



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 05:29 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

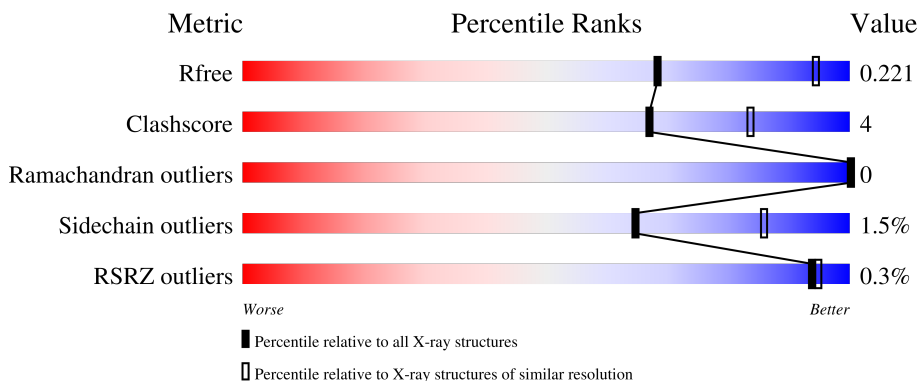
1 Overall quality at a glance

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	 91% 7% .
1	B	224	 89% 8% ..
1	C	224	 92% 7% .
1	D	224	 89% 8% ..
1	E	224	 91% 7% .

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Mol	Chain	Length	Quality of chain
1	F	224	 87% 10% ..
1	G	224	 88% 9% .
1	H	224	 90% 8% .
1	I	224	 92% 7% .
1	J	224	 89% 8% ..
1	K	224	 90% 7% ..
1	L	224	 89% 7% ..

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	220	1787	1144	304	329	10	0	0	0
1	B	220	1787	1144	304	329	10	0	0	0
1	C	220	1787	1144	304	329	10	0	0	0
1	D	220	1787	1144	304	329	10	0	0	0
1	E	220	1787	1144	304	329	10	0	0	0
1	F	220	1787	1144	304	329	10	0	0	0
1	G	220	1787	1144	304	329	10	0	0	0
1	H	220	1787	1144	304	329	10	0	0	0
1	I	220	1787	1144	304	329	10	0	0	0
1	J	220	1787	1144	304	329	10	0	0	0
1	K	220	1787	1144	304	329	10	0	0	0
1	L	220	1787	1144	304	329	10	0	0	0

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

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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

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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

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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

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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%



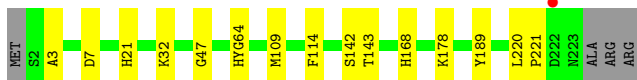
- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain B:  89% 8%




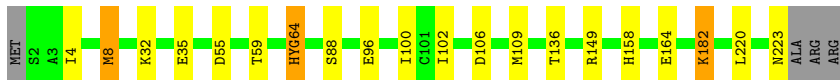
- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

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% ..




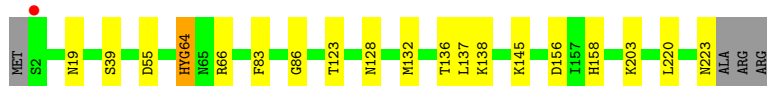
- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain G:  88% 9% .




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

Chain H:  90% 8% .




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

Chain I:  92% 7% .




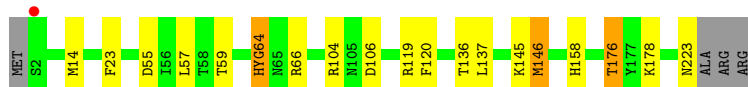
- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain J:  89% 8% ..




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

Chain K:  90% 7% ..



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

Chain L:  89% 7% ..



