



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:14 PM UTC

PDB ID : 9RYG / pdb_00009ryg
Title : Bifunctional Non-haem Iron Oxygenase NovR Involved in Novobiocin Biosynthesis with product bound
Authors : Keller, S.; Lawson, D.M.
Deposited on : 2025-07-15
Resolution : 1.79 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

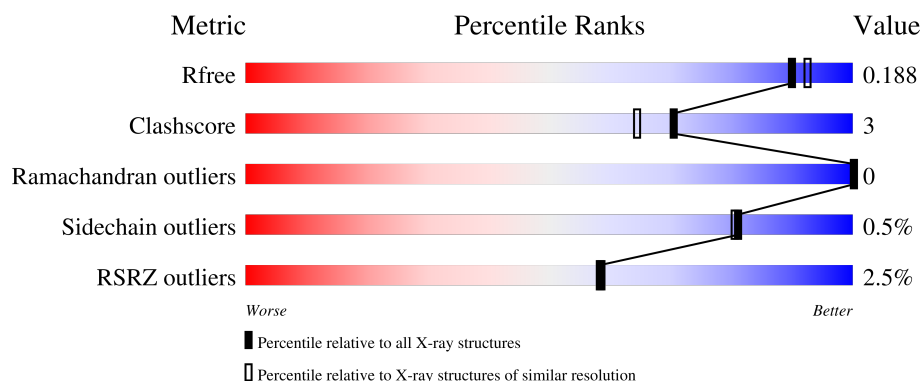
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	275	3% 84% 7% 7%
1	B	275	85% 7% 7%
1	C	275	4% 89% 6% 5%
1	D	275	2% 89% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9253 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.

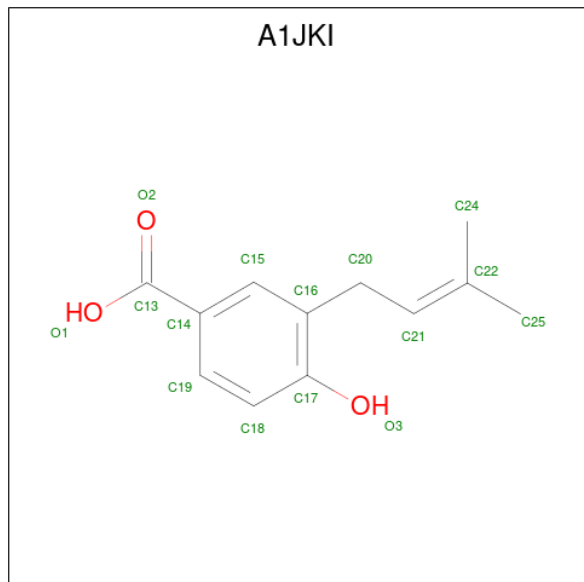
- Molecule 1 is a protein called Decarboxylase NovR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	4	0
			2055	1302	373	375	5			
1	B	255	Total	C	N	O	S	0	4	0
			2053	1305	377	367	4			
1	C	262	Total	C	N	O	S	0	1	0
			2067	1314	376	372	5			
1	D	257	Total	C	N	O	S	0	1	0
			2038	1298	370	366	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ASP	-	expression tag	UNP Q9L9F0
A	-3	HIS	-	expression tag	UNP Q9L9F0
A	-2	PRO	-	expression tag	UNP Q9L9F0
A	-1	PHE	-	expression tag	UNP Q9L9F0
A	0	THR	-	expression tag	UNP Q9L9F0
B	-4	ASP	-	expression tag	UNP Q9L9F0
B	-3	HIS	-	expression tag	UNP Q9L9F0
B	-2	PRO	-	expression tag	UNP Q9L9F0
B	-1	PHE	-	expression tag	UNP Q9L9F0
B	0	THR	-	expression tag	UNP Q9L9F0
C	-4	ASP	-	expression tag	UNP Q9L9F0
C	-3	HIS	-	expression tag	UNP Q9L9F0
C	-2	PRO	-	expression tag	UNP Q9L9F0
C	-1	PHE	-	expression tag	UNP Q9L9F0
C	0	THR	-	expression tag	UNP Q9L9F0
D	-4	ASP	-	expression tag	UNP Q9L9F0
D	-3	HIS	-	expression tag	UNP Q9L9F0
D	-2	PRO	-	expression tag	UNP Q9L9F0
D	-1	PHE	-	expression tag	UNP Q9L9F0
D	0	THR	-	expression tag	UNP Q9L9F0

