



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2014 – 11:04 PM EDT

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 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 <http://wwpdb.org/ValidationPDFNotes.html>

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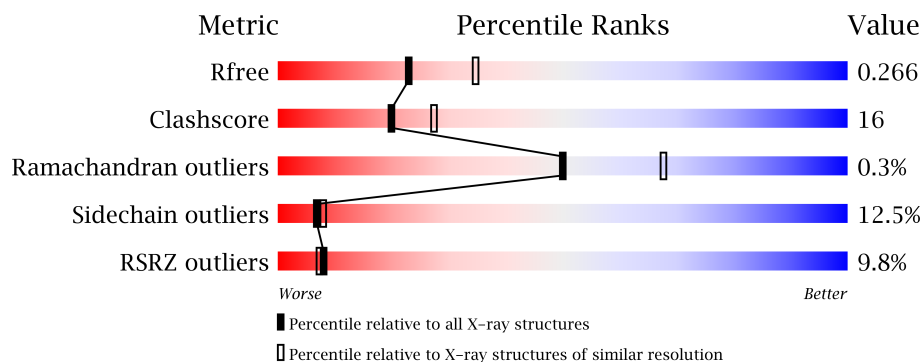
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23489  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	292	
1	B	292	
1	C	292	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	EDO	A	505	-	X
3	EDO	A	506	-	X
3	EDO	A	508	-	X
3	EDO	A	510	-	X
3	EDO	A	512	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	EDO	A	514	-	X
3	EDO	A	515	X	-
3	EDO	A	517	-	X
3	EDO	B	503	-	X
3	EDO	B	508	-	X
3	EDO	B	509	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5473 atoms, of which 0 are hydrogen and 0 are deuterium.

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:

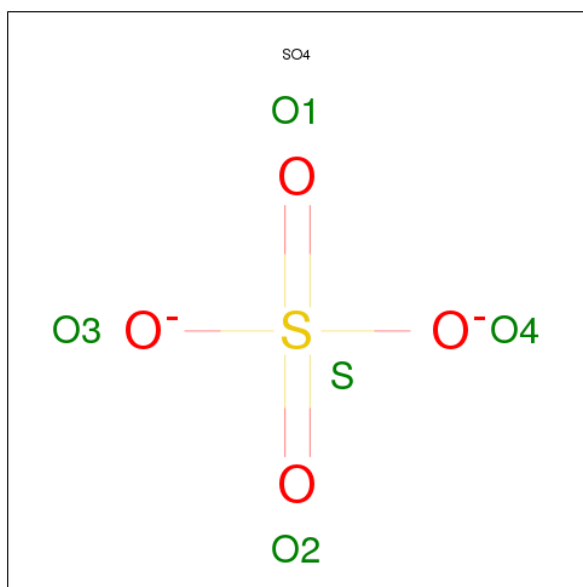
Chain	Residue	Modelled	Actual	Comment	Reference
A	147	MET	-	EXPRESSION TAG	UNP P53135
A	431	LEU	-	EXPRESSION TAG	UNP P53135
A	432	GLU	-	EXPRESSION TAG	UNP P53135
A	433	HIS	-	EXPRESSION TAG	UNP P53135
A	434	HIS	-	EXPRESSION TAG	UNP P53135
A	435	HIS	-	EXPRESSION TAG	UNP P53135
A	436	HIS	-	EXPRESSION TAG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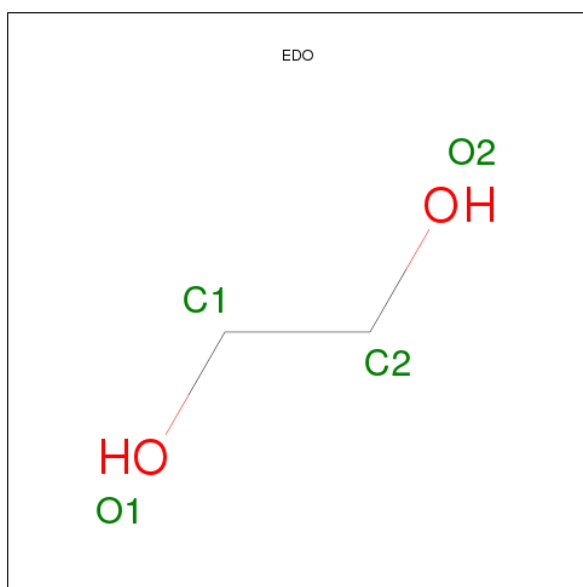
Chain	Residue	Modelled	Actual	Comment	Reference
C	435	HIS	-	EXPRESSION TAG	UNP P53135
C	436	HIS	-	EXPRESSION TAG	UNP P53135
C	437	HIS	-	EXPRESSION TAG	UNP P53135
C	438	HIS	-	EXPRESSION TAG	UNP P53135

