



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:13 AM UTC

PDB ID : 3WI3 / pdb_00003wi3
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 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

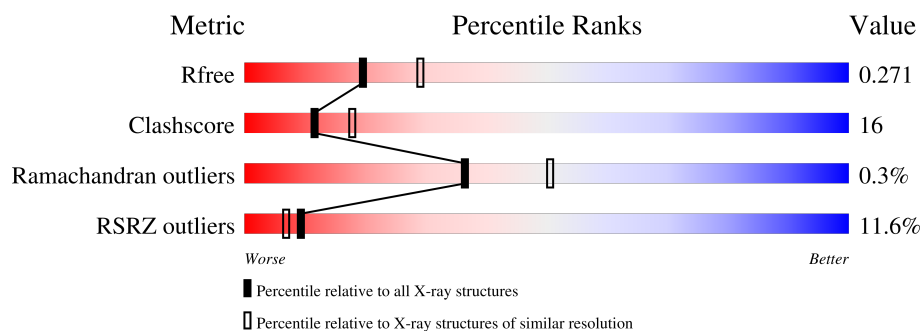
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	292	3% 57% 15% • 26%
1	B	292	3% 56% 15% • 27%
1	C	292	19% 58% 12% 30%

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	514	-	-	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:

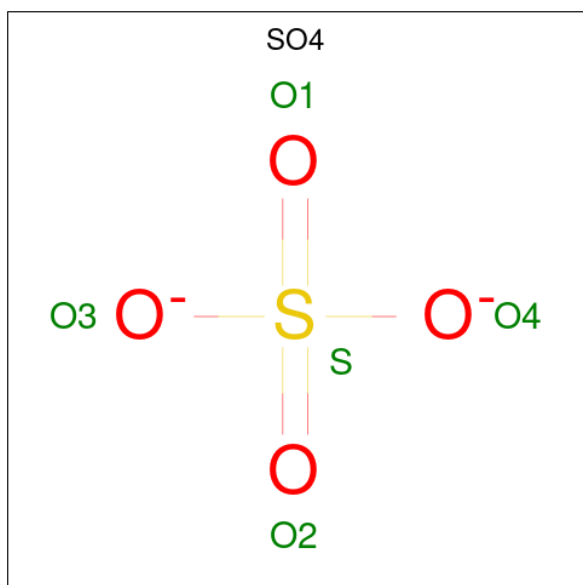
Chain	Residue	Modelled	Actual	Comment	Reference
A	147	MET	-	expression tag	UNP P53135
A	431	LEU	-	expression tag	UNP P53135
A	432	GLU	-	expression tag	UNP P53135
A	433	HIS	-	expression tag	UNP P53135
A	434	HIS	-	expression tag	UNP P53135
A	435	HIS	-	expression tag	UNP P53135
A	436	HIS	-	expression tag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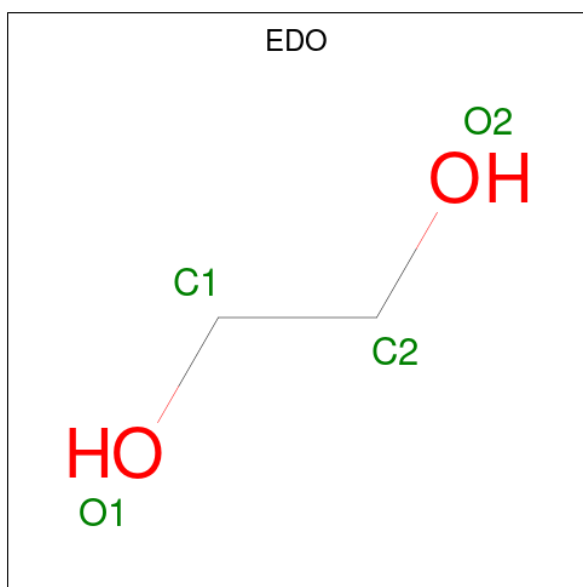
Chain	Residue	Modelled	Actual	Comment	Reference
C	435	HIS	-	expression tag	UNP P53135
C	436	HIS	-	expression tag	UNP P53135
C	437	HIS	-	expression tag	UNP P53135
C	438	HIS	-	expression tag	UNP P53135

