



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:17 am BST

PDB ID : 3WI3
Title : Crystal Structure of the Sld3/Treslin domain from yeast Sld3
Authors : Itou, H.; Araki, H.; Shirakihara, Y.
Deposited on : 2013-09-05
Resolution : 2.40 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 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

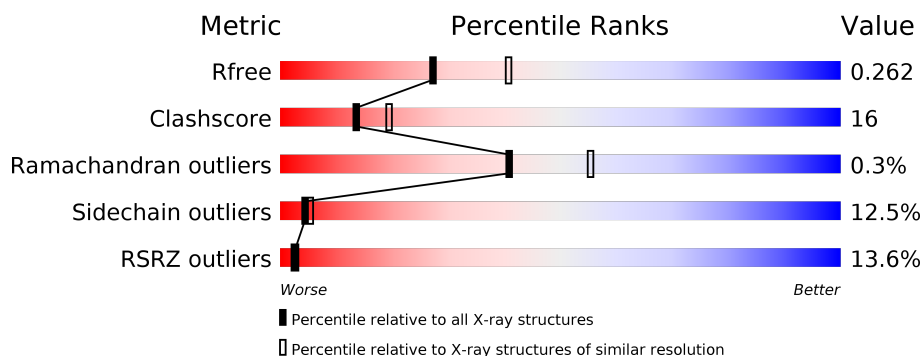
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	292	<div> <div>3%</div> <div> <div></div> <div>52%</div> <div>18%</div> <div>•</div> <div>26%</div> </div> </div>
1	B	292	<div> <div>2%</div> <div> <div></div> <div>49%</div> <div>20%</div> <div>•</div> <div>27%</div> </div> </div>
1	C	292	<div> <div>24%</div> <div> <div></div> <div>53%</div> <div>14%</div> <div>•</div> <div>30%</div> </div> </div>

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
3	EDO	A	502	-	-	X	-
3	EDO	A	503	-	-	X	-
3	EDO	A	504	-	-	X	-
3	EDO	A	505	-	-	X	-
3	EDO	A	506	-	-	X	-
3	EDO	A	507	-	-	X	-
3	EDO	A	508	-	-	X	-
3	EDO	A	514	-	-	X	-
3	EDO	A	515	-	X	-	-
3	EDO	A	516	-	-	X	-
3	EDO	A	517	-	-	X	-
3	EDO	B	502	-	-	X	-
3	EDO	B	503	-	-	X	-
3	EDO	B	504	-	-	X	-
3	EDO	B	505	-	-	X	-
3	EDO	B	506	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5473 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 DNA replication regulator SLD3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1766	1145	289	326	6			
1	B	212	Total	C	N	O	S	0	0	0
			1741	1127	287	321	6			
1	C	205	Total	C	N	O	S	0	0	0
			1686	1095	276	309	6			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	MET	-	EXPRESSION TAG	UNP P53135
A	431	LEU	-	EXPRESSION TAG	UNP P53135
A	432	GLU	-	EXPRESSION TAG	UNP P53135
A	433	HIS	-	EXPRESSION TAG	UNP P53135
A	434	HIS	-	EXPRESSION TAG	UNP P53135
A	435	HIS	-	EXPRESSION TAG	UNP P53135
A	436	HIS	-	EXPRESSION TAG	UNP P53135
A	437	HIS	-	EXPRESSION TAG	UNP P53135
A	438	HIS	-	EXPRESSION TAG	UNP P53135
B	147	MET	-	EXPRESSION TAG	UNP P53135
B	431	LEU	-	EXPRESSION TAG	UNP P53135
B	432	GLU	-	EXPRESSION TAG	UNP P53135
B	433	HIS	-	EXPRESSION TAG	UNP P53135
B	434	HIS	-	EXPRESSION TAG	UNP P53135
B	435	HIS	-	EXPRESSION TAG	UNP P53135
B	436	HIS	-	EXPRESSION TAG	UNP P53135
B	437	HIS	-	EXPRESSION TAG	UNP P53135
B	438	HIS	-	EXPRESSION TAG	UNP P53135
C	147	MET	-	EXPRESSION TAG	UNP P53135
C	431	LEU	-	EXPRESSION TAG	UNP P53135
C	432	GLU	-	EXPRESSION TAG	UNP P53135
C	433	HIS	-	EXPRESSION TAG	UNP P53135
C	434	HIS	-	EXPRESSION TAG	UNP P53135

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Chain	Residue	Modelled	Actual	Comment	Reference
C	435	HIS	-	EXPRESSION TAG	UNP P53135
C	436	HIS	-	EXPRESSION TAG	UNP P53135
C	437	HIS	-	EXPRESSION TAG	UNP P53135
C	438	HIS	-	EXPRESSION TAG	UNP P53135

