



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:59 AM UTC

PDB ID : 6ZQ5 / pdb_00006zq5
Title : Crystal structure of Chaetomium thermophilum Glycerol Kinase in P2221 space group
Authors : Wilk, P.; Wator, E.; Malecki, P.; Grudnik, P.
Deposited on : 2020-07-09
Resolution : 2.14 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

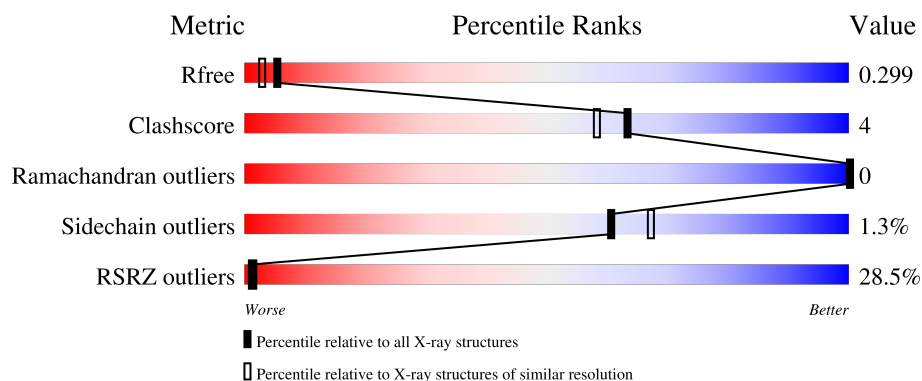
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	526	41% 87% 9% ..
1	B	526	14% 86% 11% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15910 atoms, of which 7763 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 Glycerol kinase-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	510	Total	C	H	N	O	S	0	0	0
			7755	2468	3857	674	740	16			
1	B	510	Total	C	H	N	O	S	0	0	0
			7756	2468	3858	674	740	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	GLY	-	expression tag	UNP G0SAG9
A	66	SER	-	expression tag	UNP G0SAG9
B	65	GLY	-	expression tag	UNP G0SAG9
B	66	SER	-	expression tag	UNP G0SAG9

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		

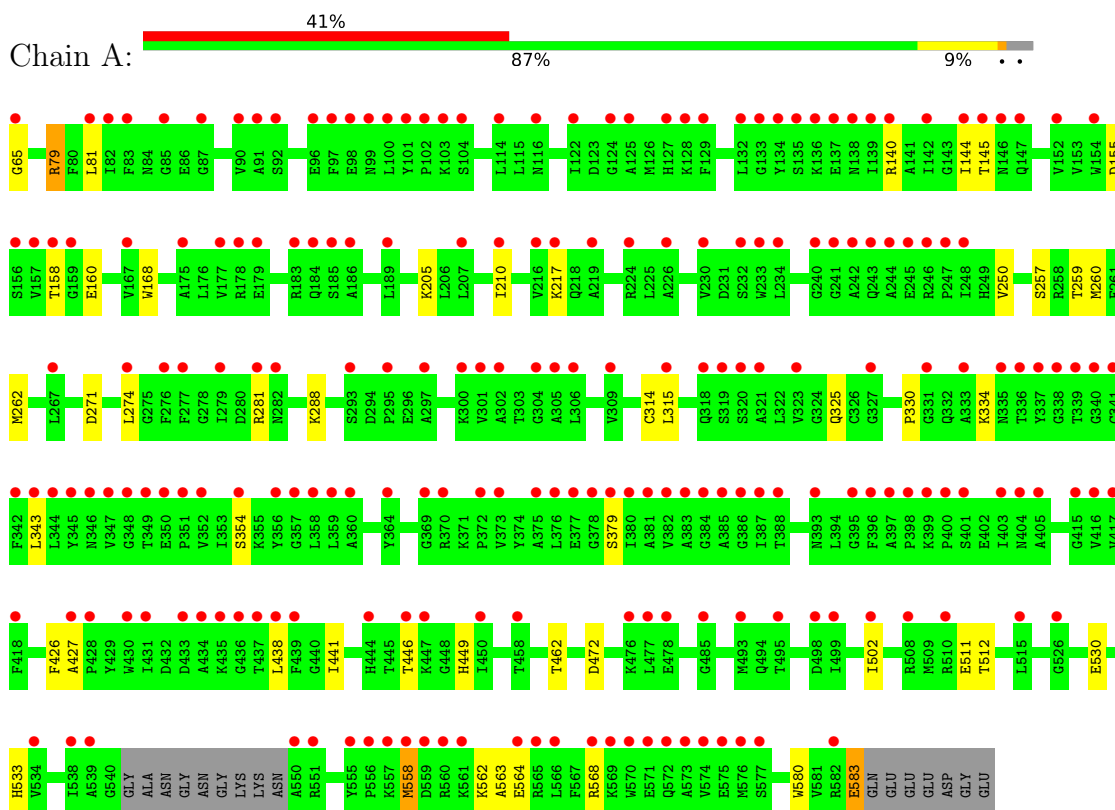
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	185	Total	O	0	1
			186	186		
3	B	133	Total	O	0	0
			133	133		