- Molecule 2 is SULFATE ION (CCD ID: 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 (CCD ID: 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

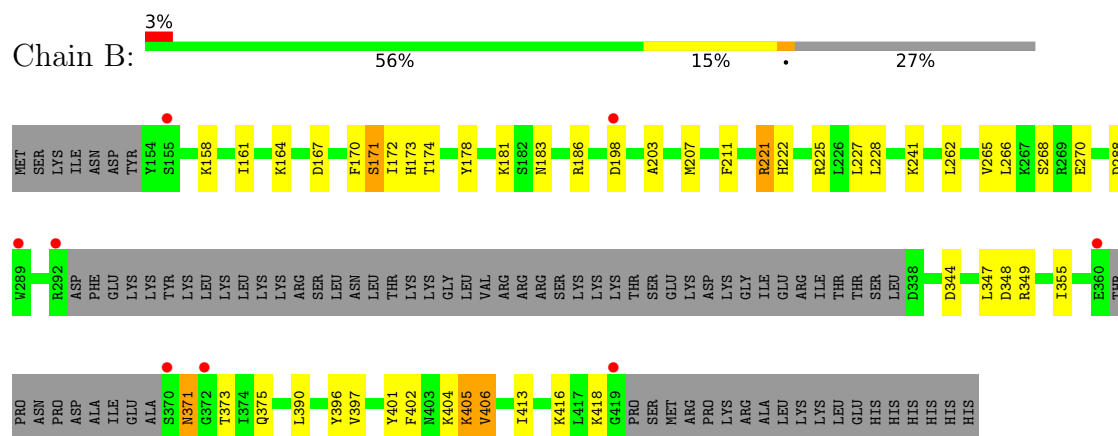
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

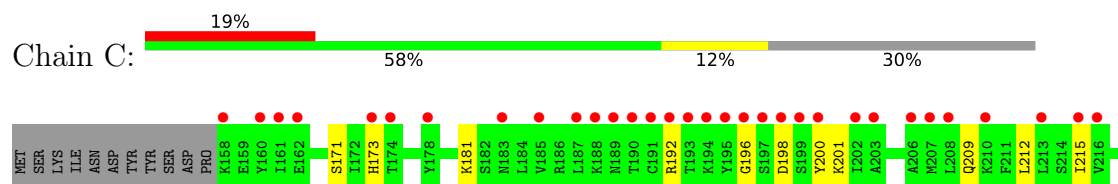
• Molecule 1: DNA replication regulator SLD3

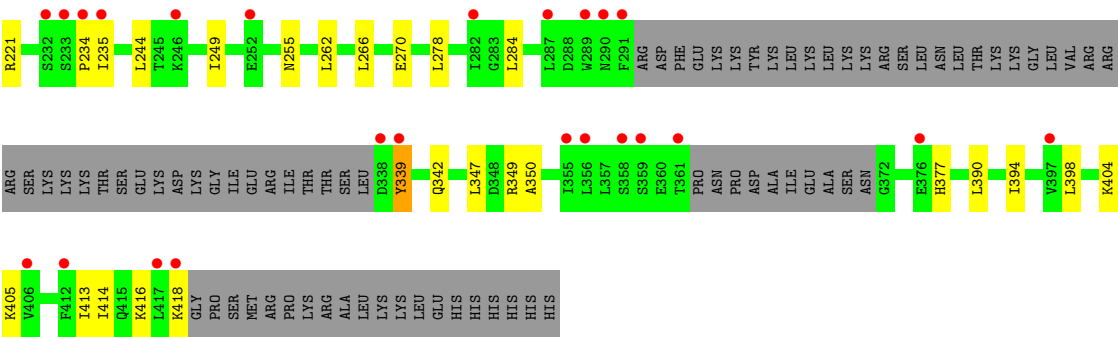


• Molecule 1: DNA replication regulator SLD3



• 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	65.26Å 92.82Å 160.87Å 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) 87.9 (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 2.41Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.217 , 0.262 (Not available) , 0.271	Depositor DCC
R_{free} test set	1714 reflections (4.40%)	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)	0.36 , 55.8	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	0.92	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: EDO, SO4

