



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2014 – 04:47 AM EST

PDB ID : 4NXL
Title : Dibenzothiophene monooxygenase (DszC) from Rhodococcus erythropolis
Authors : Zhang, L.; Duan, X.; Li, X.; Rao, Z.
Deposited on : 2013-12-09
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

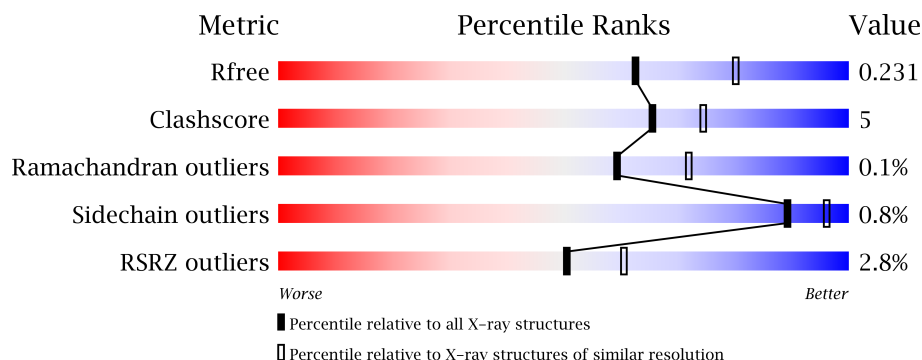
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	453	
1	B	453	
1	C	453	
1	D	453	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12786 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DszC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3041	1911	540	586	4			
1	B	399	Total	C	N	O	S	0	0	0
			3041	1911	540	586	4			
1	C	399	Total	C	N	O	S	0	0	0
			3041	1911	540	586	4			
1	D	399	Total	C	N	O	S	0	0	0
			3041	1911	540	586	4			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	EXPRESSION TAG	UNP Q64F43
A	-34	GLY	-	EXPRESSION TAG	UNP Q64F43
A	-33	SER	-	EXPRESSION TAG	UNP Q64F43
A	-32	SER	-	EXPRESSION TAG	UNP Q64F43
A	-31	HIS	-	EXPRESSION TAG	UNP Q64F43
A	-30	HIS	-	EXPRESSION TAG	UNP Q64F43
A	-29	HIS	-	EXPRESSION TAG	UNP Q64F43
A	-28	HIS	-	EXPRESSION TAG	UNP Q64F43
A	-27	HIS	-	EXPRESSION TAG	UNP Q64F43
A	-26	HIS	-	EXPRESSION TAG	UNP Q64F43
A	-25	SER	-	EXPRESSION TAG	UNP Q64F43
A	-24	SER	-	EXPRESSION TAG	UNP Q64F43
A	-23	GLY	-	EXPRESSION TAG	UNP Q64F43
A	-22	LEU	-	EXPRESSION TAG	UNP Q64F43
A	-21	VAL	-	EXPRESSION TAG	UNP Q64F43
A	-20	PRO	-	EXPRESSION TAG	UNP Q64F43
A	-19	ARG	-	EXPRESSION TAG	UNP Q64F43
A	-18	GLY	-	EXPRESSION TAG	UNP Q64F43
A	-17	SER	-	EXPRESSION TAG	UNP Q64F43
A	-16	HIS	-	EXPRESSION TAG	UNP Q64F43
A	-15	MET	-	EXPRESSION TAG	UNP Q64F43

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	ALA	-	EXPRESSION TAG	UNP Q64F43
A	-13	SER	-	EXPRESSION TAG	UNP Q64F43
A	-12	MET	-	EXPRESSION TAG	UNP Q64F43
A	-11	THR	-	EXPRESSION TAG	UNP Q64F43
A	-10	GLY	-	EXPRESSION TAG	UNP Q64F43
A	-9	GLY	-	EXPRESSION TAG	UNP Q64F43
A	-8	GLN	-	EXPRESSION TAG	UNP Q64F43
A	-7	GLN	-	EXPRESSION TAG	UNP Q64F43
A	-6	MET	-	EXPRESSION TAG	UNP Q64F43
A	-5	GLY	-	EXPRESSION TAG	UNP Q64F43
A	-4	ARG	-	EXPRESSION TAG	UNP Q64F43
A	-3	GLY	-	EXPRESSION TAG	UNP Q64F43
A	-2	SER	-	EXPRESSION TAG	UNP Q64F43
A	-1	GLU	-	EXPRESSION TAG	UNP Q64F43
