



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 12:17 am BST

PDB ID : 6BUG
Title : Crystal structure of a membrane protein, crystal form I
Authors : Ma, D.; Wang, Z.; Xu, W.
Deposited on : 2017-12-10
Resolution : 3.27 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 ⓘ 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 : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

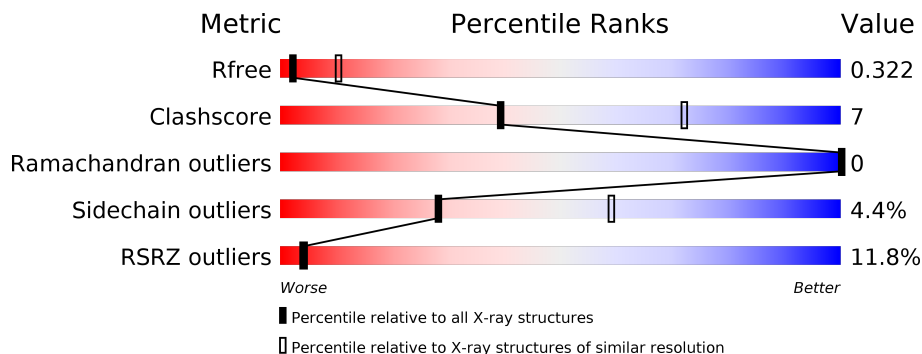
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 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.



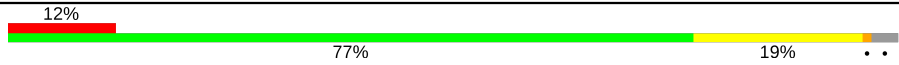
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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	82	
1	B	82	
1	E	82	
2	C	425	
2	D	425	
2	F	425	

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Mol	Chain	Length	Quality of chain
2	G	425	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '12%', a large green segment in the middle labeled '77%', and a yellow segment on the right labeled '19%'. At the far right end of the bar, there are two small black dots.</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 15679 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 D-alanyl carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	79	Total 629	C 390	N 97	O 136	P 1	S 5	0	0	0
1	B	79	Total 629	C 390	N 97	O 136	P 1	S 5	0	0	0
1	E	79	Total 629	C 390	N 97	O 136	P 1	S 5	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q5M0A6
A	-1	SER	-	expression tag	UNP Q5M0A6
A	0	HIS	-	expression tag	UNP Q5M0A6
B	-2	GLY	-	expression tag	UNP Q5M0A6
B	-1	SER	-	expression tag	UNP Q5M0A6
B	0	HIS	-	expression tag	UNP Q5M0A6
E	-2	GLY	-	expression tag	UNP Q5M0A6
E	-1	SER	-	expression tag	UNP Q5M0A6
E	0	HIS	-	expression tag	UNP Q5M0A6

- Molecule 2 is a protein called D-alanyl transfer protein DltB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	414	Total 3448	C 2327	N 548	O 553	S 20	0	0	0
2	D	414	Total 3448	C 2327	N 548	O 553	S 20	0	0	0
2	F	414	Total 3448	C 2327	N 548	O 553	S 20	0	0	0
2	G	414	Total 3448	C 2327	N 548	O 553	S 20	0	0	0

