



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:43 AM UTC

PDB ID : 3MZ1 / pdb_00003mz1
Title : The crystal structure of a possible TRANSCRIPTION REGULATOR PROTEIN from Sinorhizobium meliloti 1021
Authors : Tan, K.; Xu, X.; Cui, H.; Chin, S.; Savchenko, A.; Edwards, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2010-05-11
Resolution : 1.88 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

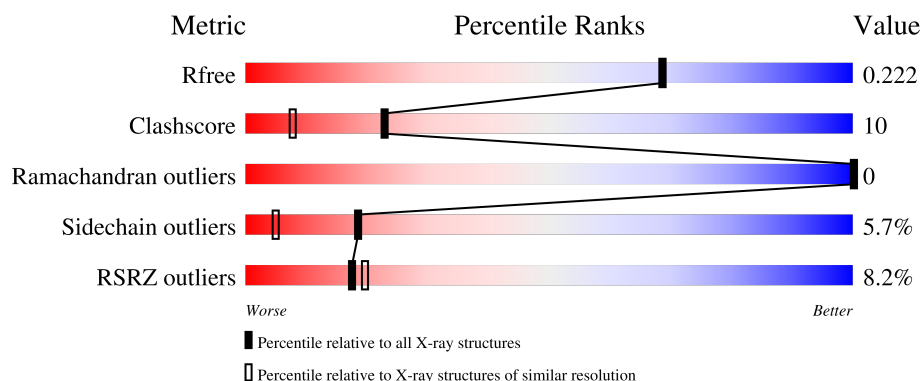
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

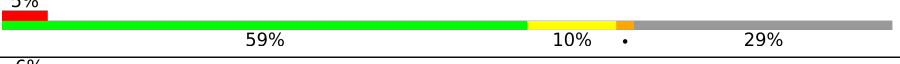
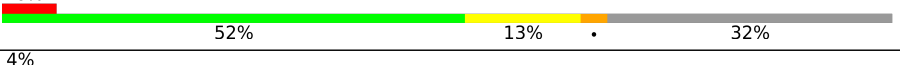
The reported resolution of this entry is 1.88 Å.

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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	300	
1	B	300	
1	C	300	
1	D	300	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7104 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 Putative transcriptional regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	Se	0	3	0
			1685	1074	303	298	3	7			
1	B	212	Total	C	N	O	S	Se	0	3	0
			1704	1088	302	304	3	7			
1	C	204	Total	C	N	O	S	Se	0	2	0
			1629	1042	288	288	4	7			
1	D	212	Total	C	N	O	S	Se	0	5	0
			1722	1099	308	305	3	7			

There are 20 discrepancies between the modelled and reference sequences:

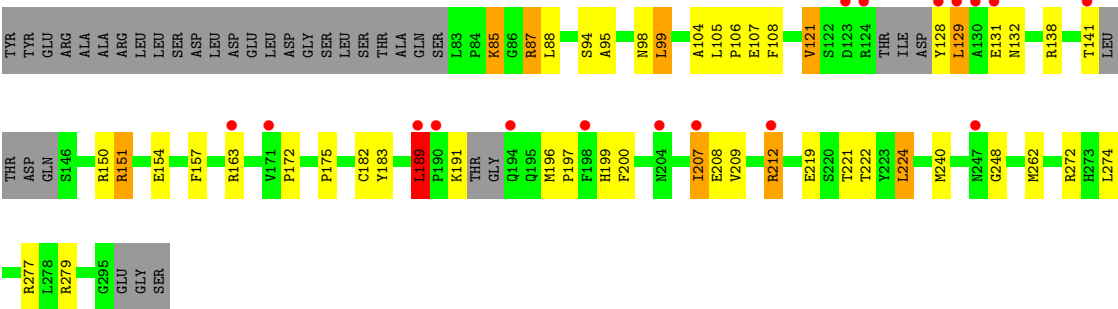
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP Q92SG7
A	0	GLY	-	expression tag	UNP Q92SG7
A	215	MSE	VAL	cloning artifact	UNP Q92SG7
A	297	GLY	-	expression tag	UNP Q92SG7
A	298	SER	-	expression tag	UNP Q92SG7
B	-1	GLN	-	expression tag	UNP Q92SG7
B	0	GLY	-	expression tag	UNP Q92SG7
B	215	MSE	VAL	cloning artifact	UNP Q92SG7
B	297	GLY	-	expression tag	UNP Q92SG7
B	298	SER	-	expression tag	UNP Q92SG7
C	-1	GLN	-	expression tag	UNP Q92SG7
C	0	GLY	-	expression tag	UNP Q92SG7
C	215	MSE	VAL	cloning artifact	UNP Q92SG7
C	297	GLY	-	expression tag	UNP Q92SG7
C	298	SER	-	expression tag	UNP Q92SG7
D	-1	GLN	-	expression tag	UNP Q92SG7
D	0	GLY	-	expression tag	UNP Q92SG7
D	215	MSE	VAL	cloning artifact	UNP Q92SG7
D	297	GLY	-	expression tag	UNP Q92SG7
D	298	SER	-	expression tag	UNP Q92SG7

