



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:05 am GMT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

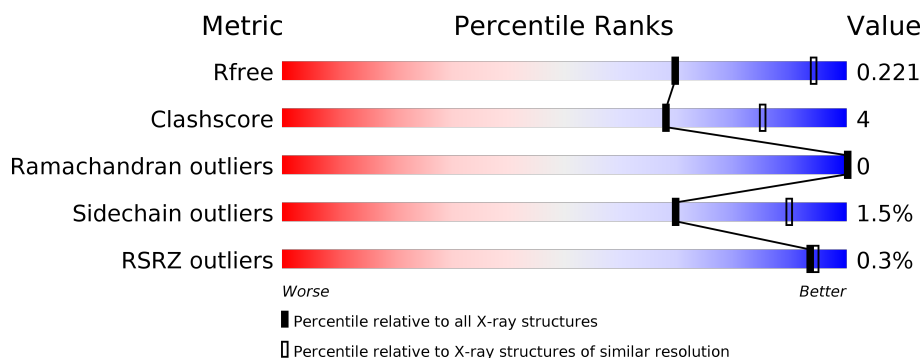
1 Overall quality at a glance

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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>92%</div> <div>7% .</div> </div>
1	B	224	<div> <div>89%</div> <div>9% .</div> </div>
1	C	224	<div> <div>91%</div> <div>7% .</div> </div>
1	D	224	<div> <div>89%</div> <div>8% ..</div> </div>
1	E	224	<div> <div>91%</div> <div>8% .</div> </div>
1	F	224	<div> <div>87%</div> <div>10% ..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	224	<div><div></div><div>88%</div><div>9%</div><div></div></div>
1	H	224	<div><div></div><div>89%</div><div>9%</div><div></div></div>
1	I	224	<div><div></div><div>91%</div><div>8%</div><div></div></div>
1	J	224	<div><div></div><div>88%</div><div>9%</div><div></div></div>
1	K	224	<div><div></div><div>89%</div><div>8%</div><div></div></div>
1	L	224	<div><div></div><div>88%</div><div>8%</div><div></div></div>

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 GPF-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	CR8	HIS	chromophore	UNP Q5S6Z9
A	64	CR8	TYR	chromophore	UNP Q5S6Z9
A	64	CR8	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	CR8	HIS	chromophore	UNP Q5S6Z9
B	64	CR8	TYR	chromophore	UNP Q5S6Z9
B	64	CR8	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	CR8	HIS	chromophore	UNP Q5S6Z9
C	64	CR8	TYR	chromophore	UNP Q5S6Z9
C	64	CR8	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	CR8	HIS	chromophore	UNP Q5S6Z9
D	64	CR8	TYR	chromophore	UNP Q5S6Z9
D	64	CR8	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	CR8	HIS	chromophore	UNP Q5S6Z9
E	64	CR8	TYR	chromophore	UNP Q5S6Z9
E	64	CR8	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	CR8	HIS	chromophore	UNP Q5S6Z9
F	64	CR8	TYR	chromophore	UNP Q5S6Z9
F	64	CR8	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	CR8	HIS	chromophore	UNP Q5S6Z9
G	64	CR8	TYR	chromophore	UNP Q5S6Z9
G	64	CR8	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	CR8	HIS	chromophore	UNP Q5S6Z9
H	64	CR8	TYR	chromophore	UNP Q5S6Z9
H	64	CR8	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	CR8	HIS	chromophore	UNP Q5S6Z9
I	64	CR8	TYR	chromophore	UNP Q5S6Z9
I	64	CR8	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	CR8	HIS	chromophore	UNP Q5S6Z9
J	64	CR8	TYR	chromophore	UNP Q5S6Z9
J	64	CR8	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	CR8	HIS	chromophore	UNP Q5S6Z9
K	64	CR8	TYR	chromophore	UNP Q5S6Z9
K	64	CR8	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	CR8	HIS	chromophore	UNP Q5S6Z9
L	64	CR8	TYR	chromophore	UNP Q5S6Z9
L	64	CR8	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	O	0	0
			40	40		
2	F	35	Total	O	0	0
			35	35		
2	G	47	Total	O	0	0
			47	47		
2	H	39	Total	O	0	0
			39	39		
2	I	53	Total	O	0	0
			53	53		
2	J	30	Total	O	0	0
			30	30		
2	K	38	Total	O	0	0
			38	38		
2	L	33	Total	O	0	0
			33	33		

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: Green to red photoconvertible GPF-like protein EosFP

Chain A: 



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

Chain B: 




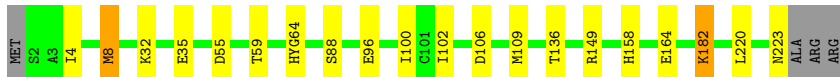
- Molecule 1: Green to red photoconvertible GPF-like protein EosFP

Chain C: 




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

Chain D: 