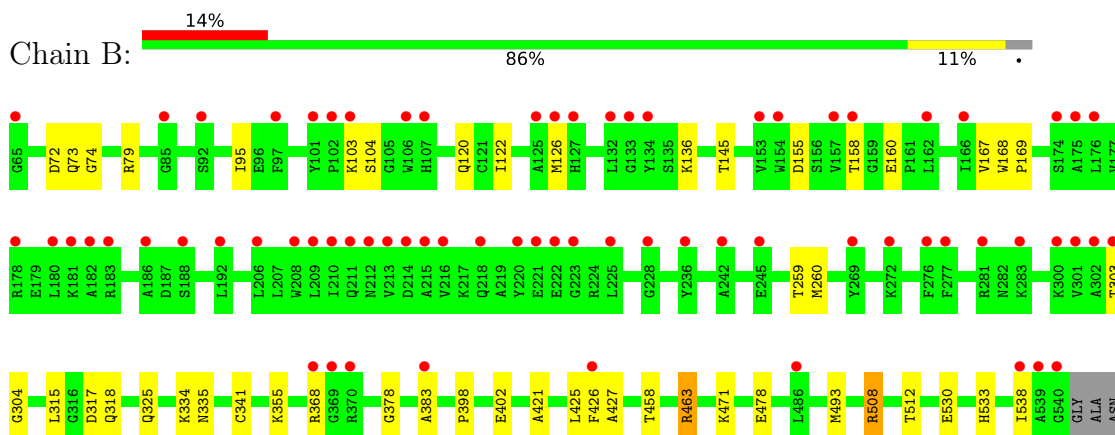
3 Residue-property plots

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: Glycerol kinase-like protein



• Molecule 1: Glycerol kinase-like protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	63.56Å 111.47Å 171.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.71 – 2.14 46.71 – 2.14	Depositor EDS
% Data completeness (in resolution range)	89.9 (46.71-2.14) 89.9 (46.71-2.14)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.215 , 0.249 0.275 , 0.299	Depositor DCC
R_{free} test set	2100 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15910	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: EDO

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	0.17	0/3980	0.39	0/5395
1	B	0.29	2/3980 (0.1%)	0.44	2/5395 (0.0%)
All	All	0.24	2/7960 (0.0%)	0.42	2/10790 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	572	GLN	C-O	-5.10	1.18	1.24
1	B	478	GLU	C-O	-5.03	1.17	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	508	ARG	N-CA-C	-6.75	103.72	112.23
1	B	463	ARG	N-CA-C	-5.22	105.67	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3898	3857	3857	32	1
1	B	3898	3858	3857	31	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	20	30	30	1	0
2	B	12	18	18	1	0
3	A	186	0	0	0	0
3	B	133	0	0	1	0
All	All	8147	7763	7762	62	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 4.

