Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:42 PM GMT

PDB ID	:	4D5B
Title	:	Crystal structure of CymA from Klebsiella oxytoca
Authors	:	vandenBerg, B.; Bhamidimarri, S.P.; Kleinekathoefer, U.; Winterhalter, M.
Deposited on	:	2014-11-03
Resolution	:	1.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

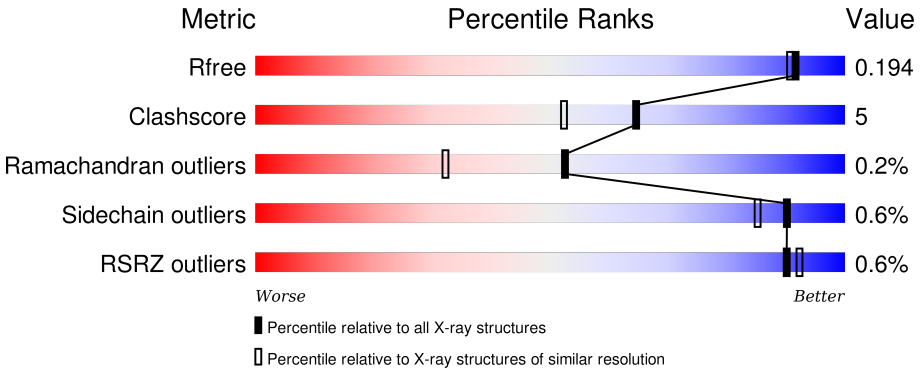
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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 <=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	339	% 84% 8% 8%
1	B	339	% 83% 8% 9%

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
2	ACX	A	1326	X	-	-	X
3	C8E	A	1327	-	-	-	X
3	C8E	A	1328	-	-	-	X
3	C8E	A	1329	-	-	-	X
3	C8E	A	1330	-	-	-	X
3	C8E	A	1332	-	-	-	X
3	C8E	A	1333	-	-	-	X
3	C8E	A	1334	-	-	-	X
3	C8E	A	1337	-	-	-	X
3	C8E	A	1338	-	-	-	X
3	C8E	B	1327	-	-	-	X
3	C8E	B	1329	-	-	-	X
3	C8E	B	1330	-	-	-	X
3	C8E	B	1331	-	-	-	X
3	C8E	B	1333	-	-	-	X
3	C8E	B	1334	-	-	-	X
3	C8E	B	1335	-	-	-	X
3	C8E	B	1337	-	-	-	X
3	C8E	B	1338	-	-	-	X
3	C8E	B	1339	-	-	-	X
3	C8E	B	1340	-	-	-	X
3	C8E	B	1343	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6657 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 CYMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	30	9	0
			2645	1689	441	513	2			
1	B	309	Total	C	N	O	S	12	6	0
			2597	1656	433	506	2			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	ALA	-	EXPRESSION TAG	UNP Q48391
A	-13	ASN	-	EXPRESSION TAG	UNP Q48391
A	-12	VAL	-	EXPRESSION TAG	UNP Q48391
A	-11	ARG	-	EXPRESSION TAG	UNP Q48391
A	-10	LEU	-	EXPRESSION TAG	UNP Q48391
A	-9	GLN	-	EXPRESSION TAG	UNP Q48391
A	-8	HIS	-	EXPRESSION TAG	UNP Q48391
A	-7	HIS	-	EXPRESSION TAG	UNP Q48391
A	-6	HIS	-	EXPRESSION TAG	UNP Q48391
A	-5	HIS	-	EXPRESSION TAG	UNP Q48391
A	-4	HIS	-	EXPRESSION TAG	UNP Q48391
A	-3	HIS	-	EXPRESSION TAG	UNP Q48391
A	-2	HIS	-	EXPRESSION TAG	UNP Q48391
A	-1	LEU	-	EXPRESSION TAG	UNP Q48391
A	0	GLU	-	EXPRESSION TAG	UNP Q48391
B	-14	ALA	-	EXPRESSION TAG	UNP Q48391
B	-13	ASN	-	EXPRESSION TAG	UNP Q48391
B	-12	VAL	-	EXPRESSION TAG	UNP Q48391
B	-11	ARG	-	EXPRESSION TAG	UNP Q48391
B	-10	LEU	-	EXPRESSION TAG	UNP Q48391
B	-9	GLN	-	EXPRESSION TAG	UNP Q48391
B	-8	HIS	-	EXPRESSION TAG	UNP Q48391
B	-7	HIS	-	EXPRESSION TAG	UNP Q48391
B	-6	HIS	-	EXPRESSION TAG	UNP Q48391
B	-5	HIS	-	EXPRESSION TAG	UNP Q48391

