



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2025 – 07:15 pm BST

PDB ID : 9FEL / pdb_00009fel
Title : LSSmCherry1 - Directionality of Optical Properties of Fluorescent Proteins
Authors : Myskova, J.; Brynda, J.; Lazar, J.
Deposited on : 2024-05-21
Resolution : 1.50 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	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

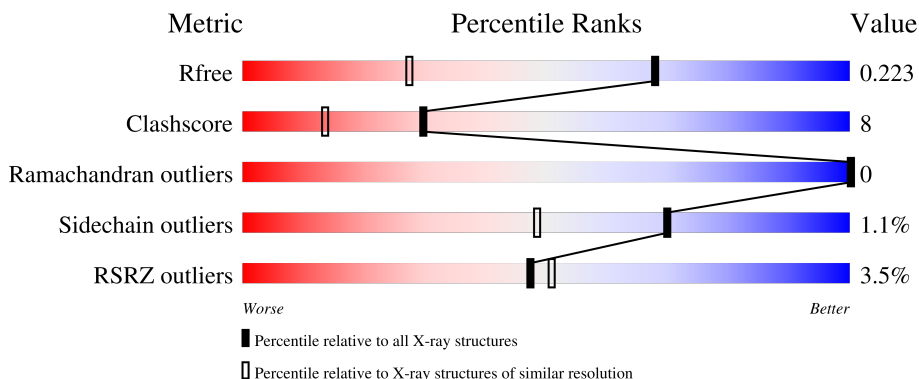
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

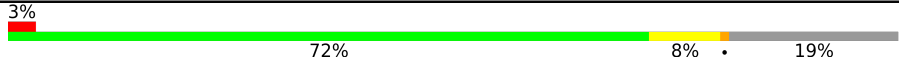

The reported resolution of this entry is 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3717 (1.50-1.50)
Clashscore	180529	4048 (1.50-1.50)
Ramachandran outliers	177936	3970 (1.50-1.50)
Sidechain outliers	177891	3967 (1.50-1.50)
RSRZ outliers	164620	3718 (1.50-1.50)

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	266	
1	L	266	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	A	304	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3916 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 PAmCherry1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	6	0
			1761	1120	296	337	8			
1	L	215	Total	C	N	O	S	0	5	0
			1767	1121	299	339	8			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-36	HIS	-	expression tag	UNP D1MPT3
A	-35	HIS	-	expression tag	UNP D1MPT3
A	-34	HIS	-	expression tag	UNP D1MPT3
A	-33	HIS	-	expression tag	UNP D1MPT3
A	-32	HIS	-	expression tag	UNP D1MPT3
A	-31	HIS	-	expression tag	UNP D1MPT3
A	-30	GLY	-	expression tag	UNP D1MPT3
A	-29	MET	-	expression tag	UNP D1MPT3
A	-28	ALA	-	expression tag	UNP D1MPT3
A	-27	SER	-	expression tag	UNP D1MPT3
A	-26	MET	-	expression tag	UNP D1MPT3
A	-25	THR	-	expression tag	UNP D1MPT3
A	-24	GLY	-	expression tag	UNP D1MPT3
A	-23	GLY	-	expression tag	UNP D1MPT3
A	-22	GLN	-	expression tag	UNP D1MPT3
A	-21	GLN	-	expression tag	UNP D1MPT3
A	-20	MET	-	expression tag	UNP D1MPT3
A	-19	GLY	-	expression tag	UNP D1MPT3
A	-18	ARG	-	expression tag	UNP D1MPT3
A	-17	ASP	-	expression tag	UNP D1MPT3
A	-16	LEU	-	expression tag	UNP D1MPT3
A	-15	TYR	-	expression tag	UNP D1MPT3
A	-14	ASP	-	expression tag	UNP D1MPT3
A	-13	ASP	-	expression tag	UNP D1MPT3
A	-12	ASP	-	expression tag	UNP D1MPT3

