



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 23, 2021 – 08:12 am BST

PDB ID : 5DTL
Title : Crystal structure of mEos2-A69T fluorescent protein
Authors : Berardozzi, R.; Adam, V.; Martins, A.; Bourgeois, D.
Deposited on : 2015-09-18
Resolution : 2.70 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 : 2.23.1
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) : 2.23.1

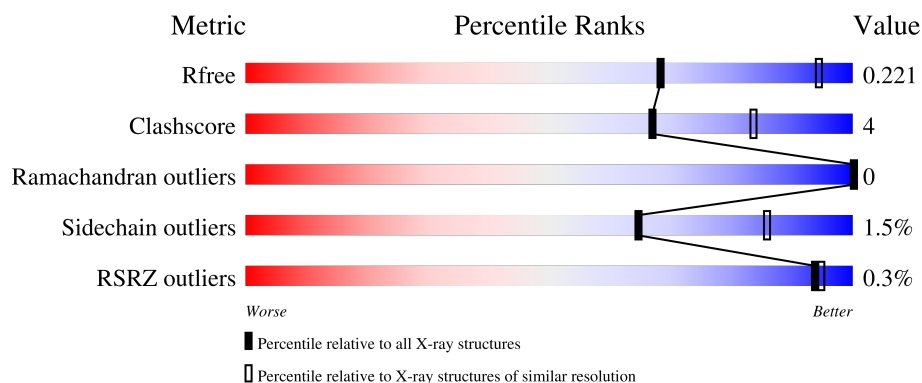
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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 $\leq 5\%$. 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	224	<div> <div>91%</div> <div>7%</div> <div>.</div> </div>
1	B	224	<div> <div>89%</div> <div>8%</div> <div>..</div> </div>
1	C	224	<div> <div>92%</div> <div>7%</div> <div>.</div> </div>
1	D	224	<div> <div>89%</div> <div>8%</div> <div>..</div> </div>
1	E	224	<div> <div>91%</div> <div>7%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	224	 87% 10% ..
1	G	224	 88% 9% .
1	H	224	 89% 8% .
1	I	224	 92% 7% .
1	J	224	 88% 9% ..
1	K	224	 89% 8% ..
1	L	224	 89% 7% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21915 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 Green to red photoconvertible GFP-like protein EosFP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1787	1144	304	329	10			
1	B	220	Total	C	N	O	S	0	0	0
			1787	1144	304	329	10			
1	C	220	Total	C	N	O	S	0	0	0
			1787	1144	304	329	10			
1	D	220	Total	C	N	O	S	0	0	0
			1787	1144	304	329	10			
1	E	220	Total	C	N	O	S	0	0	0
			1787	1144	304	329	10			
1	F	220	Total	C	N	O	S	0	0	0
			1787	1144	304	329	10			
1	G	220	Total	C	N	O	S	0	0	0
			1787	1144	304	329	10			
1	H	220	Total	C	N	O	S	0	0	0
			1787	1144	304	329	10			
1	I	220	Total	C	N	O	S	0	0	0
			1787	1144	304	329	10			
1	J	220	Total	C	N	O	S	0	0	0
			1787	1144	304	329	10			
1	K	220	Total	C	N	O	S	0	0	0
			1787	1144	304	329	10			
1	L	220	Total	C	N	O	S	0	0	0
			1787	1144	304	329	10			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	LYS	ASN	engineered mutation	UNP Q5S6Z9
A	64	5SQ	HIS	chromophore	UNP Q5S6Z9
A	64	5SQ	TYR	chromophore	UNP Q5S6Z9
A	64	5SQ	GLY	chromophore	UNP Q5S6Z9
A	69	THR	ALA	engineered mutation	UNP Q5S6Z9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	LYS	GLU	engineered mutation	UNP Q5S6Z9
A	74	ASN	HIS	engineered mutation	UNP Q5S6Z9
A	121	TYR	HIS	engineered mutation	UNP Q5S6Z9
A	123	THR	VAL	engineered mutation	UNP Q5S6Z9
A	158	HIS	THR	engineered mutation	UNP Q5S6Z9