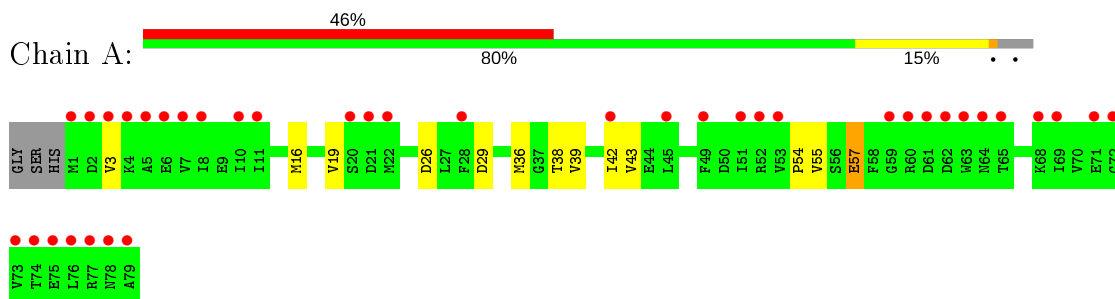
There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	416	LEU	-	expression tag	UNP Q5M4V4
C	417	GLU	-	expression tag	UNP Q5M4V4
C	418	HIS	-	expression tag	UNP Q5M4V4
C	419	HIS	-	expression tag	UNP Q5M4V4
C	420	HIS	-	expression tag	UNP Q5M4V4
C	421	HIS	-	expression tag	UNP Q5M4V4
C	422	HIS	-	expression tag	UNP Q5M4V4
C	423	HIS	-	expression tag	UNP Q5M4V4
C	424	HIS	-	expression tag	UNP Q5M4V4
C	425	HIS	-	expression tag	UNP Q5M4V4
D	416	LEU	-	expression tag	UNP Q5M4V4
D	417	GLU	-	expression tag	UNP Q5M4V4
D	418	HIS	-	expression tag	UNP Q5M4V4
D	419	HIS	-	expression tag	UNP Q5M4V4
D	420	HIS	-	expression tag	UNP Q5M4V4
D	421	HIS	-	expression tag	UNP Q5M4V4
D	422	HIS	-	expression tag	UNP Q5M4V4
D	423	HIS	-	expression tag	UNP Q5M4V4
D	424	HIS	-	expression tag	UNP Q5M4V4
D	425	HIS	-	expression tag	UNP Q5M4V4
F	416	LEU	-	expression tag	UNP Q5M4V4
F	417	GLU	-	expression tag	UNP Q5M4V4
F	418	HIS	-	expression tag	UNP Q5M4V4
F	419	HIS	-	expression tag	UNP Q5M4V4
F	420	HIS	-	expression tag	UNP Q5M4V4
F	421	HIS	-	expression tag	UNP Q5M4V4
F	422	HIS	-	expression tag	UNP Q5M4V4
F	423	HIS	-	expression tag	UNP Q5M4V4
F	424	HIS	-	expression tag	UNP Q5M4V4
F	425	HIS	-	expression tag	UNP Q5M4V4
G	416	LEU	-	expression tag	UNP Q5M4V4
G	417	GLU	-	expression tag	UNP Q5M4V4
G	418	HIS	-	expression tag	UNP Q5M4V4
G	419	HIS	-	expression tag	UNP Q5M4V4
G	420	HIS	-	expression tag	UNP Q5M4V4
G	421	HIS	-	expression tag	UNP Q5M4V4
G	422	HIS	-	expression tag	UNP Q5M4V4
G	423	HIS	-	expression tag	UNP Q5M4V4
G	424	HIS	-	expression tag	UNP Q5M4V4
G	425	HIS	-	expression tag	UNP Q5M4V4

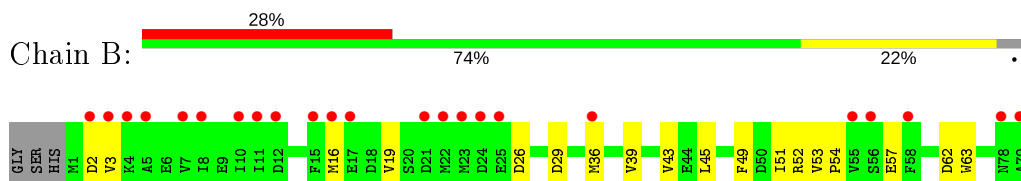
3 Residue-property plots [i](#)

