



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:29 PM GMT

PDB ID : 1XDQ  
Title : Structural and Biochemical Identification of a Novel Bacterial Oxidoreductase  
Authors : Loschi, L.; Brokx, S.J.; Hills, T.L.; Zhang, G.; Bertero, M.G.; Lovering, A.L.;  
Weiner, J.H.; Strynadka, N.C.  
Deposited on : 2004-09-07  
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

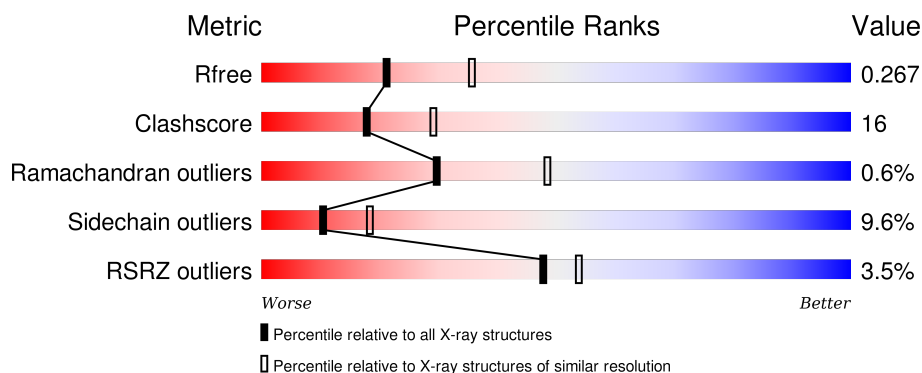
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	298	<div> <div>63%</div> <div>20%</div> <div>5%</div> <div>12%</div> </div>
1	B	298	<div> <div>4%</div> <div>61%</div> <div>23%</div> <div>•</div> <div>12%</div> </div>
1	C	298	<div> <div>3%</div> <div>59%</div> <div>25%</div> <div>•</div> <div>11%</div> </div>
1	D	298	<div> <div>3%</div> <div>58%</div> <div>22%</div> <div>7%</div> <div>12%</div> </div>
1	E	298	<div> <div>4%</div> <div>62%</div> <div>20%</div> <div>6%</div> <div>12%</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	URE	A	401	-	-	-	X
2	URE	B	402	-	-	-	X
2	URE	C	403	-	-	-	X
2	URE	D	404	-	-	-	X
2	URE	E	405	-	-	-	X
5	MTE	A	301	X	-	-	-
5	MTE	B	302	X	-	-	-
5	MTE	C	303	X	-	-	-
5	MTE	D	304	X	-	-	-
5	MTE	E	305	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10771 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 Bacterial Sulfite Oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2085	1351	353	375	6			
1	B	263	Total	C	N	O	S	0	0	0
			2093	1357	354	376	6			
1	C	264	Total	C	N	O	S	0	0	0
			2102	1363	356	377	6			
1	D	262	Total	C	N	O	S	0	0	0
			2085	1351	353	375	6			
1	E	262	Total	C	N	O	S	0	0	0
			2085	1351	353	375	6			

There are 45 discrepancies between the modelled and reference sequences:

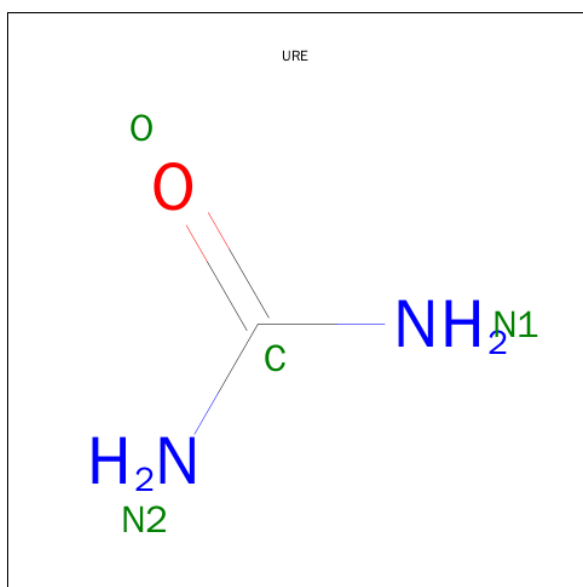
Chain	Residue	Modelled	Actual	Comment	Reference
A	275	ASP	ALA	SEE REMARK 999	UNP P76342
A	291	LEU	-	EXPRESSION TAG	UNP P76342
A	292	GLU	-	EXPRESSION TAG	UNP P76342
A	293	HIS	-	EXPRESSION TAG	UNP P76342
A	294	HIS	-	EXPRESSION TAG	UNP P76342
A	295	HIS	-	EXPRESSION TAG	UNP P76342
A	296	HIS	-	EXPRESSION TAG	UNP P76342
A	297	HIS	-	EXPRESSION TAG	UNP P76342
A	298	HIS	-	EXPRESSION TAG	UNP P76342
B	275	ASP	ALA	SEE REMARK 999	UNP P76342
B	291	LEU	-	EXPRESSION TAG	UNP P76342
B	292	GLU	-	EXPRESSION TAG	UNP P76342
B	293	HIS	-	EXPRESSION TAG	UNP P76342
B	294	HIS	-	EXPRESSION TAG	UNP P76342
B	295	HIS	-	EXPRESSION TAG	UNP P76342
B	296	HIS	-	EXPRESSION TAG	UNP P76342
B	297	HIS	-	EXPRESSION TAG	UNP P76342
B	298	HIS	-	EXPRESSION TAG	UNP P76342
C	275	ASP	ALA	SEE REMARK 999	UNP P76342

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Chain	Residue	Modelled	Actual	Comment	Reference
C	291	LEU	-	EXPRESSION TAG	UNP P76342
C	292	GLU	-	EXPRESSION TAG	UNP P76342
C	293	HIS	-	EXPRESSION TAG	UNP P76342
C	294	HIS	-	EXPRESSION TAG	UNP P76342
C	295	HIS	-	EXPRESSION TAG	UNP P76342
C	296	HIS	-	EXPRESSION TAG	UNP P76342
C	297	HIS	-	EXPRESSION TAG	UNP P76342
C	298	HIS	-	EXPRESSION TAG	UNP P76342
D	275	ASP	ALA	SEE REMARK 999	UNP P76342
D	291	LEU	-	EXPRESSION TAG	UNP P76342
D	292	GLU	-	EXPRESSION TAG	UNP P76342
D	293	HIS	-	EXPRESSION TAG	UNP P76342
D	294	HIS	-	EXPRESSION TAG	UNP P76342
D	295	HIS	-	EXPRESSION TAG	UNP P76342
D	296	HIS	-	EXPRESSION TAG	UNP P76342
D	297	HIS	-	EXPRESSION TAG	UNP P76342
D	298	HIS	-	EXPRESSION TAG	UNP P76342
E	275	ASP	ALA	SEE REMARK 999	UNP P76342
E	291	LEU	-	EXPRESSION TAG	UNP P76342
E	292	GLU	-	EXPRESSION TAG	UNP P76342
E	293	HIS	-	EXPRESSION TAG	UNP P76342
E	294	HIS	-	EXPRESSION TAG	UNP P76342
E	295	HIS	-	EXPRESSION TAG	UNP P76342
E	296	HIS	-	EXPRESSION TAG	UNP P76342
E	297	HIS	-	EXPRESSION TAG	UNP P76342
E	298	HIS	-	EXPRESSION TAG	UNP P76342

