



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 01:33 PM GMT

PDB ID : 3N86  
Title : Crystal structure of 3-dehydroquinate dehydratase from Mycobacterium tuberculosis in complex with inhibitor 4  
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 : 2010-05-27  
Resolution : 1.90 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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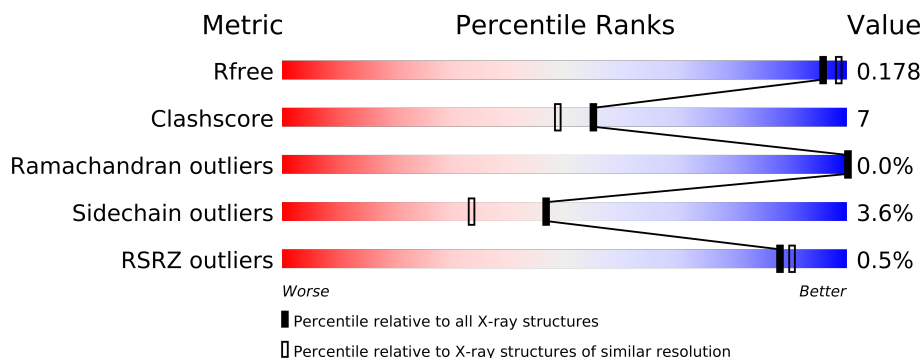
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	147	
1	B	147	
1	C	147	
1	D	147	
1	E	147	
1	F	147	
1	G	147	
1	H	147	
1	I	147	
1	J	147	
1	K	147	
1	L	147	
1	M	147	
1	N	147	

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Mol	Chain	Length	Quality of chain
1	O	147	
1	P	147	
1	Q	147	
1	R	147	
1	S	147	
1	T	147	
1	U	147	
1	V	147	
1	W	147	
1	X	147	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	RJP	C	147	-	X
2	RJP	F	147	-	X
2	RJP	H	147	-	X
2	RJP	R	147	-	X
2	RJP	S	147	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30436 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

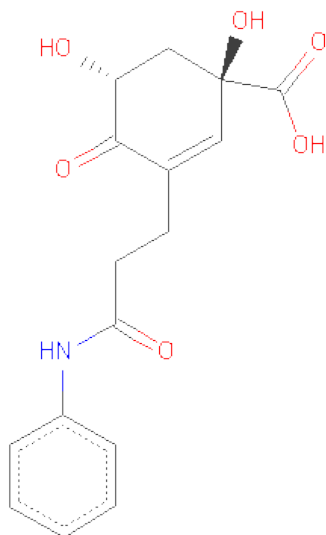
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	B	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	C	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	D	141	Total	C	N	O	S	0	1	0
			1079	679	199	200	1			
1	E	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	F	141	Total	C	N	O	S	0	0	0
			1065	671	193	200	1			
1	G	141	Total	C	N	O	S	0	0	0
			1071	674	196	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	0	0
			1071	674	196	200	1			
1	J	143	Total	C	N	O	S	0	0	0
			1086	682	198	205	1			
1	K	142	Total	C	N	O	S	0	0	0
			1080	679	197	203	1			
1	L	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	M	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	N	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	O	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	P	142	Total	C	N	O	S	0	0	0
			1080	679	197	203	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	R	142	Total	C	N	O	S	0	0	0
			1076	677	197	201	1			
1	S	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	T	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	U	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	V	144	Total	C	N	O	S	0	0	0
			1091	685	199	206	1			
1	W	143	Total	C	N	O	S	0	0	0
			1086	682	198	205	1			
1	X	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			

