



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2020 – 03:23 am BST

PDB ID : 6LVS
Title : USP14 catalytic domain mutant C114S
Authors : Lin, H.C.; Lin, T.H.; Chou, C.Y.
Deposited on : 2020-02-04
Resolution : 2.73 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

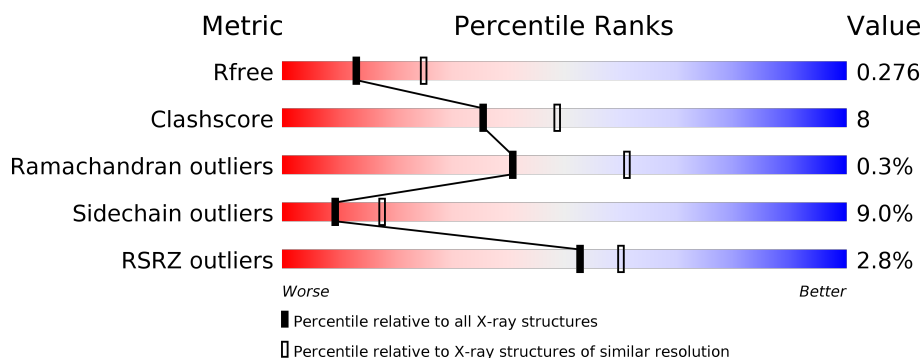
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	410	<div> <div> <div>0%</div> <div>68%</div> <div>11%</div> <div>•</div> <div>19%</div> </div> </div>
1	B	410	<div> <div> <div>0%</div> <div>66%</div> <div>13%</div> <div>•</div> <div>20%</div> </div> </div>
1	C	410	<div> <div> <div>2%</div> <div>64%</div> <div>15%</div> <div>•</div> <div>19%</div> </div> </div>
1	D	410	<div> <div> <div>4%</div> <div>65%</div> <div>14%</div> <div>•</div> <div>20%</div> </div> </div>
1	E	410	<div> <div> <div>2%</div> <div>63%</div> <div>14%</div> <div>•</div> <div>20%</div> </div> </div>
1	F	410	<div> <div> <div>4%</div> <div>61%</div> <div>17%</div> <div>•</div> <div>19%</div> </div> </div>

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
2	GOL	A	503	-	-	-	X
2	GOL	B	501	-	-	X	X
2	GOL	C	502	-	-	-	X
2	GOL	D	501	-	-	X	-
2	GOL	E	501	-	-	-	X
2	GOL	E	502	-	-	X	X
3	NA	A	509	-	-	-	X
3	NA	A	510	-	-	-	X
3	NA	B	509	-	-	-	X
3	NA	C	504	-	-	-	X
4	FMT	A	512	-	-	X	-
4	FMT	B	514	-	-	-	X
4	FMT	C	513	-	-	X	X
4	FMT	E	510	-	-	X	-
4	FMT	F	510	-	-	X	-
5	BME	C	517	-	-	X	-
5	BME	C	518	-	-	-	X
5	BME	E	517	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16510 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 Ubiquitin carboxyl-terminal hydrolase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2665	1701	445	501	18			
1	B	330	Total	C	N	O	S	0	0	0
			2651	1694	443	496	18			
1	C	333	Total	C	N	O	S	0	0	0
			2682	1714	444	505	19			
1	D	329	Total	C	N	O	S	0	0	0
			2646	1686	440	502	18			
1	E	328	Total	C	N	O	S	0	0	0
			2630	1681	441	490	18			
1	F	331	Total	C	N	O	S	0	0	0
			2651	1690	444	499	18			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	HIS	-	expression tag	UNP P54578
A	77	HIS	-	expression tag	UNP P54578
A	78	HIS	-	expression tag	UNP P54578
A	79	HIS	-	expression tag	UNP P54578
A	80	HIS	-	expression tag	UNP P54578
A	81	HIS	-	expression tag	UNP P54578
A	82	SER	-	expression tag	UNP P54578
A	83	SER	-	expression tag	UNP P54578
A	84	GLY	-	expression tag	UNP P54578
A	85	LEU	-	expression tag	UNP P54578
A	86	VAL	-	expression tag	UNP P54578
A	87	PRO	-	expression tag	UNP P54578
A	88	ARG	-	expression tag	UNP P54578
A	89	GLY	-	expression tag	UNP P54578
A	90	SER	-	expression tag	UNP P54578
A	91	HIS	-	expression tag	UNP P54578
A	114	SER	CYS	engineered mutation	UNP P54578

