



Full wwPDB X-ray Structure Validation Report ⓘ

May 6, 2024 – 06:04 pm BST

PDB ID : 4ZFS
Title : Phototoxic Fluorescent Protein KillerOrange
Authors : Pletneva, N.V.; Pletnev, V.Z.; Pletnev, S.
Deposited on : 2015-04-21
Resolution : 2.01 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	:	2.36.2
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)	:	2.36.2

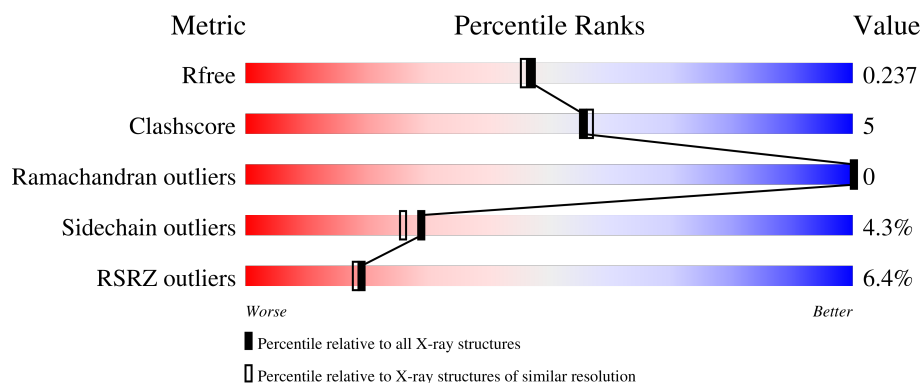
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	246	<div> <div>7%</div> <div>83% 12% • 5%</div> </div>
1	B	246	<div> <div>8%</div> <div>85% 8% • 5%</div> </div>
1	C	246	<div> <div>5%</div> <div>78% 13% • 7%</div> </div>
1	D	246	<div> <div>4%</div> <div>80% 11% • 7%</div> </div>
1	E	246	<div> <div>5%</div> <div>82% 9% • 7%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10068 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 KillerOrange.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	4	0
			1870	1173	329	352	16			
1	B	234	Total	C	N	O	S	0	2	0
			1857	1166	328	347	16			
1	C	228	Total	C	N	O	S	0	6	0
			1843	1157	322	347	17			
1	D	228	Total	C	N	O	S	0	3	0
			1820	1144	319	341	16			
1	E	228	Total	C	N	O	S	0	2	0
			1816	1142	320	338	16			