- Molecule 2 is (1R,5R)-1,5-DIHYDROXY-4-OXO-3-[3-OXO-3-(PHENYLAMINO)PROPYL]CYCLOHEX-2-ENE-1-CARBOXYLICACID (three-letter code: RJP) (formula: C<sub>16</sub>H<sub>17</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	16	1	6		
2	B	1	Total	C	N	O	0	0
			23	16	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			23	16	1	6		
2	D	1	Total	C	N	O	0	0
			23	16	1	6		
2	E	1	Total	C	N	O	0	0
			23	16	1	6		
2	F	1	Total	C	N	O	0	0
			23	16	1	6		
2	G	1	Total	C	N	O	0	0
			23	16	1	6		
2	H	1	Total	C	N	O	0	0
			23	16	1	6		
2	I	1	Total	C	N	O	0	0
			23	16	1	6		
2	J	1	Total	C	N	O	0	0
			23	16	1	6		
2	K	1	Total	C	N	O	0	0
			23	16	1	6		
2	L	1	Total	C	N	O	0	0
			23	16	1	6		
2	M	1	Total	C	N	O	0	0
			23	16	1	6		
2	N	1	Total	C	N	O	0	0
			23	16	1	6		
2	O	1	Total	C	N	O	0	0
			23	16	1	6		
2	P	1	Total	C	N	O	0	0
			23	16	1	6		
2	Q	1	Total	C	N	O	0	0
			23	16	1	6		
2	R	1	Total	C	N	O	0	0
			23	16	1	6		
2	S	1	Total	C	N	O	0	0
			23	16	1	6		
2	T	1	Total	C	N	O	0	0
			23	16	1	6		
2	U	1	Total	C	N	O	0	0
			23	16	1	6		
2	V	1	Total	C	N	O	0	0
			23	16	1	6		
2	W	1	Total	C	N	O	0	0
			23	16	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	X	1	Total	C	N	O	0	0
			23	16	1	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	169	Total	O			0	0
			169	169				
3	B	162	Total	O			0	0
			162	162				
3	C	177	Total	O			0	0
			177	177				
3	D	165	Total	O			0	0
			165	165				
3	E	169	Total	O			0	0
			169	169				
3	F	164	Total	O			0	0
			164	164				
3	G	155	Total	O			0	0
			155	155				
3	H	175	Total	O			0	0
			175	175				
3	I	159	Total	O			0	0
			159	159				
3	J	189	Total	O			0	0
			189	189				
3	K	185	Total	O			0	0
			185	185				
3	L	148	Total	O			0	0
			148	148				
3	M	181	Total	O			0	0
			181	181				
3	N	172	Total	O			0	0
			172	172				
3	O	187	Total	O			0	0
			187	187				
3	P	186	Total	O			0	0
			186	186				
3	Q	151	Total	O			0	0
			151	151				
3	R	175	Total	O			0	0
			175	175				

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	184	Total 184	O 184	0	0
3	T	204	Total 204	O 204	0	0
3	U	150	Total 150	O 150	0	0
3	V	186	Total 186	O 186	0	0
3	W	176	Total 176	O 176	0	0
3	X	136	Total 136	O 136	0	0

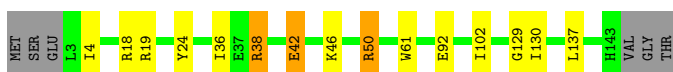


### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

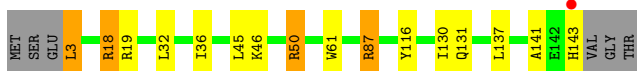
- Molecule 1: 3-dehydroquinate dehydratase

Chain A: 



- Molecule 1: 3-dehydroquinate dehydratase

Chain B: 



- Molecule 1: 3-dehydroquinate dehydratase

Chain C: 



- Molecule 1: 3-dehydroquinate dehydratase

Chain D: 



- Molecule 1: 3-dehydroquinate dehydratase

Chain E: 



- Molecule 1: 3-dehydroquinate dehydratase

Chain F: 



- Molecule 1: 3-dehydroquinate dehydratase

Chain G:



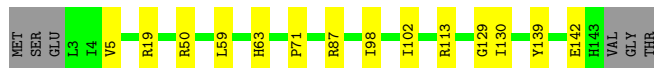
- Molecule 1: 3-dehydroquinate dehydratase

Chain H:



- Molecule 1: 3-dehydroquinate dehydratase

Chain I:



- Molecule 1: 3-dehydroquinate dehydratase

Chain J:



- Molecule 1: 3-dehydroquinate dehydratase

Chain K:



- Molecule 1: 3-dehydroquinate dehydratase

Chain L:



- Molecule 1: 3-dehydroquinate dehydratase

Chain M:



- Molecule 1: 3-dehydroquinate dehydratase

Chain N:



- Molecule 1: 3-dehydroquininate dehydratase

Chain O: 



- Molecule 1: 3-dehydroquininate dehydratase

Chain P: 



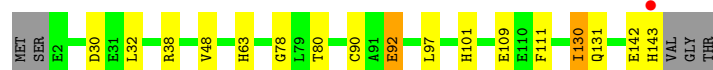
- Molecule 1: 3-dehydroquininate dehydratase