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP P54578
A	?	-	LYS	deletion	UNP P54578
A	?	-	GLU	deletion	UNP P54578
A	?	-	THR	deletion	UNP P54578
A	?	-	ASP	deletion	UNP P54578
A	?	-	SER	deletion	UNP P54578
A	?	-	SER	deletion	UNP P54578
A	?	-	SER	deletion	UNP P54578
A	?	-	ALA	deletion	UNP P54578
B	76	HIS	-	expression tag	UNP P54578
B	77	HIS	-	expression tag	UNP P54578
B	78	HIS	-	expression tag	UNP P54578
B	79	HIS	-	expression tag	UNP P54578
B	80	HIS	-	expression tag	UNP P54578
B	81	HIS	-	expression tag	UNP P54578
B	82	SER	-	expression tag	UNP P54578
B	83	SER	-	expression tag	UNP P54578
B	84	GLY	-	expression tag	UNP P54578
B	85	LEU	-	expression tag	UNP P54578
B	86	VAL	-	expression tag	UNP P54578
B	87	PRO	-	expression tag	UNP P54578
B	88	ARG	-	expression tag	UNP P54578
B	89	GLY	-	expression tag	UNP P54578
B	90	SER	-	expression tag	UNP P54578
B	91	HIS	-	expression tag	UNP P54578
B	114	SER	CYS	engineered mutation	UNP P54578
B	?	-	VAL	deletion	UNP P54578
B	?	-	LYS	deletion	UNP P54578
B	?	-	GLU	deletion	UNP P54578
B	?	-	THR	deletion	UNP P54578
B	?	-	ASP	deletion	UNP P54578
B	?	-	SER	deletion	UNP P54578
B	?	-	SER	deletion	UNP P54578
B	?	-	SER	deletion	UNP P54578
B	?	-	ALA	deletion	UNP P54578
C	76	HIS	-	expression tag	UNP P54578
C	77	HIS	-	expression tag	UNP P54578
C	78	HIS	-	expression tag	UNP P54578
C	79	HIS	-	expression tag	UNP P54578
C	80	HIS	-	expression tag	UNP P54578
C	81	HIS	-	expression tag	UNP P54578
C	82	SER	-	expression tag	UNP P54578

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	83	SER	-	expression tag	UNP P54578
C	84	GLY	-	expression tag	UNP P54578
C	85	LEU	-	expression tag	UNP P54578
C	86	VAL	-	expression tag	UNP P54578
C	87	PRO	-	expression tag	UNP P54578
C	88	ARG	-	expression tag	UNP P54578
C	89	GLY	-	expression tag	UNP P54578
C	90	SER	-	expression tag	UNP P54578
C	91	HIS	-	expression tag	UNP P54578
C	114	SER	CYS	engineered mutation	UNP P54578
C	?	-	VAL	deletion	UNP P54578
C	?	-	LYS	deletion	UNP P54578
C	?	-	GLU	deletion	UNP P54578
C	?	-	THR	deletion	UNP P54578
C	?	-	ASP	deletion	UNP P54578
C	?	-	SER	deletion	UNP P54578
C	?	-	SER	deletion	UNP P54578
C	?	-	ALA	deletion	UNP P54578
D	76	HIS	-	expression tag	UNP P54578
D	77	HIS	-	expression tag	UNP P54578
D	78	HIS	-	expression tag	UNP P54578
D	79	HIS	-	expression tag	UNP P54578
D	80	HIS	-	expression tag	UNP P54578
D	81	HIS	-	expression tag	UNP P54578
D	82	SER	-	expression tag	UNP P54578
D	83	SER	-	expression tag	UNP P54578
D	84	GLY	-	expression tag	UNP P54578
D	85	LEU	-	expression tag	UNP P54578
D	86	VAL	-	expression tag	UNP P54578
D	87	PRO	-	expression tag	UNP P54578
D	88	ARG	-	expression tag	UNP P54578
D	89	GLY	-	expression tag	UNP P54578
D	90	SER	-	expression tag	UNP P54578
D	91	HIS	-	expression tag	UNP P54578
D	114	SER	CYS	engineered mutation	UNP P54578
D	?	-	VAL	deletion	UNP P54578
D	?	-	LYS	deletion	UNP P54578
D	?	-	GLU	deletion	UNP P54578
D	?	-	THR	deletion	UNP P54578
D	?	-	ASP	deletion	UNP P54578
D	?	-	SER	deletion	UNP P54578

Continued on next page...

Continued from previous page...

