



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 03:43 PM BST

PDB ID : 5UX9
Title : The crystal structure of chloramphenicol acetyltransferase from *Vibrio fischeri* ES114
Authors : Tan, K.; Zhou, M.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2017-02-22
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

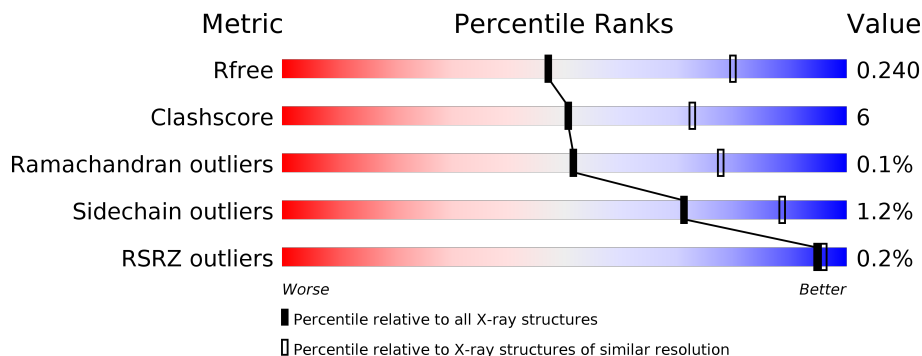
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	221	 88% 10% •
1	B	221	 84% 13% ••
1	C	221	 86% 11% •
1	D	221	 90% 8% •

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6910 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 Chloramphenicol acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	215	1674	1081	280	306	2	5	0	0	0
1	B	215	1677	1082	282	306	2	5	0	0	0
1	C	215	1670	1077	278	308	2	5	0	0	0
1	D	217	1694	1091	283	312	2	6	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q5DZD6
A	-1	ASN	-	expression tag	UNP Q5DZD6
A	0	ALA	-	expression tag	UNP Q5DZD6
B	-2	SER	-	expression tag	UNP Q5DZD6
B	-1	ASN	-	expression tag	UNP Q5DZD6
B	0	ALA	-	expression tag	UNP Q5DZD6
C	-2	SER	-	expression tag	UNP Q5DZD6
C	-1	ASN	-	expression tag	UNP Q5DZD6
C	0	ALA	-	expression tag	UNP Q5DZD6
D	-2	SER	-	expression tag	UNP Q5DZD6
D	-1	ASN	-	expression tag	UNP Q5DZD6
D	0	ALA	-	expression tag	UNP Q5DZD6

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	3	Total Cl 3 3	0	0
5	A	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



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


- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	21	Total	O	0	0
			21	21		
7	B	13	Total	O	0	0
			13	13		
7	C	24	Total	O	0	0
			24	24		
7	D	28	Total	O	0	0
			28	28		

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: Chloramphenicol acetyltransferase

Chain A: 




- Molecule 1: Chloramphenicol acetyltransferase

Chain B: 



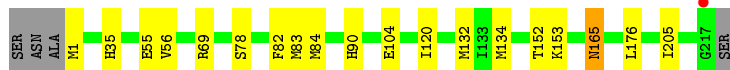
- Molecule 1: Chloramphenicol acetyltransferase

Chain C: 



- Molecule 1: Chloramphenicol acetyltransferase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	147.43Å 147.43Å 101.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.05 – 2.70 47.04 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.05-2.70) 97.6 (47.04-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.34 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.200 , 0.240 0.200 , 0.240	Depositor DCC
R_{free} test set	1625 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtrriage
Anisotropy	0.086	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6910	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ACT, FMT, MES, CL

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	0.24	0/1712	0.41	0/2312
1	B	0.33	0/1715	0.45	0/2316
1	C	0.25	0/1708	0.43	0/2309
1	D	0.25	0/1732	0.44	0/2339
All	All	0.27	0/6867	0.43	0/9276

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1674	0	1601	13	0
1	B	1677	0	1607	27	0
1	C	1670	0	1583	19	0
1	D	1694	0	1618	21	0
2	A	12	0	12	1	0
2	B	12	0	12	0	0
2	C	24	0	24	2	0
2	D	24	0	24	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	8	0	6	0	0
4	B	4	0	3	0	0
4	C	8	0	6	0	0
4	D	4	0	3	1	0
5	A	1	0	0	1	0
5	B	3	0	0	1	0
5	C	1	0	0	1	0
5	D	1	0	0	1	0
6	D	3	0	1	0	0
7	A	21	0	0	0	0
7	B	13	0	0	0	0
7	C	24	0	0	0	0
7	D	28	0	0	0	0
All	All	6910	0	6500	76	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 6.