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	1.28	3/1799 (0.2%)	1.21	10/2424 (0.4%)
1	B	1.26	2/1772 (0.1%)	1.30	16/2386 (0.7%)
1	C	0.86	0/1715	1.04	4/2309 (0.2%)
All	All	1.15	5/5286 (0.1%)	1.19	30/7119 (0.4%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	172	ILE	N-CA	16.21	1.61	1.46
1	B	406	VAL	CA-C	5.96	1.59	1.52
1	A	418	LYS	CA-C	-5.72	1.45	1.52
1	A	406	VAL	CA-C	5.69	1.58	1.52
1	A	419	GLY	N-CA	5.34	1.52	1.44

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	SER	N-CA-C	-16.18	90.50	110.41
1	B	171	SER	CA-C-N	-14.36	104.48	121.71
1	B	171	SER	C-N-CA	-14.36	104.48	121.71
1	A	418	LYS	CA-C-N	-8.11	109.14	121.87
1	A	418	LYS	C-N-CA	-8.11	109.14	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	LYS	N-CA-C	-7.50	98.01	109.41
1	B	186	ARG	CG-CD-NE	-7.06	96.46	112.00
1	A	221	ARG	NE-CZ-NH2	-7.01	112.89	119.20
1	C	405	LYS	N-CA-C	6.73	118.40	111.14
1	B	406	VAL	N-CA-CB	-6.72	101.80	111.21
1	A	405	LYS	N-CA-C	-6.63	100.65	110.46
1	A	406	VAL	N-CA-C	6.62	123.17	108.88
1	B	405	LYS	N-CA-C	-6.35	100.58	110.42
1	A	167	ASP	N-CA-C	-6.31	104.32	111.14
1	A	419	GLY	CA-C-N	6.28	126.40	119.87
1	A	419	GLY	C-N-CA	6.28	126.40	119.87
1	B	406	VAL	N-CA-C	6.14	122.14	108.88
1	B	397	VAL	N-CA-C	5.94	116.32	111.62
1	B	371	ASN	N-CA-C	5.86	118.08	108.52
1	B	397	VAL	CB-CA-C	5.86	116.27	111.05
1	B	397	VAL	N-CA-CB	5.85	116.43	111.64
1	B	172	ILE	CA-C-O	5.53	124.68	118.98
1	B	396	TYR	CA-C-N	-5.33	117.51	123.16
1	B	396	TYR	C-N-CA	-5.33	117.51	123.16
1	B	171	SER	O-C-N	-5.26	116.23	122.65
1	A	180	VAL	CB-CA-C	-5.24	105.17	112.04
1	C	404	LYS	CA-C-N	5.14	127.43	120.44
1	C	404	LYS	C-N-CA	5.14	127.43	120.44
1	B	221	ARG	NE-CZ-NH2	-5.08	114.62	119.20
1	C	339	TYR	N-CA-CB	5.05	119.02	110.49