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

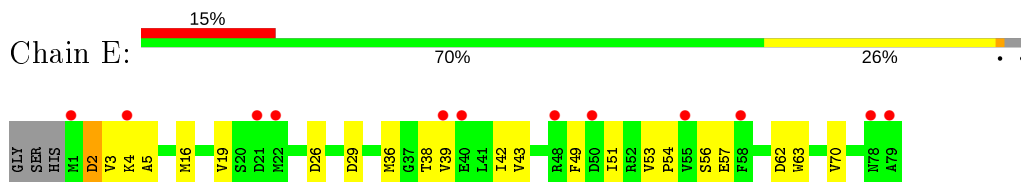
- Molecule 1: D-alanyl carrier protein



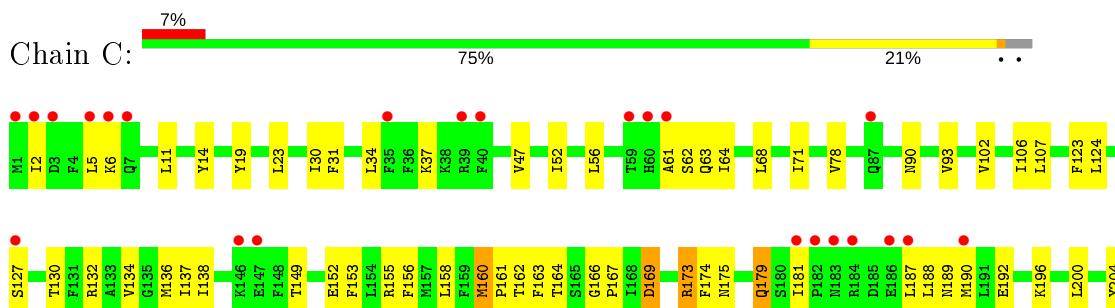
- Molecule 1: D-alanyl carrier protein

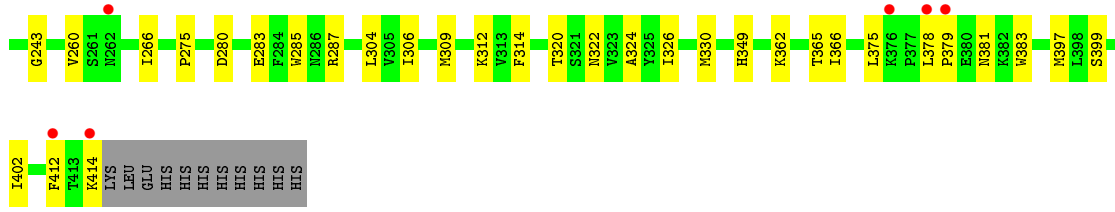


- Molecule 1: D-alanyl carrier protein

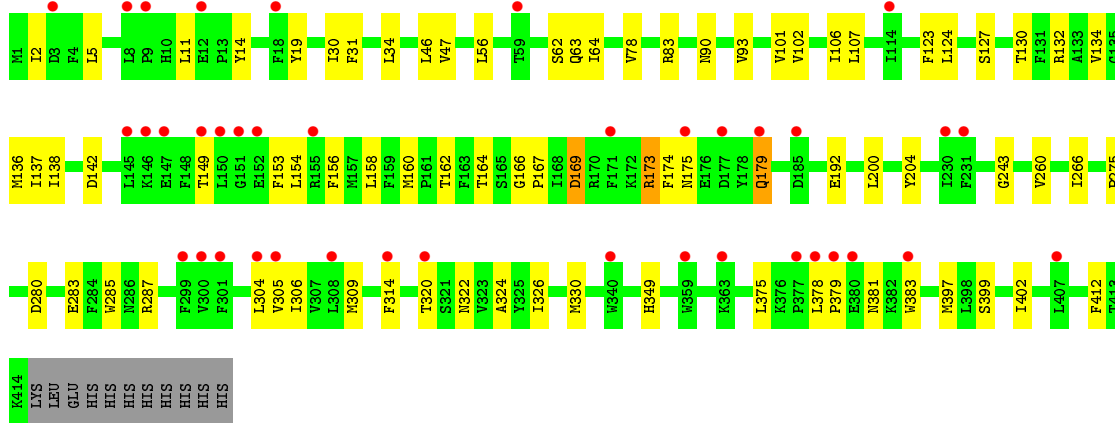
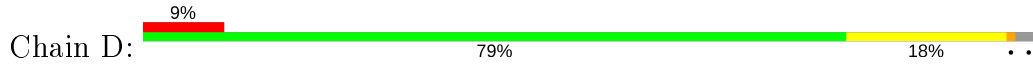