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP Q2TCH5
A	-9	ARG	-	expression tag	UNP Q2TCH5
A	-8	GLY	-	expression tag	UNP Q2TCH5
A	-7	SER	-	expression tag	UNP Q2TCH5
A	-6	HIS	-	expression tag	UNP Q2TCH5
A	-5	HIS	-	expression tag	UNP Q2TCH5
A	-4	HIS	-	expression tag	UNP Q2TCH5
A	-3	HIS	-	expression tag	UNP Q2TCH5
A	-2	HIS	-	expression tag	UNP Q2TCH5
A	-1	HIS	-	expression tag	UNP Q2TCH5
A	0	GLY	-	expression tag	UNP Q2TCH5
A	1	SER	-	expression tag	UNP Q2TCH5
A	3	CYS	GLY	conflict	UNP Q2TCH5
A	65	4M9	GLN	chromophore	UNP Q2TCH5
A	65	4M9	TYR	chromophore	UNP Q2TCH5
A	65	4M9	GLY	chromophore	UNP Q2TCH5
A	113	SER	ASP	conflict	UNP Q2TCH5
A	145	SER	ASN	conflict	UNP Q2TCH5
A	177	LEU	PHE	conflict	UNP Q2TCH5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	221	HIS	TYR	conflict	UNP Q2TCH5
A	236	GLN	GLU	conflict	UNP Q2TCH5
B	-10	MET	-	initiating methionine	UNP Q2TCH5
B	-9	ARG	-	expression tag	UNP Q2TCH5
B	-8	GLY	-	expression tag	UNP Q2TCH5
B	-7	SER	-	expression tag	UNP Q2TCH5
B	-6	HIS	-	expression tag	UNP Q2TCH5
B	-5	HIS	-	expression tag	UNP Q2TCH5
B	-4	HIS	-	expression tag	UNP Q2TCH5
B	-3	HIS	-	expression tag	UNP Q2TCH5
B	-2	HIS	-	expression tag	UNP Q2TCH5
B	-1	HIS	-	expression tag	UNP Q2TCH5
B	0	GLY	-	expression tag	UNP Q2TCH5
B	1	SER	-	expression tag	UNP Q2TCH5
B	3	CYS	GLY	conflict	UNP Q2TCH5
B	65	4M9	GLN	chromophore	UNP Q2TCH5
B	65	4M9	TYR	chromophore	UNP Q2TCH5
B	65	4M9	GLY	chromophore	UNP Q2TCH5
B	113	SER	ASP	conflict	UNP Q2TCH5
B	145	SER	ASN	conflict	UNP Q2TCH5
B	177	LEU	PHE	conflict	UNP Q2TCH5
B	221	HIS	TYR	conflict	UNP Q2TCH5
B	236	GLN	GLU	conflict	UNP Q2TCH5
C	-10	MET	-	initiating methionine	UNP Q2TCH5
C	-9	ARG	-	expression tag	UNP Q2TCH5
C	-8	GLY	-	expression tag	UNP Q2TCH5
C	-7	SER	-	expression tag	UNP Q2TCH5
C	-6	HIS	-	expression tag	UNP Q2TCH5
C	-5	HIS	-	expression tag	UNP Q2TCH5
C	-4	HIS	-	expression tag	UNP Q2TCH5
C	-3	HIS	-	expression tag	UNP Q2TCH5
C	-2	HIS	-	expression tag	UNP Q2TCH5
C	-1	HIS	-	expression tag	UNP Q2TCH5
C	0	GLY	-	expression tag	UNP Q2TCH5
C	1	SER	-	expression tag	UNP Q2TCH5
C	3	CYS	GLY	conflict	UNP Q2TCH5
C	65	4M9	GLN	chromophore	UNP Q2TCH5
C	65	4M9	TYR	chromophore	UNP Q2TCH5
C	65	4M9	GLY	chromophore	UNP Q2TCH5
C	113	SER	ASP	conflict	UNP Q2TCH5
C	145	SER	ASN	conflict	UNP Q2TCH5
C	177	LEU	PHE	conflict	UNP Q2TCH5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	221	HIS	TYR	conflict	UNP Q2TCH5
C	236	GLN	GLU	conflict	UNP Q2TCH5
D	-10	MET	-	initiating methionine	UNP Q2TCH5
D	-9	ARG	-	expression tag	UNP Q2TCH5
D	-8	GLY	-	expression tag	UNP Q2TCH5
D	-7	SER	-	expression tag	UNP Q2TCH5
D	-6	HIS	-	expression tag	UNP Q2TCH5
D	-5	HIS	-	expression tag	UNP Q2TCH5
D	-4	HIS	-	expression tag	UNP Q2TCH5
D	-3	HIS	-	expression tag	UNP Q2TCH5
D	-2	HIS	-	expression tag	UNP Q2TCH5
D	-1	HIS	-	expression tag	UNP Q2TCH5
D	0	GLY	-	expression tag	UNP Q2TCH5
D	1	SER	-	expression tag	UNP Q2TCH5
D	3	CYS	GLY	conflict	UNP Q2TCH5
D	65	4M9	GLN	chromophore	UNP Q2TCH5
D	65	4M9	TYR	chromophore	UNP Q2TCH5
D	65	4M9	GLY	chromophore	UNP Q2TCH5
D	113	SER	ASP	conflict	UNP Q2TCH5
D	145	SER	ASN	conflict	UNP Q2TCH5
D	177	LEU	PHE	conflict	UNP Q2TCH5
D	221	HIS	TYR	conflict	UNP Q2TCH5
D	236	GLN	GLU	conflict	UNP Q2TCH5
E	-10	MET	-	initiating methionine	UNP Q2TCH5
E	-9	ARG	-	expression tag	UNP Q2TCH5
E	-8	GLY	-	expression tag	UNP Q2TCH5
E	-7	SER	-	expression tag	UNP Q2TCH5
E	-6	HIS	-	expression tag	UNP Q2TCH5
E	-5	HIS	-	expression tag	UNP Q2TCH5
E	-4	HIS	-	expression tag	UNP Q2TCH5
E	-3	HIS	-	expression tag	UNP Q2TCH5
E	-2	HIS	-	expression tag	UNP Q2TCH5
E	-1	HIS	-	expression tag	UNP Q2TCH5
E	0	GLY	-	expression tag	UNP Q2TCH5
E	1	SER	-	expression tag	UNP Q2TCH5
E	3	CYS	GLY	conflict	UNP Q2TCH5
E	65	4M9	GLN	chromophore	UNP Q2TCH5
E	65	4M9	TYR	chromophore	UNP Q2TCH5
E	65	4M9	GLY	chromophore	UNP Q2TCH5
E	113	SER	ASP	conflict	UNP Q2TCH5
E	145	SER	ASN	conflict	UNP Q2TCH5
E	177	LEU	PHE	conflict	UNP Q2TCH5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	221	HIS	TYR	conflict	UNP Q2TCH5
E	236	GLN	GLU	conflict	UNP Q2TCH5