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

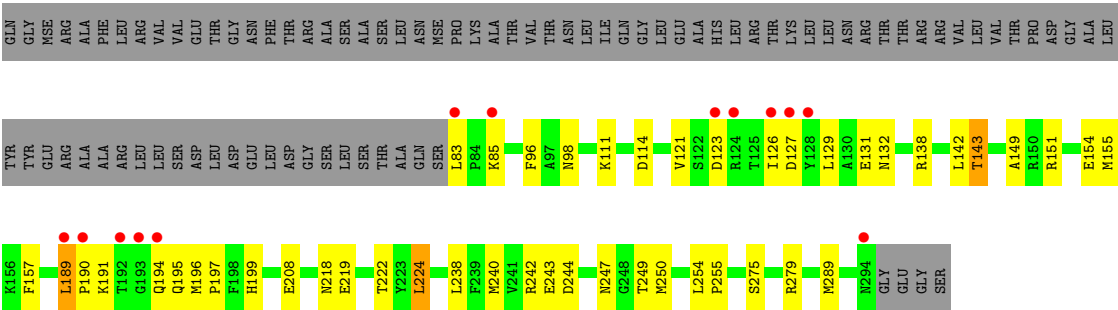
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	103	Total	O	0	0
			103	103		
3	B	90	Total	O	0	0
			90	90		
3	C	73	Total	O	0	0
			73	73		
3	D	97	Total	O	0	0
			97	97		



● Molecule 1: Putative transcriptional regulator



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.34Å 83.33Å 85.07Å 90.00° 91.65° 90.00°	Depositor
Resolution (Å)	36.42 – 1.88 36.42 – 1.88	Depositor EDS
% Data completeness (in resolution range)	93.8 (36.42-1.88) 99.2 (36.42-1.88)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.184 , 0.224 0.184 , 0.222	Depositor DCC
R_{free} test set	3817 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -h,-l,-k 0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7104	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 74.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4630e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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:
CL

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	0.46	0/1720	0.82	0/2322
1	B	0.52	1/1747 (0.1%)	0.87	0/2364
1	C	0.46	0/1666	0.82	2/2248 (0.1%)
1	D	0.49	0/1768	0.83	2/2390 (0.1%)
All	All	0.48	1/6901 (0.0%)	0.83	4/9324 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	94	SER	C-O	-5.18	1.17	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	LEU	CA-C-N	5.08	124.52	119.24
1	D	189	LEU	C-N-CA	5.08	124.52	119.24
1	C	189	LEU	CA-C-N	5.02	125.29	119.47
1	C	189	LEU	C-N-CA	5.02	125.29	119.47

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	1685	0	1690	37	0
1	B	1704	0	1720	35	0
1	C	1629	0	1631	46	0
1	D	1722	0	1744	40	0
2	D	1	0	0	0	0
3	A	103	0	0	1	0
3	B	90	0	0	1	0
3	C	73	0	0	2	0
3	D	97	0	0	1	0
All	All	7104	0	6785	141	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 10.