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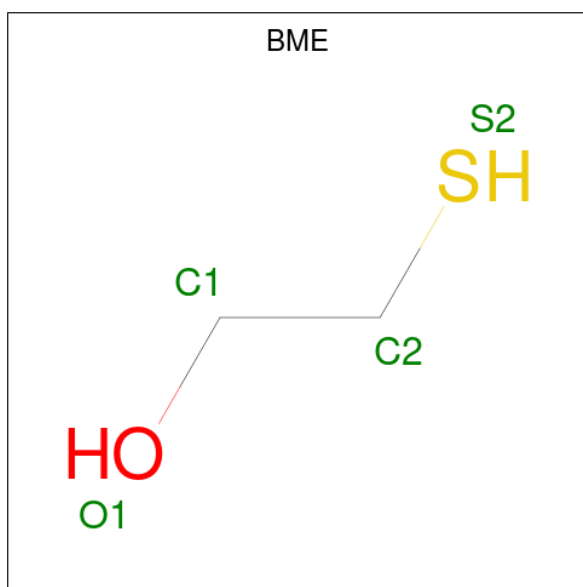
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	ASP	-	expression tag	UNP D1MPT3
A	-10	LYS	-	expression tag	UNP D1MPT3
A	-9	ASP	-	expression tag	UNP D1MPT3
A	-8	PRO	-	expression tag	UNP D1MPT3
A	-7	SER	-	expression tag	UNP D1MPT3
A	-6	SER	-	expression tag	UNP D1MPT3
A	-5	ARG	-	expression tag	UNP D1MPT3
A	6	THR	ALA	conflict	UNP D1MPT3
A	26	GLU	VAL	conflict	UNP D1MPT3
A	57	ALA	THR	conflict	UNP D1MPT3
A	66	NRQ	MET	conflict	UNP D1MPT3
A	?	-	TYR	deletion	UNP D1MPT3
A	?	-	GLY	deletion	UNP D1MPT3
A	70	LYS	ASN	conflict	UNP D1MPT3
A	83	LEU	PHE	conflict	UNP D1MPT3
A	92	ASN	LYS	conflict	UNP D1MPT3
A	98	ASN	LYS	conflict	UNP D1MPT3
A	138	CYS	LYS	conflict	UNP D1MPT3
A	139	ARG	LYS	conflict	UNP D1MPT3
A	143	LEU	TRP	conflict	UNP D1MPT3
A	146	SER	LEU	conflict	UNP D1MPT3
A	147	THR	SER	conflict	UNP D1MPT3
A	161	SER	VAL	conflict	UNP D1MPT3
A	163	GLU	PRO	conflict	UNP D1MPT3
A	165	LEU	VAL	conflict	UNP D1MPT3
A	196	ASP	ASN	conflict	UNP D1MPT3
A	197	ILE	ARG	conflict	UNP D1MPT3
A	202	LEU	THR	conflict	UNP D1MPT3
A	217	SER	ALA	conflict	UNP D1MPT3
L	-36	HIS	-	expression tag	UNP D1MPT3
L	-35	HIS	-	expression tag	UNP D1MPT3
L	-34	HIS	-	expression tag	UNP D1MPT3
L	-33	HIS	-	expression tag	UNP D1MPT3
L	-32	HIS	-	expression tag	UNP D1MPT3
L	-31	HIS	-	expression tag	UNP D1MPT3
L	-30	GLY	-	expression tag	UNP D1MPT3
L	-29	MET	-	expression tag	UNP D1MPT3
L	-28	ALA	-	expression tag	UNP D1MPT3
L	-27	SER	-	expression tag	UNP D1MPT3
L	-26	MET	-	expression tag	UNP D1MPT3
L	-25	THR	-	expression tag	UNP D1MPT3
L	-24	GLY	-	expression tag	UNP D1MPT3