All (76) 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:50:ASP:OD2	1:B:53:THR:HB	1.60	1.00
1:D:132:MSE:SE	1:D:134:MSE:HE3	2.31	0.80
1:C:68:LEU:HB2	1:C:84:MSE:HE3	1.63	0.80
1:B:90:HIS:NE2	5:B:306:CL:CL	2.52	0.79
1:A:188:TRP:HZ3	1:A:196:THR:HG21	1.52	0.74
2:A:301:MES:H22	1:B:10:GLY:HA3	1.70	0.74
1:D:152:THR:H	1:D:165:ASN:ND2	1.86	0.73
1:C:84:MSE:HE1	1:C:119:THR:OG1	1.91	0.70
1:D:55:GLU:HG2	1:D:56:VAL:N	2.09	0.67
1:C:119:THR:HG22	1:C:136:GLY:H	1.61	0.65
1:A:197:MSE:HE3	1:C:105:PHE:HB3	1.79	0.64
1:C:72:LYS:NZ	1:C:187:ASP:OD1	2.29	0.62
1:B:19:ASN:HD22	1:B:20:PRO:N	1.96	0.61
1:D:153:LYS:H	1:D:165:ASN:HD21	1.46	0.61
1:B:48:LEU:HD12	1:B:65:VAL:CG1	2.30	0.61
1:D:55:GLU:CG	1:D:56:VAL:N	2.64	0.60
1:D:152:THR:H	1:D:165:ASN:HD22	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ASN:ND2	1:B:21:ASN:H	2.00	0.59
1:C:90:HIS:NE2	5:C:306:CL:CL	2.68	0.58
1:A:38:THR:OG1	1:A:41:GLU:HG3	2.04	0.58
1:D:132:MSE:SE	1:D:134:MSE:CE	3.02	0.57
1:D:55:GLU:CD	1:D:56:VAL:H	2.07	0.57
1:C:19:ASN:HB3	1:C:22:ILE:HG13	1.86	0.57
1:D:176:LEU:HB3	1:D:205:ILE:HD12	1.88	0.55
1:B:50:ASP:O	1:B:54:GLN:N	2.40	0.55
1:B:51:ALA:N	1:B:52:PRO:CD	2.70	0.55
1:B:19:ASN:HD22	1:B:19:ASN:C	2.12	0.54
1:B:48:LEU:HD12	1:B:65:VAL:HG11	1.90	0.54
1:D:90:HIS:NE2	5:D:305:CL:CL	2.72	0.53
1:C:214:LYS:HG2	1:C:215:ASN:OD1	2.09	0.53
1:C:202:SER:OG	1:C:203:GLY:N	2.42	0.53
1:B:162:VAL:HG23	1:B:166:VAL:HB	1.91	0.53
1:D:55:GLU:CG	1:D:56:VAL:H	2.22	0.52
1:A:48:LEU:HD23	1:A:53:THR:HB	1.92	0.52
1:B:127:ILE:HA	1:B:145:ILE:HB	1.92	0.52
1:A:201:CYS:HB3	1:C:110:LYS:HB3	1.92	0.50
1:D:83:MSE:HG3	1:D:134:MSE:CE	2.40	0.50
1:D:153:LYS:H	1:D:165:ASN:ND2	2.09	0.50
2:D:302:MES:H61	4:D:304:ACT:H3	1.94	0.50
1:C:37:LYS:HB2	1:C:42:GLN:HG2	1.94	0.50
1:A:70:ILE:HD13	1:A:121:VAL:HB	1.94	0.49
1:B:50:ASP:N	1:B:50:ASP:OD2	2.41	0.49