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

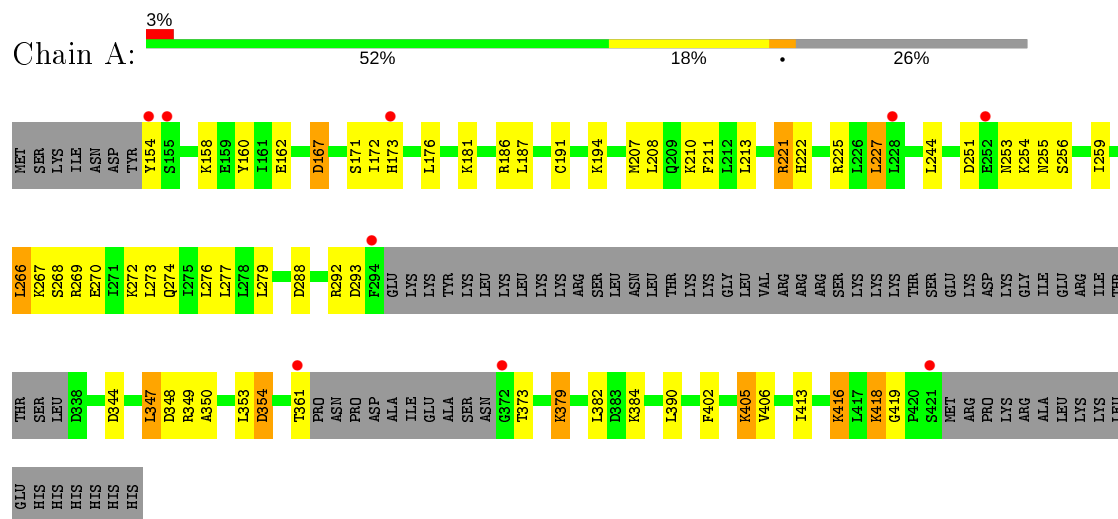
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	68	Total O 68 68	0	0
4	B	82	Total O 82 82	0	0
4	C	19	Total O 19 19	0	0

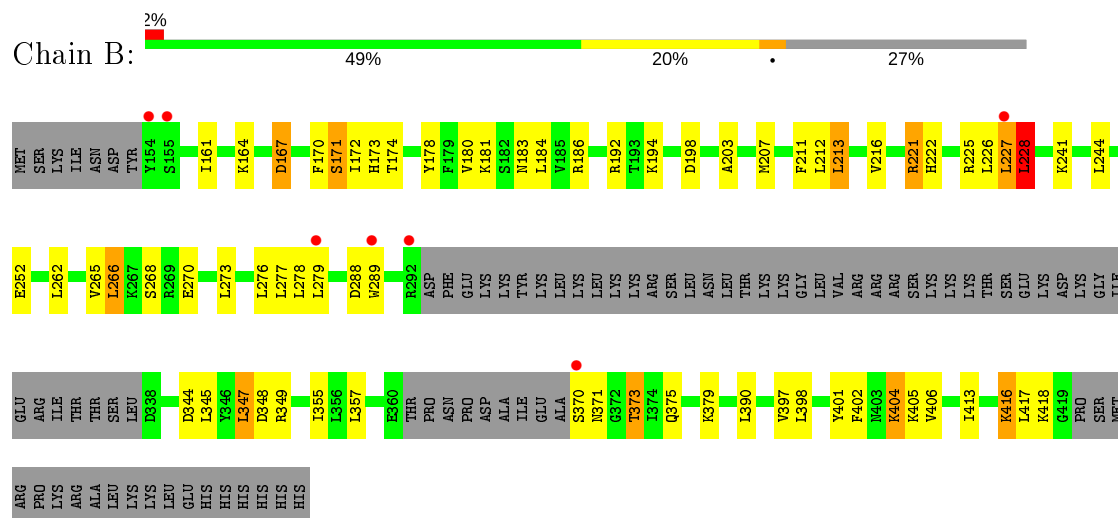
3 Residue-property plots

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: DNA replication regulator SLD3

