



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:55 pm GMT

PDB ID : 2WFL  
Title : CRYSTAL STRUCTURE OF POLYNEURIDINE ALDEHYDE ESTERASE  
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Deposited on : 2009-04-08  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

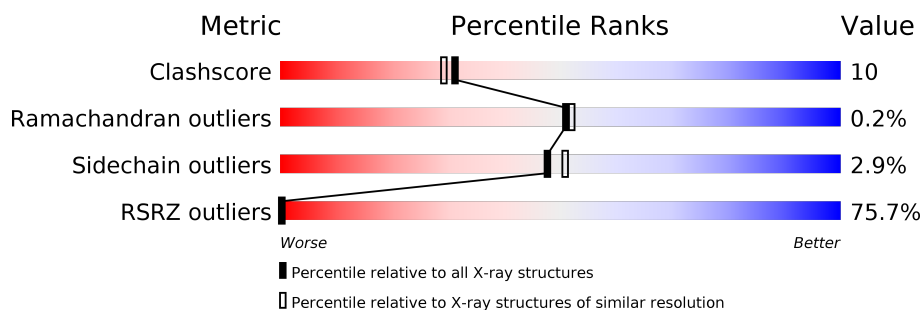
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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. 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	264	<div> <div>77%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
2	B	264	<div> <div>68%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• •</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4347 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 POLYNEURIDINE-ALDEHYDE ESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	255	2015	1292	328	372	23	0	0	0

- Molecule 2 is a protein called POLYNEURIDINE-ALDEHYDE ESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	255	2019	1294	328	373	24	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

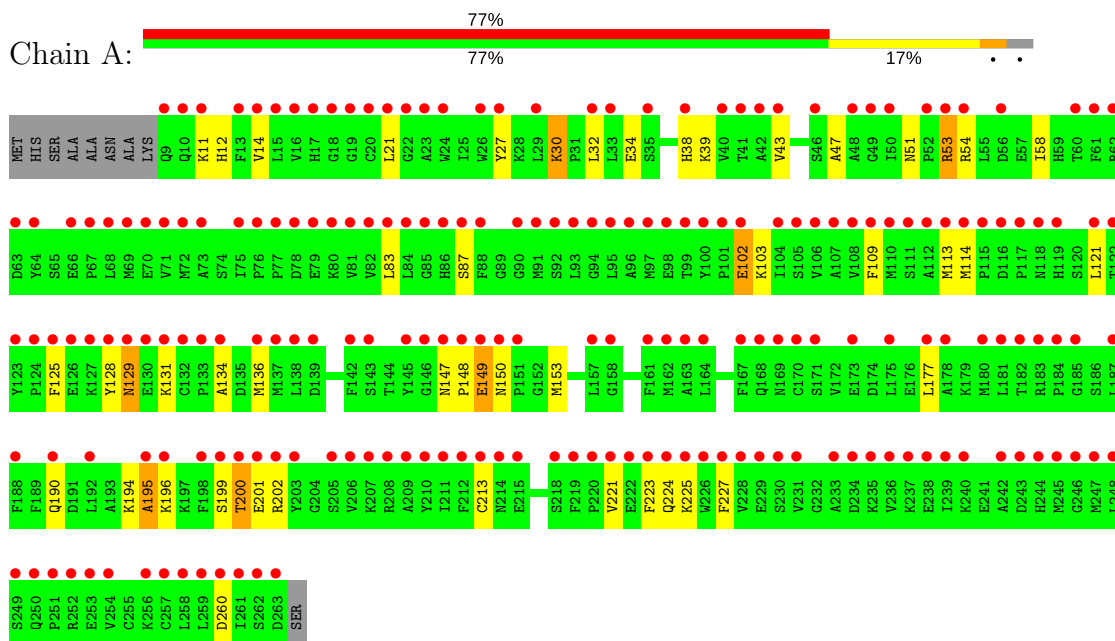
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	150	Total 150	O 150	0	0
4	B	153	Total 153	O 153	0	0