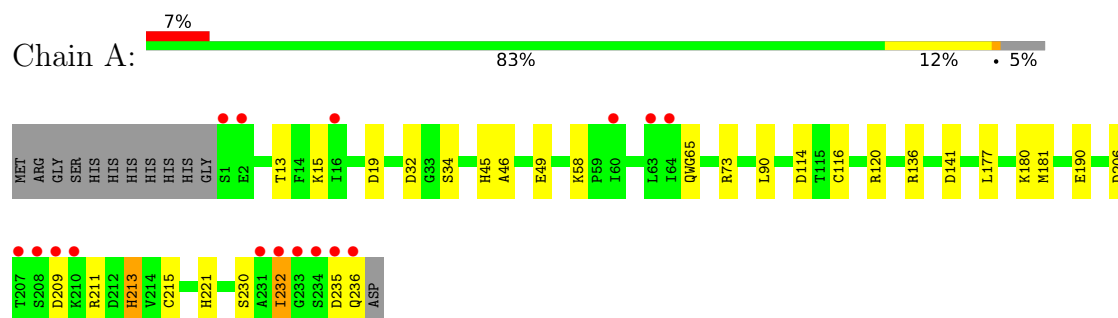
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	182	Total	O	0	0
			182	182		
2	B	185	Total	O	0	0
			185	185		
2	C	172	Total	O	0	0
			172	172		
2	D	167	Total	O	0	0
			167	167		
2	E	156	Total	O	0	0
			156	156		

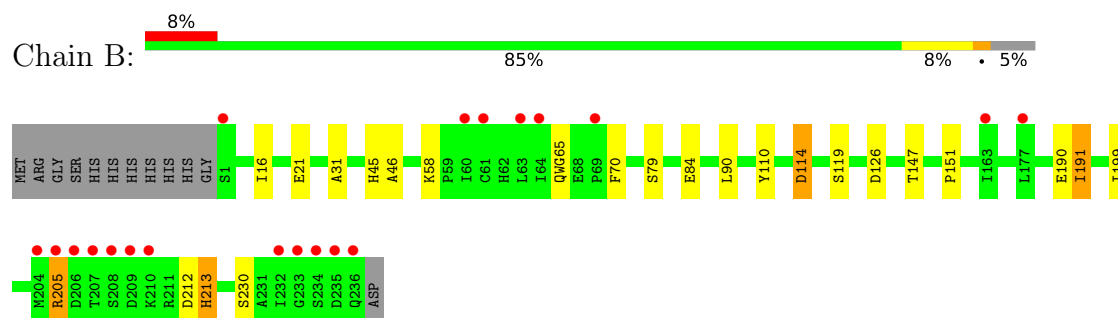
3 Residue-property plots [i](#)

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.