- Molecule 2 is UREA (three-letter code: URE) (formula: CH<sub>4</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			4	1	2	1		
2	B	1	Total	C	N	O	0	0
			4	1	2	1		
2	C	1	Total	C	N	O	0	0
			4	1	2	1		
2	D	1	Total	C	N	O	0	0
			4	1	2	1		
2	E	1	Total	C	N	O	0	0
			4	1	2	1		

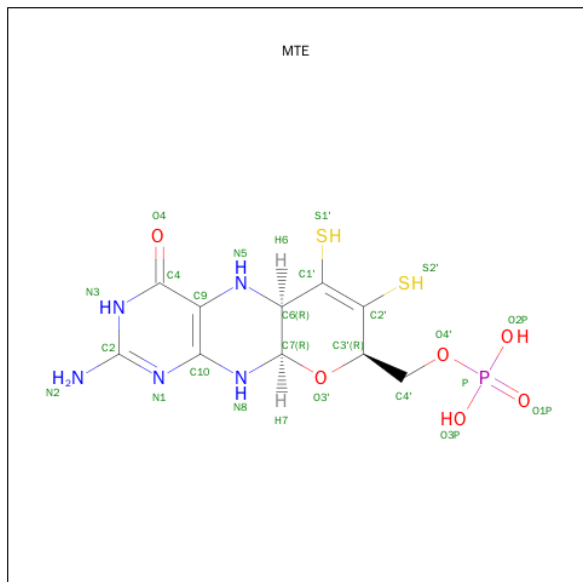
- Molecule 3 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mo	0	0
			1	1		
3	A	1	Total	Mo	0	0
			1	1		
3	D	1	Total	Mo	0	0
			1	1		
3	C	1	Total	Mo	0	0
			1	1		
3	E	1	Total	Mo	0	0
			1	1		

- Molecule 4 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O 1 1	0	0
4	A	1	Total O 1 1	0	0
4	D	1	Total O 1 1	0	0
4	C	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0

- Molecule 5 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula:  $C_{10}H_{14}N_5O_6P_2S_2$ ).



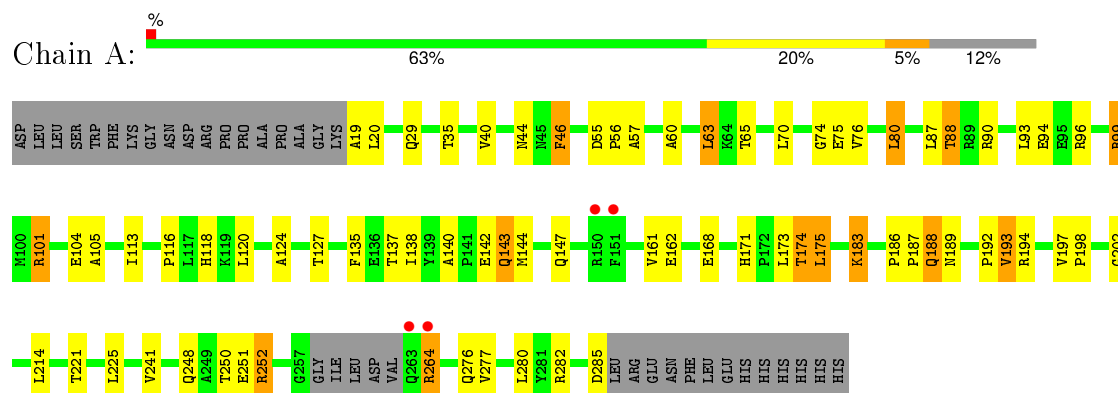
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	49	Total 49	O 49	0	0
6	B	26	Total 26	O 26	0	0
6	C	28	Total 28	O 28	0	0
6	D	36	Total 36	O 36	0	0
6	E	32	Total 32	O 32	0	0



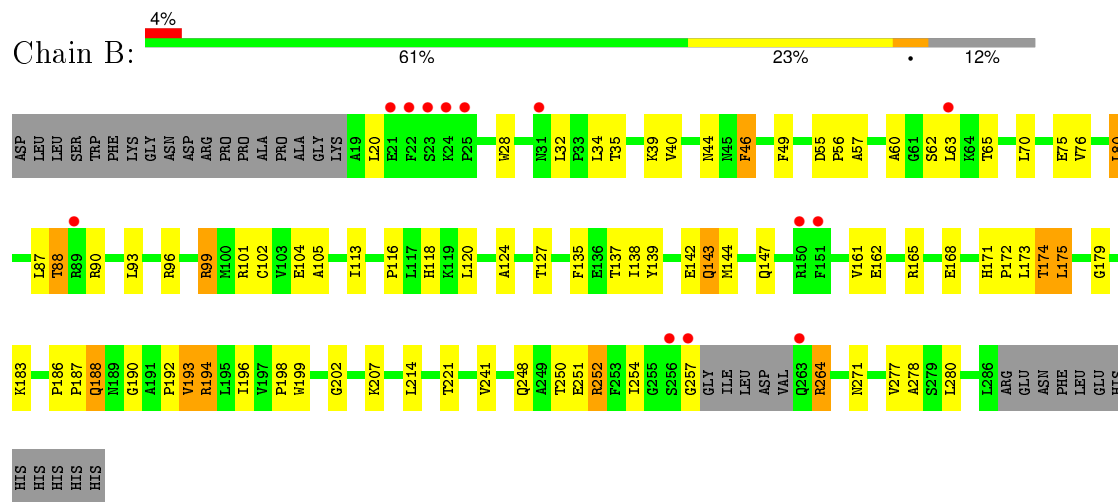
### 3 Residue-property plots

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.

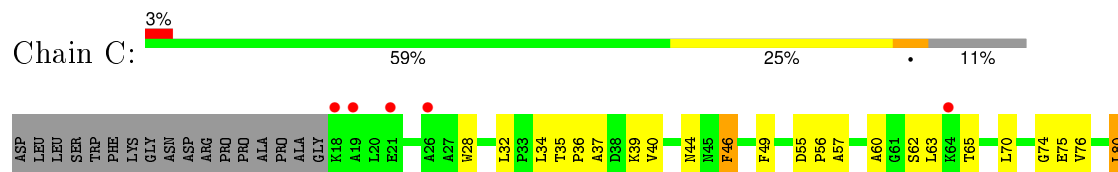
#### • Molecule 1: Bacterial Sulfite Oxidase

