



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 07:39 pm BST

PDB ID : 3CA8  
Title : Crystal structure of Escherichia coli YdcF, an S-adenosyl-L-methionine utilizing enzyme  
Authors : Lim, K.; Chao, K.; Lehmann, C.; Herzberg, O.; Structure 2 Function Project (S2F)  
Deposited on : 2008-02-19  
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

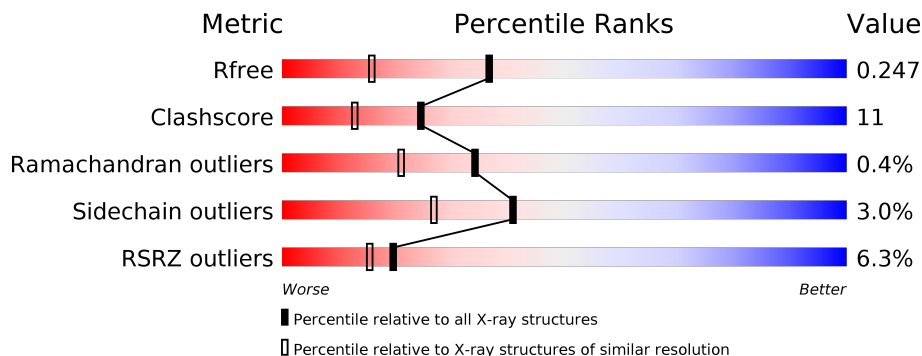
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	266	
1	B	266	

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	MPD	B	911	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5031 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 Protein ydcF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	261	Total 2092	C 1324	N 372	O 385	S 11	0	5	0
1	B	259	Total 2064	C 1306	N 365	O 382	S 11	0	4	0

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



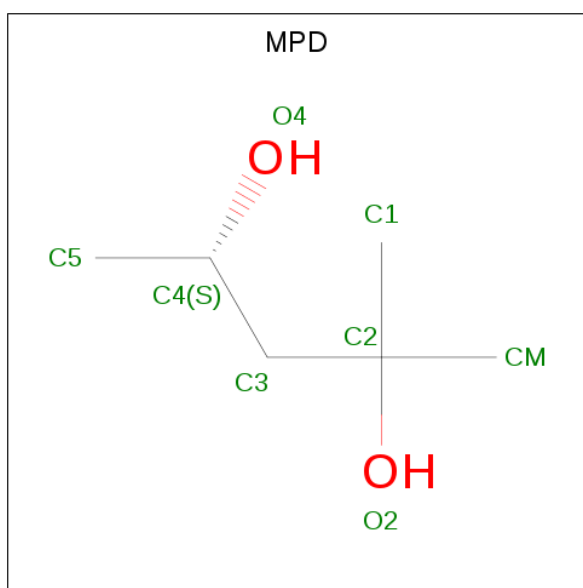
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0

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

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0

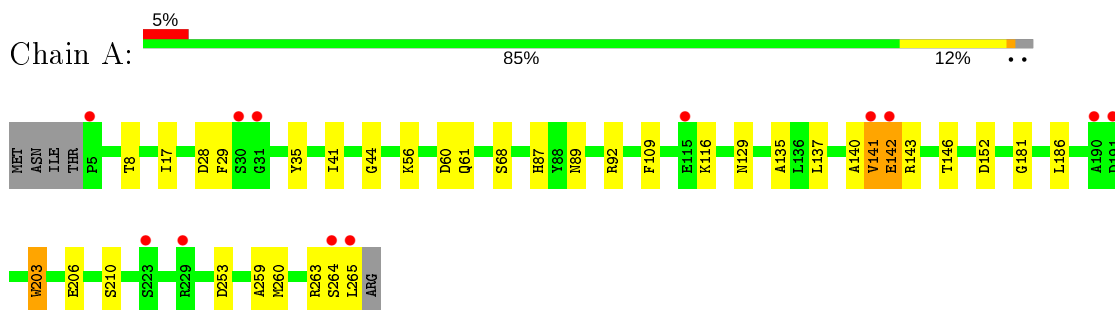
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	375	Total O 375 375	0	0
4	B	348	Total O 348 348	0	0