A	0	PHE	-	EXPRESSION TAG	UNP Q64F43
B	-35	MET	-	EXPRESSION TAG	UNP Q64F43
B	-34	GLY	-	EXPRESSION TAG	UNP Q64F43
B	-33	SER	-	EXPRESSION TAG	UNP Q64F43
B	-32	SER	-	EXPRESSION TAG	UNP Q64F43
B	-31	HIS	-	EXPRESSION TAG	UNP Q64F43
B	-30	HIS	-	EXPRESSION TAG	UNP Q64F43
B	-29	HIS	-	EXPRESSION TAG	UNP Q64F43
B	-28	HIS	-	EXPRESSION TAG	UNP Q64F43
B	-27	HIS	-	EXPRESSION TAG	UNP Q64F43
B	-26	HIS	-	EXPRESSION TAG	UNP Q64F43
B	-25	SER	-	EXPRESSION TAG	UNP Q64F43
B	-24	SER	-	EXPRESSION TAG	UNP Q64F43
B	-23	GLY	-	EXPRESSION TAG	UNP Q64F43
B	-22	LEU	-	EXPRESSION TAG	UNP Q64F43
B	-21	VAL	-	EXPRESSION TAG	UNP Q64F43
B	-20	PRO	-	EXPRESSION TAG	UNP Q64F43
B	-19	ARG	-	EXPRESSION TAG	UNP Q64F43
B	-18	GLY	-	EXPRESSION TAG	UNP Q64F43
B	-17	SER	-	EXPRESSION TAG	UNP Q64F43
B	-16	HIS	-	EXPRESSION TAG	UNP Q64F43
B	-15	MET	-	EXPRESSION TAG	UNP Q64F43
B	-14	ALA	-	EXPRESSION TAG	UNP Q64F43
B	-13	SER	-	EXPRESSION TAG	UNP Q64F43
B	-12	MET	-	EXPRESSION TAG	UNP Q64F43
B	-11	THR	-	EXPRESSION TAG	UNP Q64F43
B	-10	GLY	-	EXPRESSION TAG	UNP Q64F43
B	-9	GLY	-	EXPRESSION TAG	UNP Q64F43

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLN	-	EXPRESSION TAG	UNP Q64F43
B	-7	GLN	-	EXPRESSION TAG	UNP Q64F43
B	-6	MET	-	EXPRESSION TAG	UNP Q64F43
B	-5	GLY	-	EXPRESSION TAG	UNP Q64F43
B	-4	ARG	-	EXPRESSION TAG	UNP Q64F43
B	-3	GLY	-	EXPRESSION TAG	UNP Q64F43
B	-2	SER	-	EXPRESSION TAG	UNP Q64F43
B	-1	GLU	-	EXPRESSION TAG	UNP Q64F43
B	0	PHE	-	EXPRESSION TAG	UNP Q64F43
C	-35	MET	-	EXPRESSION TAG	UNP Q64F43
C	-34	GLY	-	EXPRESSION TAG	UNP Q64F43
C	-33	SER	-	EXPRESSION TAG	UNP Q64F43
C	-32	SER	-	EXPRESSION TAG	UNP Q64F43
C	-31	HIS	-	EXPRESSION TAG	UNP Q64F43
C	-30	HIS	-	EXPRESSION TAG	UNP Q64F43
C	-29	HIS	-	EXPRESSION TAG	UNP Q64F43
C	-28	HIS	-	EXPRESSION TAG	UNP Q64F43
C	-27	HIS	-	EXPRESSION TAG	UNP Q64F43
C	-26	HIS	-	EXPRESSION TAG	UNP Q64F43
C	-25	SER	-	EXPRESSION TAG	UNP Q64F43
C	-24	SER	-	EXPRESSION TAG	UNP Q64F43
C	-23	GLY	-	EXPRESSION TAG	UNP Q64F43
C	-22	LEU	-	EXPRESSION TAG	UNP Q64F43
C	-21	VAL	-	EXPRESSION TAG	UNP Q64F43
C	-20	PRO	-	EXPRESSION TAG	UNP Q64F43
C	-19	ARG	-	EXPRESSION TAG	UNP Q64F43
C	-18	GLY	-	EXPRESSION TAG	UNP Q64F43
C	-17	SER	-	EXPRESSION TAG	UNP Q64F43
C	-16	HIS	-	EXPRESSION TAG	UNP Q64F43
C	-15	MET	-	EXPRESSION TAG	UNP Q64F43