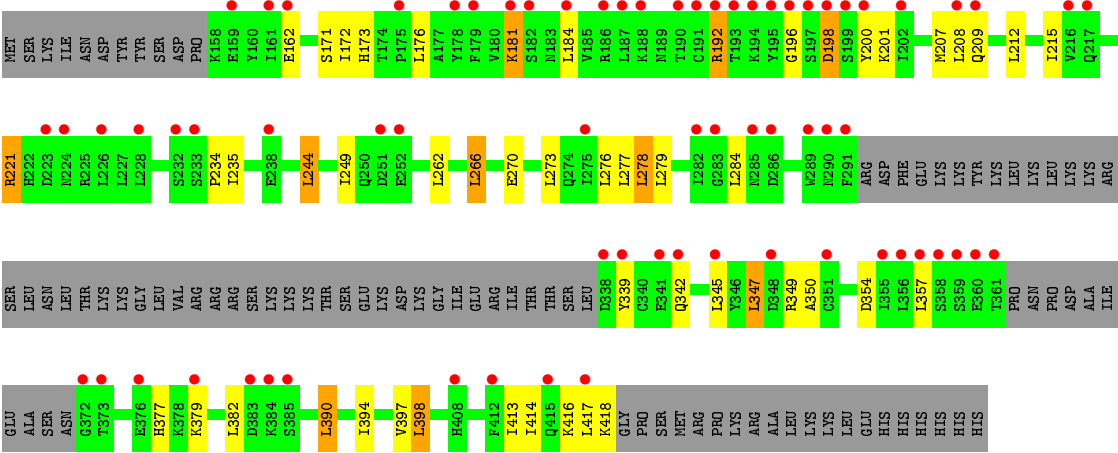


• Molecule 1: DNA replication regulator SLD3



• Molecule 1: DNA replication regulator SLD3





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.26 Å 92.82 Å 160.87 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.64 – 2.40 19.64 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.64-2.40) 88.1 (19.64-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.06 (at 2.41 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.217 , 0.262 0.218 , 0.262	Depositor DCC
R_{free} test set	1714 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5473	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: SO4, 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	0.98	0/1799	1.08	6/2424 (0.2%)
1	B	0.94	1/1772 (0.1%)	1.08	11/2386 (0.5%)
1	C	0.62	0/1715	0.88	3/2309 (0.1%)
All	All	0.87	1/5286 (0.0%)	1.02	20/7119 (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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	172	ILE	N-CA	7.57	1.61	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ARG	NE-CZ-NH2	-14.82	112.89	120.30
1	A	221	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	B	221	ARG	NE-CZ-NH2	-11.35	114.62	120.30
1	B	221	ARG	NE-CZ-NH1	10.31	125.46	120.30
1	C	221	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	C	221	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	B	171	SER	N-CA-C	-7.59	90.50	111.00
1	A	354	ASP	CB-CG-OD1	-7.55	111.50	118.30
1	B	186	ARG	CG-CD-NE	-7.30	96.46	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	SER	C-N-CA	-6.89	104.48	121.70
1	A	418	LYS	C-N-CA	-6.26	109.14	122.30
1	B	228	LEU	CA-CB-CG	6.16	129.47	115.30
1	B	213	LEU	CA-CB-CG	6.03	129.16	115.30
1	A	251	ASP	CB-CG-OD1	5.67	123.41	118.30
1	B	186	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	192	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	167	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	B	221	ARG	CD-NE-CZ	5.14	130.79	123.60
1	C	390	LEU	CA-CB-CG	5.11	127.06	115.30
1	A	292	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	171	SER	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	1766	0	1804	72	0
1	B	1741	0	1783	71	0
1	C	1686	0	1738	23	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	64	0	96	57	0
3	B	32	0	48	45	0
4	A	68	0	0	4	0
4	B	82	0	0	5	0
4	C	19	0	0	3	0
All	All	5473	0	5469	172	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 16.