- Molecule 2 is 3-(3-methylbut-2-enyl)-4-oxidanyl-benzoic acid (CCD ID: A1JKI) (formula: $C_{12}H_{14}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			15	12	3		
2	B	1	Total	C	O	0	0
			15	12	3		
2	C	1	Total	C	O	0	0
			15	12	3		
2	D	1	Total	C	O	0	0
			15	12	3		

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	B	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	D	1	Total	Fe	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		

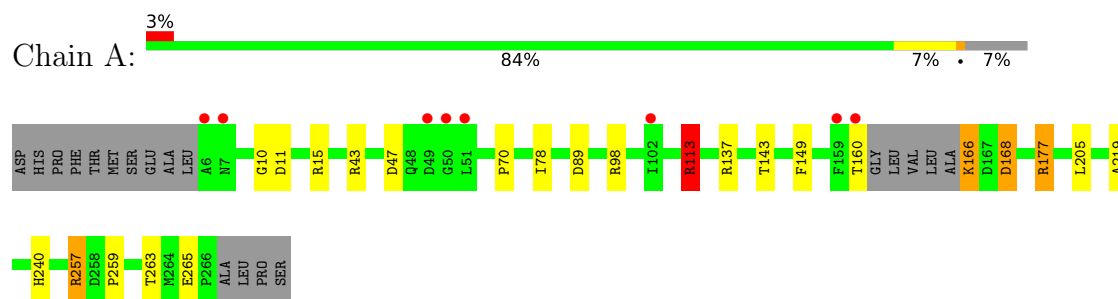
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	216	Total	O	0	1
			217	217		
6	B	246	Total	O	0	2
			248	248		
6	C	217	Total	O	0	0
			217	217		
6	D	204	Total	O	0	0
			204	204		

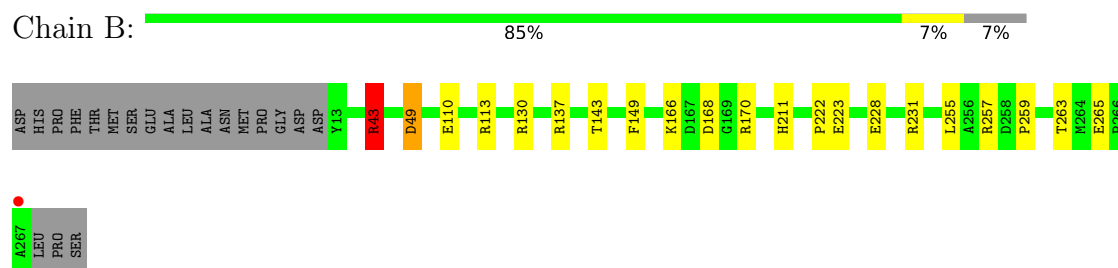
3 Residue-property plots [i](#)

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.

