wwPDB X-ray Structure Validation Summary Report (i)

Nov 5, 2023 – 04:25 PM EST

PDB ID	:	6W5O
Title	:	Class D beta-lactamase BAT-2 delta mutant
Authors	:	Smith, C.A.; Vakulenko, S.B.; Stewart, N.K.; Toth, M.
Deposited on	:	2020-03-13
Resolution	:	2.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

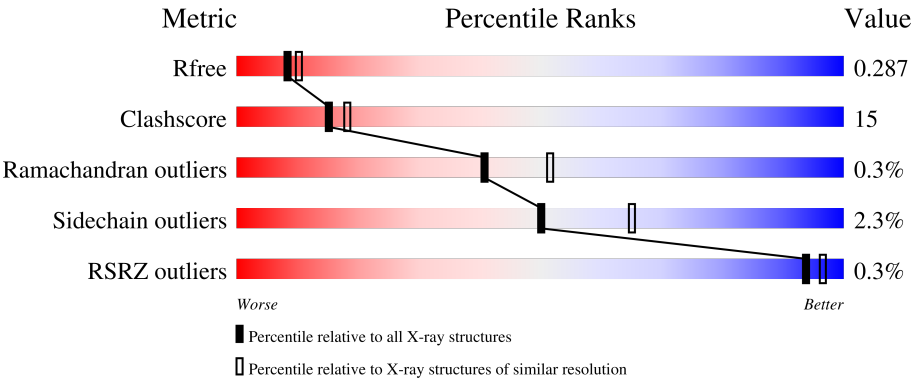
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 of 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	59% 28% • 11%
1	B	264	61% 26% • 11%
1	C	264	62% 26% • 11%
1	D	264	61% 26% • 11%
1	E	264	64% 23% • 11%

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Mol	Chain	Length	Quality of chain
1	F	264	55% 32% • 11%
1	G	264	2% 55% 32% • 11%
1	H	264	63% 25% • 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15710 atoms, of which 6 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 BAT-2 Beta-lactamase delta mutant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	2	0
			1948	1237	330	375	6			
1	B	234	Total	C	N	O	S	0	1	0
			1940	1232	327	375	6			
1	C	234	Total	C	N	O	S	0	1	0
			1940	1232	327	375	6			
1	D	234	Total	C	N	O	S	0	1	0
			1932	1226	330	370	6			
1	E	234	Total	C	N	O	S	0	0	0
			1934	1228	327	373	6			
1	F	234	Total	C	N	O	S	0	1	0
			1939	1232	330	371	6			
1	G	234	Total	C	N	O	S	0	0	0
			1934	1228	327	373	6			
1	H	234	Total	C	N	O	S	0	1	0
			1940	1232	327	375	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP A0A0H3EA14
A	?	-	LEU	deletion	UNP A0A0H3EA14
A	?	-	THR	deletion	UNP A0A0H3EA14
B	?	-	ARG	deletion	UNP A0A0H3EA14
B	?	-	LEU	deletion	UNP A0A0H3EA14
B	?	-	THR	deletion	UNP A0A0H3EA14
C	?	-	ARG	deletion	UNP A0A0H3EA14
C	?	-	LEU	deletion	UNP A0A0H3EA14
C	?	-	THR	deletion	UNP A0A0H3EA14
D	?	-	ARG	deletion	UNP A0A0H3EA14
D	?	-	LEU	deletion	UNP A0A0H3EA14
D	?	-	THR	deletion	UNP A0A0H3EA14
E	?	-	ARG	deletion	UNP A0A0H3EA14