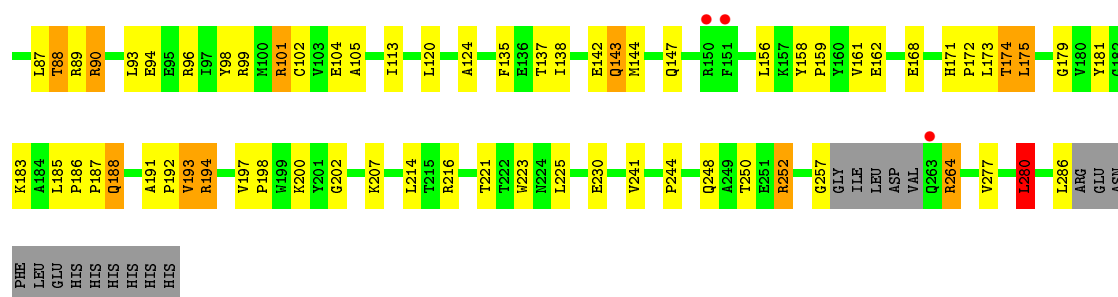


#### • Molecule 1: Bacterial Sulfite Oxidase

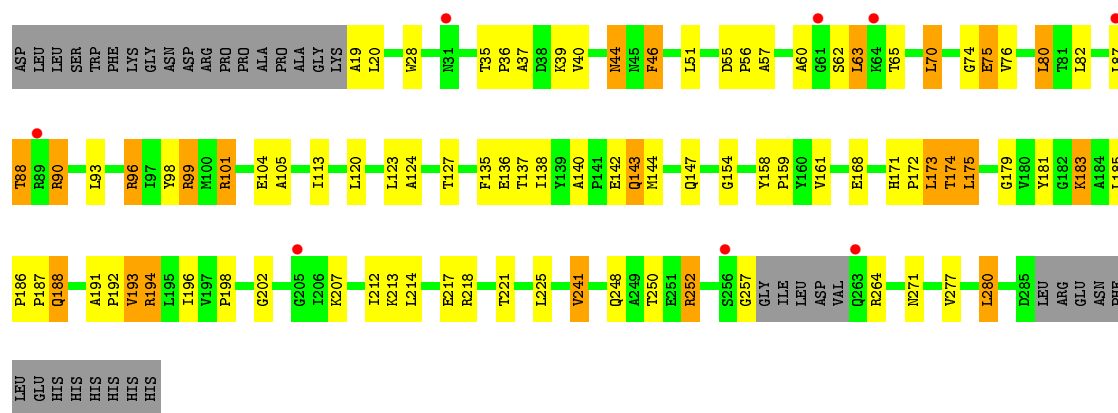


#### • Molecule 1: Bacterial Sulfite Oxidase

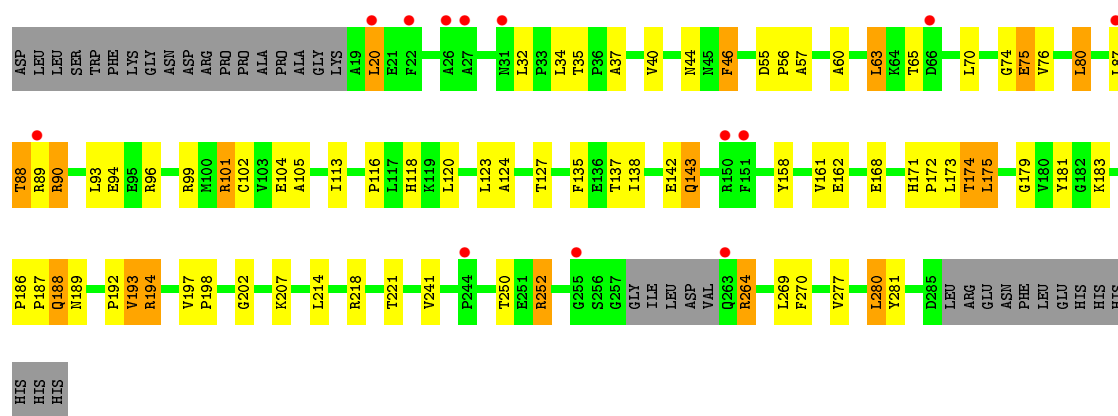




• Molecule 1: Bacterial Sulfite Oxidase



• Molecule 1: Bacterial Sulfite Oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.34Å 165.06Å 181.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.75 – 2.55 39.75 – 2.54	Depositor EDS
% Data completeness (in resolution range)	95.3 (39.75-2.55) 94.6 (39.75-2.54)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.230 , 0.274 0.227 , 0.267	Depositor DCC
$R_{free}$ test set	3650 reflections (7.59%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.2	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 51793 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10771	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: URE, MO, O, MTE

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	0.52	0/2150	0.80	2/2932 (0.1%)
1	B	0.50	0/2158	0.80	2/2943 (0.1%)
1	C	0.51	0/2167	0.81	5/2954 (0.2%)
1	D	0.51	0/2150	0.80	3/2932 (0.1%)
1	E	0.49	0/2150	0.76	1/2932 (0.0%)
All	All	0.51	0/10775	0.80	13/14693 (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	E	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	D	101	ARG	NE-CZ-NH1	-6.35	117.13	120.30
1	D	96	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	A	101	ARG	NE-CZ-NH1	-5.57	117.51	120.30
1	C	101	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	B	264	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	E	89	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	B	264	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	216	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	89	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	C	280	LEU	CA-CB-CG	5.16	127.18	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	C	101	ARG	NE-CZ-NH2	5.10	122.85	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	158	TYR	Sidechain

## 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	2085	0	2051	57	0
1	B	2093	0	2062	65	0
1	C	2102	0	2075	72	0
1	D	2085	0	2051	75	0
1	E	2085	0	2051	59	0
2	A	4	0	4	0	0
2	B	4	0	4	0	0
2	C	4	0	4	0	0
2	D	4	0	4	0	0
2	E	4	0	4	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	24	0	9	1	0
5	B	24	0	9	3	0
5	C	24	0	9	3	0
5	D	24	0	9	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	24	0	9	2	0
6	A	49	0	0	2	1
6	B	26	0	0	0	0
6	C	28	0	0	1	0
6	D	36	0	0	4	0
6	E	32	0	0	2	0
All	All	10771	0	10355	326	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 16.