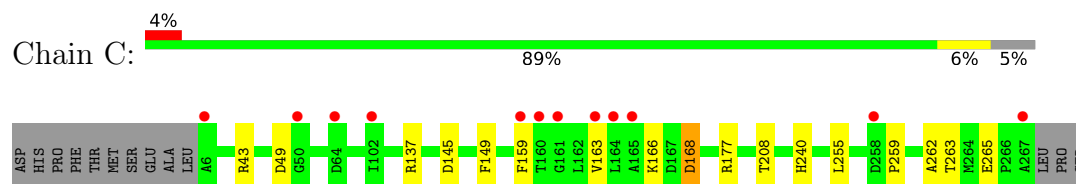
• Molecule 1: Decarboxylase NovR



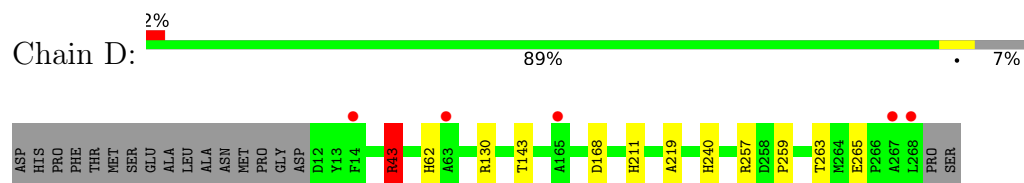
• Molecule 1: Decarboxylase NovR



• Molecule 1: Decarboxylase NovR



• Molecule 1: Decarboxylase NovR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.51Å 138.97Å 100.61Å 90.00° 101.44° 90.00°	Depositor
Resolution (Å)	49.36 – 1.79 49.36 – 1.79	Depositor EDS
% Data completeness (in resolution range)	97.4 (49.36-1.79) 97.4 (49.36-1.79)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, R_{free}	0.161 , 0.188 0.161 , 0.188	Depositor DCC
R_{free} test set	5347 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9253	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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, FE, EDO, A1JKI

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	0.68	0/2112	1.09	10/2877 (0.3%)
1	B	0.74	0/2110	1.13	9/2874 (0.3%)
1	C	0.64	0/2125	1.08	7/2897 (0.2%)
1	D	0.66	0/2095	1.09	8/2856 (0.3%)
All	All	0.68	0/8442	1.10	34/11504 (0.3%)

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	4
1	B	0	1
1	D	0	1
All	All	0	6

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	ARG	CA-CB-CG	7.33	128.76	114.10
1	B	166	LYS	CG-CD-CE	6.55	126.37	111.30
1	C	168	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	240	HIS	CA-CB-CG	-6.43	107.37	113.80
1	B	49	ASP	CA-CB-CG	6.28	118.88	112.60
1	C	159	PHE	N-CA-CB	6.02	119.92	110.71
1	A	149	PHE	CA-CB-CG	-5.95	107.85	113.80
1	B	168	ASP	CB-CA-C	5.94	120.95	110.85
1	C	43	ARG	CG-CD-NE	-5.93	98.94	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	THR	CA-CB-OG1	-5.79	100.92	109.60
1	A	10	GLY	CA-C-N	5.75	128.78	120.79
1	A	10	GLY	C-N-CA	5.75	128.78	120.79
1	B	43	ARG	CA-CB-CG	-5.72	102.67	114.10
1	D	265	GLU	CG-CD-OE1	-5.62	105.47	118.40
1	A	11	ASP	CA-CB-CG	5.62	118.22	112.60
1	D	265	GLU	CG-CD-OE2	5.58	131.23	118.40
1	D	43	ARG	CA-CB-CG	-5.57	102.97	114.10
1	A	89	ASP	CA-CB-CG	5.50	118.09	112.60
1	B	265	GLU	CB-CG-CD	5.43	121.83	112.60
1	C	240	HIS	CA-CB-CG	-5.42	108.38	113.80
1	D	240	HIS	CA-CB-CG	-5.37	108.43	113.80
1	C	43	ARG	CA-CB-CG	-5.37	103.36	114.10
1	B	149	PHE	CA-CB-CG	-5.35	108.45	113.80
1	A	168	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	166	LYS	CB-CG-CD	5.23	123.33	111.30
1	C	149	PHE	CA-CB-CG	-5.17	108.63	113.80
1	D	43	ARG	CG-CD-NE	5.14	123.30	112.00
1	D	168	ASP	CB-CA-C	5.13	119.56	110.85
1	A	143	THR	CA-CB-OG1	-5.07	101.99	109.60
1	C	177	ARG	CB-CA-C	-5.06	110.72	116.54
1	A	113	ARG	CD-NE-CZ	5.06	131.48	124.40
1	D	143	THR	CA-CB-OG1	-5.05	102.03	109.60
1	B	265	GLU	CG-CD-OE1	-5.03	106.83	118.40
1	D	62	HIS	CA-CB-CG	-5.03	108.77	113.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ARG	Sidechain
1	A	15	ARG	Sidechain
1	A	177	ARG	Sidechain
1	A	257[A]	ARG	Sidechain
1	B	43	ARG	Sidechain
1	D	43	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	2055	0	1965	14	0
1	B	2053	0	1992	20	0
1	C	2067	0	1999	16	0
1	D	2038	0	1978	8	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	1	0
2	D	15	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	D	10	0	0	0	0
5	A	8	0	12	1	0
5	B	24	0	36	6	0
5	C	12	0	18	3	0
5	D	16	0	24	4	0
6	A	217	0	0	4	1
6	B	248	0	0	2	0
6	C	217	0	0	5	0
6	D	204	0	0	0	0
All	All	9253	0	8024	55	1

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 3.