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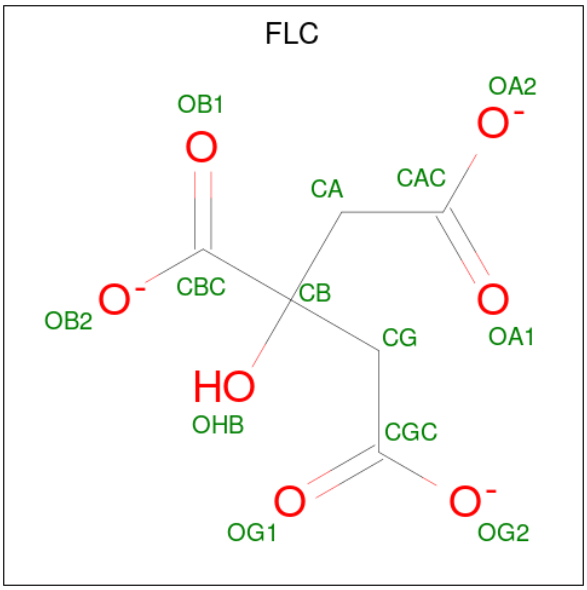
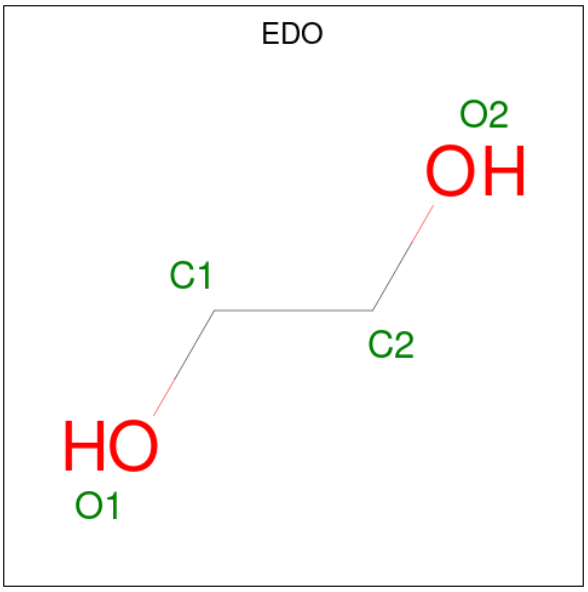
Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LEU	deletion	UNP A0A0H3EA14
E	?	-	THR	deletion	UNP A0A0H3EA14
F	?	-	ARG	deletion	UNP A0A0H3EA14
F	?	-	LEU	deletion	UNP A0A0H3EA14
F	?	-	THR	deletion	UNP A0A0H3EA14
G	?	-	ARG	deletion	UNP A0A0H3EA14
G	?	-	LEU	deletion	UNP A0A0H3EA14
G	?	-	THR	deletion	UNP A0A0H3EA14
H	?	-	ARG	deletion	UNP A0A0H3EA14
H	?	-	LEU	deletion	UNP A0A0H3EA14
H	?	-	THR	deletion	UNP A0A0H3EA14

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 13 6 7	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C H O 10 2 6 2	0	0

- Molecule 4 is water.

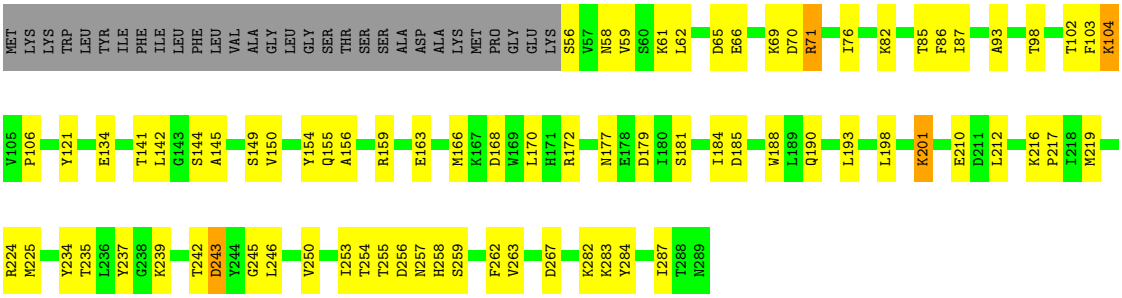
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	29	Total O 29 29	0	0
4	B	28	Total O 28 28	0	0
4	C	29	Total O 29 29	0	0
4	D	21	Total O 21 21	0	0
4	E	21	Total O 21 21	0	0
4	F	19	Total O 19 19	0	0
4	G	15	Total O 15 15	0	0
4	H	18	Total O 18 18	0	0

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.