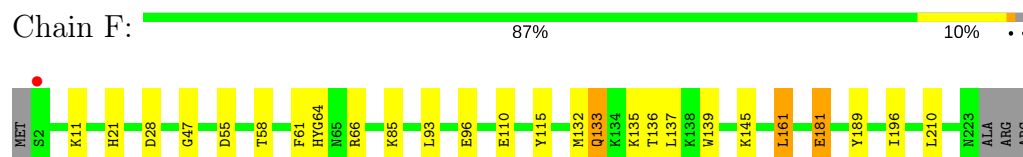


- Molecule 1: Green to red photoconvertible GPF-like protein EosFP

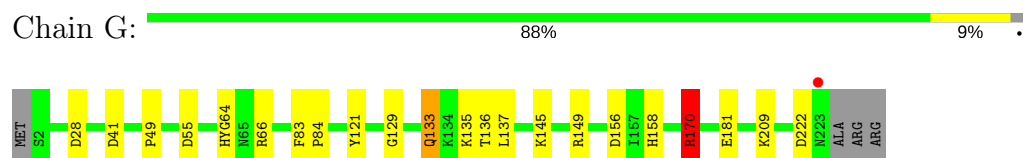
Chain E: 



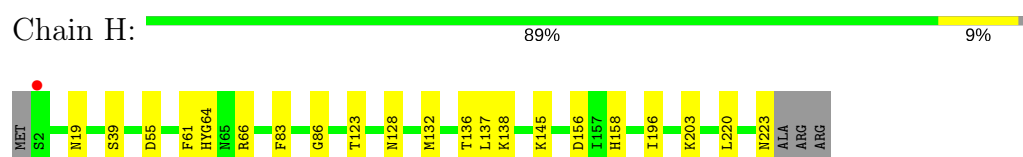
- Molecule 1: Green to red photoconvertible GPF-like protein EosFP



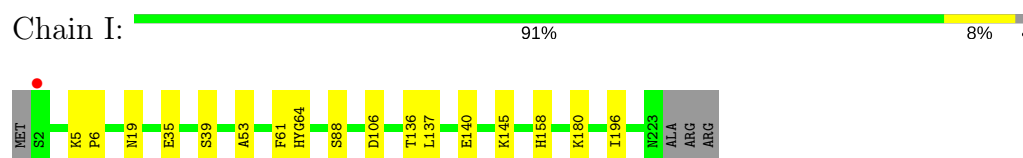
- Molecule 1: Green to red photoconvertible GPF-like protein EosFP



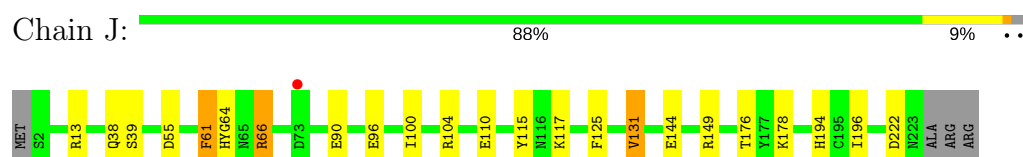
- Molecule 1: Green to red photoconvertible GPF-like protein EosFP



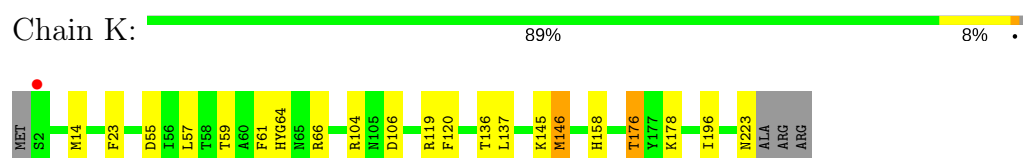
- Molecule 1: Green to red photoconvertible GPF-like protein EosFP



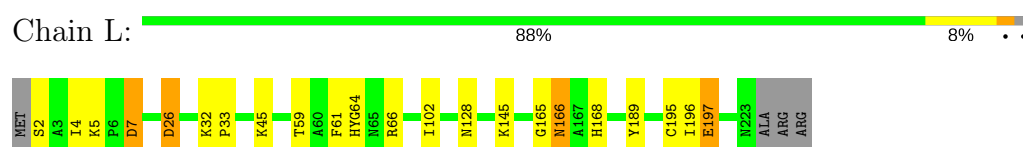
- Molecule 1: Green to red photoconvertible GPF-like protein EosFP



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



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



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) 93.3 (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 (5.16%)	DCC
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 , 38.7	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CR8

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.

All (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
1	G	149	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	D	8	MET	CG-SD-CE	5.37	108.79	100.20
1	I	137	LEU	CA-CB-CG	5.35	127.60	115.30
1	K	146	MET	CG-SD-CE	5.32	108.71	100.20
1	L	26	ASP	CB-CG-OD2	5.31	123.08	118.30
1	K	137	LEU	CA-CB-CG	5.28	127.43	115.30
1	G	137	LEU	CA-CB-CG	5.22	127.30	115.30

There are no chirality outliers.

