



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:11 PM UTC

PDB ID : 7XGB / pdb_00007xgb
Title : Crystal structure of the ctcP from Streptomyces aureofaciens
Authors : Yin, L.
Deposited on : 2022-04-04
Resolution : 2.70 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

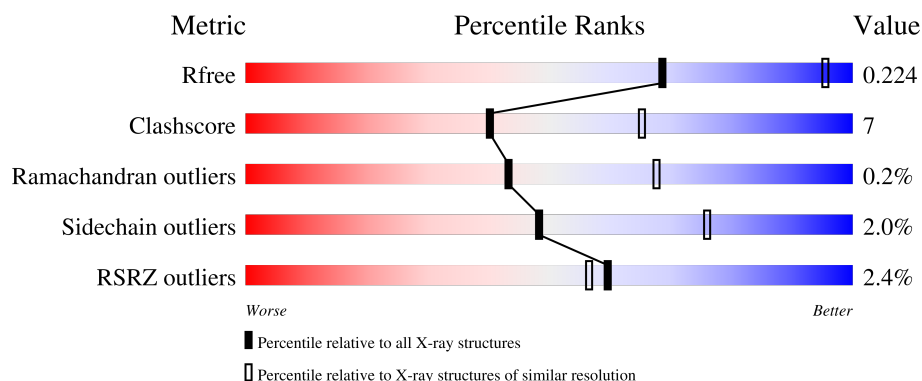
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	556	
1	B	556	
1	C	556	
1	D	556	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17330 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 Tetracycline 7-halogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	Se	0	0	0
			4278	2690	772	796	7	13			
1	B	528	Total	C	N	O	S	Se	0	0	0
			4213	2652	760	782	7	12			
1	C	544	Total	C	N	O	S	Se	0	0	0
			4332	2719	785	809	7	12			
1	D	529	Total	C	N	O	S	Se	0	0	0
			4219	2655	761	784	7	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A1E7MYN1
A	480	ARG	HIS	conflict	UNP A0A1E7MYN1
B	0	SER	-	expression tag	UNP A0A1E7MYN1
B	480	ARG	HIS	conflict	UNP A0A1E7MYN1
C	0	SER	-	expression tag	UNP A0A1E7MYN1
C	480	ARG	HIS	conflict	UNP A0A1E7MYN1
D	0	SER	-	expression tag	UNP A0A1E7MYN1
D	480	ARG	HIS	conflict	UNP A0A1E7MYN1

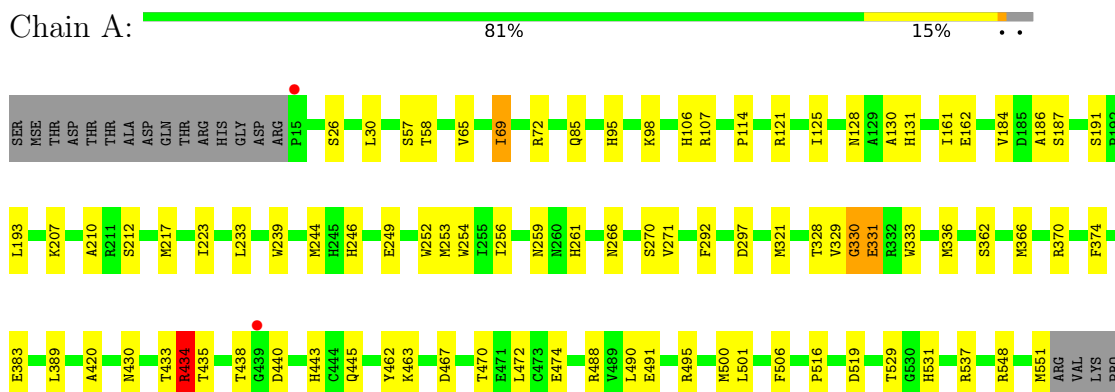
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	77	Total	O	0	0
			77	77		
2	B	79	Total	O	0	0
			79	79		
2	C	67	Total	O	0	0
			67	67		
2	D	65	Total	O	0	0
			65	65		

