wwPDB X-ray Structure Validation Summary Report (i)

Sep 28, 2024 – 08:35 pm BST

PDB ID	:	5FJW
Title	:	Yeast delta-COP-I mu-homology domain complexed with Dsl1 WxWx(MSE) peptide
Authors	:	Suckling, R.J.; Evans, P.R.; Owen, D.J.
Deposited on	:	2015-10-13
Resolution	:	2.80 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 (i)) were used in the production of this report:

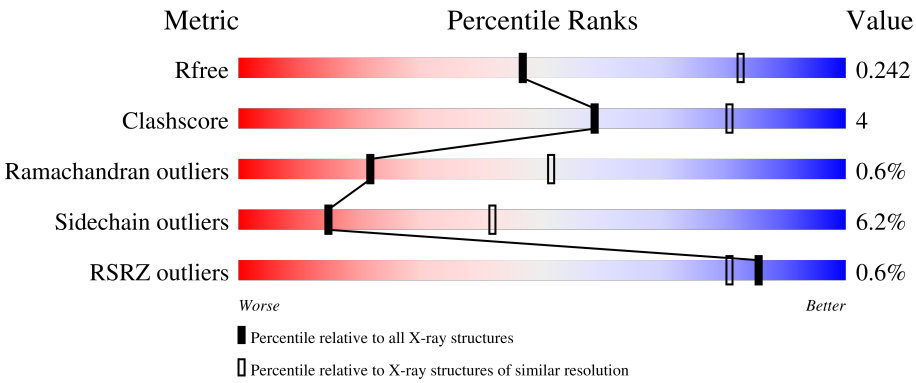
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.80 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	270	81% 14% • •
1	B	270	86% 11% • •
1	C	270	81% 16% •
1	D	270	82% 14% • •
1	E	270	% 83% 14% • •

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Mol	Chain	Length	Quality of chain
1	F	270	81% 16%
1	G	270	3% 82% 14%
1	H	270	% 77% 19%
2	L	9	100%
2	M	9	100%
2	N	9	100%
2	O	9	100%
2	P	9	78% 11% 11%
2	Q	9	89% 11%
2	R	9	67% 33%
2	S	9	78% 22%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17707 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 COATOMER SUBUNIT DELTA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	263	2066	1299	337	423	1	6	0	4	0
1	B	263	2052	1289	333	423	1	6	0	2	0
1	C	263	2047	1286	332	422	1	6	0	1	0
1	D	263	2066	1299	334	426	1	6	0	4	0
1	E	263	2047	1286	332	422	1	6	0	1	0
1	F	263	2059	1294	335	423	1	6	0	3	0
1	G	263	2059	1294	334	424	1	6	0	3	0
1	H	263	2061	1296	336	422	1	6	0	3	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	GLY	-	expression tag	UNP P43621
A	278	PRO	-	expression tag	UNP P43621
A	279	LEU	-	expression tag	UNP P43621
A	280	GLY	-	expression tag	UNP P43621
A	281	SER	-	expression tag	UNP P43621
A	282	GLU	-	expression tag	UNP P43621
A	283	GLU	-	expression tag	UNP P43621
A	284	ASP	-	expression tag	UNP P43621
A	285	VAL	-	expression tag	UNP P43621
A	286	PRO	-	expression tag	UNP P43621
A	287	GLU	-	expression tag	UNP P43621
A	404	ALA	TRP	engineered mutation	UNP P43621
B	277	GLY	-	expression tag	UNP P43621