Chain Q: 



- Molecule 1: 3-dehydroquininate dehydratase

Chain R: 



- Molecule 1: 3-dehydroquininate dehydratase

Chain S: 



- Molecule 1: 3-dehydroquininate dehydratase

Chain T: 



- Molecule 1: 3-dehydroquininate dehydratase

Chain U: 



- Molecule 1: 3-dehydroquininate dehydratase

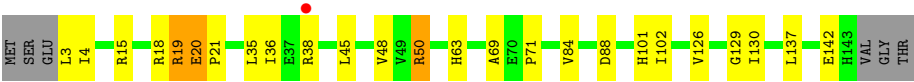
Chain V: 



● Molecule 1: 3-dehydroquinate dehydratase



● Molecule 1: 3-dehydroquinate dehydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.24Å 143.98Å 148.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.50 – 1.90 56.52 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.2 (56.50-1.90) 92.2 (56.52-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.155 , 0.212 0.150 , 0.178	Depositor DCC
$R_{free}$ test set	14004 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.9	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.6	EDS
Estimated twinning fraction	0.009 for -h,l,k 0.009 for -h,-l,-k 0.478 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 277575 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	30436	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: RJP

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	1.13	1/1089 (0.1%)	0.93	1/1483 (0.1%)
1	B	1.04	0/1089	0.89	1/1483 (0.1%)
1	C	1.10	0/1089	0.92	0/1483
1	D	1.17	0/1100	0.93	4/1497 (0.3%)
1	E	1.13	2/1089 (0.2%)	0.93	2/1483 (0.1%)
1	F	1.23	5/1083 (0.5%)	0.96	2/1476 (0.1%)
1	G	1.02	0/1089	0.99	2/1483 (0.1%)
1	H	1.12	1/1089 (0.1%)	0.92	2/1483 (0.1%)
1	I	1.03	0/1089	0.94	3/1483 (0.2%)
1	J	1.13	2/1104 (0.2%)	0.99	2/1503 (0.1%)
1	K	1.12	1/1098 (0.1%)	1.00	2/1495 (0.1%)
1	L	1.05	0/1089	0.96	2/1483 (0.1%)
1	M	1.07	1/1089 (0.1%)	0.98	3/1483 (0.2%)
1	N	1.05	1/1089 (0.1%)	0.88	0/1483
1	O	1.16	0/1089	0.98	2/1483 (0.1%)
1	P	1.14	1/1098 (0.1%)	0.90	0/1495
1	Q	1.09	1/1089 (0.1%)	0.93	3/1483 (0.2%)
1	R	1.13	5/1094 (0.5%)	0.95	1/1490 (0.1%)
1	S	1.07	4/1089 (0.4%)	0.96	0/1483
1	T	1.10	1/1089 (0.1%)	0.91	2/1483 (0.1%)
1	U	1.04	0/1089	0.91	1/1483 (0.1%)
1	V	1.15	3/1109 (0.3%)	1.03	4/1510 (0.3%)
1	W	1.09	0/1104	0.99	4/1503 (0.3%)
1	X	1.06	2/1089 (0.2%)	0.94	1/1483 (0.1%)
All	All	1.10	31/26214 (0.1%)	0.95	44/35697 (0.1%)

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	J	0	1
1	W	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	110	GLU	CB-CG	12.38	1.75	1.52
1	F	110	GLU	CD-OE2	8.86	1.35	1.25
1	V	92	GLU	CB-CG	-8.40	1.36	1.52
1	F	84	VAL	CB-CG1	6.99	1.67	1.52
1	S	124	VAL	CB-CG2	6.56	1.66	1.52