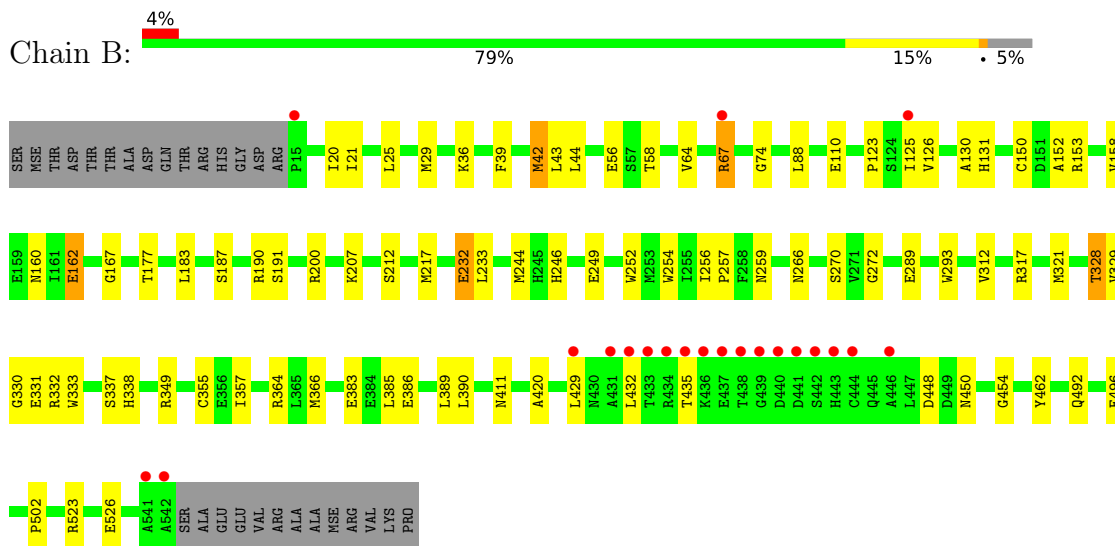
3 Residue-property plots

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.

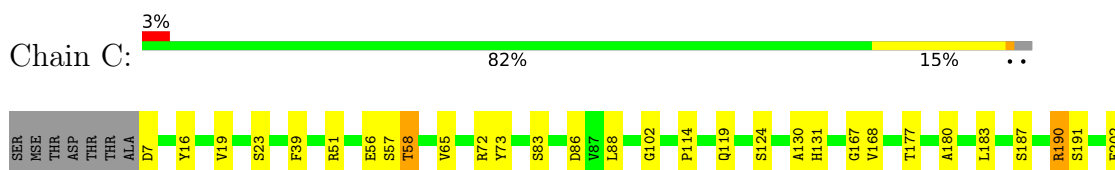
• Molecule 1: Tetracycline 7-halogenase



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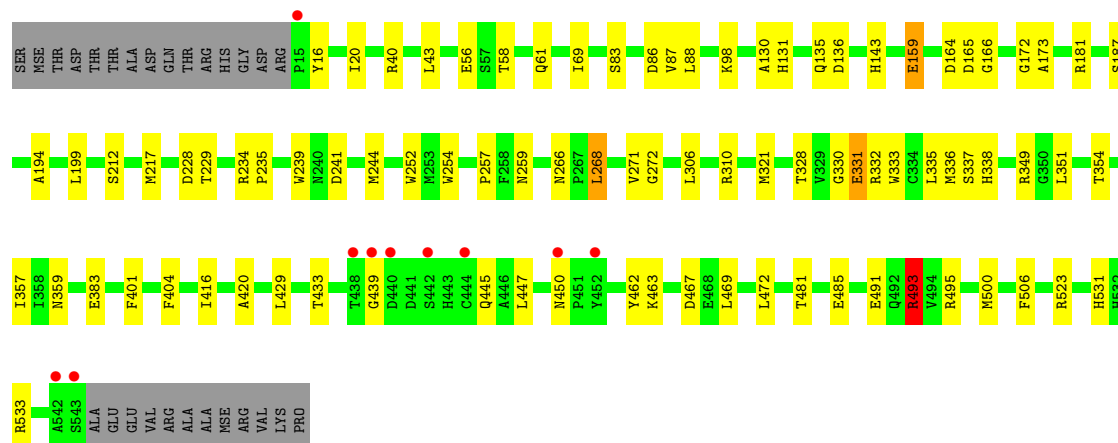
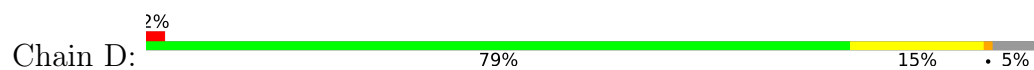