B	11	LYS	ASN	engineered mutation	UNP Q5S6Z9
B	64	5SQ	HIS	chromophore	UNP Q5S6Z9
B	64	5SQ	TYR	chromophore	UNP Q5S6Z9
B	64	5SQ	GLY	chromophore	UNP Q5S6Z9
B	69	THR	ALA	engineered mutation	UNP Q5S6Z9
B	70	LYS	GLU	engineered mutation	UNP Q5S6Z9
B	74	ASN	HIS	engineered mutation	UNP Q5S6Z9
B	121	TYR	HIS	engineered mutation	UNP Q5S6Z9
B	123	THR	VAL	engineered mutation	UNP Q5S6Z9
B	158	HIS	THR	engineered mutation	UNP Q5S6Z9
C	11	LYS	ASN	engineered mutation	UNP Q5S6Z9
C	64	5SQ	HIS	chromophore	UNP Q5S6Z9
C	64	5SQ	TYR	chromophore	UNP Q5S6Z9
C	64	5SQ	GLY	chromophore	UNP Q5S6Z9
C	69	THR	ALA	engineered mutation	UNP Q5S6Z9
C	70	LYS	GLU	engineered mutation	UNP Q5S6Z9
C	74	ASN	HIS	engineered mutation	UNP Q5S6Z9
C	121	TYR	HIS	engineered mutation	UNP Q5S6Z9
C	123	THR	VAL	engineered mutation	UNP Q5S6Z9
C	158	HIS	THR	engineered mutation	UNP Q5S6Z9
D	11	LYS	ASN	engineered mutation	UNP Q5S6Z9
D	64	5SQ	HIS	chromophore	UNP Q5S6Z9
D	64	5SQ	TYR	chromophore	UNP Q5S6Z9
D	64	5SQ	GLY	chromophore	UNP Q5S6Z9
D	69	THR	ALA	engineered mutation	UNP Q5S6Z9
D	70	LYS	GLU	engineered mutation	UNP Q5S6Z9
D	74	ASN	HIS	engineered mutation	UNP Q5S6Z9
D	121	TYR	HIS	engineered mutation	UNP Q5S6Z9
D	123	THR	VAL	engineered mutation	UNP Q5S6Z9
D	158	HIS	THR	engineered mutation	UNP Q5S6Z9
E	11	LYS	ASN	engineered mutation	UNP Q5S6Z9
E	64	5SQ	HIS	chromophore	UNP Q5S6Z9
E	64	5SQ	TYR	chromophore	UNP Q5S6Z9
E	64	5SQ	GLY	chromophore	UNP Q5S6Z9
E	69	THR	ALA	engineered mutation	UNP Q5S6Z9
E	70	LYS	GLU	engineered mutation	UNP Q5S6Z9
E	74	ASN	HIS	engineered mutation	UNP Q5S6Z9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	121	TYR	HIS	engineered mutation	UNP Q5S6Z9
E	123	THR	VAL	engineered mutation	UNP Q5S6Z9
E	158	HIS	THR	engineered mutation	UNP Q5S6Z9
F	11	LYS	ASN	engineered mutation	UNP Q5S6Z9
F	64	5SQ	HIS	chromophore	UNP Q5S6Z9
F	64	5SQ	TYR	chromophore	UNP Q5S6Z9
F	64	5SQ	GLY	chromophore	UNP Q5S6Z9
F	69	THR	ALA	engineered mutation	UNP Q5S6Z9
F	70	LYS	GLU	engineered mutation	UNP Q5S6Z9
F	74	ASN	HIS	engineered mutation	UNP Q5S6Z9
F	121	TYR	HIS	engineered mutation	UNP Q5S6Z9
F	123	THR	VAL	engineered mutation	UNP Q5S6Z9
F	158	HIS	THR	engineered mutation	UNP Q5S6Z9
G	11	LYS	ASN	engineered mutation	UNP Q5S6Z9
G	64	5SQ	HIS	chromophore	UNP Q5S6Z9
G	64	5SQ	TYR	chromophore	UNP Q5S6Z9
G	64	5SQ	GLY	chromophore	UNP Q5S6Z9
G	69	THR	ALA	engineered mutation	UNP Q5S6Z9
G	70	LYS	GLU	engineered mutation	UNP Q5S6Z9
G	74	ASN	HIS	engineered mutation	UNP Q5S6Z9