All (62) 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:79:ARG:HH11	1:A:79:ARG:HG2	1.56	0.71
1:B:421:ALA:HB2	1:B:425:LEU:HG	1.82	0.62
1:A:250:VAL:HG12	1:A:288:LYS:HB3	1.82	0.62
1:A:530:GLU:HG2	1:A:533:HIS:H	1.66	0.60
1:B:72:ASP:HB3	1:B:79:ARG:HG3	1.85	0.57
1:A:343:LEU:HD21	1:A:462:THR:HG23	1.87	0.56
1:A:271:ASP:OD1	1:A:281:ARG:HD2	2.07	0.55
1:A:65:GLY:O	1:A:140:ARG:NH2	2.36	0.55
1:B:575:GLU:O	1:B:578:ARG:HG2	2.08	0.54
1:B:158:THR:HG23	1:B:160:GLU:H	1.71	0.54
1:B:493:MET:HA	1:B:493:MET:HE2	1.90	0.54
1:B:530:GLU:HG2	1:B:533:HIS:H	1.74	0.53
1:A:274:LEU:HD13	1:A:281:ARG:HG3	1.91	0.52
1:B:155:ASP:HB3	1:B:158:THR:HG22	1.92	0.52
1:B:325:GLN:HG2	1:B:512:THR:HG21	1.92	0.51
1:B:463:ARG:NH2	1:B:564:GLU:OE2	2.33	0.51
1:A:583:GLU:OE1	1:A:583:GLU:HA	2.11	0.51
1:A:354:SER:OG	1:A:472:ASP:OD2	2.29	0.50
1:A:379:SER:HB2	2:A:605:EDO:H12	1.93	0.49
1:A:446:THR:HG22	1:A:449:HIS:ND1	2.27	0.49
1:B:95:ILE:HD12	1:B:120:GLN:HB2	1.95	0.49
1:A:79:ARG:HH11	1:A:79:ARG:CG	2.26	0.49
1:A:330:PRO:HG2	1:B:355:LYS:HE2	1.95	0.48
1:B:168:TRP:CG	1:B:169:PRO:HD3	2.48	0.48
1:A:438:LEU:HD23	1:A:441:ILE:HD11	1.95	0.48
1:A:79:ARG:HG2	1:A:79:ARG:NH1	2.20	0.48
1:B:259:THR:O	1:B:260:MET:HB2	2.15	0.47
1:B:168:TRP:CD2	1:B:169:PRO:HD3	2.50	0.47
1:B:334:LYS:HD2	1:B:334:LYS:C	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:MET:HE1	1:A:563:ALA:HA	1.97	0.47
1:B:335:ASN:OD1	1:B:341:CYS:HB3	2.15	0.47
1:A:259:THR:O	1:A:260:MET:HB2	2.16	0.46
1:B:538:ILE:HG22	1:B:538:ILE:O	2.15	0.46
1:B:167:VAL:HG12	1:B:169:PRO:HD2	1.98	0.46
1:B:378:GLY:HA2	2:B:1103:EDO:O2	2.16	0.45
1:A:325:GLN:HG2	1:A:512:THR:HG21	1.98	0.45
1:A:145:THR:HA	1:A:315:LEU:O	2.17	0.45
1:B:561:LYS:N	1:B:561:LYS:HD2	2.32	0.44
1:B:398:PRO:HD2	1:B:402:GLU:OE2	2.17	0.44
1:A:158:THR:HG23	1:A:160:GLU:H	1.83	0.44
1:A:564:GLU:O	1:A:568:ARG:HG2	2.18	0.44
1:A:168:TRP:HA	1:A:205:LYS:HE2	2.00	0.44
1:B:355:LYS:NZ	3:B:1207:HOH:O	2.49	0.44
1:A:155:ASP:HB3	1:A:158:THR:HG22	1.99	0.44
1:A:446:THR:HG22	1:A:449:HIS:CE1	2.53	0.43
1:B:303:THR:OG1	1:B:304:GLY:N	2.51	0.43
1:A:257:SER:HA	1:A:262:MET:HE2	2.01	0.43
1:A:144:ILE:O	1:A:314:CYS:HA	2.19	0.43
1:B:103:LYS:HG3	1:B:104:SER:N	2.34	0.43
1:B:122:ILE:O	1:B:126:MET:HG2	2.19	0.43
1:A:210:ILE:O	1:A:217:LYS:HG2	2.19	0.43
1:A:426:PHE:O	1:A:427:ALA:C	2.62	0.43
1:A:558:MET:HE3	1:A:562:LYS:HG2	2.01	0.42
1:B:155:ASP:HB3	1:B:158:THR:CG2	2.49	0.42
1:B:73:GLN:NE2	1:B:74:GLY:O	2.53	0.42
1:B:317:ASP:OD1	1:B:318:GLN:N	2.52	0.42
1:A:81:LEU:HD21	1:A:511:GLU:HG3	2.03	0.41
1:B:383:ALA:HA	1:B:458:THR:HG21	2.03	0.41
1:B:426:PHE:O	1:B:427:ALA:C	2.64	0.41
1:A:558:MET:CE	1:A:563:ALA:HA	2.50	0.40
1:B:145:THR:HA	1:B:315:LEU:O	2.22	0.40
1:A:334:LYS:HD2	1:A:334:LYS:C	2.47	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)
1:A:580:TRP:O	1:B:569:LYS:HZ1[4_565]	1.52	0.08