• Molecule 1: Tetracycline 7-halogenase





• Molecule 1: Tetracycline 7-halogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.39Å 121.28Å 179.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.70 48.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.80-2.70) 96.9 (48.80-2.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.176 , 0.224 0.178 , 0.224	Depositor DCC
R_{free} test set	2011 reflections (2.86%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17330	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.47	1/4380 (0.0%)	0.68	11/5928 (0.2%)
1	B	0.49	3/4316 (0.1%)	0.72	8/5844 (0.1%)
1	C	0.49	1/4436 (0.0%)	0.70	5/6007 (0.1%)
1	D	0.47	0/4322	0.69	4/5852 (0.1%)
All	All	0.48	5/17454 (0.0%)	0.70	28/23631 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	D	0	2
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	LYS	CD-CE	6.18	1.71	1.52
1	B	67	ARG	CG-CD	5.99	1.70	1.52
1	B	42	MSE	SE-CE	-5.69	1.78	1.95
1	C	327	ARG	CG-CD	5.28	1.68	1.52
1	A	434	ARG	CB-CG	5.04	1.67	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	ARG	CB-CG-CD	-8.86	90.92	111.30
1	B	162	GLU	CB-CA-C	8.84	123.76	110.14
1	B	67	ARG	N-CA-CB	-8.24	98.00	110.12
1	B	162	GLU	N-CA-CB	-7.49	98.57	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	GLY	CA-C-N	-7.06	112.77	122.30
1	A	330	GLY	C-N-CA	-7.06	112.77	122.30
1	B	67	ARG	CB-CA-C	6.69	121.89	110.79
1	A	434	ARG	CD-NE-CZ	-6.51	115.29	124.40
1	B	67	ARG	CG-CD-NE	6.38	126.04	112.00
1	D	228	ASP	CA-C-N	6.16	132.87	122.65
1	D	228	ASP	C-N-CA	6.16	132.87	122.65
1	D	493	ARG	CD-NE-CZ	6.15	133.01	124.40
1	B	232	GLU	CA-CB-CG	-6.06	101.99	114.10
1	A	434	ARG	CG-CD-NE	5.69	124.51	112.00
1	A	433	THR	CA-C-N	-5.67	111.05	120.68
1	A	433	THR	C-N-CA	-5.67	111.05	120.68
1	C	327	ARG	N-CA-CB	5.62	121.33	111.55
1	A	331	GLU	CA-CB-CG	-5.46	103.18	114.10
1	A	161	ILE	CA-C-N	5.46	130.47	122.77
1	A	161	ILE	C-N-CA	5.46	130.47	122.77
1	C	202	GLU	CB-CA-C	-5.45	104.13	110.17
1	B	67	ARG	CB-CG-CD	-5.35	98.99	111.30
1	B	67	ARG	CA-CB-CG	5.25	124.60	114.10
1	C	496	GLU	CB-CA-C	-5.18	101.43	110.09
1	C	190	ARG	CA-CB-CG	5.12	124.33	114.10
1	D	159	GLU	CB-CG-CD	5.06	121.19	112.60
1	C	190	ARG	CB-CG-CD	-5.03	99.73	111.30
1	A	434	ARG	CA-CB-CG	5.00	124.10	114.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	GLU	Sidechain
1	C	190	ARG	Sidechain
1	C	327	ARG	Sidechain
1	D	439	GLY	Mainchain
1	D	493	ARG	Sidechain

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	4278	0	4085	59	0
1	B	4213	0	4022	58	1
1	C	4332	0	4123	48	0
1	D	4219	0	4027	57	1
2	A	77	0	0	2	0
2	B	79	0	0	5	1
2	C	67	0	0	2	0
2	D	65	0	0	4	1
All	All	17330	0	16257	221	2

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 7.