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	19	ARG	NE-CZ-NH1	-10.78	114.91	120.30
1	X	88	ASP	CB-CG-OD2	9.51	126.86	118.30
1	G	19	ARG	NE-CZ-NH2	8.64	124.62	120.30
1	H	18	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	V	3	LEU	CA-CB-CG	8.45	134.74	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	19	ARG	Peptide
1	W	142	GLU	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1071	0	1079	16	0
1	B	1071	0	1079	13	0
1	C	1071	0	1079	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1079	0	1092	21	0
1	E	1071	0	1079	12	0
1	F	1065	0	1068	13	0
1	G	1071	0	1079	13	0
1	H	1071	0	1079	18	0
1	I	1071	0	1079	7	0
1	J	1086	0	1093	16	0
1	K	1080	0	1085	25	0
1	L	1071	0	1079	29	0
1	M	1071	0	1079	28	2
1	N	1071	0	1079	10	0
1	O	1071	0	1079	11	0
1	P	1080	0	1085	16	0
1	Q	1071	0	1079	11	0
1	R	1076	0	1081	11	0
1	S	1071	0	1079	14	0
1	T	1071	0	1079	20	0
1	U	1071	0	1079	13	0
1	V	1091	0	1095	12	0
1	W	1086	0	1093	18	0
1	X	1071	0	1079	24	0
2	A	23	0	16	1	0
2	B	23	0	16	1	0
2	C	23	0	16	0	0
2	D	23	0	16	1	0
2	E	23	0	16	1	0
2	F	23	0	16	0	0
2	G	23	0	16	0	0
2	H	23	0	16	0	0
2	I	23	0	16	0	0
2	J	23	0	16	0	0
2	K	23	0	16	0	0
2	L	23	0	16	1	0
2	M	23	0	16	0	0
2	N	23	0	16	0	0
2	O	23	0	16	0	0
2	P	23	0	16	1	0
2	Q	23	0	16	0	0
2	R	23	0	16	0	0
2	S	23	0	16	0	0
2	T	23	0	16	0	0
2	U	23	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	23	0	16	1	0
2	W	23	0	16	0	0
2	X	23	0	16	0	0
3	A	169	0	0	2	0
3	B	162	0	0	4	0
3	C	177	0	0	4	0
3	D	165	0	0	3	3
3	E	169	0	0	3	0
3	F	164	0	0	3	0
3	G	155	0	0	2	0
3	H	175	0	0	2	0
3	I	159	0	0	1	0
3	J	189	0	0	1	0
3	K	185	0	0	5	0
3	L	148	0	0	1	0
3	M	181	0	0	2	0
3	N	172	0	0	2	0
3	O	187	0	0	2	0
3	P	186	0	0	1	0
3	Q	151	0	0	2	2
3	R	175	0	0	2	0
3	S	184	0	0	3	0
3	T	204	0	0	3	1
3	U	150	0	0	3	0
3	V	186	0	0	6	2
3	W	176	0	0	1	0
3	X	136	0	0	3	0
All	All	30436	0	26340	353	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 353 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:110:GLU:CB	1:F:110:GLU:CG	1.75	1.63
1:F:92:GLU:OE1	1:G:19:ARG:HD2	1.27	1.31
1:D:18[B]:ARG:CG	1:D:18[B]:ARG:HH21	1.52	1.17
1:W:18:ARG:HH11	1:W:18:ARG:HG2	1.14	1.13
1:D:18[A]:ARG:HH21	1:D:18[A]:ARG:CG	1.64	1.11

All (5) 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	Distance(Å)	Clash(Å)
3:D:3503:HOH:O	3:V:3695:HOH:O[2.546]	1.54	0.66
3:D:3504:HOH:O	3:T:3696:HOH:O[2.546]	1.67	0.53
1:M:38:ARG:NH1	3:Q:3949:HOH:O[2.646]	1.72	0.48
1:M:38:ARG:NE	3:Q:3730:HOH:O[2.646]	1.97	0.23
3:D:3503:HOH:O	3:V:728:HOH:O[2.546]	2.09	0.11

## 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	139/147 (95%)	135 (97%)	4 (3%)	0	100	100
1	B	139/147 (95%)	136 (98%)	3 (2%)	0	100	100
1	C	139/147 (95%)	137 (99%)	2 (1%)	0	100	100
1	D	140/147 (95%)	137 (98%)	3 (2%)	0	100	100
1	E	139/147 (95%)	137 (99%)	2 (1%)	0	100	100
1	F	139/147 (95%)	136 (98%)	3 (2%)	0	100	100
1	G	139/147 (95%)	135 (97%)	4 (3%)	0	100	100
1	H	139/147 (95%)	136 (98%)	3 (2%)	0	100	100
1	I	139/147 (95%)	137 (99%)	2 (1%)	0	100	100
1	J	141/147 (96%)	136 (96%)	5 (4%)	0	100	100
1	K	140/147 (95%)	137 (98%)	3 (2%)	0	100	100
1	L	139/147 (95%)	134 (96%)	5 (4%)	0	100	100
1	M	139/147 (95%)	133 (96%)	6 (4%)	0	100	100
1	N	139/147 (95%)	135 (97%)	4 (3%)	0	100	100
1	O	139/147 (95%)	137 (99%)	2 (1%)	0	100	100
1	P	140/147 (95%)	138 (99%)	2 (1%)	0	100	100
1	Q	139/147 (95%)	135 (97%)	3 (2%)	1 (1%)	30	15
1	R	140/147 (95%)	137 (98%)	3 (2%)	0	100	100
1	S	139/147 (95%)	136 (98%)	3 (2%)	0	100	100
1	T	139/147 (95%)	135 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	139/147 (95%)	136 (98%)	3 (2%)	0	100	100
1	V	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
1	W	141/147 (96%)	138 (98%)	3 (2%)	0	100	100
1	X	139/147 (95%)	135 (97%)	4 (3%)	0	100	100
All	All	3347/3528 (95%)	3267 (98%)	79 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	22	ALA