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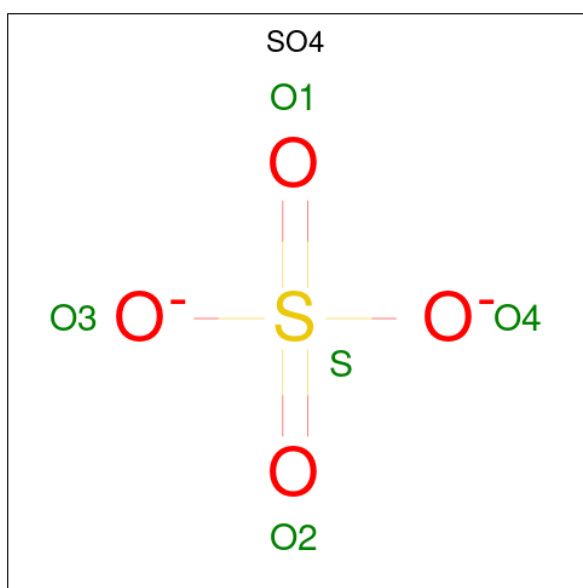
Chain	Residue	Modelled	Actual	Comment	Reference
L	-23	GLY	-	expression tag	UNP D1MPT3
L	-22	GLN	-	expression tag	UNP D1MPT3
L	-21	GLN	-	expression tag	UNP D1MPT3
L	-20	MET	-	expression tag	UNP D1MPT3
L	-19	GLY	-	expression tag	UNP D1MPT3
L	-18	ARG	-	expression tag	UNP D1MPT3
L	-17	ASP	-	expression tag	UNP D1MPT3
L	-16	LEU	-	expression tag	UNP D1MPT3
L	-15	TYR	-	expression tag	UNP D1MPT3
L	-14	ASP	-	expression tag	UNP D1MPT3
L	-13	ASP	-	expression tag	UNP D1MPT3
L	-12	ASP	-	expression tag	UNP D1MPT3
L	-11	ASP	-	expression tag	UNP D1MPT3
L	-10	LYS	-	expression tag	UNP D1MPT3
L	-9	ASP	-	expression tag	UNP D1MPT3
L	-8	PRO	-	expression tag	UNP D1MPT3
L	-7	SER	-	expression tag	UNP D1MPT3
L	-6	SER	-	expression tag	UNP D1MPT3
L	-5	ARG	-	expression tag	UNP D1MPT3
L	6	THR	ALA	conflict	UNP D1MPT3
L	26	GLU	VAL	conflict	UNP D1MPT3
L	57	ALA	THR	conflict	UNP D1MPT3
L	66	NRQ	MET	conflict	UNP D1MPT3
L	?	-	TYR	deletion	UNP D1MPT3
L	?	-	GLY	deletion	UNP D1MPT3
L	70	LYS	ASN	conflict	UNP D1MPT3
L	83	LEU	PHE	conflict	UNP D1MPT3
L	92	ASN	LYS	conflict	UNP D1MPT3
L	98	ASN	LYS	conflict	UNP D1MPT3
L	138	CYS	LYS	conflict	UNP D1MPT3
L	139	ARG	LYS	conflict	UNP D1MPT3
L	143	LEU	TRP	conflict	UNP D1MPT3
L	146	SER	LEU	conflict	UNP D1MPT3
L	147	THR	SER	conflict	UNP D1MPT3
L	161	SER	VAL	conflict	UNP D1MPT3
L	163	GLU	PRO	conflict	UNP D1MPT3
L	165	LEU	VAL	conflict	UNP D1MPT3
L	196	ASP	ASN	conflict	UNP D1MPT3
L	197	ILE	ARG	conflict	UNP D1MPT3
L	202	LEU	THR	conflict	UNP D1MPT3
L	217	SER	ALA	conflict	UNP D1MPT3

- Molecule 2 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



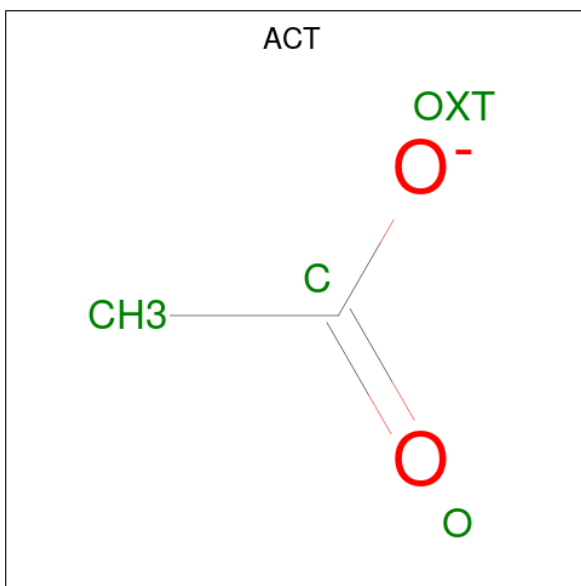
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	L	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