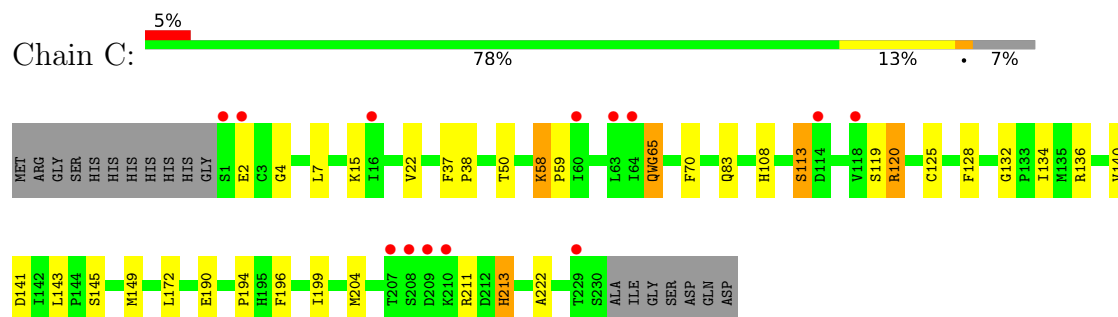
• Molecule 1: KillerOrange



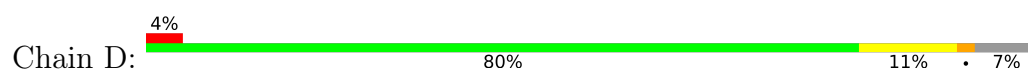
• Molecule 1: KillerOrange

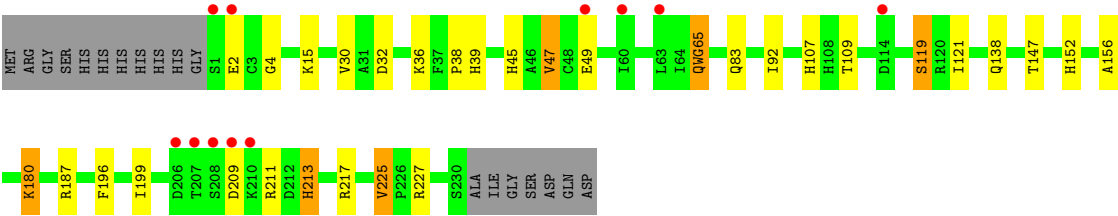


• Molecule 1: KillerOrange

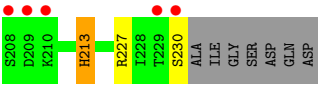
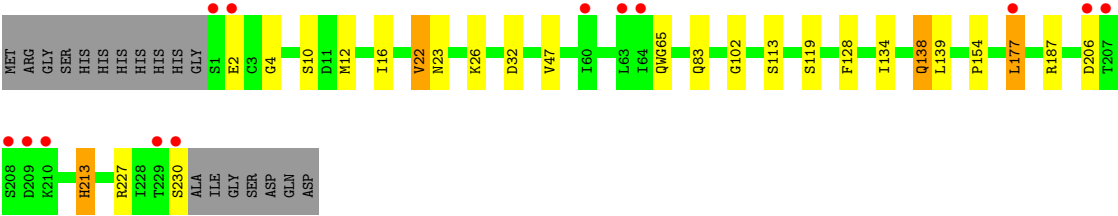
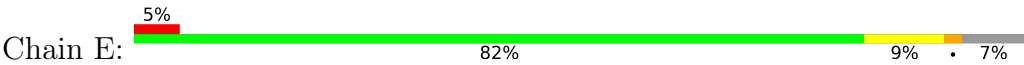


• Molecule 1: KillerOrange





• Molecule 1: KillerOrange



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	128.93Å 202.06Å 116.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.85 – 2.01 29.85 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.85-2.01) 99.4 (29.85-2.01)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.66 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.192 , 0.236 0.201 , 0.237	Depositor DCC
R_{free} test set	994 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	1.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10068	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.88% 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: 4M9

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	1.00	0/1891	0.98	0/2558
1	B	0.95	0/1879	0.99	0/2543
1	C	0.96	0/1864	0.95	0/2522
1	D	0.90	0/1842	0.90	0/2494
1	E	0.91	0/1837	0.97	1/2486 (0.0%)
All	All	0.95	0/9313	0.96	1/12603 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	177	LEU	CA-CB-CG	8.10	133.93	115.30

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	1870	0	1769	22	0
1	B	1857	0	1756	15	1
1	C	1843	0	1737	27	1
1	D	1820	0	1715	19	0
1	E	1816	0	1721	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	182	0	0	2	0
2	B	185	0	0	6	0
2	C	172	0	0	4	0
2	D	167	0	0	0	0
2	E	156	0	0	1	0
All	All	10068	0	8698	91	1

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 5.

