



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 08:09 am BST

PDB ID : 3N7A
Title : Crystal structure of 3-dehydroquinate dehydratase from Mycobacterium tuberculosis in complex with inhibitor 2
Authors : Dias, M.V.B.; Snee, W.C.; Bromfield, K.M.; Payne, R.; Palaninathan, S.K.; Ciulli, A.; Howard, N.I.; Abell, C.; Sacchettini, J.C.; Blundell, T.L.
Deposited on : 2010-05-26
Resolution : 2.00 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

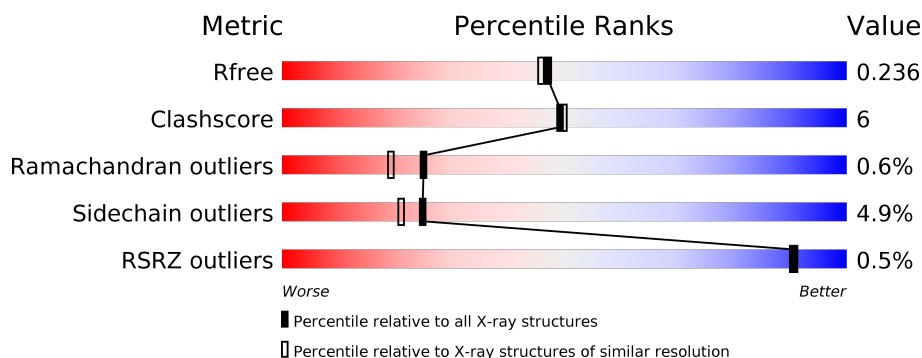
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.















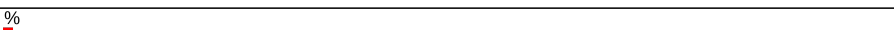


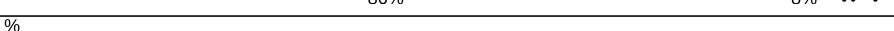


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	147	<div> <div>81%</div> <div>13%</div> <div>• •</div> </div>
1	B	147	<div> <div>84%</div> <div>11%</div> <div>• •</div> </div>
1	C	147	<div> <div>81%</div> <div>12%</div> <div>• • 5%</div> </div>
1	D	147	<div> <div>%</div> <div>88%</div> <div>6%</div> <div>• •</div> </div>
1	E	147	<div> <div>%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
1	F	147	<div> <div>82%</div> <div>7%</div> <div>• 7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	147	 84% 9% . . .
1	H	147	 80% 13% . .
1	I	147	%  80% 11% . . .
1	J	147	%  80% 10% . . .
1	K	147	 82% 12% . .
1	L	147	 78% 15% . . .
1	M	147	%  84% 8% . . .
1	N	147	%  76% 17% . .
1	O	147	%  78% 13% . . .
1	P	147	 81% 13% . . .
1	Q	147	 87% 5% . .
1	R	147	%  84% 11% . . .
1	S	147	%  79% 12% 5% .
1	T	147	 81% 13% . . .
1	U	147	%  86% 8% . . .
1	V	147	%  82% 13% . .
1	W	147	%  84% 9% . .
1	X	147	 82% 9% . . 7%

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	FA1	N	147	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 28420 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 3-dehydroquinate dehydratase.

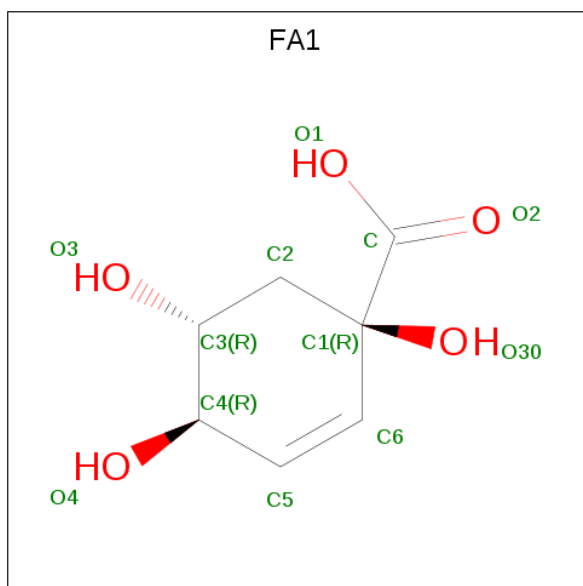
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1067	672	196	198	1			
1	B	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	C	139	Total	C	N	O	S	0	0	0
			1055	664	194	196	1			
1	D	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	E	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	F	137	Total	C	N	O	S	0	1	0
			1042	654	194	193	1			
1	G	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	H	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	I	141	Total	C	N	O	S	0	1	0
			1073	676	198	198	1			
1	J	141	Total	C	N	O	S	0	1	0
			1073	676	198	198	1			
1	K	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	L	141	Total	C	N	O	S	0	2	0
			1083	681	201	200	1			
1	M	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	N	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	O	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	P	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	141	Total	C	N	O	S	0	0	0
			1065	671	193	200	1			
1	R	141	Total	C	N	O	S	0	1	0
			1067	673	195	198	1			
1	S	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	T	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	U	141	Total	C	N	O	S	0	1	0
			1073	676	198	198	1			
1	V	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	W	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	X	137	Total	C	N	O	S	0	1	0
			1043	657	191	194	1			

- Molecule 2 is 2,3 -ANHYDRO-QUINIC ACID (three-letter code: FA1) (formula: C₇H₁₀O₅).