All (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
1	J	61	PHE	Mainchain
1	K	61	PHE	Mainchain
1	L	197	GLU	Sidechain
1	L	61	PHE	Mainchain

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	1787	0	1720	17	0
1	B	1787	0	1720	15	0
1	C	1787	0	1720	16	0
1	D	1787	0	1720	16	0
1	E	1787	0	1720	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1787	0	1720	27	0
1	G	1787	0	1720	18	0
1	H	1787	0	1720	21	0
1	I	1787	0	1720	13	0
1	J	1787	0	1720	18	0
1	K	1787	0	1720	19	0
1	L	1787	0	1720	18	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
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	20640	184	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.

All (184) 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
1:F:85:LYS:HD2	1:F:181:GLU:HG2	1.58	0.86
1:G:41:ASP:OD1	1:G:209:LYS:HD3	1.78	0.84
1:I:35:GLU:O	2:I:301:HOH:O	1.98	0.81
1:E:96:GLU:OE1	1:J:149:ARG:NH2	2.14	0.81
1:G:170:ARG:NH2	1:G:170:ARG:HG3	1.96	0.78
1:G:49:PRO:O	2:G:301:HOH:O	2.02	0.78
1:F:58:THR:HG22	1:F:196:ILE:HD11	1.66	0.77
1:H:64:CR8:N15	1:H:64:CR8:H5	2.01	0.75
1:C:220:LEU:HB2	1:C:221:PRO:HA	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:203:LYS:N	1:H:203:LYS:HD2	2.02	0.74
1:B:55:ASP:OD2	1:B:136:THR:HG22	1.88	0.73
1:H:64:CR8:H4	1:H:196:ILE:HB	1.71	0.73
1:K:55:ASP:OD2	1:K:136:THR:HG22	1.90	0.71
1:J:55:ASP:OD2	2:J:301:HOH:O	2.07	0.71
1:I:140:GLU:OE2	2:I:302:HOH:O	2.08	0.70
1:I:53:ALA:HB1	1:I:136:THR:HG21	1.74	0.69
1:A:14:MET:HE1	1:A:57:LEU:HD22	1.74	0.69
1:C:143:THR:H	1:L:145:LYS:NZ	1.89	0.69
1:B:138:LYS:HG2	1:B:139:TRP:O	1.93	0.69
1:H:55:ASP:OD2	1:H:136:THR:HG22	1.92	0.69
1:K:104:ARG:NH2	1:K:106:ASP:OD2	2.26	0.68
1:H:220:LEU:HD12	1:H:223:ASN:OD1	1.95	0.66
1:F:58:THR:CG2	1:F:196:ILE:CD1	2.74	0.64
1:D:55:ASP:OD2	1:D:136:THR:HG22	1.97	0.64
1:C:3:ALA:O	2:C:301:HOH:O	2.16	0.63
1:F:58:THR:HG23	1:F:210:LEU:HD11	1.79	0.62
1:K:14:MET:HE1	1:K:23:PHE:HE2	1.63	0.62
1:D:220:LEU:HD12	1:D:223:ASN:HB2	1.82	0.62
1:J:13:ARG:HD3	2:J:305:HOH:O	1.98	0.62
1:L:128:ASN:HB2	2:L:326:HOH:O	2.00	0.62
1:D:182:LYS:HG3	1:F:137:LEU:HD23	1.81	0.61
1:I:5:LYS:HG2	1:I:6:PRO:HD2	1.80	0.61
1:G:55:ASP:OD2	1:G:136:THR:HG22	1.99	0.61
1:D:182:LYS:HG3	1:F:137:LEU:CD2	2.31	0.60
1:J:64:CR8:H4	1:J:196:ILE:HB	1.82	0.60
1:K:14:MET:HE1	1:K:23:PHE:CE2	2.36	0.60
1:A:14:MET:CE	1:A:57:LEU:HD22	2.33	0.59
1:K:14:MET:HE1	1:K:57:LEU:HD22	1.84	0.59
1:F:55:ASP:OD2	1:F:136:THR:HG22	2.03	0.59
1:K:14:MET:CE	1:K:57:LEU:HD22	2.34	0.58
1:K:14:MET:CE	1:K:23:PHE:HE2	2.17	0.58
1:C:64:CR8:H4	1:C:196:ILE:HB	1.85	0.57
1:F:133:GLN:HB3	1:F:135:LYS:HG2	1.86	0.57
1:A:14:MET:CE	1:A:23:PHE:HE2	2.17	0.57
1:F:136:THR:HG23	1:F:161:LEU:HG	1.84	0.57
1:F:139:TRP:CE3	1:F:161:LEU:HD13	2.39	0.57
1:K:14:MET:HE2	1:K:120:PHE:HB3	1.87	0.57
1:C:7:ASP:OD1	1:C:32:LYS:HD3	2.04	0.57