C	-14	ALA	-	EXPRESSION TAG	UNP Q64F43
C	-13	SER	-	EXPRESSION TAG	UNP Q64F43
C	-12	MET	-	EXPRESSION TAG	UNP Q64F43
C	-11	THR	-	EXPRESSION TAG	UNP Q64F43
C	-10	GLY	-	EXPRESSION TAG	UNP Q64F43
C	-9	GLY	-	EXPRESSION TAG	UNP Q64F43
C	-8	GLN	-	EXPRESSION TAG	UNP Q64F43
C	-7	GLN	-	EXPRESSION TAG	UNP Q64F43
C	-6	MET	-	EXPRESSION TAG	UNP Q64F43
C	-5	GLY	-	EXPRESSION TAG	UNP Q64F43
C	-4	ARG	-	EXPRESSION TAG	UNP Q64F43
C	-3	GLY	-	EXPRESSION TAG	UNP Q64F43

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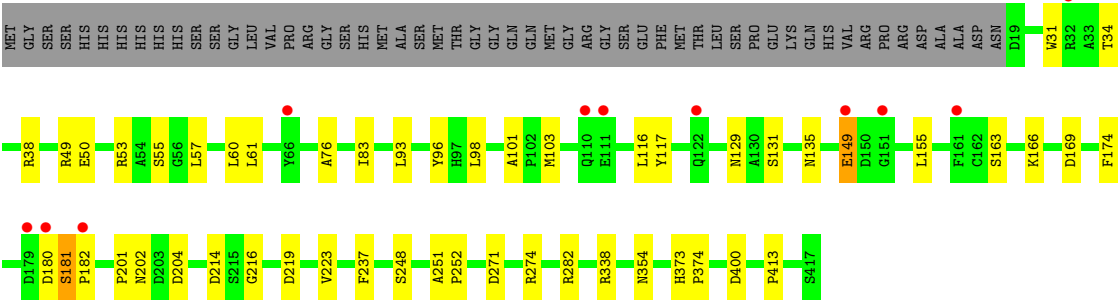
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	EXPRESSION TAG	UNP Q64F43
C	-1	GLU	-	EXPRESSION TAG	UNP Q64F43
C	0	PHE	-	EXPRESSION TAG	UNP Q64F43
D	-35	MET	-	EXPRESSION TAG	UNP Q64F43
D	-34	GLY	-	EXPRESSION TAG	UNP Q64F43
D	-33	SER	-	EXPRESSION TAG	UNP Q64F43
D	-32	SER	-	EXPRESSION TAG	UNP Q64F43
D	-31	HIS	-	EXPRESSION TAG	UNP Q64F43
D	-30	HIS	-	EXPRESSION TAG	UNP Q64F43
D	-29	HIS	-	EXPRESSION TAG	UNP Q64F43
D	-28	HIS	-	EXPRESSION TAG	UNP Q64F43
D	-27	HIS	-	EXPRESSION TAG	UNP Q64F43
D	-26	HIS	-	EXPRESSION TAG	UNP Q64F43
D	-25	SER	-	EXPRESSION TAG	UNP Q64F43
D	-24	SER	-	EXPRESSION TAG	UNP Q64F43
D	-23	GLY	-	EXPRESSION TAG	UNP Q64F43
D	-22	LEU	-	EXPRESSION TAG	UNP Q64F43
D	-21	VAL	-	EXPRESSION TAG	UNP Q64F43
D	-20	PRO	-	EXPRESSION TAG	UNP Q64F43
D	-19	ARG	-	EXPRESSION TAG	UNP Q64F43
D	-18	GLY	-	EXPRESSION TAG	UNP Q64F43
D	-17	SER	-	EXPRESSION TAG	UNP Q64F43
D	-16	HIS	-	EXPRESSION TAG	UNP Q64F43
D	-15	MET	-	EXPRESSION TAG	UNP Q64F43
D	-14	ALA	-	EXPRESSION TAG	UNP Q64F43
D	-13	SER	-	EXPRESSION TAG	UNP Q64F43
D	-12	MET	-	EXPRESSION TAG	UNP Q64F43
D	-11	THR	-	EXPRESSION TAG	UNP Q64F43
D	-10	GLY	-	EXPRESSION TAG	UNP Q64F43
D	-9	GLY	-	EXPRESSION TAG	UNP Q64F43
D	-8	GLN	-	EXPRESSION TAG	UNP Q64F43
D	-7	GLN	-	EXPRESSION TAG	UNP Q64F43
D	-6	MET	-	EXPRESSION TAG	UNP Q64F43
D	-5	GLY	-	EXPRESSION TAG	UNP Q64F43
D	-4	ARG	-	EXPRESSION TAG	UNP Q64F43
D	-3	GLY	-	EXPRESSION TAG	UNP Q64F43
D	-2	SER	-	EXPRESSION TAG	UNP Q64F43
D	-1	GLU	-	EXPRESSION TAG	UNP Q64F43
D	0	PHE	-	EXPRESSION TAG	UNP Q64F43

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	154	Total 154	O 154	0	0
2	B	145	Total 145	O 145	0	0
2	C	161	Total 161	O 161	0	0