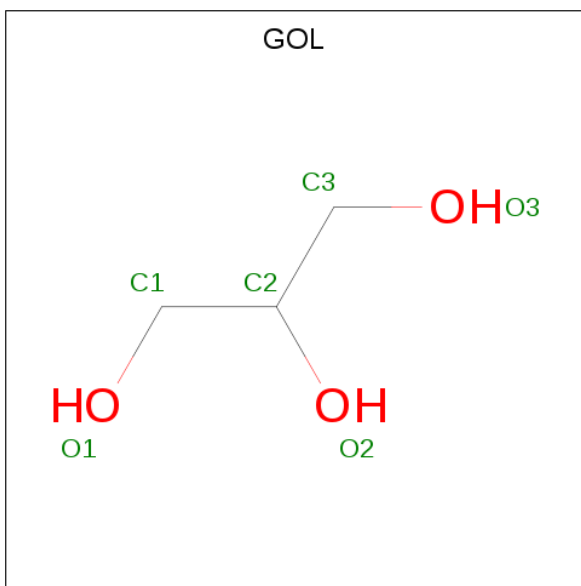
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	7	5		
2	B	1	Total	C	O	0	0
			12	7	5		
2	C	1	Total	C	O	0	0
			12	7	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			12	7	5		
2	E	1	Total	C	O	0	0
			12	7	5		
2	F	1	Total	C	O	0	0
			12	7	5		
2	G	1	Total	C	O	0	0
			12	7	5		
2	H	1	Total	C	O	0	0
			12	7	5		
2	I	1	Total	C	O	0	0
			12	7	5		
2	J	1	Total	C	O	0	0
			12	7	5		
2	K	1	Total	C	O	0	0
			12	7	5		
2	L	1	Total	C	O	0	0
			12	7	5		
2	M	1	Total	C	O	0	0
			12	7	5		
2	N	1	Total	C	O	0	0
			12	7	5		
2	O	1	Total	C	O	0	0
			12	7	5		
2	P	1	Total	C	O	0	0
			12	7	5		
2	Q	1	Total	C	O	0	0
			12	7	5		
2	R	1	Total	C	O	0	0
			12	7	5		
2	S	1	Total	C	O	0	0
			12	7	5		
2	T	1	Total	C	O	0	0
			12	7	5		
2	U	1	Total	C	O	0	0
			12	7	5		
2	V	1	Total	C	O	0	0
			12	7	5		
2	W	1	Total	C	O	0	0
			12	7	5		
2	X	1	Total	C	O	0	0
			12	7	5		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	O	1	Total	C	O	0	0
			6	3	3		
3	P	1	Total	C	O	0	0
			6	3	3		
3	Q	1	Total	C	O	0	0
			6	3	3		
3	T	1	Total	C	O	0	0
			6	3	3		
3	U	1	Total	C	O	0	0
			6	3	3		
3	V	1	Total	C	O	0	0
			6	3	3		
3	X	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	82	Total O 82 82	0	0
4	B	95	Total O 95 95	0	0
4	C	96	Total O 96 96	0	0
4	D	84	Total O 84 84	0	0
4	E	84	Total O 84 84	0	0
4	F	85	Total O 85 85	0	0
4	G	101	Total O 101 101	0	0
4	H	106	Total O 106 106	0	0
4	I	99	Total O 99 99	0	0
4	J	125	Total O 125 125	0	0
4	K	92	Total O 92 92	0	0
4	L	127	Total O 127 127	0	0
4	M	112	Total O 112 112	0	0
4	N	85	Total O 85 85	0	0
4	O	85	Total O 85 85	0	0
4	P	102	Total O 102 102	0	0
4	Q	108	Total O 108 108	0	0
4	R	83	Total O 83 83	0	0
4	S	103	Total O 103 103	0	0
4	T	112	Total O 112 112	0	0
4	U	94	Total O 94 94	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	V	81	Total 81	O 81	0	0
4	W	109	Total 109	O 109	0	0
4	X	97	Total 97	O 97	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 3-dehydroquinase dehydratase

Chain A: 




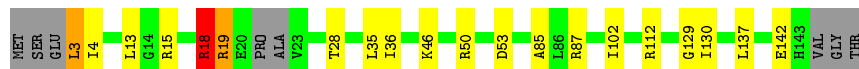
- Molecule 1: 3-dehydroquinase dehydratase

Chain B: 




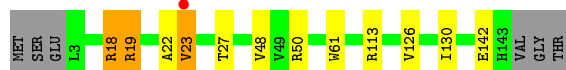
- Molecule 1: 3-dehydroquinase dehydratase