All (141) 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:98:ASN:HD21	1:B:222[B]:THR:HG22	1.01	1.08
1:B:272:ARG:HG2	1:B:272:ARG:HH11	1.10	1.08
1:C:98:ASN:HD21	1:D:222:THR:HG22	1.23	1.03
1:D:224:LEU:HD12	1:D:240:MSE:HE2	1.43	1.00
1:A:98:ASN:ND2	1:B:222[B]:THR:HG22	1.77	0.98
1:B:272:ARG:HH11	1:B:272:ARG:CG	1.88	0.85
1:D:151[A]:ARG:NH2	1:D:154:GLU:HG2	1.92	0.84
1:C:98:ASN:ND2	1:D:222:THR:HG22	1.91	0.84
1:C:224:LEU:HD12	1:C:240:MSE:HE2	1.56	0.84
1:D:151[A]:ARG:HH21	1:D:154:GLU:HG2	1.40	0.84
1:A:98:ASN:HD21	1:B:222[B]:THR:CG2	1.88	0.83
1:C:87:ARG:HH11	1:C:87:ARG:HB3	1.42	0.83
1:D:275:SER:O	1:D:279:ARG:HG3	1.78	0.83
1:B:272:ARG:HG2	1:B:272:ARG:NH1	1.92	0.82
1:A:146:SER:O	1:A:270:PRO:HG3	1.81	0.81
1:D:190:PRO:HG3	1:D:218:ASN:HD22	1.45	0.80
1:C:104:ALA:O	1:C:107:GLU:HG2	1.81	0.79
1:C:222:THR:HG22	1:D:98:ASN:HD21	1.51	0.74
1:B:272:ARG:O	1:B:274:LEU:HD13	1.91	0.70
1:A:121:VAL:HG21	1:B:222[B]:THR:HG21	1.72	0.70
1:C:189:LEU:HD13	1:C:191:LYS:HD3	1.74	0.69
1:D:155:MSE:HE3	1:D:157:PHE:CZ	2.29	0.68
1:C:222:THR:HG22	1:D:98:ASN:ND2	2.11	0.66
1:D:127:ASP:HB3	1:D:143:THR:OG1	1.95	0.66
1:C:98:ASN:HD21	1:D:222:THR:CG2	2.04	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:PRO:HG2	1:C:207:ILE:HD11	1.78	0.66
1:C:199:HIS:CD2	1:C:208:GLU:HB2	2.31	0.65
1:B:126:ILE:HD12	3:B:379:HOH:O	1.97	0.65
1:A:107:GLU:HG3	1:A:108:PHE:N	2.11	0.64
1:B:219:GLU:OE1	1:B:222[B]:THR:HG23	1.98	0.64
1:D:190:PRO:HG3	1:D:218:ASN:ND2	2.13	0.62
1:D:151[A]:ARG:HH21	1:D:154:GLU:CG	2.11	0.62
1:A:224:LEU:HD22	1:A:240:MSE:HE2	1.81	0.61
1:A:104:ALA:O	1:A:107:GLU:HG2	2.02	0.59
1:A:125:THR:HG22	1:A:189:LEU:HD23	1.85	0.59
1:C:87:ARG:HB3	1:C:87:ARG:NH1	2.17	0.59
1:C:172:PRO:HG3	1:C:182[A]:CYS:SG	2.43	0.58
1:B:94:SER:OG	1:B:219:GLU:OE2	2.21	0.58
1:D:189:LEU:HB2	1:D:194:GLN:HG2	1.84	0.58
1:C:212:ARG:HB3	1:C:212:ARG:NH2	2.18	0.57
1:C:85:LYS:NZ	1:C:85:LYS:HB3	2.19	0.57
1:A:222:THR:HG23	1:B:102:ILE:HD11	1.86	0.57
1:A:158:VAL:HG21	1:A:238:LEU:HD13	1.89	0.55
1:D:238:LEU:O	1:D:242[A]:ARG:HG3	2.07	0.55
1:D:224:LEU:HD11	1:D:240:MSE:HB3	1.89	0.55
1:A:189:LEU:HG	1:A:190:PRO:HD2	1.89	0.55
1:A:187:TYR:HE2	1:A:189:LEU:HD12	1.71	0.54
1:B:272:ARG:CG	1:B:272:ARG:NH1	2.56	0.54
1:C:121:VAL:HG21	1:D:222:THR:HG21	1.88	0.54