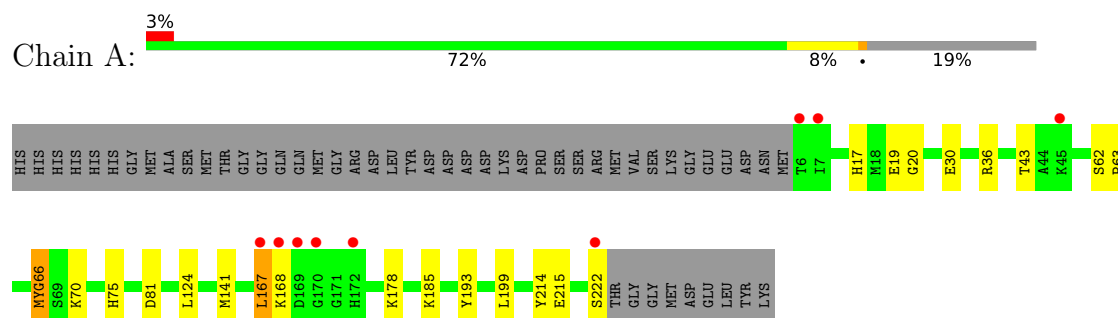
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	168	Total	O	0	0
			168	168		
5	L	198	Total	O	0	0
			198	198		

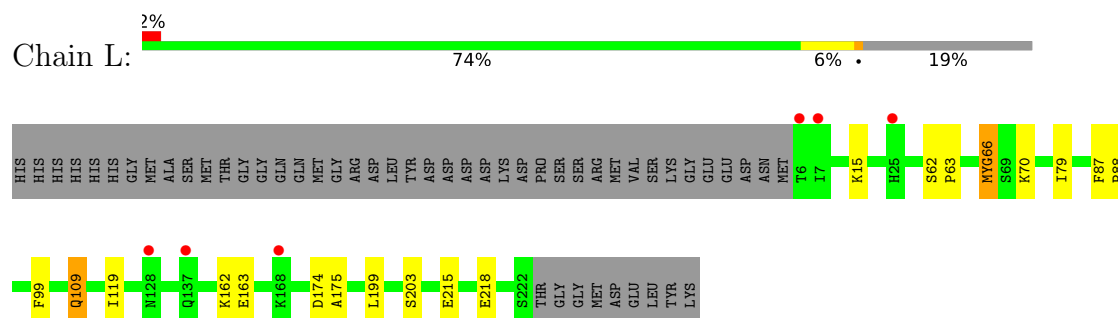
3 Residue-property plots [i](#)

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: PAmCherry1 protein



- Molecule 1: PAmCherry1 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.54Å 107.98Å 58.73Å 90.00° 103.95° 90.00°	Depositor
Resolution (Å)	39.20 – 1.50 39.20 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.20-1.50) 100.0 (39.20-1.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.189 , 0.213 0.198 , 0.223	Depositor DCC
R_{free} test set	2100 reflections (2.75%)	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 28.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3916	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.49% 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: ACT, SO4, NRQ, BME

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	1.02	0/1797	1.13	2/2421 (0.1%)
1	L	1.07	2/1794 (0.1%)	1.14	0/2415
All	All	1.05	2/3591 (0.1%)	1.14	2/4836 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	79	ILE	N-CA	6.10	1.50	1.46
1	L	203	SER	C-O	5.11	1.29	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ASP	CA-C-N	5.80	128.38	120.54
1	A	81	ASP	C-N-CA	5.80	128.38	120.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1761	0	1716	34	0
1	L	1767	0	1711	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	5	0	0
2	L	4	0	5	0	0
3	A	10	0	0	0	0
4	A	4	0	3	4	0
5	A	168	0	0	11	0
5	L	198	0	0	13	0
All	All	3916	0	3440	59	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 8.

