



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 08:40 pm BST

PDB ID : 2QMW  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

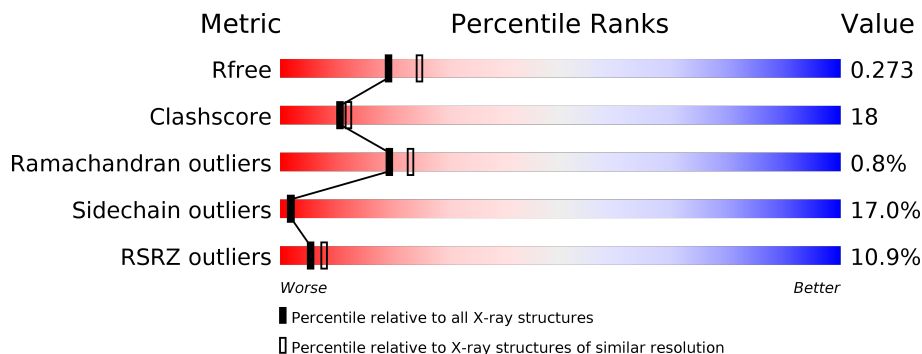
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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  $\geq 3$ , 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	
1	B	267	

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 [i](#)

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
			Total	C	N	O	S	Se			
1	A	264	2081	1339	334	402	1	5	0	0	0
1	B	249	1961	1270	315	370	1	5	0	0	0

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 (three-letter code: NA) (formula: Na).

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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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 (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

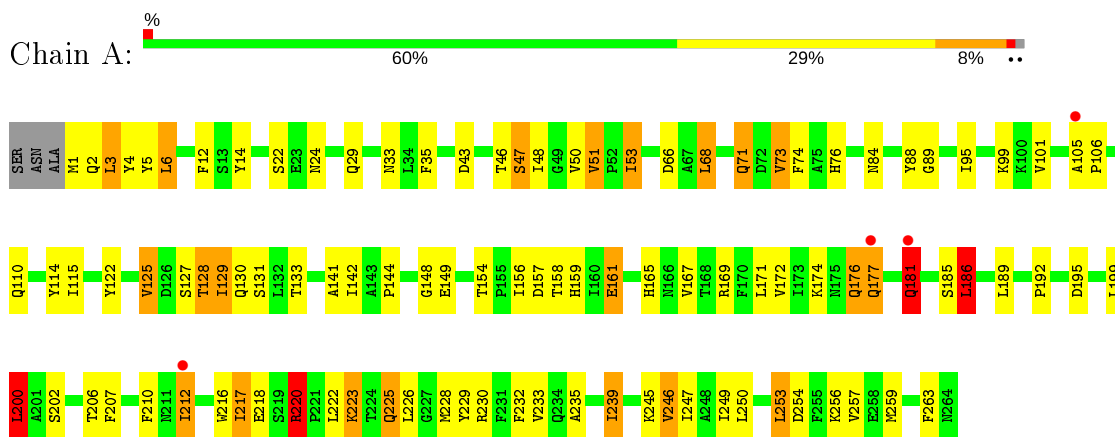
- Molecule 6 is water.

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

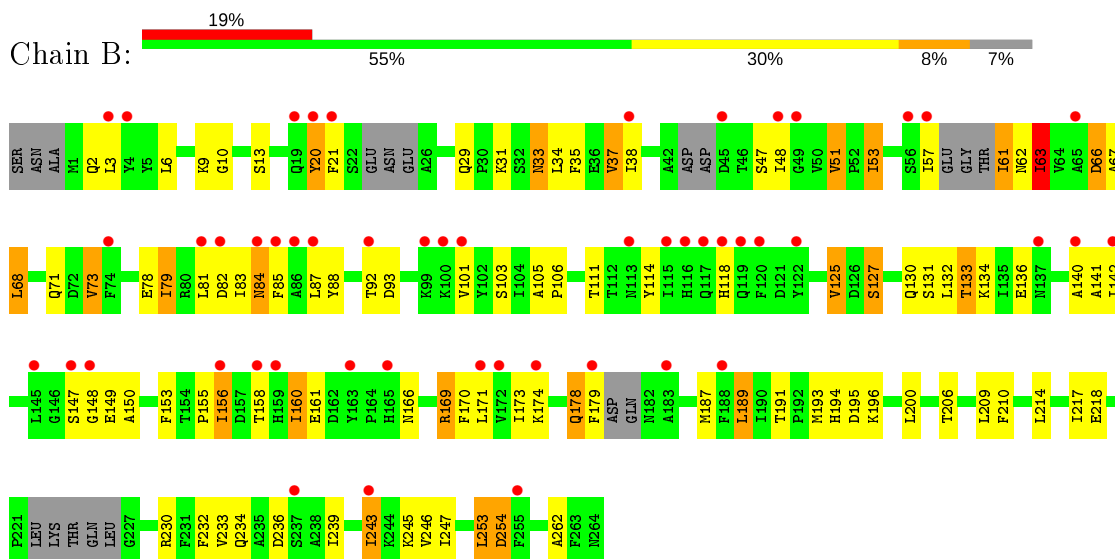
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	60.86Å 87.41Å 107.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.88 – 2.30 45.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.1 (45.88-2.30) 98.1 (45.86-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.13 (at 2.29Å)	Xtrriage
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 (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtrriage
Anisotropy	0.188	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 67.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4159	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NA, PEG, EDO, ACT