1:F:11:LYS:HD3	1:F:115:TYR:CE1	2.41	0.56
1:K:64:CR8:H4	1:K:196:ILE:HB	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:THR:CG2	1:F:210:LEU:HD11	2.36	0.55
1:L:2:SER:N	2:L:302:HOH:O	2.39	0.54
1:J:90:GLU:HG2	1:J:104:ARG:HG2	1.88	0.54
1:J:110:GLU:HB2	1:J:115:TYR:HE2	1.73	0.54
1:B:55:ASP:HB2	1:B:136:THR:HG21	1.89	0.54
1:C:178:LYS:NZ	2:C:303:HOH:O	2.40	0.53
1:C:143:THR:H	1:L:145:LYS:HZ1	1.57	0.53
1:H:55:ASP:HB2	1:H:136:THR:HG21	1.90	0.53
1:A:14:MET:HE2	1:A:120:PHE:HB3	1.90	0.53
1:I:64:CR8:H5	1:I:64:CR8:N15	2.24	0.53
1:A:14:MET:CE	1:A:120:PHE:HB3	2.38	0.53
1:G:133:GLN:HB3	1:G:135:LYS:HG2	1.91	0.53
1:L:7:ASP:OD2	1:L:32:LYS:NZ	2.34	0.53
1:K:64:CR8:N15	1:K:64:CR8:H5	2.24	0.52
1:F:58:THR:CG2	1:F:196:ILE:HD11	2.37	0.52
1:A:14:MET:HE1	1:A:23:PHE:CE2	2.46	0.51
1:A:14:MET:HE1	1:A:23:PHE:HE2	1.74	0.51
1:K:14:MET:CE	1:K:120:PHE:HB3	2.41	0.51
1:B:64:CR8:N15	1:B:64:CR8:H5	2.25	0.50
1:D:32:LYS:HD3	1:D:35:GLU:OE1	2.12	0.50
1:J:13:ARG:CD	2:J:305:HOH:O	2.58	0.50
1:C:143:THR:H	1:L:145:LYS:HZ3	1.56	0.50
1:K:55:ASP:HB2	1:K:136:THR:HG21	1.94	0.50
1:L:64:CR8:H4	1:L:196:ILE:HB	1.94	0.50
1:G:158:HIS:HB2	1:K:145:LYS:HE3	1.94	0.49
1:D:64:CR8:N15	1:D:64:CR8:H5	2.27	0.49
1:A:14:MET:CE	1:A:23:PHE:CE2	2.96	0.49
1:A:19:ASN:HB3	2:A:338:HOH:O	2.11	0.49
1:H:19:ASN:HB2	1:H:132:MET:CE	2.42	0.49
1:H:55:ASP:OD2	1:H:136:THR:CG2	2.60	0.49
1:J:64:CR8:N15	1:J:64:CR8:H5	2.28	0.48
1:L:165:GLY:C	1:L:166:ASN:OD1	2.52	0.48
1:J:117:LYS:HE2	2:J:328:HOH:O	2.12	0.48
1:C:142:SER:HA	1:L:145:LYS:HZ3	1.79	0.48
1:G:181:GLU:HA	1:G:181:GLU:OE1	2.14	0.48
1:H:128:ASN:ND2	2:H:304:HOH:O	2.47	0.48
1:F:110:GLU:C	1:F:110:GLU:OE1	2.52	0.47
1:C:64:CR8:H5	1:C:64:CR8:N15	2.29	0.47
1:A:14:MET:HE3	1:A:120:PHE:CB	2.44	0.47
1:C:220:LEU:HD12	1:L:195:CYS:HB2	1.96	0.47
1:I:136:THR:HG23	2:I:303:HOH:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:THR:CG2	1:F:196:ILE:HD13	2.33	0.47
1:F:58:THR:HG23	1:F:210:LEU:CD1	2.44	0.47
1:J:61:PHE:O	1:J:64:CR8:H23	2.15	0.47
1:E:85:LYS:HD2	1:E:181:GLU:HB2	1.97	0.47
1:L:59:THR:O	1:L:64:CR8:C12	2.64	0.46
1:D:59:THR:O	1:D:64:CR8:C12	2.63	0.46
1:G:156:ASP:HB3	1:K:158:HIS:CE1	2.50	0.46
1:D:4:ILE:HD13	1:D:109:MET:CE	2.46	0.46
1:K:14:MET:CE	1:K:23:PHE:CE2	2.96	0.46
1:G:129:GLY:O	1:G:133:GLN:HB2	2.16	0.46
1:B:168:HIS:CE1	1:F:189:TYR:HB2	2.51	0.46
1:J:125:PHE:CE1	1:J:131:VAL:HG11	2.51	0.46
1:A:150:ASP:N	2:A:306:HOH:O	2.49	0.46
1:I:64:CR8:H4	1:I:196:ILE:HB	1.98	0.46
1:E:64:CR8:H23	1:E:212:GLU:HB2	1.99	0.45
1:E:149:ARG:HD3	2:J:322:HOH:O	2.16	0.45
1:G:170:ARG:HH21	1:G:170:ARG:HG3	1.81	0.45
1:A:158:HIS:NE2	1:D:158:HIS:CE1	2.85	0.45
1:F:64:CR8:H4	1:F:196:ILE:HB	1.99	0.45
1:H:137:LEU:O	1:H:138:LYS:HG3	2.16	0.45
1:F:139:TRP:CD2	1:F:161:LEU:HD13	2.52	0.45
1:J:178:LYS:NZ	2:J:304:HOH:O	2.37	0.44
1:E:149:ARG:HD2	1:E:150:ASP:N	2.32	0.44