All (172) 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:256:SER:O	3:A:502:EDO:H21	1.04	1.22
1:B:222:HIS:CD2	3:B:506:EDO:H22	1.78	1.19
1:A:256:SER:O	3:A:502:EDO:C2	1.93	1.17
1:B:222:HIS:HD2	3:B:506:EDO:C2	1.74	1.00
1:B:222:HIS:CD2	3:B:506:EDO:C2	2.45	0.99
1:B:222:HIS:HD2	3:B:506:EDO:H22	1.24	0.98
1:B:167:ASP:HB2	3:B:503:EDO:H22	1.51	0.93
1:A:256:SER:C	3:A:502:EDO:H21	1.90	0.90
1:A:256:SER:HA	3:A:502:EDO:H22	1.51	0.90
1:B:174:THR:HG21	3:B:502:EDO:H21	1.55	0.89
1:B:174:THR:HB	3:B:502:EDO:H22	1.55	0.86
1:A:348:ASP:OD1	1:A:416:LYS:NZ	2.10	0.84
1:A:160:TYR:OH	2:A:501:SO4:O4	1.94	0.84
1:A:227:LEU:HD22	3:A:504:EDO:H21	1.59	0.84
1:B:401:TYR:HA	3:B:504:EDO:H22	1.60	0.82
3:A:516:EDO:H22	1:B:225:ARG:CD	2.09	0.82
1:A:402:PHE:O	1:A:405:LYS:O	1.97	0.82
1:A:344:ASP:OD1	1:A:416:LYS:HE3	1.79	0.82
1:B:344:ASP:OD1	1:B:416:LYS:HE3	1.80	0.82
1:B:402:PHE:O	1:B:405:LYS:O	1.98	0.81
3:B:502:EDO:H12	3:B:503:EDO:H21	1.62	0.80
1:B:348:ASP:OD1	1:B:416:LYS:NZ	2.15	0.80
1:A:361:THR:HG21	4:A:662:HOH:O	1.81	0.79
1:B:174:THR:CB	3:B:502:EDO:H22	2.11	0.79
1:B:167:ASP:HB3	3:B:503:EDO:H21	1.65	0.77
3:A:516:EDO:H22	1:B:225:ARG:HD2	1.64	0.77
1:B:174:THR:HG21	3:B:502:EDO:C2	2.14	0.77
1:A:213:LEU:H	1:A:274:GLN:HE22	1.35	0.75
1:A:256:SER:HA	3:A:502:EDO:C2	2.17	0.74
1:A:222:HIS:HA	3:A:504:EDO:H22	1.70	0.74
3:A:516:EDO:C2	1:B:225:ARG:HD2	2.18	0.73
3:A:505:EDO:H11	3:A:514:EDO:C1	2.19	0.72
1:B:181:LYS:NZ	3:B:504:EDO:H11	2.06	0.71
1:B:167:ASP:CB	3:B:503:EDO:C2	2.70	0.69
1:A:353:LEU:HD13	3:A:517:EDO:C2	2.23	0.68
1:B:265:VAL:O	3:B:505:EDO:H22	1.93	0.68
3:A:516:EDO:H22	1:B:225:ARG:HD3	1.76	0.68
1:C:212:LEU:HD11	1:C:278:LEU:HD13	1.74	0.68
1:B:167:ASP:HB2	3:B:503:EDO:C2	2.24	0.67
1:B:167:ASP:CB	3:B:503:EDO:H22	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:TYR:HE2	4:A:642:HOH:O	1.78	0.67
1:A:353:LEU:HD13	3:A:517:EDO:H21	1.78	0.66
1:A:213:LEU:H	1:A:274:GLN:NE2	1.94	0.64
3:A:505:EDO:C1	3:A:514:EDO:H12	2.28	0.64
1:B:418:LYS:NZ	4:B:671:HOH:O	2.32	0.63
1:B:355:ILE:HG22	1:C:249:ILE:HD11	1.81	0.63
1:A:419:GLY:HA3	4:B:601:HOH:O	2.00	0.62
1:B:401:TYR:CA	3:B:504:EDO:H22	2.29	0.62
1:B:225:ARG:HA	3:B:506:EDO:H12	1.82	0.62
1:A:255:ASN:O	3:A:502:EDO:O1	2.15	0.62
1:B:181:LYS:HZ2	3:B:504:EDO:H11	1.65	0.62
1:B:222:HIS:CD2	3:B:506:EDO:H21	2.34	0.61
1:A:210:LYS:CD	3:A:506:EDO:H11	2.31	0.61
1:A:221:ARG:HD3	1:A:270:GLU:OE1	2.00	0.61
1:A:191:CYS:SG	1:A:207:MET:CE	2.89	0.60
1:A:191:CYS:SG	1:A:207:MET:HE1	2.41	0.60
1:B:167:ASP:HB3	3:B:503:EDO:C2	2.30	0.60
1:A:210:LYS:HD3	3:A:506:EDO:H11	1.85	0.59
1:A:405:LYS:NZ	4:A:660:HOH:O	2.35	0.59
1:A:256:SER:C	3:A:502:EDO:C2	2.61	0.59
3:A:505:EDO:H11	3:A:514:EDO:C2	2.34	0.58
3:B:505:EDO:O1	3:B:507:EDO:H12	2.02	0.58
1:B:164:LYS:CD	3:B:503:EDO:H11	2.33	0.58
3:A:516:EDO:C2	1:B:225:ARG:HH11	2.17	0.58
1:B:164:LYS:HD2	3:B:503:EDO:C1	2.34	0.57
1:A:158:LYS:HB3	3:A:506:EDO:H12	1.86	0.57
1:B:178:TYR:HE2	3:B:503:EDO:H12	1.69	0.57
1:B:181:LYS:NZ	3:B:504:EDO:C1	2.68	0.57
1:B:167:ASP:CB	3:B:503:EDO:H21	2.33	0.57
1:C:173:HIS:HB3	1:C:377:HIS:CE1	2.41	0.56
1:C:347:LEU:HB3	1:C:416:LYS:HG2	1.88	0.56
1:A:256:SER:CA	3:A:502:EDO:C2	2.84	0.56
3:A:505:EDO:H11	3:A:514:EDO:H12	1.87	0.56
1:A:353:LEU:CD1	3:A:517:EDO:H21	2.36	0.55
1:A:353:LEU:HD13	3:A:517:EDO:H22	1.89	0.55
1:B:174:THR:CG2	3:B:502:EDO:C2	2.84	0.55
1:C:414:ILE:O	1:C:418:LYS:HE2	2.07	0.55
1:B:227:LEU:HB2	3:B:506:EDO:H11	1.88	0.54
1:B:181:LYS:HZ3	3:B:504:EDO:C1	2.20	0.54
1:C:201:LYS:HD3	1:C:284:LEU:HD11	1.90	0.54
1:A:253:ASN:O	1:A:254:LYS:C	2.46	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ARG:HD3	1:B:270:GLU:OE1	2.09	0.53
1:A:213:LEU:HD21	3:A:510:EDO:H11	1.91	0.52
3:A:502:EDO:O2	3:A:515:EDO:H21	2.08	0.52
1:A:225:ARG:HH21	3:A:505:EDO:H21	1.74	0.52
1:B:174:THR:CG2	3:B:502:EDO:H22	2.39	0.52
1:B:183:ASN:ND2	3:B:503:EDO:O2	2.42	0.52
1:C:192:ARG:HG3	1:C:200:TYR:CE2	2.45	0.52
1:B:170:PHE:C	1:B:171:SER:O	2.41	0.51