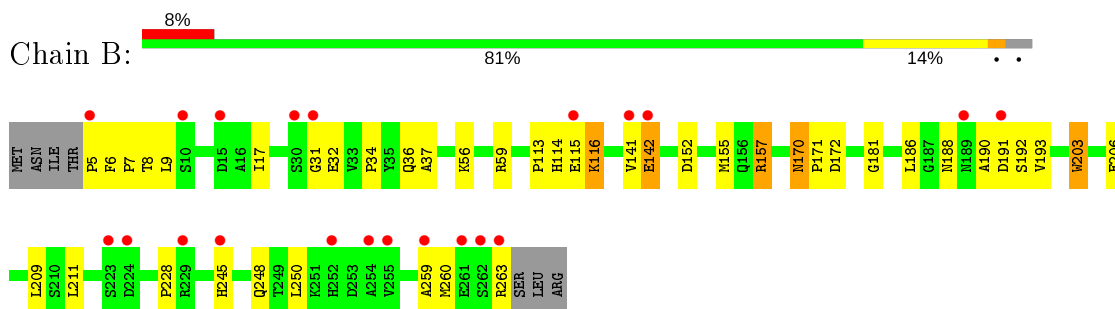
### 3 Residue-property plots [i](#)

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

- Molecule 1: Protein ydcF



- Molecule 1: Protein ydcF



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.80Å 39.71Å 122.64Å 90.00° 96.34° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 42.01 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-1.80) 93.1 (42.01-1.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.21 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.195 , 0.238 0.205 , 0.247	Depositor DCC
$R_{free}$ test set	4161 reflections (7.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.2	Xtrriage
Anisotropy	0.611	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 78.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, 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	0.85	0/2146	0.84	2/2928 (0.1%)
1	B	0.75	0/2118	0.77	2/2892 (0.1%)
All	All	0.80	0/4264	0.81	4/5820 (0.1%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	157	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	B	157	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	A	92	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	A	152	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	ALA	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	2092	0	2039	33	0
1	B	2064	0	2003	53	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
3	A	56	0	98	8	0
3	B	56	0	98	11	0
4	A	375	0	0	14	0
4	B	348	0	0	19	0
All	All	5031	0	4238	93	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 11.