1:B:51:ALA:N	1:B:52:PRO:HD3	2.28	0.48
1:C:119:THR:HG22	1:C:136:GLY:N	2.27	0.48
1:D:83:MSE:HG3	1:D:134:MSE:HE2	1.94	0.48
1:A:94:TRP:O	1:B:171:ARG:NH2	2.47	0.48
1:C:62:PHE:CD1	2:C:302:MES:H81	2.49	0.48
1:A:90:HIS:NE2	5:A:305:CL:CL	2.75	0.46
1:B:53:THR:O	1:B:53:THR:HG22	2.16	0.46
1:D:82:PHE:HB3	1:D:84:MSE:HE3	1.99	0.45
1:A:32:GLY:HA2	1:A:78:SER:HB2	1.97	0.45
1:B:175:ASN:O	1:B:179:THR:HG23	2.17	0.45
1:B:51:ALA:HB3	1:B:52:PRO:HD3	1.99	0.44
1:B:19:ASN:HD22	1:B:20:PRO:CD	2.31	0.44
1:B:152:THR:N	1:B:165:ASN:OD1	2.44	0.44
1:A:148:ARG:NH1	1:C:130:GLU:O	2.46	0.44
1:D:69:ARG:CZ	1:D:120:ILE:HD12	2.48	0.43
1:A:106:GLY:N	1:B:194:LYS:HG2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:VAL:HG22	1:B:167:VAL:HG22	1.99	0.43
1:C:48:LEU:HD22	2:C:302:MES:H62	2.01	0.43
1:B:13:LEU:HB2	1:B:24:VAL:HG11	2.01	0.42
1:D:153:LYS:HG2	1:D:165:ASN:ND2	2.34	0.42
1:C:151:ILE:HA	1:C:165:ASN:HD22	1.83	0.42
1:B:91:ARG:HE	1:B:91:ARG:HB3	1.74	0.42
1:A:185:TRP:HA	1:A:188:TRP:CE2	2.55	0.42
1:D:132:MSE:HG2	1:D:134:MSE:HE3	2.01	0.42
1:C:30:TYR:CZ	1:C:32:GLY:HA3	2.54	0.42
1:D:82:PHE:HB3	1:D:84:MSE:CE	2.50	0.42
1:D:132:MSE:CG	1:D:134:MSE:HE3	2.50	0.41
1:D:35:HIS:HD2	1:D:78:SER:OG	2.03	0.41
1:A:134:MSE:HG3	1:A:152:THR:HG22	2.03	0.41
1:B:196:THR:HG22	1:B:199:ILE:HD12	2.02	0.41
1:C:48:LEU:HD21	1:C:62:PHE:CD2	2.56	0.41
1:B:51:ALA:C	1:B:53:THR:H	2.25	0.40
1:B:53:THR:O	1:B:53:THR:CG2	2.69	0.40
1:C:168:VAL:HG12	1:C:169:LYS:HG2	2.04	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	213/221 (96%)	204 (96%)	9 (4%)	0	100	100
1	B	213/221 (96%)	195 (92%)	17 (8%)	1 (0%)	29	54
1	C	213/221 (96%)	203 (95%)	10 (5%)	0	100	100
1	D	215/221 (97%)	206 (96%)	9 (4%)	0	100	100
All	All	854/884 (97%)	808 (95%)	45 (5%)	1 (0%)	51	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	36	SER