All (221) 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:B:123:PRO:HB2	1:B:125:ILE:HG22	1.46	0.97
1:A:184:VAL:HG11	1:A:336:MSE:HE2	1.58	0.86
1:B:64:VAL:HG12	1:B:67:ARG:HH21	1.40	0.85
1:D:383:GLU:OE2	2:D:601:HOH:O	1.99	0.80
1:D:337:SER:OG	1:D:338:HIS:N	2.16	0.78
1:C:328:THR:HB	1:C:383:GLU:HG3	1.64	0.77
1:B:42:MSE:HE2	1:B:44:LEU:HD23	1.66	0.76
1:D:61:GLN:HE21	1:D:349:ARG:HH22	1.31	0.76
1:C:239:TRP:CE3	1:C:244:MSE:HE1	2.23	0.74
1:D:58:THR:HG22	1:D:130:ALA:H	1.52	0.73
1:B:160:ASN:HD21	1:B:162:GLU:HG3	1.54	0.72
1:D:239:TRP:HB3	1:D:244:MSE:HE3	1.71	0.72
1:B:39:PHE:CE2	1:B:366:MSE:HG2	2.24	0.72
1:A:212:SER:HB2	1:A:321:MSE:SE	2.38	0.72
1:B:58:THR:HG22	1:B:130:ALA:H	1.53	0.71
1:D:239:TRP:CE3	1:D:244:MSE:HE1	2.26	0.71
1:D:194:ALA:HA	1:D:199:LEU:HD12	1.74	0.70
1:C:239:TRP:HB3	1:C:244:MSE:HE3	1.75	0.69
1:C:330:GLY:HA3	1:C:333:TRP:CE2	2.26	0.69
1:A:434:ARG:O	1:A:438:THR:HG22	1.92	0.68
1:C:420:ALA:HB2	1:C:462:TYR:CE1	2.29	0.68
1:B:123:PRO:HB2	1:B:125:ILE:CG2	2.21	0.67
1:D:447:LEU:O	1:D:450:ASN:ND2	2.28	0.66
1:B:160:ASN:ND2	2:B:603:HOH:O	2.23	0.66
1:B:420:ALA:HB2	1:B:462:TYR:CE1	2.30	0.65
1:B:259:ASN:HB3	1:B:266:ASN:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLY:HA3	1:A:333:TRP:CE2	2.32	0.65
1:A:297:ASP:OD1	2:A:601:HOH:O	2.14	0.63
1:C:477:ASP:OD1	2:C:601:HOH:O	2.15	0.63
1:C:488:ARG:HH21	1:C:492:GLN:HE22	1.46	0.63
1:D:61:GLN:NE2	1:D:349:ARG:HH22	1.95	0.63
1:B:67:ARG:HH22	1:B:429:LEU:HD11	1.64	0.62
1:B:328:THR:HB	1:B:383:GLU:HG3	1.80	0.62
1:D:328:THR:HB	1:D:383:GLU:HG3	1.82	0.62
1:A:58:THR:HG22	1:A:130:ALA:H	1.65	0.61
1:A:186:ALA:HB2	1:A:336:MSE:HE3	1.83	0.61
1:B:337:SER:N	1:B:386:GLU:OE2	2.32	0.60
1:A:430:ASN:HB3	1:A:434:ARG:NH1	2.16	0.60
1:B:212:SER:HB2	1:B:321:MSE:SE	2.51	0.60
1:B:328:THR:HG22	1:B:329:VAL:HG13	1.83	0.60
1:B:337:SER:OG	1:B:338:HIS:N	2.33	0.60
1:D:420:ALA:HB2	1:D:462:TYR:CZ	2.37	0.59
1:C:212:SER:HB2	1:C:321:MSE:SE	2.52	0.59
1:B:244:MSE:HE2	1:B:246:HIS:CE1	2.38	0.59
1:D:331:GLU:CD	1:D:331:GLU:H	2.08	0.59
1:A:58:THR:CG2	1:A:130:ALA:H	2.16	0.58
1:B:25:LEU:O	1:B:29:MSE:HG3	2.02	0.58
1:A:239:TRP:CE3	1:A:244:MSE:HE1	2.38	0.58
1:C:114:PRO:HB2	1:C:233:LEU:HD13	1.85	0.58
1:A:106:HIS:HE1	1:A:246:HIS:ND1	2.01	0.58
1:B:432:LEU:O	1:B:435:THR:HG22	2.04	0.58
1:C:58:THR:HG22	1:C:130:ALA:H	1.69	0.58
1:A:252:TRP:CZ3	1:A:254:TRP:HB3	2.39	0.57
1:C:337:SER:OG	1:C:338:HIS:N	2.29	0.57
1:D:181:ARG:O	1:D:332:ARG:HD3	2.04	0.57
1:B:20:ILE:HB	1:B:43:LEU:HD23	1.87	0.56
1:A:420:ALA:HB2	1:A:462:TYR:CE1	2.40	0.56
1:B:232:GLU:HG2	1:B:233:LEU:N	2.19	0.56
1:C:434:ARG:HB3	1:C:443:HIS:ND1	2.20	0.56
1:D:491:GLU:OE2	1:D:495:ARG:NH1	2.38	0.56
1:A:217:MSE:HE1	1:A:292:PHE:CE2	2.40	0.56
1:D:212:SER:HB2	1:D:321:MSE:SE	2.54	0.56
1:C:420:ALA:HB2	1:C:462:TYR:CZ	2.40	0.56
1:A:438:THR:HG21	1:A:443:HIS:CE1	2.42	0.55
1:C:467:ASP:O	1:C:471:GLU:HG3	2.06	0.55
1:A:184:VAL:HG11	1:A:336:MSE:CE	2.33	0.55
1:D:58:THR:CG2	1:D:130:ALA:H	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:LYS:NZ	1:C:467:ASP:OD2	2.34	0.55
1:B:36:LYS:HE3	1:B:74:GLY:O	2.06	0.55
1:B:42:MSE:HE3	1:B:43:LEU:O	2.07	0.54
1:B:357:ILE:HD13	1:B:385:LEU:HD23	1.89	0.54
1:C:488:ARG:HE	1:C:492:GLN:NE2	2.05	0.54
1:B:150:CYS:O	1:D:310:ARG:NH2	2.41	0.54