All (93) 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:B:211:LEU:HD13	4:B:1601:HOH:O	1.62	0.98
1:B:209:LEU:HD13	1:B:260[B]:MET:CE	1.94	0.96
1:A:260[B]:MET:CE	1:A:265:LEU:HD22	1.95	0.95
1:A:181:GLY:O	3:A:901:MPD:H13	1.65	0.95
1:A:260[A]:MET:O	1:A:265:LEU:HD21	1.67	0.94
1:A:259:ALA:O	1:A:263:ARG:HD2	1.69	0.92
1:A:260[B]:MET:HE1	1:A:265:LEU:HD22	1.49	0.92
1:B:209:LEU:HD13	1:B:260[B]:MET:HE3	1.50	0.90
1:B:209:LEU:CD1	1:B:260[B]:MET:CE	2.53	0.86
1:A:260[B]:MET:O	1:A:265:LEU:HD21	1.77	0.83
1:B:181:GLY:O	3:B:904:MPD:H13	1.76	0.83
3:A:901:MPD:H11	4:A:1017:HOH:O	1.80	0.81
1:B:209:LEU:HD12	1:B:260[B]:MET:HE1	1.66	0.76
1:B:209:LEU:CD1	1:B:260[B]:MET:HE1	2.16	0.76
3:B:904:MPD:H11	4:B:1053:HOH:O	1.85	0.75
1:A:260[B]:MET:HE3	1:A:265:LEU:HD22	1.71	0.72
1:B:37:ALA:HA	3:B:911:MPD:H53	1.74	0.69
1:B:8:THR:HA	4:B:1101:HOH:O	1.93	0.68
1:B:155:MET:HE2	4:B:1601:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:LEU:CD1	1:B:260[B]:MET:HE3	2.20	0.67
1:B:188:ASN:ND2	4:B:1101:HOH:O	2.21	0.66
1:A:56[A]:LYS:NZ	1:A:60:ASP:OD2	2.27	0.66
1:B:141:VAL:HG23	1:B:142:GLU:H	1.60	0.66
1:B:37:ALA:CA	3:B:911:MPD:H53	2.27	0.65
1:B:259:ALA:O	1:B:263:ARG:HD2	1.96	0.64
1:B:203:TRP:HA	3:B:905:MPD:H4	1.79	0.64
1:B:206:GLU:OE1	1:B:263:ARG:NH1	2.33	0.62
1:A:203:TRP:HA	3:A:902:MPD:H4	1.82	0.62
1:A:141:VAL:HG23	1:A:142:GLU:H	1.65	0.61
1:A:29:PHE:HA	4:A:1068:HOH:O	2.02	0.60
1:A:68:SER:O	4:A:1533:HOH:O	2.16	0.60
1:A:87:HIS:CD2	3:A:908:MPD:HM3	2.37	0.59
3:B:911:MPD:H51	4:B:1178:HOH:O	2.02	0.59
1:A:206:GLU:CD	1:A:206:GLU:H	2.05	0.59
3:B:911:MPD:HM1	4:B:1333:HOH:O	2.01	0.58
1:A:265:LEU:HD13	4:A:1551:HOH:O	2.04	0.58
1:A:129:ASN:ND2	4:A:1041:HOH:O	2.36	0.57
1:A:44:GLY:N	4:A:1533:HOH:O	2.23	0.57
1:A:141:VAL:HA	4:A:1649:HOH:O	2.06	0.56
1:A:17:ILE:HG21	1:A:186:LEU:HD12	1.87	0.56
1:B:193:VAL:HG22	4:B:1101:HOH:O	2.06	0.54
1:A:8:THR:HG22	4:A:1263:HOH:O	2.07	0.54
1:B:170:ASN:ND2	1:B:172:ASP:H	2.06	0.53
1:A:8:THR:HG23	4:A:1586:HOH:O	2.08	0.53
1:B:116:LYS:HB3	4:B:1290:HOH:O	2.08	0.53
1:A:259:ALA:O	1:A:263:ARG:CD	2.50	0.53
1:B:193:VAL:CG2	4:B:1101:HOH:O	2.57	0.52
1:B:115:GLU:CG	1:B:116:LYS:HD2	2.40	0.51
1:B:6:PHE:CZ	1:B:260[B]:MET:HE2	2.45	0.51
1:B:113:PRO:HB2	1:B:116:LYS:HD3	1.94	0.49
1:B:228:PRO:HG3	4:B:1345:HOH:O	2.13	0.49
1:B:141:VAL:HG23	1:B:142:GLU:N	2.26	0.48
1:B:56:LYS:NZ	1:B:59:ARG:NH2	2.61	0.47
1:A:109:PHE:HD2	3:A:908:MPD:H11	1.79	0.47
1:B:8:THR:HG22	4:B:1560:HOH:O	2.14	0.47
1:B:170:ASN:HD22	1:B:171:PRO:HD2	1.80	0.47
1:B:34:PRO:HB3	3:B:910:MPD:H12	1.97	0.47
1:B:17:ILE:HG21	1:B:186:LEU:HD12	1.96	0.47
1:A:146:THR:HG22	4:A:1036:HOH:O	2.15	0.46
1:B:37:ALA:HA	3:B:911:MPD:C5	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:910:MPD:H12	4:B:1545:HOH:O	2.15	0.46
1:B:250:LEU:HD12	4:B:1567:HOH:O	2.14	0.46
1:B:115:GLU:HG2	1:B:116:LYS:HD2	1.97	0.46
1:B:6:PHE:HZ	1:B:260[B]:MET:HE2	1.81	0.46
1:B:7:PRO:O	1:B:193:VAL:HG23	2.15	0.45
1:A:135:ALA:HB3	3:A:912:MPD:H13	1.98	0.45
1:B:152:ASP:CG	4:B:1601:HOH:O	2.54	0.45
1:A:35:TYR:N	4:A:1162:HOH:O	2.50	0.44
1:A:35:TYR:O	1:A:61:GLN:NE2	2.49	0.44
1:B:5:PRO:HB2	1:B:192:SER:HB3	1.99	0.44
1:B:9:LEU:H	1:B:188:ASN:HD21	1.64	0.44
1:A:87:HIS:CG	3:A:908:MPD:HM3	2.52	0.44
1:B:114:HIS:HD2	4:B:1221:HOH:O	2.00	0.44
1:B:170:ASN:HD22	1:B:171:PRO:CD	2.32	0.43
1:B:36:GLN:HG3	4:B:1545:HOH:O	2.19	0.43
3:B:904:MPD:H4	3:B:904:MPD:H12	1.82	0.43
1:B:245:HIS:CE1	4:B:1188:HOH:O	2.71	0.43
1:B:56:LYS:HZ3	1:B:59:ARG:NH2	2.16	0.43
1:B:206:GLU:HG2	1:B:263:ARG:HD3	2.01	0.42
1:A:210:SER:HB2	1:A:265:LEU:HB3	2.01	0.42
1:B:115:GLU:HG3	1:B:116:LYS:HD2	2.00	0.42
1:A:253:ASP:C	1:A:253:ASP:OD2	2.58	0.42
1:A:41:ILE:HD11	1:A:137:LEU:HD11	2.01	0.42
3:A:907:MPD:HM2	4:A:1512:HOH:O	2.19	0.42
1:B:190:ALA:O	1:B:191:ASP:CB	2.67	0.42
1:A:265:LEU:CD1	4:A:1551:HOH:O	2.63	0.42
1:B:248:GLN:NE2	4:B:1317:HOH:O	2.52	0.41
1:B:170:ASN:C	1:B:170:ASN:HD22	2.24	0.40
1:B:209:LEU:CB	1:B:260[B]:MET:HE3	2.50	0.40
1:B:209:LEU:HB3	1:B:260[B]:MET:HE3	2.02	0.40
1:B:56:LYS:HZ3	1:B:59:ARG:HH22	1.68	0.40
1:A:129:ASN:CG	4:A:1533:HOH:O	2.59	0.40
1:B:5:PRO:HB2	1:B:192:SER:CB	2.50	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	264/266 (99%)	257 (97%)	6 (2%)	1 (0%)	34	21
1	B	261/266 (98%)	253 (97%)	7 (3%)	1 (0%)	34	21
All	All	525/532 (99%)	510 (97%)	13 (2%)	2 (0%)	34	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	VAL
1	B	31	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	224/224 (100%)	216 (96%)	8 (4%)	35	20
1	B	221/224 (99%)	215 (97%)	6 (3%)	44	31
All	All	445/448 (99%)	431 (97%)	14 (3%)	41	25