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)	Xtrriage
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	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: 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	G	0	1
1	L	0	1
All	All	0	4

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 (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	GLU	Mainchain
1	B	202	ASP	Mainchain
1	G	170	ARG	Sidechain
1	L	197	GLU	Sidechain

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	1706	17	0
1	B	1787	0	1706	13	0
1	C	1787	0	1706	14	0
1	D	1787	0	1706	15	0
1	E	1787	0	1706	10	0
1	F	1787	0	1706	26	0
1	G	1787	0	1706	17	0
1	H	1787	0	1706	19	0
1	I	1787	0	1706	10	0
1	J	1787	0	1706	15	0
1	K	1787	0	1706	17	0
1	L	1787	0	1706	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	20472	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.

All (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
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:HG3	1:G:170:ARG:NH2	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:C:220:LEU:HB2	1:C:221:PRO:HA	1.69	0.74
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:143:THR:H	1:L:145:LYS:HZ3	1.56	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:H:64:5SQ:N2	1:H:64:5SQ:CD1	2.74	0.50
1:K:55:ASP:HB2	1:K:136:THR:HG21	1.94	0.50
1:G:158:HIS:HB2	1:K:145:LYS:HE3	1.94	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:L:165:GLY:C	1:L:166:ASN:OD1	2.52	0.48
1:C:142:SER:HA	1:L:145:LYS:HZ3	1.79	0.48
1:J:117:LYS:HE2	2:J:328:HOH:O	2.12	0.48
1:G:181:GLU:OE1	1:G:181:GLU:HA	2.14	0.48
1:H:128:ASN:ND2	2:H:304:HOH:O	2.47	0.48
1:F:110:GLU:OE1	1:F:110:GLU:C	2.52	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
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:E:85:LYS:HD2	1:E:181:GLU:HB2	1.97	0.47
1:L:59:THR:O	1:L:64:5SQ:C2	2.64	0.46
1:D:59:THR:O	1:D:64:5SQ:C2	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:E:149:ARG:HD3	2:J:322:HOH:O	2.16	0.45
1:G:170:ARG:HG3	1:G:170:ARG:HH21	1.81	0.45
1:A:158:HIS:NE2	1:D:158:HIS:CE1	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:ARG:HD2	1:E:150:ASP:N	2.32	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:I:88:SER:OG	1:I:106:ASP:OD1	2.31	0.44
1:B:38:GLN:HG2	1:B:64:5SQ:C1H	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: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:OD1	1:A:222:ASP:N	2.52	0.43
1:B:121:TYR:CE1	1:G:121:TYR:CE1	3.06	0.43
1:E:66:ARG:CZ	1:E:66:ARG:HA	2.49	0.43
1:F:58:THR:HG23	1:F:210:LEU:HD21	2.01	0.43
1:J:144:GLU:OE1	1:J:194:HIS:HE1	2.02	0.43
1:J:222:ASP:N	1:J:222:ASP:OD1	2.52	0.42
1:C:21:HIS:HE1	1:C:47:GLY:O	2.00	0.42
1:E:64:5SQ:C2H	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: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:CZ	1:J:66:ARG:HA	2.50	0.42
1:G:66:ARG:CZ	1:G:66:ARG:HA	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:N	1:B:93:LEU:HD12	2.35	0.41
1:F:66:ARG:CZ	1:F:66:ARG:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:64:5SQ:CD1	2.51	0.41
1:B:158:HIS:HB2	1:F:145:LYS:HE2	2.03	0.40
1:H:66:ARG:HA	1:H:66:ARG:CZ	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
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	215/224 (96%)	214 (100%)	1 (0%)	0	100	100
1	B	215/224 (96%)	213 (99%)	2 (1%)	0	100	100
1	C	215/224 (96%)	213 (99%)	2 (1%)	0	100	100
1	D	215/224 (96%)	214 (100%)	1 (0%)	0	100	100
1	E	215/224 (96%)	212 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	215/224 (96%)	214 (100%)	1 (0%)	0	100	100
1	G	215/224 (96%)	214 (100%)	1 (0%)	0	100	100
1	H	215/224 (96%)	214 (100%)	1 (0%)	0	100	100
1	I	215/224 (96%)	215 (100%)	0	0	100	100
1	J	215/224 (96%)	214 (100%)	1 (0%)	0	100	100
1	K	215/224 (96%)	213 (99%)	2 (1%)	0	100	100
1	L	215/224 (96%)	213 (99%)	2 (1%)	0	100	100
All	All	2580/2688 (96%)	2563 (99%)	17 (1%)	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	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
All	All	2268/2304 (98%)	2235 (98%)	33 (2%)	65	86