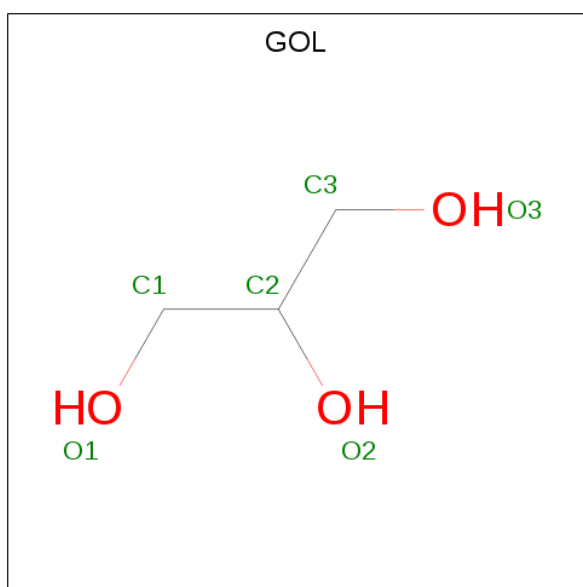
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	SER	deletion	UNP P54578
D	?	-	SER	deletion	UNP P54578
D	?	-	ALA	deletion	UNP P54578
E	76	HIS	-	expression tag	UNP P54578
E	77	HIS	-	expression tag	UNP P54578
E	78	HIS	-	expression tag	UNP P54578
E	79	HIS	-	expression tag	UNP P54578
E	80	HIS	-	expression tag	UNP P54578
E	81	HIS	-	expression tag	UNP P54578
E	82	SER	-	expression tag	UNP P54578
E	83	SER	-	expression tag	UNP P54578
E	84	GLY	-	expression tag	UNP P54578
E	85	LEU	-	expression tag	UNP P54578
E	86	VAL	-	expression tag	UNP P54578
E	87	PRO	-	expression tag	UNP P54578
E	88	ARG	-	expression tag	UNP P54578
E	89	GLY	-	expression tag	UNP P54578
E	90	SER	-	expression tag	UNP P54578
E	91	HIS	-	expression tag	UNP P54578
E	114	SER	CYS	engineered mutation	UNP P54578
E	?	-	VAL	deletion	UNP P54578
E	?	-	LYS	deletion	UNP P54578
E	?	-	GLU	deletion	UNP P54578
E	?	-	THR	deletion	UNP P54578
E	?	-	ASP	deletion	UNP P54578
E	?	-	SER	deletion	UNP P54578
E	?	-	SER	deletion	UNP P54578
E	?	-	SER	deletion	UNP P54578
E	?	-	ALA	deletion	UNP P54578
F	76	HIS	-	expression tag	UNP P54578
F	77	HIS	-	expression tag	UNP P54578
F	78	HIS	-	expression tag	UNP P54578
F	79	HIS	-	expression tag	UNP P54578
F	80	HIS	-	expression tag	UNP P54578
F	81	HIS	-	expression tag	UNP P54578
F	82	SER	-	expression tag	UNP P54578
F	83	SER	-	expression tag	UNP P54578
F	84	GLY	-	expression tag	UNP P54578
F	85	LEU	-	expression tag	UNP P54578
F	86	VAL	-	expression tag	UNP P54578
F	87	PRO	-	expression tag	UNP P54578
F	88	ARG	-	expression tag	UNP P54578

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	89	GLY	-	expression tag	UNP P54578
F	90	SER	-	expression tag	UNP P54578
F	91	HIS	-	expression tag	UNP P54578
F	114	SER	CYS	engineered mutation	UNP P54578
F	?	-	VAL	deletion	UNP P54578
F	?	-	LYS	deletion	UNP P54578
F	?	-	GLU	deletion	UNP P54578
F	?	-	THR	deletion	UNP P54578
F	?	-	ASP	deletion	UNP P54578
F	?	-	SER	deletion	UNP P54578
F	?	-	SER	deletion	UNP P54578
F	?	-	SER	deletion	UNP P54578
F	?	-	ALA	deletion	UNP P54578

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

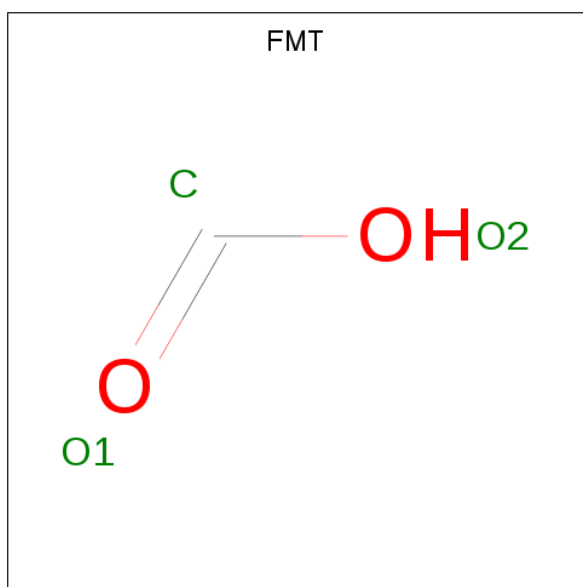
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	5	Total	Na	0	0
			5	5		
3	E	7	Total	Na	0	0
			7	7		
3	B	8	Total	Na	0	0
			8	8		
3	C	8	Total	Na	0	0
			8	8		
3	A	7	Total	Na	0	0
			7	7		
3	F	6	Total	Na	0	0
			6	6		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



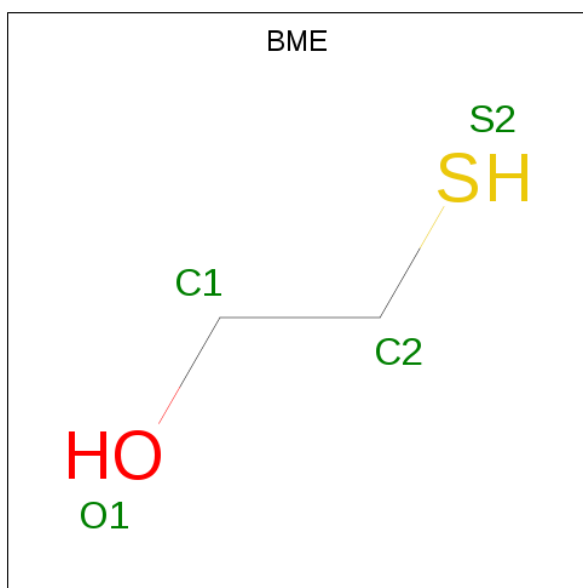
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		

Continued on next page...

Continued from previous page...