All (91) 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:136[B]:ARG:HH11	1:A:136[B]:ARG:CG	1.63	1.11
1:A:136[B]:ARG:HG2	1:A:136[B]:ARG:NH1	1.49	0.96
1:C:2:GLU:HG2	1:C:7:LEU:HD21	1.66	0.77
1:A:32:ASP:OD2	1:C:113:SER:OG	2.02	0.76
1:C:2:GLU:CG	1:C:7:LEU:HD21	2.18	0.72
1:B:213:HIS:CD2	2:B:323:HOH:O	2.48	0.66
1:A:136[B]:ARG:HH11	1:A:136[B]:ARG:HG2	0.68	0.66
1:C:2:GLU:N	2:C:301:HOH:O	2.25	0.65
1:E:227[A]:ARG:NH1	2:E:301:HOH:O	2.29	0.65
1:B:45[A]:HIS:NE2	2:B:301:HOH:O	2.30	0.65
1:C:140:VAL:HG12	1:C:141:ASP:OD1	1.98	0.64
1:D:209:ASP:HB3	1:D:211:ARG:H	1.64	0.62
1:A:73:ARG:HB3	1:A:221:HIS:HD2	1.66	0.61
1:B:151:PRO:CB	1:B:191:ILE:HD11	2.31	0.60
1:C:136:ARG:HD3	2:C:416:HOH:O	2.01	0.60
1:D:196:PHE:HE2	1:D:225:VAL:HG13	1.66	0.60
1:A:177:LEU:C	1:A:177:LEU:HD23	2.24	0.57
2:A:319:HOH:O	1:C:120:ARG:HG3	2.05	0.55
1:C:143:LEU:HD11	1:C:172:LEU:HD21	1.89	0.55
1:B:114:ASP:HA	2:B:428:HOH:O	2.05	0.55
1:C:50:THR:HG21	2:C:406:HOH:O	2.07	0.54
1:C:65:4M9:H10	1:C:65:4M9:O2	2.09	0.53
1:B:205:ARG:NH2	2:B:304:HOH:O	2.41	0.53
1:A:45:HIS:CD2	1:A:215:CYS:SG	3.03	0.52
1:B:151:PRO:HB3	1:B:191:ILE:HD11	1.92	0.51
1:D:209:ASP:HB2	1:D:213:HIS:NE2	2.25	0.51
1:C:2:GLU:HG3	1:C:7:LEU:HD21	1.93	0.51
1:D:4:GLY:HA2	1:D:83:GLN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ALA:O	1:A:213:HIS:HB2	2.12	0.50
1:A:235:ASP:O	1:A:236:GLN:CB	2.58	0.50
1:E:206:ASP:O	1:E:213:HIS:CD2	2.65	0.50
1:C:4:GLY:HA2	1:C:83:GLN:O	2.10	0.50
1:A:136[B]:ARG:CG	1:A:136[B]:ARG:NH1	2.36	0.50
1:C:211:ARG:O	1:C:213:HIS:CD2	2.66	0.49
1:A:235:ASP:O	1:A:236:GLN:HB2	2.13	0.48
1:B:230:SER:HB3	2:B:375:HOH:O	2.13	0.48
1:E:4:GLY:HA2	1:E:83:GLN:O	2.13	0.48
1:D:196:PHE:CE2	1:D:225:VAL:HG13	2.48	0.48
1:D:227:ARG:NH2	1:E:187:ARG:O	2.48	0.47
1:A:49:GLU:HA	1:A:49:GLU:OE1	2.13	0.47
1:A:141:ASP:OD2	1:E:154:PRO:HG3	2.15	0.47
1:B:16:ILE:HB	1:B:31:ALA:HB3	1.97	0.47
1:B:110:TYR:CD2	1:B:119:SER:HB3	2.51	0.46
1:D:65:4M9:H10	1:D:65:4M9:O2	2.16	0.46
1:D:211:ARG:O	1:D:213:HIS:HD2	1.99	0.46
1:D:196:PHE:CE2	1:D:225:VAL:CG1	2.99	0.45
1:C:132:GLY:O	1:C:136:ARG:HG3	2.16	0.45
1:A:45:HIS:CD2	1:A:215:CYS:HG	2.35	0.45
1:C:22:VAL:HA	1:C:125:CYS:HB2	1.98	0.45
1:E:206:ASP:HB3	1:E:213:HIS:CD2	2.52	0.44
1:D:152:HIS:O	1:D:156:ALA:HB3	2.18	0.44
1:A:19[B]:ASP:OD2	1:C:120:ARG:NH1	2.51	0.44
1:A:13:THR:HA	1:A:34:SER:HA	2.00	0.44
1:E:10:SER:O	1:E:12:MET:HG3	2.17	0.44
1:C:58:LYS:CB	1:C:59:PRO:HD3	2.48	0.44
1:C:196:PHE:O	1:C:222:ALA:HA	2.18	0.44
1:A:90:LEU:HD11	1:A:181:MET:HB3	1.99	0.44
1:C:108:HIS:CD2	1:C:108:HIS:N	2.86	0.44
1:E:47:VAL:HG22	1:E:213:HIS:HB3	2.00	0.43
1:E:16:ILE:HG12	1:E:119:SER:OG	2.18	0.43
1:C:128:PHE:HE2	1:C:134:ILE:HD13	1.83	0.43
1:D:147:THR:HG21	1:D:199:ILE:HD12	2.01	0.43
1:D:45[A]:HIS:CE1	1:D:213:HIS:HD1	2.36	0.43
1:A:116:CYS:SG	1:C:15:LYS:HE3	2.59	0.43
1:A:206:ASP:O	1:A:213:HIS:CD2	2.71	0.43
1:A:232:ILE:HG13	1:D:217:ARG:NH1	2.33	0.42
1:B:46:ALA:O	1:B:213:HIS:HB2	2.19	0.42
1:D:30:VAL:HG12	1:D:49:GLU:OE2	2.19	0.42
1:B:205:ARG:NH1	1:B:212:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ARG:HD3	1:C:120:ARG:C	2.40	0.42
1:A:180:LYS:HE2	2:A:307:HOH:O	2.20	0.42
1:B:45[A]:HIS:CE1	2:B:301:HOH:O	2.71	0.42
1:D:109:THR:O	1:D:119:SER:HA	2.20	0.42
1:C:37:PHE:CD1	1:C:38:PRO:HA	2.56	0.41
1:C:199:ILE:HD13	1:C:199:ILE:HG21	1.83	0.41
1:E:102:GLY:HA3	1:E:128:PHE:CD1	2.56	0.41
1:D:38:PRO:O	1:D:39:HIS:HB2	2.20	0.41
1:D:107:HIS:O	1:D:121:ILE:HA	2.21	0.41
1:E:134:ILE:HG12	1:E:139:LEU:HD11	2.01	0.41
1:D:47:VAL:HB	1:D:213:HIS:HB3	2.03	0.41
1:D:92:ILE:HA	1:D:180:LYS:O	2.21	0.41
1:A:120:ARG:HD2	1:A:120:ARG:C	2.40	0.41
1:E:138[A]:GLN:HE21	1:E:138[A]:GLN:HB2	1.62	0.41
1:B:21:GLU:OE1	1:B:126:ASP:OD1	2.39	0.41
1:C:50:THR:CG2	2:C:406:HOH:O	2.66	0.41
1:C:120:ARG:C	1:C:120:ARG:CD	2.89	0.41
1:C:149:MET:O	1:C:194:PRO:HA	2.21	0.40
1:E:22:VAL:O	1:E:23:ASN:C	2.60	0.40
1:B:147:THR:HG21	1:B:199:ILE:HD12	2.02	0.40
1:E:26:LYS:HB3	1:E:26:LYS:HE3	1.84	0.40
1:B:84:GLU:OE1	1:B:190:GLU:O	2.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:SER:OG	1:C:190[A]:GLU:OE2[6_445]	1.94	0.26