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
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

Sometimes 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

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	C	64	1	23,27,28	4.53	6 (26%)	29,37,39	3.90	9 (31%)
1	5SQ	K	64	1	23,27,28	4.56	6 (26%)	29,37,39	4.14	9 (31%)
1	5SQ	D	64	1	23,27,28	4.44	6 (26%)	29,37,39	4.17	10 (34%)
1	5SQ	L	64	1	23,27,28	4.65	6 (26%)	29,37,39	4.20	9 (31%)
1	5SQ	A	64	1	23,27,28	4.50	6 (26%)	29,37,39	4.19	10 (34%)
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	G	64	1	23,27,28	4.67	6 (26%)	29,37,39	3.82	11 (37%)
1	5SQ	J	64	1	23,27,28	4.57	6 (26%)	29,37,39	3.79	11 (37%)
1	5SQ	E	64	1	23,27,28	4.59	6 (26%)	29,37,39	4.01	11 (37%)
1	5SQ	H	64	1	23,27,28	4.50	6 (26%)	29,37,39	4.09	9 (31%)
1	5SQ	I	64	1	23,27,28	4.51	6 (26%)	29,37,39	4.02	9 (31%)

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

All (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
1	L	64	5SQ	CB2-CA2	17.00	1.49	1.35
1	A	64	5SQ	CB2-CA2	16.89	1.49	1.35
1	K	64	5SQ	CB2-CA2	16.58	1.49	1.35
1	C	64	5SQ	CB2-CA2	16.51	1.48	1.35
1	I	64	5SQ	CB2-CA2	16.20	1.48	1.35
1	H	64	5SQ	CB2-CA2	15.91	1.48	1.35
1	B	64	5SQ	CB2-CA2	15.71	1.48	1.35
1	D	64	5SQ	CB2-CA2	15.63	1.48	1.35
1	B	64	5SQ	CA2-C2	-12.43	1.36	1.48
1	H	64	5SQ	CA2-C2	-12.15	1.36	1.48
1	L	64	5SQ	CA2-C2	-12.04	1.36	1.48
1	D	64	5SQ	CA2-C2	-11.93	1.36	1.48
1	I	64	5SQ	CA2-C2	-11.86	1.36	1.48
1	K	64	5SQ	CA2-C2	-11.81	1.37	1.48
1	C	64	5SQ	CA2-C2	-11.61	1.37	1.48
1	F	64	5SQ	CA2-C2	-11.51	1.37	1.48
1	G	64	5SQ	CA2-C2	-11.34	1.37	1.48
1	E	64	5SQ	CA2-C2	-11.33	1.37	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	5SQ	CA2-C2	-10.69	1.38	1.48
