



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:13 PM UTC

PDB ID : 2QMW / pdb_00002qmw
Title : The crystal structure of the prephenate dehydratase (PDT) from *Staphylococcus aureus* subsp. *aureus* Mu50
Authors : Tan, K.; Zhang, R.; Li, H.; Gu, M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2007-07-17
Resolution : 2.30 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

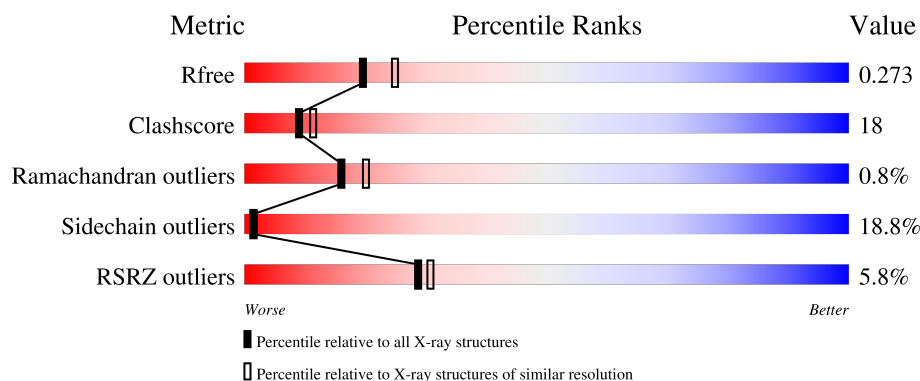
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	267	 54% 32% 10% ..
1	B	267	 10% 54% 30% 9% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	A	331	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4159 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 Prephenate dehydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	Se	0	0	0
			2081	1339	334	402	1	5			
1	B	249	Total	C	N	O	S	Se	0	0	0
			1961	1270	315	370	1	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	cloning artifact	UNP Q99SX2
A	-1	ASN	-	cloning artifact	UNP Q99SX2
A	0	ALA	-	cloning artifact	UNP Q99SX2
A	1	MSE	MET	modified residue	UNP Q99SX2
A	187	MSE	MET	modified residue	UNP Q99SX2
A	193	MSE	MET	modified residue	UNP Q99SX2
A	228	MSE	MET	modified residue	UNP Q99SX2
A	259	MSE	MET	modified residue	UNP Q99SX2
B	-2	SER	-	cloning artifact	UNP Q99SX2
B	-1	ASN	-	cloning artifact	UNP Q99SX2
B	0	ALA	-	cloning artifact	UNP Q99SX2
B	1	MSE	MET	modified residue	UNP Q99SX2
B	187	MSE	MET	modified residue	UNP Q99SX2
B	193	MSE	MET	modified residue	UNP Q99SX2
B	228	MSE	MET	modified residue	UNP Q99SX2
B	259	MSE	MET	modified residue	UNP Q99SX2

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

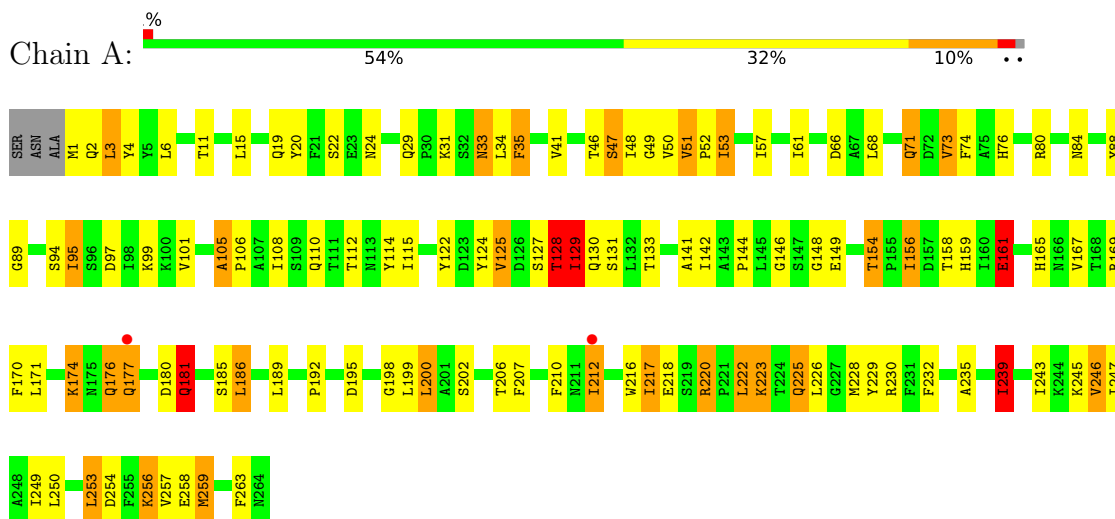
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	73	Total	O	0	0
			73	73		
6	B	24	Total	O	0	0
			24	24		