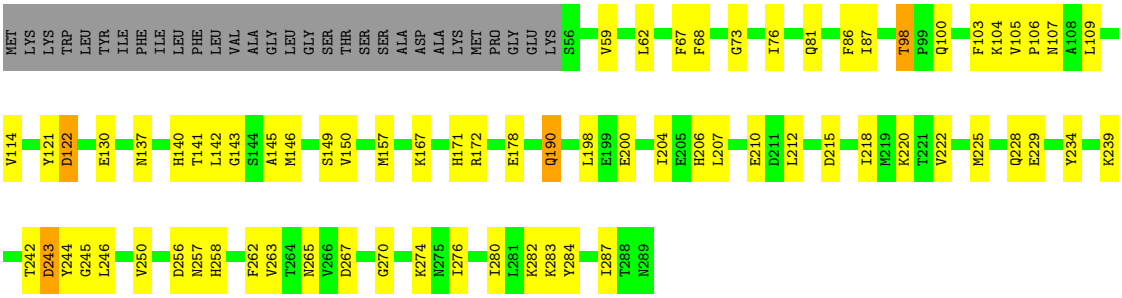
• Molecule 1: BAT-2 Beta-lactamase delta mutant

Chain A:



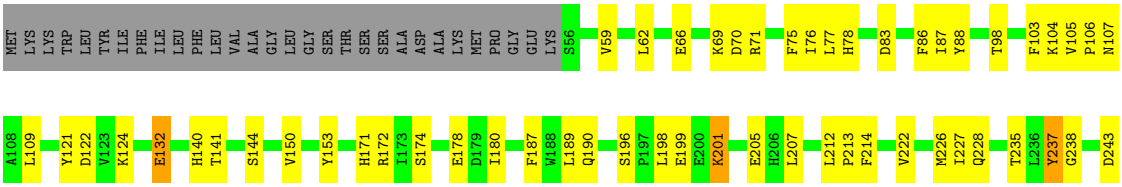
• Molecule 1: BAT-2 Beta-lactamase delta mutant

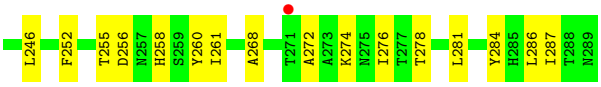
Chain B:



• Molecule 1: BAT-2 Beta-lactamase delta mutant

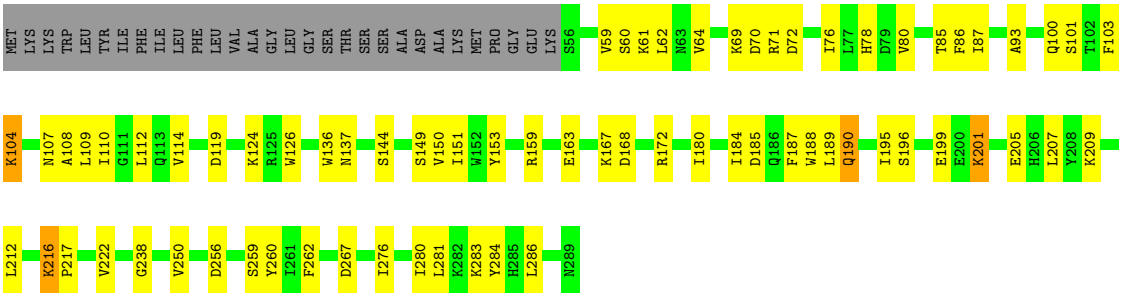
Chain C:





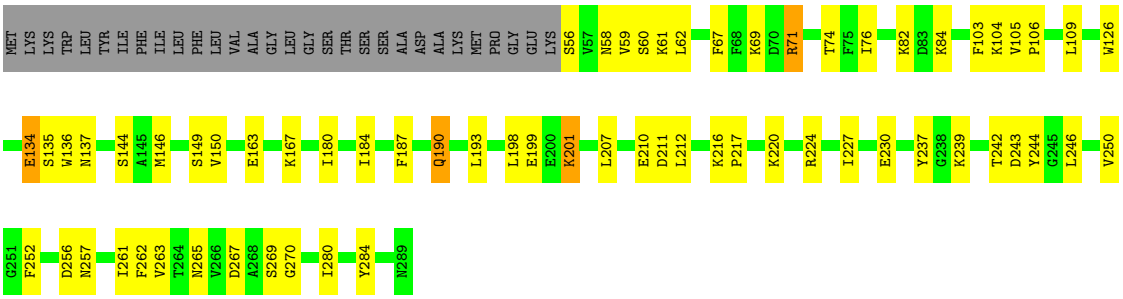
• Molecule 1: BAT-2 Beta-lactamase delta mutant