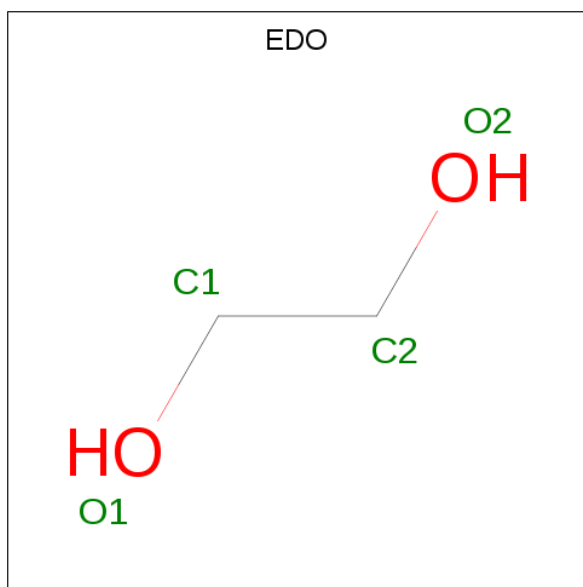
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	E	1	Total	C	O	S	0	0
			4	2	1	1		
5	E	1	Total	C	O	S	0	0
			4	2	1	1		
5	E	1	Total	C	O	S	0	0
			4	2	1	1		
5	F	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

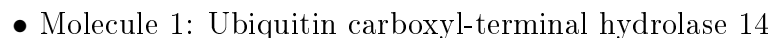
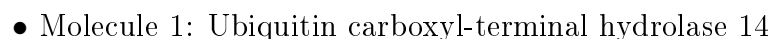


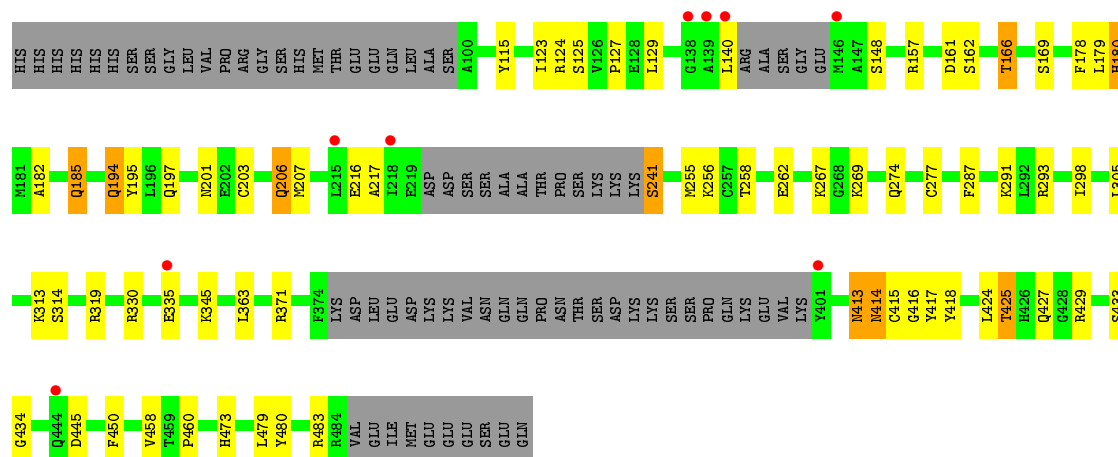
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

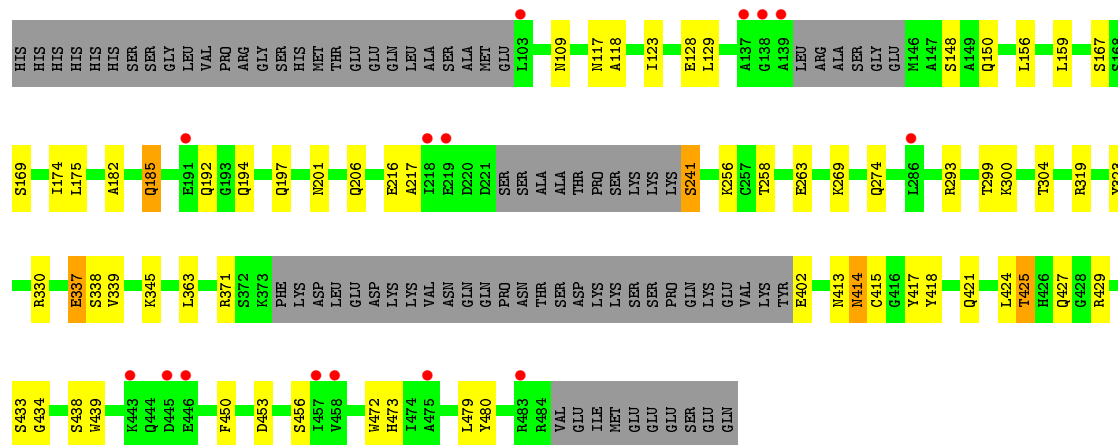
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	27	Total 27	O 27	0	0
7	B	52	Total 52	O 52	0	0
7	C	98	Total 98	O 98	0	0
7	D	40	Total 40	O 40	0	0
7	E	109	Total 109	O 109	0	0
7	F	28	Total 28	O 28	0	0