- Molecule 2: D-alanyl transfer protein DltB

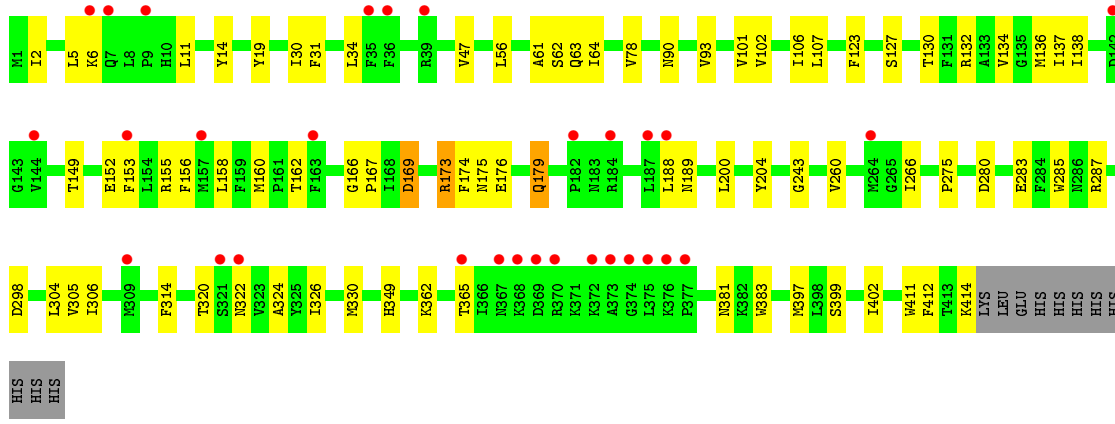
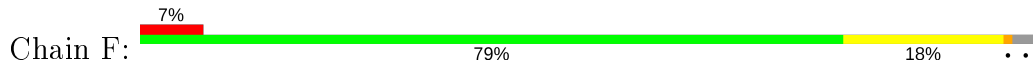




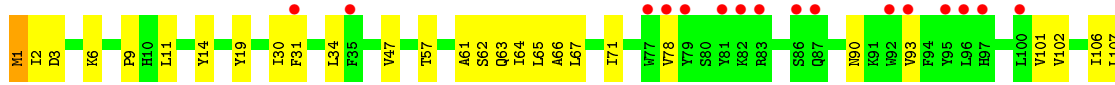
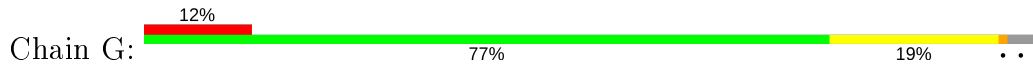
• Molecule 2: D-alanyl transfer protein DltB

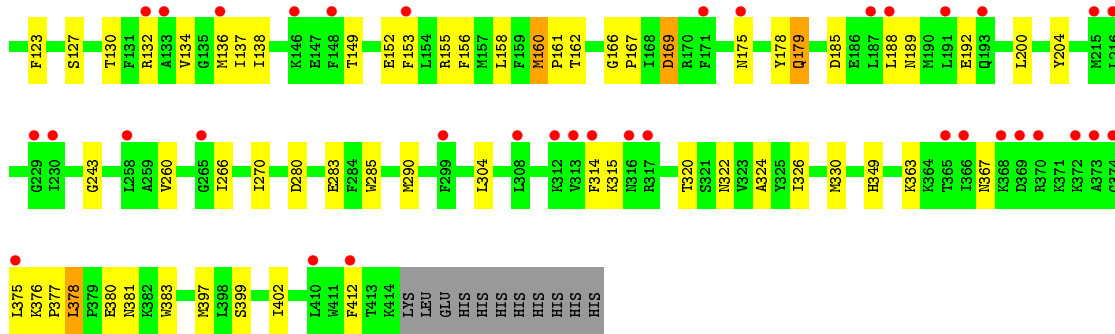


• Molecule 2: D-alanyl transfer protein DltB



• Molecule 2: D-alanyl transfer protein DltB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.71Å 121.12Å 126.53Å 90.00° 101.58° 90.00°	Depositor
Resolution (Å)	123.95 – 3.27 49.43 – 3.27	Depositor EDS
% Data completeness (in resolution range)	98.1 (123.95-3.27) 98.1 (49.43-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.25Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.289 , 0.311 0.303 , 0.322	Depositor DCC
R_{free} test set	2428 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	111.2	Xtrriage
Anisotropy	0.142	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 78.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	15679	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: SEP

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	0.50	0/624	0.68	0/841
1	B	0.47	0/624	0.67	0/841
1	E	0.47	0/624	0.65	0/841
2	C	0.48	0/3556	0.68	0/4811
2	D	0.48	0/3556	0.67	0/4811
2	F	0.48	0/3556	0.68	0/4811
2	G	0.47	0/3556	0.67	0/4811
All	All	0.48	0/16096	0.67	0/21767

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	629	0	600	10	0
1	B	629	0	600	10	0
1	E	629	0	600	12	0
2	C	3448	0	3527	65	0
2	D	3448	0	3527	48	0
2	F	3448	0	3527	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	3448	0	3527	61	0
All	All	15679	0	15908	233	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 7.