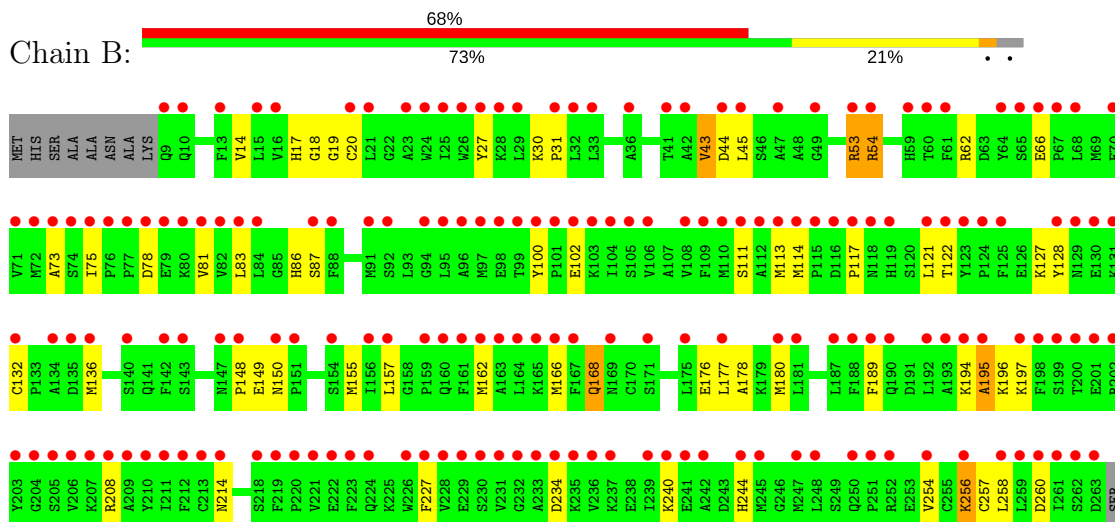
### 3 Residue-property plots

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: POLYNEURIDINE-ALDEHYDE ESTERASE



#### • Molecule 2: POLYNEURIDINE-ALDEHYDE ESTERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.76Å 176.92Å 75.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.10) 100.0 (19.83-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.98 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, $R_{free}$	0.182 , 0.231 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.75	EDS
Total number of atoms	4347	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CME, 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	0.94	7/2055 (0.3%)	0.89	5/2769 (0.2%)
2	B	0.99	5/2048 (0.2%)	0.92	7/2758 (0.3%)
All	All	0.96	12/4103 (0.3%)	0.90	12/5527 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	3
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	53	ARG	CG-CD	-8.86	1.29	1.51
1	A	43	VAL	CB-CG2	-7.92	1.36	1.52
1	A	53	ARG	CG-CD	-7.77	1.32	1.51
1	A	102	GLU	CD-OE1	-6.91	1.18	1.25
2	B	53	ARG	CD-NE	-6.80	1.34	1.46
2	B	43	VAL	CB-CG2	-6.21	1.39	1.52
1	A	30	LYS	CE-NZ	-6.10	1.33	1.49
1	A	53	ARG	CD-NE	-5.47	1.37	1.46
1	A	190	GLN	CB-CG	-5.45	1.37	1.52
2	B	102	GLU	CD-OE1	-5.41	1.19	1.25
1	A	43	VAL	CB-CG1	-5.24	1.41	1.52
2	B	43	VAL	CB-CG1	-5.12	1.42	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	53	ARG	NE-CZ-NH1	9.36	124.98	120.30
2	B	234	ASP	CB-CG-OD2	8.06	125.56	118.30
1	A	53	ARG	NE-CZ-NH1	8.06	124.33	120.30
2	B	43	VAL	CG1-CB-CG2	-7.01	99.69	110.90
1	A	102	GLU	OE1-CD-OE2	-6.07	116.01	123.30
1	A	53	ARG	NE-CZ-NH2	-5.95	117.32	120.30
2	B	102	GLU	OE1-CD-OE2	-5.92	116.19	123.30
1	A	30	LYS	CD-CE-NZ	5.82	125.08	111.70
2	B	53	ARG	CB-CG-CD	-5.59	97.08	111.60
1	A	43	VAL	CG1-CB-CG2	-5.40	102.25	110.90
2	B	166	MET	CG-SD-CE	5.39	108.83	100.20
2	B	44	ASP	CB-CG-OD1	5.12	122.90	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	ALA	Peptide
2	B	195	ALA	Peptide
2	B	256	LYS	Mainchain
2	B	257	CME	Mainchain

## 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	2015	0	1991	40	70
2	B	2019	0	1994	50	72
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	150	0	0	2	7
4	B	153	0	0	5	4
All	All	4347	0	3985	83	77

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 10.