G	121	TYR	HIS	engineered mutation	UNP Q5S6Z9
G	123	THR	VAL	engineered mutation	UNP Q5S6Z9
G	158	HIS	THR	engineered mutation	UNP Q5S6Z9
H	11	LYS	ASN	engineered mutation	UNP Q5S6Z9
H	64	5SQ	HIS	chromophore	UNP Q5S6Z9
H	64	5SQ	TYR	chromophore	UNP Q5S6Z9
H	64	5SQ	GLY	chromophore	UNP Q5S6Z9
H	69	THR	ALA	engineered mutation	UNP Q5S6Z9
H	70	LYS	GLU	engineered mutation	UNP Q5S6Z9
H	74	ASN	HIS	engineered mutation	UNP Q5S6Z9
H	121	TYR	HIS	engineered mutation	UNP Q5S6Z9
H	123	THR	VAL	engineered mutation	UNP Q5S6Z9
H	158	HIS	THR	engineered mutation	UNP Q5S6Z9
I	11	LYS	ASN	engineered mutation	UNP Q5S6Z9
I	64	5SQ	HIS	chromophore	UNP Q5S6Z9
I	64	5SQ	TYR	chromophore	UNP Q5S6Z9
I	64	5SQ	GLY	chromophore	UNP Q5S6Z9
I	69	THR	ALA	engineered mutation	UNP Q5S6Z9
I	70	LYS	GLU	engineered mutation	UNP Q5S6Z9
I	74	ASN	HIS	engineered mutation	UNP Q5S6Z9
I	121	TYR	HIS	engineered mutation	UNP Q5S6Z9
I	123	THR	VAL	engineered mutation	UNP Q5S6Z9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	158	HIS	THR	engineered mutation	UNP Q5S6Z9
J	11	LYS	ASN	engineered mutation	UNP Q5S6Z9
J	64	5SQ	HIS	chromophore	UNP Q5S6Z9
J	64	5SQ	TYR	chromophore	UNP Q5S6Z9
J	64	5SQ	GLY	chromophore	UNP Q5S6Z9
J	69	THR	ALA	engineered mutation	UNP Q5S6Z9
J	70	LYS	GLU	engineered mutation	UNP Q5S6Z9
J	74	ASN	HIS	engineered mutation	UNP Q5S6Z9
J	121	TYR	HIS	engineered mutation	UNP Q5S6Z9
J	123	THR	VAL	engineered mutation	UNP Q5S6Z9
J	158	HIS	THR	engineered mutation	UNP Q5S6Z9
K	11	LYS	ASN	engineered mutation	UNP Q5S6Z9
K	64	5SQ	HIS	chromophore	UNP Q5S6Z9
K	64	5SQ	TYR	chromophore	UNP Q5S6Z9
K	64	5SQ	GLY	chromophore	UNP Q5S6Z9
K	69	THR	ALA	engineered mutation	UNP Q5S6Z9
K	70	LYS	GLU	engineered mutation	UNP Q5S6Z9
K	74	ASN	HIS	engineered mutation	UNP Q5S6Z9
K	121	TYR	HIS	engineered mutation	UNP Q5S6Z9
K	123	THR	VAL	engineered mutation	UNP Q5S6Z9
K	158	HIS	THR	engineered mutation	UNP Q5S6Z9
L	11	LYS	ASN	engineered mutation	UNP Q5S6Z9
L	64	5SQ	HIS	chromophore	UNP Q5S6Z9
L	64	5SQ	TYR	chromophore	UNP Q5S6Z9
L	64	5SQ	GLY	chromophore	UNP Q5S6Z9
L	69	THR	ALA	engineered mutation	UNP Q5S6Z9
L	70	LYS	GLU	engineered mutation	UNP Q5S6Z9
L	74	ASN	HIS	engineered mutation	UNP Q5S6Z9
L	121	TYR	HIS	engineered mutation	UNP Q5S6Z9
L	123	THR	VAL	engineered mutation	UNP Q5S6Z9
L	158	HIS	THR	engineered mutation	UNP Q5S6Z9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	49	Total O 49 49	0	0
2	B	41	Total O 41 41	0	0
2	C	37	Total O 37 37	0	0
2	D	29	Total O 29 29	0	0