1:E:64:CR8:H4	1:E:196:ILE:HB	1.99	0.44
1:L:4:ILE:HD11	1:L:33:PRO:HG2	1.98	0.44
1:H:156:ASP:HB3	1:I:158:HIS:CE1	2.53	0.44
1:E:184:VAL:O	2:E:301:HOH:O	2.21	0.44
1:C:109:MET:HE2	1:C:114:PHE:CE1	2.53	0.44
1:C:189:TYR:HB2	1:L:168:HIS:CE1	2.53	0.44
1:E:64:CR8:H5	1:E:64:CR8:N15	2.32	0.44
1:I:88:SER:OG	1:I:106:ASP:OD1	2.31	0.44
1:B:38:GLN:HG2	1:B:64:CR8:C10	2.47	0.44
1:H:19:ASN:CB	1:H:132:MET:CE	2.95	0.44
1:H:123:THR:HG23	1:L:102:ILE:HD12	2.00	0.44
1:H:145:LYS:HG3	1:I:158:HIS:HB2	2.00	0.43
1:A:96:GLU:OE1	1:D:149:ARG:NH2	2.51	0.43
1:B:64:CR8:H4	1:B:196:ILE:HB	2.00	0.43
1:B:83:PHE:CE1	1:B:86:GLY:HA2	2.53	0.43
1:K:66:ARG:CZ	1:K:66:ARG:HA	2.49	0.43
1:A:222:ASP:N	1:A:222:ASP:OD1	2.52	0.43
1:E:66:ARG:HA	1:E:66:ARG:CZ	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:THR:HG23	1:F:210:LEU:HD21	2.01	0.43
1:B:121:TYR:CE1	1:G:121:TYR:CE1	3.06	0.43
1:J:144:GLU:OE1	1:J:194:HIS:HE1	2.02	0.43
1:J:222:ASP:OD1	1:J:222:ASP:N	2.52	0.42
1:C:21:HIS:HE1	1:C:47:GLY:O	2.00	0.42
1:E:64:CR8:C23	1:E:212:GLU:HB2	2.49	0.42
1:D:4:ILE:HD13	1:D:109:MET:HE2	2.01	0.42
1:G:55:ASP:HB2	1:G:136:THR:HG21	2.02	0.42
1:C:168:HIS:CE1	1:L:189:TYR:HB2	2.54	0.42
1:E:50:LEU:O	1:E:134:LYS:HE2	2.19	0.42
1:H:136:THR:HB	2:H:324:HOH:O	2.20	0.42
1:H:64:CR8:N15	1:H:64:CR8:C5	2.74	0.42
1:H:158:HIS:HB2	1:I:145:LYS:HG3	2.01	0.42
1:D:88:SER:OG	1:D:106:ASP:OD1	2.31	0.42
1:J:66:ARG:HA	1:J:66:ARG:CZ	2.50	0.42
1:G:64:CR8:N15	1:G:64:CR8:H5	2.35	0.42
1:G:66:ARG:HA	1:G:66:ARG:CZ	2.49	0.42
1:L:66:ARG:HA	1:L:66:ARG:CZ	2.50	0.42
1:I:53:ALA:HB1	1:I:136:THR:CG2	2.47	0.42
1:L:26:ASP:OD2	1:L:45:LYS:CG	2.47	0.42
1:B:93:LEU:HD12	1:B:93:LEU:N	2.35	0.41
1:F:66:ARG:HA	1:F:66:ARG:CZ	2.51	0.41
1:B:128:ASN:ND2	2:B:301:HOH:O	2.36	0.41
1:A:149:ARG:CZ	1:D:96:GLU:OE2	2.69	0.41
1:F:21:HIS:HE1	1:F:47:GLY:O	2.03	0.41
1:G:145:LYS:HG3	1:K:158:HIS:HB2	2.01	0.41
1:D:102:ILE:HD11	1:J:100:ILE:CG2	2.51	0.41
1:J:90:GLU:OE2	1:J:104:ARG:NH2	2.51	0.41
1:C:220:LEU:CB	1:C:221:PRO:HA	2.41	0.41
1:H:137:LEU:O	1:H:138:LYS:CG	2.69	0.41
1:I:61:PHE:O	1:I:64:CR8:H23	2.21	0.41
1:A:215:VAL:HG23	1:D:220:LEU:HD21	2.03	0.41
1:E:204:ASP:OD1	1:E:204:ASP:N	2.52	0.41
2:E:326:HOH:O	1:G:136:THR:HB	2.20	0.41
1:A:174:ARG:NH2	2:A:310:HOH:O	2.54	0.41
1:B:93:LEU:HB2	1:B:101:CYS:HB2	2.03	0.41
1:K:59:THR:HG22	1:K:64:CR8:C5	2.51	0.41
1:B:158:HIS:HB2	1:F:145:LYS:HE2	2.03	0.40
1:H:66:ARG:CZ	1:H:66:ARG:HA	2.51	0.40
1:K:176:THR:HG21	1:K:178:LYS:HE3	2.02	0.40
1:F:93:LEU:HD12	1:F:93:LEU:N	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:19:ASN:HB2	1:H:132:MET:HE1	2.03	0.40
1:G:222:ASP:N	1:G:222:ASP:OD1	2.53	0.40
1:H:83:PHE:CE1	1:H:86:GLY:HA2	2.57	0.40
1:B:176:THR:HG21	1:B:178:LYS:HE3	2.03	0.40
1:E:108:THR:HG23	1:E:115:TYR:HB2	2.04	0.40
1:G:83:PHE:HB3	1:G:84:PRO:HA	2.03	0.40