All (83) 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)
2:B:54:ARG:NH1	4:B:2035:HOH:O	1.87	1.08
1:A:131:LYS:HD2	1:A:131:LYS:O	1.55	1.05
2:B:114:MET:CE	2:B:208:ARG:HD2	1.87	1.04
1:A:21:LEU:HD12	4:A:2060:HOH:O	1.62	0.97
2:B:114:MET:HE1	2:B:208:ARG:HD2	1.49	0.93
2:B:17:HIS:HE1	2:B:45:LEU:H	1.19	0.91
2:B:114:MET:HE1	2:B:208:ARG:CD	2.04	0.87
1:A:51:ASN:HD21	1:A:53:ARG:HG2	1.42	0.85
1:A:121:LEU:HD12	1:A:195:ALA:HB3	1.59	0.82
1:A:213:CYS:H	1:A:224:GLN:HE22	1.31	0.79
2:B:114:MET:CE	2:B:208:ARG:CD	2.63	0.77
2:B:114:MET:HE3	2:B:208:ARG:HD2	1.65	0.77
1:A:11:LYS:H	1:A:38:HIS:HD2	1.34	0.77
2:B:17:HIS:CE1	2:B:45:LEU:H	2.03	0.76
1:A:121:LEU:HD12	1:A:195:ALA:CB	2.17	0.74
1:A:11:LYS:H	1:A:38:HIS:CD2	2.06	0.73
1:A:131:LYS:CD	1:A:131:LYS:O	2.38	0.71
2:B:86:HIS:HE1	2:B:244:HIS:O	1.74	0.70
2:B:117:PRO:O	2:B:197:LYS:HD3	1.91	0.70
1:A:47:ALA:H	1:A:51:ASN:ND2	1.90	0.70
1:A:21:LEU:CD1	4:A:2060:HOH:O	2.26	0.70
1:A:47:ALA:H	1:A:51:ASN:HD22	1.42	0.68
2:B:114:MET:HE1	2:B:208:ARG:NE	2.09	0.67
2:B:177:LEU:HA	2:B:180:MET:HE2	1.80	0.62
1:A:54:ARG:O	1:A:58:ILE:HD12	2.00	0.62
2:B:196:LYS:O	4:B:2126:HOH:O	2.16	0.61
1:A:27:TYR:CB	2:B:180:MET:HE1	2.31	0.60
1:A:129:ASN:OD1	1:A:129:ASN:C	2.42	0.58
1:A:149:GLU:O	1:A:149:GLU:HG2	2.04	0.58
2:B:114:MET:HE1	2:B:208:ARG:HE	1.69	0.58
2:B:177:LEU:HA	2:B:180:MET:CE	2.33	0.58
2:B:168:GLN:H	2:B:168:GLN:HE21	1.53	0.56
1:A:109:PHE:CG	1:A:114:MET:HG2	2.42	0.55
2:B:132:CYS:HB3	2:B:136:MET:HG3	1.89	0.55
1:A:51:ASN:ND2	1:A:53:ARG:HG2	2.16	0.55
2:B:30:LYS:HB3	2:B:31:PRO:HD3	1.89	0.54
1:A:147:ASN:HD22	1:A:148:PRO:HD2	1.73	0.53
1:A:51:ASN:HD21	1:A:53:ARG:CG	2.18	0.53
1:A:14:VAL:HB	1:A:83:LEU:HD23	1.91	0.53
1:A:129:ASN:OD1	1:A:129:ASN:O	2.27	0.52
2:B:162:MET:CE	2:B:178:ALA:HB1	2.40	0.52
1:A:27:TYR:HB3	2:B:180:MET:CE	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:HIS:HE1	2:B:45:LEU:N	1.99	0.51
1:A:27:TYR:HB3	2:B:180:MET:HE3	1.93	0.51
2:B:114:MET:CE	2:B:208:ARG:NE	2.71	0.50
2:B:17:HIS:HD2	2:B:18:GLY:O	1.93	0.50
2:B:256:LYS:O	2:B:260:ASP:HB2	2.12	0.49
2:B:155:MET:HE3	2:B:157:LEU:HD23	1.94	0.49
2:B:86:HIS:CE1	2:B:244:HIS:O	2.60	0.49
1:A:30:LYS:HE2	2:B:176:GLU:CD	2.33	0.49
2:B:122:THR:HB	2:B:189:PHE:CE1	2.48	0.48
1:A:221:VAL:HG22	1:A:225:LYS:HE3	1.95	0.48
1:A:27:TYR:HB2	2:B:180:MET:HE1	1.96	0.47
2:B:113:MET:HG2	2:B:227:PHE:CZ	2.49	0.47
1:A:53:ARG:CB	1:A:58:ILE:HD11	2.45	0.47
2:B:155:MET:CE	2:B:157:LEU:HD23	2.45	0.46
2:B:54:ARG:HD2	2:B:54:ARG:HH11	1.56	0.46
1:A:30:LYS:HE3	1:A:34:GLU:OE2	2.15	0.46
2:B:19:GLY:O	2:B:20:CYS:HB2	2.15	0.46
1:A:27:TYR:CB	2:B:180:MET:CE	2.94	0.45
1:A:51:ASN:ND2	1:A:53:ARG:H	2.14	0.45
2:B:14:VAL:HB	2:B:83:LEU:HD23	1.99	0.45
2:B:66:GLU:OE1	4:B:2052:HOH:O	2.21	0.44
1:A:53:ARG:HA	1:A:53:ARG:HD2	1.80	0.44
2:B:214:ASN:HB2	2:B:240:LYS:O	2.18	0.44
1:A:103:LYS:HD2	1:A:103:LYS:HA	1.57	0.43
2:B:87:SER:HA	2:B:111:SER:O	2.19	0.43
2:B:168:GLN:H	2:B:168:GLN:NE2	2.15	0.42
2:B:127:LYS:HD2	2:B:127:LYS:HA	1.67	0.42
1:A:113:MET:HG2	1:A:227:PHE:CZ	2.55	0.42
2:B:75:ILE:HD13	2:B:81:VAL:HG13	2.01	0.42
1:A:150:ASN:HD21	1:A:194:LYS:NZ	2.17	0.42
1:A:12:HIS:CD2	1:A:39:LYS:HG2	2.55	0.42
2:B:254:VAL:O	2:B:258:LEU:HB2	2.20	0.42
1:A:11:LYS:N	1:A:38:HIS:HD2	2.10	0.42
2:B:128:TYR:O	2:B:132:CYS:HB2	2.20	0.41
1:A:177:LEU:HD13	2:B:27:TYR:CG	2.54	0.41
2:B:194:LYS:HB2	2:B:194:LYS:HE2	1.82	0.41
2:B:121:LEU:HD12	2:B:195:ALA:HB3	2.02	0.41
2:B:54:ARG:NH2	4:B:2037:HOH:O	2.52	0.41
2:B:113:MET:HE2	4:B:2075:HOH:O	2.20	0.41
1:A:128:TYR:HA	1:A:223:PHE:CE2	2.56	0.40
1:A:113:MET:CE	1:A:125:PHE:CE1	3.04	0.40