1	J	64	5SQ	CA2-C2	-10.62	1.38	1.48
1	C	64	5SQ	OH-CZ1	-5.10	1.25	1.37
1	F	64	5SQ	OH-CZ1	-5.09	1.25	1.37
1	G	64	5SQ	OH-CZ1	-5.03	1.25	1.37
1	D	64	5SQ	OH-CZ1	-5.03	1.25	1.37
1	E	64	5SQ	OH-CZ1	-5.00	1.25	1.37
1	K	64	5SQ	OH-CZ1	-5.00	1.25	1.37
1	I	64	5SQ	OH-CZ1	-4.99	1.25	1.37
1	H	64	5SQ	OH-CZ1	-4.95	1.25	1.37
1	B	64	5SQ	OH-CZ1	-4.93	1.25	1.37
1	A	64	5SQ	OH-CZ1	-4.92	1.25	1.37
1	J	64	5SQ	OH-CZ1	-4.69	1.26	1.37
1	L	64	5SQ	OH-CZ1	-4.67	1.26	1.37
1	I	64	5SQ	C1-N2	4.20	1.38	1.32
1	L	64	5SQ	C1-N2	4.04	1.38	1.32
1	E	64	5SQ	C1-N2	4.03	1.38	1.32
1	K	64	5SQ	C1-N2	4.03	1.38	1.32
1	H	64	5SQ	C1-N2	4.02	1.38	1.32
1	A	64	5SQ	C1-N2	4.00	1.38	1.32
1	F	64	5SQ	C1-N2	4.00	1.38	1.32
1	J	64	5SQ	C1-N2	3.96	1.38	1.32
1	G	64	5SQ	C1-N2	3.77	1.37	1.32
1	B	64	5SQ	C1-N2	3.74	1.37	1.32
1	D	64	5SQ	C1-N2	3.73	1.37	1.32
1	C	64	5SQ	C1-N2	3.73	1.37	1.32
1	F	64	5SQ	C2-N3	-3.38	1.31	1.39
1	C	64	5SQ	C2-N3	-3.31	1.32	1.39
1	G	64	5SQ	C2-N3	-3.27	1.32	1.39
1	L	64	5SQ	C2-N3	-3.17	1.32	1.39
1	D	64	5SQ	C2-N3	-3.06	1.32	1.39
1	I	64	5SQ	C2-N3	-3.00	1.32	1.39
1	H	64	5SQ	C2-N3	-3.00	1.32	1.39
1	J	64	5SQ	O2-C2	2.99	1.29	1.23
1	B	64	5SQ	C2-N3	-2.98	1.32	1.39
1	J	64	5SQ	C2-N3	-2.98	1.32	1.39
1	E	64	5SQ	C2-N3	-2.93	1.33	1.39
1	H	64	5SQ	O2-C2	2.90	1.29	1.23
1	K	64	5SQ	C2-N3	-2.83	1.33	1.39
1	K	64	5SQ	O2-C2	2.80	1.29	1.23
1	A	64	5SQ	C2-N3	-2.80	1.33	1.39
1	I	64	5SQ	O2-C2	2.71	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	64	5SQ	O2-C2	2.71	1.28	1.23
1	A	64	5SQ	O2-C2	2.66	1.28	1.23
1	G	64	5SQ	O2-C2	2.65	1.28	1.23
1	F	64	5SQ	O2-C2	2.64	1.28	1.23
1	C	64	5SQ	O2-C2	2.63	1.28	1.23
1	E	64	5SQ	O2-C2	2.63	1.28	1.23
1	L	64	5SQ	O2-C2	2.59	1.28	1.23
1	B	64	5SQ	O2-C2	2.46	1.28	1.23
1	B	64	5SQ	CA2-N2	-2.03	1.34	1.38