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	506/526 (96%)	493 (97%)	13 (3%)	0	100	100
1	B	506/526 (96%)	491 (97%)	15 (3%)	0	100	100
All	All	1012/1052 (96%)	984 (97%)	28 (3%)	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	409/420 (97%)	405 (99%)	4 (1%)	68	74
1	B	409/420 (97%)	402 (98%)	7 (2%)	53	58
All	All	818/840 (97%)	807 (99%)	11 (1%)	61	67

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
1	A	502	ILE
1	A	558	MET
1	A	583	GLU
1	B	136	LYS
1	B	368	ARG
1	B	471	LYS
1	B	508	ARG

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Mol	Chain	Res	Type
1	B	551	ARG
1	B	552	GLU
1	B	559	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	494	GLN
1	B	88	ASN
1	B	116	ASN
1	B	120	GLN
1	B	211	GLN
1	B	243	GLN
1	B	475	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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	603	-	3,3,3	0.43	0	2,2,2	0.33	0
2	EDO	B	1102	-	3,3,3	0.43	0	2,2,2	0.33	0
2	EDO	B	1101	-	3,3,3	0.44	0	2,2,2	0.34	0
2	EDO	A	605	-	3,3,3	0.45	0	2,2,2	0.43	0
2	EDO	A	601	-	3,3,3	0.43	0	2,2,2	0.40	0
2	EDO	A	604	-	3,3,3	0.42	0	2,2,2	0.45	0
2	EDO	B	1103	-	3,3,3	0.49	0	2,2,2	0.88	0
2	EDO	A	602	-	3,3,3	0.41	0	2,2,2	0.39	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
2	EDO	A	603	-	-	0/1/1/1	-
2	EDO	B	1102	-	-	0/1/1/1	-
2	EDO	B	1101	-	-	1/1/1/1	-
2	EDO	A	605	-	-	0/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	A	604	-	-	0/1/1/1	-
2	EDO	B	1103	-	-	1/1/1/1	-
2	EDO	A	602	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	EDO	O1-C1-C2-O2
2	A	602	EDO	O1-C1-C2-O2
2	B	1103	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	605	EDO	1	0
2	B	1103	EDO	1	0

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	510/526 (96%)	1.91	215 (42%) 0 1	31, 53, 85, 107	0
1	B	510/526 (96%)	1.05	76 (14%) 5 7	30, 59, 86, 102	0
All	All	1020/1052 (96%)	1.48	291 (28%) 1 1	30, 56, 86, 107	0