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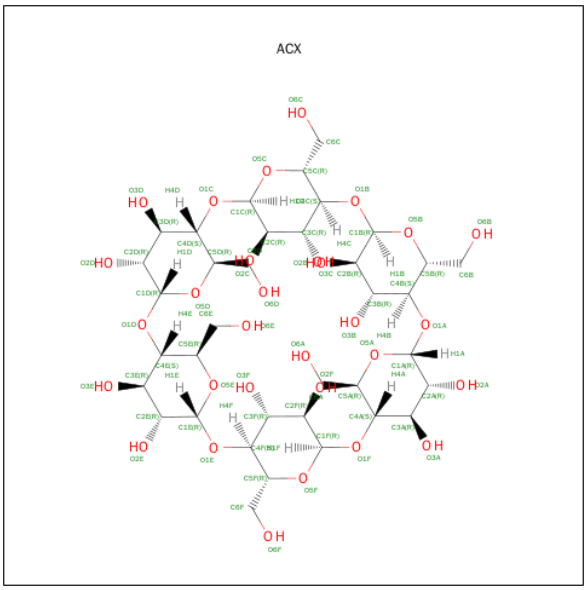
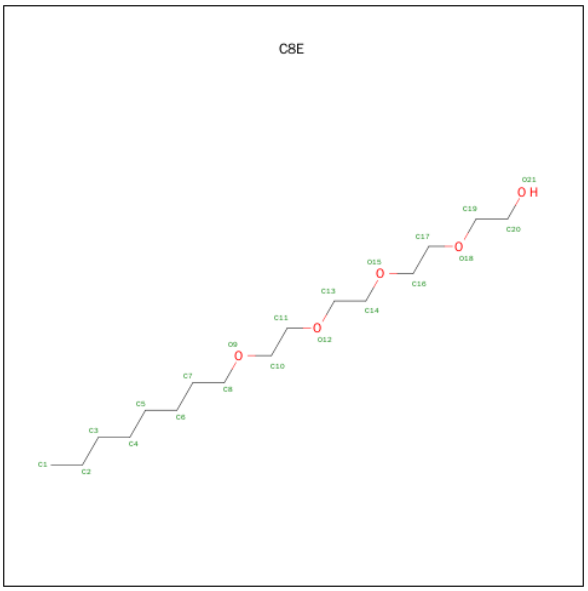
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	EXPRESSION TAG	UNP Q48391
B	-3	HIS	-	EXPRESSION TAG	UNP Q48391
B	-2	HIS	-	EXPRESSION TAG	UNP Q48391
B	-1	LEU	-	EXPRESSION TAG	UNP Q48391
B	0	GLU	-	EXPRESSION TAG	UNP Q48391

- Molecule 2 is SUGAR (ALPHA-CYCLODEXTRIN (CYCLOHEXA-AMYLOSE)) (three-letter code: ACX) (formula: $C_{36}H_{60}O_{30}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 66 36 30	0	0
2	A	1	Total C O 66 36 30	0	0
2	B	1	Total C O 66 36 30	0	0
2	B	1	Total C O 66 36 30	0	0