### 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	110/115 (96%)	106 (96%)	4 (4%)	47	33
1	B	110/115 (96%)	106 (96%)	4 (4%)	47	33
1	C	110/115 (96%)	106 (96%)	4 (4%)	47	33
1	D	111/115 (96%)	108 (97%)	3 (3%)	57	47
1	E	110/115 (96%)	105 (96%)	5 (4%)	38	24
1	F	109/115 (95%)	106 (97%)	3 (3%)	56	45
1	G	110/115 (96%)	106 (96%)	4 (4%)	47	33
1	H	110/115 (96%)	105 (96%)	5 (4%)	38	24
1	I	110/115 (96%)	108 (98%)	2 (2%)	71	66
1	J	112/115 (97%)	105 (94%)	7 (6%)	25	12
1	K	111/115 (96%)	106 (96%)	5 (4%)	38	24
1	L	110/115 (96%)	106 (96%)	4 (4%)	47	33
1	M	110/115 (96%)	105 (96%)	5 (4%)	38	24
1	N	110/115 (96%)	106 (96%)	4 (4%)	47	33
1	O	110/115 (96%)	108 (98%)	2 (2%)	71	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	111/115 (96%)	105 (95%)	6 (5%)	31	17
1	Q	110/115 (96%)	107 (97%)	3 (3%)	57	47
1	R	110/115 (96%)	109 (99%)	1 (1%)	87	86
1	S	110/115 (96%)	106 (96%)	4 (4%)	47	33
1	T	110/115 (96%)	108 (98%)	2 (2%)	71	66
1	U	110/115 (96%)	107 (97%)	3 (3%)	57	47
1	V	112/115 (97%)	105 (94%)	7 (6%)	25	12
1	W	112/115 (97%)	109 (97%)	3 (3%)	57	47
1	X	110/115 (96%)	105 (96%)	5 (4%)	38	24
All	All	2648/2760 (96%)	2553 (96%)	95 (4%)	47	33

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	23	VAL
1	M	50	ARG
1	W	18	ARG
1	K	46	LYS
1	L	130	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	131	GLN
1	M	63	HIS
1	R	131	GLN
1	G	57	GLN
1	I	63	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