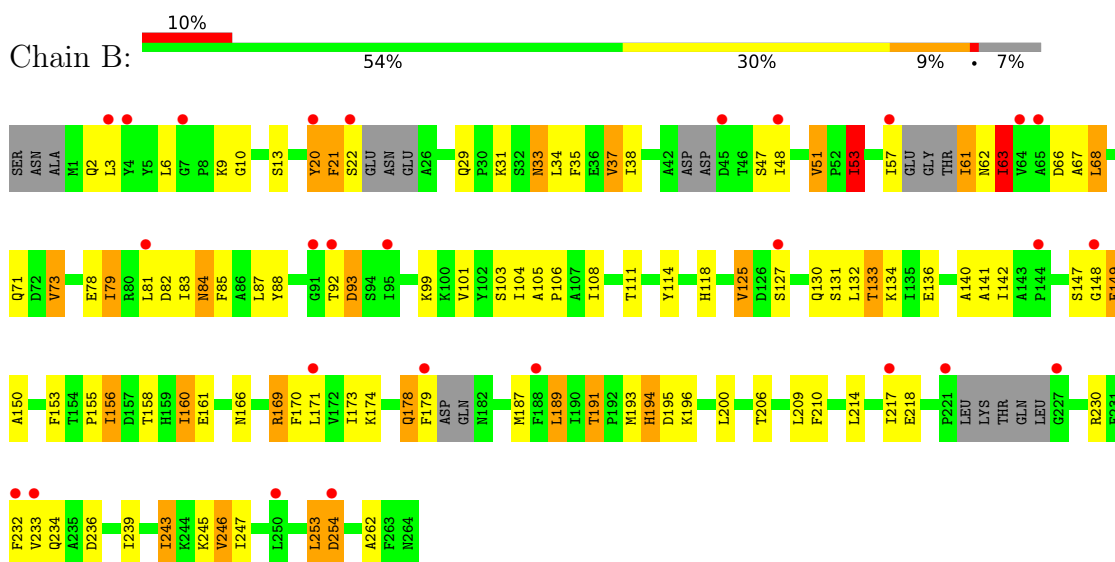
3 Residue-property plots

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: Prephenate dehydratase



• Molecule 1: Prephenate dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	60.86Å 87.41Å 107.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.88 – 2.30 45.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.1 (45.88-2.30) 98.3 (45.88-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.13 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.276 0.222 , 0.273	Depositor DCC
R_{free} test set	1320 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4159	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, PEG, NA, 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	1.61	18/2123 (0.8%)	1.55	32/2881 (1.1%)
1	B	0.93	0/1998	1.09	4/2704 (0.1%)
All	All	1.32	18/4121 (0.4%)	1.35	36/5585 (0.6%)