Chain D:



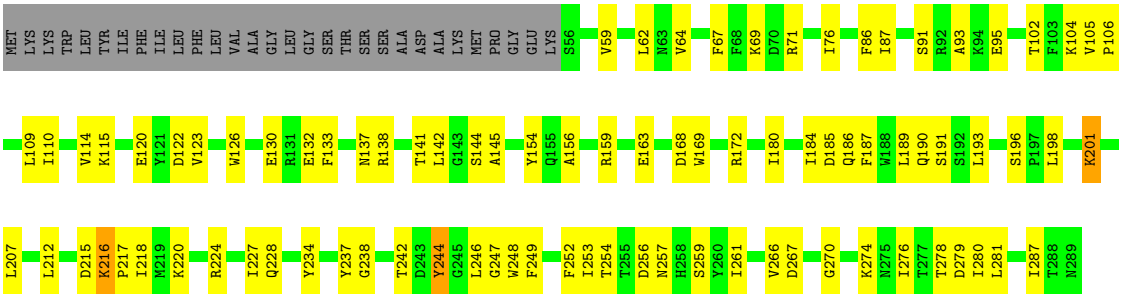
• Molecule 1: BAT-2 Beta-lactamase delta mutant

Chain E:



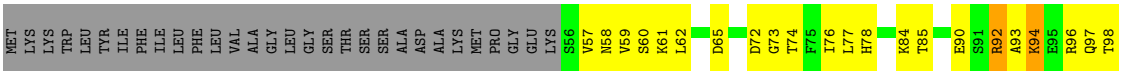
• Molecule 1: BAT-2 Beta-lactamase delta mutant

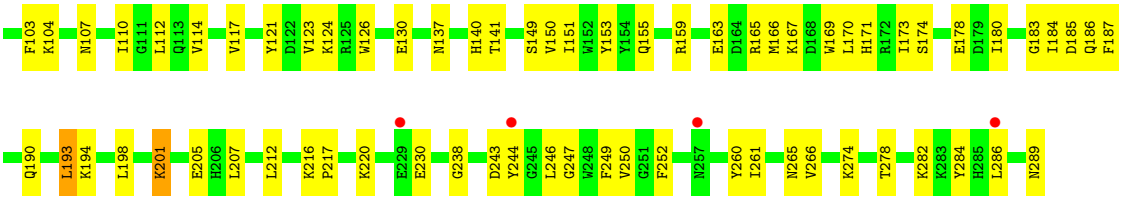
Chain F:



• Molecule 1: BAT-2 Beta-lactamase delta mutant

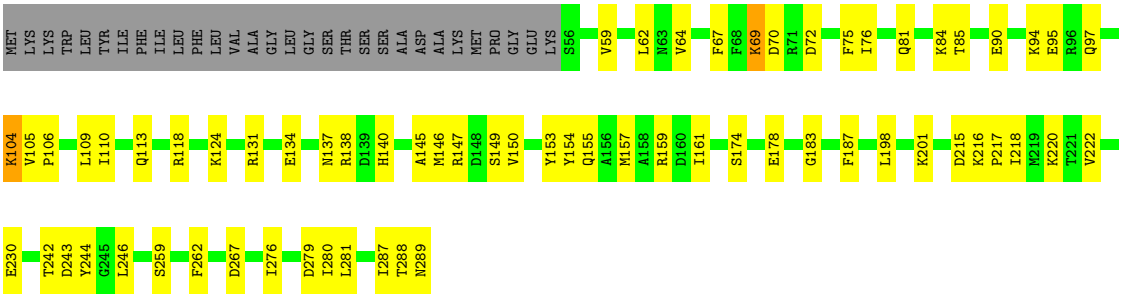
Chain G:





• Molecule 1: BAT-2 Beta-lactamase delta mutant

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	133.43Å 66.18Å 134.01Å 90.00° 91.66° 90.00°	Depositor
Resolution (Å)	60.56 – 2.55 133.95 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.6 (60.56-2.55) 89.6 (133.95-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.217 , 0.290 0.218 , 0.287	Depositor DCC
R_{free} test set	3574 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 22.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.140 for l,k,-h 0.053 for h,-k,-l 0.043 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	15710	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2864e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: EDO, FLC, KCX