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Chain	Residue	Modelled	Actual	Comment	Reference
B	278	PRO	-	expression tag	UNP P43621
B	279	LEU	-	expression tag	UNP P43621
B	280	GLY	-	expression tag	UNP P43621
B	281	SER	-	expression tag	UNP P43621
B	282	GLU	-	expression tag	UNP P43621
B	283	GLU	-	expression tag	UNP P43621
B	284	ASP	-	expression tag	UNP P43621
B	285	VAL	-	expression tag	UNP P43621
B	286	PRO	-	expression tag	UNP P43621
B	287	GLU	-	expression tag	UNP P43621
B	404	ALA	TRP	engineered mutation	UNP P43621
C	277	GLY	-	expression tag	UNP P43621
C	278	PRO	-	expression tag	UNP P43621
C	279	LEU	-	expression tag	UNP P43621
C	280	GLY	-	expression tag	UNP P43621
C	281	SER	-	expression tag	UNP P43621
C	282	GLU	-	expression tag	UNP P43621
C	283	GLU	-	expression tag	UNP P43621
C	284	ASP	-	expression tag	UNP P43621
C	285	VAL	-	expression tag	UNP P43621
C	286	PRO	-	expression tag	UNP P43621
C	287	GLU	-	expression tag	UNP P43621
C	404	ALA	TRP	engineered mutation	UNP P43621
D	277	GLY	-	expression tag	UNP P43621
D	278	PRO	-	expression tag	UNP P43621
D	279	LEU	-	expression tag	UNP P43621
D	280	GLY	-	expression tag	UNP P43621
D	281	SER	-	expression tag	UNP P43621
D	282	GLU	-	expression tag	UNP P43621
D	283	GLU	-	expression tag	UNP P43621
D	284	ASP	-	expression tag	UNP P43621
D	285	VAL	-	expression tag	UNP P43621
D	286	PRO	-	expression tag	UNP P43621
D	287	GLU	-	expression tag	UNP P43621
D	404	ALA	TRP	engineered mutation	UNP P43621
E	277	GLY	-	expression tag	UNP P43621
E	278	PRO	-	expression tag	UNP P43621
E	279	LEU	-	expression tag	UNP P43621
E	280	GLY	-	expression tag	UNP P43621
E	281	SER	-	expression tag	UNP P43621
E	282	GLU	-	expression tag	UNP P43621
E	283	GLU	-	expression tag	UNP P43621

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Chain	Residue	Modelled	Actual	Comment	Reference
E	284	ASP	-	expression tag	UNP P43621
E	285	VAL	-	expression tag	UNP P43621
E	286	PRO	-	expression tag	UNP P43621
E	287	GLU	-	expression tag	UNP P43621
E	404	ALA	TRP	engineered mutation	UNP P43621
F	277	GLY	-	expression tag	UNP P43621
F	278	PRO	-	expression tag	UNP P43621
F	279	LEU	-	expression tag	UNP P43621
F	280	GLY	-	expression tag	UNP P43621
F	281	SER	-	expression tag	UNP P43621
F	282	GLU	-	expression tag	UNP P43621
F	283	GLU	-	expression tag	UNP P43621
F	284	ASP	-	expression tag	UNP P43621
F	285	VAL	-	expression tag	UNP P43621
F	286	PRO	-	expression tag	UNP P43621
F	287	GLU	-	expression tag	UNP P43621
F	404	ALA	TRP	engineered mutation	UNP P43621
G	277	GLY	-	expression tag	UNP P43621
G	278	PRO	-	expression tag	UNP P43621
G	279	LEU	-	expression tag	UNP P43621
G	280	GLY	-	expression tag	UNP P43621
G	281	SER	-	expression tag	UNP P43621
G	282	GLU	-	expression tag	UNP P43621
G	283	GLU	-	expression tag	UNP P43621
G	284	ASP	-	expression tag	UNP P43621
G	285	VAL	-	expression tag	UNP P43621
G	286	PRO	-	expression tag	UNP P43621
G	287	GLU	-	expression tag	UNP P43621
G	404	ALA	TRP	engineered mutation	UNP P43621
H	277	GLY	-	expression tag	UNP P43621
H	278	PRO	-	expression tag	UNP P43621
H	279	LEU	-	expression tag	UNP P43621
H	280	GLY	-	expression tag	UNP P43621
H	281	SER	-	expression tag	UNP P43621
H	282	GLU	-	expression tag	UNP P43621
H	283	GLU	-	expression tag	UNP P43621
H	284	ASP	-	expression tag	UNP P43621
H	285	VAL	-	expression tag	UNP P43621
H	286	PRO	-	expression tag	UNP P43621
H	287	GLU	-	expression tag	UNP P43621
H	404	ALA	TRP	engineered mutation	UNP P43621