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	B	0	1
All	All	0	2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	ILE	CA-CB	7.64	1.63	1.54
1	A	34	LEU	C-O	6.45	1.32	1.24
1	A	61	ILE	C-O	-6.29	1.17	1.24
1	A	35	PHE	C-O	-6.29	1.16	1.24
1	A	11	THR	CA-C	-6.20	1.44	1.53
1	A	94	SER	N-CA	-6.03	1.37	1.45
1	A	239	ILE	CA-CB	5.94	1.59	1.53
1	A	124	TYR	CA-C	-5.94	1.45	1.52
1	A	169	ARG	CD-NE	-5.89	1.38	1.46
1	A	41	VAL	C-O	5.87	1.30	1.24
1	A	33	ASN	CA-C	-5.79	1.45	1.52
1	A	47	SER	CA-C	-5.52	1.45	1.52
1	A	112	THR	CA-C	5.52	1.59	1.52
1	A	170	PHE	CA-C	-5.51	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	ILE	N-CA	5.14	1.52	1.46
1	A	167	VAL	CA-CB	5.11	1.60	1.54
1	A	114	TYR	CG-CD1	5.07	1.50	1.39
1	A	19	GLN	C-O	-5.02	1.18	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ARG	NE-CZ-NH2	-8.74	111.33	119.20
1	A	239	ILE	CB-CA-C	7.13	119.36	111.80
1	A	94	SER	N-CA-C	-7.12	99.70	109.95
1	A	181	GLN	N-CA-C	6.56	121.12	111.87
1	A	57	ILE	N-CA-C	-6.42	106.74	112.90
1	B	93	ASP	N-CA-C	-6.24	100.80	110.10
1	A	161	GLU	CB-CG-CD	6.15	123.06	112.60
1	A	180	ASP	N-CA-C	-6.07	102.35	110.24
1	A	51	VAL	N-CA-CB	-6.00	102.80	111.21
1	A	156	ILE	N-CA-C	-5.96	103.45	111.44
1	A	129	ILE	CB-CA-C	-5.93	102.97	112.16
1	A	128	THR	N-CA-CB	5.85	118.72	110.12
1	B	194	HIS	N-CA-C	5.81	118.01	109.24
1	A	95	ILE	CB-CG1-CD1	-5.79	101.64	113.80
1	A	114	TYR	N-CA-C	5.64	117.10	111.07
1	A	105	ALA	CA-C-N	5.58	125.25	119.05
1	A	105	ALA	C-N-CA	5.58	125.25	119.05
1	B	108	ILE	N-CA-C	-5.53	105.14	110.72
1	A	198	GLY	N-CA-C	5.51	121.52	113.48
1	A	20	TYR	N-CA-C	5.44	120.07	113.38
1	A	52	PRO	N-CA-C	5.39	119.55	111.14
1	A	95	ILE	CB-CA-C	5.39	120.98	112.26
1	A	15	LEU	N-CA-C	5.31	117.76	111.33
1	A	146	GLY	N-CA-C	-5.29	107.24	114.64
1	A	80	ARG	CA-C-N	-5.29	115.54	122.99
1	A	80	ARG	C-N-CA	-5.29	115.54	122.99
1	A	154	THR	CB-CA-C	-5.28	100.96	108.88
1	A	95	ILE	N-CA-CB	-5.26	101.25	110.77
1	A	49	GLY	N-CA-C	-5.17	103.00	110.90
1	B	53	ILE	CB-CA-C	-5.16	105.85	110.91
1	A	97	ASP	N-CA-C	5.15	119.41	113.18
1	A	73	VAL	CB-CA-C	5.09	118.58	111.40
1	A	11	THR	N-CA-C	-5.06	103.72	110.55
1	A	220	ARG	NE-CZ-NH2	-5.05	114.65	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	VAL	CG1-CB-CG2	5.04	121.90	110.80
1	A	128	THR	CB-CA-C	5.03	119.14	110.79

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	GLN	Peptide
1	B	92	THR	Peptide

