Full wwPDB X-ray Structure Validation Report (i)

Feb 7, 2017 – 12:38 PM EST

PDB ID	:	5B12
Title	:	Crystal structure of the B-type halohydrin hydrogen-halide-lyase mutant F71W/Q125T/D199H from Corynebacterium sp. N-1074
Authors	:	Watanabe, F.; Yu, F.; Ohtaki, A.; Yamanaka, Y.; Noguchi, K.; Odaka, M.; Yohda, M.
Deposited on	:	2015-11-17
Resolution	:	1.72 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:

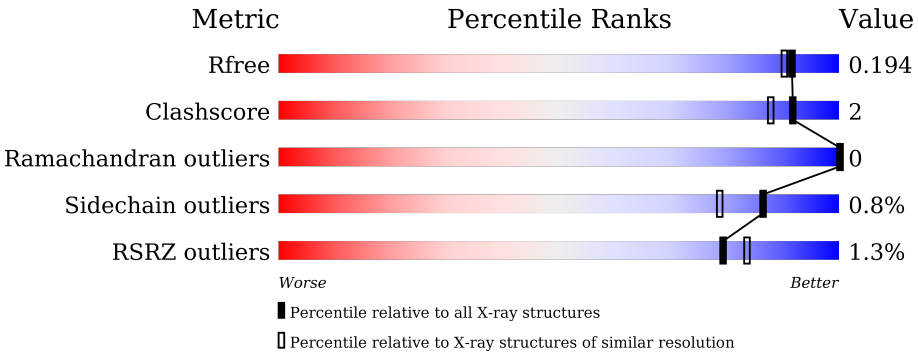
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 1.72 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	3998 (1.74-1.70)
Clashscore	102246	4425 (1.74-1.70)
Ramachandran outliers	100387	4360 (1.74-1.70)
Sidechain outliers	100360	4360 (1.74-1.70)
RSRZ outliers	91569	4010 (1.74-1.70)

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	227	3% 93% 6% ·
1	B	227	2% 94% 5% ·
1	C	227	93% 5% ·
1	D	227	93% 5% ·
1	E	227	94% · ·
1	F	227	2% 93% 6% ·

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12157 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 Halohydrin epoxidase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	1	0
			1767	1121	310	332	4			
1	B	225	Total	C	N	O	S	0	2	0
			1780	1130	311	335	4			
1	C	224	Total	C	N	O	S	0	1	0
			1765	1120	310	331	4			
1	D	224	Total	C	N	O	S	0	3	0
			1770	1125	310	331	4			
1	E	225	Total	C	N	O	S	0	2	0
			1774	1127	312	331	4			
1	F	224	Total	C	N	O	S	0	2	0
			1771	1123	310	334	4			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q46347
A	2	LYS	-	expression tag	UNP Q46347
A	71	TRP	PHE	engineered mutation	UNP Q46347
A	125	THR	GLN	engineered mutation	UNP Q46347
A	199	HIS	ASP	engineered mutation	UNP Q46347
B	1	MET	-	initiating methionine	UNP Q46347
B	2	LYS	-	expression tag	UNP Q46347
B	71	TRP	PHE	engineered mutation	UNP Q46347
B	125	THR	GLN	engineered mutation	UNP Q46347
B	199	HIS	ASP	engineered mutation	UNP Q46347
C	1	MET	-	initiating methionine	UNP Q46347
C	2	LYS	-	expression tag	UNP Q46347
C	71	TRP	PHE	engineered mutation	UNP Q46347
C	125	THR	GLN	engineered mutation	UNP Q46347
C	199	HIS	ASP	engineered mutation	UNP Q46347
D	1	MET	-	initiating methionine	UNP Q46347
D	2	LYS	-	expression tag	UNP Q46347

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Chain	Residue	Modelled	Actual	Comment	Reference
D	71	TRP	PHE	engineered mutation	UNP Q46347
D	125	THR	GLN	engineered mutation	UNP Q46347
D	199	HIS	ASP	engineered mutation	UNP Q46347
E	1	MET	-	initiating methionine	UNP Q46347
E	2	LYS	-	expression tag	UNP Q46347
E	71	TRP	PHE	engineered mutation	UNP Q46347
E	125	THR	GLN	engineered mutation	UNP Q46347
E	199	HIS	ASP	engineered mutation	UNP Q46347
F	1	MET	-	initiating methionine	UNP Q46347
F	2	LYS	-	expression tag	UNP Q46347
F	71	TRP	PHE	engineered mutation	UNP Q46347
F	125	THR	GLN	engineered mutation	UNP Q46347
F	199	HIS	ASP	engineered mutation	UNP Q46347