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 14

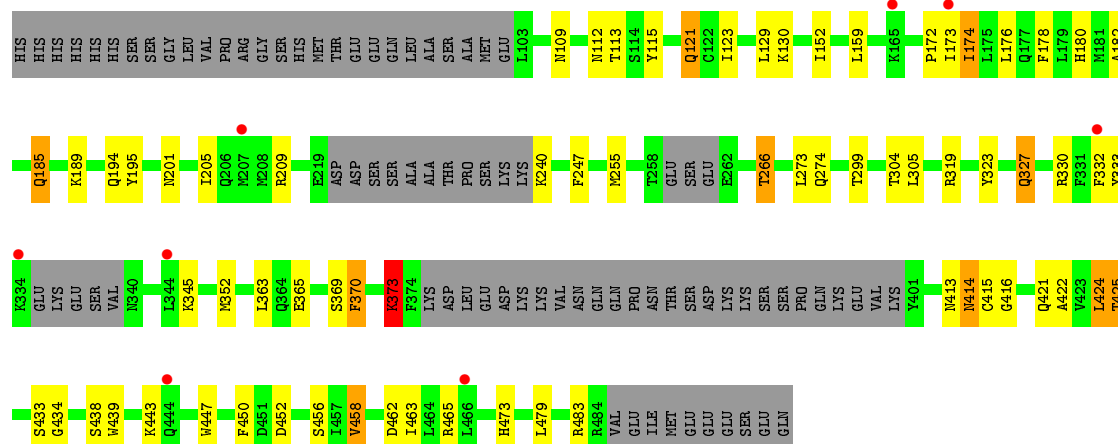




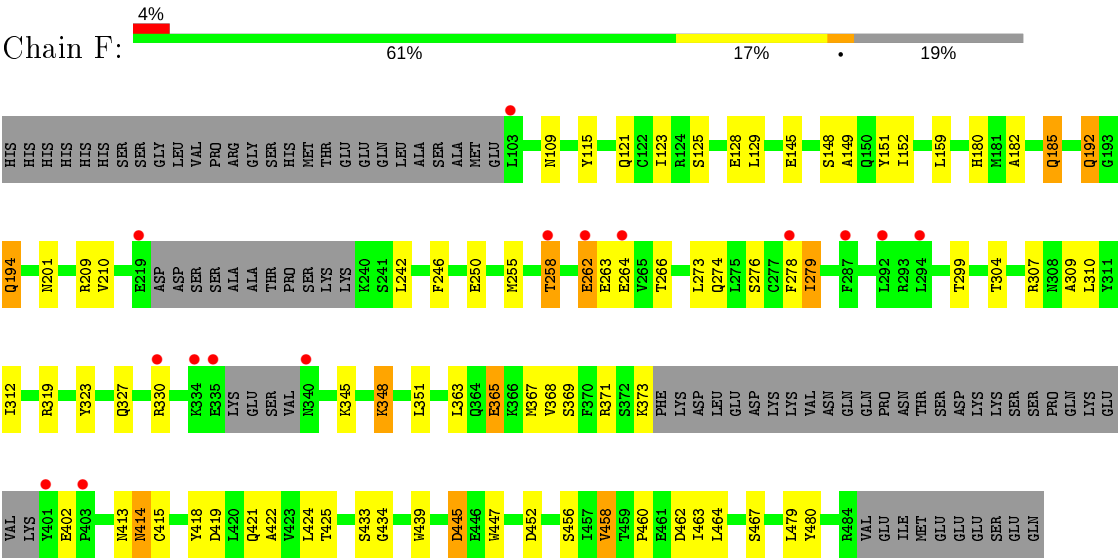
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 14



• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 14



• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 14



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.51Å 160.42Å 90.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.49 – 2.73 28.47 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.0 (28.49-2.73) 98.1 (28.47-2.73)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.197 , 0.277 0.199 , 0.276	Depositor DCC
R_{free} test set	3065 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 14.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.459 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16510	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: GOL, FMT, EDO, NA, 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	0.65	0/2716	0.75	0/3658
1	B	0.64	0/2702	0.75	0/3640
1	C	0.65	0/2734	0.75	0/3682
1	D	0.66	0/2696	0.74	0/3631
1	E	0.65	0/2680	0.76	0/3608
1	F	0.66	0/2702	0.77	0/3640
All	All	0.65	0/16230	0.75	0/21859

There are no bond length outliers.

There are no bond angle outliers.

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	2665	0	2650	38	0
1	B	2651	0	2634	43	0
1	C	2682	0	2664	42	0
1	D	2646	0	2625	36	0
1	E	2630	0	2618	63	0
1	F	2651	0	2622	38	0
2	A	18	0	24	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	18	0	24	6	0
2	C	12	0	16	0	0
2	D	12	0	16	4	0
2	E	12	0	16	16	0
3	A	7	0	0	0	0
3	B	8	0	0	1	0
3	C	8	0	0	0	0
3	D	5	0	0	0	0
3	E	7	0	0	0	0
3	F	6	0	0	0	0
4	A	6	0	2	3	0
4	B	21	0	7	5	0
4	C	18	0	6	3	0
4	D	6	0	2	2	0
4	E	15	0	5	3	0
4	F	12	0	4	5	0
5	A	4	0	6	2	0
5	B	8	0	12	0	0
5	C	8	0	12	6	0
5	E	12	0	18	3	0
5	F	4	0	6	0	0
6	E	4	0	6	3	0
7	A	27	0	0	2	0
7	B	52	0	0	4	0
7	C	98	0	0	5	0
7	D	40	0	0	3	0
7	E	109	0	0	9	0
7	F	28	0	0	1	0
All	All	16510	0	15995	260	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.