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	1.33	10/2123 (0.5%)	1.27	14/2881 (0.5%)
1	B	0.73	0/1998	0.79	0/2704
All	All	1.08	10/4121 (0.2%)	1.07	14/5585 (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	1
1	B	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	TYR	CG-CD1	8.34	1.50	1.39
1	A	14	TYR	CD2-CE2	7.12	1.50	1.39
1	A	172	VAL	CB-CG2	6.80	1.67	1.52
1	A	12	PHE	CD2-CE2	5.56	1.50	1.39
1	A	167	VAL	CB-CG2	5.44	1.64	1.52
1	A	233	VAL	CB-CG1	-5.43	1.41	1.52
1	A	51	VAL	CB-CG1	-5.35	1.41	1.52
1	A	14	TYR	CD1-CE1	5.24	1.47	1.39
1	A	5	TYR	CD1-CE1	5.18	1.47	1.39
1	A	12	PHE	CD1-CE1	5.04	1.49	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ARG	NE-CZ-NH2	-17.93	111.33	120.30
1	A	220	ARG	NE-CZ-NH2	-11.30	114.65	120.30
1	A	220	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	A	169	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	A	51	VAL	CG1-CB-CG2	6.87	121.90	110.90
1	A	157	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	157	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	43	ASP	CB-CG-OD2	6.35	124.02	118.30
1	A	68	LEU	CA-CB-CG	5.75	128.54	115.30
1	A	6	LEU	CB-CG-CD1	-5.73	101.27	111.00
1	A	200	LEU	CB-CG-CD2	5.50	120.36	111.00
1	A	186	LEU	CA-CB-CG	5.26	127.41	115.30
1	A	73	VAL	CG1-CB-CG2	5.22	119.26	110.90
1	A	220	ARG	CD-NE-CZ	5.17	130.84	123.60

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	84	0
1	B	1961	0	1934	65	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
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: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:A:195:ASP:CG	1:A:228:MSE:HE1	1.99	0.83
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:78:GLU:CD	1:B:169:ARG:HE	2.01	0.63
1:B:178:GLN:HG2	1:B:178:GLN:O	1.99	0.62
1:B:243:ILE:O	1:B:247:ILE:HG13	1.99	0.62
1:A:127:SER:OG	1:A:129:ILE:HD12	2.00	0.62
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:A:161:GLU:CD	1:A:161:GLU:H	2.08	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:176:GLN:O	1:A:176:GLN:HG2	2.06	0.56
1:A:33:ASN:CA	5:A:331:PEG:H41	2.35	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:B:125:VAL:HG22	1:B:130:GLN:HB3	1.90	0.54
1:A:181:GLN:HA	1:A:181:GLN:NE2	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:A:4:TYR:HE2	1:A:47:SER:HG	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:O	1:A:223:LYS:HB3	2.10	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:A:200:LEU:HD11	1:A:217:ILE:HD11	1.93	0.50
1:A:2:GLN:HG3	1:A:29:GLN:HG3	1.93	0.50
1:A:247:ILE:HG12	1:A:257:VAL:HG11	1.93	0.50
1:B:178:GLN:CG	1:B:178:GLN:O	2.60	0.50
1:A:33:ASN:HA	5:A:331:PEG:C4	2.42	0.50
1:A:225:GLN:CD	1:A:228:MSE:HG3	2.31	0.49
1:A:230:ARG:CD	6:A:358:HOH:O	2.61	0.49
1:A:186:LEU:HD11	1:A:239:ILE:HG22	1.94	0.49
1:A:53:ILE:CD1	1:A:216:TRP:CZ2	2.95	0.49
1:A:200:LEU:HD21	1:A:217:ILE:HD12	1.94	0.49
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:214:LEU:HD22	1:B:233:VAL:CG1	2.46	0.45
1:B:33:ASN:HD22	1:B:34:LEU:H	1.64	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:84:ASN:C	1:B:84:ASN:HD22	2.20	0.44
1:B:103:SER:OG	1:B:142:ILE:O	2.27	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:127:SER:HB3	1:B:130:GLN:H	1.84	0.42
1:A:212:ILE:HG13	1:A:212:ILE:O	2.15	0.42
1:A:3:LEU:HD21	1:A:50:VAL:HG23	2.00	0.42
1:A:245:LYS:O	1:A:249:ILE:HG13	2.20	0.42
1:A:71:GLN:HG2	1:A:74:PHE:CE1	2.55	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:217:ILE:HA	1:A:232:PHE:O	2.19	0.41
1:A:88:TYR:CE1	1:A:148:GLY:HA3	2.55	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:125:VAL:CG1	1:B:127:SER:O	2.68	0.41
1:B:53:ILE:HD13	1:B:169:ARG:NH1	2.35	0.41
1:A:53:ILE:HD11	1:A:216:TRP:CZ2	2.55	0.41
1:A:259:MSE:HB3	1:A:259:MSE:HE2	1.93	0.41
1:A:129:ILE:H	1:A:129:ILE:HD12	1.86	0.41
1:A:1:MSE:HE2	1:A:46:THR:C	2.41	0.40
1:A:46:THR:OG1	1:A:46:THR:O	2.35	0.40
1:B:160:ILE:HD12	1:B:160:ILE:HA	1.79	0.40
1:A:129:ILE:H	1:A:129:ILE:CD1	2.35	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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%)	19	23
1	B	237/267 (89%)	219 (92%)	16 (7%)	2 (1%)	19	23
All	All	499/534 (93%)	465 (93%)	30 (6%)	4 (1%)	19	23