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	252	Total O 252 252	0	0
3	B	288	Total O 288 288	0	0
3	C	266	Total O 266 266	0	0
3	D	259	Total O 259 259	0	0
3	E	289	Total O 289 289	0	0

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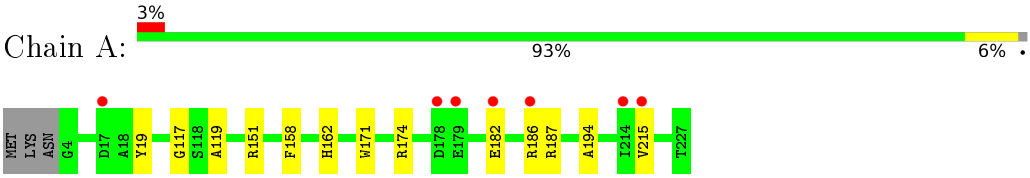
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	170	Total	O	0	0
			170	170		

3 Residue-property plots

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

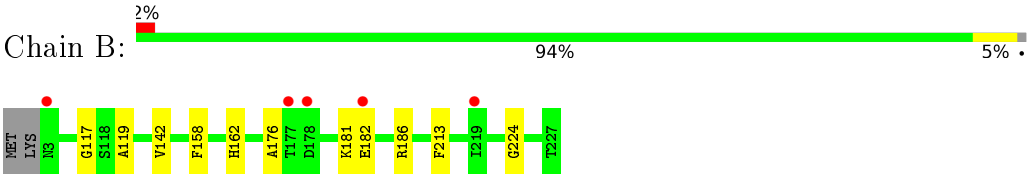
- Molecule 1: Halohydrin epoxidase B

Chain A:



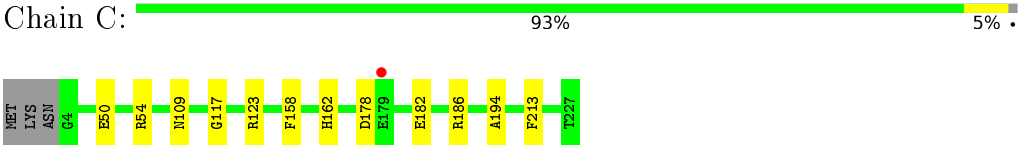
- Molecule 1: Halohydrin epoxidase B

Chain B:



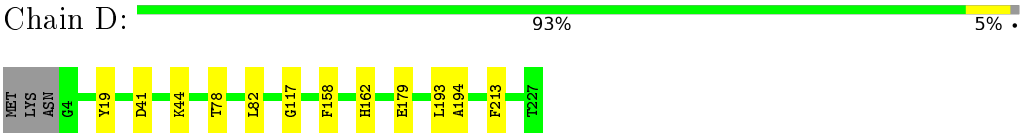
- Molecule 1: Halohydrin epoxidase B

Chain C:



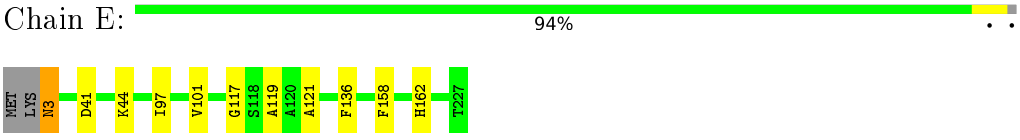
- Molecule 1: Halohydrin epoxidase B

Chain D:



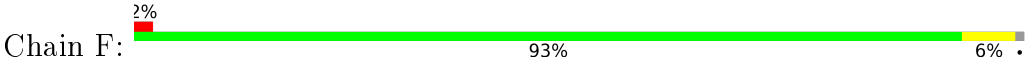
- Molecule 1: Halohydrin epoxidase B

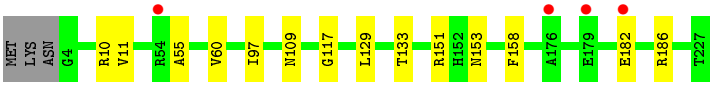
Chain E:



- Molecule 1: Halohydrin epoxidase B

Chain F:




MET
LYS
ASN
G4
R10
V11
R54
A55
V60
I97
N109
G117
L129
T133
R151
H152
N153
F158
A176
E179
E182
R186
T227

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	120.91Å 215.00Å 104.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.13 – 1.72 35.13 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.13-1.72) 99.8 (35.13-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	9.44 (at 1.72Å)	Xtriage
Refinement program	PHENIX (1.10_2152: 000)	Depositor
R, R_{free}	0.162 , 0.194 0.162 , 0.194	Depositor DCC
R_{free} test set	7211 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.005 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.011 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12157	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.05% 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, 0.333 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: 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	0.44	0/1810	0.64	0/2459
1	B	0.47	0/1826	0.63	0/2481
1	C	0.48	0/1808	0.66	0/2456
1	D	0.44	0/1819	0.64	0/2472
1	E	0.49	0/1820	0.66	0/2473
1	F	0.42	0/1817	0.60	0/2468
All	All	0.46	0/10900	0.64	0/14809

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	1767	0	1706	8	0
1	B	1780	0	1721	7	0
1	C	1765	0	1707	10	0
1	D	1770	0	1716	8	0
1	E	1774	0	1720	8	0
1	F	1771	0	1714	8	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	252	0	0	1	1
3	B	288	0	0	0	0
3	C	266	0	0	2	0
3	D	259	0	0	0	0
3	E	289	0	0	2	0
3	F	170	0	0	1	0
All	All	12157	0	10284	44	1

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 2.

All (44) 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:E:41:ASP:O	1:E:44:LYS:HE2	1.95	0.67
1:E:3:ASN:OD1	3:E:401:HOH:O	2.12	0.67
1:D:41:ASP:HB3	1:D:44:LYS:HE3	1.78	0.66
1:F:10:ARG:NH2	1:F:55:ALA:O	2.30	0.65
1:B:176:ALA:O	1:B:181:LYS:NZ	2.35	0.59
1:C:123:ARG:NH1	3:C:404:HOH:O	2.36	0.59
1:E:44:LYS:NZ	3:E:403:HOH:O	2.36	0.57
1:C:186:ARG:NH2	3:C:403:HOH:O	2.32	0.56
1:D:179:GLU:CD	1:D:179:GLU:H	2.12	0.53
1:C:117:GLY:HA3	1:C:158:PHE:CZ	2.44	0.53
1:A:182:GLU:OE2	1:A:186:ARG:HG3	2.09	0.52
1:C:178:ASP:O	1:C:182:GLU:HG3	2.10	0.52
1:F:11:VAL:HG22	1:F:60:VAL:HB	1.93	0.50
1:C:50:GLU:HG3	1:C:54:ARG:NH1	2.25	0.49
1:C:213:PHE:CD2	1:D:194:ALA:HB2	2.48	0.49
1:C:117:GLY:HA3	1:C:158:PHE:CE1	2.49	0.48
1:B:182:GLU:OE1	1:B:186:ARG:HD3	2.14	0.48
1:B:119:ALA:HB3	1:B:162:HIS:HB2	1.95	0.47
1:A:117:GLY:HA3	1:A:158:PHE:CZ	2.50	0.47
1:A:117:GLY:HA3	1:A:158:PHE:CE1	2.51	0.46
1:A:119:ALA:HB3	1:A:162:HIS:HB2	1.97	0.46
1:A:194:ALA:HB2	1:B:213:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:GLY:HA3	1:D:158:PHE:CZ	2.52	0.45
1:C:182:GLU:O	1:C:186:ARG:HG3	2.17	0.45
1:E:117:GLY:HA3	1:E:158:PHE:CZ	2.53	0.43
1:E:119:ALA:HB3	1:E:162:HIS:HB2	1.99	0.43
1:E:3:ASN:ND2	1:E:3:ASN:N	2.66	0.43
1:E:97:ILE:O	1:E:101[A]:VAL:HG23	2.18	0.43
1:C:194:ALA:HB2	1:D:213:PHE:CD2	2.54	0.42
1:B:142:VAL:HG21	1:B:158:PHE:HB2	2.00	0.42
1:F:117:GLY:HA3	1:F:158:PHE:CZ	2.55	0.42
1:A:215:VAL:HG22	1:B:224:GLY:HA3	2.00	0.42
1:F:97:ILE:HD12	1:F:97:ILE:HA	1.92	0.42
1:A:171:TRP:CE2	1:A:174:ARG:HB2	2.55	0.41
1:F:109:ASN:O	1:F:153:ASN:HB3	2.20	0.41
1:F:182:GLU:O	1:F:186:ARG:HG3	2.20	0.41
1:B:117:GLY:HA3	1:B:158:PHE:CZ	2.55	0.41
1:D:117:GLY:HA3	1:D:158:PHE:CE1	2.55	0.41
1:C:213:PHE:CE2	1:D:194:ALA:HB2	2.55	0.41
1:D:78:THR:HG23	1:D:82:LEU:HD22	2.01	0.41
1:A:187:ARG:NH1	3:A:403:HOH:O	2.40	0.41
1:F:129:LEU:O	1:F:133:THR:HG23	2.21	0.41
1:E:121:ALA:HA	1:E:136:PHE:CD1	2.56	0.40
1:F:151:ARG:NH1	3:F:415:HOH:O	2.54	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:542:HOH:O	3:A:542:HOH:O[4_555]	2.12	0.08