Chain C: 




- Molecule 1: 3-dehydroquinase dehydratase

Chain D: 




- Molecule 1: 3-dehydroquinase dehydratase

Chain E: 




- Molecule 1: 3-dehydroquinase dehydratase

Chain F:  82% 7% 7%



- Molecule 1: 3-dehydroquinase dehydratase

Chain G:  84% 9% 7%




- Molecule 1: 3-dehydroquinase dehydratase

Chain H:  80% 13% 7%




- Molecule 1: 3-dehydroquinase dehydratase

Chain I:  80% 11% 7%




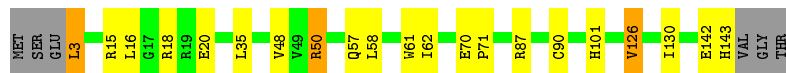
- Molecule 1: 3-dehydroquinase dehydratase

Chain J:  80% 10% 7%




- Molecule 1: 3-dehydroquinase dehydratase

Chain K:  82% 12% 7%

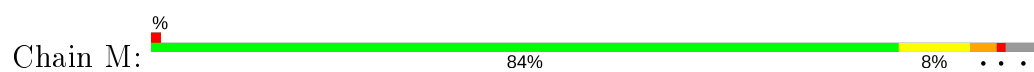


- Molecule 1: 3-dehydroquinase dehydratase

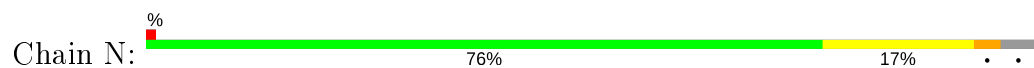
Chain L:  78% 15% 7%



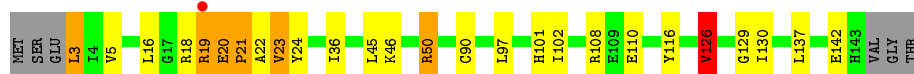
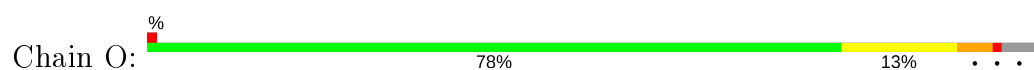
- Molecule 1: 3-dehydroquinase dehydratase



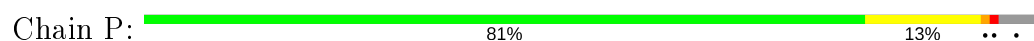
- Molecule 1: 3-dehydroquinase dehydratase



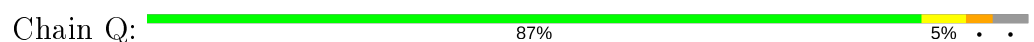
- Molecule 1: 3-dehydroquinase dehydratase



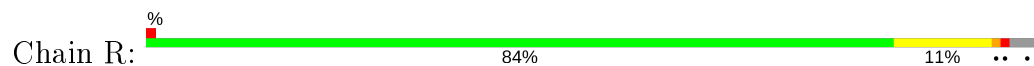
- Molecule 1: 3-dehydroquinase dehydratase



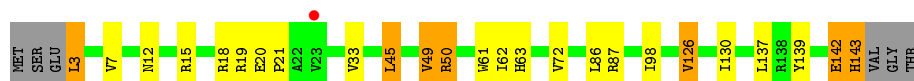
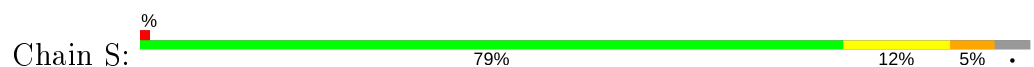
- Molecule 1: 3-dehydroquinase dehydratase




- Molecule 1: 3-dehydroquinase dehydratase



- Molecule 1: 3-dehydroquinase dehydratase




- Molecule 1: 3-dehydroquininate dehydratase

Chain T:  81% 13% ..




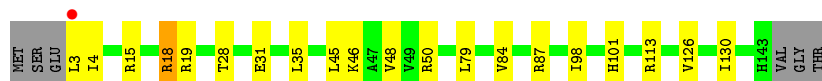
- Molecule 1: 3-dehydroquininate dehydratase

Chain U:  86% 8% ..




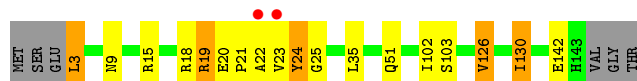
- Molecule 1: 3-dehydroquininate dehydratase

Chain V:  82% 13% ..




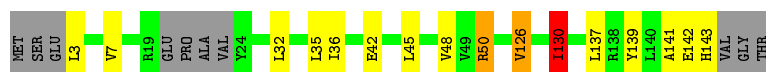
- Molecule 1: 3-dehydroquininate dehydratase

Chain W:  84% 9% ..