Continued on next page...

Continued from previous page...

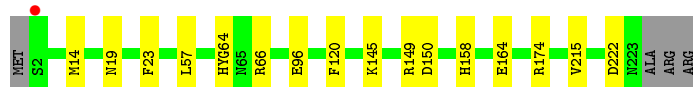
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	40	Total 40	O 40	0	0
2	F	35	Total 35	O 35	0	0
2	G	47	Total 47	O 47	0	0
2	H	39	Total 39	O 39	0	0
2	I	53	Total 53	O 53	0	0
2	J	30	Total 30	O 30	0	0
2	K	38	Total 38	O 38	0	0
2	L	33	Total 33	O 33	0	0

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: Green to red photoconvertible GFP-like protein EosFP

Chain A:  91% 7% .



- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain B:  89% 8% ..




- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain C:  92% 7% .



- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain D:  89% 8% ..




- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain E:  91% 7% .




- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain F:  87% 10% ..



- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain G:  88% 9% .



- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain H:  89% 8% .




- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain I:  92% 7% .



- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain J:  88% 9% ..




- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain K:  89% 8% ..



- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain L:  89% 7% ..

MET	S2	A3	I4	K5	P6	D7	D26	K32	P33	K45	T59	A60	F61	HYG64	R65	R66	I102	H128	K145	G165	N166	A167	H168	Y189	C195	I196	E197	M223	ALA	ARG	ARG
-----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-------	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.37Å 96.50Å 100.06Å 91.68° 107.83° 97.38°	Depositor
Resolution (Å)	95.45 – 2.70 47.72 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.4 (95.45-2.70) 95.4 (47.72-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.211 , 0.232 0.212 , 0.221	Depositor DCC
R_{free} test set	3325 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21915	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.52% 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: 5SQ

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	0.31	0/1809	0.59	2/2437 (0.1%)
1	B	0.33	0/1809	0.52	0/2437
1	C	0.34	0/1809	0.57	0/2437
1	D	0.32	0/1809	0.56	1/2437 (0.0%)
1	E	0.32	0/1809	0.52	0/2437
1	F	0.34	0/1809	0.55	0/2437
1	G	0.34	0/1809	0.62	3/2437 (0.1%)
1	H	0.33	0/1809	0.54	0/2437
1	I	0.34	0/1809	0.54	1/2437 (0.0%)
1	J	0.32	0/1809	0.58	2/2437 (0.1%)
1	K	0.33	0/1809	0.56	2/2437 (0.1%)
1	L	0.32	0/1809	0.55	1/2437 (0.0%)
All	All	0.33	0/21708	0.56	12/29244 (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	B	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	J	0	1
1	K	0	1
1	L	0	2
All	All	0	9

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	170	ARG	CG-CD-NE	-8.73	93.47	111.80
1	A	66	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	A	66	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	J	66	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	J	66	ARG	NE-CZ-NH1	6.95	123.77	120.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	GLU	Mainchain
1	B	202	ASP	Mainchain
1	F	61	PHE	Mainchain
1	G	170	ARG	Sidechain
1	H	61	PHE	Mainchain

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	1787	0	1707	17	0
1	B	1787	0	1707	13	0
1	C	1787	0	1707	14	0
1	D	1787	0	1707	15	0
1	E	1787	0	1707	10	0
1	F	1787	0	1707	26	0
1	G	1787	0	1707	17	0
1	H	1787	0	1707	19	0
1	I	1787	0	1707	10	0
1	J	1787	0	1707	15	0
1	K	1787	0	1707	17	0
1	L	1787	0	1707	17	0
2	A	49	0	0	3	0
2	B	41	0	0	1	0
2	C	37	0	0	2	0
2	D	29	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	40	0	0	2	0
2	F	35	0	0	0	0
2	G	47	0	0	1	0
2	H	39	0	0	2	0
2	I	53	0	0	3	0
2	J	30	0	0	6	0
2	K	38	0	0	0	0
2	L	33	0	0	2	0
All	All	21915	0	20484	163	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 163 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:149:ARG:NH2	1:F:96:GLU:OE1	1.80	1.15
1:D:100:ILE:HD11	1:J:100:ILE:HD11	1.15	1.13
1:L:26:ASP:OD2	1:L:45:LYS:HG3	1.57	1.05
1:F:58:THR:HG22	1:F:196:ILE:CD1	1.92	1.00
1:F:58:THR:HG22	1:F:196:ILE:HD13	1.50	0.93