The worst 5 of 260 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:E:180:HIS:CE1	2:E:502:GOL:H31	1.88	1.07
1:E:180:HIS:HE1	2:E:502:GOL:H31	0.96	1.06
1:E:180:HIS:HE1	2:E:502:GOL:C3	1.74	1.01
1:D:217:ALA:HB2	1:D:241:SER:HB3	1.41	0.99
1:C:217:ALA:HB2	1:C:241:SER:HB3	1.48	0.96

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	323/410 (79%)	305 (94%)	17 (5%)	1 (0%)	41	61
1	B	322/410 (78%)	306 (95%)	16 (5%)	0	100	100
1	C	325/410 (79%)	307 (94%)	18 (6%)	0	100	100
1	D	321/410 (78%)	308 (96%)	13 (4%)	0	100	100
1	E	318/410 (78%)	293 (92%)	23 (7%)	2 (1%)	25	44
1	F	323/410 (79%)	305 (94%)	16 (5%)	2 (1%)	25	44
All	All	1932/2460 (78%)	1824 (94%)	103 (5%)	5 (0%)	41	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	279	ILE
1	E	373	LYS
1	A	169	SER
1	F	452	ASP
1	E	452	ASP

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	294/368 (80%)	276 (94%)	18 (6%)	18	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	291/368 (79%)	268 (92%)	23 (8%)	12	22
1	C	296/368 (80%)	267 (90%)	29 (10%)	8	14
1	D	293/368 (80%)	268 (92%)	25 (8%)	10	20
1	E	288/368 (78%)	263 (91%)	25 (9%)	10	19
1	F	290/368 (79%)	253 (87%)	37 (13%)	4	6
All	All	1752/2208 (79%)	1595 (91%)	157 (9%)	9	18

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	167	SER
1	D	363	LEU
1	F	369	SER
1	D	185	GLN
1	D	258	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	274	GLN
1	D	185	GLN
1	F	201	ASN
1	C	308	ASN
1	C	414	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 89 ligands modelled in this entry, 41 are monoatomic - leaving 48 for Mogul analysis.

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	$\# Z > 2$
2	GOL	A	502	-	5,5,5	0.12	0	5,5,5	0.35	0
4	FMT	F	508	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	518	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	516	-	0,2,2	0.00	-	0,1,1	0.00	-
2	GOL	D	502	-	5,5,5	0.11	0	5,5,5	0.28	0
4	FMT	E	514	-	0,2,2	0.00	-	0,1,1	0.00	-
2	GOL	B	502	-	5,5,5	0.17	0	5,5,5	0.39	0
4	FMT	B	514	3	0,2,2	0.00	-	0,1,1	0.00	-
2	GOL	C	502	-	5,5,5	0.10	0	5,5,5	0.28	0
4	FMT	C	511	-	0,2,2	0.00	-	0,1,1	0.00	-
5	BME	C	517	-	3,3,3	0.17	0	1,2,2	0.20	0
5	BME	F	511	-	3,3,3	0.15	0	1,2,2	0.17	0
4	FMT	B	517	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	E	512	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	D	508	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	512	3	0,2,2	0.00	-	0,1,1	0.00	-
5	BME	E	515	-	3,3,3	0.14	0	1,2,2	0.01	0
4	FMT	D	509	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	C	514	3	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	513	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	F	510	-	0,2,2	0.00	-	0,1,1	0.00	-
5	BME	B	520	-	3,3,3	0.13	0	1,2,2	0.05	0
5	BME	C	518	-	3,3,3	0.12	0	1,2,2	0.43	0
5	BME	E	517	-	3,3,3	0.07	0	1,2,2	0.21	0
4	FMT	C	512	3	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	511	-	0,2,2	0.00	-	0,1,1	0.00	-
2	GOL	B	503	-	5,5,5	0.12	0	5,5,5	0.40	0
4	FMT	A	512	3	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	C	516	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	515	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	E	513	3	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	F	509	3	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BME	B	519	-	3,3,3	0.15	0	1,2,2	0.07	0
2	GOL	B	501	-	5,5,5	0.07	0	5,5,5	0.28	0
2	GOL	A	501	-	5,5,5	0.10	0	5,5,5	0.31	0
2	GOL	C	501	-	5,5,5	0.11	0	5,5,5	0.29	0
4	FMT	E	511	-	0,2,2	0.00	-	0,1,1	0.00	-
5	BME	A	513	-	3,3,3	0.13	0	1,2,2	0.35	0
4	FMT	C	515	-	0,2,2	0.00	-	0,1,1	0.00	-
2	GOL	E	502	-	5,5,5	0.09	0	5,5,5	0.32	0
2	GOL	A	503	-	5,5,5	0.10	0	5,5,5	0.30	0
4	FMT	C	513	-	0,2,2	0.00	-	0,1,1	0.00	-
5	BME	E	516	-	3,3,3	0.13	0	1,2,2	0.07	0
6	EDO	E	518	-	3,3,3	0.05	0	2,2,2	0.30	0
4	FMT	F	507	-	0,2,2	0.00	-	0,1,1	0.00	-
2	GOL	D	501	-	5,5,5	0.11	0	5,5,5	0.39	0
4	FMT	E	510	-	0,2,2	0.00	-	0,1,1	0.00	-
2	GOL	E	501	-	5,5,5	0.12	0	5,5,5	0.30	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	GOL	A	502	-	-	4/4/4/4	-
6	EDO	E	518	-	-	0/1/1/1	-
2	GOL	D	502	-	-	2/4/4/4	-
2	GOL	B	502	-	-	3/4/4/4	-
2	GOL	C	502	-	-	2/4/4/4	-
5	BME	C	517	-	-	1/1/1/1	-
5	BME	F	511	-	-	1/1/1/1	-
5	BME	E	516	-	-	1/1/1/1	-
5	BME	E	515	-	-	0/1/1/1	-
5	BME	B	520	-	-	1/1/1/1	-
5	BME	C	518	-	-	1/1/1/1	-
5	BME	E	517	-	-	0/1/1/1	-
2	GOL	B	503	-	-	2/4/4/4	-
5	BME	B	519	-	-	1/1/1/1	-
2	GOL	B	501	-	-	3/4/4/4	-
2	GOL	A	501	-	-	4/4/4/4	-
2	GOL	C	501	-	-	0/4/4/4	-
5	BME	A	513	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	E	502	-	-	3/4/4/4	-
2	GOL	A	503	-	-	4/4/4/4	-
2	GOL	D	501	-	-	2/4/4/4	-
2	GOL	E	501	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	511	BME	O1-C1-C2-S2
2	B	501	GOL	C1-C2-C3-O3
5	C	517	BME	O1-C1-C2-S2
2	B	503	GOL	O1-C1-C2-C3
2	A	503	GOL	O1-C1-C2-C3