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	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1741	0	1783	73	0
1	C	1686	0	1738	24	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	55	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:A:256:SER:C	3:A:502:EDO:H21	1.90	0.95
1:B:167:ASP:HB2	3:B:503:EDO:H22	1.51	0.93
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:207:MET:HA	1:B:207:MET:HE2	1.67	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:158:LYS:HG2	1:B:207:MET:HE1	1.73	0.70
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
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:A:191:CYS:SG	1:A:207:MET:HE2	2.39	0.63
1:A:256:SER:C	3:A:502:EDO:C2	2.61	0.63
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:225:ARG:HA	3:B:506:EDO:H12	1.82	0.62
1:B:401:TYR:CA	3:B:504:EDO:H22	2.29	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: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
3:A:505:EDO:H11	3:A:514:EDO:C2	2.34	0.58
1:A:253:ASN:O	1:A:254:LYS:C	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:PHE:C	1:B:171:SER:O	2.41	0.58
3:B:505:EDO:O1	3:B:507:EDO:H12	2.02	0.58
3:A:516:EDO:C2	1:B:225:ARG:HH11	2.17	0.58
1:B:164:LYS:CD	3:B:503:EDO:H11	2.33	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:A:272:LYS:HZ2	3:A:503:EDO:C2	2.20	0.54
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: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: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: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:268:SER:C	3:A:507:EDO:H22	2.38	0.49
1:A:167:ASP:O	1:A:171:SER:HB3	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:288:ASP:CG	1:B:406:VAL:HA	2.39	0.47
1:B:262:LEU:HG	1:B:266:LEU:HD22	1.95	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:C:347:LEU:HD21	1:C:413:ILE:HG12	1.97	0.47
1:A:186:ARG:HD3	3:A:513:EDO:O2	2.14	0.47
1:A:191:CYS:SG	1:A:207:MET:HE1	2.55	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:HA	1:C:181:LYS:HE2	1.97	0.46
1:B:167:ASP:HB3	3:B:502:EDO:H12	1.98	0.46
1:A:288:ASP:CG	1:A:406:VAL:HA	2.41	0.46
1:A:225:ARG:HA	3:A:504:EDO:O2	2.16	0.46
1:A:361:THR:HB	1:B:241:LYS:NZ	2.31	0.46
3:A:516:EDO:H21	1:B:225:ARG:HD2	1.95	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: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:B:348:ASP:CG	1:C:255:ASN:HB2	2.43	0.44
1:A:210:LYS:HD2	3:A:506:EDO:H11	1.99	0.43
1:A:213:LEU:N	1:A:274:GLN:HE22	2.09	0.43
1:A:268:SER:OG	3:A:507:EDO:H21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ASN:C	1:B:373:THR:H	2.25	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:HD23	1:B:390:LEU:HA	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: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:A:256:SER:CA	3:A:502:EDO:H21	2.46	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: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:A:187:LEU:HD11	1:A:207:MET:HE1	2.03	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%)	24	37
1	C	199/292 (68%)	192 (96%)	6 (3%)	1 (0%)	24	37
All	All	614/876 (70%)	598 (97%)	14 (2%)	2 (0%)	36	50

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](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