All (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
1	I	64	5SQ	CA2-C2-N3	15.19	110.55	103.37
1	F	64	5SQ	CA2-C2-N3	15.18	110.55	103.37
1	H	64	5SQ	CA2-C2-N3	15.16	110.54	103.37
1	C	64	5SQ	CA2-C2-N3	15.03	110.48	103.37
1	J	64	5SQ	CA2-C2-N3	14.99	110.46	103.37
1	G	64	5SQ	CA2-C2-N3	14.87	110.40	103.37
1	D	64	5SQ	CA2-C2-N3	14.57	110.26	103.37
1	B	64	5SQ	O2-C2-CA2	-13.09	123.61	130.96
1	D	64	5SQ	O2-C2-CA2	-13.05	123.63	130.96
1	K	64	5SQ	O2-C2-CA2	-12.41	123.99	130.96
1	L	64	5SQ	O2-C2-CA2	-12.29	124.06	130.96
1	A	64	5SQ	O2-C2-CA2	-10.99	124.79	130.96
1	E	64	5SQ	O2-C2-CA2	-10.98	124.80	130.96
1	I	64	5SQ	O2-C2-CA2	-10.82	124.89	130.96
1	H	64	5SQ	O2-C2-CA2	-10.79	124.90	130.96
1	C	64	5SQ	O2-C2-CA2	-9.72	125.50	130.96
1	F	64	5SQ	O2-C2-CA2	-9.27	125.76	130.96
1	G	64	5SQ	O2-C2-CA2	-9.19	125.80	130.96
1	J	64	5SQ	O2-C2-CA2	-8.67	126.09	130.96
1	H	64	5SQ	CG2-CB2-CA2	-6.83	121.57	129.94
1	B	64	5SQ	C2-N3-C1	-6.82	104.51	107.97
1	A	64	5SQ	C2-N3-C1	-6.45	104.70	107.97
1	D	64	5SQ	C2-N3-C1	-6.27	104.79	107.97
1	B	64	5SQ	CG2-CB2-CA2	-5.79	122.85	129.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	64	5SQ	CG2-CB2-CA2	-5.62	123.06	129.94
1	K	64	5SQ	C2-N3-C1	-5.16	105.36	107.97
1	B	64	5SQ	CB2-CA2-C2	5.14	128.41	122.28
1	J	64	5SQ	CB2-CA2-C2	5.14	128.41	122.28
1	I	64	5SQ	CG2-CB2-CA2	-5.13	123.66	129.94
1	K	64	5SQ	CG2-CB2-CA2	-5.08	123.72	129.94
1	H	64	5SQ	CB2-CA2-C2	4.94	128.18	122.28
1	A	64	5SQ	CB2-CA2-C2	4.91	128.14	122.28
1	G	64	5SQ	CB2-CA2-C2	4.80	128.01	122.28
1	L	64	5SQ	C2-N3-C1	-4.71	105.58	107.97
1	E	64	5SQ	CG2-CB2-CA2	-4.45	124.49	129.94
1	C	64	5SQ	CB2-CA2-C2	4.44	127.58	122.28
1	C	64	5SQ	C2-N3-C1	-4.40	105.74	107.97
1	I	64	5SQ	CB2-CA2-C2	4.36	127.48	122.28
1	E	64	5SQ	CB2-CA2-C2	4.36	127.48	122.28
1	G	64	5SQ	CG2-CB2-CA2	-4.34	124.62	129.94
1	E	64	5SQ	C2-N3-C1	-4.33	105.77	107.97
1	J	64	5SQ	C2-N3-C1	-4.30	105.79	107.97
1	J	64	5SQ	CG2-CB2-CA2	-4.18	124.82	129.94
1	H	64	5SQ	C2-N3-C1	-4.16	105.86	107.97
1	D	64	5SQ	CG2-CB2-CA2	-4.11	124.91	129.94
1	F	64	5SQ	C2-N3-C1	-3.98	105.95	107.97
1	I	64	5SQ	C2-N3-C1	-3.74	106.07	107.97
1	A	64	5SQ	CG2-CB2-CA2	-3.73	125.37	129.94
1	K	64	5SQ	CB2-CA2-C2	3.64	126.62	122.28
1	B	64	5SQ	CB2-CA2-N2	-3.54	123.92	128.83
1	I	64	5SQ	CA1-C1-N3	-3.54	120.24	124.85
1	G	64	5SQ	CA1-C1-N3	-3.52	120.26	124.85
1	L	64	5SQ	CB2-CA2-C2	3.50	126.46	122.28
1	H	64	5SQ	CB2-CA2-N2	-3.48	124.00	128.83