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	0.52	0/1987	0.53	0/2680
1	B	0.50	0/1976	0.53	0/2666
1	C	0.65	2/1976 (0.1%)	0.57	0/2666
1	D	0.40	0/1967	0.50	0/2653
1	E	0.58	0/1967	0.56	0/2654
1	F	0.55	0/1975	0.53	0/2664
1	G	0.65	0/1967	0.61	1/2654 (0.0%)
1	H	0.44	0/1976	0.52	0/2666
All	All	0.54	2/15791 (0.0%)	0.55	1/21303 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	237	TYR	CE1-CZ	-5.67	1.31	1.38
1	C	237	TYR	CE2-CZ	-5.05	1.31	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	193	LEU	CB-CG-CD2	-5.17	102.20	111.00

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	1948	0	1878	75	0
1	B	1940	0	1865	58	0
1	C	1940	0	1865	59	0
1	D	1932	0	1863	52	0
1	E	1934	0	1859	58	0
1	F	1939	0	1870	54	0
1	G	1934	0	1859	80	0
1	H	1940	0	1865	44	0
2	B	13	0	5	0	0
3	F	4	6	6	0	0
4	A	29	0	0	2	0
4	B	28	0	0	2	0
4	C	29	0	0	1	0
4	D	21	0	0	0	0
4	E	21	0	0	1	0
4	F	19	0	0	0	0
4	G	15	0	0	1	0
4	H	18	0	0	2	0
All	All	15704	6	14935	458	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 15.

The worst 5 of 458 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:G:59:VAL:HA	1:G:62:LEU:HD13	1.36	1.07
1:A:98:THR:HG21	1:A:190:GLN:H	1.18	1.07
1:E:59:VAL:HA	1:E:62:LEU:HD13	1.42	1.02
1:A:76:ILE:HD13	1:A:198:LEU:HD23	1.42	0.98
1:B:100:GLN:HE21	1:B:100:GLN:HA	1.32	0.95

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	233/264 (88%)	210 (90%)	22 (9%)	1 (0%)	34 46
1	B	232/264 (88%)	209 (90%)	21 (9%)	2 (1%)	17 24
1	C	232/264 (88%)	213 (92%)	18 (8%)	1 (0%)	34 46
1	D	232/264 (88%)	212 (91%)	19 (8%)	1 (0%)	34 46
1	E	231/264 (88%)	215 (93%)	16 (7%)	0	100 100
1	F	232/264 (88%)	217 (94%)	15 (6%)	0	100 100
1	G	231/264 (88%)	215 (93%)	15 (6%)	1 (0%)	34 46
1	H	232/264 (88%)	214 (92%)	18 (8%)	0	100 100
All	All	1855/2112 (88%)	1705 (92%)	144 (8%)	6 (0%)	41 51

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ASP
1	B	243	ASP
1	G	244	TYR
1	B	122	ASP
1	D	256	ASP

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	211/233 (91%)	209 (99%)	2 (1%)	78 86
1	B	210/233 (90%)	206 (98%)	4 (2%)	57 72
1	C	210/233 (90%)	206 (98%)	4 (2%)	57 72
1	D	208/233 (89%)	203 (98%)	5 (2%)	49 64
1	E	209/233 (90%)	203 (97%)	6 (3%)	42 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	209/233 (90%)	201 (96%)	8 (4%)	33 45
1	G	209/233 (90%)	203 (97%)	6 (3%)	42 57
1	H	210/233 (90%)	206 (98%)	4 (2%)	57 72
All	All	1676/1864 (90%)	1637 (98%)	39 (2%)	50 65

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	244	TYR
1	H	69	LYS
1	G	65	ASP
1	G	149	SER
1	H	201	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	100	GLN
1	D	58	ASN
1	D	190	GLN
1	G	289	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)