All (55) 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:265:GLU:OE2	6:C:401:HOH:O	1.90	0.89
1:A:265:GLU:OE2	6:A:401:HOH:O	1.90	0.88
1:C:163:VAL:HG13	1:C:168:ASP:HB3	1.56	0.87
1:B:130[B]:ARG:HH12	1:C:208:THR:CG2	1.87	0.86
1:D:211:HIS:NE2	5:D:307:EDO:H12	1.91	0.85
1:B:211:HIS:NE2	5:B:308:EDO:H21	1.92	0.83
1:B:130[B]:ARG:HH12	1:C:208:THR:HG21	1.45	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:ASP:OD1	6:C:402:HOH:O	2.05	0.74
1:C:166:LYS:HE3	6:C:587:HOH:O	1.96	0.66
1:D:43:ARG:HD2	1:D:257[A]:ARG:CZ	2.27	0.64
1:B:130[B]:ARG:NH1	1:C:208:THR:CG2	2.62	0.61
1:B:137:ARG:HH11	5:B:305:EDO:H11	1.67	0.59
1:B:130[B]:ARG:HH12	1:C:208:THR:HG22	1.64	0.57
1:B:43:ARG:HD2	1:B:257[B]:ARG:CZ	2.35	0.56
1:D:130:ARG:NH2	5:D:308:EDO:O1	2.39	0.55
5:C:304:EDO:H22	1:D:219:ALA:HB1	1.89	0.53
1:B:130[B]:ARG:NH1	1:C:208:THR:HG22	2.22	0.53
1:B:228:GLU:CD	1:B:228:GLU:H	2.16	0.53
1:B:49:ASP:HA	5:B:309:EDO:H12	1.92	0.52
1:C:163:VAL:HG22	1:C:168:ASP:OD2	2.11	0.50
1:C:259:PRO:O	1:C:263:THR:HG23	2.12	0.50
1:D:43:ARG:HH11	1:D:43:ARG:HG3	1.75	0.50
1:B:43:ARG:HD2	1:B:257[B]:ARG:NE	2.27	0.50
1:A:219:ALA:HB1	5:D:305:EDO:H22	1.93	0.50
1:B:43:ARG:HG2	1:B:43:ARG:O	2.13	0.49
1:A:259:PRO:O	1:A:263:THR:HG23	2.13	0.48
1:B:137:ARG:HH11	5:B:305:EDO:C1	2.26	0.48
1:A:160:THR:HB	6:A:586:HOH:O	2.14	0.48
1:C:49:ASP:HA	5:C:305:EDO:O1	2.13	0.48
1:D:43:ARG:HD2	1:D:257[A]:ARG:NE	2.30	0.47
1:A:137:ARG:NH1	5:A:305:EDO:O1	2.47	0.47
1:B:222:PRO:HG2	5:B:310:EDO:H12	1.96	0.47
1:D:43:ARG:O	1:D:43:ARG:HG2	2.15	0.47
1:B:43:ARG:HH11	1:B:43:ARG:HG3	1.80	0.46
1:A:205:LEU:HA	5:D:308:EDO:H22	1.98	0.46
1:D:259:PRO:O	1:D:263:THR:HG23	2.15	0.46
2:C:301:A1JKI:C13	6:C:410:HOH:O	2.64	0.45
1:B:43:ARG:HD3	6:B:588:HOH:O	2.16	0.45
1:B:259:PRO:O	1:B:263:THR:HG23	2.16	0.45
1:A:43:ARG:HG3	1:A:43:ARG:HH11	1.83	0.44
1:A:43:ARG:HD2	1:A:257[A]:ARG:CZ	2.49	0.43
1:A:98:ARG:HD3	6:A:496:HOH:O	2.17	0.42
5:B:307:EDO:H11	5:B:308:EDO:H11	1.99	0.42
1:A:70:PRO:HD2	1:A:78:ILE:HD11	2.01	0.42
1:A:47[B]:ASP:CG	1:A:47[B]:ASP:O	2.59	0.42
1:C:166:LYS:HG2	6:C:587:HOH:O	2.20	0.41
1:B:110:GLU:OE1	1:B:113:ARG:NH1	2.54	0.41
1:B:170[B]:ARG:HG2	6:B:552:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ARG:NH1	5:C:304:EDO:O1	2.51	0.41
1:C:255:LEU:HD23	1:C:255:LEU:HA	1.79	0.41
1:A:113:ARG:HG2	6:A:593:HOH:O	2.21	0.41
1:A:177:ARG:HH11	1:A:177:ARG:HG3	1.86	0.41
1:B:255:LEU:HA	1:B:255:LEU:HD23	1.80	0.40
1:A:43:ARG:HD2	1:A:257[A]:ARG:NE	2.36	0.40
1:C:255:LEU:HD22	1:C:262:ALA:HA	2.03	0.40