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
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%)	91	97
1	B	189/192 (98%)	186 (98%)	3 (2%)	68	89
1	C	189/192 (98%)	189 (100%)	0	100	100
1	D	189/192 (98%)	186 (98%)	3 (2%)	68	89
1	E	189/192 (98%)	187 (99%)	2 (1%)	78	93
1	F	189/192 (98%)	184 (97%)	5 (3%)	51	81
1	G	189/192 (98%)	187 (99%)	2 (1%)	78	93
1	H	189/192 (98%)	188 (100%)	1 (0%)	91	97
1	I	189/192 (98%)	186 (98%)	3 (2%)	68	89
1	J	189/192 (98%)	184 (97%)	5 (3%)	51	81
1	K	189/192 (98%)	185 (98%)	4 (2%)	59	85
1	L	189/192 (98%)	185 (98%)	4 (2%)	59	85
All	All	2268/2304 (98%)	2235 (98%)	33 (2%)	70	90

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	LYS
1	B	19	ASN
1	B	92	SER
1	B	176	THR
1	D	8	MET
1	D	164	GLU
1	D	182	LYS
1	E	39	SER
1	E	185	LYS
1	F	28	ASP
1	F	132	MET
1	F	133	GLN
1	F	161	LEU
1	F	181	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	28	ASP
1	G	133	GLN
1	H	39	SER
1	I	19	ASN
1	I	39	SER
1	I	180	LYS
1	J	38	GLN
1	J	39	SER
1	J	96	GLU
1	J	131	VAL
1	J	176	THR
1	K	119	ARG
1	K	146	MET
1	K	176	THR
1	K	223	ASN
1	L	5	LYS
1	L	7	ASP
1	L	166	ASN
1	L	197	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	124	ASN
1	C	21	HIS
1	C	206	ASN
1	D	133	GLN
1	F	21	HIS
1	H	128	ASN
1	H	133	GLN
1	I	124	ASN
1	J	194	HIS

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	CR8	A	64	1	18,27,28	1.96	5 (27%)	16,37,39	1.59	3 (18%)
1	CR8	B	64	1	18,27,28	1.85	4 (22%)	16,37,39	1.48	3 (18%)
1	CR8	C	64	1	18,27,28	1.85	4 (22%)	16,37,39	1.60	2 (12%)
1	CR8	D	64	1	18,27,28	1.84	4 (22%)	16,37,39	1.78	4 (25%)
1	CR8	E	64	1	18,27,28	1.89	5 (27%)	16,37,39	1.61	3 (18%)
1	CR8	F	64	1	18,27,28	1.89	5 (27%)	16,37,39	1.69	4 (25%)
1	CR8	G	64	1	18,27,28	1.89	4 (22%)	16,37,39	1.65	4 (25%)
1	CR8	H	64	1	18,27,28	1.78	5 (27%)	16,37,39	1.58	4 (25%)
1	CR8	I	64	1	18,27,28	1.88	5 (27%)	16,37,39	1.62	4 (25%)
1	CR8	J	64	1	18,27,28	1.91	5 (27%)	16,37,39	1.39	3 (18%)
1	CR8	K	64	1	18,27,28	1.85	5 (27%)	16,37,39	1.59	3 (18%)
1	CR8	L	64	1	18,27,28	1.89	5 (27%)	16,37,39	1.52	2 (12%)