2	D	162	Total 162	O 162	0	0

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	130.98Å 136.18Å 174.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.35 – 2.30 41.66 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.35-2.30) 99.9 (41.66-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1525)	Depositor
R, R_{free}	0.179 , 0.231 0.179 , 0.231	Depositor DCC
R_{free} test set	3508 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.2	EDS
Estimated twinning fraction	0.046 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 69353 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12786	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.45	0/3116	0.60	0/4248
1	B	0.43	0/3116	0.59	1/4248 (0.0%)
1	C	0.46	0/3116	0.64	3/4248 (0.1%)
1	D	0.43	0/3116	0.58	0/4248
All	All	0.44	0/12464	0.60	4/16992 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	338	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	C	290	GLN	CA-CB-CG	5.92	126.42	113.40
1	B	106	LEU	CA-CB-CG	5.84	128.73	115.30
1	C	338	ARG	NE-CZ-NH1	5.28	122.94	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3041	0	2918	28	0
1	B	3041	0	2918	34	0
1	C	3041	0	2918	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3041	0	2918	34	0
2	A	154	0	0	7	0
2	B	145	0	0	10	0
2	C	161	0	0	8	0
2	D	162	0	0	6	0
All	All	12786	0	11672	124	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (124) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:200:THR:OG1	2:C:650:HOH:O	1.81	0.98
1:B:244:SER:OG	2:B:602:HOH:O	1.83	0.97
1:C:358:ASN:ND2	2:C:634:HOH:O	2.12	0.83
1:B:34:THR:OG1	1:B:38:ARG:NH1	2.12	0.82
1:D:413:PRO:O	2:D:563:HOH:O	1.97	0.82
1:C:34:THR:OG1	1:C:38:ARG:NH1	2.12	0.82
1:B:318:GLU:OE1	2:B:625:HOH:O	2.02	0.77
1:A:105:GLU:HG2	1:A:246:ARG:HH12	1.50	0.77
1:A:106:LEU:HB3	1:A:247:GLY:HA2	1.67	0.76
1:D:248:SER:O	1:D:338:ARG:NH1	2.18	0.75
1:A:282:ARG:NH1	1:D:135:ASN:HD22	1.85	0.75
1:D:354:ASN:OD1	2:D:544:HOH:O	2.05	0.74
1:D:34:THR:OG1	1:D:38:ARG:NH1	2.21	0.74
1:C:354:ASN:ND2	2:C:600:HOH:O	2.23	0.71
1:B:246:ARG:NH2	2:B:635:HOH:O	2.23	0.70
1:B:53:ARG:NH2	1:B:169:ASP:OD2	2.24	0.70
1:C:290:GLN:HE21	1:C:290:GLN:HA	1.56	0.70
1:D:50:GLU:OE1	2:D:644:HOH:O	2.09	0.69
1:B:271:ASP:OD1	1:B:274:ARG:NH2	2.26	0.68