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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 errors 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.

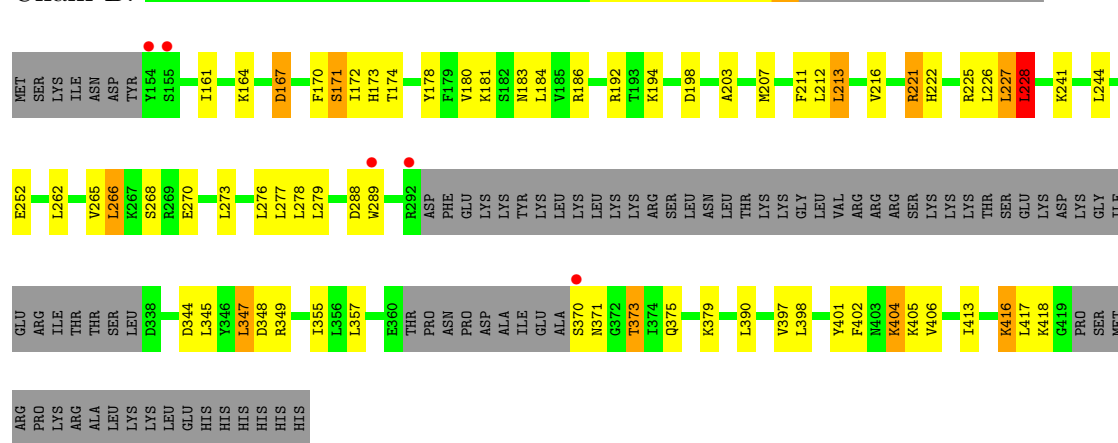
#### • Molecule 1: DNA replication regulator SLD3

Chain A:



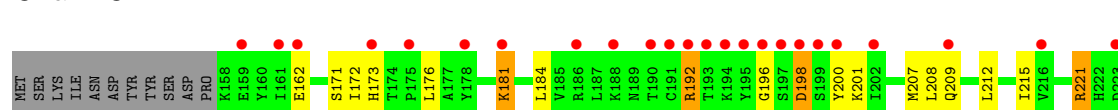
#### • Molecule 1: DNA replication regulator SLD3

Chain B:

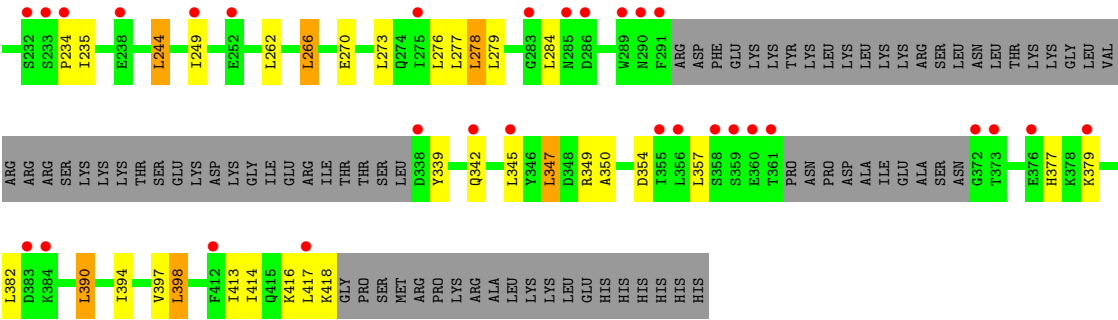


#### • Molecule 1: DNA replication regulator SLD3

Chain C:







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 88.1 (19.64-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.06 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.217 , 0.262 0.220 , 0.266	Depositor DCC
$R_{free}$ test set	1714 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.4	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 34298 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5473	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

## 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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	1
4	B	82	0	0	5	1
4	C	19	0	0	3	0
All	All	5473	0	5469	172	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (172) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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: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
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: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	Distance(Å)	Clash(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:183:ASN:ND2	3:B:503:EDO:O2	2.42	0.52
1:B:174:THR:CG2	3:B:502:EDO:H22	2.39	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:186:ARG:HD3	3:A:513:EDO:O2	2.14	0.47
1:A:187:LEU:HD11	1:A:207:MET:HE3	1.97	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
1:A:267:LYS:HZ1	3:A:508:EDO:H22	1.80	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:624:HOH:O	4:B:624:HOH:O[3_656]	1.71	0.49

## 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	209/292 (72%)	205 (98%)	4 (2%)	0	100	100
1	B	206/292 (70%)	201 (98%)	4 (2%)	1 (0%)	38	53
1	C	199/292 (68%)	192 (96%)	6 (3%)	1 (0%)	38	53
All	All	614/876 (70%)	598 (97%)	14 (2%)	2 (0%)	50	68

All (2) Ramachandran outliers are listed below:

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

### 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	201/273 (74%)	181 (90%)	20 (10%)	11	16
1	B	198/273 (72%)	169 (85%)	29 (15%)	5	5
1	C	192/273 (70%)	167 (87%)	25 (13%)	6	7
All	All	591/819 (72%)	517 (88%)	74 (12%)	7	8

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

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Mol	Chain	Res	Type
1	B	227	LEU
1	B	228	LEU
1	B	244	LEU
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