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 5 3	0	0
3	A	1	Total C O 19 14 5	0	0
3	A	1	Total C O 17 12 5	0	0
3	A	1	Total C O 16 12 4	0	0
3	A	1	Total C O 16 11 5	0	0
3	A	1	Total C O 12 9 3	0	0
3	A	1	Total C O 11 10 1	0	0
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C 7 7	0	0
3	A	1	Total C O 10 9 1	0	0
3	A	1	Total C O 21 16 5	0	0
3	A	1	Total C O 13 9 4	0	0
3	A	1	Total C O 9 8 1	0	0
3	B	1	Total C O 21 16 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 16 12 4	0	0
3	B	1	Total C O 12 10 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 14 12 2	0	0
3	B	1	Total C O 9 6 3	0	0
3	B	1	Total C O 14 12 2	0	0
3	B	1	Total C O 13 9 4	0	0
3	B	1	Total C O 9 6 3	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C O 19 16 3	0	0
3	B	1	Total C O 13 8 5	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C O 7 6 1	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C O 13 10 3	3	0

- Molecule 4 is water.

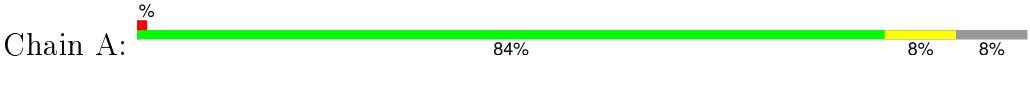
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	423	Total O 423 423	0	0
4	B	362	Total O 362 362	0	0

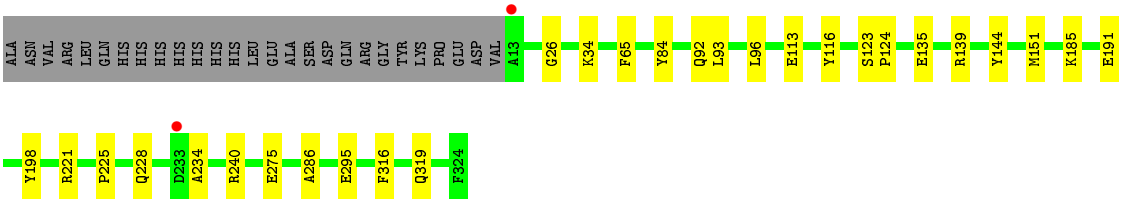
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: CYMA

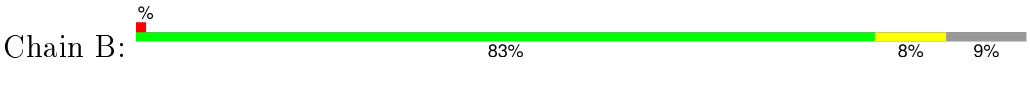
Chain A:

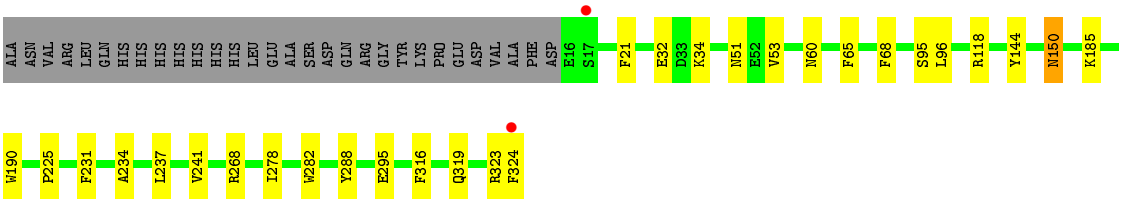




- Molecule 1: CYMA

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	140.56Å 77.40Å 110.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.05 – 1.70 47.10 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.05-1.70) 96.1 (47.10-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 1.70Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.167 , 0.190 0.181 , 0.194	Depositor DCC
R_{free} test set	2000 reflections (1.58%)	DCC
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	10 of 132414 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6657	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ACX, C8E

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	0.39	0/2734	0.52	0/3689
1	B	0.37	0/2685	0.53	0/3620
All	All	0.38	0/5419	0.53	0/7309

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

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	2645	0	2488	24	0
1	B	2597	0	2436	27	0
2	A	132	0	120	6	0
2	B	132	0	120	1	0
3	A	169	0	236	13	0
3	B	197	0	290	15	0
4	A	423	0	0	8	4
4	B	362	0	0	5	4
All	All	6657	0	5690	58	4

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 5.