- Molecule 1: 3-dehydroquininate dehydratase

Chain X:  82% 9% .. 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.91Å 95.56Å 124.47Å 79.93° 80.30° 77.60°	Depositor
Resolution (Å)	79.21 – 2.00 79.21 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (79.21-2.00) 95.0 (79.21-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.178 , 0.238 0.178 , 0.236	Depositor DCC
R_{free} test set	12908 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	28420	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: GOL, FA1

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	1.05	0/1085	0.99	2/1478 (0.1%)
1	B	1.00	0/1100	0.97	1/1498 (0.1%)
1	C	1.04	1/1071 (0.1%)	0.99	6/1456 (0.4%)
1	D	0.99	1/1100 (0.1%)	0.94	0/1498
1	E	0.99	0/1100	0.96	4/1498 (0.3%)
1	F	1.05	2/1062 (0.2%)	0.92	3/1443 (0.2%)
1	G	1.10	0/1100	1.02	2/1498 (0.1%)
1	H	1.10	0/1089	1.02	2/1483 (0.1%)
1	I	1.10	0/1096	1.04	5/1493 (0.3%)
1	J	1.31	5/1096 (0.5%)	1.10	5/1493 (0.3%)
1	K	1.02	1/1100 (0.1%)	0.96	4/1498 (0.3%)
1	L	1.28	6/1111 (0.5%)	1.05	2/1512 (0.1%)
1	M	1.18	2/1100 (0.2%)	1.04	4/1498 (0.3%)
1	N	1.09	1/1100 (0.1%)	0.95	1/1498 (0.1%)
1	O	1.06	1/1100 (0.1%)	0.94	3/1498 (0.2%)
1	P	1.13	1/1089 (0.1%)	0.94	2/1483 (0.1%)
1	Q	1.17	2/1083 (0.2%)	0.98	1/1476 (0.1%)
1	R	1.02	0/1090	0.93	3/1486 (0.2%)
1	S	1.19	1/1100 (0.1%)	1.08	6/1498 (0.4%)
1	T	1.14	4/1100 (0.4%)	1.01	4/1498 (0.3%)
1	U	0.99	1/1096 (0.1%)	0.94	1/1493 (0.1%)
1	V	0.99	1/1100 (0.1%)	0.95	3/1498 (0.2%)
1	W	1.16	1/1100 (0.1%)	1.01	3/1498 (0.2%)
1	X	1.00	0/1064	0.95	3/1447 (0.2%)
All	All	1.09	31/26232 (0.1%)	0.99	70/35719 (0.2%)

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	D	0	1
1	G	0	1
1	I	0	2
1	J	0	1
1	K	0	1
1	L	0	2
1	M	0	1
1	Q	0	1
1	U	0	2
1	X	0	1
All	All	0	13

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	126	VAL	CB-CG1	-9.90	1.32	1.52
1	U	90	CYS	CB-SG	-7.45	1.69	1.82
1	V	84	VAL	CB-CG2	7.14	1.67	1.52
1	T	84	VAL	CB-CG2	7.04	1.67	1.52
1	F	126	VAL	CB-CG1	-5.88	1.40	1.52

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ASP	CB-CG-OD1	8.19	125.67	118.30
1	I	20	GLU	C-N-CD	-8.01	102.98	120.60
1	S	87	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	M	53	ASP	CB-CG-OD1	7.54	125.09	118.30
1	G	23	VAL	C-N-CA	7.50	140.45	121.70

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	19	ARG	Peptide
1	G	23	VAL	Peptide
1	I	20	GLU	Peptide
1	I	22	ALA	Peptide
1	J	22	ALA	Peptide