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	2081	0	2043	83	0
1	B	1961	0	1934	66	0
2	A	1	0	0	0	0
3	A	4	0	3	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	7	0	10	6	0
6	A	73	0	0	6	0
6	B	24	0	0	1	0
All	All	4159	0	4002	148	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (148) 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:212:ILE:HD11	1:A:235:ALA:HB1	1.35	1.06
1:A:195:ASP:HB2	1:A:228:MSE:HE1	1.38	1.02
1:A:195:ASP:CB	1:A:228:MSE:HE1	1.95	0.95
1:A:6:LEU:HD11	5:A:331:PEG:H32	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ILE:HG13	1:B:170:PHE:HB2	1.50	0.93
1:A:115:ILE:HD11	1:A:142:ILE:CD1	2.03	0.89
1:A:195:ASP:CG	1:A:228:MSE:HE1	1.99	0.88
1:A:105:ALA:HB3	1:A:106:PRO:HD3	1.56	0.87
1:A:66:ASP:OD1	1:A:220:ARG:HD3	1.75	0.86
1:B:253:LEU:O	1:B:254:ASP:HB2	1.77	0.85
1:B:47:SER:HA	6:B:336:HOH:O	1.75	0.85
1:A:84:ASN:HA	1:A:161:GLU:HG3	1.59	0.84
1:B:53:ILE:HG12	1:B:171:LEU:HG	1.62	0.82
1:B:2:GLN:OE1	1:B:29:GLN:NE2	2.13	0.81
1:A:84:ASN:HA	1:A:161:GLU:CG	2.11	0.81
1:A:33:ASN:CB	5:A:331:PEG:H41	2.14	0.77
1:A:125:VAL:CG2	1:A:130:GLN:HB3	2.16	0.76
1:A:115:ILE:HD11	1:A:142:ILE:HD12	1.66	0.76
1:A:125:VAL:HG22	1:A:130:GLN:HB3	1.69	0.75
1:B:20:TYR:CD2	1:B:79:ILE:HG22	2.21	0.74
1:B:87:LEU:O	1:B:156:ILE:N	2.20	0.73
1:A:222:LEU:O	1:A:223:LYS:CB	2.35	0.73
1:A:128:THR:O	1:A:131:SER:HB2	1.87	0.73
1:A:33:ASN:HB2	5:A:331:PEG:H41	1.71	0.73
1:A:74:PHE:CE1	1:A:177:GLN:HB3	2.24	0.73
1:B:169:ARG:NH2	1:B:234:GLN:OE1	2.22	0.72
1:A:149:GLU:HB2	6:A:395:HOH:O	1.89	0.71
1:A:131:SER:HB3	1:A:141:ALA:HB1	1.72	0.71
1:B:9:LYS:HE3	1:B:150:ALA:HB1	1.71	0.70
1:A:195:ASP:HB2	1:A:228:MSE:CE	2.21	0.69
1:A:76:HIS:HD2	1:A:174:LYS:HB2	1.57	0.69
1:A:89:GLY:HA3	1:A:156:ILE:HD11	1.75	0.68
1:A:1:MSE:HE2	1:A:47:SER:N	2.09	0.68
1:B:78:GLU:CD	1:B:169:ARG:HE	2.01	0.68
1:B:57:ILE:HG23	1:B:106:PRO:HB2	1.75	0.66
1:A:222:LEU:O	6:A:398:HOH:O	2.15	0.65
1:A:74:PHE:CD1	1:A:177:GLN:HB3	2.32	0.64
1:B:133:THR:HG22	1:B:134:LYS:HD3	1.78	0.64
1:B:34:LEU:HD22	1:B:51:VAL:HG22	1.79	0.63
1:B:61:ILE:O	1:B:61:ILE:HD13	1.98	0.63
1:A:33:ASN:HA	5:A:331:PEG:H41	1.80	0.63
1:B:178:GLN:O	1:B:178:GLN:HG2	1.99	0.62
1:B:243:ILE:O	1:B:247:ILE:HG13	1.99	0.62
1:A:161:GLU:H	1:A:161:GLU:CD	2.08	0.62
1:A:127:SER:OG	1:A:129:ILE:HD12	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LEU:HD23	1:B:156:ILE:HG21	1.83	0.61