All (77) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:MET:CG	2:B:78:ASP:OD2[6_564]	0.53	1.67
1:A:153:MET:CE	2:B:78:ASP:CB[6_564]	0.55	1.65
1:A:201:GLU:OE1	2:B:150:ASN:N[3_655]	0.57	1.63
1:A:134:ALA:CB	2:B:73:ALA:O[6_564]	0.58	1.62
1:A:201:GLU:CD	2:B:149:GLU:C[3_655]	0.66	1.54
1:A:200:THR:OG1	4:B:2091:HOH:O[3_655]	0.75	1.45
1:A:153:MET:SD	2:B:78:ASP:CG[6_564]	0.85	1.35
1:A:201:GLU:CB	2:B:149:GLU:CB[3_655]	0.87	1.33
1:A:202:ARG:CD	2:B:148:PRO:CB[3_655]	0.90	1.30
1:A:201:GLU:OE1	2:B:149:GLU:C[3_655]	0.91	1.29
1:A:200:THR:C	2:B:149:GLU:OE2[3_655]	0.94	1.26
1:A:153:MET:SD	2:B:78:ASP:OD1[6_564]	0.94	1.26
1:A:201:GLU:CB	2:B:149:GLU:CA[3_655]	1.05	1.15
1:A:202:ARG:CD	2:B:148:PRO:CG[3_655]	1.05	1.15
1:A:200:THR:CA	2:B:149:GLU:OE2[3_655]	1.10	1.10
1:A:202:ARG:CG	2:B:148:PRO:CB[3_655]	1.21	0.99
1:A:153:MET:CE	2:B:78:ASP:CG[6_564]	1.22	0.98
1:A:201:GLU:CD	2:B:149:GLU:O[3_655]	1.25	0.95
1:A:201:GLU:CG	2:B:149:GLU:CA[3_655]	1.30	0.90
1:A:201:GLU:N	2:B:149:GLU:CD[3_655]	1.32	0.88
1:A:201:GLU:N	2:B:149:GLU:OE2[3_655]	1.32	0.88
1:A:199:SER:C	2:B:149:GLU:OE1[3_655]	1.41	0.79
1:A:201:GLU:N	2:B:149:GLU:CG[3_655]	1.42	0.78
1:A:201:GLU:CD	2:B:150:ASN:N[3_655]	1.44	0.76
1:A:202:ARG:CG	2:B:148:PRO:CG[3_655]	1.45	0.75
1:A:202:ARG:NE	2:B:148:PRO:CB[3_655]	1.45	0.75
1:A:153:MET:SD	2:B:78:ASP:OD2[6_564]	1.49	0.71
1:A:202:ARG:CD	2:B:148:PRO:CD[3_655]	1.49	0.71
1:A:201:GLU:CG	2:B:149:GLU:C[3_655]	1.52	0.68
1:A:201:GLU:CA	2:B:149:GLU:CG[3_655]	1.53	0.67
1:A:200:THR:N	2:B:149:GLU:OE1[3_655]	1.56	0.64
1:A:200:THR:N	2:B:149:GLU:OE2[3_655]	1.56	0.64
1:A:202:ARG:CD	2:B:148:PRO:CA[3_655]	1.58	0.62
1:A:201:GLU:CG	2:B:149:GLU:O[3_655]	1.67	0.53
1:A:153:MET:CB	2:B:78:ASP:OD2[6_564]	1.68	0.52
1:A:200:THR:N	2:B:149:GLU:CD[3_655]	1.69	0.51
1:A:153:MET:CG	2:B:78:ASP:CG[6_564]	1.72	0.48
1:A:199:SER:CA	2:B:149:GLU:OE1[3_655]	1.73	0.47
1:A:134:ALA:CB	2:B:73:ALA:C[6_564]	1.74	0.46
1:A:202:ARG:CD	2:B:148:PRO:N[3_655]	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:SER:CB	2:B:149:GLU:OE1[3_655]	1.76	0.44
2:B:148:PRO:O	4:A:2131:HOH:O[3_655]	1.76	0.44
1:A:200:THR:CB	4:B:2091:HOH:O[3_655]	1.77	0.43
1:A:202:ARG:CB	2:B:148:PRO:CG[3_655]	1.79	0.41
1:A:201:GLU:CA	2:B:149:GLU:CB[3_655]	1.83	0.37
1:A:201:GLU:CD	2:B:149:GLU:CA[3_655]	1.83	0.37
2:B:100:TYR:OH	4:A:2076:HOH:O[6_565]	1.84	0.36
1:A:153:MET:CE	2:B:78:ASP:CA[6_564]	1.84	0.36
1:A:202:ARG:CG	2:B:148:PRO:CA[3_655]	1.84	0.36
1:A:202:ARG:NE	2:B:148:PRO:CG[3_655]	1.85	0.35
1:A:201:GLU:CB	2:B:149:GLU:CG[3_655]	1.86	0.34
1:A:201:GLU:OE2	2:B:149:GLU:C[3_655]	1.88	0.32
2:B:148:PRO:CA	4:A:2131:HOH:O[3_655]	1.88	0.32
1:A:201:GLU:OE2	2:B:149:GLU:O[3_655]	1.88	0.32
1:A:200:THR:C	2:B:149:GLU:CD[3_655]	1.89	0.31
2:B:148:PRO:C	4:A:2131:HOH:O[3_655]	1.89	0.31
1:A:201:GLU:OE1	2:B:149:GLU:O[3_655]	1.90	0.30
1:A:201:GLU:OE1	2:B:150:ASN:CA[3_655]	1.91	0.29
1:A:199:SER:C	2:B:149:GLU:CD[3_655]	1.92	0.28
1:A:134:ALA:CA	2:B:73:ALA:O[6_564]	1.95	0.25
1:A:202:ARG:N	2:B:149:GLU:CG[3_655]	1.96	0.24
1:A:201:GLU:OE1	2:B:149:GLU:CA[3_655]	1.97	0.23
1:A:201:GLU:C	2:B:149:GLU:CG[3_655]	2.01	0.19
1:A:153:MET:CE	2:B:78:ASP:OD1[6_564]	2.01	0.19
1:A:200:THR:C	4:B:2094:HOH:O[3_655]	2.04	0.16
2:B:73:ALA:CA	4:A:2036:HOH:O[6_565]	2.05	0.15
2:B:100:TYR:OH	4:A:2036:HOH:O[6_565]	2.06	0.14
1:A:201:GLU:CB	2:B:149:GLU:C[3_655]	2.08	0.12
1:A:201:GLU:OE2	2:B:150:ASN:N[3_655]	2.09	0.11
1:A:148:PRO:CD	1:A:148:PRO:CD[3_655]	2.10	0.10
1:A:202:ARG:CZ	2:B:148:PRO:CB[3_655]	2.12	0.08
1:A:202:ARG:CG	2:B:148:PRO:C[3_655]	2.12	0.08
1:A:200:THR:O	4:B:2094:HOH:O[3_655]	2.14	0.06
1:A:200:THR:O	2:B:149:GLU:OE2[3_655]	2.14	0.06
1:A:201:GLU:N	2:B:149:GLU:CB[3_655]	2.15	0.05
2:B:100:TYR:CZ	4:A:2036:HOH:O[6_565]	2.16	0.04
1:A:200:THR:CA	2:B:149:GLU:CD[3_655]	2.16	0.04