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	CR8	A	64	1	-	0/8/25/26	0/3/3/3
1	CR8	B	64	1	-	0/8/25/26	0/3/3/3
1	CR8	C	64	1	-	0/8/25/26	0/3/3/3
1	CR8	D	64	1	-	0/8/25/26	0/3/3/3
1	CR8	E	64	1	-	0/8/25/26	0/3/3/3
1	CR8	F	64	1	-	0/8/25/26	0/3/3/3
1	CR8	G	64	1	-	0/8/25/26	0/3/3/3
1	CR8	H	64	1	-	0/8/25/26	0/3/3/3
1	CR8	I	64	1	-	0/8/25/26	0/3/3/3
1	CR8	J	64	1	-	0/8/25/26	0/3/3/3
1	CR8	K	64	1	-	0/8/25/26	0/3/3/3
1	CR8	L	64	1	-	0/8/25/26	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	CR8	C2-C1	-3.19	1.38	1.46
1	I	64	CR8	C2-C1	-3.19	1.38	1.46
1	G	64	CR8	C2-C1	-3.10	1.38	1.46
1	E	64	CR8	C2-C1	-3.07	1.38	1.46
1	F	64	CR8	C2-C1	-3.05	1.38	1.46
1	D	64	CR8	C2-C1	-3.04	1.38	1.46
1	C	64	CR8	C2-C1	-3.03	1.38	1.46
1	K	64	CR8	C2-C1	-2.97	1.38	1.46
1	B	64	CR8	C2-C1	-2.91	1.39	1.46
1	J	64	CR8	C2-C1	-2.84	1.39	1.46
1	L	64	CR8	C2-C1	-2.82	1.39	1.46
1	F	64	CR8	C4-C1	-2.78	1.39	1.46
1	H	64	CR8	C2-C1	-2.74	1.39	1.46
1	D	64	CR8	C4-C1	-2.70	1.39	1.46
1	H	64	CR8	C4-C1	-2.67	1.39	1.46
1	A	64	CR8	C4-C1	-2.66	1.39	1.46
1	I	64	CR8	C4-C1	-2.64	1.39	1.46
1	B	64	CR8	C4-C1	-2.63	1.39	1.46
1	K	64	CR8	C4-C1	-2.62	1.39	1.46
1	G	64	CR8	C4-C1	-2.60	1.39	1.46
1	J	64	CR8	C4-C1	-2.58	1.39	1.46
1	C	64	CR8	C4-C1	-2.56	1.39	1.46
1	E	64	CR8	C4-C1	-2.56	1.39	1.46
1	L	64	CR8	C4-C1	-2.40	1.40	1.46
1	D	64	CR8	C9-C8	2.07	1.48	1.40
1	B	64	CR8	C9-C8	2.08	1.48	1.40
1	H	64	CR8	C9-C8	2.13	1.48	1.40
1	J	64	CR8	C14-N15	2.17	1.38	1.34
1	I	64	CR8	C9-C8	2.19	1.48	1.40
1	F	64	CR8	C14-N15	2.21	1.38	1.34
1	A	64	CR8	C14-N15	2.21	1.38	1.34
1	H	64	CR8	C14-N15	2.23	1.38	1.34
1	K	64	CR8	C14-N15	2.24	1.38	1.34
1	E	64	CR8	C14-N15	2.25	1.38	1.34
1	L	64	CR8	C14-N15	2.25	1.38	1.34
1	C	64	CR8	C9-C8	2.26	1.48	1.40
1	K	64	CR8	C9-C8	2.28	1.49	1.40
1	A	64	CR8	C9-C8	2.35	1.49	1.40
1	L	64	CR8	C9-C8	2.37	1.49	1.40
1	E	64	CR8	C9-C8	2.39	1.49	1.40
1	F	64	CR8	C9-C8	2.42	1.49	1.40
1	I	64	CR8	C14-N15	2.42	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	64	CR8	C9-C8	2.46	1.49	1.40
1	G	64	CR8	C9-C8	2.49	1.49	1.40
1	H	64	CR8	C8-C7	4.34	1.47	1.36
1	D	64	CR8	C8-C7	4.64	1.48	1.36
1	C	64	CR8	C8-C7	4.72	1.48	1.36
1	K	64	CR8	C8-C7	4.72	1.48	1.36
1	I	64	CR8	C8-C7	4.76	1.48	1.36
1	F	64	CR8	C8-C7	4.78	1.48	1.36
1	B	64	CR8	C8-C7	4.79	1.48	1.36
1	G	64	CR8	C8-C7	4.89	1.48	1.36
1	J	64	CR8	C8-C7	4.94	1.49	1.36
1	L	64	CR8	C8-C7	4.95	1.49	1.36
1	E	64	CR8	C8-C7	4.96	1.49	1.36
1	A	64	CR8	C8-C7	5.07	1.49	1.36