All (326) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ALA:HA	1:A:188:GLN:HG2	1.27	1.14
1:D:57:ALA:HA	1:D:188:GLN:HG2	1.30	1.11
1:B:57:ALA:HA	1:B:188:GLN:HG2	1.29	1.07
1:E:57:ALA:HA	1:E:188:GLN:HG2	1.35	1.06
1:C:57:ALA:HA	1:C:188:GLN:HG2	1.38	1.05
1:D:57:ALA:HA	1:D:188:GLN:CG	2.03	0.86
1:B:57:ALA:HA	1:B:188:GLN:CG	2.06	0.85
1:A:277:VAL:O	1:A:280:LEU:HD23	1.79	0.83
1:A:57:ALA:HA	1:A:188:GLN:CG	2.07	0.83
1:C:87:LEU:HD13	1:C:193:VAL:HG22	1.61	0.83
1:B:87:LEU:HD13	1:B:193:VAL:HG22	1.60	0.82
1:A:87:LEU:HD13	1:A:193:VAL:HG22	1.60	0.81
1:B:39:LYS:HZ1	1:B:257:GLY:H	1.26	0.80
1:A:75:GLU:HG3	1:A:127:THR:OG1	1.78	0.80
1:A:57:ALA:CA	1:A:188:GLN:HG2	2.10	0.80
1:B:57:ALA:CA	1:B:188:GLN:HG2	2.11	0.79
1:C:57:ALA:HA	1:C:188:GLN:CG	2.12	0.78
1:D:57:ALA:CA	1:D:188:GLN:HG2	2.12	0.78
1:C:76:VAL:HG13	1:C:124:ALA:O	1.82	0.78
1:E:75:GLU:HG3	1:E:127:THR:OG1	1.84	0.77
1:A:76:VAL:HG13	1:A:124:ALA:O	1.85	0.77
1:B:75:GLU:HG3	1:B:127:THR:OG1	1.83	0.77
1:D:65:THR:HB	1:D:192:PRO:HD3	1.67	0.77
1:E:57:ALA:HA	1:E:188:GLN:CG	2.14	0.76
1:E:87:LEU:HD13	1:E:193:VAL:HG22	1.66	0.75
1:E:60:ALA:HB1	1:E:187:PRO:HB2	1.68	0.75
1:E:96:ARG:HD2	1:E:175:LEU:HD13	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:LEU:HD13	1:D:193:VAL:HG22	1.69	0.74
1:C:35:THR:HG22	1:C:40:VAL:HG23	1.69	0.73
1:D:76:VAL:HG13	1:D:124:ALA:O	1.89	0.72
1:E:76:VAL:HG13	1:E:124:ALA:O	1.90	0.71
1:E:280:LEU:H	1:E:280:LEU:HD23	1.55	0.71
1:D:280:LEU:HD23	1:D:280:LEU:H	1.56	0.71
1:B:76:VAL:HG13	1:B:124:ALA:O	1.91	0.70
1:E:277:VAL:O	1:E:280:LEU:HD23	1.90	0.70
1:C:57:ALA:CA	1:C:188:GLN:HG2	2.20	0.70
1:A:96:ARG:HD2	1:A:175:LEU:HD13	1.74	0.70
1:C:60:ALA:HB1	1:C:187:PRO:HB2	1.73	0.70
1:D:213:LYS:HD2	6:D:614:HOH:O	1.90	0.70
1:B:60:ALA:HB1	1:B:187:PRO:HB2	1.73	0.69
1:C:101:ARG:NH1	1:C:248:GLN:OE1	2.25	0.69
1:C:76:VAL:HG11	1:C:124:ALA:HB1	1.75	0.69
1:A:65:THR:HB	1:A:192:PRO:HD3	1.74	0.68
1:D:277:VAL:O	1:D:280:LEU:HD23	1.93	0.68
1:C:44:ASN:HB2	1:C:56:PRO:HG3	1.75	0.68
1:D:168:GLU:O	1:D:174:THR:HG21	1.94	0.68
1:A:252:ARG:HD3	1:A:264:ARG:NH1	2.08	0.68
1:B:39:LYS:NZ	1:B:257:GLY:H	1.92	0.68
1:E:80:LEU:H	1:E:80:LEU:HD23	1.58	0.68
1:B:88:THR:HG22	1:B:93:LEU:HD21	1.76	0.68
1:C:96:ARG:HD2	1:C:175:LEU:HD13	1.76	0.67
1:A:168:GLU:O	1:A:174:THR:HG21	1.95	0.66
1:C:252:ARG:HD3	1:C:264:ARG:NH1	2.11	0.66
1:E:252:ARG:HD3	1:E:264:ARG:NH1	2.10	0.66
1:E:168:GLU:O	1:E:174:THR:HG21	1.96	0.66
1:A:280:LEU:HD23	1:A:280:LEU:H	1.61	0.65
1:D:76:VAL:HG11	1:D:124:ALA:HB1	1.77	0.65
1:D:75:GLU:HG3	1:D:127:THR:OG1	1.96	0.65
1:C:80:LEU:H	1:C:80:LEU:HD23	1.61	0.65
1:A:75:GLU:HG3	1:A:127:THR:HG1	1.60	0.65
1:D:221:THR:HG21	6:D:640:HOH:O	1.96	0.65
1:B:277:VAL:O	1:B:280:LEU:HD23	1.96	0.65
1:B:44:ASN:HB2	1:B:56:PRO:HG3	1.78	0.65
1:D:28:TRP:CG	1:D:96:ARG:HG2	2.32	0.65
1:D:96:ARG:HD3	1:D:175:LEU:HD13	1.79	0.65
1:B:280:LEU:HD23	1:B:280:LEU:H	1.62	0.64
1:E:88:THR:HG22	1:E:93:LEU:HD21	1.79	0.64
1:D:213:LYS:NZ	6:D:626:HOH:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:VAL:O	1:C:280:LEU:HD23	1.98	0.64
1:E:162:GLU:OE2	1:E:221:THR:HG23	1.97	0.64
1:B:80:LEU:H	1:B:80:LEU:HD23	1.62	0.63
1:B:168:GLU:O	1:B:174:THR:HG21	1.98	0.63
1:E:65:THR:HB	1:E:192:PRO:HD3	1.80	0.63
1:B:252:ARG:HD3	1:B:264:ARG:HH12	1.64	0.63
1:A:101:ARG:HD3	1:A:251:GLU:OE2	1.99	0.62
1:B:101:ARG:NH1	1:B:105:ALA:HA	2.14	0.62
1:D:186:PRO:HB2	1:D:188:GLN:OE1	2.00	0.62
1:E:57:ALA:CA	1:E:188:GLN:HG2	2.19	0.62
1:D:171:HIS:CE1	1:D:173:LEU:HB2	2.35	0.62
1:C:186:PRO:HB2	1:C:188:GLN:OE1	1.99	0.61
1:D:80:LEU:HD23	1:D:80:LEU:H	1.65	0.61
1:C:280:LEU:H	1:C:280:LEU:HD23	1.64	0.61
1:E:56:PRO:HG2	6:E:636:HOH:O	2.01	0.61
1:C:76:VAL:CG1	1:C:124:ALA:HB1	2.31	0.61
1:A:104:GLU:O	1:A:105:ALA:HB3	2.00	0.61
1:B:101:ARG:NH1	1:B:248:GLN:OE1	2.33	0.61
1:D:101:ARG:NH1	1:D:105:ALA:HA	2.16	0.60
1:A:252:ARG:HD3	1:A:264:ARG:HH11	1.66	0.60
1:A:88:THR:HG22	1:A:93:LEU:HD21	1.84	0.60
1:D:60:ALA:HB1	1:D:187:PRO:HB2	1.81	0.60
1:C:32:LEU:O	1:C:34:LEU:HD23	2.02	0.60
1:D:171:HIS:O	1:D:174:THR:HG23	2.02	0.60
1:C:88:THR:HG22	1:C:93:LEU:HD21	1.83	0.60
1:A:186:PRO:HB2	1:A:188:GLN:OE1	2.02	0.60
1:E:76:VAL:HG11	1:E:124:ALA:HB1	1.84	0.59
1:E:80:LEU:N	1:E:80:LEU:HD23	2.16	0.59
1:B:80:LEU:N	1:B:80:LEU:HD23	2.17	0.59
1:A:29:GLN:NE2	6:A:650:HOH:O	2.35	0.59
1:D:80:LEU:N	1:D:80:LEU:HD23	2.17	0.59
1:D:88:THR:HG22	1:D:93:LEU:HD21	1.84	0.59
1:B:76:VAL:HG11	1:B:124:ALA:HB1	1.84	0.58
1:C:168:GLU:O	1:C:174:THR:HG21	2.03	0.58
1:B:75:GLU:HG3	1:B:127:THR:HG1	1.69	0.58
1:D:76:VAL:CG1	1:D:124:ALA:HB1	2.33	0.58
1:C:104:GLU:O	1:C:105:ALA:HB3	2.03	0.58
1:E:32:LEU:O	1:E:34:LEU:HD23	2.04	0.57
1:C:80:LEU:N	1:C:80:LEU:HD23	2.19	0.57
1:B:65:THR:HB	1:B:192:PRO:HD3	1.86	0.57