1:C:19:VAL:HG13	1:C:183:LEU:HD23	1.89	0.54
1:D:217:MSE:CE	1:D:306:LEU:HD22	2.38	0.54
1:A:72:ARG:NH2	1:A:445:GLN:OE1	2.41	0.54
1:A:435:THR:HG23	1:A:440:ASP:O	2.07	0.53
1:D:69:ILE:HG22	1:D:359:ASN:HB2	1.91	0.53
1:D:217:MSE:HE2	1:D:271:VAL:HG21	1.90	0.53
1:D:429:LEU:O	1:D:433:THR:HG23	2.08	0.53
1:B:420:ALA:HB2	1:B:462:TYR:CZ	2.44	0.53
1:B:312:VAL:O	2:B:601:HOH:O	2.18	0.53
1:C:254:TRP:CZ2	1:C:272:GLY:HA3	2.45	0.52
1:A:470:THR:O	1:A:474:GLU:HG3	2.09	0.52
1:B:39:PHE:HE2	1:B:366:MSE:HG2	1.74	0.52
1:C:252:TRP:CZ3	1:C:254:TRP:HB3	2.44	0.51
1:C:515:ASN:O	1:C:520:LYS:HE3	2.11	0.51
1:B:317:ARG:HG3	2:B:614:HOH:O	2.10	0.51
1:C:259:ASN:HB3	1:C:266:ASN:O	2.10	0.51
1:B:523:ARG:HH21	1:B:526:GLU:HB2	1.75	0.50
1:C:39:PHE:CE2	1:C:366:MSE:HG2	2.45	0.50
1:B:58:THR:CG2	1:B:130:ALA:H	2.22	0.50
1:A:239:TRP:HB3	1:A:244:MSE:CE	2.40	0.50
1:B:331:GLU:HG3	1:B:332:ARG:HG3	1.93	0.50
1:A:472:LEU:HD12	1:A:490:LEU:HG	1.94	0.50
1:B:252:TRP:CZ3	1:B:254:TRP:HB3	2.47	0.50
1:B:42:MSE:HE1	1:B:152:ALA:C	2.37	0.50
1:C:131:HIS:CE1	1:C:257:PRO:HD2	2.47	0.50
1:D:491:GLU:O	1:D:495:ARG:HG3	2.12	0.50
1:D:266:ASN:OD1	1:D:268:LEU:HB2	2.12	0.49
1:D:330:GLY:HA3	1:D:333:TRP:CE2	2.47	0.49
1:C:73:TYR:CZ	1:C:362:SER:HB2	2.47	0.49
1:B:411:ASN:HB3	2:B:613:HOH:O	2.12	0.48
1:D:254:TRP:CZ2	1:D:272:GLY:HA3	2.49	0.48
1:A:98:LYS:HG3	1:A:131:HIS:HE2	1.78	0.48
1:A:548:ARG:HA	1:A:551:MSE:HE3	1.94	0.48
1:B:29:MSE:HE1	1:B:355:CYS:SG	2.53	0.48
1:B:42:MSE:HE1	1:B:153:ARG:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:TRP:CZ3	1:D:254:TRP:HB3	2.49	0.48
1:A:217:MSE:HE3	1:A:271:VAL:HB	1.96	0.48
1:C:23:SER:OG	1:C:51:ARG:NH2	2.46	0.47
1:B:289:GLU:HG3	1:B:293:TRP:CD1	2.49	0.47
1:D:328:THR:HG23	1:D:335:LEU:O	2.14	0.47
1:D:420:ALA:HB2	1:D:462:TYR:CE1	2.48	0.47
1:A:210:ALA:O	1:A:321:MSE:HG2	2.14	0.47
1:C:72:ARG:NH1	1:C:359:ASN:OD1	2.47	0.47
1:D:259:ASN:HB3	1:D:266:ASN:O	2.14	0.47
1:D:463:LYS:HD3	1:D:467:ASP:OD2	2.14	0.47
1:C:57:SER:HB2	1:C:348:SER:OG	2.14	0.47
1:D:164:ASP:OD1	1:D:166:GLY:N	2.40	0.47
1:C:254:TRP:CH2	1:C:272:GLY:HA3	2.50	0.47
1:C:283:ARG:NH1	1:C:285:ASP:OD2	2.48	0.47
1:C:375:ALA:HB1	1:C:377:GLU:OE1	2.15	0.47
1:A:217:MSE:HE3	1:A:271:VAL:HG11	1.97	0.47
1:A:259:ASN:HB3	1:A:266:ASN:O	2.15	0.47
1:A:434:ARG:HH21	1:A:434:ARG:HD2	1.39	0.47
1:C:7:ASP:N	2:C:610:HOH:O	2.48	0.47
1:D:165:ASP:O	1:D:332:ARG:NH2	2.44	0.47
1:C:83:SER:HB3	1:C:86:ASP:HB2	1.97	0.47
1:D:159:GLU:CD	1:D:173:ALA:HA	2.40	0.47
1:B:254:TRP:CZ2	1:B:272:GLY:HA3	2.50	0.46
1:C:102:GLY:O	1:C:245:HIS:HD2	1.98	0.46
1:C:484:GLU:H	1:C:484:GLU:CD	2.24	0.46
1:B:357:ILE:HD13	1:B:357:ILE:HA	1.69	0.46
1:A:217:MSE:HE3	1:A:271:VAL:CB	2.46	0.46
1:B:330:GLY:HA3	1:B:333:TRP:CE2	2.50	0.46
1:C:450:ASN:H	1:C:450:ASN:HD22	1.61	0.46
1:D:401:PHE:HA	1:D:404:PHE:CD2	2.50	0.46
1:B:21:ILE:HD13	1:B:158:VAL:HG21	1.97	0.46
1:A:463:LYS:NZ	1:A:467:ASP:OD2	2.46	0.46
1:B:502:PRO:O	2:B:602:HOH:O	2.21	0.46
1:C:235:PRO:HG3	1:C:239:TRP:CE2	2.51	0.46
1:C:244:MSE:HA	1:C:244:MSE:HE2	1.97	0.46
1:B:125:ILE:HG23	1:B:126:VAL:N	2.30	0.46
1:A:193:LEU:HD21	1:A:333:TRP:CE3	2.50	0.46
1:D:83:SER:HB3	1:D:86:ASP:HB2	1.97	0.46
1:A:366:MSE:O	1:A:370:ARG:HG2	2.16	0.46
1:B:131:HIS:CE1	1:B:257:PRO:HD2	2.50	0.45