All (58) 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:295:GLU:OE2	4:B:2323:HOH:O	1.93	0.86
1:A:139:ARG:NH2	2:A:1326:ACX:H6D2	1.97	0.80
1:B:51:ASN:HD21	3:B:1334:C8E:H102	1.48	0.79
1:A:34:LYS:HD2	4:A:2026:HOH:O	1.87	0.75
1:B:316:PHE:HB2	3:B:1333:C8E:H71	1.72	0.72
1:B:118:ARG:NH1	4:B:2169:HOH:O	2.24	0.70
1:B:144:TYR:HE2	3:B:1340:C8E:H52	1.60	0.67
1:A:295:GLU:OE2	4:A:2373:HOH:O	2.14	0.65
1:A:135:GLU:OE2	4:A:2203:HOH:O	2.14	0.65
1:B:288:TYR:CE1	3:B:1332:C8E:H112	2.32	0.64
1:A:139:ARG:HH22	2:A:1326:ACX:H6D2	1.61	0.63
1:A:198:TYR:HB2	3:A:1330:C8E:H171	1.81	0.63
3:A:1327:C8E:H142	1:B:53:VAL:HB	1.82	0.62
2:B:1326:ACX:H6D2	4:B:2142:HOH:O	2.04	0.56
1:B:278:ILE:HG22	3:B:1329:C8E:H82	1.89	0.54
1:B:150:ASN:ND2	4:B:2189:HOH:O	2.40	0.53
1:A:144:TYR:HE2	3:A:1332:C8E:H102	1.73	0.52
1:A:92:GLN:HE21	3:A:1331:C8E:H171	1.75	0.52
1:B:51:ASN:ND2	3:B:1334:C8E:H102	2.22	0.52
1:A:275:GLU:OE1	4:A:2353:HOH:O	2.18	0.51
1:B:288:TYR:CZ	3:B:1332:C8E:H112	2.46	0.50
1:A:185:LYS:NZ	3:A:1334:C8E:H161	2.27	0.50
4:A:2183:HOH:O	1:B:324:PHE:OXT	2.18	0.50
1:A:116:TYR:HB2	3:A:1331:C8E:H172	1.94	0.49
2:A:1326:ACX:H6E1	4:A:2149:HOH:O	2.12	0.49
1:A:65:PHE:HZ	1:A:96:LEU:HD22	1.78	0.49
1:B:323:ARG:NH2	4:B:2314:HOH:O	2.45	0.49
1:A:191:GLU:HB3	1:A:228:GLN:HG2	1.95	0.48
3:A:1331:C8E:H112	1:B:21:PHE:HB2	1.94	0.48
1:A:151:MET:HG2	1:A:185:LYS:HG3	1.96	0.48
1:B:51:ASN:ND2	3:B:1334:C8E:H71	2.27	0.48
1:B:32[A]:GLU:OE2	1:B:34:LYS:HD2	2.14	0.48
1:A:26:GLY:HA2	3:A:1327:C8E:H101	1.95	0.48
1:B:268:ARG:HB3	3:B:1343:C8E:H42	1.95	0.47
1:A:319:GLN:OE1	2:A:1326:ACX:H2B	2.14	0.47
1:B:185:LYS:HD2	3:B:1338:C8E:H161	1.96	0.47
1:B:190:TRP:CH2	3:B:1339:C8E:H41	2.50	0.46
1:B:68:PHE:HB3	1:B:95:SER:HB3	1.98	0.46
1:A:93:LEU:HD11	1:A:113:GLU:HG2	1.98	0.45
3:A:1328:C8E:H142	3:A:1328:C8E:H171	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1326:ACX:H6E1	4:A:2150:HOH:O	2.17	0.44
3:A:1327:C8E:H102	3:A:1327:C8E:H132	1.69	0.44
1:A:316:PHE:CD2	3:A:1336:C8E:H71	2.53	0.44
1:A:286:ALA:HB1	3:A:1328:C8E:H191	1.99	0.43
1:B:237:LEU:HD23	3:B:1339:C8E:H51	2.01	0.42
1:A:84:TYR:CE1	1:A:124:PRO:HD3	2.55	0.42
1:B:231:PHE:HB2	1:B:234:ALA:HB3	2.00	0.42
3:A:1331:C8E:H102	3:A:1331:C8E:H202	2.02	0.42
3:B:1327:C8E:H31	3:B:1331:C8E:H51	2.01	0.42
1:B:65:PHE:HZ	1:B:96:LEU:HD22	1.84	0.41
1:B:225:PRO:HD2	1:B:241:VAL:O	2.19	0.41
1:A:139:ARG:HH22	2:A:1326:ACX:C6D	2.31	0.41
1:A:123:SER:HB2	1:A:124:PRO:HD2	2.03	0.41
1:B:21:PHE:CE2	1:B:60:ASN:HB2	2.55	0.41
1:B:282:TRP:CD1	3:B:1329:C8E:H71	2.56	0.41
1:B:185:LYS:HD3	3:B:1338:C8E:H201	2.02	0.41
1:A:240:ARG:NH2	4:A:2308:HOH:O	2.54	0.41