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	KCX	A	104	1	9,11,12	0.89	0	5,12,14	1.68	1 (20%)
1	KCX	F	104	1	9,11,12	0.98	0	5,12,14	1.17	1 (20%)
1	KCX	E	104	1	9,11,12	0.89	0	5,12,14	1.75	2 (40%)
1	KCX	D	104	1	9,11,12	1.04	0	5,12,14	0.99	1 (20%)
1	KCX	G	104	1	9,11,12	0.97	0	5,12,14	1.53	1 (20%)
1	KCX	B	104	1	9,11,12	0.80	0	5,12,14	1.73	2 (40%)
1	KCX	H	104	1	9,11,12	0.93	0	5,12,14	1.60	1 (20%)
1	KCX	C	104	1	9,11,12	0.92	0	5,12,14	1.46	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	A	104	1	-	1/9/10/12	-
1	KCX	F	104	1	-	0/9/10/12	-
1	KCX	E	104	1	-	0/9/10/12	-
1	KCX	D	104	1	-	0/9/10/12	-
1	KCX	G	104	1	-	0/9/10/12	-
1	KCX	B	104	1	-	0/9/10/12	-
1	KCX	H	104	1	-	1/9/10/12	-
1	KCX	C	104	1	-	0/9/10/12	-

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	104	KCX	OQ1-CX-NZ	-3.62	119.34	124.96
1	H	104	KCX	OQ1-CX-NZ	-3.50	119.53	124.96
1	G	104	KCX	OQ1-CX-NZ	-3.24	119.93	124.96
1	C	104	KCX	OQ1-CX-NZ	-3.16	120.06	124.96
1	B	104	KCX	OQ1-CX-NZ	-2.92	120.44	124.96

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	104	KCX	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	H	104	KCX	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	104	KCX	2	0
1	D	104	KCX	1	0
1	H	104	KCX	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	F	301	-	3,3,3	0.51	0	2,2,2	0.24	0
2	FLC	B	301	-	12,12,12	0.99	0	17,17,17	1.46	2 (11%)

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	EDO	F	301	-	-	0/1/1/1	-
2	FLC	B	301	-	-	6/16/16/16	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	FLC	OB2-CBC-CB	3.94	119.89	113.05
2	B	301	FLC	OB1-CBC-CB	-2.70	118.44	122.25

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	FLC	CA-CB-CBC-OB1
2	B	301	FLC	CA-CB-CBC-OB2
2	B	301	FLC	OHB-CB-CBC-OB1
2	B	301	FLC	OHB-CB-CBC-OB2
2	B	301	FLC	CB-CA-CAC-OA1

There are no ring outliers.

No monomer is involved in short contacts.

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^{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	233/264 (88%)	-0.18	0 100 100	20, 31, 44, 52	3 (1%)
1	B	233/264 (88%)	-0.22	0 100 100	15, 27, 41, 48	3 (1%)
1	C	233/264 (88%)	-0.15	1 (0%) 92 96	19, 30, 54, 67	3 (1%)
1	D	233/264 (88%)	-0.15	0 100 100	16, 31, 54, 63	3 (1%)
1	E	233/264 (88%)	-0.26	0 100 100	15, 27, 38, 50	3 (1%)
1	F	233/264 (88%)	-0.19	0 100 100	22, 31, 43, 59	3 (1%)
1	G	233/264 (88%)	-0.03	4 (1%) 70 76	15, 32, 58, 70	3 (1%)
1	H	233/264 (88%)	-0.16	0 100 100	18, 31, 56, 71	3 (1%)
All	All	1864/2112 (88%)	-0.17	5 (0%) 94 96	15, 30, 52, 71	24 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	244	TYR	3.3
1	C	271	THR	2.9
1	G	286	LEU	2.4
1	G	257	ASN	2.2
1	G	229	GLU	2.0

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

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^{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	B-factors(Å^2)	Q<0.9
1	KCX	F	104	12/13	0.94	0.13	20,23,32,32	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KCX	B	104	12/13	0.95	0.14	13,21,24,27	0
1	KCX	G	104	12/13	0.95	0.13	14,21,24,24	1
1	KCX	D	104	12/13	0.96	0.10	15,21,24,28	1
1	KCX	H	104	12/13	0.96	0.13	19,22,26,26	1
1	KCX	C	104	12/13	0.97	0.10	18,22,23,25	1
1	KCX	A	104	12/13	0.97	0.13	19,24,27,32	2
1	KCX	E	104	12/13	0.97	0.12	19,21,23,25	1

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(Å^2)	Q<0.9
2	FLC	B	301	13/13	0.85	0.18	34,42,53,53	0
3	EDO	F	301	4/4	0.87	0.12	33,47,51,57	0

6.5 Other polymers (i)

There are no such residues in this entry.