1:C:167:GLY:HA2	1:C:332:ARG:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:TRP:CD2	1:A:244:MSE:HE1	2.51	0.45
1:D:159:GLU:HG3	1:D:172:GLY:C	2.42	0.45
1:D:351:LEU:O	1:D:354:THR:HB	2.16	0.45
1:D:493:ARG:HA	1:D:493:ARG:HD3	1.68	0.45
1:B:64:VAL:HA	1:B:67:ARG:HE	1.82	0.45
1:B:167:GLY:HA2	1:B:332:ARG:HD3	1.98	0.45
1:A:30:LEU:HD22	1:A:336:MSE:CE	2.47	0.45
1:A:256:ILE:HB	1:A:270:SER:HB3	1.99	0.45
1:A:531:HIS:O	1:A:537:ARG:HD3	2.17	0.45
1:D:472:LEU:HD23	1:D:472:LEU:HA	1.84	0.45
1:D:20:ILE:HB	1:D:43:LEU:HD23	1.97	0.44
1:D:143:HIS:HE1	2:D:663:HOH:O	1.99	0.44
1:A:329:VAL:HG22	1:A:383:GLU:HB2	1.99	0.44
1:A:420:ALA:HB2	1:A:462:TYR:CZ	2.53	0.44
1:A:331:GLU:HG3	1:A:374:PHE:O	2.17	0.44
1:A:491:GLU:OE2	1:A:495:ARG:NH1	2.50	0.44
1:C:429:LEU:O	1:C:433:THR:HG23	2.17	0.44
1:A:223:ILE:HG21	1:A:244:MSE:HE3	2.00	0.44
1:C:330:GLY:HA3	1:C:333:TRP:NE1	2.33	0.44
1:C:16:TYR:O	1:C:180:ALA:HA	2.17	0.43
1:D:235:PRO:HG3	1:D:239:TRP:CE2	2.53	0.43
1:D:16:TYR:CD1	1:D:40:ARG:HG2	2.53	0.43
1:A:207:LYS:O	2:A:602:HOH:O	2.21	0.43
1:B:349:ARG:HE	1:B:349:ARG:HB3	1.67	0.43
1:B:429:LEU:HD23	1:B:429:LEU:HA	1.78	0.43
1:D:229:THR:HG22	1:D:234:ARG:HG3	2.01	0.43
1:B:450:ASN:OD1	1:B:450:ASN:N	2.52	0.43
1:D:131:HIS:CE1	1:D:257:PRO:HD2	2.54	0.43
1:B:390:LEU:HD12	1:B:390:LEU:HA	1.85	0.43
1:D:135:GLN:HG3	1:D:136:ASP:N	2.34	0.43
1:D:199:LEU:HD13	1:D:335:LEU:HD22	2.00	0.42
1:A:58:THR:HG22	1:A:130:ALA:O	2.19	0.42
1:A:519:ASP:OD2	1:A:519:ASP:N	2.53	0.42
1:C:23:SER:HG	1:C:51:ARG:NH2	2.17	0.42
1:D:481:THR:HG22	1:D:485:GLU:HB3	2.02	0.42
1:B:200:ARG:HA	1:B:200:ARG:HD3	1.83	0.42
1:A:500:MSE:O	1:A:506:PHE:HB2	2.20	0.42
1:D:401:PHE:HB3	2:D:640:HOH:O	2.20	0.42
1:B:256:ILE:HB	1:B:270:SER:HB3	2.01	0.42
1:B:492:GLN:O	1:B:496:GLU:HG2	2.19	0.42
1:A:98:LYS:HG3	1:A:131:HIS:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:SER:O	1:A:366:MSE:HG3	2.19	0.42
1:D:500:MSE:O	1:D:506:PHE:HB2	2.19	0.42
1:D:416:ILE:HD12	1:D:469:LEU:HD13	2.02	0.42
1:B:364:ARG:NH1	1:B:448:ASP:OD2	2.41	0.42
1:C:65:VAL:HG12	1:C:355:CYS:HB3	2.00	0.42
1:C:413:VAL:HG22	1:C:469:LEU:HD11	2.02	0.42
1:C:452:TYR:CE1	1:C:463:LYS:HD3	2.55	0.41
1:A:246:HIS:HB2	1:A:253:MSE:HB3	2.02	0.41
1:A:95:HIS:O	1:A:261:HIS:HE1	2.03	0.41
1:A:389:LEU:HA	1:A:389:LEU:HD23	1.83	0.41
1:C:499:TRP:CZ3	1:C:500:MSE:HG2	2.56	0.41
1:A:65:VAL:O	1:A:69:ILE:HG23	2.20	0.41
1:B:183:LEU:O	1:B:333:TRP:HA	2.21	0.41
1:C:254:TRP:HD1	1:C:256:ILE:HG13	1.84	0.41
1:D:445:GLN:NE2	1:D:445:GLN:HA	2.35	0.41
1:A:106:HIS:CE1	1:A:246:HIS:ND1	2.86	0.41
1:D:336:MSE:HG2	1:D:357:ILE:HG21	2.02	0.41
1:A:85:GLN:HE22	1:A:128:ASN:HD22	1.66	0.41
1:A:217:MSE:HE3	1:A:271:VAL:CG1	2.50	0.41
1:D:83:SER:O	1:D:87:VAL:HG23	2.21	0.41
1:D:241:ASP:HB3	2:D:604:HOH:O	2.21	0.41
1:D:531:HIS:CE1	1:D:533:ARG:HG3	2.56	0.41
1:A:121:ARG:HB3	1:A:516:PRO:HD2	2.03	0.41
1:B:389:LEU:HD23	1:B:454:GLY:HA2	2.02	0.41
1:C:119:GLN:OE1	1:C:236:PRO:HD2	2.21	0.41
1:A:125:ILE:HD12	1:A:125:ILE:HA	1.84	0.40
1:D:331:GLU:OE1	1:D:331:GLU:N	2.46	0.40
1:A:114:PRO:HB2	1:A:233:LEU:HD13	2.03	0.40
1:A:239:TRP:HB3	1:A:244:MSE:HE3	2.03	0.40
1:A:500:MSE:O	1:A:501:LEU:C	2.64	0.40
1:B:217:MSE:HE1	1:B:293:TRP:CZ2	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:665:HOH:O	2:D:653:HOH:O[4_555]	1.94	0.26
1:B:496:GLU:OE1	1:D:523:ARG:NH2[4_555]	2.02	0.18