1:A:162:GLU:OE2	1:A:221:THR:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:GLY:O	1:E:76:VAL:N	2.38	0.57
1:B:76:VAL:CG1	1:B:124:ALA:HB1	2.35	0.56
1:E:168:GLU:OE2	1:E:281:TYR:OH	2.18	0.56
1:C:37:ALA:HB2	1:C:181:TYR:CD2	2.40	0.56
1:A:171:HIS:O	1:A:174:THR:HG23	2.06	0.56
1:E:101:ARG:HD2	1:E:102:CYS:O	2.06	0.56
1:A:76:VAL:HG11	1:A:124:ALA:HB1	1.87	0.56
1:D:221:THR:O	1:D:225:LEU:HD13	2.06	0.55
1:B:104:GLU:O	1:B:105:ALA:HB3	2.07	0.55
1:B:116:PRO:HB2	1:B:118:HIS:CD2	2.41	0.55
1:D:99:ARG:HD3	1:D:271:ASN:O	2.07	0.55
1:C:44:ASN:HB2	1:C:56:PRO:CG	2.36	0.54
1:B:194:ARG:HG3	1:B:194:ARG:NH1	2.22	0.54
1:A:87:LEU:CD1	1:A:193:VAL:HG22	2.36	0.54
1:A:80:LEU:HD23	1:A:80:LEU:N	2.23	0.54
1:A:101:ARG:NH1	1:A:248:GLN:OE1	2.35	0.54
1:D:37:ALA:HB2	1:D:181:TYR:CD2	2.43	0.54
1:E:104:GLU:O	1:E:105:ALA:HB3	2.07	0.54
1:B:171:HIS:CE1	1:B:173:LEU:HB2	2.43	0.54
1:C:171:HIS:CE1	1:C:173:LEU:HB2	2.43	0.53
1:E:186:PRO:HB2	1:E:188:GLN:OE1	2.07	0.53
1:B:32:LEU:O	1:B:34:LEU:HD23	2.07	0.53
1:E:252:ARG:HD3	1:E:264:ARG:HH11	1.74	0.53
1:D:62:SER:O	1:D:143:GLN:HG3	2.09	0.53
1:C:221:THR:O	1:C:225:LEU:HD13	2.09	0.53
1:D:142:GLU:O	1:D:143:GLN:HB2	2.08	0.53
1:D:241:VAL:HG22	6:D:607:HOH:O	2.09	0.53
1:C:74:GLY:O	1:C:76:VAL:N	2.39	0.53
1:A:76:VAL:CG1	1:A:124:ALA:HB1	2.39	0.53
1:B:44:ASN:HB2	1:B:56:PRO:CG	2.38	0.53
1:D:137:THR:HG22	1:D:138:ILE:N	2.23	0.53
1:C:252:ARG:HD3	1:C:264:ARG:HH11	1.72	0.52
1:C:28:TRP:HB3	1:C:96:ARG:HA	1.92	0.52
1:E:75:GLU:HG3	1:E:127:THR:HG1	1.70	0.52
1:A:221:THR:O	1:A:225:LEU:HD13	2.10	0.52
1:D:35:THR:HG22	1:D:40:VAL:HG23	1.91	0.52
1:A:142:GLU:O	1:A:142:GLU:HG3	2.09	0.52
1:E:241:VAL:HG22	1:E:241:VAL:O	2.10	0.52
1:C:194:ARG:NH1	1:C:194:ARG:HG3	2.25	0.52
1:E:101:ARG:NH1	1:E:105:ALA:HA	2.26	0.52
1:C:39:LYS:NZ	1:C:257:GLY:H	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:HIS:CG	1:E:172:PRO:HD2	2.45	0.51
1:E:94:GLU:O	1:E:113:ILE:HA	2.10	0.51
1:D:171:HIS:ND1	1:D:173:LEU:HB2	2.26	0.51
1:D:104:GLU:O	1:D:105:ALA:HB3	2.11	0.51
1:D:202:GLY:HA3	5:D:304:MTE:S2'	2.51	0.51
1:D:80:LEU:HD21	1:D:124:ALA:HB2	1.93	0.51
1:D:19:ALA:HA	1:D:183:LYS:HB3	1.93	0.51
1:C:142:GLU:O	1:C:143:GLN:HB2	2.11	0.51
1:A:276:GLN:NE2	6:A:610:HOH:O	2.28	0.51
1:C:241:VAL:O	1:C:241:VAL:HG22	2.11	0.50
1:E:44:ASN:HB2	1:E:56:PRO:CG	2.42	0.50
1:A:137:THR:HG22	1:A:138:ILE:N	2.27	0.50
1:C:87:LEU:CD1	1:C:193:VAL:HG22	2.39	0.50
1:E:171:HIS:CE1	1:E:173:LEU:HB2	2.47	0.50
1:D:113:ILE:N	1:D:179:GLY:O	2.44	0.50
1:E:46:PHE:HB3	1:E:56:PRO:HB3	1.94	0.50
1:B:102:CYS:HB2	5:B:302:MTE:S2'	2.51	0.50
1:A:171:HIS:ND1	1:A:173:LEU:HB2	2.27	0.49
1:B:96:ARG:HD2	1:B:175:LEU:HD13	1.93	0.49
1:B:137:THR:HG22	1:B:138:ILE:N	2.26	0.49
1:C:162:GLU:OE2	1:C:221:THR:HG23	2.12	0.49
1:D:74:GLY:O	1:D:76:VAL:N	2.42	0.49
1:E:171:HIS:O	1:E:174:THR:HG23	2.12	0.49
1:A:144:MET:HE3	1:A:147:GLN:OE1	2.13	0.49
1:E:202:GLY:HA3	5:E:305:MTE:S2'	2.53	0.49
1:C:171:HIS:CG	1:C:172:PRO:HD2	2.48	0.49
1:D:241:VAL:HG22	1:D:241:VAL:O	2.13	0.49
1:C:135:PHE:O	1:C:161:VAL:HG23	2.12	0.49
1:B:162:GLU:OE2	1:B:221:THR:HG23	2.12	0.49
1:C:35:THR:CG2	1:C:40:VAL:HG23	2.41	0.49
1:A:142:GLU:O	1:A:143:GLN:HB2	2.12	0.49
1:A:202:GLY:HA3	5:A:301:MTE:S2'	2.53	0.49
1:E:142:GLU:O	1:E:142:GLU:HG3	2.12	0.49
1:A:63:LEU:HA	1:A:143:GLN:HG2	1.95	0.48
1:E:113:ILE:N	1:E:179:GLY:O	2.46	0.48
1:E:116:PRO:HB2	1:E:118:HIS:CD2	2.48	0.48
1:E:76:VAL:CG1	1:E:124:ALA:HB1	2.42	0.48
1:E:20:LEU:HB2	6:E:631:HOH:O	2.12	0.48
1:D:55:ASP:N	1:D:56:PRO:HD2	2.29	0.48
1:A:282:ARG:NH2	1:D:136:GLU:OE1	2.44	0.48
1:A:171:HIS:CE1	1:A:173:LEU:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:TRP:CD1	1:D:96:ARG:HG2	2.49	0.48
1:B:39:LYS:NZ	1:B:257:GLY:N	2.61	0.48
1:A:80:LEU:HD23	1:A:80:LEU:H	1.78	0.48
1:B:194:ARG:HH11	1:B:194:ARG:HG3	1.78	0.48
1:C:65:THR:HB	1:C:192:PRO:HD3	1.95	0.48
1:D:90:ARG:CZ	1:D:123:LEU:HD11	2.43	0.48
1:E:44:ASN:HB2	1:E:56:PRO:HG3	1.96	0.47
1:B:62:SER:O	1:B:143:GLN:HG3	2.14	0.47
1:A:186:PRO:HG2	1:A:189:ASN:OD1	2.13	0.47
1:C:241:VAL:HG22	6:C:625:HOH:O	2.14	0.47
1:A:46:PHE:HB3	1:A:56:PRO:HB3	1.95	0.47
1:C:49:PHE:O	1:C:55:ASP:HB3	2.15	0.47
1:C:76:VAL:CG1	1:C:124:ALA:O	2.56	0.47
1:C:36:PRO:HG2	1:C:39:LYS:HG3	1.96	0.47
1:D:158:TYR:HB3	1:D:159:PRO:HA	1.96	0.47
1:A:80:LEU:HD21	1:A:124:ALA:HB2	1.96	0.47
1:B:171:HIS:ND1	1:B:173:LEU:HB2	2.28	0.47
1:C:113:ILE:N	1:C:179:GLY:O	2.47	0.47
1:E:142:GLU:O	1:E:143:GLN:HB2	2.13	0.47
1:C:202:GLY:HA3	5:C:303:MTE:S2'	2.54	0.47
1:B:186:PRO:HB2	1:B:188:GLN:OE1	2.15	0.47
1:C:171:HIS:ND1	1:C:173:LEU:HB2	2.30	0.47
1:D:46:PHE:HB3	1:D:56:PRO:HB3	1.96	0.47
1:C:102:CYS:HB2	5:C:303:MTE:S2'	2.55	0.47
1:E:63:LEU:HA	1:E:143:GLN:HG2	1.96	0.47
1:D:101:ARG:NH1	1:D:248:GLN:OE1	2.44	0.46
1:D:207:LYS:HE3	5:D:304:MTE:O3'	2.15	0.46