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	217/224 (97%)	216 (100%)	1 (0%)	0	100	100
1	B	217/224 (97%)	215 (99%)	2 (1%)	0	100	100
1	C	217/224 (97%)	215 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	217/224 (97%)	216 (100%)	1 (0%)	0	100	100
1	E	217/224 (97%)	214 (99%)	3 (1%)	0	100	100
1	F	217/224 (97%)	216 (100%)	1 (0%)	0	100	100
1	G	217/224 (97%)	216 (100%)	1 (0%)	0	100	100
1	H	217/224 (97%)	216 (100%)	1 (0%)	0	100	100
1	I	217/224 (97%)	217 (100%)	0	0	100	100
1	J	217/224 (97%)	216 (100%)	1 (0%)	0	100	100
1	K	217/224 (97%)	215 (99%)	2 (1%)	0	100	100
1	L	217/224 (97%)	215 (99%)	2 (1%)	0	100	100
All	All	2604/2688 (97%)	2587 (99%)	17 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	189/192 (98%)	188 (100%)	1 (0%)	88	96
1	B	189/192 (98%)	186 (98%)	3 (2%)	62	85
1	C	189/192 (98%)	189 (100%)	0	100	100
1	D	189/192 (98%)	186 (98%)	3 (2%)	62	85
1	E	189/192 (98%)	187 (99%)	2 (1%)	73	90
1	F	189/192 (98%)	184 (97%)	5 (3%)	46	75
1	G	189/192 (98%)	187 (99%)	2 (1%)	73	90
1	H	189/192 (98%)	188 (100%)	1 (0%)	88	96
1	I	189/192 (98%)	186 (98%)	3 (2%)	62	85
1	J	189/192 (98%)	184 (97%)	5 (3%)	46	75
1	K	189/192 (98%)	185 (98%)	4 (2%)	53	80
1	L	189/192 (98%)	185 (98%)	4 (2%)	53	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2268/2304 (98%)	2235 (98%)	33 (2%)	65 86

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	223	ASN
1	L	5	LYS
1	L	197	GLU
1	F	161	LEU
1	F	133	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	124	ASN
1	J	194	HIS
1	D	133	GLN
1	F	21	HIS
1	H	128	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	5SQ	L	64	1	23,27,28	4.65	6 (26%)	29,37,39	4.20	9 (31%)
1	5SQ	I	64	1	23,27,28	4.51	6 (26%)	29,37,39	4.02	9 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5SQ	K	64	1	23,27,28	4.56	6 (26%)	29,37,39	4.14	9 (31%)
1	5SQ	B	64	1	23,27,28	4.49	7 (30%)	29,37,39	4.54	7 (24%)
1	5SQ	F	64	1	23,27,28	4.64	6 (26%)	29,37,39	3.74	9 (31%)
1	5SQ	C	64	1	23,27,28	4.53	6 (26%)	29,37,39	3.90	9 (31%)
1	5SQ	D	64	1	23,27,28	4.44	6 (26%)	29,37,39	4.17	10 (34%)
1	5SQ	H	64	1	23,27,28	4.50	6 (26%)	29,37,39	4.09	9 (31%)
1	5SQ	E	64	1	23,27,28	4.59	6 (26%)	29,37,39	4.01	11 (37%)
1	5SQ	J	64	1	23,27,28	4.57	6 (26%)	29,37,39	3.79	11 (37%)
1	5SQ	G	64	1	23,27,28	4.67	6 (26%)	29,37,39	3.82	11 (37%)
1	5SQ	A	64	1	23,27,28	4.50	6 (26%)	29,37,39	4.19	10 (34%)