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Mol	Chain	Res	Type
1	C	379	LYS
1	C	382	LEU
1	C	397	VAL
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 chains 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	$\# Z  > 2$
2	SO4	A	501	-	4,4,4	2.18	2 (50%)	6,6,6	0.46	0
3	EDO	A	502	-	3,3,3	1.12	0	2,2,2	0.69	0
3	EDO	A	503	-	3,3,3	0.99	0	2,2,2	0.77	0
3	EDO	A	504	-	3,3,3	0.86	0	2,2,2	0.65	0
3	EDO	A	505	-	3,3,3	1.03	0	2,2,2	1.22	0
3	EDO	A	506	-	3,3,3	0.77	0	2,2,2	0.70	0
3	EDO	A	507	-	3,3,3	0.55	0	2,2,2	0.62	0
3	EDO	A	508	-	3,3,3	1.52	1 (33%)	2,2,2	0.28	0
3	EDO	A	509	-	3,3,3	0.86	0	2,2,2	0.60	0
3	EDO	A	510	-	3,3,3	0.85	0	2,2,2	0.08	0
3	EDO	A	511	-	3,3,3	0.46	0	2,2,2	0.70	0
3	EDO	A	512	-	3,3,3	0.80	0	2,2,2	0.86	0
3	EDO	A	513	-	3,3,3	0.40	0	2,2,2	1.28	0
3	EDO	A	514	-	3,3,3	0.64	0	2,2,2	0.52	0
3	EDO	A	515	-	3,3,3	2.31	2 (66%)	2,2,2	1.53	1 (50%)
3	EDO	A	516	-	3,3,3	0.38	0	2,2,2	0.32	0
3	EDO	A	517	-	3,3,3	0.76	0	2,2,2	0.49	0
2	SO4	B	501	-	4,4,4	1.44	0	6,6,6	0.84	0
3	EDO	B	502	-	3,3,3	0.73	0	2,2,2	0.02	0
3	EDO	B	503	-	3,3,3	1.30	0	2,2,2	1.50	1 (50%)
3	EDO	B	504	-	3,3,3	0.53	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	B	505	-	3,3,3	1.32	0	2,2,2	1.17	0
3	EDO	B	506	-	3,3,3	0.72	0	2,2,2	0.35	0
3	EDO	B	507	-	3,3,3	0.60	0	2,2,2	0.29	0
3	EDO	B	508	-	3,3,3	0.97	0	2,2,2	0.35	0
3	EDO	B	509	-	3,3,3	0.75	0	2,2,2	0.17	0
2	SO4	C	501	-	4,4,4	1.91	2 (50%)	6,6,6	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	501	-	-	0/0/0/0	0/0/0/0
3	EDO	A	502	-	-	0/1/1/1	0/0/0/0
3	EDO	A	503	-	-	0/1/1/1	0/0/0/0
3	EDO	A	504	-	-	0/1/1/1	0/0/0/0
3	EDO	A	505	-	-	0/1/1/1	0/0/0/0
3	EDO	A	506	-	-	0/1/1/1	0/0/0/0
3	EDO	A	507	-	-	0/1/1/1	0/0/0/0
3	EDO	A	508	-	-	0/1/1/1	0/0/0/0
3	EDO	A	509	-	-	0/1/1/1	0/0/0/0
3	EDO	A	510	-	-	0/1/1/1	0/0/0/0
3	EDO	A	511	-	-	0/1/1/1	0/0/0/0
3	EDO	A	512	-	-	0/1/1/1	0/0/0/0
3	EDO	A	513	-	-	0/1/1/1	0/0/0/0
3	EDO	A	514	-	-	0/1/1/1	0/0/0/0
3	EDO	A	515	-	-	0/1/1/1	0/0/0/0
3	EDO	A	516	-	-	0/1/1/1	0/0/0/0
3	EDO	A	517	-	-	0/1/1/1	0/0/0/0
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
3	EDO	B	502	-	-	0/1/1/1	0/0/0/0
3	EDO	B	503	-	-	0/1/1/1	0/0/0/0
3	EDO	B	504	-	-	0/1/1/1	0/0/0/0
3	EDO	B	505	-	-	0/1/1/1	0/0/0/0
3	EDO	B	506	-	-	0/1/1/1	0/0/0/0
3	EDO	B	507	-	-	0/1/1/1	0/0/0/0
3	EDO	B	508	-	-	0/1/1/1	0/0/0/0
3	EDO	B	509	-	-	0/1/1/1	0/0/0/0
2	SO4	C	501	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	515	EDO	O1-C1	3.01	1.58	1.42
2	A	501	SO4	O2-S	2.65	1.56	1.47
2	A	501	SO4	O3-S	2.44	1.56	1.47
3	A	515	EDO	C2-C1	2.31	1.63	1.47
2	C	501	SO4	O1-S	2.06	1.54	1.47
2	C	501	SO4	O3-S	2.01	1.54	1.47
3	A	508	EDO	O1-C1	2.01	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	2.14	127.56	112.35