There are no ring outliers.

28 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	GOL	3	0
4	F	508	FMT	1	0
4	B	518	FMT	1	0
4	B	516	FMT	1	0
4	E	514	FMT	1	0
4	B	514	FMT	1	0
5	C	517	BME	4	0
4	D	508	FMT	1	0
4	D	509	FMT	1	0
4	B	513	FMT	1	0
4	F	510	FMT	3	0
5	C	518	BME	2	0
4	C	512	FMT	1	0
4	A	511	FMT	1	0
4	A	512	FMT	2	0
4	B	515	FMT	1	0
2	B	501	GOL	6	0
2	A	501	GOL	3	0
5	A	513	BME	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	502	GOL	15	0
2	A	503	GOL	2	0
4	C	513	FMT	2	0
5	E	516	BME	3	0
6	E	518	EDO	3	0
4	F	507	FMT	1	0
2	D	501	GOL	4	0
4	E	510	FMT	2	0
2	E	501	GOL	1	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	331/410 (80%)	0.14	4 (1%) 79 83	22, 39, 70, 102	0
1	B	330/410 (80%)	0.20	4 (1%) 79 83	23, 39, 70, 89	0
1	C	333/410 (81%)	0.27	9 (2%) 54 61	29, 50, 87, 107	0
1	D	329/410 (80%)	0.34	15 (4%) 32 35	29, 50, 80, 112	0
1	E	328/410 (80%)	0.33	8 (2%) 59 66	30, 51, 79, 105	0
1	F	331/410 (80%)	0.35	15 (4%) 33 36	32, 53, 80, 112	0
All	All	1982/2460 (80%)	0.27	55 (2%) 53 60	22, 48, 79, 112	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	334	LYS	7.2
1	D	139	ALA	5.4
1	F	335	GLU	5.3
1	C	140	LEU	5.2
1	D	138	GLY	5.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(Å ²)	Q<0.9
3	NA	B	511	1/1	0.49	0.27	57,57,57,57	0
3	NA	C	504	1/1	0.55	1.39	85,85,85,85	0
3	NA	B	509	1/1	0.56	0.44	68,68,68,68	0
2	GOL	E	502	6/6	0.62	1.35	107,115,118,118	0
2	GOL	E	501	6/6	0.63	1.49	163,167,170,173	0
2	GOL	C	502	6/6	0.67	0.65	106,107,114,115	0
2	GOL	A	503	6/6	0.70	0.44	81,86,88,92	0
6	EDO	E	518	4/4	0.70	0.27	82,85,87,90	0
4	FMT	B	514	3/3	0.70	0.55	59,59,61,63	0
4	FMT	E	510	3/3	0.71	0.24	74,74,75,77	0
3	NA	A	510	1/1	0.74	1.15	78,78,78,78	0
4	FMT	C	513	3/3	0.75	0.50	89,89,90,91	0
2	GOL	B	501	6/6	0.76	1.03	121,126,126,130	0
3	NA	D	503	1/1	0.77	0.23	61,61,61,61	0
2	GOL	D	502	6/6	0.77	0.25	69,70,72,73	0
5	BME	E	517	4/4	0.77	0.45	69,70,71,74	0
5	BME	C	518	4/4	0.79	0.42	94,94,96,102	0
5	BME	B	519	4/4	0.80	0.30	70,71,72,76	0
3	NA	A	509	1/1	0.80	0.54	54,54,54,54	0
4	FMT	C	514	3/3	0.81	1.32	123,123,125,126	0
2	GOL	D	501	6/6	0.81	0.81	93,96,97,101	0
4	FMT	B	517	3/3	0.82	0.52	87,87,88,89	0
2	GOL	A	502	6/6	0.82	0.35	57,61,62,64	0
3	NA	F	501	1/1	0.82	0.53	49,49,49,49	0
2	GOL	B	503	6/6	0.83	0.26	56,62,63,64	0
4	FMT	E	513	3/3	0.83	0.54	91,91,93,93	0
4	FMT	D	509	3/3	0.83	0.32	88,88,89,90	0
3	NA	D	506	1/1	0.83	0.24	68,68,68,68	0
2	GOL	A	501	6/6	0.84	0.92	74,88,91,93	0
4	FMT	E	511	3/3	0.84	0.60	61,61,64,66	0
3	NA	E	507	1/1	0.85	0.22	85,85,85,85	0