1:C:221:ARG:HD3	1:C:270:GLU:OE1	2.11	0.51
1:A:418:LYS:HA	3:A:516:EDO:H21	1.93	0.51
1:A:268:SER:OG	3:A:503:EDO:H21	2.11	0.51
1:B:164:LYS:HA	3:B:503:EDO:H22	1.93	0.50
1:A:191:CYS:SG	1:A:207:MET:HE2	2.52	0.49
1:A:225:ARG:HH12	3:A:515:EDO:H11	1.76	0.49
1:C:173:HIS:HB3	1:C:377:HIS:HE1	1.77	0.49
1:C:209:GLN:OE1	1:C:339:TYR:OH	2.30	0.49
3:A:509:EDO:O2	3:A:510:EDO:H21	2.12	0.49
1:A:167:ASP:O	1:A:171:SER:HB3	2.13	0.48
1:A:272:LYS:HZ2	3:A:503:EDO:C2	2.26	0.48
1:A:272:LYS:NZ	3:A:503:EDO:C2	2.76	0.48
1:A:390:LEU:HD21	3:A:503:EDO:H22	1.94	0.48
1:A:187:LEU:HD11	1:A:207:MET:CE	2.44	0.48
1:B:173:HIS:O	3:B:509:EDO:H12	2.14	0.48
1:B:225:ARG:HB3	1:B:228:LEU:HD22	1.96	0.48
1:B:349:ARG:HG2	3:B:508:EDO:H12	1.96	0.48
1:A:256:SER:O	3:A:502:EDO:C1	2.60	0.47
1:B:178:TYR:CE2	3:B:503:EDO:H12	2.49	0.47
1:A:172:ILE:HD11	1:A:266:LEU:HD13	1.95	0.47
1:A:350:ALA:O	3:A:503:EDO:H11	2.15	0.47
1:B:401:TYR:HA	3:B:504:EDO:C2	2.38	0.47
1:A:186:ARG:HG2	3:A:513:EDO:O2	2.14	0.47
1:B:265:VAL:HG13	3:B:505:EDO:C1	2.45	0.47
1:C:235:ILE:HG13	4:C:612:HOH:O	2.14	0.47
1:B:262:LEU:HG	1:B:266:LEU:HD22	1.95	0.47
1:C:347:LEU:HD21	1:C:413:ILE:HG12	1.97	0.47
1:A:187:LEU:HD11	1:A:207:MET:HE3	1.97	0.47
1:A:186:ARG:HD3	3:A:513:EDO:O2	2.14	0.47
1:B:161:ILE:HG23	1:B:211:PHE:HE2	1.80	0.47
1:C:196:GLY:O	1:C:200:TYR:HB3	2.15	0.47
1:C:215:ILE:HG12	1:C:342:GLN:HE22	1.80	0.47
1:C:181:LYS:HE2	1:C:181:LYS:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LYS:HZ1	3:A:508:EDO:H22	1.80	0.46
1:B:167:ASP:HB3	3:B:502:EDO:H12	1.98	0.46
1:A:225:ARG:HA	3:A:504:EDO:O2	2.16	0.46
3:A:516:EDO:H21	1:B:225:ARG:HD2	1.95	0.46
1:A:361:THR:HB	1:B:241:LYS:NZ	2.31	0.46
1:B:355:ILE:HG23	1:C:244:LEU:HG	1.98	0.46
1:A:384:LYS:HE3	4:B:612:HOH:O	2.15	0.45
1:A:269:ARG:N	3:A:507:EDO:H22	2.31	0.45
1:B:164:LYS:HD3	3:B:503:EDO:H11	1.97	0.45
1:A:162:GLU:HA	1:A:211:PHE:CZ	2.51	0.45
1:C:192:ARG:HG3	1:C:200:TYR:CZ	2.51	0.45
1:B:347:LEU:HD21	1:B:413:ILE:HG12	1.99	0.45
1:A:349:ARG:HG2	3:A:508:EDO:H12	1.99	0.45
1:B:203:ALA:O	1:B:207:MET:HG2	2.17	0.45
1:B:164:LYS:CD	3:B:503:EDO:C1	2.95	0.45
1:A:268:SER:C	3:A:507:EDO:H22	2.38	0.45
1:B:405:LYS:HG2	4:B:651:HOH:O	2.17	0.44
1:B:222:HIS:HA	3:B:506:EDO:H21	1.99	0.44
1:A:213:LEU:N	1:A:274:GLN:HE22	2.09	0.43
1:A:210:LYS:HD2	3:A:506:EDO:H11	1.99	0.43
1:A:268:SER:OG	3:A:507:EDO:H21	2.18	0.43
1:B:373:THR:CG2	1:B:375:GLN:HB2	2.49	0.43
1:B:404:LYS:N	1:B:404:LYS:HE3	2.32	0.43
1:C:262:LEU:HG	1:C:266:LEU:HD22	2.00	0.43
1:B:373:THR:HG23	4:B:620:HOH:O	2.18	0.43
1:A:167:ASP:O	1:A:171:SER:CB	2.67	0.43
1:A:268:SER:OG	3:A:507:EDO:C2	2.67	0.43
1:A:347:LEU:HD21	1:A:413:ILE:HG12	2.01	0.43
1:C:212:LEU:HD11	1:C:278:LEU:CD1	2.44	0.42
1:C:394:ILE:HA	1:C:398:LEU:HB2	2.01	0.42
1:B:390:LEU:HA	1:B:390:LEU:HD23	1.84	0.42
1:C:349:ARG:NH2	4:C:613:HOH:O	2.44	0.42
1:B:265:VAL:HG13	3:B:505:EDO:H11	2.02	0.42
1:B:288:ASP:CG	1:B:406:VAL:HA	2.39	0.42
1:A:379:LYS:HE3	4:A:648:HOH:O	2.20	0.42
3:A:505:EDO:C1	3:A:514:EDO:C1	2.89	0.42
1:A:418:LYS:NZ	3:A:516:EDO:H12	2.34	0.42
1:C:234:PRO:HG2	4:C:612:HOH:O	2.20	0.42
1:A:222:HIS:ND1	3:A:504:EDO:H22	2.34	0.42
1:A:225:ARG:HH21	3:A:505:EDO:C2	2.33	0.42
1:B:207:MET:CE	1:B:207:MET:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:SER:CA	3:A:502:EDO:H21	2.46	0.41
1:A:288:ASP:CG	1:A:406:VAL:HA	2.41	0.41
1:A:173:HIS:CD2	1:A:173:HIS:H	2.38	0.40
1:A:259:ILE:HB	3:A:515:EDO:H22	2.03	0.40
1:A:267:LYS:HE2	3:A:508:EDO:H11	2.03	0.40
1:A:267:LYS:HZ1	3:A:508:EDO:C2	2.34	0.40
1:B:268:SER:HB3	3:B:505:EDO:C2	2.52	0.40
1:C:350:ALA:HB1	1:C:390:LEU:HD11	2.02	0.40
1:B:371:ASN:C	1:B:373:THR:H	2.25	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	209/292 (72%)	205 (98%)	4 (2%)	0	100	100
1	B	206/292 (70%)	201 (98%)	4 (2%)	1 (0%)	29	41
1	C	199/292 (68%)	192 (96%)	6 (3%)	1 (0%)	29	41
All	All	614/876 (70%)	598 (97%)	14 (2%)	2 (0%)	41	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	198	ASP
1	B	198	ASP