All (59) 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:A:141:MET:CE	1:A:168:LYS:HA	1.76	1.15
1:L:218[A]:GLU:HG3	5:L:418:HOH:O	1.63	0.97
1:A:141:MET:HE3	1:A:168:LYS:HA	1.43	0.97
1:A:36[B]:ARG:HH22	4:A:304:ACT:H2	1.28	0.96
1:L:119:ILE:CD1	5:L:558:HOH:O	2.16	0.92
1:L:15:LYS:NZ	5:L:403:HOH:O	2.04	0.91
1:A:66:NRQ:HD2	5:A:508:HOH:O	1.80	0.81
1:A:141:MET:HE1	1:A:168:LYS:HA	1.62	0.79
1:L:119:ILE:HD13	5:L:558:HOH:O	1.75	0.79
1:A:141:MET:HE3	1:A:168:LYS:CA	2.15	0.76
1:A:36[B]:ARG:HH22	4:A:304:ACT:CH3	1.99	0.76
1:A:75:HIS:HE1	1:A:193:TYR:OH	1.71	0.74
1:A:36[B]:ARG:NH2	4:A:304:ACT:H2	2.03	0.72
1:L:162[B]:LYS:HG2	5:L:402:HOH:O	1.93	0.68
1:L:119:ILE:HD11	5:L:558:HOH:O	1.86	0.66
1:L:162[B]:LYS:CE	1:L:174:ASP:HB3	2.27	0.63
1:L:162[B]:LYS:HD2	1:L:163:GLU:N	2.13	0.63
1:L:119:ILE:HD11	5:L:414:HOH:O	2.01	0.61
1:L:162[B]:LYS:HE3	1:L:174:ASP:HB3	1.84	0.59
1:A:141:MET:CE	1:A:168:LYS:CA	2.66	0.58
1:A:70:LYS:HG2	5:A:437:HOH:O	2.04	0.58
1:A:36[A]:ARG:NE	5:A:402:HOH:O	2.30	0.56
1:A:36[A]:ARG:NH2	5:A:402:HOH:O	2.29	0.55
1:A:43[A]:THR:HG22	1:A:214:TYR:HD1	1.71	0.55
1:A:141:MET:HE2	1:A:168:LYS:CG	2.36	0.55
1:L:162[B]:LYS:CG	5:L:402:HOH:O	2.51	0.54
1:A:17:HIS:NE2	1:A:19:GLU:HG3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LYS:HB2	5:A:437:HOH:O	2.09	0.52
1:A:36[A]:ARG:HH12	4:A:304:ACT:H2	1.75	0.50
1:A:185[A]:LYS:HD2	5:A:554:HOH:O	2.09	0.50
1:L:162[B]:LYS:NZ	5:L:402:HOH:O	1.95	0.50
1:L:162[B]:LYS:HE2	1:L:174:ASP:HB3	1.93	0.49
1:L:70:LYS:HG2	5:L:508:HOH:O	2.12	0.48
1:L:87:PHE:HB3	1:L:88:PRO:HA	1.96	0.48
1:L:109:GLN:HE21	1:L:109:GLN:C	2.21	0.48
1:A:17:HIS:ND1	1:A:30:GLU:OE2	2.35	0.48
1:A:185[A]:LYS:HG2	5:A:518:HOH:O	2.13	0.48
1:L:162[B]:LYS:HE2	1:L:163:GLU:O	2.14	0.47
1:A:141:MET:HE2	1:A:168:LYS:HG2	1.97	0.47
1:A:70:LYS:CG	5:A:437:HOH:O	2.60	0.46
1:A:70:LYS:CB	5:A:437:HOH:O	2.64	0.45
1:L:66:NRQ:HD1	1:L:199:LEU:HD12	1.97	0.45
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.85	0.44
1:A:141:MET:HE2	1:A:168:LYS:HG3	1.98	0.44
1:L:218[A]:GLU:CG	5:L:418:HOH:O	2.43	0.44
1:A:185[A]:LYS:HG3	5:A:554:HOH:O	2.17	0.44
1:L:162[B]:LYS:HE3	5:L:578:HOH:O	2.16	0.43
1:L:99:PHE:CD2	1:L:175:ALA:HB2	2.53	0.43
1:A:20:GLY:HA2	1:A:124:LEU:O	2.19	0.43
1:A:199:LEU:C	1:A:199:LEU:HD23	2.45	0.42
1:L:162[B]:LYS:HD3	5:L:578:HOH:O	2.19	0.42
1:L:66:NRQ:HD1	1:L:215:GLU:OE1	2.20	0.42
1:A:66:NRQ:HD1	1:A:215:GLU:OE1	2.20	0.41
1:A:185[A]:LYS:CD	5:A:554:HOH:O	2.68	0.41
1:A:62:SER:OG	1:A:63:PRO:HD3	2.21	0.41
1:A:66:NRQ:HD1	1:A:199:LEU:HD12	2.03	0.41
1:L:62:SER:N	1:L:63:PRO:CD	2.84	0.40
1:A:62:SER:N	1:A:63:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	216/266 (81%)	213 (99%)	3 (1%)	0	100	100
1	L	215/266 (81%)	213 (99%)	2 (1%)	0	100	100
All	All	431/532 (81%)	426 (99%)	5 (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	190/227 (84%)	187 (98%)	3 (2%)	58	32
1	L	189/227 (83%)	188 (100%)	1 (0%)	86	75
All	All	379/454 (84%)	375 (99%)	4 (1%)	70	48