All (4) 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)
4:A:2088:HOH:O	4:B:2201:HOH:O[2_765]	1.93	0.27
4:A:2210:HOH:O	4:B:2327:HOH:O[4_555]	2.00	0.20
4:A:2086:HOH:O	4:B:2166:HOH:O[4_555]	2.09	0.11
4:A:2144:HOH:O	4:B:2069:HOH:O[2_755]	2.10	0.10

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	319/339 (94%)	315 (99%)	3 (1%)	1 (0%)	46 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	313/339 (92%)	309 (99%)	4 (1%)	0	100 100
All	All	632/678 (93%)	624 (99%)	7 (1%)	1 (0%)	52 32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	ALA

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	280/295 (95%)	279 (100%)	1 (0%)	93 90
1	B	274/295 (93%)	272 (99%)	2 (1%)	88 82
All	All	554/590 (94%)	551 (100%)	3 (0%)	90 88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ARG
1	B	150	ASN
1	B	319	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	51	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 (i)

34 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	ACX	A	1325	-	72,72,72	0.44	0	108,108,108	0.96	4 (3%)
2	ACX	A	1326	-	72,72,72	0.48	0	108,108,108	1.52	18 (16%)
3	C8E	A	1327	-	7,7,20	0.36	0	6,6,19	0.26	0
3	C8E	A	1328	-	18,18,20	0.37	0	17,17,19	0.49	0
3	C8E	A	1329	-	15,15,20	0.35	0	13,13,19	0.36	0
3	C8E	A	1330	-	14,14,20	0.34	0	12,12,19	0.37	0
3	C8E	A	1331	-	15,15,20	0.44	0	14,14,19	0.40	0
3	C8E	A	1332	-	11,11,20	0.45	0	10,10,19	0.46	0
3	C8E	A	1333	-	10,10,20	0.35	0	9,9,19	0.53	0
3	C8E	A	1334	-	9,9,20	0.42	0	8,8,19	0.27	0
3	C8E	A	1335	-	6,6,20	0.23	0	5,5,19	0.46	0
3	C8E	A	1336	-	9,9,20	0.25	0	8,8,19	0.61	0
3	C8E	A	1337	-	20,20,20	0.44	0	19,19,19	0.35	0
3	C8E	A	1338	-	12,12,20	0.47	0	11,11,19	0.19	0
3	C8E	A	1339	-	8,8,20	0.25	0	7,7,19	0.49	0
2	ACX	B	1325	-	72,72,72	0.44	0	108,108,108	1.07	8 (7%)
2	ACX	B	1326	-	72,72,72	0.49	0	108,108,108	1.20	12 (11%)
3	C8E	B	1327	-	20,20,20	0.38	0	19,19,19	0.46	0
3	C8E	B	1328	-	15,15,20	0.38	0	14,14,19	0.36	0
3	C8E	B	1329	-	11,11,20	0.29	0	10,10,19	0.52	0