The worst 5 of 233 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)
2:G:376:LYS:HG3	2:G:377:PRO:CD	1.67	1.23
2:D:158:LEU:HD12	2:D:158:LEU:O	1.45	1.15
2:F:158:LEU:O	2:F:158:LEU:HD12	1.48	1.12
2:C:52:ILE:HG23	2:C:163:PHE:HE2	1.08	1.12
2:C:378:LEU:CD1	2:C:379:PRO:HD2	1.81	1.09

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	76/82 (93%)	67 (88%)	9 (12%)	0	100	100
1	B	76/82 (93%)	68 (90%)	8 (10%)	0	100	100
1	E	76/82 (93%)	67 (88%)	9 (12%)	0	100	100
2	C	412/425 (97%)	385 (93%)	27 (7%)	0	100	100
2	D	412/425 (97%)	385 (93%)	27 (7%)	0	100	100
2	F	412/425 (97%)	383 (93%)	29 (7%)	0	100	100
2	G	412/425 (97%)	385 (93%)	27 (7%)	0	100	100
All	All	1876/1946 (96%)	1740 (93%)	136 (7%)	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	70/72 (97%)	65 (93%)	5 (7%)	14	42
1	B	70/72 (97%)	63 (90%)	7 (10%)	7	28
1	E	70/72 (97%)	64 (91%)	6 (9%)	10	34
2	C	370/381 (97%)	355 (96%)	15 (4%)	30	61
2	D	370/381 (97%)	357 (96%)	13 (4%)	36	64
2	F	370/381 (97%)	358 (97%)	12 (3%)	39	67
2	G	370/381 (97%)	354 (96%)	16 (4%)	29	59
All	All	1690/1740 (97%)	1616 (96%)	74 (4%)	28	59

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	173	ARG
1	E	3	VAL
2	G	315	LYS
2	D	179	GLN
2	D	322	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	381	ASN
2	F	183	ASN
2	G	356	ASN
2	D	394	ASN
2	F	90	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](#)

3 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	SEP	A	35	1	8,9,10	0.78	0	8,12,14	1.14	0
1	SEP	B	35	1	8,9,10	0.77	0	8,12,14	1.13	0
1	SEP	E	35	1	8,9,10	0.77	0	8,12,14	1.14	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
1	SEP	A	35	1	-	5/5/8/10	-
1	SEP	B	35	1	-	5/5/8/10	-
1	SEP	E	35	1	-	5/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	35	SEP	N-CA-CB-OG
1	A	35	SEP	CB-OG-P-O1P
1	A	35	SEP	CB-OG-P-O2P
1	A	35	SEP	CB-OG-P-O3P
1	B	35	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 [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	78/82 (95%)	3.26	38 (48%) 0 0	154, 225, 276, 305	1 (1%)
1	B	78/82 (95%)	1.89	23 (29%) 0 0	178, 236, 281, 325	1 (1%)
1	E	78/82 (95%)	0.76	12 (15%) 2 2	136, 209, 240, 259	1 (1%)
2	C	414/425 (97%)	0.33	29 (7%) 16 16	71, 117, 176, 238	0
2	D	414/425 (97%)	0.42	39 (9%) 8 9	73, 122, 184, 231	0
2	F	414/425 (97%)	0.23	30 (7%) 15 15	66, 124, 174, 219	0
2	G	414/425 (97%)	0.50	52 (12%) 3 3	68, 133, 193, 241	0
All	All	1890/1946 (97%)	0.57	223 (11%) 4 4	66, 128, 231, 325	3 (0%)

The worst 5 of 223 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	LEU	17.0
1	A	72	GLY	15.1
1	B	21	ASP	14.5
1	A	79	ALA	14.1
1	A	7	VAL	13.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	E	35	10/11	0.87	0.35	58,58,58,58	0
1	SEP	B	35	10/11	0.88	0.24	52,52,52,52	0
1	SEP	A	35	10/11	0.89	0.30	49,49,49,49	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.