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	201/273 (74%)	181 (90%)	20 (10%)	7	11
1	B	198/273 (72%)	169 (85%)	29 (15%)	3	3
1	C	192/273 (70%)	167 (87%)	25 (13%)	4	4
All	All	591/819 (72%)	517 (88%)	74 (12%)	4	5

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	ASP
1	A	176	LEU
1	A	181	LYS
1	A	194	LYS
1	A	208	LEU
1	A	227	LEU
1	A	244	LEU
1	A	266	LEU
1	A	273	LEU
1	A	276	LEU
1	A	277	LEU
1	A	279	LEU
1	A	293	ASP
1	A	347	LEU
1	A	354	ASP
1	A	373	THR
1	A	379	LYS
1	A	382	LEU
1	A	405	LYS
1	A	416	LYS
1	B	180	VAL
1	B	184	LEU
1	B	194	LYS
1	B	212	LEU
1	B	213	LEU
1	B	216	VAL
1	B	226	LEU
1	B	227	LEU
1	B	228	LEU
1	B	244	LEU

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Mol	Chain	Res	Type
1	B	252	GLU
1	B	266	LEU
1	B	273	LEU
1	B	276	LEU
1	B	277	LEU
1	B	278	LEU
1	B	279	LEU
1	B	289	TRP
1	B	345	LEU
1	B	347	LEU
1	B	357	LEU
1	B	370	SER
1	B	373	THR
1	B	379	LYS
1	B	397	VAL
1	B	398	LEU
1	B	404	LYS
1	B	416	LYS
1	B	417	LEU
1	C	162	GLU
1	C	172	ILE
1	C	176	LEU
1	C	181	LYS
1	C	184	LEU
1	C	192	ARG
1	C	198	ASP
1	C	207	MET
1	C	208	LEU
1	C	244	LEU
1	C	266	LEU
1	C	273	LEU
1	C	276	LEU
1	C	277	LEU
1	C	278	LEU
1	C	279	LEU
1	C	345	LEU
1	C	347	LEU
1	C	354	ASP
1	C	357	LEU
1	C	379	LYS
1	C	382	LEU
1	C	397	VAL

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Mol	Chain	Res	Type
1	C	398	LEU
1	C	417	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	HIS
1	A	189	ASN
1	A	250	GLN
1	A	274	GLN
1	A	380	ASN
1	A	395	ASN
1	A	415	GLN
1	B	183	ASN
1	B	189	ASN
1	B	209	GLN
1	B	222	HIS
1	B	285	ASN
1	B	371	ASN
1	B	375	GLN
1	B	380	ASN
1	B	395	ASN
1	B	415	GLN
1	C	183	ASN
1	C	189	ASN
1	C	285	ASN
1	C	342	GLN
1	C	375	GLN
1	C	377	HIS
1	C	395	ASN
1	C	415	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