1:B:122:SER:OG	1:B:124:ARG:HG2	2.07	0.54
1:B:130:ALA:HB3	1:B:133:VAL:HG23	1.90	0.53
1:C:219:GLU:OE1	1:C:222:THR:HG23	2.08	0.53
1:D:199:HIS:HE1	1:D:208:GLU:OE1	1.91	0.53
1:C:189:LEU:HB3	1:C:191:LYS:HG3	1.91	0.53
1:C:212:ARG:HB3	1:C:212:ARG:CZ	2.40	0.52
1:D:142:LEU:HD11	1:D:149:ALA:CB	2.40	0.51
1:A:274:LEU:HG	1:A:279:ARG:CG	2.41	0.51
1:C:163:ARG:HG3	1:C:248:GLY:O	2.11	0.51
1:C:107:GLU:HG3	1:C:108:PHE:N	2.25	0.50
1:C:222:THR:HG21	1:D:121:VAL:HG11	1.93	0.50
1:A:222:THR:HG23	1:B:102:ILE:CD1	2.41	0.50
1:D:194:GLN:O	1:D:194:GLN:HG3	2.12	0.50
1:C:129:LEU:HD12	1:C:129:LEU:H	1.77	0.49
1:B:143:THR:HG23	1:B:144:ASP:OD1	2.13	0.49
1:C:222:THR:HA	1:D:98:ASN:HD21	1.77	0.49
1:A:254:LEU:N	1:A:255:PRO:HD3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:PRO:HG3	1:B:182:CYS:SG	2.53	0.48
1:D:244:ASP:HB3	1:D:250:MSE:HG2	1.95	0.48
1:A:154:GLU:HG2	1:A:261:PRO:HB2	1.95	0.48
1:D:142:LEU:HD11	1:D:149:ALA:HB2	1.95	0.48
1:C:272:ARG:HD3	1:C:272:ARG:HA	1.69	0.47
1:D:243:GLU:HB3	3:D:333:HOH:O	2.14	0.47
1:D:199:HIS:CE1	1:D:208:GLU:OE1	2.68	0.47
1:B:155:MSE:HE2	1:B:264:ILE:HD11	1.97	0.47
1:A:111[B]:LYS:HG3	3:A:328:HOH:O	2.14	0.46
1:C:212:ARG:CZ	1:C:212:ARG:CB	2.93	0.46
1:D:155:MSE:HE3	1:D:157:PHE:HZ	1.78	0.46
1:C:151:ARG:NH1	1:C:154:GLU:HG3	2.31	0.46
1:B:126:ILE:O	1:B:138:ARG:NH2	2.47	0.46
1:A:185:VAL:HB	1:A:234:ILE:HG22	1.98	0.45
1:C:189:LEU:HB3	1:C:191:LYS:CG	2.46	0.45
1:D:126:ILE:HG13	1:D:138:ARG:HB2	1.98	0.45
1:D:275:SER:O	1:D:279:ARG:CG	2.57	0.45
1:A:224:LEU:CD2	1:A:240:MSE:HE2	2.48	0.44
1:A:213:TYR:O	1:B:116:GLN:HG2	2.16	0.44
1:D:194:GLN:O	1:D:194:GLN:CG	2.66	0.44
1:A:102:ILE:HD11	1:A:119:LEU:CD2	2.47	0.44
1:B:126:ILE:O	1:B:126:ILE:HG22	2.17	0.44
1:D:85:LYS:HD2	1:D:114:ASP:HB3	1.99	0.44
1:D:247[B]:ASN:HD22	1:D:249:THR:H	1.66	0.44
1:A:137:ILE:HD12	1:A:137:ILE:N	2.33	0.43
1:C:219:GLU:CD	1:C:221:THR:HG1	2.26	0.43
1:C:183:TYR:HE1	1:C:212:ARG:HH22	1.57	0.43
1:B:243:GLU:HA	1:B:246:ARG:NH2	2.34	0.43
1:A:142:LEU:HD13	1:A:142:LEU:HA	1.67	0.43
1:A:196:MSE:HA	1:A:197:PRO:HD3	1.94	0.43
1:A:238:LEU:HG	1:A:242[A]:ARG:HE	1.84	0.43
1:B:132:ASN:OD1	1:B:132:ASN:N	2.52	0.43
1:C:200:PHE:HB2	1:C:207:ILE:CD1	2.49	0.43
1:D:254:LEU:N	1:D:255:PRO:HD3	2.34	0.43