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
2	SO4	A	501	-	4,4,4	1.33	0	6,6,6	0.49	0
3	EDO	A	507	-	3,3,3	0.49	0	2,2,2	0.58	0
3	EDO	B	504	-	3,3,3	0.55	0	2,2,2	0.27	0
3	EDO	A	511	-	3,3,3	0.40	0	2,2,2	0.66	0
2	SO4	B	501	-	4,4,4	1.01	0	6,6,6	1.16	0
3	EDO	A	509	-	3,3,3	0.86	0	2,2,2	0.56	0
3	EDO	A	504	-	3,3,3	0.80	0	2,2,2	0.60	0
3	EDO	A	512	-	3,3,3	0.80	0	2,2,2	0.80	0
3	EDO	B	502	-	3,3,3	0.65	0	2,2,2	0.02	0
2	SO4	C	501	-	4,4,4	1.17	0	6,6,6	0.31	0
3	EDO	A	510	-	3,3,3	0.80	0	2,2,2	0.08	0
3	EDO	A	515	-	3,3,3	2.26	1 (33%)	2,2,2	1.42	0
3	EDO	B	509	-	3,3,3	0.68	0	2,2,2	0.16	0
3	EDO	A	502	-	3,3,3	1.01	0	2,2,2	0.65	0
3	EDO	A	516	-	3,3,3	0.37	0	2,2,2	0.30	0
3	EDO	A	513	-	3,3,3	0.33	0	2,2,2	1.20	0
3	EDO	A	506	-	3,3,3	0.70	0	2,2,2	0.66	0
3	EDO	A	508	-	3,3,3	1.51	1 (33%)	2,2,2	0.26	0
3	EDO	B	506	-	3,3,3	0.62	0	2,2,2	0.33	0
3	EDO	B	503	-	3,3,3	1.17	0	2,2,2	1.39	0
3	EDO	B	508	-	3,3,3	0.90	0	2,2,2	0.32	0
3	EDO	A	505	-	3,3,3	0.95	0	2,2,2	1.14	0
3	EDO	B	507	-	3,3,3	0.57	0	2,2,2	0.27	0
3	EDO	A	503	-	3,3,3	0.95	0	2,2,2	0.72	0
3	EDO	A	514	-	3,3,3	0.60	0	2,2,2	0.48	0
3	EDO	A	517	-	3,3,3	0.67	0	2,2,2	0.46	0
3	EDO	B	505	-	3,3,3	1.28	0	2,2,2	1.09	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
3	EDO	A	507	-	-	1/1/1/1	-
3	EDO	B	504	-	-	1/1/1/1	-
3	EDO	A	511	-	-	1/1/1/1	-
3	EDO	A	509	-	-	0/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	A	512	-	-	1/1/1/1	-
3	EDO	B	502	-	-	0/1/1/1	-
3	EDO	A	515	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	510	-	-	1/1/1/1	-
3	EDO	B	509	-	-	1/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
3	EDO	A	516	-	-	0/1/1/1	-
3	EDO	A	513	-	-	0/1/1/1	-
3	EDO	A	506	-	-	1/1/1/1	-
3	EDO	A	508	-	-	1/1/1/1	-
3	EDO	B	506	-	-	0/1/1/1	-
3	EDO	B	503	-	-	1/1/1/1	-
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	A	503	-	-	1/1/1/1	-
3	EDO	A	514	-	-	1/1/1/1	-
3	EDO	A	517	-	-	1/1/1/1	-
3	EDO	B	505	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	515	EDO	O1-C1	3.14	1.58	1.42
3	A	508	EDO	O1-C1	2.08	1.52	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	B	504	EDO	O1-C1-C2-O2
3	A	511	EDO	O1-C1-C2-O2
3	A	517	EDO	O1-C1-C2-O2

There are no ring outliers.