3	C8E	B	1330	-	7,7,20	0.50	0	6,6,19	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	C8E	B	1331	-	13,13,20	0.39	0	12,12,19	0.44	0
3	C8E	B	1332	-	8,8,20	0.46	0	7,7,19	0.44	0
3	C8E	B	1333	-	13,13,20	0.38	0	12,12,19	0.58	0
3	C8E	B	1334	-	12,12,20	0.44	0	11,11,19	0.22	0
3	C8E	B	1335	-	8,8,20	0.48	0	7,7,19	0.57	0
3	C8E	B	1336	-	6,6,20	0.25	0	5,5,19	0.40	0
3	C8E	B	1337	-	16,16,20	0.41	0	13,13,19	0.38	0
3	C8E	B	1338	-	12,12,20	0.43	0	11,11,19	0.25	0
3	C8E	B	1339	-	6,6,20	0.26	0	5,5,19	0.44	0
3	C8E	B	1340	-	6,6,20	0.25	0	5,5,19	0.41	0
3	C8E	B	1341	-	7,7,20	0.25	0	6,6,19	0.53	0
3	C8E	B	1342	-	6,6,20	0.25	0	5,5,19	0.51	0
3	C8E	B	1343	-	12,12,20	0.38	0	11,11,19	0.26	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	ACX	A	1325	-	-	0/36/156/156	0/0/7/7
2	ACX	A	1326	-	3/3/30/30	0/36/156/156	0/0/7/7
3	C8E	A	1327	-	-	0/5/5/18	0/0/0/0
3	C8E	A	1328	-	-	0/16/16/18	0/0/0/0
3	C8E	A	1329	-	-	0/11/11/18	0/0/0/0
3	C8E	A	1330	-	-	0/10/10/18	0/0/0/0
3	C8E	A	1331	-	-	0/13/13/18	0/0/0/0
3	C8E	A	1332	-	-	0/9/9/18	0/0/0/0
3	C8E	A	1333	-	-	0/8/8/18	0/0/0/0
3	C8E	A	1334	-	-	0/7/7/18	0/0/0/0
3	C8E	A	1335	-	-	0/4/4/18	0/0/0/0
3	C8E	A	1336	-	-	0/7/7/18	0/0/0/0
3	C8E	A	1337	-	-	0/18/18/18	0/0/0/0
3	C8E	A	1338	-	-	0/10/10/18	0/0/0/0
3	C8E	A	1339	-	-	0/6/6/18	0/0/0/0
2	ACX	B	1325	-	-	0/36/156/156	0/0/7/7
2	ACX	B	1326	-	-	0/36/156/156	0/0/7/7
3	C8E	B	1327	-	-	0/18/18/18	0/0/0/0
3	C8E	B	1328	-	-	0/13/13/18	0/0/0/0
3	C8E	B	1329	-	-	0/9/9/18	0/0/0/0
3	C8E	B	1330	-	-	0/5/5/18	0/0/0/0
3	C8E	B	1331	-	-	0/11/11/18	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	B	1332	-	-	0/6/6/18	0/0/0/0
3	C8E	B	1333	-	-	0/11/11/18	0/0/0/0
3	C8E	B	1334	-	-	0/10/10/18	0/0/0/0
3	C8E	B	1335	-	-	0/6/6/18	0/0/0/0
3	C8E	B	1336	-	-	0/4/4/18	0/0/0/0
3	C8E	B	1337	-	-	0/10/10/18	0/0/0/0
3	C8E	B	1338	-	-	0/10/10/18	0/0/0/0
3	C8E	B	1339	-	-	0/4/4/18	0/0/0/0
3	C8E	B	1340	-	-	0/4/4/18	0/0/0/0
3	C8E	B	1341	-	-	0/5/5/18	0/0/0/0
3	C8E	B	1342	-	-	0/4/4/18	0/0/0/0
3	C8E	B	1343	-	-	0/10/10/18	0/0/0/0