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	169/178 (95%)	167 (99%)	2 (1%)	71	88
1	B	170/178 (96%)	168 (99%)	2 (1%)	71	88
1	C	168/178 (94%)	167 (99%)	1 (1%)	86	95
1	D	172/178 (97%)	169 (98%)	3 (2%)	60	84
All	All	679/712 (95%)	671 (99%)	8 (1%)	71	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	114	GLN
1	B	19	ASN
1	B	165	ASN
1	C	202	SER
1	D	1	MSE
1	D	104	GLU
1	D	165	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	ASN
1	C	165	ASN
1	C	195	ASN
1	D	35	HIS
1	D	165	ASN
1	D	178	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 10 are monoatomic - leaving 13 for Mogul analysis.

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	MES	A	301	-	12,12,12	2.32	1 (8%)	14,16,16	2.32	7 (50%)
4	ACT	C	304	-	1,3,3	1.30	0	0,3,3	0.00	-
2	MES	C	301	-	12,12,12	2.28	1 (8%)	14,16,16	2.04	6 (42%)
4	ACT	A	303	-	1,3,3	1.28	0	0,3,3	0.00	-
4	ACT	A	304	-	1,3,3	1.36	0	0,3,3	0.00	-
4	ACT	C	305	-	1,3,3	1.35	0	0,3,3	0.00	-
2	MES	D	301	-	12,12,12	2.29	1 (8%)	14,16,16	2.39	7 (50%)
4	ACT	D	304	-	1,3,3	1.28	0	0,3,3	0.00	-
2	MES	B	301	-	12,12,12	2.28	1 (8%)	14,16,16	2.44	8 (57%)
2	MES	D	302	-	12,12,12	2.31	1 (8%)	14,16,16	2.15	5 (35%)
4	ACT	B	303	-	1,3,3	1.45	0	0,3,3	0.00	-
2	MES	C	302	-	12,12,12	2.30	1 (8%)	14,16,16	2.17	7 (50%)
6	FMT	D	306	-	0,2,2	0.00	-	0,1,1	0.00	-

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	MES	A	301	-	-	0/6/14/14	0/1/1/1
2	MES	C	301	-	-	4/6/14/14	0/1/1/1
2	MES	D	301	-	-	3/6/14/14	0/1/1/1
2	MES	B	301	-	-	1/6/14/14	0/1/1/1
2	MES	D	302	-	-	5/6/14/14	0/1/1/1
2	MES	C	302	-	-	1/6/14/14	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	MES	C8-S	-7.77	1.66	1.77
2	D	302	MES	C8-S	-7.71	1.66	1.77
2	C	302	MES	C8-S	-7.71	1.66	1.77
2	D	301	MES	C8-S	-7.65	1.66	1.77
2	B	301	MES	C8-S	-7.62	1.66	1.77
2	C	301	MES	C8-S	-7.62	1.66	1.77

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	MES	C5-N4-C3	5.24	120.63	108.83
2	D	301	MES	C5-N4-C3	5.13	120.38	108.83
2	D	302	MES	C5-N4-C3	5.09	120.29	108.83
2	A	301	MES	C5-N4-C3	4.89	119.84	108.83
2	C	301	MES	C5-N4-C3	4.83	119.71	108.83
2	C	302	MES	C5-N4-C3	4.57	119.12	108.83
2	A	301	MES	C2-C3-N4	-3.34	105.04	110.10
2	B	301	MES	C7-N4-C5	3.17	119.35	111.23
2	D	301	MES	C6-C5-N4	-3.15	105.33	110.10
2	B	301	MES	C7-N4-C3	3.10	119.17	111.23
2	D	301	MES	C7-N4-C3	3.08	119.11	111.23
2	C	302	MES	C2-C3-N4	-2.94	105.64	110.10
2	B	301	MES	C6-C5-N4	-2.81	105.84	110.10
2	A	301	MES	C7-N4-C5	2.78	118.36	111.23
2	B	301	MES	C2-C3-N4	-2.75	105.94	110.10
2	C	302	MES	C7-N4-C5	2.70	118.15	111.23
2	A	301	MES	C7-N4-C3	2.68	118.08	111.23
2	D	301	MES	C7-N4-C5	2.61	117.90	111.23
2	D	302	MES	C7-N4-C5	2.56	117.79	111.23
2	D	301	MES	C2-C3-N4	-2.52	106.28	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	302	MES	O2S-S-C8	2.52	109.94	106.92
2	A	301	MES	C6-C5-N4	-2.50	106.31	110.10
2	D	301	MES	O3S-S-C8	2.49	109.80	105.77
2	D	302	MES	C7-N4-C3	2.43	117.46	111.23
2	C	301	MES	O1S-S-C8	2.43	109.84	106.92
2	C	301	MES	C7-N4-C5	2.36	117.28	111.23
2	B	301	MES	O3S-S-C8	2.33	109.54	105.77
2	C	301	MES	O2S-S-C8	2.32	109.71	106.92
2	C	302	MES	O2S-S-C8	2.32	109.70	106.92
2	A	301	MES	O3S-S-C8	2.31	109.51	105.77
2	C	302	MES	C6-C5-N4	-2.30	106.61	110.10
2	C	302	MES	C7-N4-C3	2.28	117.07	111.23
2	C	302	MES	O3S-S-C8	2.25	109.40	105.77
2	D	302	MES	O3S-S-C8	2.25	109.40	105.77
2	C	301	MES	C7-N4-C3	2.23	116.94	111.23
2	A	301	MES	O2S-S-C8	2.16	109.52	106.92
2	D	301	MES	O1S-S-C8	2.13	109.48	106.92
2	B	301	MES	O1S-S-C8	2.12	109.47	106.92
2	B	301	MES	O2S-S-C8	2.08	109.42	106.92
2	C	301	MES	O3S-S-C8	2.05	109.08	105.77