- Molecule 2 is a protein called PROTEIN TRANSPORT PROTEIN DSL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
2	L	9	87	53	12	21	1	0	0	0
2	M	9	87	53	12	21	1	0	0	0
2	N	9	87	53	12	21	1	0	0	0
2	O	9	87	53	12	21	1	0	0	0
2	P	9	87	53	12	21	1	0	0	0
2	Q	9	87	53	12	21	1	0	0	0
2	R	9	87	53	12	21	1	0	0	0
2	S	9	87	53	12	21	1	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	417	MSE	VAL	conflict	UNP P53847
M	417	MSE	VAL	conflict	UNP P53847
N	417	MSE	VAL	conflict	UNP P53847
O	417	MSE	VAL	conflict	UNP P53847
P	417	MSE	VAL	conflict	UNP P53847
Q	417	MSE	VAL	conflict	UNP P53847
R	417	MSE	VAL	conflict	UNP P53847
S	417	MSE	VAL	conflict	UNP P53847

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	100	100	100	0	0
3	B	106	106	106	0	0
3	C	90	90	90	0	0
3	D	97	97	97	0	0
3	E	50	50	50	0	0
3	F	42	42	42	0	0

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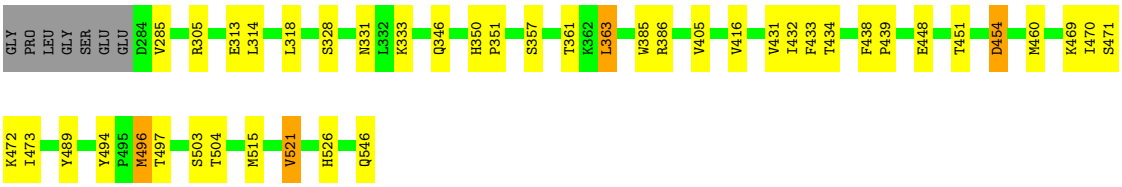
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	43	Total O 43 43	0	0
3	H	21	Total O 21 21	0	0
3	L	3	Total O 3 3	0	0
3	M	2	Total O 2 2	0	0

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.

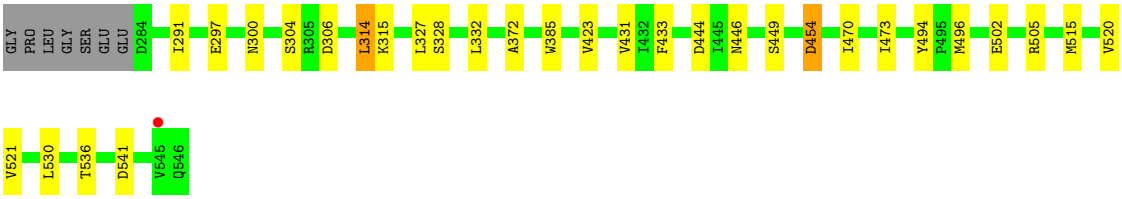
• Molecule 1: COATOMER SUBUNIT DELTA

Chain A:



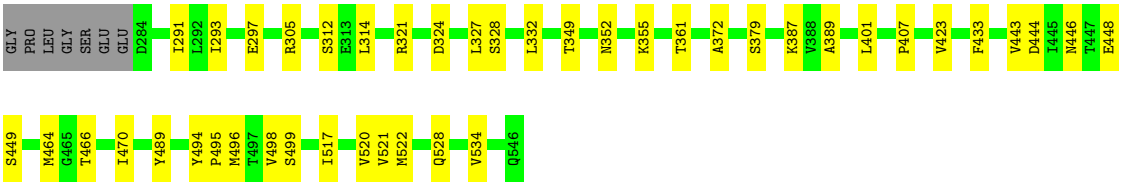
• Molecule 1: COATOMER SUBUNIT DELTA

Chain B:



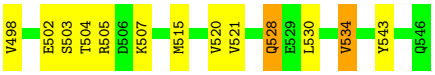
• Molecule 1: COATOMER SUBUNIT DELTA

Chain C:



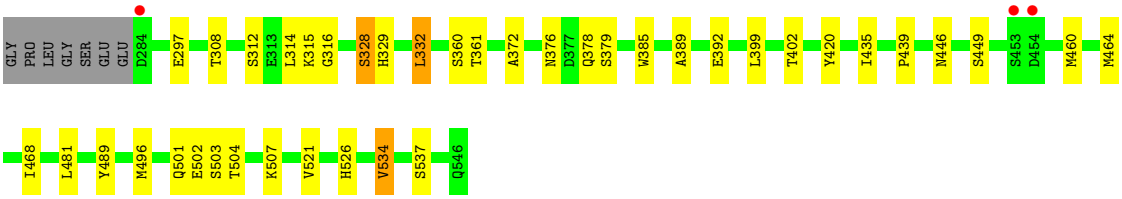
• Molecule 1: COATOMER SUBUNIT DELTA

Chain D:



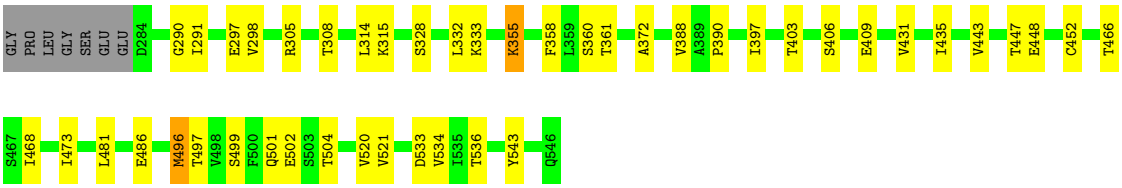
• Molecule 1: COATOMER SUBUNIT DELTA

Chain E:



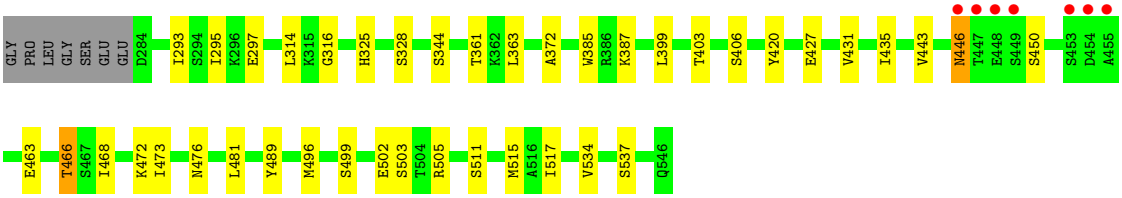
• Molecule 1: COATOMER SUBUNIT DELTA

Chain F:



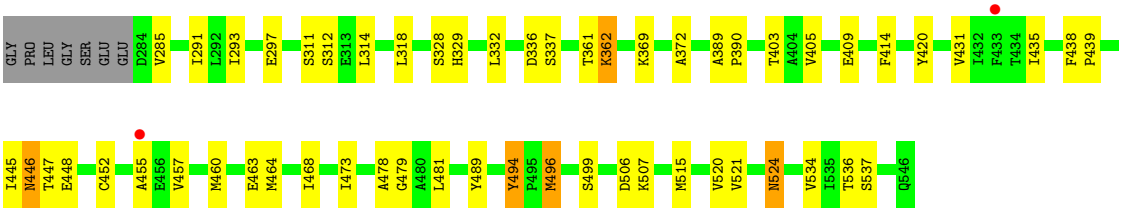
• Molecule 1: COATOMER SUBUNIT DELTA

Chain G:



• Molecule 1: COATOMER SUBUNIT DELTA

Chain H:



• Molecule 2: PROTEIN TRANSPORT PROTEIN DSL1

Chain L:

There are no outlier residues recorded for this chain.

• Molecule 2: PROTEIN TRANSPORT PROTEIN DSL1

Chain M: 100%

There are no outlier residues recorded for this chain.

• Molecule 2: PROTEIN TRANSPORT PROTEIN DSL1

Chain N: 100%

There are no outlier residues recorded for this chain.

• Molecule 2: PROTEIN TRANSPORT PROTEIN DSL1

Chain O: 100%

There are no outlier residues recorded for this chain.