5	BME	F	511	4/4	0.85	0.24	66,71,73,79	0
3	NA	E	509	1/1	0.85	0.39	54,54,54,54	0
4	FMT	C	515	3/3	0.86	0.16	65,65,65,66	0
3	NA	C	510	1/1	0.87	0.19	66,66,66,66	0
3	NA	A	506	1/1	0.87	0.34	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	FMT	C	516	3/3	0.88	0.19	62,62,65,65	0
2	GOL	C	501	6/6	0.88	0.18	59,62,65,66	0
5	BME	B	520	4/4	0.88	0.16	95,99,100,101	0
3	NA	E	506	1/1	0.89	0.14	55,55,55,55	0
4	FMT	F	508	3/3	0.89	0.46	88,88,89,89	0
5	BME	E	516	4/4	0.90	0.22	91,96,98,100	0
4	FMT	A	511	3/3	0.90	1.31	69,69,76,80	0
3	NA	D	507	1/1	0.90	0.59	69,69,69,69	0
5	BME	A	513	4/4	0.90	0.70	117,120,123,127	0
3	NA	A	504	1/1	0.90	0.24	36,36,36,36	0
4	FMT	B	518	3/3	0.90	0.22	58,58,61,62	0
3	NA	C	509	1/1	0.91	0.22	63,63,63,63	0
3	NA	F	504	1/1	0.91	0.18	68,68,68,68	0
4	FMT	F	507	3/3	0.91	0.20	71,71,75,78	0
4	FMT	A	512	3/3	0.92	0.39	61,61,63,63	0
3	NA	E	508	1/1	0.92	0.14	60,60,60,60	0
4	FMT	C	512	3/3	0.92	0.40	53,53,56,57	0
3	NA	B	506	1/1	0.92	0.16	91,91,91,91	0
3	NA	A	505	1/1	0.93	0.32	46,46,46,46	0
3	NA	C	503	1/1	0.93	0.30	61,61,61,61	0
3	NA	B	504	1/1	0.93	0.27	52,52,52,52	0
3	NA	F	503	1/1	0.93	0.15	54,54,54,54	0
4	FMT	E	514	3/3	0.93	1.04	89,89,91,92	0
3	NA	E	503	1/1	0.93	0.19	46,46,46,46	0
4	FMT	B	515	3/3	0.94	0.47	72,72,80,84	0
5	BME	C	517	4/4	0.94	0.21	61,63,64,65	0
5	BME	E	515	4/4	0.94	0.12	70,73,73,73	0
4	FMT	C	511	3/3	0.94	0.19	44,44,47,49	0
3	NA	B	508	1/1	0.94	0.31	35,35,35,35	0
4	FMT	F	510	3/3	0.95	0.46	75,75,75,80	0
2	GOL	B	502	6/6	0.95	0.28	47,48,50,50	0
4	FMT	B	513	3/3	0.95	0.29	52,52,58,63	0
3	NA	C	507	1/1	0.95	0.48	64,64,64,64	0
3	NA	B	507	1/1	0.95	0.64	52,52,52,52	0
3	NA	F	506	1/1	0.95	0.31	52,52,52,52	0
3	NA	A	508	1/1	0.95	0.47	95,95,95,95	0
3	NA	C	505	1/1	0.95	0.19	44,44,44,44	0
4	FMT	E	512	3/3	0.95	0.44	89,89,89,90	0
3	NA	F	502	1/1	0.95	0.34	51,51,51,51	0
3	NA	E	504	1/1	0.95	0.15	41,41,41,41	0
4	FMT	F	509	3/3	0.95	0.35	55,55,57,58	0
4	FMT	D	508	3/3	0.96	0.24	45,45,46,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	FMT	B	512	3/3	0.97	0.17	47,47,52,57	0
3	NA	D	505	1/1	0.97	0.37	47,47,47,47	0
4	FMT	B	516	3/3	0.97	0.47	63,63,66,67	0
3	NA	D	504	1/1	0.97	1.16	52,52,52,52	0
3	NA	F	505	1/1	0.98	0.27	63,63,63,63	0
3	NA	C	506	1/1	0.98	0.31	45,45,45,45	0
3	NA	B	510	1/1	0.98	0.16	66,66,66,66	0
3	NA	E	505	1/1	0.98	0.55	55,55,55,55	0
3	NA	B	505	1/1	0.98	0.72	55,55,55,55	0
3	NA	A	507	1/1	0.98	0.57	53,53,53,53	0
3	NA	C	508	1/1	0.98	0.22	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.