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	89	ASN
1	A	116	LYS
1	A	142	GLU

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Mol	Chain	Res	Type
1	A	143[A]	ARG
1	A	143[B]	ARG
1	A	203	TRP
1	A	264	SER
1	B	32	GLU
1	B	116	LYS
1	B	142	GLU
1	B	157	ARG
1	B	170	ASN
1	B	203	TRP

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	22	GLN
1	A	26	GLN
1	A	89	ASN
1	A	139	GLN
1	A	200	GLN
1	B	22	GLN
1	B	36	GLN
1	B	108	GLN
1	B	114	HIS
1	B	170	ASN
1	B	188	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

22 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	B	803	-	4,4,4	0.07	0	6,6,6	0.36	0
2	SO4	A	807	-	4,4,4	0.15	0	6,6,6	0.17	0
3	MPD	A	903	-	7,7,7	0.38	0	9,10,10	0.50	0
3	MPD	B	911	-	7,7,7	0.31	0	9,10,10	0.38	0
3	MPD	B	914	-	7,7,7	0.30	0	9,10,10	0.72	0
2	SO4	A	805	-	4,4,4	0.13	0	6,6,6	0.14	0
3	MPD	A	909	-	7,7,7	0.42	0	9,10,10	0.50	0
2	SO4	B	806	-	4,4,4	0.15	0	6,6,6	0.15	0
3	MPD	B	905	-	7,7,7	0.40	0	9,10,10	0.61	0
2	SO4	B	804	-	4,4,4	0.22	0	6,6,6	0.38	0
2	SO4	B	808	-	4,4,4	0.18	0	6,6,6	0.09	0
3	MPD	A	908	-	7,7,7	0.23	0	9,10,10	0.49	0
3	MPD	B	904	-	7,7,7	0.54	0	9,10,10	0.36	0
2	SO4	A	801	-	4,4,4	0.16	0	6,6,6	0.41	0
3	MPD	A	901	-	7,7,7	0.71	0	9,10,10	0.46	0
3	MPD	B	906	-	7,7,7	0.52	0	9,10,10	0.37	0
3	MPD	A	907	-	7,7,7	0.32	0	9,10,10	0.41	0
2	SO4	A	802	-	4,4,4	0.27	0	6,6,6	0.93	0
3	MPD	B	910	-	7,7,7	0.34	0	9,10,10	0.59	0
3	MPD	A	912	-	7,7,7	0.31	0	9,10,10	0.32	0
3	MPD	A	902	-	7,7,7	0.60	0	9,10,10	0.90	0
3	MPD	B	913	-	7,7,7	0.33	0	9,10,10	0.55	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	MPD	B	905	-	-	3/5/5/5	-
3	MPD	A	901	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	B	906	-	-	0/5/5/5	-
3	MPD	A	907	-	-	1/5/5/5	-
3	MPD	A	909	-	-	0/5/5/5	-
3	MPD	A	903	-	-	0/5/5/5	-
3	MPD	A	908	-	-	0/5/5/5	-
3	MPD	B	911	-	-	0/5/5/5	-
3	MPD	B	904	-	-	0/5/5/5	-
3	MPD	B	910	-	-	0/5/5/5	-
3	MPD	B	914	-	-	0/5/5/5	-
3	MPD	A	912	-	-	0/5/5/5	-
3	MPD	A	902	-	-	1/5/5/5	-
3	MPD	B	913	-	-	3/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	905	MPD	O2-C2-C3-C4
3	B	913	MPD	O2-C2-C3-C4
3	B	905	MPD	C1-C2-C3-C4
3	B	905	MPD	CM-C2-C3-C4
3	A	907	MPD	C1-C2-C3-C4
3	A	902	MPD	C1-C2-C3-C4
3	B	913	MPD	C1-C2-C3-C4
3	B	913	MPD	CM-C2-C3-C4