1:D:140:ALA:H	1:D:144:MET:CE	2.28	0.46
1:A:135:PHE:O	1:A:161:VAL:HG23	2.15	0.46
1:D:142:GLU:HG3	1:D:142:GLU:O	2.15	0.46
1:A:101:ARG:NH1	1:A:105:ALA:HA	2.30	0.46
1:A:282:ARG:NH2	1:D:136:GLU:CD	2.69	0.46
1:B:241:VAL:O	1:B:241:VAL:HG22	2.15	0.46
1:B:101:ARG:HD3	1:B:251:GLU:OE2	2.15	0.46
1:C:142:GLU:HG3	1:C:142:GLU:O	2.15	0.46
1:B:87:LEU:CD1	1:B:193:VAL:HG22	2.39	0.46
1:C:80:LEU:HD21	1:C:124:ALA:HB2	1.96	0.46
1:E:80:LEU:HD21	1:E:124:ALA:HB2	1.96	0.46
1:D:194:ARG:NH1	1:D:194:ARG:HG3	2.31	0.46
1:C:28:TRP:CD1	1:C:96:ARG:HG2	2.51	0.46
1:D:20:LEU:HD13	1:D:93:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:PHE:O	1:D:161:VAL:HG23	2.16	0.46
1:D:39:LYS:NZ	1:D:257:GLY:H	2.14	0.46
1:A:60:ALA:HB1	1:A:187:PRO:HB2	1.97	0.45
1:C:98:TYR:HE1	1:C:175:LEU:HD22	1.80	0.45
1:B:46:PHE:HB3	1:B:56:PRO:HB3	1.98	0.45
1:D:87:LEU:CD1	1:D:193:VAL:HG22	2.44	0.45
1:B:202:GLY:HA3	5:B:302:MTE:S2'	2.57	0.45
1:D:36:PRO:HG2	1:D:39:LYS:HD2	1.97	0.45
1:A:248:GLN:OE1	1:A:248:GLN:HA	2.16	0.45
1:A:44:ASN:HB2	1:A:56:PRO:HG3	1.98	0.45
1:B:196:ILE:HG22	1:B:198:PRO:HD3	1.99	0.45
1:B:138:ILE:HG12	1:B:139:TYR:N	2.32	0.45
1:B:135:PHE:O	1:B:161:VAL:HG23	2.16	0.45
1:C:168:GLU:OE2	1:C:200:LYS:NZ	2.48	0.45
1:A:74:GLY:O	1:A:76:VAL:N	2.49	0.45
1:B:49:PHE:O	1:B:55:ASP:HB3	2.17	0.45
1:D:63:LEU:HA	1:D:143:GLN:HG2	1.99	0.45
1:B:190:GLY:HA3	1:B:207:LYS:HB3	1.99	0.44
1:D:185:LEU:O	1:D:191:ALA:HB2	2.18	0.44
1:A:35:THR:HG22	1:A:40:VAL:HG23	1.99	0.44
1:A:252:ARG:CD	1:A:264:ARG:HH11	2.28	0.44
1:E:55:ASP:N	1:E:56:PRO:HD2	2.31	0.44
1:C:194:ARG:HG3	1:C:194:ARG:HH11	1.82	0.44
1:D:51:LEU:HD21	1:D:154:GLY:CA	2.48	0.44
1:C:137:THR:HG22	1:C:138:ILE:N	2.31	0.44
1:B:101:ARG:CZ	1:B:105:ALA:HA	2.48	0.44
1:E:186:PRO:HG2	1:E:189:ASN:OD1	2.17	0.44
1:B:207:LYS:HE3	5:B:302:MTE:O3'	2.17	0.44
1:C:94:GLU:O	1:C:113:ILE:HA	2.17	0.44
1:B:113:ILE:N	1:B:179:GLY:O	2.50	0.44
1:E:197:VAL:HA	1:E:198:PRO:HD2	1.77	0.44
1:C:46:PHE:HB3	1:C:56:PRO:HB3	1.99	0.44
1:A:44:ASN:HB2	1:A:56:PRO:CG	2.48	0.44
1:C:207:LYS:HE3	5:C:303:MTE:O3'	2.17	0.44
1:E:90:ARG:CZ	1:E:123:LEU:HD11	2.47	0.44
1:E:63:LEU:HD13	1:E:65:THR:HG22	2.00	0.44
1:B:142:GLU:O	1:B:142:GLU:HG3	2.18	0.44
1:C:90:ARG:HD3	1:C:90:ARG:O	2.18	0.43
1:A:94:GLU:O	1:A:113:ILE:HA	2.18	0.43
1:E:35:THR:HG22	1:E:40:VAL:HG23	2.00	0.43
1:D:28:TRP:HB3	1:D:96:ARG:HA	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:TRP:HB3	1:B:96:ARG:HA	2.00	0.43
1:B:142:GLU:O	1:B:143:GLN:HB2	2.18	0.43
1:D:98:TYR:HE1	1:D:175:LEU:HD22	1.84	0.43
1:C:241:VAL:CG2	1:C:241:VAL:O	2.66	0.43
1:D:194:ARG:HH11	1:D:194:ARG:HG3	1.84	0.43
1:D:252:ARG:HD3	1:D:264:ARG:HH12	1.83	0.43
1:C:171:HIS:O	1:C:174:THR:HG23	2.19	0.43
1:B:138:ILE:CG1	1:B:139:TYR:N	2.82	0.43
1:E:269:LEU:O	1:E:270:PHE:HB2	2.18	0.43
1:A:19:ALA:HA	1:A:183:LYS:HB3	2.01	0.43
1:D:171:HIS:CG	1:D:172:PRO:HD2	2.53	0.43
1:C:49:PHE:CZ	1:C:144:MET:HG2	2.54	0.43
1:C:158:TYR:HB3	1:C:159:PRO:HA	2.00	0.43
1:D:28:TRP:CB	1:D:96:ARG:HG2	2.49	0.42
1:D:144:MET:HE1	1:D:147:GLN:NE2	2.34	0.42
1:B:99:ARG:HG3	1:B:271:ASN:ND2	2.34	0.42
1:C:104:GLU:O	1:C:105:ALA:CB	2.67	0.42
1:E:194:ARG:HG3	1:E:194:ARG:NH1	2.35	0.42
1:B:277:VAL:O	1:B:278:ALA:C	2.57	0.42
1:B:171:HIS:CG	1:B:172:PRO:HD2	2.55	0.42
1:E:241:VAL:CG2	1:E:241:VAL:O	2.67	0.42
1:E:135:PHE:O	1:E:161:VAL:HG23	2.20	0.42
1:E:137:THR:HG22	1:E:138:ILE:N	2.35	0.42
1:B:144:MET:HE3	1:B:147:GLN:OE1	2.19	0.42
1:C:156:LEU:HD21	1:C:223:TRP:CZ2	2.55	0.42
1:C:62:SER:O	1:C:143:GLN:HG3	2.19	0.42
1:C:144:MET:HE1	1:C:147:GLN:NE2	2.34	0.42
1:D:144:MET:HE3	1:D:147:GLN:OE1	2.20	0.42
1:D:196:ILE:HG22	1:D:198:PRO:HD3	2.01	0.42
1:B:35:THR:HG22	1:B:40:VAL:HG23	2.02	0.42
1:B:137:THR:CG2	1:B:138:ILE:N	2.83	0.41
1:B:39:LYS:HD3	1:B:254:ILE:CG2	2.50	0.41
1:A:116:PRO:HB2	1:A:118:HIS:CD2	2.55	0.41
1:C:197:VAL:HA	1:C:198:PRO:HD2	1.77	0.41
1:C:230:GLU:HG2	1:C:244:PRO:HG2	2.03	0.41
1:C:248:GLN:HA	1:C:248:GLN:OE1	2.21	0.41
1:B:93:LEU:CD1	1:B:93:LEU:N	2.84	0.41
1:C:185:LEU:O	1:C:191:ALA:HB2	2.21	0.41
1:E:87:LEU:CD1	1:E:193:VAL:HG22	2.44	0.41
1:C:28:TRP:CG	1:C:96:ARG:HG2	2.56	0.41
1:B:55:ASP:N	1:B:56:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:LYS:HB2	5:E:305:MTE:N1	2.36	0.41
1:A:197:VAL:HA	1:A:198:PRO:HD2	1.84	0.41
1:D:143:GLN:HB2	1:D:143:GLN:HE21	1.77	0.41
1:D:82:LEU:HD12	1:D:82:LEU:N	2.35	0.40
1:A:140:ALA:H	1:A:144:MET:CE	2.34	0.40
1:D:70:LEU:HD21	1:D:212:ILE:HG13	2.03	0.40
1:D:44:ASN:HB2	1:D:56:PRO:HG3	2.03	0.40
1:A:55:ASP:N	1:A:56:PRO:HD2	2.35	0.40
1:B:174:THR:HG22	1:B:199:TRP:CH2	2.57	0.40
1:D:248:GLN:HA	1:D:248:GLN:OE1	2.21	0.40
1:E:37:ALA:HB2	1:E:181:TYR:CD2	2.56	0.40
1:C:191:ALA:HB1	1:C:192:PRO:HA	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:646:HOH:O	6:A:646:HOH:O[6_445]	2.10	0.10