1:B:87:LEU:HD23	1:B:156:ILE:CG2	2.31	0.61
1:A:165:HIS:HD2	6:A:353:HOH:O	1.84	0.60
1:B:10:GLY:O	1:B:147:SER:HB2	2.01	0.60
1:B:206:THR:HG22	1:B:246:VAL:HB	1.83	0.59
1:A:222:LEU:O	1:A:223:LYS:HB2	2.03	0.59
1:A:115:ILE:CD1	1:A:142:ILE:CD1	2.80	0.58
1:B:35:PHE:HB2	1:B:63:ILE:HD11	1.85	0.58
1:B:210:PHE:HE1	1:B:245:LYS:HD3	1.69	0.58
1:A:48:ILE:HG22	1:A:174:LYS:HG3	1.85	0.58
1:B:34:LEU:HD22	1:B:51:VAL:CG2	2.33	0.58
1:A:218:GLU:HB3	1:A:232:PHE:HB2	1.86	0.57
1:B:84:ASN:HD22	1:B:85:PHE:N	2.01	0.57
1:B:31:LYS:HB2	1:B:37:VAL:HG12	1.85	0.57
1:A:129:ILE:O	1:A:133:THR:HG23	2.03	0.57
1:A:53:ILE:HD11	1:A:216:TRP:CH2	2.39	0.57
1:B:34:LEU:HA	1:B:37:VAL:HG13	1.86	0.56
1:A:33:ASN:CA	5:A:331:PEG:H41	2.35	0.56
1:A:176:GLN:O	1:A:176:GLN:HG2	2.06	0.56
1:B:131:SER:HB3	1:B:141:ALA:HB1	1.87	0.55
1:A:206:THR:HG22	1:A:246:VAL:HB	1.88	0.55
1:A:115:ILE:CD1	1:A:142:ILE:HD11	2.37	0.55
1:A:125:VAL:HG21	1:A:130:GLN:HB3	1.89	0.55
1:B:79:ILE:CG1	1:B:170:PHE:HB2	2.29	0.55
1:A:225:GLN:OE1	1:A:228:MSE:HG3	2.07	0.54
1:A:225:GLN:CD	1:A:228:MSE:HG3	2.31	0.54
1:B:125:VAL:HG22	1:B:130:GLN:HB3	1.90	0.54
1:A:181:GLN:NE2	1:A:181:GLN:HA	2.22	0.54
1:B:83:ILE:HG22	1:B:161:GLU:OE1	2.07	0.53
1:B:88:TYR:OH	1:B:149:GLU:OE2	2.19	0.53
1:B:73:VAL:HG13	1:B:173:ILE:HB	1.91	0.53
1:B:218:GLU:HB3	1:B:232:PHE:HB2	1.91	0.52
1:B:171:LEU:HD21	1:B:187:MSE:HE1	1.90	0.52
1:A:207:PHE:HD1	1:A:212:ILE:HG12	1.74	0.52
1:A:222:LEU:O	1:A:223:LYS:HB3	2.10	0.51
1:A:4:TYR:HE2	1:A:47:SER:HG	1.57	0.51
1:A:53:ILE:HB	1:A:171:LEU:HG	1.92	0.51
1:B:191:THR:HG23	1:B:230:ARG:HB3	1.92	0.51
1:B:103:SER:OG	1:B:142:ILE:O	2.27	0.51
1:A:2:GLN:HG3	1:A:29:GLN:HG3	1.93	0.50
1:A:200:LEU:HD11	1:A:217:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ILE:HG12	1:A:257:VAL:HG11	1.93	0.50
1:B:178:GLN:O	1:B:178:GLN:CG	2.60	0.50
1:A:33:ASN:HA	5:A:331:PEG:C4	2.42	0.50
1:A:230:ARG:CD	6:A:358:HOH:O	2.61	0.49
1:A:53:ILE:CD1	1:A:216:TRP:CZ2	2.95	0.49
1:A:186:LEU:HD11	1:A:239:ILE:HG22	1.94	0.49
1:A:200:LEU:HD21	1:A:217:ILE:HD12	1.94	0.49
1:B:84:ASN:HD22	1:B:84:ASN:C	2.20	0.48
1:B:114:TYR:O	1:B:118:HIS:HD2	1.96	0.48
1:B:105:ALA:N	1:B:106:PRO:CD	2.77	0.48
1:A:210:PHE:CD2	1:A:246:VAL:HG12	2.48	0.47
1:A:230:ARG:HD3	6:A:358:HOH:O	2.13	0.47
1:B:53:ILE:CG1	1:B:171:LEU:HG	2.38	0.47
1:B:179:PHE:HB3	1:B:262:ALA:HB3	1.95	0.47