1	F	64	5SQ	CB2-CA2-C2	3.41	126.35	122.28
1	F	64	5SQ	CA1-C1-N3	-3.40	120.42	124.85
1	J	64	5SQ	CB2-CA2-N2	-3.34	124.19	128.83
1	D	64	5SQ	CB2-CA2-C2	3.27	126.18	122.28
1	A	64	5SQ	CB2-CA2-N2	-3.22	124.35	128.83
1	G	64	5SQ	C2-N3-C1	-3.22	106.33	107.97
1	F	64	5SQ	O3-C3-CA3	-3.19	116.77	126.39
1	C	64	5SQ	CB2-CA2-N2	-3.13	124.49	128.83
1	D	64	5SQ	CA1-C1-N3	-3.11	120.79	124.85
1	A	64	5SQ	CA1-C1-N3	-3.10	120.82	124.85
1	E	64	5SQ	CA1-C1-N3	-3.05	120.88	124.85
1	E	64	5SQ	O3-C3-CA3	-3.04	117.21	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	64	5SQ	CG2-CB2-CA2	-2.99	126.28	129.94
1	G	64	5SQ	O3-C3-CA3	-2.97	117.42	126.39
1	G	64	5SQ	CB2-CA2-N2	-2.95	124.74	128.83
1	I	64	5SQ	CA1-C1-N2	2.94	129.48	123.56
1	J	64	5SQ	CA1-C1-N3	-2.91	121.05	124.85
1	G	64	5SQ	CA1-C1-N2	2.89	129.38	123.56
1	D	64	5SQ	CB2-CA2-N2	-2.89	124.82	128.83
1	K	64	5SQ	O3-C3-CA3	-2.87	117.73	126.39
1	I	64	5SQ	CB2-CA2-N2	-2.81	124.92	128.83
1	L	64	5SQ	O3-C3-CA3	-2.76	118.06	126.39
1	D	64	5SQ	O3-C3-CA3	-2.74	118.11	126.39
1	J	64	5SQ	O3-C3-CA3	-2.74	118.12	126.39
1	C	64	5SQ	CA1-C1-N3	-2.72	121.31	124.85
1	F	64	5SQ	CA1-C1-N2	2.71	129.02	123.56
1	A	64	5SQ	CA3-N3-C2	2.71	130.01	123.80
1	F	64	5SQ	CG2-CB2-CA2	-2.70	126.63	129.94
1	C	64	5SQ	O3-C3-CA3	-2.69	118.28	126.39
1	L	64	5SQ	C2-CA2-N2	-2.67	107.06	108.93
1	I	64	5SQ	O3-C3-CA3	-2.66	118.35	126.39
1	E	64	5SQ	CB2-CA2-N2	-2.66	125.14	128.83
1	A	64	5SQ	O3-C3-CA3	-2.63	118.44	126.39
1	H	64	5SQ	CB1-CA1-C1	2.56	115.87	110.85
1	K	64	5SQ	CA1-C1-N3	-2.54	121.55	124.85
1	H	64	5SQ	O3-C3-CA3	-2.52	118.79	126.39
1	K	64	5SQ	CB2-CA2-N2	-2.50	125.36	128.83
1	E	64	5SQ	CA1-C1-N2	2.46	128.51	123.56
1	G	64	5SQ	C2-CA2-N2	-2.46	107.21	108.93
1	J	64	5SQ	CA1-C1-N2	2.35	128.29	123.56
1	B	64	5SQ	O3-C3-CA3	-2.27	119.52	126.39
1	J	64	5SQ	C2-CA2-N2	-2.25	107.36	108.93
1	L	64	5SQ	CA1-C1-N3	-2.22	121.95	124.85
1	E	64	5SQ	C2-CA2-N2	-2.22	107.38	108.93
1	H	64	5SQ	N3-C1-N2	-2.21	109.92	111.45
1	J	64	5SQ	CB1-CA1-C1	2.19	115.14	110.85
1	D	64	5SQ	CA3-N3-C2	2.17	128.78	123.80
1	C	64	5SQ	CA1-C1-N2	2.16	127.92	123.56
1	G	64	5SQ	CA3-N3-C2	2.10	128.60	123.80
1	L	64	5SQ	CA1-C1-N2	2.07	127.73	123.56
1	A	64	5SQ	C2-CA2-N2	-2.04	107.51	108.93
1	D	64	5SQ	CA1-C1-N2	2.04	127.66	123.56
1	K	64	5SQ	CA1-C1-N2	2.02	127.63	123.56
1	F	64	5SQ	CB2-CA2-N2	-2.01	126.04	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	64	5SQ	CA3-N3-C2	2.00	128.39	123.80