• Molecule 2: PROTEIN TRANSPORT PROTEIN DSL1

Chain P: 78% 11% 11%

D411 D412 D419

• Molecule 2: PROTEIN TRANSPORT PROTEIN DSL1

Chain Q: 89% 11%

D411 D419

• Molecule 2: PROTEIN TRANSPORT PROTEIN DSL1

Chain R: 67% 33%

D411 N414 W415 E416 D419

• Molecule 2: PROTEIN TRANSPORT PROTEIN DSL1

Chain S: 78% 22%

D411 D412 W413 M417 E418 D419

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	68.41Å 79.30Å 163.35Å 79.71° 87.50° 83.60°	Depositor
Resolution (Å)	160.67 – 2.80 160.67 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (160.67-2.80) 97.8 (160.67-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.170 , 0.239 0.179 , 0.242	Depositor DCC
R_{free} test set	4059 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	73.8	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17707	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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 (i)

5.1 Standard geometry (i)

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	0.67	0/2107	0.87	2/2849 (0.1%)
1	B	0.64	0/2087	0.85	1/2824 (0.0%)
1	C	0.66	0/2079	0.85	1/2813 (0.0%)
1	D	0.61	0/2107	0.83	0/2849
1	E	0.55	0/2079	0.80	0/2813
1	F	0.56	0/2098	0.77	1/2839 (0.0%)
1	G	0.56	0/2098	0.78	1/2839 (0.0%)
1	H	0.55	0/2101	0.76	0/2843
2	L	0.87	0/89	0.94	0/118
2	M	0.67	0/89	0.78	0/118
2	N	0.80	0/89	0.71	0/118
2	O	0.75	0/89	1.00	0/118
2	P	0.64	0/89	0.79	0/118
2	Q	0.69	0/89	0.71	0/118
2	R	0.53	0/89	0.73	0/118
2	S	0.68	0/89	0.70	0/118
All	All	0.61	0/17468	0.81	6/23613 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	2
1	H	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	444	ASP	CB-CG-OD1	5.51	123.26	118.30
1	G	505	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	363	LEU	CA-CB-CG	5.10	127.04	115.30
1	A	496	MSE	N-CA-CB	5.10	119.78	110.60
1	C	444	ASP	CB-CG-OD1	5.07	122.86	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	285	VAL	Peptide
1	D	446	ASN	Peptide
1	D	454	ASP	Peptide
1	H	285	VAL	Peptide

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	2066	0	2048	23	0
1	B	2052	0	2022	15	0
1	C	2047	0	2016	17	0
1	D	2066	0	2035	18	0
1	E	2047	0	2016	17	0
1	F	2059	0	2029	15	0
1	G	2059	0	2027	17	0
1	H	2061	0	2030	27	0
2	L	87	0	58	0	0
2	M	87	0	58	0	0
2	N	87	0	58	0	0
2	O	87	0	58	0	0
2	P	87	0	58	1	0
2	Q	87	0	58	0	0
2	R	87	0	58	0	0
2	S	87	0	58	0	0
3	A	100	0	0	1	0
3	B	106	0	0	0	0
3	C	90	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	97	0	0	1	0
3	E	50	0	0	2	0
3	F	42	0	0	0	0
3	G	43	0	0	1	0
3	H	21	0	0	0	0
3	L	3	0	0	0	0
3	M	2	0	0	0	0
All	All	17707	0	16687	147	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 4.

The worst 5 of 147 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:H:468:ILE:HG21	1:H:481:LEU:HD21	1.74	0.69
1:A:494:TYR:CZ	1:A:496:MSE:HE3	2.32	0.65
1:A:494:TYR:CE1	1:A:496:MSE:HE3	2.32	0.65
1:H:403:THR:HG21	1:H:496:MSE:CE	2.26	0.64
1:A:346:GLN:HE22	1:A:386[A]:ARG:HE	1.45	0.63