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	233/246 (95%)	224 (96%)	9 (4%)	0	100	100
1	B	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
1	C	229/246 (93%)	221 (96%)	8 (4%)	0	100	100
1	D	226/246 (92%)	217 (96%)	9 (4%)	0	100	100
1	E	225/246 (92%)	216 (96%)	9 (4%)	0	100	100
All	All	1144/1230 (93%)	1100 (96%)	44 (4%)	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	206/212 (97%)	197 (96%)	9 (4%)	28	25
1	B	204/212 (96%)	197 (97%)	7 (3%)	37	36
1	C	204/212 (96%)	196 (96%)	8 (4%)	32	30
1	D	201/212 (95%)	189 (94%)	12 (6%)	19	14
1	E	200/212 (94%)	191 (96%)	9 (4%)	27	24
All	All	1015/1060 (96%)	970 (96%)	45 (4%)	29	25

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	58	LYS
1	A	114	ASP
1	A	190	GLU
1	A	209	ASP
1	A	211	ARG
1	A	213	HIS
1	A	230	SER
1	A	232	ILE
1	B	58	LYS

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Mol	Chain	Res	Type
1	B	70	PHE
1	B	90	LEU
1	B	114	ASP
1	B	191	ILE
1	B	205	ARG
1	B	213	HIS
1	C	58	LYS
1	C	70	PHE
1	C	113	SER
1	C	119	SER
1	C	120	ARG
1	C	145	SER
1	C	204	MET
1	C	213	HIS
1	D	2	GLU
1	D	15	LYS
1	D	32[A]	ASP
1	D	32[B]	ASP
1	D	36	LYS
1	D	47	VAL
1	D	119	SER
1	D	138	GLN
1	D	180	LYS
1	D	187	ARG
1	D	213	HIS
1	D	225	VAL
1	E	2	GLU
1	E	22	VAL
1	E	32	ASP
1	E	113	SER
1	E	138[A]	GLN
1	E	138[B]	GLN
1	E	177	LEU
1	E	213	HIS
1	E	230	SER

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

Mol	Chain	Res	Type
1	A	138	GLN
1	A	221	HIS
1	B	25	GLN

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Mol	Chain	Res	Type
1	B	213	HIS
1	C	45	HIS
1	C	124	ASN
1	D	43	ASN
1	D	124	ASN
1	D	221	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	4M9	E	65	1	26,28,28	1.43	5 (19%)	29,39,39	3.54	8 (27%)
1	4M9	C	65	1	26,28,28	1.44	5 (19%)	29,39,39	3.27	10 (34%)
1	4M9	B	65	1	26,28,28	1.60	4 (15%)	29,39,39	2.91	11 (37%)
1	4M9	A	65	1	26,28,28	1.41	5 (19%)	29,39,39	3.28	8 (27%)
1	4M9	D	65	1	26,28,28	1.22	2 (7%)	29,39,39	2.58	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	4M9	E	65	1	-	2/8/32/32	0/3/3/3
1	4M9	C	65	1	-	3/8/32/32	0/3/3/3
1	4M9	B	65	1	-	5/8/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4M9	A	65	1	-	2/8/32/32	0/3/3/3
1	4M9	D	65	1	-	3/8/32/32	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	65	4M9	C1-N2	-3.69	1.25	1.33
1	D	65	4M9	CA1-N1	3.60	1.36	1.27
1	A	65	4M9	CA1-N1	3.48	1.35	1.27
1	E	65	4M9	CB2-CA2	-3.36	1.32	1.35
1	C	65	4M9	CA1-N1	3.27	1.35	1.27
1	E	65	4M9	CA1-N1	3.22	1.35	1.27
1	C	65	4M9	CA2-C2	3.18	1.51	1.48
1	B	65	4M9	CA1-N1	3.14	1.35	1.27
1	B	65	4M9	CB2-CA2	-3.09	1.32	1.35
1	A	65	4M9	C1-N2	-2.95	1.26	1.33
1	E	65	4M9	C1-N2	-2.91	1.26	1.33
1	B	65	4M9	CZ2-CE2	-2.70	1.37	1.41
1	C	65	4M9	C1-N2	-2.63	1.27	1.33
1	D	65	4M9	C1-N2	-2.38	1.28	1.33
1	A	65	4M9	CA3-N3	-2.27	1.42	1.47
1	A	65	4M9	CZ2-CE2	-2.23	1.38	1.41
1	C	65	4M9	CH2-CZ2	2.15	1.41	1.36
1	E	65	4M9	CD1-NE1	2.14	1.41	1.36
1	E	65	4M9	CG2-CB2	-2.07	1.42	1.46
1	A	65	4M9	CB2-CA2	-2.06	1.33	1.35
1	C	65	4M9	CB2-CA2	-2.05	1.33	1.35