## 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	252/264 (96%)	242 (96%)	9 (4%)	1 (0%)	38	35
2	B	251/264 (95%)	242 (96%)	9 (4%)	0	100	100
All	All	503/528 (95%)	484 (96%)	18 (4%)	1 (0%)	51	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	LYS

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	221/227 (97%)	213 (96%)	8 (4%)	40	41
2	B	220/226 (97%)	215 (98%)	5 (2%)	56	60
All	All	441/453 (97%)	428 (97%)	13 (3%)	48	51

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	87	SER
1	A	102	GLU
1	A	129	ASN
1	A	136	MET

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Mol	Chain	Res	Type
1	A	149	GLU
1	A	200	THR
1	A	260	ASP
2	B	43	VAL
2	B	53	ARG
2	B	54	ARG
2	B	62	ARG
2	B	168	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	51	ASN
1	A	118	ASN
1	A	147	ASN
1	A	150	ASN
1	A	224	GLN
1	A	250	GLN
2	B	17	HIS
2	B	59	HIS
2	B	86	HIS
2	B	168	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues 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
1	CME	A	255	1	9,9,10	1.19	1 (11%)	6,9,11	1.43	0
2	CME	B	255	2	9,9,10	1.29	1 (11%)	6,9,11	1.97	2 (33%)
2	CME	B	257	2	9,9,10	0.41	0	6,9,11	1.78	3 (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
1	CME	A	255	1	-	0/5/8/10	0/0/0/0
2	CME	B	255	2	-	0/5/8/10	0/0/0/0
2	CME	B	257	2	-	0/5/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	CME	CA-C	3.20	1.54	1.50
2	B	255	CME	CA-C	3.64	1.55	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	255	CME	O-C-CA	-2.92	116.95	125.02
2	B	257	CME	O-C-CA	-2.11	119.20	125.02
2	B	257	CME	CB-SG-SD	2.25	108.22	103.83
2	B	257	CME	CE-SD-SG	2.93	118.15	103.40
2	B	255	CME	CB-SG-SD	3.40	110.44	103.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 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	SO4	A	1264	-	4,4,4	0.33	0	6,6,6	0.59	0
3	SO4	B	1264	-	4,4,4	0.83	0	6,6,6	1.33	1 (16%)

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	SO4	A	1264	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1264	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	B	1264	SO4	O4-S-O3	2.88	121.94	108.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	254/264 (96%)	3.21	204 (80%)  	27, 38, 48, 64	0
2	B	253/264 (95%)	3.08	180 (71%)  	24, 38, 48, 66	0
All	All	507/528 (96%)	3.14	384 (75%)  	24, 38, 48, 66	0