All (1) 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)
6:A:577:HOH:O	6:A:577:HOH:O[2_656]	1.51	0.69

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	256/275 (93%)	252 (98%)	4 (2%)	0	100	100
1	B	257/275 (94%)	253 (98%)	4 (2%)	0	100	100
1	C	261/275 (95%)	255 (98%)	6 (2%)	0	100	100
1	D	256/275 (93%)	249 (97%)	7 (3%)	0	100	100
All	All	1030/1100 (94%)	1009 (98%)	21 (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	208/220 (94%)	206 (99%)	2 (1%)	68	64
1	B	207/220 (94%)	206 (100%)	1 (0%)	81	80
1	C	208/220 (94%)	208 (100%)	0	100	100
1	D	206/220 (94%)	205 (100%)	1 (0%)	81	80
All	All	829/880 (94%)	825 (100%)	4 (0%)	81	80

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	LYS
1	A	168	ASP
1	B	223	GLU
1	D	43	ARG

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

Mol	Chain	Res	Type
1	A	144	GLN
1	A	175	GLN
1	A	186	ASN
1	B	16	GLN
1	D	186	ASN

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

Of 29 ligands modelled in this entry, 4 are monoatomic - leaving 25 for Mogul analysis.

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
5	EDO	C	306	-	3,3,3	0.33	0	2,2,2	0.44	0
4	SO4	B	304	-	4,4,4	0.37	0	6,6,6	0.16	0
5	EDO	D	308	-	3,3,3	0.63	0	2,2,2	0.88	0
4	SO4	D	303	-	4,4,4	0.22	0	6,6,6	0.41	0
5	EDO	B	305	-	3,3,3	0.23	0	2,2,2	0.83	0
2	A1JKI	B	301	3	15,15,15	1.40	2 (13%)	20,20,20	3.33	8 (40%)
5	EDO	D	307	-	3,3,3	0.74	0	2,2,2	1.13	0
2	A1JKI	D	301	3	15,15,15	1.18	1 (6%)	20,20,20	2.83	8 (40%)
5	EDO	B	306	-	3,3,3	0.10	0	2,2,2	0.40	0
4	SO4	C	303	-	4,4,4	0.25	0	6,6,6	0.22	0
4	SO4	D	304	-	4,4,4	0.33	0	6,6,6	0.06	0
5	EDO	D	306	-	3,3,3	0.43	0	2,2,2	0.83	0
5	EDO	C	304	-	3,3,3	0.19	0	2,2,2	0.49	0
5	EDO	A	304	-	3,3,3	0.47	0	2,2,2	0.06	0
5	EDO	C	305	-	3,3,3	0.36	0	2,2,2	0.35	0
2	A1JKI	A	301	3	15,15,15	1.32	2 (13%)	20,20,20	1.53	4 (20%)
5	EDO	B	309	-	3,3,3	0.30	0	2,2,2	0.40	0
2	A1JKI	C	301	3	15,15,15	0.85	0	20,20,20	1.83	5 (25%)
5	EDO	B	310	-	3,3,3	0.42	0	2,2,2	0.59	0
5	EDO	B	308	-	3,3,3	0.84	0	2,2,2	1.07	0
4	SO4	A	303	-	4,4,4	0.28	0	6,6,6	0.12	0
5	EDO	B	307	-	3,3,3	0.34	0	2,2,2	0.21	0
4	SO4	B	303	-	4,4,4	0.24	0	6,6,6	0.18	0
5	EDO	A	305	-	3,3,3	0.21	0	2,2,2	0.96	0
5	EDO	D	305	-	3,3,3	0.25	0	2,2,2	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	306	-	-	1/1/1/1	-
5	EDO	B	305	-	-	0/1/1/1	-
2	A1JKI	B	301	3	-	0/9/9/9	0/1/1/1
5	EDO	D	307	-	-	1/1/1/1	-
5	EDO	D	305	-	-	0/1/1/1	-
2	A1JKI	D	301	3	-	0/9/9/9	0/1/1/1
5	EDO	B	306	-	-	1/1/1/1	-
5	EDO	D	306	-	-	1/1/1/1	-
5	EDO	C	304	-	-	0/1/1/1	-
5	EDO	A	304	-	-	1/1/1/1	-
5	EDO	C	305	-	-	1/1/1/1	-
2	A1JKI	A	301	3	-	0/9/9/9	0/1/1/1
5	EDO	B	309	-	-	0/1/1/1	-
2	A1JKI	C	301	3	-	0/9/9/9	0/1/1/1
5	EDO	B	310	-	-	1/1/1/1	-
5	EDO	B	308	-	-	1/1/1/1	-
5	EDO	B	307	-	-	0/1/1/1	-
5	EDO	A	305	-	-	0/1/1/1	-
5	EDO	D	308	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	A1JKI	C19-C18	3.95	1.45	1.38
2	A	301	A1JKI	C15-C14	2.52	1.43	1.39
2	B	301	A1JKI	C15-C14	2.51	1.43	1.39
2	D	301	A1JKI	C19-C18	2.31	1.42	1.38
2	A	301	A1JKI	C14-C13	2.21	1.54	1.49