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	223/227 (98%)	216 (97%)	7 (3%)	0	100	100
1	B	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
1	C	223/227 (98%)	217 (97%)	6 (3%)	0	100	100
1	D	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
1	E	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
1	F	224/227 (99%)	216 (96%)	8 (4%)	0	100	100
All	All	1345/1362 (99%)	1306 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	175/178 (98%)	173 (99%)	2 (1%)	80	68
1	B	177/178 (99%)	177 (100%)	0	100	100
1	C	175/178 (98%)	173 (99%)	2 (1%)	80	68
1	D	176/178 (99%)	173 (98%)	3 (2%)	68	50
1	E	176/178 (99%)	175 (99%)	1 (1%)	90	84
1	F	177/178 (99%)	177 (100%)	0	100	100
All	All	1056/1068 (99%)	1048 (99%)	8 (1%)	86	79

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

Mol	Chain	Res	Type
1	A	19	TYR
1	A	151	ARG
1	C	109	ASN
1	C	162	HIS
1	D	19	TYR
1	D	162	HIS
1	D	193	LEU

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Mol	Chain	Res	Type
1	E	3	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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^{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	224/227 (98%)	0.00	7 (3%) 52 57	11, 18, 30, 43	0
1	B	225/227 (99%)	-0.20	5 (2%) 65 70	10, 15, 27, 48	0
1	C	224/227 (98%)	-0.20	1 (0%) 93 94	11, 16, 30, 35	0
1	D	224/227 (98%)	0.05	0 100 100	13, 19, 29, 40	0
1	E	225/227 (99%)	-0.36	0 100 100	9, 14, 26, 41	0
1	F	224/227 (98%)	0.29	4 (1%) 71 76	13, 23, 40, 53	0
All	All	1346/1362 (98%)	-0.07	17 (1%) 79 83	9, 17, 33, 53	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ASN	4.7
1	B	178	ASP	3.6
1	A	182	GLU	3.0
1	A	178	ASP	2.9
1	B	182	GLU	2.9
1	A	186	ARG	2.7
1	A	17	ASP	2.6
1	F	179	GLU	2.5
1	F	182	GLU	2.4
1	F	176	ALA	2.3
1	B	219	ILE	2.2
1	F	54	ARG	2.1
1	A	179	GLU	2.1
1	B	177	THR	2.1
1	A	214	ILE	2.1
1	C	179	GLU	2.1
1	A	215	VAL	2.1

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. 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
2	CL	B	301	1/1	0.99	0.05	-1.47	28,28,28,28	0
2	CL	D	301	1/1	0.98	0.06	-1.83	22,22,22,22	0
2	CL	A	301	1/1	0.98	0.04	-2.85	22,22,22,22	0
2	CL	F	301	1/1	0.98	0.05	-3.21	28,28,28,28	0
2	CL	E	301	1/1	0.99	0.03	-3.60	17,17,17,17	0
2	CL	C	301	1/1	1.00	0.04	-3.97	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.