All (384) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	SER	10.3
1	A	263	ASP	9.8
1	A	78	ASP	8.6
2	B	74	SER	8.3
2	B	123	TYR	8.2
2	B	210	TYR	8.2
2	B	88	PHE	7.4
2	B	219	PHE	7.4
1	A	235	LYS	7.3
1	A	77	PRO	7.3
1	A	221	VAL	7.2
2	B	218	SER	7.0
1	A	76	PRO	7.0
1	A	258	LEU	7.0
2	B	206	VAL	7.0
1	A	203	TYR	6.9
2	B	254	VAL	6.8
2	B	54	ARG	6.7
1	A	227	PHE	6.6
2	B	117	PRO	6.6
2	B	227	PHE	6.5
2	B	229	GLU	6.3
1	A	178	ALA	6.3
2	B	201	GLU	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	198	PHE	6.2
1	A	234	ASP	6.0
1	A	131	LYS	6.0
2	B	258	LEU	6.0
2	B	27	TYR	5.9
2	B	129	ASN	5.9
1	A	79	GLU	5.8
1	A	13	PHE	5.8
1	A	210	TYR	5.8
2	B	226	TRP	5.8
1	A	223	PHE	5.7
1	A	187	LEU	5.7
2	B	198	PHE	5.6
1	A	213	CYS	5.6
2	B	148	PRO	5.6
1	A	199	SER	5.5
1	A	261	ILE	5.4
1	A	132	CYS	5.4
1	A	254	VAL	5.4
1	A	226	TRP	5.4
2	B	163	ALA	5.4
1	A	96	ALA	5.4
2	B	36	ALA	5.4
1	A	206	VAL	5.3
2	B	143	SER	5.3
2	B	211	ILE	5.3
2	B	25	ILE	5.2
1	A	211	ILE	5.2
1	A	240	LYS	5.2
1	A	184	PRO	5.1
2	B	187	LEU	5.1
2	B	81	VAL	5.1
2	B	200	THR	5.0
2	B	109	PHE	5.0
2	B	248	LEU	5.0
1	A	40	VAL	4.9
1	A	128	TYR	4.9
2	B	128	TYR	4.9
1	A	149	GLU	4.9
1	A	75	ILE	4.8
2	B	204	GLY	4.8
2	B	221	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	115	PRO	4.8
1	A	150	ASN	4.8
1	A	242	ALA	4.8
2	B	209	ALA	4.8
1	A	38	HIS	4.7
2	B	228	VAL	4.7
1	A	113	MET	4.7
2	B	252	ARG	4.7
1	A	177	LEU	4.6
2	B	9	GLN	4.6
2	B	24	TRP	4.6
2	B	114	MET	4.6
2	B	164	LEU	4.6
1	A	133	PRO	4.6
2	B	94	GLY	4.6
2	B	177	LEU	4.6
1	A	256	LYS	4.6
1	A	26	TRP	4.6
1	A	84	LEU	4.6
1	A	66	GLU	4.5
1	A	126	GLU	4.5
2	B	208	ARG	4.5
2	B	82	VAL	4.5
1	A	219	PHE	4.5
2	B	259	LEU	4.5
1	A	97	MET	4.5
2	B	199	SER	4.5
1	A	233	ALA	4.5
2	B	131	LYS	4.5
2	B	29	LEU	4.5
2	B	106	VAL	4.5
2	B	220	PRO	4.5
1	A	108	VAL	4.4
2	B	103	LYS	4.4
2	B	235	LYS	4.4
1	A	212	PHE	4.4
1	A	104	ILE	4.4
1	A	130	GLU	4.4
2	B	116	ASP	4.4
2	B	122	THR	4.4
1	A	237	LYS	4.4
2	B	80	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	95	LEU	4.4
2	B	132	CYS	4.4
1	A	52	PRO	4.4
1	A	95	LEU	4.4
2	B	83	LEU	4.3
1	A	147	ASN	4.3
1	A	105	SER	4.3
2	B	102	GLU	4.3
2	B	108	VAL	4.3
2	B	101	PRO	4.3
1	A	209	ALA	4.3
1	A	200	THR	4.2
1	A	201	GLU	4.2
1	A	14	VAL	4.2
1	A	72	MET	4.2
2	B	234	ASP	4.2
2	B	41	THR	4.1
2	B	72	MET	4.1
2	B	135	ASP	4.1
1	A	167	PHE	4.1
2	B	263	ASP	4.1
2	B	16	VAL	4.1
1	A	122	THR	4.1
2	B	250	GLN	4.0