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	CR8	C4-C5-C7	-3.28	119.16	121.95
1	F	64	CR8	O19-C-C17	-3.04	116.77	126.26
1	L	64	CR8	C4-C5-C7	-2.96	119.43	121.95
1	H	64	CR8	C4-C5-C7	-2.95	119.44	121.95
1	C	64	CR8	C4-C5-C7	-2.93	119.46	121.95
1	E	64	CR8	O19-C-C17	-2.89	117.21	126.26
1	G	64	CR8	O19-C-C17	-2.83	117.42	126.26
1	E	64	CR8	C4-C5-C7	-2.79	119.58	121.95
1	I	64	CR8	C4-C5-C7	-2.78	119.59	121.95
1	K	64	CR8	O19-C-C17	-2.73	117.73	126.26
1	B	64	CR8	C4-C5-C7	-2.67	119.68	121.95
1	K	64	CR8	C4-C5-C7	-2.63	119.72	121.95
1	L	64	CR8	O19-C-C17	-2.62	118.06	126.26
1	D	64	CR8	O19-C-C17	-2.61	118.11	126.26
1	J	64	CR8	O19-C-C17	-2.60	118.12	126.26
1	F	64	CR8	C4-C5-C7	-2.58	119.76	121.95
1	C	64	CR8	O19-C-C17	-2.55	118.28	126.26
1	I	64	CR8	O19-C-C17	-2.53	118.35	126.26
1	A	64	CR8	O19-C-C17	-2.50	118.44	126.26
1	G	64	CR8	C4-C5-C7	-2.46	119.86	121.95
1	H	64	CR8	O19-C-C17	-2.39	118.79	126.26
1	J	64	CR8	C4-C5-C7	-2.37	119.94	121.95
1	H	64	CR8	C2-C6-C7	-2.34	119.96	121.95
1	A	64	CR8	C4-C5-C7	-2.27	120.03	121.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	CR8	O19-C-C17	-2.15	119.52	126.26
1	D	64	CR8	C6-C7-C8	-2.02	116.19	121.90
1	J	64	CR8	C17-N13-C12	2.04	127.65	124.32
1	F	64	CR8	C16-C14-N15	2.07	129.02	124.88
1	H	64	CR8	C6-C7-C5	2.08	120.58	116.20
1	B	64	CR8	C17-N13-C12	2.12	127.79	124.32
1	G	64	CR8	C16-C14-N15	2.26	129.38	124.88
1	I	64	CR8	C16-C14-N15	2.31	129.48	124.88
1	F	64	CR8	C17-N13-C12	2.32	128.11	124.32
1	I	64	CR8	C17-N13-C12	2.44	128.31	124.32
1	K	64	CR8	C17-N13-C12	2.48	128.36	124.32
1	E	64	CR8	C17-N13-C12	2.50	128.39	124.32
1	G	64	CR8	C17-N13-C12	2.62	128.60	124.32
1	D	64	CR8	C17-N13-C12	2.73	128.78	124.32
1	A	64	CR8	C17-N13-C12	3.49	130.01	124.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	64	CR8	3	0
1	C	64	CR8	2	0
1	D	64	CR8	2	0
1	E	64	CR8	4	0
1	F	64	CR8	1	0
1	G	64	CR8	1	0
1	H	64	CR8	3	0
1	I	64	CR8	3	0
1	J	64	CR8	3	0
1	K	64	CR8	3	0
1	L	64	CR8	2	0

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 ⓘ

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, 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%)	-0.42	1 (0%) 90 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%) 90 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%) 90 92	23, 32, 51, 74	0
1	F	219/224 (97%)	-0.41	1 (0%) 90 92	25, 34, 50, 75	0
1	G	219/224 (97%)	-0.38	1 (0%) 90 92	20, 31, 49, 86	0
1	H	219/224 (97%)	-0.29	1 (0%) 90 92	25, 35, 55, 75	0
1	I	219/224 (97%)	-0.35	1 (0%) 90 92	21, 33, 54, 74	0
1	J	219/224 (97%)	-0.28	1 (0%) 90 92	26, 37, 59, 82	0
1	K	219/224 (97%)	-0.28	1 (0%) 90 92	24, 36, 56, 81	0
1	L	219/224 (97%)	-0.25	0 100 100	25, 38, 58, 75	0
All	All	2628/2688 (97%)	-0.34	9 (0%) 93 94	20, 34, 54, 86	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2	SER	4.0
1	E	2	SER	3.6
1	K	2	SER	3.3
1	I	2	SER	3.1
1	G	223	ASN	3.0
1	J	73	ASP	2.8
1	A	2	SER	2.7
1	H	2	SER	2.7
1	C	222	ASP	2.3

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
1	CR8	H	64	25/26	0.96	0.12	-	28,32,36,39	0
1	CR8	G	64	25/26	0.96	0.14	-	25,28,37,38	0
1	CR8	B	64	25/26	0.96	0.17	-	27,30,36,38	0
1	CR8	A	64	25/26	0.94	0.15	-	26,30,33,34	0
1	CR8	D	64	25/26	0.97	0.13	-	25,27,37,37	0
1	CR8	C	64	25/26	0.96	0.15	-	27,30,32,32	0
1	CR8	J	64	25/26	0.93	0.16	-	33,38,46,48	0
1	CR8	I	64	25/26	0.95	0.17	-	27,33,40,41	0
1	CR8	L	64	25/26	0.94	0.15	-	30,34,41,41	0
1	CR8	K	64	25/26	0.96	0.14	-	26,31,34,35	0
1	CR8	F	64	25/26	0.97	0.14	-	24,27,30,32	0
1	CR8	E	64	25/26	0.95	0.14	-	27,31,36,38	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.