## 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	258/298 (87%)	245 (95%)	12 (5%)	1 (0%)	39	60
1	B	259/298 (87%)	240 (93%)	18 (7%)	1 (0%)	39	60
1	C	260/298 (87%)	244 (94%)	14 (5%)	2 (1%)	24	40
1	D	258/298 (87%)	242 (94%)	14 (5%)	2 (1%)	24	40
1	E	258/298 (87%)	241 (93%)	15 (6%)	2 (1%)	24	40
All	All	1293/1490 (87%)	1212 (94%)	73 (6%)	8 (1%)	30	48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	B	143	GLN
1	C	143	GLN
1	D	143	GLN
1	E	143	GLN
1	C	75	GLU
1	D	75	GLU
1	E	75	GLU

### 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	218/249 (88%)	197 (90%)	21 (10%)	10	18
1	B	219/249 (88%)	200 (91%)	19 (9%)	13	22
1	C	220/249 (88%)	200 (91%)	20 (9%)	12	20
1	D	218/249 (88%)	195 (89%)	23 (11%)	8	15
1	E	218/249 (88%)	196 (90%)	22 (10%)	9	16
All	All	1093/1245 (88%)	988 (90%)	105 (10%)	10	18

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	46	PHE
1	A	63	LEU
1	A	70	LEU
1	A	80	LEU
1	A	88	THR
1	A	90	ARG
1	A	99	ARG
1	A	120	LEU
1	A	174	THR

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Mol	Chain	Res	Type
1	A	175	LEU
1	A	183	LYS
1	A	188	GLN
1	A	193	VAL
1	A	194	ARG
1	A	214	LEU
1	A	241	VAL
1	A	250	THR
1	A	252	ARG
1	A	264	ARG
1	A	285	ASP
1	B	20	LEU
1	B	46	PHE
1	B	63	LEU
1	B	70	LEU
1	B	80	LEU
1	B	88	THR
1	B	90	ARG
1	B	99	ARG
1	B	120	LEU
1	B	165	ARG
1	B	174	THR
1	B	175	LEU
1	B	183	LYS
1	B	188	GLN
1	B	193	VAL
1	B	194	ARG
1	B	214	LEU
1	B	250	THR
1	B	252	ARG
1	C	46	PHE
1	C	63	LEU
1	C	70	LEU
1	C	80	LEU
1	C	88	THR
1	C	90	ARG
1	C	99	ARG
1	C	120	LEU
1	C	174	THR
1	C	175	LEU
1	C	183	LYS
1	C	188	GLN