All (291) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	540	GLY	7.1
1	A	416	VAL	6.9
1	A	417	VAL	6.5
1	A	383	ALA	6.4
1	A	550	ALA	6.4
1	A	437	THR	6.1
1	A	184	GLN	5.9
1	A	341	CYS	5.9
1	B	550	ALA	5.7
1	A	343	LEU	5.6
1	A	382	VAL	5.6
1	A	158	THR	5.5
1	A	380	ILE	5.5
1	A	344	LEU	5.3
1	A	378	GLY	5.3
1	A	375	ALA	5.1
1	A	436	GLY	4.8
1	A	538	ILE	4.7
1	A	318	GLN	4.7
1	A	342	PHE	4.6
1	A	327	GLY	4.3
1	A	246	ARG	4.3
1	A	384	GLY	4.3
1	A	560	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	216	VAL	4.2
1	A	386	GLY	4.2
1	A	398	PRO	4.2
1	A	572	GLN	4.1
1	A	337	TYR	4.1
1	A	418	PHE	4.1
1	A	574	VAL	4.1
1	A	573	ALA	4.0
1	A	87	GLY	4.0
1	A	157	VAL	4.0
1	A	137	GLU	4.0
1	A	319	SER	3.9
1	A	306	LEU	3.9
1	A	508	ARG	3.9
1	A	345	TYR	3.9
1	B	127	HIS	3.9
1	A	335	ASN	3.9
1	A	370	ARG	3.9
1	A	400	PRO	3.9
1	A	582	ARG	3.8
1	A	102	PRO	3.8
1	A	338	GLY	3.8
1	B	539	ALA	3.8
1	A	376	LEU	3.8
1	A	446	THR	3.7
1	A	495	THR	3.7
1	A	377	GLU	3.7
1	A	346	ASN	3.7
1	A	577	SER	3.7
1	A	539	ALA	3.7
1	A	114	LEU	3.6
1	A	85	GLY	3.6
1	A	132	LEU	3.5
1	A	357	GLY	3.5
1	A	415	GLY	3.5
1	B	369	GLY	3.5
1	A	569	LYS	3.5
1	A	146	ASN	3.5
1	A	279	ILE	3.5
1	A	431	ILE	3.5
1	A	381	ALA	3.5
1	A	477	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	132	LEU	3.5
1	A	336	THR	3.5
1	A	65	GLY	3.4
1	A	438	LEU	3.4
1	B	125	ALA	3.4
1	B	215	ALA	3.4
1	B	180	LEU	3.4
1	A	245	GLU	3.4
1	A	403	ILE	3.4
1	A	434	ALA	3.4
1	A	510	ARG	3.4
1	A	360	ALA	3.4
1	A	127	HIS	3.3
1	A	404	ASN	3.3
1	A	356	TYR	3.3
1	A	242	ALA	3.3
1	B	210	ILE	3.3
1	A	186	ALA	3.3
1	A	304	GLY	3.2
1	A	379	SER	3.2
1	A	82	ILE	3.2
1	A	135	SER	3.2
1	A	142	ILE	3.2
1	A	575	GLU	3.2
1	A	576	MET	3.2
1	B	162	LEU	3.1
1	A	369	GLY	3.1
1	A	138	ASN	3.1
1	A	315	LEU	3.1
1	A	373	VAL	3.1
1	A	555	TYR	3.1
1	A	348	GLY	3.1
1	A	156	SER	3.1
1	B	277	PHE	3.0
1	A	300	LYS	3.0
1	A	385	ALA	3.0
1	B	134	TYR	3.0
1	A	349	THR	3.0
1	B	303	THR	3.0
1	A	134	TYR	3.0
1	A	217	LYS	3.0
1	B	272	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	211	GLN	3.0
1	A	305	ALA	3.0
1	A	405	ALA	3.0
1	B	182	ALA	3.0
1	B	551	ARG	3.0
1	A	243	GLN	2.9
1	A	359	LEU	2.9
1	A	566	LEU	2.9
1	B	225	LEU	2.9
1	A	309	VAL	2.9
1	A	323	VAL	2.9
1	A	551	ARG	2.9
1	A	232	SER	2.9
1	A	207	LEU	2.9
1	A	241	GLY	2.9
1	B	65	GLY	2.9
1	A	144	ILE	2.9
1	A	339	THR	2.9
1	A	103	LYS	2.9
1	A	175	ALA	2.9
1	B	216	VAL	2.9
1	B	218	GLN	2.9
1	A	230	VAL	2.8
1	A	556	PRO	2.8
1	A	358	LEU	2.8
1	A	282	ASN	2.8
1	B	236	TYR	2.8
1	A	224	ARG	2.8
1	A	428	PRO	2.8
1	A	99	ASN	2.7
1	A	147	GLN	2.7
1	A	100	LEU	2.7
1	A	247	PRO	2.7
1	B	370	ARG	2.7
1	B	106	TRP	2.7
1	A	340	GLY	2.7
1	A	129	PHE	2.7
1	A	297	ALA	2.7
1	A	570	TRP	2.7
1	A	136	LYS	2.7
1	A	240	GLY	2.7
1	B	383	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	347	VAL	2.7
1	A	354	SER	2.7
1	A	333	ALA	2.6
1	A	558	MET	2.6
1	B	486	LEU	2.6
1	A	395	GLY	2.6