23 monomers are involved in 101 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SO4	1	0
3	A	507	EDO	4	0
3	B	504	EDO	7	0
3	A	509	EDO	1	0
3	A	504	EDO	4	0
3	B	502	EDO	8	0
3	A	510	EDO	2	0
3	A	515	EDO	3	0
3	B	509	EDO	1	0
3	A	502	EDO	11	0
3	A	516	EDO	8	0
3	A	513	EDO	2	0
3	A	506	EDO	4	0
3	A	508	EDO	2	0
3	B	506	EDO	8	0
3	B	503	EDO	16	0
3	B	508	EDO	1	0
3	A	505	EDO	7	0
3	B	507	EDO	1	0
3	A	503	EDO	5	0
3	A	514	EDO	5	0
3	A	517	EDO	4	0
3	B	505	EDO	5	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%)	-0.07	9 (4%) 40 36	14, 31, 59, 86	0
1	B	212/292 (72%)	-0.12	8 (3%) 44 40	13, 33, 68, 84	0
1	C	205/292 (70%)	1.33	56 (27%) 1 1	44, 75, 128, 170	0
All	All	632/876 (72%)	0.37	73 (11%) 9 7	13, 42, 104, 170	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	195	TYR	5.8
1	C	199	SER	4.8
1	C	194	LYS	4.4
1	C	197	SER	4.4
1	C	356	LEU	4.1
1	C	158	LYS	3.9
1	C	289	TRP	3.8
1	A	361	THR	3.8
1	B	198	ASP	3.6
1	C	234	PRO	3.5
1	C	193	THR	3.4
1	C	287	LEU	3.4
1	C	215	ILE	3.4
1	C	216	VAL	3.4
1	C	417	LEU	3.4
1	C	232	SER	3.3
1	C	178	TYR	3.2
1	A	252	GLU	3.2
1	C	206	ALA	3.1
1	C	190	THR	3.1
1	C	202	ILE	3.1
1	C	246	LYS	3.0
1	C	290	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	376	GLU	2.9
1	C	235	ILE	2.9
1	B	289	TRP	2.9
1	C	191	CYS	2.8
1	C	161	ILE	2.8
1	C	361	THR	2.8
1	A	338	ASP	2.7
1	A	421	SER	2.7
1	C	174	THR	2.7
1	C	213	LEU	2.6
1	B	370	SER	2.6
1	C	196	GLY	2.6
1	C	210	LYS	2.6
1	C	203	ALA	2.6
1	C	198	ASP	2.5
1	C	338	ASP	2.5
1	C	187	LEU	2.5
1	C	189	ASN	2.5
1	B	292	ARG	2.5
1	C	173	HIS	2.4
1	B	372	GLY	2.4
1	A	178	TYR	2.4
1	C	185	VAL	2.4
1	C	418	LYS	2.4
1	C	358	SER	2.4
1	C	233	SER	2.3
1	C	355	ILE	2.3
1	C	412	PHE	2.3
1	C	160	TYR	2.3
1	C	200	TYR	2.3
1	C	359	SER	2.3
1	C	208	LEU	2.3
1	B	360	GLU	2.3
1	C	162	GLU	2.3
1	C	188	LYS	2.3
1	C	397	VAL	2.3
1	A	405	LYS	2.2
1	C	183	ASN	2.2
1	A	154	TYR	2.2
1	C	339	TYR	2.2
1	C	192	ARG	2.2
1	C	291	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	419	GLY	2.1
1	C	282	ILE	2.1
1	C	252	GLU	2.1
1	B	155	SER	2.1
1	C	406	VAL	2.0
1	A	419	GLY	2.0
1	C	207	MET	2.0
1	A	372	GLY	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	SO4	C	501	5/5	0.58	0.15	118,121,128,130	0
3	EDO	A	509	4/4	0.79	0.19	57,60,64,64	0
3	EDO	A	513	4/4	0.79	0.17	52,54,57,62	0
2	SO4	A	501	5/5	0.80	0.17	66,72,92,105	0
3	EDO	A	510	4/4	0.83	0.12	51,51,54,58	0
3	EDO	B	508	4/4	0.83	0.16	62,62,70,77	0
3	EDO	B	505	4/4	0.86	0.18	26,30,32,44	0
3	EDO	A	508	4/4	0.86	0.17	34,43,45,54	0
3	EDO	A	506	4/4	0.87	0.25	28,31,32,34	0
3	EDO	A	517	4/4	0.88	0.21	44,49,51,52	0
3	EDO	B	509	4/4	0.88	0.16	39,44,44,54	0
3	EDO	B	506	4/4	0.89	0.21	28,33,35,36	0
3	EDO	A	511	4/4	0.89	0.14	39,46,49,54	0
3	EDO	A	505	4/4	0.89	0.15	29,31,32,34	0
3	EDO	A	515	4/4	0.90	0.14	25,28,29,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	503	4/4	0.90	0.16	28,35,40,47	0
3	EDO	A	512	4/4	0.91	0.11	38,40,45,47	0
3	EDO	A	514	4/4	0.91	0.25	30,32,35,36	0
3	EDO	A	502	4/4	0.93	0.17	31,35,37,37	0
3	EDO	B	503	4/4	0.93	0.21	21,28,28,28	0
3	EDO	A	507	4/4	0.93	0.16	35,39,44,48	0
3	EDO	A	516	4/4	0.94	0.13	35,36,36,38	0
3	EDO	B	504	4/4	0.94	0.14	32,33,42,45	0
3	EDO	A	504	4/4	0.95	0.20	20,21,24,25	0
3	EDO	B	507	4/4	0.95	0.15	29,34,36,37	0
3	EDO	B	502	4/4	0.97	0.13	21,22,23,24	0
2	SO4	B	501	5/5	0.99	0.04	19,19,22,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.