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	5SQ	L	64	1	-	4/12/31/32	0/3/3/3
1	5SQ	I	64	1	-	3/12/31/32	0/3/3/3
1	5SQ	K	64	1	-	3/12/31/32	0/3/3/3
1	5SQ	B	64	1	-	4/12/31/32	0/3/3/3
1	5SQ	F	64	1	-	4/12/31/32	0/3/3/3
1	5SQ	C	64	1	-	4/12/31/32	0/3/3/3
1	5SQ	D	64	1	-	3/12/31/32	0/3/3/3
1	5SQ	H	64	1	-	4/12/31/32	0/3/3/3
1	5SQ	E	64	1	-	4/12/31/32	0/3/3/3
1	5SQ	J	64	1	-	3/12/31/32	0/3/3/3
1	5SQ	G	64	1	-	4/12/31/32	0/3/3/3
1	5SQ	A	64	1	-	4/12/31/32	0/3/3/3

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	64	5SQ	CB2-CA2	17.53	1.49	1.35
1	J	64	5SQ	CB2-CA2	17.40	1.49	1.35
1	F	64	5SQ	CB2-CA2	17.21	1.49	1.35
1	E	64	5SQ	CB2-CA2	17.08	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	64	5SQ	CB2-CA2	17.00	1.49	1.35

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	5SQ	CA2-C2-N3	16.88	111.35	103.37
1	L	64	5SQ	CA2-C2-N3	16.49	111.17	103.37
1	A	64	5SQ	CA2-C2-N3	15.96	110.92	103.37
1	K	64	5SQ	CA2-C2-N3	15.37	110.64	103.37
1	E	64	5SQ	CA2-C2-N3	15.29	110.60	103.37

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	64	5SQ	C-CA3-N3-C1
1	A	64	5SQ	C-CA3-N3-C2
1	A	64	5SQ	CA1-CB1-CG1-C2H
1	A	64	5SQ	CA1-CB1-CG1-N1H
1	B	64	5SQ	C-CA3-N3-C2

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L	64	5SQ	1	0
1	K	64	5SQ	1	0
1	B	64	5SQ	1	0
1	D	64	5SQ	1	0
1	H	64	5SQ	1	0
1	E	64	5SQ	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	219/224 (97%)	-0.41	1 (0%) 91 92	23, 32, 51, 67	0
1	B	219/224 (97%)	-0.40	0 100 100	21, 31, 54, 67	0
1	C	219/224 (97%)	-0.41	1 (0%) 91 92	21, 32, 50, 74	0
1	D	219/224 (97%)	-0.35	0 100 100	23, 36, 52, 68	0
1	E	219/224 (97%)	-0.31	1 (0%) 91 92	23, 32, 51, 74	0
1	F	219/224 (97%)	-0.41	1 (0%) 91 92	25, 34, 50, 75	0
1	G	219/224 (97%)	-0.38	1 (0%) 91 92	20, 31, 49, 86	0
1	H	219/224 (97%)	-0.28	1 (0%) 91 92	25, 35, 55, 75	0
1	I	219/224 (97%)	-0.35	1 (0%) 91 92	21, 33, 54, 74	0
1	J	219/224 (97%)	-0.28	1 (0%) 91 92	26, 37, 59, 82	0
1	K	219/224 (97%)	-0.28	1 (0%) 91 92	24, 36, 56, 81	0
1	L	219/224 (97%)	-0.24	0 100 100	25, 38, 58, 75	0
All	All	2628/2688 (97%)	-0.34	9 (0%) 94 95	20, 34, 54, 86	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2	SER	4.0
1	E	2	SER	3.5
1	K	2	SER	3.3
1	I	2	SER	3.1
1	G	223	ASN	3.0

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	5SQ	J	64	25/26	0.93	0.16	33,38,46,48	0
1	5SQ	A	64	25/26	0.94	0.15	26,30,33,34	0
1	5SQ	L	64	25/26	0.94	0.15	30,34,41,41	0
1	5SQ	I	64	25/26	0.95	0.17	27,33,40,41	0
1	5SQ	B	64	25/26	0.95	0.17	27,30,36,38	0
1	5SQ	E	64	25/26	0.95	0.14	27,31,36,38	0
1	5SQ	C	64	25/26	0.96	0.15	27,30,32,32	0
1	5SQ	G	64	25/26	0.96	0.14	25,28,37,38	0
1	5SQ	K	64	25/26	0.96	0.14	26,31,34,35	0
1	5SQ	H	64	25/26	0.96	0.12	28,32,36,39	0
1	5SQ	D	64	25/26	0.97	0.13	25,27,37,37	0
1	5SQ	F	64	25/26	0.97	0.14	24,27,30,32	0

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.