1:A:158:VAL:CG2	1:A:238:LEU:HD13	2.48	0.42
1:A:85:LYS:HG2	1:A:114:ASP:HB2	2.01	0.42
1:A:144:ASP:CG	1:A:147:LEU:HG	2.44	0.42
1:C:189:LEU:CD1	1:C:191:LYS:HD3	2.44	0.42
1:C:274:LEU:HG	1:C:279:ARG:HG3	2.00	0.42
1:C:95:ALA:O	1:C:99:LEU:HB2	2.19	0.42
1:D:96:PHE:CD1	1:D:289:MSE:HE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:PRO:HB2	1:D:208:GLU:HG3	2.02	0.42
1:C:182[B]:CYS:HA	3:C:305:HOH:O	2.18	0.42
1:B:124:ARG:O	1:B:124:ARG:HG3	2.18	0.42
1:C:183:TYR:CE1	1:C:212:ARG:NH2	2.73	0.42
1:C:85:LYS:HB3	1:C:85:LYS:HZ2	1.83	0.42
1:B:126:ILE:HG21	1:B:129:LEU:HD21	2.02	0.42
1:C:222:THR:CG2	1:D:98:ASN:HD21	2.26	0.42
1:A:131:GLU:OE2	1:A:271:ASN:ND2	2.53	0.42
1:A:222:THR:CG2	1:B:102:ILE:HD11	2.49	0.42
1:B:243:GLU:HG2	1:B:247:ASN:HD21	1.84	0.42
1:B:91:GLU:OE2	1:B:120:GLY:HA3	2.20	0.41
1:B:164:ASP:OD2	1:B:168:ARG:NH1	2.53	0.41
1:C:94:SER:OG	1:C:219:GLU:OE2	2.38	0.41
1:C:105:LEU:N	1:C:106:PRO:CD	2.83	0.41
1:B:137:ILE:HD12	1:B:137:ILE:N	2.35	0.41
1:C:200:PHE:HB2	1:C:207:ILE:HD11	2.01	0.41
1:A:138:ARG:HD3	1:A:138:ARG:HA	1.84	0.41
1:A:274:LEU:HG	1:A:279:ARG:HD3	2.02	0.41
1:C:157:PHE:HE2	1:C:262:MSE:HB2	1.85	0.41
1:C:197:PRO:HB2	1:C:208:GLU:HG3	2.03	0.41
1:A:144:ASP:HB3	1:A:147:LEU:CD1	2.51	0.41
1:B:199:HIS:CE1	1:B:208:GLU:HB2	2.56	0.41
1:A:215:MSE:HE3	1:A:217:ALA:HB2	2.03	0.41
1:B:143:THR:HG23	1:B:144:ASP:N	2.36	0.41
1:D:247[B]:ASN:ND2	1:D:249:THR:H	2.19	0.41
1:D:131:GLU:O	1:D:132:ASN:HB2	2.20	0.40
1:A:244:ASP:HB3	1:A:250:MSE:HG2	2.02	0.40
1:B:105:LEU:N	1:B:106:PRO:CD	2.84	0.40
1:A:269:PRO:HG2	1:A:272:ARG:HH21	1.86	0.40
1:C:88:LEU:HD21	1:C:277:ARG:HG3	2.02	0.40
1:C:182[A]:CYS:HA	3:C:305:HOH:O	2.20	0.40
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.72	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	205/300 (68%)	200 (98%)	5 (2%)	0	100	100
1	B	213/300 (71%)	209 (98%)	4 (2%)	0	100	100
1	C	198/300 (66%)	193 (98%)	5 (2%)	0	100	100
1	D	215/300 (72%)	212 (99%)	3 (1%)	0	100	100
All	All	831/1200 (69%)	814 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	182/246 (74%)	174 (96%)	8 (4%)	25	9
1	B	186/246 (76%)	181 (97%)	5 (3%)	39	23
1	C	176/246 (72%)	158 (90%)	18 (10%)	7	1
1	D	188/246 (76%)	177 (94%)	11 (6%)	18	5
All	All	732/984 (74%)	690 (94%)	42 (6%)	18	5