1:A:159:HIS:HA	1:A:161:GLU:OE2	2.14	0.47
1:B:125:VAL:HG13	1:B:127:SER:O	2.14	0.47
1:B:101:VAL:HA	1:B:140:ALA:O	2.14	0.46
1:A:199:LEU:O	1:A:202:SER:HB2	2.16	0.46
1:B:53:ILE:HD12	1:B:169:ARG:HB3	1.96	0.46
1:B:33:ASN:HD22	1:B:34:LEU:H	1.64	0.45
1:B:214:LEU:HD22	1:B:233:VAL:CG1	2.46	0.45
1:A:1:MSE:HE2	1:A:46:THR:C	2.41	0.45
1:A:256:LYS:HE3	1:A:256:LYS:HB2	1.39	0.45
1:B:62:ASN:O	1:B:66:ASP:OD1	2.34	0.45
1:B:171:LEU:CD2	1:B:187:MSE:HE1	2.46	0.45
1:B:189:LEU:HD11	1:B:230:ARG:HD2	1.99	0.45
1:A:246:VAL:O	1:A:250:LEU:HG	2.17	0.45
1:A:192:PRO:HD2	1:A:229:TYR:O	2.17	0.44
1:A:106:PRO:O	1:A:110:GLN:HG2	2.17	0.44
1:B:38:ILE:HG21	1:B:67:ALA:CB	2.48	0.44
1:A:253:LEU:HD11	1:B:209:LEU:HD13	1.99	0.44
1:B:87:LEU:O	1:B:155:PRO:HA	2.18	0.44
1:B:114:TYR:CZ	1:B:160:ILE:HG13	2.53	0.43
1:B:68:LEU:HD13	1:B:73:VAL:HG12	2.00	0.43
1:A:101:VAL:O	1:A:122:TYR:HA	2.18	0.43
1:A:4:TYR:HE2	1:A:47:SER:OG	1.99	0.43
1:B:114:TYR:CE2	1:B:160:ILE:HG13	2.53	0.43
1:B:210:PHE:CE1	1:B:245:LYS:HD3	2.52	0.43
1:A:127:SER:OG	1:A:129:ILE:CD1	2.67	0.42
1:B:174:LYS:NZ	1:B:178:GLN:HE22	2.17	0.42
1:B:148:GLY:O	1:B:153:PHE:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:SER:HB3	1:B:130:GLN:H	1.84	0.42
1:A:212:ILE:O	1:A:212:ILE:HG13	2.15	0.42
1:A:3:LEU:HD21	1:A:50:VAL:HG23	2.00	0.42
1:A:71:GLN:HG2	1:A:74:PHE:CE1	2.55	0.42
1:A:245:LYS:O	1:A:249:ILE:HG13	2.20	0.42
1:A:185:SER:HB2	6:A:365:HOH:O	2.18	0.42
1:B:132:LEU:HB3	1:B:153:PHE:CE2	2.55	0.42
1:B:111:THR:HG22	1:B:161:GLU:HA	2.00	0.41
1:A:88:TYR:CE1	1:A:148:GLY:HA3	2.55	0.41
1:A:217:ILE:HA	1:A:232:PHE:O	2.19	0.41
1:A:33:ASN:OD1	1:A:35:PHE:HB3	2.21	0.41
1:A:131:SER:HB3	1:A:141:ALA:CB	2.47	0.41
1:A:185:SER:HA	1:A:235:ALA:O	2.20	0.41
1:B:53:ILE:HD13	1:B:169:ARG:NH1	2.35	0.41
1:B:125:VAL:CG1	1:B:127:SER:O	2.68	0.41
1:A:53:ILE:HD11	1:A:216:TRP:CZ2	2.55	0.41
1:A:259:MSE:HE2	1:A:259:MSE:HB3	1.93	0.41
1:A:129:ILE:HD12	1:A:129:ILE:H	1.86	0.41
1:B:160:ILE:HA	1:B:160:ILE:HD12	1.79	0.40
1:A:129:ILE:CD1	1:A:129:ILE:H	2.35	0.40
1:B:21:PHE:O	1:B:22:SER:C	2.64	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	262/267 (98%)	246 (94%)	14 (5%)	2 (1%)	16	20
1	B	237/267 (89%)	219 (92%)	16 (7%)	2 (1%)	16	20
All	All	499/534 (93%)	465 (93%)	30 (6%)	4 (1%)	16	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	63	ILE
1	B	254	ASP
1	A	263	PHE
1	A	223	LYS