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	64	5SQ	C3-CA3-N3-C1
1	A	64	5SQ	C3-CA3-N3-C2
1	A	64	5SQ	CA1-CB1-CG1-C2H
1	A	64	5SQ	CA1-CB1-CG1-N1H
1	B	64	5SQ	C3-CA3-N3-C2
1	B	64	5SQ	CA1-CB1-CG1-N1H
1	C	64	5SQ	C3-CA3-N3-C1
1	C	64	5SQ	C3-CA3-N3-C2
1	C	64	5SQ	CA1-CB1-CG1-C2H
1	C	64	5SQ	CA1-CB1-CG1-N1H
1	D	64	5SQ	C3-CA3-N3-C1
1	D	64	5SQ	C3-CA3-N3-C2
1	D	64	5SQ	CA1-CB1-CG1-N1H
1	E	64	5SQ	C3-CA3-N3-C1
1	E	64	5SQ	C3-CA3-N3-C2
1	E	64	5SQ	CA1-CB1-CG1-C2H
1	E	64	5SQ	CA1-CB1-CG1-N1H
1	F	64	5SQ	C3-CA3-N3-C1
1	F	64	5SQ	C3-CA3-N3-C2
1	F	64	5SQ	CA1-CB1-CG1-C2H
1	F	64	5SQ	CA1-CB1-CG1-N1H
1	G	64	5SQ	C3-CA3-N3-C1
1	G	64	5SQ	C3-CA3-N3-C2
1	G	64	5SQ	CA1-CB1-CG1-C2H
1	G	64	5SQ	CA1-CB1-CG1-N1H
1	H	64	5SQ	C3-CA3-N3-C1
1	H	64	5SQ	C3-CA3-N3-C2
1	H	64	5SQ	CA1-CB1-CG1-C2H
1	H	64	5SQ	CA1-CB1-CG1-N1H
1	I	64	5SQ	C3-CA3-N3-C1
1	I	64	5SQ	C3-CA3-N3-C2
1	I	64	5SQ	CA1-CB1-CG1-N1H
1	J	64	5SQ	C3-CA3-N3-C1
1	J	64	5SQ	C3-CA3-N3-C2
1	J	64	5SQ	CA1-CB1-CG1-N1H
1	K	64	5SQ	C3-CA3-N3-C1

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Mol	Chain	Res	Type	Atoms
1	K	64	5SQ	C3-CA3-N3-C2
1	K	64	5SQ	CA1-CB1-CG1-N1H
1	L	64	5SQ	C3-CA3-N3-C2
1	L	64	5SQ	CA1-CB1-CG1-C2H
1	L	64	5SQ	CA1-CB1-CG1-N1H
1	L	64	5SQ	C3-CA3-N3-C1
1	B	64	5SQ	CA1-CB1-CG1-C2H
1	B	64	5SQ	C3-CA3-N3-C1

There are no ring outliers.

6 monomers are involved in 6 short contacts:

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

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%)	-0.41	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

All (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
1	H	2	SER	2.8
1	A	2	SER	2.7
1	J	73	ASP	2.7
1	C	222	ASP	2.4

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.