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	65	4M9	O2-C2-CA2	10.58	136.90	130.96
1	E	65	4M9	CB2-CA2-C2	9.74	133.90	122.28
1	E	65	4M9	CB2-CA2-N2	-9.50	115.65	128.83
1	A	65	4M9	CA2-C2-N3	-9.44	98.91	103.37
1	A	65	4M9	CB2-CA2-N2	-8.54	116.98	128.83
1	C	65	4M9	CB2-CA2-N2	-8.27	117.36	128.83
1	C	65	4M9	CA2-C2-N3	-7.95	99.61	103.37
1	C	65	4M9	O2-C2-CA2	7.49	135.17	130.96
1	A	65	4M9	CB2-CA2-C2	7.35	131.05	122.28
1	D	65	4M9	CB2-CA2-C2	6.93	130.54	122.28
1	D	65	4M9	CB2-CA2-N2	-6.92	119.23	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	4M9	O2-C2-CA2	6.81	134.78	130.96
1	B	65	4M9	CB2-CA2-C2	6.75	130.34	122.28
1	B	65	4M9	CB2-CA2-N2	-6.43	119.91	128.83
1	C	65	4M9	CB2-CA2-C2	6.34	129.84	122.28
1	A	65	4M9	O2-C2-CA2	5.96	134.31	130.96
1	E	65	4M9	CA2-C2-N3	-5.24	100.89	103.37
1	C	65	4M9	C2-CA2-N2	5.02	112.45	108.93
1	D	65	4M9	CA2-C2-N3	-4.92	101.04	103.37
1	B	65	4M9	CG-CD-N4	4.91	131.78	116.51
1	B	65	4M9	CA2-C2-N3	-4.41	101.28	103.37
1	A	65	4M9	C2-CA2-N2	4.16	111.85	108.93
1	D	65	4M9	CG-CB1-CA1	4.11	126.25	113.53
1	B	65	4M9	O5-CD-CG	-3.60	110.49	121.07
1	C	65	4M9	O3-C3-CA3	-3.59	115.55	126.39
1	B	65	4M9	CE3-CD2-CE2	3.32	122.58	118.17
1	A	65	4M9	CE3-CD2-CE2	3.24	122.47	118.17
1	C	65	4M9	CE3-CD2-CE2	3.23	122.45	118.17
1	A	65	4M9	O3-C3-CA3	-3.21	116.70	126.39
1	D	65	4M9	O3-C3-CA3	-3.18	116.80	126.39
1	B	65	4M9	O3-C3-CA3	-3.13	116.93	126.39
1	E	65	4M9	O3-C3-CA3	-3.11	117.00	126.39
1	B	65	4M9	CE3-CD2-CG2	-3.03	130.31	135.45
1	D	65	4M9	CG-CD-N4	2.96	125.74	116.51
1	D	65	4M9	O5-CD-N4	-2.89	114.61	122.50
1	E	65	4M9	CE3-CD2-CE2	2.71	121.76	118.17
1	D	65	4M9	CE3-CD2-CE2	2.51	121.50	118.17
1	D	65	4M9	O2-C2-CA2	2.50	132.37	130.96
1	B	65	4M9	CB1-CG-CD	2.50	126.70	114.16
1	A	65	4M9	CE3-CD2-CG2	-2.44	131.31	135.45
1	B	65	4M9	N3-C1-N2	2.33	116.35	113.28
1	C	65	4M9	O5-CD-CG	-2.32	114.24	121.07
1	C	65	4M9	N3-C1-N2	2.24	116.23	113.28
1	C	65	4M9	CE3-CD2-CG2	-2.23	131.67	135.45
1	E	65	4M9	C2-CA2-N2	2.06	110.37	108.93
1	E	65	4M9	CE3-CD2-CG2	-2.05	131.96	135.45