24 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	RJP	A	147	-	24,24,24	2.35	7 (29%)	34,34,34	1.68	9 (26%)
2	RJP	B	147	-	24,24,24	2.19	4 (16%)	34,34,34	1.33	5 (14%)
2	RJP	C	147	-	24,24,24	2.14	5 (20%)	34,34,34	1.55	7 (20%)
2	RJP	D	147	-	24,24,24	2.30	4 (16%)	34,34,34	1.53	7 (20%)
2	RJP	E	147	-	24,24,24	2.38	5 (20%)	34,34,34	0.95	1 (2%)
2	RJP	F	147	-	24,24,24	2.41	6 (25%)	34,34,34	1.39	6 (17%)
2	RJP	G	147	-	24,24,24	2.31	4 (16%)	34,34,34	1.58	5 (14%)
2	RJP	H	147	-	24,24,24	2.53	6 (25%)	34,34,34	1.65	7 (20%)
2	RJP	I	147	-	24,24,24	2.22	4 (16%)	34,34,34	1.29	3 (8%)
2	RJP	J	147	-	24,24,24	1.87	4 (16%)	34,34,34	1.63	7 (20%)
2	RJP	K	147	-	24,24,24	2.21	4 (16%)	34,34,34	1.39	6 (17%)
2	RJP	L	147	-	24,24,24	2.06	4 (16%)	34,34,34	1.16	3 (8%)
2	RJP	M	147	-	24,24,24	2.45	5 (20%)	34,34,34	1.56	5 (14%)
2	RJP	N	147	-	24,24,24	2.44	4 (16%)	34,34,34	1.53	7 (20%)
2	RJP	O	147	-	24,24,24	2.00	4 (16%)	34,34,34	1.30	3 (8%)
2	RJP	P	147	-	24,24,24	2.36	7 (29%)	34,34,34	1.52	9 (26%)
2	RJP	Q	147	-	24,24,24	2.18	5 (20%)	34,34,34	1.27	2 (5%)
2	RJP	R	147	-	24,24,24	2.17	6 (25%)	34,34,34	1.30	4 (11%)
2	RJP	S	147	-	24,24,24	2.27	4 (16%)	34,34,34	1.42	3 (8%)
2	RJP	T	147	-	24,24,24	2.33	4 (16%)	34,34,34	1.59	7 (20%)
2	RJP	U	147	-	24,24,24	2.38	5 (20%)	34,34,34	1.32	4 (11%)
2	RJP	V	147	-	24,24,24	1.90	5 (20%)	34,34,34	1.73	6 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	RJP	W	147	-	24,24,24	2.24	4 (16%)	34,34,34	1.34	3 (8%)
2	RJP	X	147	-	24,24,24	2.48	5 (20%)	34,34,34	1.19	3 (8%)

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	RJP	A	147	-	-	0/15/33/33	0/2/2/2
2	RJP	B	147	-	-	0/15/33/33	0/2/2/2
2	RJP	C	147	-	-	0/15/33/33	0/2/2/2
2	RJP	D	147	-	-	0/15/33/33	0/2/2/2
2	RJP	E	147	-	-	0/15/33/33	0/2/2/2
2	RJP	F	147	-	-	0/15/33/33	0/2/2/2
2	RJP	G	147	-	-	0/15/33/33	0/2/2/2
2	RJP	H	147	-	-	0/15/33/33	0/2/2/2
2	RJP	I	147	-	-	0/15/33/33	0/2/2/2
2	RJP	J	147	-	-	0/15/33/33	0/2/2/2
2	RJP	K	147	-	-	0/15/33/33	0/2/2/2
2	RJP	L	147	-	-	0/15/33/33	0/2/2/2
2	RJP	M	147	-	-	0/15/33/33	0/2/2/2
2	RJP	N	147	-	-	0/15/33/33	0/2/2/2
2	RJP	O	147	-	-	0/15/33/33	0/2/2/2
2	RJP	P	147	-	-	0/15/33/33	0/2/2/2
2	RJP	Q	147	-	-	0/15/33/33	0/2/2/2
2	RJP	R	147	-	-	0/15/33/33	0/2/2/2
2	RJP	S	147	-	-	0/15/33/33	0/2/2/2
2	RJP	T	147	-	-	0/15/33/33	0/2/2/2
2	RJP	U	147	-	-	0/15/33/33	0/2/2/2
2	RJP	V	147	-	-	0/15/33/33	0/2/2/2
2	RJP	W	147	-	-	0/15/33/33	0/2/2/2
2	RJP	X	147	-	-	0/15/33/33	0/2/2/2

The worst 5 of 115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	147	RJP	OAE-CAV	8.61	1.37	1.22
2	M	147	RJP	OAE-CAV	8.35	1.37	1.22
2	H	147	RJP	OAE-CAV	8.27	1.37	1.22
2	I	147	RJP	OAE-CAV	8.08	1.37	1.22
2	D	147	RJP	OAE-CAV	7.90	1.36	1.22