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	265/270 (98%)	253 (96%)	12 (4%)	0	100	100
1	B	263/270 (97%)	249 (95%)	14 (5%)	0	100	100
1	C	262/270 (97%)	248 (95%)	13 (5%)	1 (0%)	30	61
1	D	265/270 (98%)	248 (94%)	15 (6%)	2 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	262/270 (97%)	242 (92%)	20 (8%)	0	100	100
1	F	264/270 (98%)	247 (94%)	16 (6%)	1 (0%)	30	61
1	G	264/270 (98%)	248 (94%)	13 (5%)	3 (1%)	12	37
1	H	264/270 (98%)	233 (88%)	27 (10%)	4 (2%)	8	29
2	L	7/9 (78%)	7 (100%)	0	0	100	100
2	M	7/9 (78%)	7 (100%)	0	0	100	100
2	N	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	O	7/9 (78%)	7 (100%)	0	0	100	100
2	P	7/9 (78%)	5 (71%)	1 (14%)	1 (14%)	0	0
2	Q	7/9 (78%)	7 (100%)	0	0	100	100
2	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	S	7/9 (78%)	7 (100%)	0	0	100	100
All	All	2165/2232 (97%)	2020 (93%)	133 (6%)	12 (1%)	22	51

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	352	ASN
1	D	476	ASN
1	G	446	ASN
1	G	476	ASN
2	P	412	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	239/236 (101%)	225 (94%)	14 (6%)	16	44
1	B	237/236 (100%)	229 (97%)	8 (3%)	32	66
1	C	236/236 (100%)	223 (94%)	13 (6%)	18	47
1	D	239/236 (101%)	225 (94%)	14 (6%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	236/236 (100%)	219 (93%)	17 (7%)	12	34
1	F	238/236 (101%)	215 (90%)	23 (10%)	6	21
1	G	238/236 (101%)	226 (95%)	12 (5%)	20	51
1	H	238/236 (101%)	221 (93%)	17 (7%)	12	35
2	L	9/8 (112%)	9 (100%)	0	100	100
2	M	9/8 (112%)	9 (100%)	0	100	100
2	N	9/8 (112%)	9 (100%)	0	100	100
2	O	9/8 (112%)	9 (100%)	0	100	100
2	P	9/8 (112%)	9 (100%)	0	100	100
2	Q	9/8 (112%)	8 (89%)	1 (11%)	5	16
2	R	9/8 (112%)	6 (67%)	3 (33%)	0	0
2	S	9/8 (112%)	7 (78%)	2 (22%)	1	2
All	All	1973/1952 (101%)	1849 (94%)	124 (6%)	15	42

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	464	MSE
1	H	494	TYR
1	F	360	SER
1	H	489	TYR
2	Q	419	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	546	GLN
1	E	331	ASN
1	H	528	GLN
1	H	462	GLN
1	H	524	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	258/270 (95%)	-0.85	0	100	100	31, 62, 103, 142	3 (1%)
1	B	258/270 (95%)	-0.75	1 (0%)	89	85	36, 65, 106, 154	2 (0%)
1	C	258/270 (95%)	-0.60	0	100	100	26, 73, 122, 153	0
1	D	258/270 (95%)	-0.67	0	100	100	43, 72, 120, 161	3 (1%)
1	E	258/270 (95%)	-0.36	3 (1%)	76	69	53, 87, 170, 198	0
1	F	258/270 (95%)	-0.38	0	100	100	41, 92, 168, 188	2 (0%)
1	G	258/270 (95%)	-0.21	7 (2%)	56	47	46, 94, 177, 211	2 (0%)
1	H	258/270 (95%)	-0.13	2 (0%)	82	77	57, 109, 184, 208	2 (0%)
2	L	8/9 (88%)	-0.40	0	100	100	59, 88, 120, 124	0
2	M	8/9 (88%)	-0.49	0	100	100	63, 95, 119, 121	0
2	N	8/9 (88%)	-0.23	0	100	100	76, 109, 130, 147	0
2	O	8/9 (88%)	-0.25	0	100	100	59, 103, 127, 132	0
2	P	8/9 (88%)	-0.80	0	100	100	83, 106, 112, 113	0
2	Q	8/9 (88%)	-0.37	0	100	100	73, 104, 118, 128	0
2	R	8/9 (88%)	-0.46	0	100	100	78, 106, 124, 137	0
2	S	8/9 (88%)	-0.29	0	100	100	104, 128, 136, 158	0
All	All	2128/2232 (95%)	-0.49	13 (0%)	85	81	26, 81, 157, 211	14 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	545	VAL	3.8
1	G	449	SER	3.5
1	G	453	SER	3.3
1	G	455	ALA	3.1
1	G	448	GLU	2.3

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.