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1326	ACX	O1D-C1D-O5D	-2.93	103.26	110.68
2	A	1326	ACX	C1E-O1E-C4F	-2.87	110.50	118.01
2	A	1326	ACX	C1C-O1C-C4D	-2.74	110.85	118.01
2	B	1326	ACX	C1E-O1E-C4F	-2.56	111.31	118.01
2	A	1326	ACX	O1F-C4A-C5A	-2.56	102.60	109.32
2	A	1325	ACX	O6F-C6F-C5F	-2.25	103.90	111.33
2	B	1325	ACX	O6E-C6E-C5E	-2.22	104.00	111.33
2	B	1325	ACX	O1D-C1D-O5D	-2.07	105.44	110.68
2	B	1325	ACX	O1F-C1F-O5F	-2.04	105.52	110.68
2	B	1326	ACX	C1C-O1C-C4D	-2.02	112.72	118.01
2	B	1326	ACX	C1F-O5F-C5F	2.01	117.65	113.75
2	A	1326	ACX	C3E-C4E-C5E	2.10	115.59	110.84
2	B	1326	ACX	O5D-C5D-C4D	2.25	114.50	109.75
2	A	1326	ACX	C2E-C3E-C4E	2.26	114.57	109.60
2	A	1326	ACX	O5D-C1D-C2D	2.27	114.94	110.28
2	A	1326	ACX	C1D-C2D-C3D	2.30	114.51	109.97
2	B	1325	ACX	O5F-C5F-C6F	2.35	112.29	106.36
2	B	1326	ACX	C3E-C4E-C5E	2.36	116.19	110.84
2	B	1325	ACX	C1E-O5E-C5E	2.46	118.53	113.75
2	B	1326	ACX	C2D-C3D-C4D	2.48	115.05	109.60
2	B	1325	ACX	C1D-O5D-C5D	2.50	118.60	113.75
2	A	1326	ACX	O5D-C5D-C4D	2.50	115.04	109.75
2	B	1326	ACX	C3D-C4D-C5D	2.58	116.68	110.84
2	B	1326	ACX	C3F-C4F-C5F	2.59	116.70	110.84
2	B	1326	ACX	C1D-O5D-C5D	2.60	118.80	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1326	ACX	C1E-O5E-C5E	2.68	118.95	113.75
2	A	1325	ACX	C1D-O5D-C5D	2.71	119.01	113.75
2	A	1325	ACX	O5F-C5F-C4F	2.75	115.55	109.75
2	B	1325	ACX	O5B-C5B-C4B	2.78	115.62	109.75
2	A	1326	ACX	O5B-C5B-C4B	2.79	115.64	109.75
2	B	1326	ACX	O5B-C5B-C4B	2.89	115.85	109.75
2	A	1325	ACX	C1F-O5F-C5F	2.90	119.38	113.75
2	A	1326	ACX	C3A-C4A-C5A	2.92	117.44	110.84
2	A	1326	ACX	O5F-C5F-C6F	3.18	114.40	106.36
2	A	1326	ACX	C2A-C3A-C4A	3.20	116.62	109.60
2	B	1326	ACX	C1E-O5E-C5E	3.28	120.11	113.75
2	A	1326	ACX	C1F-O5F-C5F	3.54	120.62	113.75
2	A	1326	ACX	O5D-C5D-C6D	3.54	115.31	106.36
2	A	1326	ACX	C1D-O5D-C5D	3.64	120.81	113.75
2	B	1326	ACX	O5E-C5E-C4E	3.96	118.11	109.75
2	A	1326	ACX	O5E-C5E-C4E	4.21	118.63	109.75
2	B	1325	ACX	O5E-C5E-C4E	4.26	118.73	109.75

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1326	ACX	C2D
2	A	1326	ACX	C3F
2	A	1326	ACX	C2F