5.2 Too-close contacts ⓘ

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	1067	0	1075	11	0
1	B	1077	0	1082	11	0
1	C	1055	0	1062	13	0
1	D	1077	0	1082	10	0
1	E	1077	0	1082	14	0
1	F	1042	0	1047	10	0
1	G	1077	0	1082	8	0
1	H	1071	0	1079	15	0
1	I	1073	0	1078	34	0
1	J	1073	0	1078	20	0
1	K	1077	0	1082	7	0
1	L	1083	0	1091	16	1
1	M	1077	0	1082	9	0
1	N	1077	0	1082	19	0
1	O	1077	0	1082	18	0
1	P	1071	0	1079	11	0
1	Q	1065	0	1068	4	0
1	R	1067	0	1067	11	0
1	S	1077	0	1082	18	0
1	T	1077	0	1082	13	0
1	U	1073	0	1078	6	0
1	V	1077	0	1082	14	0
1	W	1077	0	1082	19	0
1	X	1043	0	1043	8	0
2	A	12	0	10	0	0
2	B	12	0	10	1	0
2	C	12	0	10	0	0
2	D	12	0	10	0	0
2	E	12	0	10	0	0
2	F	12	0	10	0	0
2	G	12	0	10	0	0
2	H	12	0	10	0	0
2	I	12	0	10	0	0
2	J	12	0	9	0	0
2	K	12	0	10	0	0
2	L	12	0	10	0	0
2	M	12	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	12	0	10	2	0
2	O	12	0	10	0	0
2	P	12	0	10	0	0
2	Q	12	0	10	0	0
2	R	12	0	8	0	0
2	S	12	0	10	0	0
2	T	12	0	10	0	0
2	U	12	0	10	0	0
2	V	12	0	10	0	0
2	W	12	0	10	0	0
2	X	12	0	10	0	0
3	B	6	0	8	0	0
3	E	6	0	8	1	0
3	G	6	0	8	1	0
3	H	6	0	8	0	0
3	I	6	0	8	0	0
3	L	6	0	8	0	0
3	O	6	0	8	2	0
3	P	6	0	8	0	0
3	Q	6	0	8	0	0
3	T	6	0	8	0	0
3	U	6	0	8	0	0
3	V	6	0	8	0	0
3	X	6	0	8	0	0
4	A	82	0	0	3	0
4	B	95	0	0	5	0
4	C	96	0	0	2	0
4	D	84	0	0	2	0
4	E	84	0	0	2	0
4	F	85	0	0	4	0
4	G	101	0	0	2	0
4	H	106	0	0	2	0
4	I	99	0	0	1	0
4	J	125	0	0	3	0
4	K	92	0	0	3	0
4	L	127	0	0	7	0
4	M	112	0	0	1	0
4	N	85	0	0	4	0
4	O	85	0	0	3	0
4	P	102	0	0	1	0
4	Q	108	0	0	0	0
4	R	83	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	103	0	0	3	0
4	T	112	0	0	5	0
4	U	94	0	0	4	0
4	V	81	0	0	3	0
4	W	109	0	0	5	1
4	X	97	0	0	2	0
All	All	28420	0	26170	309	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 6.

The worst 5 of 309 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:W:23:VAL:HG21	1:W:103:SER:CB	1.80	1.12
1:J:21:PRO:HB3	1:J:23:VAL:H	0.96	1.10
1:J:21:PRO:HB3	1:J:23:VAL:N	1.65	1.10
1:O:50:ARG:HG3	1:O:50:ARG:HH11	0.98	1.09
1:L:3:LEU:HD12	4:L:1155:HOH:O	1.57	1.05

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:L:46:LYS:NZ	4:W:1243:HOH:O[1_655]	2.15	0.05

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	139/147 (95%)	131 (94%)	6 (4%)	2 (1%)	11 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	140/147 (95%)	138 (99%)	2 (1%)	0	100	100
1	C	135/147 (92%)	128 (95%)	6 (4%)	1 (1%)	22	16
1	D	140/147 (95%)	136 (97%)	4 (3%)	0	100	100
1	E	140/147 (95%)	132 (94%)	7 (5%)	1 (1%)	22	16
1	F	134/147 (91%)	131 (98%)	2 (2%)	1 (1%)	22	16
1	G	140/147 (95%)	135 (96%)	4 (3%)	1 (1%)	22	16
1	H	139/147 (95%)	137 (99%)	2 (1%)	0	100	100
1	I	140/147 (95%)	132 (94%)	5 (4%)	3 (2%)	7	2
1	J	140/147 (95%)	134 (96%)	4 (3%)	2 (1%)	11	5
1	K	140/147 (95%)	137 (98%)	3 (2%)	0	100	100
1	L	141/147 (96%)	137 (97%)	3 (2%)	1 (1%)	22	16
1	M	140/147 (95%)	137 (98%)	3 (2%)	0	100	100
1	N	140/147 (95%)	134 (96%)	5 (4%)	1 (1%)	22	16
1	O	140/147 (95%)	135 (96%)	3 (2%)	2 (1%)	11	5
1	P	139/147 (95%)	135 (97%)	4 (3%)	0	100	100
1	Q	139/147 (95%)	135 (97%)	3 (2%)	1 (1%)	22	16
1	R	140/147 (95%)	137 (98%)	3 (2%)	0	100	100
1	S	140/147 (95%)	137 (98%)	3 (2%)	0	100	100
1	T	140/147 (95%)	138 (99%)	2 (1%)	0	100	100
1	U	140/147 (95%)	134 (96%)	5 (4%)	1 (1%)	22	16
1	V	140/147 (95%)	135 (96%)	5 (4%)	0	100	100
1	W	140/147 (95%)	133 (95%)	5 (4%)	2 (1%)	11	5
1	X	134/147 (91%)	132 (98%)	2 (2%)	0	100	100
All	All	3340/3528 (95%)	3230 (97%)	91 (3%)	19 (1%)	25	19

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	C	19	ARG
1	E	19	ARG
1	I	21	PRO
1	J	21	PRO