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	65	4M9	C2-CA2-CB2-CG2
1	B	65	4M9	C1-CA1-CB1-CG

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Mol	Chain	Res	Type	Atoms
1	C	65	4M9	C2-CA2-CB2-CG2
1	D	65	4M9	C1-CA1-CB1-CG
1	B	65	4M9	C2-CA2-CB2-CG2
1	D	65	4M9	C2-CA2-CB2-CG2
1	E	65	4M9	C2-CA2-CB2-CG2
1	A	65	4M9	N2-CA2-CB2-CG2
1	B	65	4M9	N2-CA2-CB2-CG2
1	C	65	4M9	N2-CA2-CB2-CG2
1	D	65	4M9	N2-CA2-CB2-CG2
1	E	65	4M9	N2-CA2-CB2-CG2
1	B	65	4M9	O5-CD-CG-CB1
1	B	65	4M9	N4-CD-CG-CB1
1	C	65	4M9	CA1-CB1-CG-CD

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	65	4M9	1	0
1	D	65	4M9	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	233/246 (94%)	0.33	16 (6%) 16 16	27, 39, 67, 117	0
1	B	233/246 (94%)	0.35	20 (8%) 10 9	29, 40, 77, 112	0
1	C	227/246 (92%)	0.24	13 (5%) 23 23	32, 42, 63, 115	0
1	D	227/246 (92%)	0.39	11 (4%) 30 29	31, 45, 70, 142	0
1	E	227/246 (92%)	0.41	13 (5%) 23 23	30, 46, 74, 114	0
All	All	1147/1230 (93%)	0.34	73 (6%) 19 18	27, 42, 71, 142	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	SER	19.3
1	C	1	SER	9.1
1	B	232	ILE	7.5
1	A	232	ILE	7.2
1	A	234	SER	7.1
1	A	233	GLY	6.9
1	E	1	SER	6.6
1	A	1	SER	6.4
1	B	233	GLY	6.3
1	A	235	ASP	6.1
1	E	207	THR	6.0
1	A	236	GLN	5.9
1	B	1	SER	5.6
1	E	210	LYS	5.2
1	B	236	GLN	5.1
1	B	207	THR	5.0
1	C	207	THR	4.7
1	E	209	ASP	4.7
1	A	207	THR	4.6
1	C	210	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	235	ASP	4.5
1	E	208	SER	4.4
1	E	64	ILE	4.4
1	D	208	SER	4.2
1	A	210	LYS	3.7
1	E	229	THR	3.7
1	E	60	ILE	3.6
1	C	2	GLU	3.5
1	A	231	ALA	3.5
1	C	209	ASP	3.5
1	B	209	ASP	3.4
1	B	210	LYS	3.4
1	E	63	LEU	3.4
1	A	209	ASP	3.3
1	B	208	SER	3.3
1	C	208	SER	3.2
1	B	234	SER	3.1
1	B	63	LEU	3.1
1	E	2	GLU	3.1
1	A	63	LEU	3.0
1	A	64	ILE	3.0
1	D	2	GLU	3.0
1	C	64	ILE	3.0
1	E	206	ASP	2.9
1	A	16	ILE	2.8
1	A	208	SER	2.8
1	A	2	GLU	2.7
1	C	60	ILE	2.7
1	B	205	ARG	2.7
1	B	206	ASP	2.6
1	C	63	LEU	2.6
1	D	207	THR	2.5
1	B	61	CYS	2.5
1	D	210	LYS	2.4
1	D	60	ILE	2.4
1	D	114	ASP	2.3
1	B	204	MET	2.3
1	B	163	ILE	2.3
1	D	209	ASP	2.3
1	B	177	LEU	2.3
1	E	177	LEU	2.3
1	C	118	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	229	THR	2.2
1	B	69	PRO	2.2
1	D	63	LEU	2.2
1	E	230	SER	2.2
1	B	64	ILE	2.2
1	D	49	GLU	2.2
1	C	114	ASP	2.2
1	C	16	ILE	2.2
1	D	206	ASP	2.1
1	B	60	ILE	2.1
1	A	60	ILE	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(Å ²)	Q<0.9
1	4M9	B	65	26/26	0.92	0.22	36,39,44,45	0
1	4M9	D	65	26/26	0.92	0.18	40,46,52,57	0
1	4M9	C	65	26/26	0.93	0.19	40,48,63,65	0
1	4M9	A	65	26/26	0.93	0.20	31,38,43,44	0
1	4M9	E	65	26/26	0.94	0.25	39,47,53,58	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.