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1326	ACX	6	0
3	A	1327	C8E	3	0
3	A	1328	C8E	2	0
3	A	1330	C8E	1	0
3	A	1331	C8E	4	0
3	A	1332	C8E	1	0
3	A	1334	C8E	1	0
3	A	1336	C8E	1	0
2	B	1326	ACX	1	0
3	B	1327	C8E	1	0
3	B	1329	C8E	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1331	C8E	1	0
3	B	1332	C8E	2	0
3	B	1333	C8E	1	0
3	B	1334	C8E	3	0
3	B	1338	C8E	2	0
3	B	1339	C8E	2	0
3	B	1340	C8E	1	0
3	B	1343	C8E	1	0

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^{th} 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	312/339 (92%)	-0.24	2 (0%)	90	92	16, 23, 41, 66	8 (2%)
1	B	309/339 (91%)	-0.19	2 (0%)	90	92	16, 26, 42, 62	4 (1%)
All	All	621/678 (91%)	-0.21	4 (0%)	90	92	16, 24, 42, 66	12 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	ALA	2.8
1	A	233	ASP	2.3
1	B	17	SER	2.2
1	B	324	PHE	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^{th} 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^2)	Q<0.9
3	C8E	A	1337	21/21	0.58	0.25	15.90	38,54,67,77	0
3	C8E	B	1330	8/21	0.91	0.18	10.88	33,41,49,51	0
3	C8E	A	1329	17/21	0.88	0.15	10.86	41,58,66,69	0
3	C8E	A	1332	12/21	0.74	0.18	10.38	41,60,67,68	0
3	C8E	B	1329	12/21	0.84	0.25	9.06	39,47,59,60	0
3	C8E	B	1339	7/21	0.79	0.19	8.81	32,48,51,52	0
3	C8E	B	1334	13/21	0.75	0.19	7.79	47,51,66,69	0
3	C8E	B	1340	7/21	0.69	0.19	7.69	51,55,57,58	0
3	C8E	A	1328	19/21	0.87	0.22	7.63	39,56,72,75	0
3	C8E	B	1331	14/21	0.71	0.21	7.49	45,52,66,66	0
3	C8E	B	1338	13/21	0.79	0.23	7.37	54,61,75,76	0
3	C8E	A	1338	13/21	0.82	0.21	6.77	38,66,73,75	0
3	C8E	A	1330	16/21	0.81	0.20	6.71	33,49,69,71	0
3	C8E	A	1333	11/21	0.80	0.12	6.55	51,55,60,63	0
3	C8E	B	1333	14/21	0.82	0.16	6.08	29,46,56,59	0
3	C8E	A	1327	8/21	0.84	0.16	6.08	37,51,59,68	0
3	C8E	B	1335	9/21	0.64	0.22	5.74	54,73,79,80	0
3	C8E	B	1327	21/21	0.80	0.20	5.74	41,52,64,68	0
3	C8E	A	1334	10/21	0.67	0.13	4.99	62,67,69,72	0
3	C8E	B	1337	19/21	0.80	0.16	3.71	34,45,64,65	0
3	C8E	B	1343	13/21	0.74	0.15	3.70	45,48,53,60	3
2	ACX	A	1326	66/66	0.80	0.16	3.55	32,62,79,84	0
3	C8E	B	1328	16/21	0.90	0.14	1.04	31,46,59,61	0
3	C8E	A	1331	16/21	0.89	0.13	0.81	28,38,49,59	0
2	ACX	B	1326	66/66	0.90	0.11	0.41	23,38,52,79	0
2	ACX	B	1325	66/66	0.94	0.10	0.01	20,31,40,45	0
2	ACX	A	1325	66/66	0.96	0.07	-0.70	17,23,30,34	0
3	C8E	A	1336	10/21	0.78	0.21	-	48,55,66,67	0
3	C8E	B	1332	9/21	0.72	0.19	-	52,61,69,69	0
3	C8E	B	1336	7/21	0.87	0.12	-	38,40,43,45	0
3	C8E	A	1339	9/21	0.70	0.21	-	57,65,77,77	0
3	C8E	A	1335	7/21	0.92	0.12	-	31,33,37,42	0
3	C8E	B	1342	7/21	0.84	0.25	-	52,53,57,58	0
3	C8E	B	1341	8/21	0.88	0.12	-	42,43,48,49	0

6.5 Other polymers

There are no such residues in this entry.