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	228/225 (101%)	190 (83%)	38 (17%)	2	2
1	B	214/225 (95%)	169 (79%)	45 (21%)	1	1
All	All	442/450 (98%)	359 (81%)	83 (19%)	1	1

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	22	SER
1	A	24	ASN
1	A	31	LYS
1	A	51	VAL
1	A	53	ILE
1	A	68	LEU
1	A	71	GLN
1	A	73	VAL
1	A	95	ILE
1	A	99	LYS
1	A	125	VAL
1	A	128	THR
1	A	129	ILE
1	A	144	PRO
1	A	154	THR
1	A	158	THR
1	A	161	GLU
1	A	174	LYS

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Mol	Chain	Res	Type
1	A	176	GLN
1	A	177	GLN
1	A	181	GLN
1	A	186	LEU
1	A	189	LEU
1	A	200	LEU
1	A	212	ILE
1	A	217	ILE
1	A	222	LEU
1	A	225	GLN
1	A	226	LEU
1	A	239	ILE
1	A	243	ILE
1	A	246	VAL
1	A	253	LEU
1	A	254	ASP
1	A	256	LYS
1	A	258	GLU
1	A	259	MSE
1	B	3	LEU
1	B	6	LEU
1	B	13	SER
1	B	20	TYR
1	B	21	PHE
1	B	33	ASN
1	B	37	VAL
1	B	48	ILE
1	B	51	VAL
1	B	53	ILE
1	B	61	ILE
1	B	63	ILE
1	B	68	LEU
1	B	71	GLN
1	B	73	VAL
1	B	79	ILE
1	B	81	LEU
1	B	82	ASP
1	B	84	ASN
1	B	93	ASP
1	B	99	LYS
1	B	104	ILE
1	B	125	VAL

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Mol	Chain	Res	Type
1	B	133	THR
1	B	136	GLU
1	B	149	GLU
1	B	156	ILE
1	B	158	THR
1	B	160	ILE
1	B	166	ASN
1	B	169	ARG
1	B	178	GLN
1	B	189	LEU
1	B	191	THR
1	B	193	MSE
1	B	194	HIS
1	B	195	ASP
1	B	196	LYS
1	B	200	LEU
1	B	217	ILE
1	B	236	ASP
1	B	239	ILE
1	B	243	ILE
1	B	246	VAL
1	B	253	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	117	GLN
1	A	118	HIS
1	A	177	GLN
1	A	181	GLN
1	A	194	HIS
1	B	33	ASN
1	B	55	ASN
1	B	62	ASN
1	B	113	ASN
1	B	118	HIS
1	B	119	GLN
1	B	137	ASN
1	B	178	GLN
1	B	264	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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	PEG	A	331	-	6,6,6	0.78	0	5,5,5	0.56	0
4	EDO	B	322	-	3,3,3	0.60	0	2,2,2	0.47	0
3	ACT	A	311	-	3,3,3	0.87	0	3,3,3	1.22	0
4	EDO	A	321	-	3,3,3	0.52	0	2,2,2	0.67	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
4	EDO	B	322	-	-	1/1/1/1	-
5	PEG	A	331	-	-	1/4/4/4	-
4	EDO	A	321	-	-	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
4	B	322	EDO	O1-C1-C2-O2
4	A	321	EDO	O1-C1-C2-O2
5	A	331	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	331	PEG	6	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	259/267 (97%)	0.32	2 (0%) 82 83	29, 46, 67, 80	1 (0%)
1	B	244/267 (91%)	1.15	27 (11%) 10 11	57, 79, 96, 114	1 (0%)
All	All	503/534 (94%)	0.72	29 (5%) 29 31	29, 64, 92, 114	2 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	LEU	5.5
1	A	212	ILE	4.5
1	B	171	LEU	4.0
1	B	48	ILE	3.8
1	B	227	GLY	3.4
1	B	188	PHE	3.1
1	B	221	PRO	3.1
1	B	20	TYR	2.8
1	B	64	VAL	2.6
1	B	91	GLY	2.5
1	B	7	GLY	2.5
1	B	179	PHE	2.5
1	B	254	ASP	2.5
1	B	92	THR	2.4
1	B	233	VAL	2.4
1	B	65	ALA	2.4
1	B	22	SER	2.4
1	B	144	PRO	2.3
1	B	95	ILE	2.3
1	B	232	PHE	2.3
1	B	148	GLY	2.2
1	B	250	LEU	2.1
1	B	3	LEU	2.1
1	A	177	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	127	SER	2.0
1	B	4	TYR	2.0
1	B	45	ASP	2.0
1	B	57	ILE	2.0
1	B	217	ILE	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	PEG	A	331	7/7	0.74	0.20	35,53,71,73	0
4	EDO	B	322	4/4	0.77	0.14	69,72,72,73	0
4	EDO	A	321	4/4	0.83	0.15	37,40,42,46	0
3	ACT	A	311	4/4	0.85	0.14	98,98,98,98	0
2	NA	A	301	1/1	0.96	0.06	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.