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	302	MES	N4-C7-C8-S
2	D	302	MES	C7-C8-S-O2S
2	D	302	MES	C7-C8-S-O3S
2	C	301	MES	C7-C8-S-O2S
2	D	301	MES	C7-C8-S-O1S
2	D	301	MES	C7-C8-S-O3S
2	C	301	MES	C7-C8-S-O3S
2	B	301	MES	C8-C7-N4-C3
2	D	302	MES	C8-C7-N4-C5
2	C	302	MES	C8-C7-N4-C5
2	D	302	MES	C7-C8-S-O1S
2	C	301	MES	C7-C8-S-O1S
2	D	301	MES	C7-C8-S-O2S
2	C	301	MES	C8-C7-N4-C5

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	MES	1	0
4	D	304	ACT	1	0
2	D	302	MES	1	0
2	C	302	MES	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	210/221 (95%)	-0.35	0 100 100	27, 43, 70, 81	0
1	B	210/221 (95%)	-0.23	0 100 100	27, 50, 82, 99	0
1	C	210/221 (95%)	-0.38	1 (0%) 91 92	28, 46, 68, 83	0
1	D	211/221 (95%)	-0.49	1 (0%) 91 92	17, 32, 59, 82	0
All	All	841/884 (95%)	-0.36	2 (0%) 95 96	17, 43, 74, 99	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	GLY	3.0
1	D	217	GLY	2.6

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 monosaccharides 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(\AA^2)	Q<0.9
4	ACT	C	305	4/4	0.61	0.33	82,88,89,89	0
5	CL	C	306	1/1	0.76	0.35	94,94,94,94	0
2	MES	D	302	12/12	0.77	0.28	147,150,168,169	0
3	MG	D	303	1/1	0.83	0.14	86,86,86,86	0
6	FMT	D	306	3/3	0.84	0.14	55,55,56,59	0
2	MES	C	302	12/12	0.85	0.28	82,90,113,113	0
5	CL	B	304	1/1	0.86	0.12	70,70,70,70	0
3	MG	C	303	1/1	0.86	0.27	51,51,51,51	0
4	ACT	A	304	4/4	0.86	0.19	64,69,69,69	0
2	MES	B	301	12/12	0.86	0.28	94,97,104,110	0
5	CL	D	305	1/1	0.88	0.26	77,77,77,77	0
5	CL	A	305	1/1	0.88	0.30	86,86,86,86	0
5	CL	B	306	1/1	0.88	0.29	92,92,92,92	0
4	ACT	D	304	4/4	0.88	0.25	69,69,71,71	0
3	MG	A	302	1/1	0.88	0.07	79,79,79,79	0
2	MES	A	301	12/12	0.89	0.21	73,82,99,101	0
2	MES	C	301	12/12	0.91	0.23	59,68,87,94	0
3	MG	B	302	1/1	0.92	0.15	71,71,71,71	0
4	ACT	C	304	4/4	0.92	0.17	72,73,77,79	0
4	ACT	B	303	4/4	0.93	0.13	61,64,65,66	0
5	CL	B	305	1/1	0.94	0.05	63,63,63,63	0
2	MES	D	301	12/12	0.94	0.28	66,74,86,89	0
4	ACT	A	303	4/4	0.96	0.19	53,62,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.