1:D:400:ASP:OD1	2:D:623:HOH:O	2.12	0.67
1:B:214:ASP:O	2:B:582:HOH:O	2.13	0.66
1:A:318:GLU:OE1	2:A:583:HOH:O	2.14	0.66
1:D:202:ASN:ND2	1:D:219:ASP:OD2	2.22	0.65
1:B:282:ARG:NH1	1:B:370:ARG:HD2	2.12	0.65
1:D:271:ASP:OD1	1:D:274:ARG:NH2	2.29	0.64
1:A:338:ARG:NH2	2:A:630:HOH:O	2.17	0.64
1:D:214:ASP:O	2:D:612:HOH:O	2.15	0.64
1:A:282:ARG:HH12	1:D:135:ASN:HD22	1.47	0.61
1:B:131:SER:OG	1:B:132:SER:N	2.34	0.60
1:D:101:ALA:HB1	1:D:117:TYR:HE1	1.67	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:31:TRP:HZ3	1:D:83:ILE:HG23	1.68	0.59
1:A:135:ASN:HB3	1:D:282:ARG:NH2	2.17	0.59
1:B:30:LYS:NZ	1:B:51:ASP:OD2	2.35	0.59
1:C:204:ASP:HB3	1:C:216:GLY:HA3	1.85	0.58
1:B:32:ARG:NH1	2:B:596:HOH:O	1.94	0.58
1:A:53:ARG:NH2	1:A:169:ASP:OD2	2.37	0.57
1:D:338:ARG:NH2	1:D:413:PRO:HA	2.19	0.57
1:C:30:LYS:NZ	1:C:51:ASP:OD2	2.34	0.56
1:A:317:ARG:NH2	2:A:635:HOH:O	2.27	0.56
1:C:290:GLN:HE21	1:C:290:GLN:CA	2.19	0.56
1:B:101:ALA:HB3	1:B:102:PRO:HD3	1.88	0.55
1:A:360:SER:HB3	1:A:382:TRP:HB2	1.88	0.55
1:A:405:THR:O	1:B:274:ARG:HD3	2.08	0.54
1:B:77:ILE:HG21	2:B:523:HOH:O	2.07	0.54
1:C:282:ARG:HH11	1:C:370:ARG:HE	1.55	0.54
1:D:149:GLU:H	1:D:149:GLU:CD	2.12	0.53
1:C:149:GLU:H	1:C:149:GLU:CD	2.11	0.52
1:C:265:ILE:HG21	1:C:385:VAL:HG23	1.91	0.52
1:B:135:ASN:HB3	1:C:282:ARG:HH21	1.75	0.52
1:C:106:LEU:HD22	1:C:246:ARG:O	2.10	0.52
1:C:40:ARG:NH1	2:C:626:HOH:O	2.43	0.52
1:B:179:ASP:OD1	1:B:181:SER:HB3	2.10	0.51
1:C:106:LEU:HB3	1:C:247:GLY:HA2	1.91	0.51
1:C:60:LEU:HD21	1:C:76:ALA:HA	1.93	0.51
1:C:248:SER:O	1:C:338:ARG:NE	2.33	0.51
1:A:77:ILE:HG21	2:A:523:HOH:O	2.11	0.51
1:C:166:LYS:HA	1:C:201:PRO:HB2	1.93	0.50
1:C:329:LYS:NZ	2:C:660:HOH:O	2.20	0.50
1:C:31:TRP:HZ3	1:C:83:ILE:HG23	1.76	0.50
1:A:205:TRP:CD2	1:A:215:SER:HB2	2.47	0.50
1:B:135:ASN:CB	1:C:282:ARG:HH21	2.25	0.50
1:B:103:MET:HG3	1:B:237:PHE:HZ	1.75	0.50
1:B:239:LEU:O	1:B:243:GLN:HG2	2.12	0.50
1:D:204:ASP:HB3	1:D:216:GLY:HA3	1.94	0.50
1:A:105:GLU:HG2	1:A:246:ARG:NH1	2.22	0.49
1:B:201:PRO:HA	1:B:218:THR:HG22	1.93	0.49
1:D:55:SER:OG	1:D:57:LEU:HB2	2.12	0.49
1:D:223:VAL:HA	2:D:655:HOH:O	2.14	0.48
1:A:101:ALA:HB3	1:A:102:PRO:HD3	1.95	0.48
1:B:72:ASP:HB2	1:B:324:GLN:OE1	2.13	0.48
1:C:204:ASP:OD2	1:C:217:SER:OG	2.20	0.48