3	B	503	EDO	O2-C2-C1	2.10	127.22	112.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	215/292 (73%)	-0.19	3 (1%) 72 71	14, 31, 59, 86	0
1	B	212/292 (72%)	-0.25	5 (2%) 56 54	13, 33, 68, 84	0
1	C	205/292 (70%)	1.15	54 (26%) 1 1	44, 75, 128, 170	0
All	All	632/876 (72%)	0.22	62 (9%) 8 7	13, 42, 104, 170	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	195	TYR	9.8
1	C	199	SER	9.1
1	C	178	TYR	6.4
1	C	193	THR	6.2
1	C	194	LYS	5.9
1	C	361	THR	5.9
1	C	289	TRP	5.9
1	C	198	ASP	5.1
1	C	232	SER	5.0
1	C	359	SER	4.7
1	C	191	CYS	4.4
1	C	196	GLY	4.2
1	C	202	ILE	4.1
1	C	355	ILE	3.9
1	C	192	ARG	3.9
1	C	216	VAL	3.9
1	C	233	SER	3.8
1	C	372	GLY	3.6
1	C	376	GLU	3.6
1	C	342	GLN	3.4
1	C	159	GLU	3.4
1	C	356	LEU	3.4
1	B	292	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	200	TYR	3.2
1	C	190	THR	3.2
1	C	197	SER	3.1
1	C	286	ASP	3.0
1	C	360	GLU	3.0
1	C	162	GLU	3.0
1	C	384	LYS	2.9
1	C	252	GLU	2.9
1	C	358	SER	2.8
1	C	173	HIS	2.8
1	C	290	ASN	2.7
1	B	370	SER	2.7
1	C	175	PRO	2.6
1	C	188	LYS	2.6
1	C	379	LYS	2.6
1	A	421	SER	2.5
1	C	345	LEU	2.5
1	B	289	TRP	2.5
1	C	417	LEU	2.4
1	C	283	GLY	2.4
1	C	373	THR	2.4
1	C	161	ILE	2.3
1	C	291	PHE	2.3
1	A	252	GLU	2.3
1	C	338	ASP	2.2
1	C	209	GLN	2.2
1	C	181	LYS	2.2
1	C	186	ARG	2.2
1	C	223	ASP	2.2
1	C	412	PHE	2.1
1	B	155	SER	2.1
1	C	275	ILE	2.1
1	A	361	THR	2.1
1	C	383	ASP	2.1
1	C	285	ASN	2.1
1	C	238	GLU	2.1
1	C	234	PRO	2.0
1	C	249	ILE	2.0
1	B	154	TYR	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	A	512	4/4	0.29	13.30	38,40,45,47	0
3	EDO	A	514	4/4	0.30	7.55	30,32,35,36	0
3	EDO	B	503	4/4	0.27	6.97	21,28,28,28	0
3	EDO	B	508	4/4	0.27	6.86	62,62,70,77	0
3	EDO	A	517	4/4	0.30	6.65	44,49,51,52	0
3	EDO	A	506	4/4	0.29	4.28	28,31,32,34	0
3	EDO	B	509	4/4	0.19	4.16	39,44,44,54	0
3	EDO	A	505	4/4	0.20	4.00	29,31,32,34	0
3	EDO	A	510	4/4	0.21	2.47	51,51,54,58	0
3	EDO	A	508	4/4	0.20	2.17	34,43,45,54	0
3	EDO	A	503	4/4	0.19	1.99	28,35,40,47	0
3	EDO	A	515	4/4	0.16	1.87	25,28,29,32	0
3	EDO	B	502	4/4	0.15	1.84	21,22,23,24	0
3	EDO	B	504	4/4	0.22	1.66	32,33,42,45	0
3	EDO	B	505	4/4	0.18	1.51	26,30,32,44	0
3	EDO	A	509	4/4	0.16	1.44	57,60,64,64	0
3	EDO	A	502	4/4	0.16	1.43	31,35,37,37	0
3	EDO	B	506	4/4	0.21	1.41	28,33,35,36	0
3	EDO	A	513	4/4	0.24	1.30	52,54,57,62	0
2	SO4	C	501	5/5	0.39	0.93	118,121,128,130	0
3	EDO	B	507	4/4	0.13	0.08	29,34,36,37	0
3	EDO	A	504	4/4	0.16	0.06	20,21,24,25	0
3	EDO	A	507	4/4	0.14	0.04	35,39,44,48	0
3	EDO	A	511	4/4	0.16	-0.10	39,46,49,54	0
2	SO4	A	501	5/5	0.18	-0.21	66,72,92,105	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	516	4/4	0.14	-0.61	35,36,36,38	0
2	SO4	B	501	5/5	0.11	-0.96	19,19,22,23	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.