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	535/556 (96%)	519 (97%)	15 (3%)	1 (0%)	43	68
1	B	526/556 (95%)	511 (97%)	14 (3%)	1 (0%)	43	68
1	C	542/556 (98%)	523 (96%)	18 (3%)	1 (0%)	43	68
1	D	527/556 (95%)	512 (97%)	14 (3%)	1 (0%)	43	68
All	All	2130/2224 (96%)	2065 (97%)	61 (3%)	4 (0%)	43	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	SER
1	C	187	SER
1	B	187	SER
1	D	187	SER

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	452/455 (99%)	442 (98%)	10 (2%)	45	74
1	B	446/455 (98%)	438 (98%)	8 (2%)	51	78
1	C	457/455 (100%)	444 (97%)	13 (3%)	38	68
1	D	447/455 (98%)	442 (99%)	5 (1%)	65	85
All	All	1802/1820 (99%)	1766 (98%)	36 (2%)	48	76

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	57	SER
1	A	69	ILE
1	A	107	ARG
1	A	191	SER
1	A	249	GLU
1	A	328	THR
1	A	434	ARG
1	A	488	ARG
1	A	529	THR
1	B	56	GLU
1	B	88	LEU
1	B	110	GLU
1	B	177	THR
1	B	190	ARG
1	B	191	SER
1	B	249	GLU
1	B	328	THR
1	C	56	GLU
1	C	58	THR
1	C	88	LEU
1	C	124	SER
1	C	168	VAL
1	C	177	THR
1	C	191	SER
1	C	328	THR
1	C	337	SER
1	C	426	LYS
1	C	450	ASN
1	C	529	THR
1	C	545	GLU
1	D	56	GLU
1	D	88	LEU
1	D	98	LYS
1	D	268	LEU
1	D	331	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS

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Mol	Chain	Res	Type
1	A	115	ASN
1	A	128	ASN
1	A	209	HIS
1	A	261	HIS
1	A	303	GLN
1	A	399	ASN
1	A	443	HIS
1	B	90	ASN
1	B	240	ASN
1	C	209	HIS
1	C	303	GLN
1	C	393	ASN
1	C	450	ASN
1	C	492	GLN
1	C	512	HIS
1	D	61	GLN
1	D	90	ASN
1	D	143	HIS
1	D	338	HIS
1	D	353	ASN
1	D	393	ASN
1	D	445	GLN
1	D	450	ASN
1	D	492	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	524/556 (94%)	-0.49	2 (0%) 88 87	18, 33, 60, 116	0
1	B	516/556 (92%)	-0.34	21 (4%) 41 37	18, 31, 61, 198	0
1	C	532/556 (95%)	-0.32	18 (3%) 48 44	18, 33, 71, 139	0
1	D	517/556 (92%)	-0.25	10 (1%) 66 63	19, 38, 73, 136	0
All	All	2089/2224 (93%)	-0.35	51 (2%) 59 56	18, 33, 68, 198	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	444	CYS	8.9
1	B	542	ALA	7.9
1	B	438	THR	5.7
1	B	441	ASP	5.4
1	B	443	HIS	5.1
1	B	434	ARG	5.0
1	B	437	GLU	4.9
1	B	431	ALA	4.9
1	D	542	ALA	4.8
1	C	441	ASP	4.7
1	B	541	ALA	4.7
1	B	432	LEU	4.6
1	D	543	SER	4.6
1	C	443	HIS	4.6
1	B	435	THR	4.5
1	C	444	CYS	4.4
1	B	433	THR	4.4
1	C	439	GLY	4.3
1	C	438	THR	4.1
1	B	442	SER	4.0
1	B	436	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	439	GLY	3.9
1	C	544	ALA	3.6
1	C	436	LYS	3.5
1	C	435	THR	3.4
1	B	125	ILE	3.0
1	B	440	ASP	3.0
1	C	433	THR	3.0
1	A	15	PRO	2.9
1	C	437	GLU	2.9
1	C	442	SER	2.9
1	C	542	ALA	2.8
1	C	440	ASP	2.7
1	C	434	ARG	2.6
1	C	548	ARG	2.6
1	C	550	ALA	2.5
1	D	444	CYS	2.5
1	D	438	THR	2.5
1	D	15	PRO	2.5
1	C	549	ALA	2.4
1	D	450	ASN	2.4
1	D	442	SER	2.4
1	B	67	ARG	2.3
1	A	439	GLY	2.3
1	B	446	ALA	2.2
1	B	429	LEU	2.2
1	B	15	PRO	2.1
1	D	452	TYR	2.1
1	D	439	GLY	2.1
1	D	440	ASP	2.0
1	C	547	VAL	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.