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	LEU
1	A	178	LYS
1	A	222	SER
1	L	109	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	L	109	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 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	NRQ	L	66	1	23,24,25	0.99	1 (4%)	23,32,34	2.00	6 (26%)
1	NRQ	A	66	1	23,24,25	1.18	1 (4%)	23,32,34	1.78	5 (21%)

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	NRQ	L	66	1	-	4/9/31/32	0/2/2/2
1	NRQ	A	66	1	-	5/9/31/32	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	NRQ	C1-N2	3.99	1.42	1.33
1	L	66	NRQ	C1-N2	3.26	1.40	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	66	NRQ	CA2-C2-N3	4.67	105.58	103.37
1	A	66	NRQ	CA2-C2-N3	4.51	105.50	103.37
1	L	66	NRQ	CB2-CA2-C2	-3.92	117.59	122.28
1	L	66	NRQ	O2-C2-CA2	-3.73	128.86	130.96
1	A	66	NRQ	CB2-CA2-C2	-3.72	117.83	122.28
1	A	66	NRQ	O3-C3-CA3	-3.59	115.54	126.39
1	L	66	NRQ	O3-C3-CA3	-3.48	115.89	126.39
1	L	66	NRQ	CG2-CB2-CA2	3.32	134.01	129.94
1	A	66	NRQ	CB2-CA2-N2	2.87	132.80	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	66	NRQ	CB2-CA2-N2	2.81	132.72	128.83
1	A	66	NRQ	CG2-CB2-CA2	2.04	132.45	129.94

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	NRQ	C3-CA3-N3-C2
1	L	66	NRQ	C2-CA2-CB2-CG2
1	L	66	NRQ	N2-CA2-CB2-CG2
1	A	66	NRQ	CB1-CG1-SD-CE
1	A	66	NRQ	C3-CA3-N3-C1
1	A	66	NRQ	N2-CA2-CB2-CG2
1	L	66	NRQ	CB1-CG1-SD-CE
1	A	66	NRQ	C2-CA2-CB2-CG2
1	L	66	NRQ	C3-CA3-N3-C1

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L	66	NRQ	2	0
1	A	66	NRQ	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands 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
4	ACT	A	304	-	3,3,3	0.60	0	3,3,3	1.45	0
2	BME	A	301	1	3,3,3	0.22	0	1,2,2	0.64	0
3	SO4	A	302	-	4,4,4	0.31	0	6,6,6	0.11	0
3	SO4	A	303	-	4,4,4	0.24	0	6,6,6	0.14	0
2	BME	L	301	1	3,3,3	0.22	0	1,2,2	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BME	A	301	1	-	0/1/1/1	-
2	BME	L	301	1	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	301	BME	O1-C1-C2-S2

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304	ACT	4	0

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	214/266 (80%)	0.15	9 (4%)	41 44	10, 20, 35, 58	6 (2%)
1	L	214/266 (80%)	0.13	6 (2%)	55 58	10, 20, 34, 58	5 (2%)
All	All	428/532 (80%)	0.14	15 (3%)	47 51	10, 20, 35, 58	11 (2%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	THR	4.4
1	A	170	GLY	4.3
1	L	6	THR	4.3
1	A	169	ASP	3.8
1	L	7	ILE	3.7
1	A	7	ILE	3.6
1	L	25[A]	HIS	3.1
1	A	168	LYS	3.1
1	L	168	LYS	3.0
1	A	167	LEU	2.8
1	A	45	LYS	2.6
1	A	222	SER	2.2
1	A	172	HIS	2.1
1	L	128[A]	ASN	2.1
1	L	137	GLN	2.1

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(\AA^2)	Q<0.9
1	NRQ	A	66	23/24	0.94	0.14	20,26,41,44	0
1	NRQ	L	66	23/24	0.94	0.13	20,25,34,38	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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(\AA^2)	Q<0.9
2	BME	A	301	4/4	0.73	0.30	33,35,37,42	4
2	BME	L	301	4/4	0.79	0.28	39,39,40,41	4
3	SO4	A	303	5/5	0.81	0.11	51,56,64,65	0
3	SO4	A	302	5/5	0.83	0.11	55,56,59,60	0
4	ACT	A	304	4/4	0.85	0.14	30,32,34,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.