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	ILE
1	A	125	THR
1	A	142	LEU
1	A	189	LEU
1	A	208	GLU
1	A	219	GLU
1	A	268	TYR
1	A	271	ASN

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Mol	Chain	Res	Type
1	B	125	THR
1	B	126	ILE
1	B	138	ARG
1	B	272	ARG
1	B	274	LEU
1	C	85	LYS
1	C	87	ARG
1	C	99	LEU
1	C	121	VAL
1	C	128	TYR
1	C	129	LEU
1	C	131	GLU
1	C	132	ASN
1	C	138	ARG
1	C	141	THR
1	C	150	ARG
1	C	151	ARG
1	C	189	LEU
1	C	196	MSE
1	C	207	ILE
1	C	209	VAL
1	C	212	ARG
1	C	224	LEU
1	D	83	LEU
1	D	111[A]	LYS
1	D	111[B]	LYS
1	D	123	ASP
1	D	129	LEU
1	D	143	THR
1	D	191	LYS
1	D	195	GLN
1	D	196	MSE
1	D	219	GLU
1	D	224	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	145	GLN
1	A	173	GLN
1	A	181	ASN

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Mol	Chain	Res	Type
1	A	271	ASN
1	B	98	ASN
1	B	235	GLN
1	B	247	ASN
1	B	258	GLN
1	B	293	GLN
1	C	98	ASN
1	C	116	GLN
1	C	132	ASN
1	C	181	ASN
1	C	194	GLN
1	D	98	ASN
1	D	116	GLN
1	D	199	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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	201/300 (67%)	0.38	20 (9%)	12 14	16, 30, 75, 119	3 (1%)
1	B	205/300 (68%)	0.30	16 (7%)	19 21	11, 30, 73, 108	3 (1%)
1	C	197/300 (65%)	0.50	17 (8%)	16 18	20, 36, 81, 99	2 (1%)
1	D	205/300 (68%)	0.26	13 (6%)	26 28	14, 28, 68, 104	5 (2%)
All	All	808/1200 (67%)	0.36	66 (8%)	17 20	11, 31, 77, 119	13 (1%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	LEU	7.4
1	C	128	TYR	5.7
1	D	189	LEU	5.7
1	A	189	LEU	5.6
1	C	190	PRO	5.3
1	D	83	LEU	5.1
1	C	129	LEU	4.9
1	C	124	ARG	4.8
1	B	128	TYR	4.8
1	A	273	HIS	4.7
1	C	130	ALA	4.6
1	D	193	GLY	4.2
1	A	125	THR	4.2
1	C	189	LEU	4.0
1	D	190	PRO	3.6
1	C	123	ASP	3.5
1	D	126	ILE	3.5
1	D	123	ASP	3.5
1	D	128	TYR	3.4
1	C	141	THR	3.4
1	D	192	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	189	LEU	3.4
1	B	192	THR	3.3
1	B	126	ILE	3.2
1	A	272	ARG	3.2
1	A	128	TYR	3.1
1	A	83	LEU	3.1
1	B	271	ASN	3.0
1	A	190	PRO	3.0
1	B	130	ALA	2.9
1	C	171	VAL	2.9
1	A	194	GLN	2.9
1	B	193	GLY	2.8
1	D	127	ASP	2.7
1	C	204	ASN	2.7
1	B	131	GLU	2.6
1	C	194	GLN	2.6
1	A	143	THR	2.6
1	B	143	THR	2.6
1	A	270	PRO	2.5
1	B	83	LEU	2.5
1	D	124	ARG	2.5
1	B	274	LEU	2.5
1	C	247	ASN	2.5
1	C	131	GLU	2.5
1	A	154	GLU	2.5
1	C	207	ILE	2.4
1	C	163	ARG	2.4
1	A	144	ASP	2.4
1	B	107	GLU	2.4
1	A	130	ALA	2.3
1	A	85	LYS	2.3
1	B	194	GLN	2.3
1	A	271	ASN	2.3
1	D	85	LYS	2.3
1	B	272	ARG	2.2
1	C	212	ARG	2.2
1	A	142	LEU	2.2
1	A	124	ARG	2.2
1	D	194	GLN	2.1
1	A	294	ASN	2.1
1	B	142	LEU	2.1
1	B	125	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	294	ASN	2.0
1	A	111[A]	LYS	2.0
1	C	198	PHE	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(Å ²)	Q<0.9
2	CL	D	299	1/1	0.99	0.06	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.