27 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	$\# Z > 2$
3	EDO	B	508	-	3,3,3	0.94	0	2,2,2	0.39	0
3	EDO	A	505	-	3,3,3	1.00	0	2,2,2	1.21	0
3	EDO	B	507	-	3,3,3	0.58	0	2,2,2	0.27	0
3	EDO	B	509	-	3,3,3	0.72	0	2,2,2	0.15	0
3	EDO	A	508	-	3,3,3	1.53	1 (33%)	2,2,2	0.28	0
3	EDO	A	513	-	3,3,3	0.35	0	2,2,2	1.20	0
2	SO4	A	501	-	4,4,4	1.31	0	6,6,6	0.52	0
3	EDO	B	505	-	3,3,3	1.31	0	2,2,2	1.17	0
2	SO4	C	501	-	4,4,4	1.13	0	6,6,6	0.30	0
3	EDO	A	507	-	3,3,3	0.52	0	2,2,2	0.58	0
3	EDO	A	506	-	3,3,3	0.75	0	2,2,2	0.66	0
3	EDO	A	503	-	3,3,3	0.97	0	2,2,2	0.76	0
3	EDO	B	506	-	3,3,3	0.67	0	2,2,2	0.29	0
3	EDO	A	502	-	3,3,3	1.09	0	2,2,2	0.67	0
3	EDO	B	504	-	3,3,3	0.55	0	2,2,2	0.25	0
3	EDO	A	517	-	3,3,3	0.72	0	2,2,2	0.44	0
3	EDO	B	502	-	3,3,3	0.70	0	2,2,2	0.06	0
3	EDO	A	512	-	3,3,3	0.80	0	2,2,2	0.82	0
3	EDO	A	516	-	3,3,3	0.37	0	2,2,2	0.26	0
2	SO4	B	501	-	4,4,4	0.96	0	6,6,6	1.15	0
3	EDO	A	504	-	3,3,3	0.84	0	2,2,2	0.68	0
3	EDO	A	510	-	3,3,3	0.82	0	2,2,2	0.02	0
3	EDO	A	511	-	3,3,3	0.43	0	2,2,2	0.67	0
3	EDO	A	514	-	3,3,3	0.61	0	2,2,2	0.54	0
3	EDO	A	509	-	3,3,3	0.85	0	2,2,2	0.53	0
3	EDO	A	515	-	3,3,3	2.32	2 (66%)	2,2,2	1.56	1 (50%)
3	EDO	B	503	-	3,3,3	1.27	0	2,2,2	1.53	1 (50%)

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
3	EDO	B	508	-	-	0/1/1/1	-
3	EDO	A	505	-	-	1/1/1/1	-
3	EDO	B	507	-	-	1/1/1/1	-
3	EDO	B	509	-	-	1/1/1/1	-
3	EDO	A	508	-	-	1/1/1/1	-
3	EDO	A	513	-	-	0/1/1/1	-
3	EDO	B	505	-	-	1/1/1/1	-
3	EDO	A	507	-	-	1/1/1/1	-
3	EDO	A	506	-	-	1/1/1/1	-
3	EDO	A	503	-	-	1/1/1/1	-
3	EDO	B	506	-	-	0/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
3	EDO	B	504	-	-	1/1/1/1	-
3	EDO	A	517	-	-	0/1/1/1	-
3	EDO	A	509	-	-	0/1/1/1	-
3	EDO	A	512	-	-	1/1/1/1	-
3	EDO	A	516	-	-	0/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	A	510	-	-	1/1/1/1	-
3	EDO	A	511	-	-	1/1/1/1	-
3	EDO	A	514	-	-	1/1/1/1	-
3	EDO	B	502	-	-	0/1/1/1	-
3	EDO	A	515	-	-	1/1/1/1	-
3	EDO	B	503	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	515	EDO	O1-C1	3.10	1.58	1.42
3	A	515	EDO	C2-C1	2.22	1.63	1.48
3	A	508	EDO	O1-C1	2.06	1.52	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	515	EDO	O2-C2-C1	2.17	127.56	111.91
3	B	503	EDO	O2-C2-C1	2.13	127.22	111.91

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	505	EDO	O1-C1-C2-O2
3	B	503	EDO	O1-C1-C2-O2
3	B	505	EDO	O1-C1-C2-O2
3	A	506	EDO	O1-C1-C2-O2
3	A	508	EDO	O1-C1-C2-O2
3	A	514	EDO	O1-C1-C2-O2
3	A	510	EDO	O1-C1-C2-O2
3	B	509	EDO	O1-C1-C2-O2
3	A	512	EDO	O1-C1-C2-O2
3	A	503	EDO	O1-C1-C2-O2
3	B	507	EDO	O1-C1-C2-O2
3	A	507	EDO	O1-C1-C2-O2
3	B	504	EDO	O1-C1-C2-O2
3	A	515	EDO	O1-C1-C2-O2
3	A	511	EDO	O1-C1-C2-O2

There are no ring outliers.