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	109/115 (95%)	104 (95%)	5 (5%)	27	23
1	B	111/115 (96%)	108 (97%)	3 (3%)	44	46
1	C	108/115 (94%)	103 (95%)	5 (5%)	27	23
1	D	111/115 (96%)	106 (96%)	5 (4%)	27	24
1	E	111/115 (96%)	106 (96%)	5 (4%)	27	24
1	F	107/115 (93%)	104 (97%)	3 (3%)	43	44
1	G	111/115 (96%)	102 (92%)	9 (8%)	11	7
1	H	110/115 (96%)	104 (94%)	6 (6%)	21	17
1	I	110/115 (96%)	104 (94%)	6 (6%)	21	17
1	J	110/115 (96%)	103 (94%)	7 (6%)	17	13
1	K	111/115 (96%)	103 (93%)	8 (7%)	14	9
1	L	112/115 (97%)	108 (96%)	4 (4%)	35	34
1	M	111/115 (96%)	106 (96%)	5 (4%)	27	24
1	N	111/115 (96%)	106 (96%)	5 (4%)	27	24
1	O	111/115 (96%)	100 (90%)	11 (10%)	8	4
1	P	110/115 (96%)	105 (96%)	5 (4%)	27	24
1	Q	109/115 (95%)	103 (94%)	6 (6%)	21	17
1	R	109/115 (95%)	104 (95%)	5 (5%)	27	23
1	S	111/115 (96%)	105 (95%)	6 (5%)	22	18
1	T	111/115 (96%)	109 (98%)	2 (2%)	59	63
1	U	110/115 (96%)	105 (96%)	5 (4%)	27	24
1	V	111/115 (96%)	108 (97%)	3 (3%)	44	46
1	W	111/115 (96%)	106 (96%)	5 (4%)	27	24
1	X	107/115 (93%)	103 (96%)	4 (4%)	34	32
All	All	2643/2760 (96%)	2515 (95%)	128 (5%)	25	22

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	20	GLU
1	N	16	LEU
1	V	130	ILE
1	K	50	ARG
1	L	143	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	64	GLN
1	J	143	HIS
1	T	131	GLN
1	I	131	GLN
1	U	131	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

37 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
2	FA1	W	147	-	7,12,12	4.53	6 (85%)	7,18,18	1.65	2 (28%)
2	FA1	A	147	-	7,12,12	4.15	3 (42%)	7,18,18	1.31	0
2	FA1	P	148	-	7,12,12	4.15	3 (42%)	7,18,18	1.89	4 (57%)
2	FA1	F	147	-	7,12,12	4.04	3 (42%)	7,18,18	1.29	1 (14%)
2	FA1	T	148	-	7,12,12	3.79	5 (71%)	7,18,18	1.03	0
3	GOL	I	147	-	5,5,5	0.35	0	5,5,5	0.32	0
3	GOL	T	147	-	5,5,5	0.28	0	5,5,5	0.74	0
3	GOL	U	147	-	5,5,5	0.43	0	5,5,5	0.56	0
3	GOL	Q	147	-	5,5,5	0.38	0	5,5,5	0.49	0
2	FA1	H	148	-	7,12,12	4.14	3 (42%)	7,18,18	1.42	1 (14%)
2	FA1	N	147	-	7,12,12	5.70	6 (85%)	7,18,18	3.70	5 (71%)
2	FA1	O	148	-	7,12,12	4.34	3 (42%)	7,18,18	0.92	0
2	FA1	D	147	-	7,12,12	4.87	5 (71%)	7,18,18	1.11	0
2	FA1	Q	148	-	7,12,12	4.11	5 (71%)	7,18,18	1.12	1 (14%)
3	GOL	O	147	-	5,5,5	0.58	0	5,5,5	0.89	0
2	FA1	C	147	-	7,12,12	4.21	3 (42%)	7,18,18	1.76	2 (28%)
2	FA1	X	148	-	7,12,12	4.20	4 (57%)	7,18,18	1.42	1 (14%)