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	A1JKI	C20-C21-C22	9.14	143.22	127.52
2	B	301	A1JKI	C25-C22-C21	-5.68	105.62	122.66
2	D	301	A1JKI	C20-C21-C22	5.55	137.05	127.52
2	B	301	A1JKI	C20-C16-C17	-5.39	110.36	120.78
2	D	301	A1JKI	C25-C22-C21	-5.38	106.52	122.66
2	D	301	A1JKI	C20-C16-C17	-5.32	110.49	120.78
2	B	301	A1JKI	C20-C16-C15	4.45	129.81	121.02
2	D	301	A1JKI	C20-C16-C15	4.39	129.70	121.02
2	B	301	A1JKI	C24-C22-C21	4.00	134.65	122.66
2	B	301	A1JKI	C16-C20-C21	3.90	121.09	112.67
2	C	301	A1JKI	C20-C16-C17	-3.65	113.73	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	A1JKI	C20-C16-C15	3.53	127.99	121.02
2	A	301	A1JKI	C16-C20-C21	3.41	120.03	112.67
2	D	301	A1JKI	C24-C22-C21	3.32	132.62	122.66
2	D	301	A1JKI	C16-C20-C21	3.18	119.54	112.67
2	D	301	A1JKI	C25-C22-C24	2.71	120.83	114.59
2	C	301	A1JKI	C16-C20-C21	2.61	118.31	112.67
2	D	301	A1JKI	O1-C13-C14	2.59	121.49	114.84
2	B	301	A1JKI	O1-C13-C14	2.56	121.39	114.84
2	A	301	A1JKI	C20-C16-C15	2.49	125.95	121.02
2	A	301	A1JKI	O1-C13-C14	2.48	121.20	114.84
2	A	301	A1JKI	C20-C16-C17	-2.32	116.31	120.78
2	B	301	A1JKI	C25-C22-C24	2.23	119.72	114.59
2	C	301	A1JKI	O2-C13-C14	-2.19	115.73	121.46
2	C	301	A1JKI	C25-C22-C24	2.01	119.21	114.59