23 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	508	EDO	1	0
3	A	505	EDO	7	0
3	B	507	EDO	1	0
3	B	509	EDO	1	0
3	A	508	EDO	4	0
3	A	513	EDO	2	0
2	A	501	SO4	1	0
3	B	505	EDO	5	0
3	A	507	EDO	4	0
3	A	506	EDO	4	0
3	A	503	EDO	5	0
3	B	506	EDO	8	0
3	A	502	EDO	11	0
3	B	504	EDO	7	0
3	A	517	EDO	4	0
3	B	502	EDO	8	0
3	A	516	EDO	8	0
3	A	504	EDO	4	0
3	A	510	EDO	2	0
3	A	514	EDO	5	0
3	A	509	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	515	EDO	3	0
3	B	503	EDO	16	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	215/292 (73%)	0.01	9 (4%) 36 35	14, 31, 59, 86	0
1	B	212/292 (72%)	-0.07	7 (3%) 46 45	13, 33, 68, 84	0
1	C	205/292 (70%)	1.75	70 (34%) 0 0	44, 75, 128, 170	0
All	All	632/876 (72%)	0.55	86 (13%) 3 2	13, 42, 104, 170	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	199	SER	8.9
1	C	178	TYR	8.3
1	C	193	THR	7.8
1	C	195	TYR	7.6
1	C	289	TRP	7.5
1	C	361	THR	7.2
1	C	198	ASP	6.8
1	C	194	LYS	6.6
1	C	192	ARG	6.6
1	C	216	VAL	6.5
1	C	372	GLY	5.7
1	C	191	CYS	5.7
1	C	355	ILE	5.5
1	C	190	THR	5.4
1	C	200	TYR	5.4
1	C	232	SER	4.9
1	C	359	SER	4.7
1	C	197	SER	4.4
1	C	233	SER	4.3
1	C	161	ILE	4.2
1	C	202	ILE	4.1
1	C	159	GLU	4.0
1	C	283	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	196	GLY	3.9
1	C	290	ASN	3.8
1	C	356	LEU	3.6
1	C	342	GLN	3.6
1	C	376	GLU	3.5
1	C	224	ASN	3.5
1	A	421	SER	3.5
1	C	360	GLU	3.5
1	C	379	LYS	3.5
1	C	187	LEU	3.4
1	B	292	ARG	3.4
1	C	351	CYS	3.4
1	C	417	LEU	3.3
1	C	358	SER	3.3
1	C	175	PRO	3.3
1	C	252	GLU	3.3
1	C	162	GLU	3.2
1	C	282	ILE	3.2
1	C	188	LYS	3.2
1	C	383	ASP	3.1
1	C	373	THR	3.1
1	C	338	ASP	3.1
1	C	385	SER	3.1
1	C	339	TYR	3.0
1	C	223	ASP	2.9
1	C	384	LYS	2.9
1	C	275	ILE	2.9
1	C	184	LEU	2.9
1	C	286	ASP	2.8
1	C	186	ARG	2.8
1	C	291	PHE	2.8
1	A	294	PHE	2.7
1	C	238	GLU	2.7
1	B	289	TRP	2.7
1	C	209	GLN	2.7
1	B	370	SER	2.6
1	C	348	ASP	2.6
1	A	154	TYR	2.6
1	C	415	GLN	2.5
1	C	208	LEU	2.5
1	C	285	ASN	2.4
1	A	155	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	182	SER	2.4
1	C	408	HIS	2.4
1	C	357	LEU	2.3
1	C	341	GLU	2.3
1	A	372	GLY	2.3
1	B	155	SER	2.2
1	C	179	PHE	2.2
1	B	227	LEU	2.2
1	A	252	GLU	2.2
1	B	279	LEU	2.1
1	C	181	LYS	2.1
1	C	412	PHE	2.1
1	C	226	LEU	2.1
1	B	154	TYR	2.1
1	C	228	LEU	2.1
1	A	361	THR	2.1
1	A	228	LEU	2.0
1	C	217	GLN	2.0
1	C	345	LEU	2.0
1	A	173	HIS	2.0
1	C	251	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
2	SO4	C	501	5/5	0.62	0.39	118,121,128,130	0
3	EDO	A	510	4/4	0.67	0.24	51,51,54,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	B	508	4/4	0.75	0.30	62,62,70,77	0
3	EDO	A	513	4/4	0.79	0.22	52,54,57,62	0
3	EDO	A	509	4/4	0.79	0.21	57,60,64,64	0
2	SO4	A	501	5/5	0.83	0.21	66,72,92,105	0
3	EDO	A	512	4/4	0.83	0.29	38,40,45,47	0
3	EDO	A	517	4/4	0.86	0.32	44,49,51,52	0
3	EDO	B	505	4/4	0.87	0.24	26,30,32,44	0
3	EDO	B	509	4/4	0.88	0.26	39,44,44,54	0
3	EDO	A	508	4/4	0.89	0.23	34,43,45,54	0
3	EDO	A	503	4/4	0.90	0.21	28,35,40,47	0
3	EDO	B	503	4/4	0.90	0.33	21,28,28,28	0
3	EDO	A	506	4/4	0.90	0.31	28,31,32,34	0
3	EDO	B	506	4/4	0.91	0.25	28,33,35,36	0
3	EDO	A	507	4/4	0.91	0.16	35,39,44,48	0
3	EDO	B	504	4/4	0.92	0.22	32,33,42,45	0
3	EDO	A	515	4/4	0.92	0.18	25,28,29,32	0
3	EDO	A	505	4/4	0.93	0.20	29,31,32,34	0
3	EDO	A	511	4/4	0.93	0.23	39,46,49,54	0
3	EDO	A	516	4/4	0.94	0.12	35,36,36,38	0
3	EDO	A	514	4/4	0.94	0.36	30,32,35,36	0
3	EDO	A	504	4/4	0.96	0.20	20,21,24,25	0
3	EDO	A	502	4/4	0.96	0.18	31,35,37,37	0
3	EDO	B	502	4/4	0.96	0.16	21,22,23,24	0
3	EDO	B	507	4/4	0.97	0.14	29,34,36,37	0
2	SO4	B	501	5/5	1.00	0.12	19,19,22,23	0

6.5 Other polymers

There are no such residues in this entry.