3	GOL	L	147	-	5,5,5	0.48	0	5,5,5	0.95	0
2	FA1	E	148	-	7,12,12	3.94	2 (28%)	7,18,18	1.64	1 (14%)
2	FA1	G	148	-	7,12,12	4.07	3 (42%)	7,18,18	1.66	1 (14%)
2	FA1	S	147	-	7,12,12	3.76	2 (28%)	7,18,18	1.45	1 (14%)
2	FA1	R	147	-	7,12,12	15.38	5 (71%)	7,18,18	2.89	4 (57%)
2	FA1	V	148	-	7,12,12	4.60	2 (28%)	7,18,18	1.83	2 (28%)
3	GOL	E	147	-	5,5,5	0.38	0	5,5,5	0.56	0
2	FA1	J	147	-	7,12,12	3.67	2 (28%)	7,18,18	2.31	3 (42%)
2	FA1	M	147	-	7,12,12	3.70	3 (42%)	7,18,18	1.35	1 (14%)
2	FA1	U	148	-	7,12,12	4.64	3 (42%)	7,18,18	1.02	1 (14%)
2	FA1	L	148	-	7,12,12	4.26	4 (57%)	7,18,18	1.74	1 (14%)
3	GOL	B	147	-	5,5,5	0.35	0	5,5,5	0.79	0
3	GOL	G	147	-	5,5,5	0.45	0	5,5,5	0.36	0
3	GOL	H	147	-	5,5,5	0.16	0	5,5,5	0.83	0
2	FA1	B	148	-	7,12,12	4.28	4 (57%)	7,18,18	1.69	3 (42%)
3	GOL	V	147	-	5,5,5	0.43	0	5,5,5	0.24	0
2	FA1	I	148	-	7,12,12	4.38	3 (42%)	7,18,18	1.53	1 (14%)
2	FA1	K	147	-	7,12,12	4.13	4 (57%)	7,18,18	1.66	1 (14%)
3	GOL	P	147	-	5,5,5	0.33	0	5,5,5	0.76	0
3	GOL	X	147	-	5,5,5	0.42	0	5,5,5	0.52	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	FA1	W	147	-	-	0/0/21/21	0/1/1/1
2	FA1	A	147	-	-	0/0/21/21	0/1/1/1
2	FA1	P	148	-	-	0/0/21/21	0/1/1/1
2	FA1	F	147	-	-	0/0/21/21	0/1/1/1
2	FA1	T	148	-	-	0/0/21/21	0/1/1/1
3	GOL	I	147	-	-	3/4/4/4	-
2	FA1	N	147	-	1/1/4/6	0/0/21/21	0/1/1/1
3	GOL	U	147	-	-	4/4/4/4	-
3	GOL	Q	147	-	-	2/4/4/4	-
2	FA1	H	148	-	-	0/0/21/21	0/1/1/1
3	GOL	T	147	-	-	1/4/4/4	-
2	FA1	O	148	-	-	0/0/21/21	0/1/1/1
2	FA1	D	147	-	-	0/0/21/21	0/1/1/1
2	FA1	Q	148	-	-	0/0/21/21	0/1/1/1
3	GOL	O	147	-	-	0/4/4/4	-
2	FA1	C	147	-	-	0/0/21/21	0/1/1/1
2	FA1	X	148	-	-	0/0/21/21	0/1/1/1
3	GOL	L	147	-	-	4/4/4/4	-
2	FA1	E	148	-	-	0/0/21/21	0/1/1/1
2	FA1	G	148	-	-	0/0/21/21	0/1/1/1
2	FA1	S	147	-	-	0/0/21/21	0/1/1/1
2	FA1	R	147	-	-	0/0/21/21	0/1/1/1
2	FA1	V	148	-	-	0/0/21/21	0/1/1/1
3	GOL	E	147	-	-	0/4/4/4	-
2	FA1	J	147	-	-	0/0/21/21	0/1/1/1
2	FA1	M	147	-	-	0/0/21/21	0/1/1/1
2	FA1	U	148	-	-	0/0/21/21	0/1/1/1
2	FA1	L	148	-	-	0/0/21/21	0/1/1/1
3	GOL	B	147	-	-	4/4/4/4	-
3	GOL	G	147	-	-	2/4/4/4	-
3	GOL	H	147	-	-	2/4/4/4	-
2	FA1	B	148	-	-	0/0/21/21	0/1/1/1
3	GOL	V	147	-	-	4/4/4/4	-
2	FA1	I	148	-	-	0/0/21/21	0/1/1/1
2	FA1	K	147	-	-	0/0/21/21	0/1/1/1
3	GOL	P	147	-	-	1/4/4/4	-
3	GOL	X	147	-	-	2/4/4/4	-