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	306	EDO	O1-C1-C2-O2
5	C	306	EDO	O1-C1-C2-O2
5	A	304	EDO	O1-C1-C2-O2
5	B	308	EDO	O1-C1-C2-O2
5	B	310	EDO	O1-C1-C2-O2
5	D	308	EDO	O1-C1-C2-O2
5	D	307	EDO	O1-C1-C2-O2
5	C	305	EDO	O1-C1-C2-O2
5	D	306	EDO	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	308	EDO	2	0
5	B	305	EDO	2	0
5	D	307	EDO	1	0
5	C	304	EDO	2	0
5	C	305	EDO	1	0
5	B	309	EDO	1	0
2	C	301	A1JKI	1	0
5	B	310	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	308	EDO	2	0
5	B	307	EDO	1	0
5	A	305	EDO	1	0
5	D	305	EDO	1	0

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	256/275 (93%)	-0.11	8 (3%) 51 51	13, 27, 57, 82	4 (1%)
1	B	255/275 (92%)	-0.31	1 (0%) 88 89	12, 23, 45, 67	4 (1%)
1	C	262/275 (95%)	-0.04	12 (4%) 37 36	18, 30, 63, 83	1 (0%)
1	D	257/275 (93%)	-0.10	5 (1%) 66 66	17, 29, 54, 91	1 (0%)
All	All	1030/1100 (93%)	-0.14	26 (2%) 58 58	12, 27, 55, 91	10 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	268	LEU	5.9
1	A	6	ALA	5.4
1	C	6	ALA	5.2
1	D	63	ALA	4.3
1	C	267	ALA	4.2
1	C	159	PHE	4.1
1	C	163	VAL	3.6
1	A	50	GLY	3.6
1	C	50	GLY	3.5
1	B	267	ALA	3.5
1	C	165	ALA	3.5
1	C	160	THR	3.5
1	C	164	LEU	3.0
1	D	267	ALA	2.9
1	C	161	GLY	2.9
1	A	160	THR	2.8
1	A	102	ILE	2.6
1	A	7	ASN	2.6
1	A	49	ASP	2.5
1	A	51	LEU	2.3
1	D	14	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	102	ILE	2.1
1	D	165	ALA	2.1
1	A	159	PHE	2.0
1	C	64	ASP	2.0
1	C	258	ASP	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
5	EDO	B	307	4/4	0.80	0.21	35,36,43,48	0
4	SO4	C	303	5/5	0.82	0.10	64,70,73,80	0
2	A1JKI	A	301	15/15	0.82	0.17	45,66,75,78	0
4	SO4	D	304	5/5	0.83	0.10	64,80,85,88	0
4	SO4	A	303	5/5	0.83	0.12	75,84,93,99	0
5	EDO	D	308	4/4	0.84	0.16	38,45,49,52	0
5	EDO	B	308	4/4	0.87	0.10	24,29,30,39	0
5	EDO	B	309	4/4	0.87	0.13	43,48,50,51	0
5	EDO	B	306	4/4	0.87	0.12	42,47,52,53	0
4	SO4	B	304	5/5	0.89	0.09	49,61,66,73	0
5	EDO	C	305	4/4	0.89	0.13	51,53,57,57	0
2	A1JKI	C	301	15/15	0.89	0.13	51,55,62,65	0
5	EDO	D	307	4/4	0.90	0.10	25,31,34,44	0
4	SO4	B	303	5/5	0.91	0.08	48,50,60,60	0
5	EDO	A	304	4/4	0.92	0.10	35,37,40,48	0
5	EDO	C	306	4/4	0.92	0.11	40,42,45,51	0
5	EDO	A	305	4/4	0.93	0.11	32,34,38,41	0
5	EDO	D	306	4/4	0.93	0.11	21,33,33,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	C	304	4/4	0.94	0.10	35,37,39,42	0
2	A1JKI	B	301	15/15	0.94	0.08	28,32,41,41	0
5	EDO	B	305	4/4	0.95	0.10	30,36,39,51	0
5	EDO	B	310	4/4	0.95	0.09	38,40,41,43	0
2	A1JKI	D	301	15/15	0.96	0.08	32,34,44,44	0
5	EDO	D	305	4/4	0.97	0.06	37,39,43,43	0
4	SO4	D	303	5/5	0.98	0.06	38,39,41,41	0
3	FE	A	302	1/1	0.99	0.13	38,38,38,38	0
3	FE	B	302	1/1	1.00	0.02	23,23,23,23	0
3	FE	C	302	1/1	1.00	0.04	33,33,33,33	0
3	FE	D	302	1/1	1.00	0.03	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.