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	911	MPD	5	0
3	B	905	MPD	1	0
3	A	908	MPD	3	0
3	B	904	MPD	3	0
3	A	901	MPD	2	0
3	A	907	MPD	1	0
3	B	910	MPD	2	0
3	A	912	MPD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	MPD	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	261/266 (98%)	0.25	12 (4%) 32 26	11, 18, 33, 47	0
1	B	259/266 (97%)	0.42	21 (8%) 12 9	14, 22, 39, 51	0
All	All	520/532 (97%)	0.33	33 (6%) 20 15	11, 20, 36, 51	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	SER	8.5
1	A	265	LEU	5.4
1	B	191	ASP	5.1
1	B	5	PRO	5.0
1	B	31	GLY	4.9
1	A	5	PRO	4.3
1	A	141	VAL	4.2
1	B	223	SER	4.2
1	B	245	HIS	3.8
1	B	141	VAL	3.6
1	B	229	ARG	3.3
1	A	191	ASP	3.1
1	B	30	SER	3.1
1	A	115	GLU	3.0
1	A	223	SER	2.9
1	A	229	ARG	2.8
1	B	142	GLU	2.8
1	B	115	GLU	2.8
1	B	263	ARG	2.7
1	A	30	SER	2.6
1	B	252	HIS	2.5
1	A	142	GLU	2.4
1	B	224	ASP	2.4
1	A	190	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	10	SER	2.3
1	B	261	GLU	2.3
1	B	255	VAL	2.3
1	A	31	GLY	2.2
1	B	262	SER	2.2
1	B	259	ALA	2.2
1	B	189	ASN	2.1
1	B	15	ASP	2.1
1	B	254	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

## 6.3 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MPD	B	911	8/8	0.55	0.40	72,72,73,74	0
3	MPD	B	914	8/8	0.63	0.23	39,45,46,48	0
3	MPD	B	913	8/8	0.63	0.24	51,51,52,52	0
3	MPD	A	907	8/8	0.65	0.23	47,48,48,48	0
2	SO4	A	805	5/5	0.77	0.25	87,87,88,88	0
3	MPD	A	908	8/8	0.79	0.22	46,47,47,50	0
3	MPD	A	912	8/8	0.80	0.19	64,65,65,65	0
3	MPD	A	909	8/8	0.81	0.18	29,32,35,35	0
3	MPD	B	910	8/8	0.81	0.24	33,37,41,43	0
2	SO4	B	806	5/5	0.82	0.35	74,75,76,76	0
3	MPD	A	903	8/8	0.82	0.17	31,37,38,38	0
3	MPD	B	905	8/8	0.86	0.16	31,34,37,38	0
3	MPD	B	906	8/8	0.87	0.15	30,33,34,34	0
3	MPD	A	902	8/8	0.90	0.16	25,27,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	808	5/5	0.90	0.36	74,75,75,75	0
2	SO4	A	807	5/5	0.92	0.32	74,74,75,76	0
2	SO4	A	801	5/5	0.92	0.15	63,63,64,64	0
2	SO4	B	803	5/5	0.93	0.15	49,49,51,53	0
3	MPD	B	904	8/8	0.95	0.15	11,16,19,21	0
3	MPD	A	901	8/8	0.95	0.17	8,13,17,18	0
2	SO4	B	804	5/5	0.98	0.07	32,32,35,36	0
2	SO4	A	802	5/5	0.98	0.09	29,29,31,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.