1	A	123	TYR	4.0
1	A	68	LEU	4.0
2	B	64	TYR	4.0
1	A	83	LEU	4.0
2	B	188	PHE	4.0
1	A	157	LEU	4.0
2	B	192	LEU	4.0
1	A	107	ALA	4.0
2	B	130	GLU	4.0
1	A	35	SER	3.9
1	A	29	LEU	3.9
2	B	203	TYR	3.9
2	B	262	SER	3.9
1	A	49	GLY	3.9
2	B	26	TRP	3.9
2	B	33	LEU	3.9
1	A	129	ASN	3.8
1	A	94	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	124	PRO	3.8
1	A	192	LEU	3.8
1	A	117	PRO	3.8
2	B	92	SER	3.8
1	A	90	GLY	3.8
2	B	75	ILE	3.8
2	B	194	LYS	3.8
2	B	256	LYS	3.8
2	B	113	MET	3.8
2	B	166	MET	3.8
1	A	181	LEU	3.8
1	A	32	LEU	3.7
2	B	125	PHE	3.7
2	B	193	ALA	3.7
1	A	17	HIS	3.7
1	A	142	PHE	3.7
1	A	100	TYR	3.7
1	A	145	TYR	3.6
1	A	115	PRO	3.6
1	A	71	VAL	3.6
2	B	68	LEU	3.6
1	A	161	PHE	3.5
1	A	10	GLN	3.5
1	A	24	TRP	3.5
1	A	88	PHE	3.5
2	B	65	SER	3.5
1	A	259	LEU	3.5
1	A	252	ARG	3.5
1	A	195	ALA	3.5
2	B	240	LYS	3.5
2	B	214	ASN	3.5
2	B	134	ALA	3.5
2	B	60	THR	3.4
1	A	81	VAL	3.4
2	B	10	GLN	3.4
1	A	16	VAL	3.4
1	A	27	TYR	3.4
1	A	43	VAL	3.4
1	A	246	GLY	3.4
1	A	9	GLN	3.4
2	B	236	VAL	3.4
2	B	61	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	223	PHE	3.3
1	A	248	LEU	3.3
1	A	20	CYS	3.3
2	B	237	LYS	3.3
1	A	238	GLU	3.3
2	B	175	LEU	3.3
2	B	189	PHE	3.3
2	B	77	PRO	3.3
2	B	118	ASN	3.3
1	A	136	MET	3.2
1	A	93	LEU	3.2
2	B	119	HIS	3.2
1	A	207	LYS	3.2
2	B	247	MET	3.2
2	B	13	PHE	3.2
2	B	232	GLY	3.2
1	A	112	ALA	3.2
2	B	244	HIS	3.2
2	B	154	SER	3.2
2	B	156	ILE	3.2
2	B	224	GLN	3.2
2	B	142	PHE	3.2
2	B	167	PHE	3.2
2	B	213	CYS	3.2
1	A	11	LYS	3.2
2	B	66	GLU	3.2
1	A	109	PHE	3.1
2	B	157	LEU	3.1
2	B	161	PHE	3.1
1	A	239	ILE	3.1
2	B	71	VAL	3.1
2	B	231	VAL	3.1
1	A	87	SER	3.1
1	A	86	HIS	3.1
1	A	127	LYS	3.1
2	B	151	PRO	3.1
2	B	70	GLU	3.1
2	B	251	PRO	3.1
1	A	196	LYS	3.1
2	B	242	ALA	3.1
1	A	15	LEU	3.1
2	B	190	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	116	ASP	3.1
2	B	261	ILE	3.1
2	B	159	PRO	3.0
2	B	53	ARG	3.0
1	A	121	LEU	3.0
1	A	42	ALA	3.0
2	B	105	SER	3.0
1	A	170	CYS	3.0
1	A	162	MET	3.0
1	A	18	GLY	3.0
1	A	151	PRO	2.9
2	B	47	ALA	2.9
2	B	104	ILE	2.9
1	A	70	GLU	2.9
1	A	228	VAL	2.9
2	B	150	ASN	2.9
2	B	73	ALA	2.9
2	B	121	LEU	2.9
2	B	222	GLU	2.9
1	A	218	SER	2.9
1	A	243	ASP	2.9
2	B	205	SER	2.9
1	A	183	ARG	2.8
2	B	180	MET	2.8
2	B	245	MET	2.8
1	A	67	PRO	2.8
1	A	73	ALA	2.8
1	A	202	ARG	2.8
1	A	85	GLY	2.8
1	A	146	GLY	2.8
2	B	49	GLY	2.8
1	A	98	GLU	2.8
2	B	91	MET	2.8
1	A	251	PRO	2.8
1	A	118	ASN	2.8
2	B	197	LYS	2.7
