22 (8%)	11	26
1	B	279/285 (98%)	262 (94%)	17 (6%)	17	37
1	C	277/285 (97%)	249 (90%)	28 (10%)	7	15
1	D	272/285 (95%)	237 (87%)	35 (13%)	4	8
All	All	1106/1140 (97%)	1004 (91%)	102 (9%)	8	19

All (102) 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
1	A	114	ILE
1	A	116	ASN
1	A	118	LEU
1	A	124	ILE
1	A	185	ARG
1	A	201	THR
1	A	214	THR
1	A	219	VAL
1	A	220	LYS
1	A	260	LEU
1	A	291	GLU
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	14	MET
1	B	55	LYS
1	B	56	THR
1	B	59	ARG
1	B	81	ASN
1	B	114	ILE

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Mol	Chain	Res	Type
1	B	130	LEU
1	B	133	GLU
1	B	137	THR
1	B	147	ARG
1	B	208	GLU
1	B	242	GLU
1	B	291	GLU
1	B	324	THR
1	C	27	MET
1	C	55	LYS
1	C	59	ARG
1	C	94	THR
1	C	99	SER
1	C	113	GLU
1	C	114	ILE
1	C	116	ASN
1	C	130	LEU
1	C	132	ASN
1	C	148	GLU
1	C	153	SER
1	C	171	ARG
1	C	207	LYS
1	C	209	SER
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	260	LEU
1	C	261	ILE
1	C	287	LYS
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

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Mol	Chain	Res	Type
1	D	113	GLU
1	D	114	ILE
1	D	120	GLU
1	D	124	ILE
1	D	130	LEU
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	233	VAL
1	D	242	GLU
1	D	243	SER
1	D	252	MET
1	D	255	GLN
1	D	260	LEU
1	D	264	THR
1	D	282	ASP
1	D	287	LYS
1	D	293	TYR
1	D	301	GLU
1	D	302	VAL
1	D	304	GLU
1	D	317	GLN
1	D	324	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	168	ASN
1	B	116	ASN
1	B	132	ASN
1	B	135	HIS
1	B	138	GLN
1	C	112	GLN
1	C	116	ASN
1	C	230	HIS

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Mol	Chain	Res	Type
1	D	128	ASN
1	D	138	GLN
1	D	149	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 oligosaccharides 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	0.34	0	6,6,6	0.35	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.05	8 (2%)	59 54	36, 67, 124, 176	0
1	B	330/336 (98%)	-0.05	7 (2%)	63 58	41, 64, 139, 191	0
1	C	328/336 (97%)	0.57	19 (5%)	29 23	47, 92, 149, 182	0
1	D	325/336 (96%)	0.59	23 (7%)	22 17	49, 92, 153, 177	0
All	All	1312/1344 (97%)	0.29	57 (4%)	40 34	36, 77, 148, 191	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	336	ILE	6.4
1	B	134	PHE	5.2
1	C	336	ILE	5.1
1	B	336	ILE	4.8
1	A	134	PHE	4.5
1	D	130	LEU	3.7
1	A	118	LEU	3.6
1	A	11	LEU	3.4
1	D	135	HIS	3.4
1	D	134	PHE	3.3
1	C	134	PHE	3.3
1	B	118	LEU	3.1
1	C	235	VAL	3.0
1	A	121	TYR	2.9
1	B	119	ALA	2.9
1	B	9	ASP	2.8
1	C	174	TYR	2.7
1	D	240	PRO	2.5
1	D	192	LEU	2.5
1	C	107	TYR	2.5
1	A	10	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	10	LEU	2.5
1	D	132	ASN	2.5
1	D	82	SER	2.5
1	A	336	ILE	2.4
1	D	162	PHE	2.4
1	D	241	ILE	2.4
1	D	118	LEU	2.4
1	C	109	GLY	2.4
1	C	121	TYR	2.4
1	D	258	MET	2.4
1	C	159	TYR	2.4
1	C	11	LEU	2.3
1	C	226	VAL	2.3
1	C	250	ALA	2.3
1	D	195	GLU	2.3
1	C	192	LEU	2.3
1	D	256	VAL	2.3
1	C	196	ALA	2.2
1	A	8	ARG	2.2
1	D	296	LEU	2.2
1	D	136	PRO	2.2
1	B	114	ILE	2.1
1	D	254	TYR	2.1
1	D	14	MET	2.1
1	A	81	ASN	2.1
1	B	12	SER	2.1
1	D	186	LEU	2.1
1	D	56	THR	2.1
1	C	241	ILE	2.1
1	D	244	TRP	2.1
1	C	114	ILE	2.1
1	C	248	ILE	2.1
1	D	226	VAL	2.0
1	C	277	ALA	2.0
1	D	250	ALA	2.0
1	C	234	TRP	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 [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
2	SO4	A	401	5/5	0.96	0.11	57,62,75,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.