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	147	RJP	CAH-CAG-CAQ	-5.00	105.38	112.65
2	V	147	RJP	CAH-CAG-CAQ	-4.99	105.39	112.65
2	D	147	RJP	CAH-CAG-CAQ	-4.67	105.84	112.65
2	H	147	RJP	CAW-CAO-CAU	-4.45	103.79	111.85
2	S	147	RJP	CAH-CAG-CAQ	-4.45	106.17	112.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	141/147 (95%)	-0.61	0 100 100	11, 16, 29, 49	0
1	B	141/147 (95%)	-0.59	1 (0%) 84 87	7, 13, 34, 52	0
1	C	141/147 (95%)	-0.62	0 100 100	9, 14, 29, 48	0
1	D	141/147 (95%)	-0.59	1 (0%) 84 87	9, 13, 34, 46	0
1	E	141/147 (95%)	-0.56	1 (0%) 84 87	9, 14, 33, 51	0
1	F	141/147 (95%)	-0.59	1 (0%) 84 87	8, 14, 28, 53	0
1	G	141/147 (95%)	-0.58	1 (0%) 84 87	10, 16, 30, 53	1 (0%)
1	H	141/147 (95%)	-0.61	1 (0%) 84 87	9, 14, 29, 56	0
1	I	141/147 (95%)	-0.54	0 100 100	9, 14, 38, 49	0
1	J	143/147 (97%)	-0.58	1 (0%) 84 87	9, 13, 32, 51	0
1	K	142/147 (96%)	-0.63	0 100 100	10, 14, 29, 44	0
1	L	141/147 (95%)	-0.55	0 100 100	10, 16, 36, 53	0
1	M	141/147 (95%)	-0.59	0 100 100	10, 16, 29, 46	0
1	N	141/147 (95%)	-0.59	0 100 100	8, 13, 35, 48	0
1	O	141/147 (95%)	-0.61	0 100 100	9, 13, 28, 47	0
1	P	142/147 (96%)	-0.59	1 (0%) 84 87	8, 13, 31, 49	0
1	Q	141/147 (95%)	-0.58	1 (0%) 84 87	9, 15, 33, 53	0
1	R	142/147 (96%)	-0.57	1 (0%) 84 87	9, 14, 29, 54	0
1	S	141/147 (95%)	-0.60	1 (0%) 84 87	10, 15, 28, 51	1 (0%)
1	T	141/147 (95%)	-0.62	1 (0%) 84 87	9, 13, 29, 54	0
1	U	141/147 (95%)	-0.52	0 100 100	9, 15, 36, 52	0
1	V	144/147 (97%)	-0.54	1 (0%) 84 87	8, 14, 32, 51	0
1	W	143/147 (97%)	-0.60	1 (0%) 84 87	10, 14, 28, 47	0
1	X	141/147 (95%)	-0.48	1 (0%) 84 87	9, 17, 36, 56	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3394/3528 (96%)	-0.58	15 (0%) 88 91	7, 14, 34, 56	2 (0%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	143	HIS	3.6
1	R	143	HIS	3.6
1	H	143	HIS	3.5
1	F	143	HIS	3.4
1	Q	143	HIS	3.1

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	RJP	H	147	23/23	0.10	3.54	9,13,17,21	0
2	RJP	F	147	23/23	0.10	2.73	10,14,21,27	0
2	RJP	C	147	23/23	0.08	2.39	8,13,19,20	0
2	RJP	S	147	23/23	0.09	2.01	11,16,21,27	0
2	RJP	R	147	23/23	0.10	2.01	9,15,18,25	0
2	RJP	O	147	23/23	0.09	1.98	10,14,17,23	0
2	RJP	A	147	23/23	0.09	1.63	13,16,26,26	0
2	RJP	U	147	23/23	0.12	1.29	10,17,25,30	0
2	RJP	W	147	23/23	0.10	1.20	11,18,25,27	0
2	RJP	T	147	23/23	0.08	1.13	8,13,17,26	0
2	RJP	L	147	23/23	0.09	0.92	12,18,23,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	RJP	G	147	23/23	0.08	0.90	11,16,21,26	0
2	RJP	X	147	23/23	0.10	0.79	11,17,24,24	0
2	RJP	Q	147	23/23	0.10	0.79	10,17,23,28	0
2	RJP	I	147	23/23	0.09	0.51	10,18,24,27	0
2	RJP	P	147	23/23	0.10	0.49	11,18,25,28	0
2	RJP	V	147	23/23	0.09	0.47	9,17,29,30	0
2	RJP	K	147	23/23	0.08	0.35	10,16,24,26	0
2	RJP	N	147	23/23	0.09	0.34	9,14,26,28	0
2	RJP	D	147	23/23	0.09	0.32	12,16,26,27	0
2	RJP	E	147	23/23	0.08	0.26	9,17,25,26	0
2	RJP	B	147	23/23	0.09	0.20	8,15,25,28	0
2	RJP	M	147	23/23	0.08	0.16	12,17,23,25	0
2	RJP	J	147	23/23	0.08	0.11	10,18,26,27	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.