1	A	260	ASP	2.7
1	A	119	HIS	2.7
1	A	190	GLN	2.7
1	A	231	VAL	2.7
2	B	97	MET	2.7
1	A	205	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	230	SER	2.7
1	A	101	PRO	2.7
1	A	236	VAL	2.7
2	B	162	MET	2.7
1	A	114	MET	2.7
1	A	148	PRO	2.7
1	A	106	VAL	2.6
1	A	244	HIS	2.6
1	A	48	ALA	2.6
1	A	134	ALA	2.6
2	B	99	THR	2.6
1	A	22	GLY	2.6
2	B	202	ARG	2.6
1	A	41	THR	2.6
1	A	137	MET	2.6
2	B	181	LEU	2.6
1	A	225	LYS	2.6
1	A	139	ASP	2.6
1	A	69	MET	2.6
1	A	138	LEU	2.6
1	A	220	PRO	2.6
2	B	241	GLU	2.6
2	B	233	ALA	2.6
1	A	110	MET	2.6
1	A	125	PHE	2.6
1	A	54	ARG	2.5
2	B	112	ALA	2.5
2	B	212	PHE	2.5
2	B	15	LEU	2.5
1	A	249	SER	2.5
2	B	100	TYR	2.5
2	B	136	MET	2.5
1	A	50	ILE	2.5
1	A	124	PRO	2.5
2	B	84	LEU	2.5
2	B	110	MET	2.5
2	B	28	LYS	2.5
1	A	21	LEU	2.5
1	A	99	THR	2.5
1	A	102	GLU	2.5
1	A	169	ASN	2.5
2	B	79	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	230	SER	2.5
2	B	239	ILE	2.5
2	B	21	LEU	2.4
1	A	208	ARG	2.4
1	A	214	ASN	2.4
2	B	67	PRO	2.4
1	A	173	GLU	2.4
2	B	42	ALA	2.4
1	A	56	ASP	2.4
2	B	165	LYS	2.4
2	B	32	LEU	2.4
2	B	260	ASP	2.4
1	A	60	THR	2.4
1	A	253	GLU	2.4
2	B	207	LYS	2.4
2	B	147	ASN	2.4
1	A	163	ALA	2.4
1	A	80	LYS	2.4
2	B	45	LEU	2.3
1	A	82	VAL	2.3
1	A	182	THR	2.3
1	A	64	TYR	2.3
1	A	188	PHE	2.3
2	B	44	ASP	2.3
2	B	195	ALA	2.3
2	B	98	GLU	2.3
1	A	247	MET	2.3
2	B	31	PRO	2.3
2	B	111	SER	2.3
1	A	91	MET	2.2
2	B	169	ASN	2.2
1	A	62	ARG	2.2
1	A	92	SER	2.2
2	B	59	HIS	2.2
1	A	46	SER	2.2
1	A	222	GLU	2.2
1	A	158	GLY	2.2
1	A	185	GLY	2.2
1	A	257	CYS	2.2
1	A	61	PHE	2.2
1	A	250	GLN	2.2
1	A	215	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	143	SER	2.2
1	A	224	GLN	2.1
1	A	33	LEU	2.1
1	A	164	LEU	2.1
1	A	180	MET	2.1
1	A	175	LEU	2.1
1	A	229	GLU	2.1
2	B	76	PRO	2.1
2	B	140	SER	2.1
2	B	96	ALA	2.1
1	A	63	ASP	2.1
2	B	78	ASP	2.1
1	A	168	GLN	2.1
1	A	19	GLY	2.1
2	B	87	SER	2.1
1	A	245	MET	2.1
1	A	23	ALA	2.1
2	B	160	GLN	2.1
1	A	171	SER	2.1
1	A	53	ARG	2.1
1	A	111	SER	2.0
2	B	23	ALA	2.0
2	B	171	SER	2.0
2	B	20	CYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CME	A	255	10/11	0.42	0.38	-	35,35,47,49	0
2	CME	B	255	10/11	0.80	0.25	-	35,35,46,47	4
2	CME	B	257	10/11	0.41	0.37	-	34,37,52,53	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	1264	5/5	0.78	0.32	1.39	26,37,46,47	5
3	SO4	B	1264	5/5	0.90	0.19	-0.79	36,37,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.