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	147	FA1	O30-C1	31.55	1.94	1.43
2	R	147	FA1	C5-C6	22.61	1.65	1.32
2	N	147	FA1	C1-C6	-11.56	1.40	1.50
2	D	147	FA1	C1-C6	-11.02	1.40	1.50
2	R	147	FA1	C1-C6	-10.11	1.41	1.50

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	147	FA1	C4-C5-C6	-5.94	116.15	123.55
2	N	147	FA1	O30-C1-C2	5.02	119.63	107.98
2	N	147	FA1	O4-C4-C5	-4.82	98.91	109.92
2	N	147	FA1	C3-C4-C5	-4.82	104.53	111.65
2	J	147	FA1	O4-C4-C5	4.50	120.19	109.92

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	N	147	FA1	C1

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	147	GOL	O1-C1-C2-C3
3	U	147	GOL	O1-C1-C2-C3
3	U	147	GOL	C1-C2-C3-O3
3	Q	147	GOL	O1-C1-C2-C3
3	L	147	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	147	FA1	2	0
3	O	147	GOL	2	0
3	E	147	GOL	1	0
3	G	147	GOL	1	0
2	B	148	FA1	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

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	141/147 (95%)	-0.49	0  	18, 29, 50, 63	3 (2%)
1	B	141/147 (95%)	-0.61	0  	18, 26, 38, 51	3 (2%)
1	C	139/147 (94%)	-0.48	0  	19, 28, 53, 72	5 (3%)
1	D	141/147 (95%)	-0.39	1 (0%)  	18, 29, 54, 65	5 (3%)
1	E	141/147 (95%)	-0.40	2 (1%)  	19, 29, 53, 69	4 (2%)
1	F	137/147 (93%)	-0.47	0  	18, 28, 46, 70	3 (2%)
1	G	141/147 (95%)	-0.42	0  	19, 26, 47, 67	1 (0%)
1	H	141/147 (95%)	-0.50	0  	17, 25, 39, 59	5 (3%)
1	I	141/147 (95%)	-0.39	2 (1%)  	17, 26, 51, 68	5 (3%)
1	J	141/147 (95%)	-0.44	2 (1%)  	13, 19, 43, 61	4 (2%)
1	K	141/147 (95%)	-0.41	0  	19, 29, 55, 70	4 (2%)
1	L	141/147 (95%)	-0.48	0  	11, 21, 38, 59	8 (5%)
1	M	141/147 (95%)	-0.44	1 (0%)  	15, 21, 46, 62	8 (5%)
1	N	141/147 (95%)	-0.42	1 (0%)  	18, 29, 51, 65	7 (4%)
1	O	141/147 (95%)	-0.44	1 (0%)  	14, 25, 49, 68	7 (4%)
1	P	141/147 (95%)	-0.43	0  	19, 27, 43, 58	9 (6%)
1	Q	141/147 (95%)	-0.48	0  	15, 22, 41, 63	9 (6%)
1	R	141/147 (95%)	-0.36	1 (0%)  	18, 27, 57, 65	8 (5%)
1	S	141/147 (95%)	-0.43	1 (0%)  	15, 23, 45, 68	1 (0%)
1	T	141/147 (95%)	-0.59	0  	16, 24, 36, 58	8 (5%)
1	U	141/147 (95%)	-0.37	2 (1%)  	20, 30, 53, 67	8 (5%)
1	V	141/147 (95%)	-0.41	1 (0%)  	18, 29, 55, 67	8 (5%)
1	W	141/147 (95%)	-0.49	2 (1%)  	15, 23, 49, 72	8 (5%)
1	X	137/147 (93%)	-0.48	0  	17, 27, 47, 58	8 (5%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3374/3528 (95%)	-0.45	17 (0%) 91 90	11, 26, 51, 72	139 (4%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	23	VAL	3.7
1	J	23	VAL	3.2
1	W	22	ALA	2.8
1	D	23	VAL	2.7
1	V	3	LEU	2.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	GOL	I	147	6/6	0.81	0.14	69,73,73,74	0
3	GOL	O	147	6/6	0.85	0.19	49,53,55,56	0
3	GOL	V	147	6/6	0.85	0.23	74,75,75,75	0
3	GOL	E	147	6/6	0.87	0.21	58,59,61,61	0
3	GOL	L	147	6/6	0.88	0.14	53,54,56,58	0
3	GOL	X	147	6/6	0.89	0.12	51,56,56,58	0
3	GOL	P	147	6/6	0.90	0.17	42,46,47,49	0
3	GOL	H	147	6/6	0.90	0.13	41,46,48,49	0
3	GOL	Q	147	6/6	0.93	0.09	61,63,63,64	0
2	FA1	R	147	12/12	0.93	0.11	28,33,35,35	0
3	GOL	U	147	6/6	0.93	0.13	56,60,61,61	0
2	FA1	N	147	12/12	0.94	0.12	22,26,29,31	0
3	GOL	T	147	6/6	0.95	0.11	40,40,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	B	147	6/6	0.95	0.10	31,39,43,43	0
2	FA1	T	148	12/12	0.95	0.11	21,22,25,27	0
2	FA1	C	147	12/12	0.96	0.09	26,28,31,34	0
3	GOL	G	147	6/6	0.96	0.11	48,51,53,54	0
2	FA1	V	148	12/12	0.97	0.11	26,29,32,35	0
2	FA1	M	147	12/12	0.97	0.10	18,21,27,28	0
2	FA1	U	148	12/12	0.97	0.09	23,32,34,35	0
2	FA1	A	147	12/12	0.97	0.10	23,24,26,31	0
2	FA1	X	148	12/12	0.97	0.09	26,30,31,34	0
2	FA1	F	147	12/12	0.97	0.09	26,30,34,34	0
2	FA1	B	148	12/12	0.97	0.10	21,24,26,28	0
2	FA1	E	148	12/12	0.97	0.11	21,27,28,32	0
2	FA1	I	148	12/12	0.97	0.08	22,29,32,34	0
2	FA1	K	147	12/12	0.97	0.10	24,31,34,35	0
2	FA1	S	147	12/12	0.97	0.10	22,24,25,26	0
2	FA1	W	147	12/12	0.97	0.11	21,23,26,26	0
2	FA1	H	148	12/12	0.98	0.08	18,23,25,27	0
2	FA1	P	148	12/12	0.98	0.09	23,24,27,27	0
2	FA1	O	148	12/12	0.98	0.11	21,24,26,29	0
2	FA1	L	148	12/12	0.98	0.08	16,22,25,27	0
2	FA1	J	147	12/12	0.98	0.10	16,19,23,26	0
2	FA1	D	147	12/12	0.98	0.10	22,27,29,30	0
2	FA1	Q	148	12/12	0.98	0.10	18,22,30,30	0
2	FA1	G	148	12/12	0.98	0.10	20,26,31,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.