1	A	98	GLU	2.6
1	A	351	PRO	2.6
1	B	102	PRO	2.6
1	A	435	LYS	2.6
1	A	139	ILE	2.6
1	A	321	ALA	2.6
1	B	208	TRP	2.6
1	A	439	PHE	2.6
1	A	498	ASP	2.6
1	B	209	LEU	2.6
1	B	281	ARG	2.6
1	A	352	VAL	2.6
1	A	534	VAL	2.6
1	B	157	VAL	2.6
1	B	133	GLY	2.6
1	A	281	ARG	2.6
1	A	401	SER	2.6
1	B	174	SER	2.6
1	A	248	ILE	2.5
1	A	226	ALA	2.5
1	A	244	ALA	2.5
1	A	234	LEU	2.5
1	A	96	GLU	2.5
1	B	276	PHE	2.5
1	A	90	VAL	2.5
1	A	101	TYR	2.5
1	B	368	ARG	2.5
1	B	186	ALA	2.5
1	B	176	LEU	2.5
1	A	159	GLY	2.5
1	A	444	HIS	2.5
1	A	447	LYS	2.5
1	A	387	ILE	2.5
1	A	92	SER	2.5
1	A	293	SER	2.5
1	A	372	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	427	ALA	2.5
1	A	267	LEU	2.5
1	A	210	ILE	2.5
1	B	101	TYR	2.4
1	A	97	PHE	2.4
1	A	277	PHE	2.4
1	B	426	PHE	2.4
1	A	350	GLU	2.4
1	A	301	VAL	2.4
1	A	364	TYR	2.4
1	B	213	VAL	2.4
1	B	283	LYS	2.4
1	A	219	ALA	2.4
1	A	485	GLY	2.4
1	A	499	ILE	2.4
1	A	502	ILE	2.4
1	A	104	SER	2.4
1	A	128	LYS	2.4
1	B	181	LYS	2.4
1	A	295	PRO	2.4
1	A	179	GLU	2.3
1	B	206	LEU	2.3
1	A	399	LYS	2.3
1	A	476	LYS	2.3
1	A	167	VAL	2.3
1	A	564	GLU	2.3
1	B	154	TRP	2.3
1	A	397	ALA	2.3
1	A	140	ARG	2.3
1	A	493	MET	2.3
1	B	103	LYS	2.3
1	A	396	PHE	2.3
1	A	122	ILE	2.3
1	B	212	ASN	2.3
1	A	91	ALA	2.3
1	A	274	LEU	2.3
1	A	83	PHE	2.3
1	A	450	ILE	2.3
1	A	152	VAL	2.3
1	A	565	ARG	2.3
1	B	582	ARG	2.3
1	A	559	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	478	GLU	2.2
1	A	458	THR	2.2
1	B	178	ARG	2.2
1	B	300	LYS	2.2
1	A	133	GLY	2.2
1	A	302	ALA	2.2
1	B	223	GLY	2.2
1	B	220	TYR	2.2
1	A	557	LYS	2.2
1	B	166	ILE	2.2
1	B	153	VAL	2.2
1	B	301	VAL	2.2
1	B	561	LYS	2.2
1	A	526	GLY	2.2
1	B	188	SER	2.2
1	A	178	ARG	2.2
1	A	568	ARG	2.2
1	A	571	GLU	2.2
1	A	125	ALA	2.2
1	B	183	ARG	2.2
1	A	276	PHE	2.1
1	B	221	GLU	2.1
1	A	177	VAL	2.1
1	B	85	GLY	2.1
1	B	107	HIS	2.1
1	A	189	LEU	2.1
1	A	320	SER	2.1
1	A	331	GLY	2.1
1	B	126	MET	2.1
1	B	214	ASP	2.1
1	B	269	TYR	2.1
1	A	124	GLY	2.1
1	A	183	ARG	2.1
1	B	228	GLY	2.1
1	B	97	PHE	2.1
1	B	175	ALA	2.1
1	B	242	ALA	2.1
1	B	302	ALA	2.1
1	A	185	SER	2.1
1	A	515	LEU	2.1
1	A	116	ASN	2.1
1	A	393	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	559	ASP	2.1
1	A	145	THR	2.1
1	A	388	THR	2.1
1	B	538	ILE	2.1
1	A	154	TRP	2.1
1	B	92	SER	2.1
1	B	222	GLU	2.0
1	B	245	GLU	2.0
1	B	192	LEU	2.0
1	A	433	ASP	2.0
1	B	158	THR	2.0
1	A	233	TRP	2.0
1	A	430	TRP	2.0
1	A	81	LEU	2.0
1	A	561	LYS	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($\text{\AA}^2$)	Q<0.9
2	EDO	A	604	4/4	0.70	0.23	63,76,77,78	0
2	EDO	A	603	4/4	0.77	0.19	60,73,73,73	0
2	EDO	B	1101	4/4	0.79	0.38	55,67,69,70	0
2	EDO	A	605	4/4	0.80	0.26	66,80,84,84	0
2	EDO	A	602	4/4	0.87	0.16	64,77,78,78	0
2	EDO	B	1102	4/4	0.89	0.12	51,62,62,62	0
2	EDO	A	601	4/4	0.90	0.17	36,44,45,46	0
2	EDO	B	1103	4/4	0.94	0.18	69,83,89,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.