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 [i](#)

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%)	195 (86%)	33 (14%)	3	3
1	B	214/225 (95%)	172 (80%)	42 (20%)	1	1
All	All	442/450 (98%)	367 (83%)	75 (17%)	2	2

All (75) 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	47	SER
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	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	220	ARG
1	A	225	GLN
1	A	226	LEU
1	A	239	ILE
1	A	246	VAL
1	A	253	LEU
1	A	254	ASP
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	66	ASP
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

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Mol	Chain	Res	Type
1	B	125	VAL
1	B	127	SER
1	B	133	THR
1	B	136	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	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	253	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	117	GLN
1	A	181	GLN
1	B	33	ASN
1	B	62	ASN
1	B	84	ASN
1	B	113	ASN
1	B	118	HIS
1	B	119	GLN
1	B	137	ASN
1	B	166	ASN
1	B	178	GLN

### 5.3.3 RNA

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
3	ACT	A	311	-	1,3,3	1.38	0	0,3,3	0.00	-
4	EDO	A	321	-	3,3,3	0.53	0	2,2,2	0.68	0
5	PEG	A	331	-	6,6,6	0.78	0	5,5,5	0.57	0
4	EDO	B	322	-	3,3,3	0.62	0	2,2,2	0.45	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	A	321	-	-	1/1/1/1	-
5	PEG	A	331	-	-	1/4/4/4	-
4	EDO	B	322	-	-	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	A	321	EDO	O1-C1-C2-O2
4	B	322	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	259/267 (97%)	0.32	4 (1%) 73 79	29, 46, 67, 80	1 (0%)
1	B	244/267 (91%)	1.10	51 (20%) 1 1	57, 79, 96, 114	1 (0%)
All	All	503/534 (94%)	0.70	55 (10%) 5 8	29, 64, 92, 114	2 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	LEU	9.0
1	B	20	TYR	4.7
1	B	117	GLN	4.5
1	B	85	PHE	4.3
1	B	179	PHE	4.3
1	B	49	GLY	4.3
1	B	116	HIS	4.2
1	B	113	ASN	4.1
1	B	115	ILE	4.1
1	B	48	ILE	4.0
1	B	21	PHE	3.8
1	B	156	ILE	3.6
1	B	148	GLY	3.4
1	B	3	LEU	3.4
1	B	183	ALA	3.4
1	B	65	ALA	3.3
1	B	137	ASN	3.2
1	B	92	THR	3.2
1	B	45	ASP	3.1
1	B	19	GLN	3.1
1	B	163	TYR	3.0
1	B	86	ALA	3.0
1	B	120	PHE	3.0
1	B	174	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	99	LYS	2.9
1	B	84	ASN	2.8
1	B	237	SER	2.8
1	B	56	SER	2.8
1	B	147	SER	2.7
1	B	118	HIS	2.7
1	B	122	TYR	2.7
1	B	119	GLN	2.6
1	B	172	VAL	2.6
1	B	165	HIS	2.6
1	B	57	ILE	2.6
1	A	105	ALA	2.5
1	B	38	ILE	2.5
1	B	255	PHE	2.5
1	B	87	LEU	2.5
1	B	158	THR	2.4
1	B	101	VAL	2.4
1	A	212	ILE	2.4
1	B	140	ALA	2.4
1	B	82	ASP	2.3
1	B	100	LYS	2.3
1	A	177	GLN	2.3
1	B	159	HIS	2.3
1	B	243	ILE	2.3
1	B	171	LEU	2.2
1	B	142	ILE	2.2
1	B	145	LEU	2.2
1	B	74	PHE	2.1
1	B	188	PHE	2.1
1	B	4	TYR	2.0
1	A	181	GLN	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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	EDO	B	322	4/4	0.69	0.19	69,72,72,73	0
5	PEG	A	331	7/7	0.69	0.30	35,53,71,73	0
3	ACT	A	311	4/4	0.79	0.32	98,98,98,98	0
4	EDO	A	321	4/4	0.93	0.13	37,40,42,46	0
2	NA	A	301	1/1	0.94	0.04	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.