1:D:181:SER:OG	1:D:182:PRO:HD2	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:160:HIS:O	2:A:640:HOH:O	2.20	0.47
1:D:131:SER:HB2	1:D:174:PHE:CE1	2.49	0.47
1:D:61:LEU:HD12	1:D:98:LEU:HB3	1.96	0.47
1:A:60:LEU:HD21	1:A:76:ALA:HA	1.96	0.47
1:B:113:GLU:O	1:B:117:TYR:HB2	2.15	0.47
1:C:290:GLN:HG2	2:C:636:HOH:O	2.15	0.47
1:D:251:ALA:HB3	1:D:252:PRO:HD3	1.97	0.46
1:D:166:LYS:HA	1:D:201:PRO:HB2	1.97	0.46
1:B:354:ASN:OD1	2:B:638:HOH:O	2.20	0.46
1:B:245:GLU:HB3	2:B:511:HOH:O	2.16	0.46
1:B:103:MET:HA	1:B:106:LEU:HG	1.98	0.45
1:D:103:MET:HG3	1:D:237:PHE:HZ	1.81	0.45
1:A:181:SER:OG	1:A:182:PRO:HD2	2.17	0.45
1:A:27:LEU:HD22	1:A:51:ASP:HB3	1.98	0.45
1:D:129:ASN:HB3	1:D:163:SER:HB2	1.99	0.45
1:B:200:THR:HB	1:B:219:ASP:HB3	1.98	0.44
1:B:103:MET:HG3	1:B:237:PHE:CZ	2.52	0.44
1:C:40:ARG:CZ	2:C:626:HOH:O	2.65	0.44
1:A:130:ALA:O	1:A:159:LYS:HE3	2.18	0.44
1:C:55:SER:OG	1:C:57:LEU:HB2	2.18	0.44
1:D:49:ARG:HH11	1:D:93:LEU:HD21	1.83	0.44
1:A:110:GLN:O	1:A:114:GLU:HG3	2.18	0.43
1:C:166:LYS:HA	1:C:201:PRO:CB	2.47	0.43
1:D:60:LEU:HD21	1:D:76:ALA:HA	2.00	0.43
1:B:112:GLN:NE2	1:B:230:VAL:O	2.43	0.43
1:C:273:ALA:HB2	1:C:363:VAL:HG13	2.00	0.43
1:D:53:ARG:NH2	1:D:169:ASP:OD2	2.51	0.43
1:A:360:SER:HB3	1:A:382:TRP:CB	2.49	0.43
1:B:49:ARG:NH1	1:B:214:ASP:OD2	2.51	0.42
1:C:282:ARG:NH1	1:C:370:ARG:HE	2.16	0.42
1:C:64:ARG:HA	1:C:68:GLY:O	2.19	0.42
1:C:266:ALA:HB2	1:C:356:ALA:HA	2.02	0.42
1:D:49:ARG:NH1	1:D:93:LEU:HD21	2.35	0.42
1:A:135:ASN:HB3	1:D:282:ARG:HH21	1.83	0.42
1:B:61:LEU:HA	1:B:61:LEU:HD23	1.74	0.41
1:C:81:ARG:HH22	1:C:313:ASP:CG	2.23	0.41
1:D:373:HIS:HA	1:D:374:PRO:HD3	1.96	0.41
1:A:239:LEU:O	1:A:243:GLN:HG2	2.20	0.41
1:B:135:ASN:HD22	1:C:282:ARG:NH2	2.18	0.41
1:D:155:LEU:HB2	1:D:223:VAL:HB	2.02	0.41
1:C:245:GLU:HB3	2:C:644:HOH:O	2.20	0.41
1:C:101:ALA:HB3	1:C:102:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:103:MET:HG3	1:C:237:PHE:HZ	1.86	0.41
1:A:338:ARG:NH1	2:A:596:HOH:O	2.54	0.41
1:B:93:LEU:HD23	2:B:562:HOH:O	2.20	0.41
1:D:116:LEU:HD23	1:D:116:LEU:HA	1.84	0.41
1:A:360:SER:HB3	1:A:382:TRP:CA	2.51	0.41
1:A:58:LEU:HB2	2:A:560:HOH:O	2.21	0.40
1:A:93:LEU:HA	1:A:93:LEU:HD23	1.99	0.40
1:C:116:LEU:HA	1:C:116:LEU:HD23	1.95	0.40
1:B:37:GLU:HG2	2:B:626:HOH:O	2.20	0.40
1:B:85:ALA:HA	1:B:264:GLY:O	2.22	0.40

There are no symmetry-related clashes.

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	397/453 (88%)	393 (99%)	4 (1%)	0	100	100
1	B	397/453 (88%)	392 (99%)	5 (1%)	0	100	100
1	C	397/453 (88%)	391 (98%)	6 (2%)	0	100	100
1	D	397/453 (88%)	391 (98%)	5 (1%)	1 (0%)	50	60
All	All	1588/1812 (88%)	1567 (99%)	20 (1%)	1 (0%)	59	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	180	ASP

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	307/351 (88%)	305 (99%)	2 (1%)	91	97
1	B	307/351 (88%)	304 (99%)	3 (1%)	85	94
1	C	307/351 (88%)	305 (99%)	2 (1%)	91	97
1	D	307/351 (88%)	304 (99%)	3 (1%)	85	94
All	All	1228/1404 (88%)	1218 (99%)	10 (1%)	89	96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	TYR
1	A	363	VAL
1	B	96	TYR
1	B	181	SER
1	B	363	VAL
1	C	65	GLU
1	C	290	GLN
1	D	96	TYR
1	D	149	GLU
1	D	181	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	290	GLN
1	D	354	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	399/453 (88%)	-0.09	16 (4%)	36 47	17, 29, 63, 97	0
1	B	399/453 (88%)	0.12	14 (3%)	42 52	18, 35, 68, 88	0
1	C	399/453 (88%)	-0.26	3 (0%)	83 90	19, 27, 51, 70	0
1	D	399/453 (88%)	-0.03	11 (2%)	50 60	18, 35, 63, 89	0
All	All	1596/1812 (88%)	-0.07	44 (2%)	50 60	17, 31, 62, 97	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	LEU	6.2
1	A	182	PRO	4.4
1	D	180	ASP	4.4
1	A	180	ASP	4.4
1	A	179	ASP	4.4
1	B	182	PRO	3.9
1	A	137	HIS	3.9
1	B	138	VAL	3.9
1	B	161	PHE	3.8
1	A	183	GLN	3.4
1	D	179	ASP	3.3
1	C	242	ILE	3.3
1	B	332	ALA	3.2
1	B	101	ALA	3.0
1	D	161	PHE	3.0
1	A	149	GLU	2.9
1	A	242	ILE	2.9
1	B	180	ASP	2.9
1	D	182	PRO	2.9
1	D	149	GLU	2.7
1	A	140	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	139	LEU	2.6
1	D	110	GLN	2.5
1	D	151	GLY	2.5
1	D	32	ARG	2.5
1	A	178	GLN	2.5
1	A	161	PHE	2.5
1	C	239	LEU	2.4
1	A	151	GLY	2.4
1	B	151	GLY	2.4
1	A	181	SER	2.3
1	D	66	TYR	2.3
1	B	291	GLN	2.3
1	C	161	PHE	2.3
1	B	65	GLU	2.2
1	B	40	ARG	2.2
1	A	134	ASN	2.2
1	A	280	GLN	2.2
1	B	149	GLU	2.2
1	A	160	HIS	2.1
1	D	111	GLU	2.1
1	D	122	GLN	2.1
1	B	242	ILE	2.0
1	B	106	LEU	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 carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.