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Mol	Chain	Res	Type
1	C	193	VAL
1	C	194	ARG
1	C	214	LEU
1	C	250	THR
1	C	252	ARG
1	C	264	ARG
1	C	280	LEU
1	C	286	LEU
1	D	44	ASN
1	D	46	PHE
1	D	63	LEU
1	D	70	LEU
1	D	80	LEU
1	D	88	THR
1	D	90	ARG
1	D	99	ARG
1	D	120	LEU
1	D	173	LEU
1	D	174	THR
1	D	175	LEU
1	D	183	LYS
1	D	188	GLN
1	D	193	VAL
1	D	194	ARG
1	D	214	LEU
1	D	217	GLU
1	D	218	ARG
1	D	241	VAL
1	D	250	THR
1	D	252	ARG
1	D	280	LEU
1	E	20	LEU
1	E	46	PHE
1	E	63	LEU
1	E	70	LEU
1	E	80	LEU
1	E	88	THR
1	E	90	ARG
1	E	99	ARG
1	E	101	ARG
1	E	120	LEU
1	E	174	THR

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Mol	Chain	Res	Type
1	E	175	LEU
1	E	183	LYS
1	E	188	GLN
1	E	193	VAL
1	E	194	ARG
1	E	214	LEU
1	E	218	ARG
1	E	250	THR
1	E	252	ARG
1	E	264	ARG
1	E	280	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	224	ASN
1	B	148	GLN
1	C	148	GLN
1	D	148	GLN
1	E	148	GLN
1	E	224	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 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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$
5	MTE	A	301	3	19,26,26	4.36	13 (68%)	19,40,40	6.53	12 (63%)
2	URE	A	401	-	3,3,3	0.88	0	3,3,3	1.76	1 (33%)
5	MTE	B	302	3	19,26,26	3.97	13 (68%)	19,40,40	6.53	13 (68%)
2	URE	B	402	-	3,3,3	0.78	0	3,3,3	1.69	1 (33%)
5	MTE	C	303	3	19,26,26	4.51	13 (68%)	19,40,40	6.22	13 (68%)
2	URE	C	403	-	3,3,3	0.73	0	3,3,3	1.74	1 (33%)
5	MTE	D	304	3	19,26,26	4.65	13 (68%)	19,40,40	6.30	12 (63%)
2	URE	D	404	-	3,3,3	1.04	0	3,3,3	1.69	1 (33%)
5	MTE	E	305	3	19,26,26	4.44	12 (63%)	19,40,40	6.51	14 (73%)
2	URE	E	405	-	3,3,3	0.77	0	3,3,3	1.74	1 (33%)

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
5	MTE	A	301	3	1/1/6/8	0/6/34/34	0/3/3/3
2	URE	A	401	-	-	0/0/0/0	0/0/0/0
5	MTE	B	302	3	1/1/6/8	0/6/34/34	0/3/3/3
2	URE	B	402	-	-	0/0/0/0	0/0/0/0
5	MTE	C	303	3	1/1/6/8	0/6/34/34	0/3/3/3
2	URE	C	403	-	-	0/0/0/0	0/0/0/0
5	MTE	D	304	3	1/1/6/8	0/6/34/34	0/3/3/3
2	URE	D	404	-	-	0/0/0/0	0/0/0/0
5	MTE	E	305	3	1/1/6/8	0/6/34/34	0/3/3/3
2	URE	E	405	-	-	0/0/0/0	0/0/0/0

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	301	MTE	P-O4'	-5.45	1.42	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	304	MTE	P-O4'	-5.31	1.42	1.60
5	C	303	MTE	P-O4'	-5.22	1.42	1.60
5	E	305	MTE	P-O4'	-4.89	1.43	1.60
5	B	302	MTE	P-O4'	-4.83	1.44	1.60
5	D	304	MTE	P-O2P	-4.67	1.37	1.54
5	E	305	MTE	P-O2P	-4.59	1.38	1.54
5	A	301	MTE	P-O2P	-4.56	1.38	1.54
5	C	303	MTE	P-O2P	-4.54	1.38	1.54
5	B	302	MTE	P-O1P	-4.47	1.36	1.51
5	B	302	MTE	P-O2P	-4.35	1.39	1.54
5	E	305	MTE	P-O1P	-4.02	1.37	1.51
5	C	303	MTE	P-O1P	-4.00	1.38	1.51
5	A	301	MTE	P-O1P	-3.96	1.38	1.51
5	D	304	MTE	P-O1P	-3.74	1.38	1.51
5	A	301	MTE	C2-N3	-2.99	1.30	1.35
5	C	303	MTE	C2-N2	-2.87	1.28	1.34
5	D	304	MTE	C2-N2	-2.84	1.28	1.34
5	B	302	MTE	C2-N3	-2.82	1.30	1.35
5	B	302	MTE	C2-N2	-2.76	1.28	1.34
5	A	301	MTE	C2-N2	-2.71	1.28	1.34
5	E	305	MTE	C2-N2	-2.68	1.28	1.34
5	D	304	MTE	C2-N3	-2.58	1.30	1.35
5	C	303	MTE	C2-N3	-2.29	1.31	1.35
5	A	301	MTE	O4-C4	2.18	1.30	1.24
5	B	302	MTE	O4-C4	2.30	1.30	1.24
5	D	304	MTE	O3'-C7	2.61	1.47	1.43
5	B	302	MTE	C9-N5	2.89	1.44	1.38
5	D	304	MTE	C9-N5	2.92	1.44	1.38
5	A	301	MTE	C4-N3	3.05	1.38	1.33
5	B	302	MTE	O3'-C7	3.15	1.48	1.43
5	C	303	MTE	O4-C4	3.23	1.32	1.24
5	E	305	MTE	O4-C4	3.40	1.32	1.24
5	A	301	MTE	C9-N5	3.61	1.46	1.38
5	D	304	MTE	O3'-C3'	3.64	1.49	1.43
5	B	302	MTE	C4-N3	3.65	1.39	1.33
5	E	305	MTE	C9-N5	3.66	1.46	1.38
5	E	305	MTE	O3'-C7	3.73	1.49	1.43
5	C	303	MTE	O3'-C7	3.76	1.49	1.43
5	C	303	MTE	C9-N5	3.79	1.46	1.38
5	D	304	MTE	O4-C4	3.86	1.34	1.24
5	C	303	MTE	O3'-C3'	3.89	1.49	1.43
5	A	301	MTE	O3'-C7	3.93	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	304	MTE	C4-N3	3.98	1.40	1.33
5	B	302	MTE	O3'-C3'	4.03	1.49	1.43
5	C	303	MTE	C4-N3	4.19	1.40	1.33
5	A	301	MTE	O3'-C3'	4.25	1.49	1.43
5	B	302	MTE	C6-N5	4.71	1.52	1.45
5	E	305	MTE	C4-N3	4.74	1.41	1.33
5	E	305	MTE	O3'-C3'	4.97	1.50	1.43
5	D	304	MTE	C6-N5	5.26	1.52	1.45
5	C	303	MTE	C6-N5	5.60	1.53	1.45
5	E	305	MTE	C6-N5	5.68	1.53	1.45
5	B	302	MTE	C9-C10	5.94	1.53	1.41
5	A	301	MTE	C9-C10	6.36	1.54	1.41
5	D	304	MTE	C9-C10	6.45	1.54	1.41
5	A	301	MTE	C6-N5	6.51	1.54	1.45
5	E	305	MTE	C9-C10	6.64	1.55	1.41
5	C	303	MTE	C9-C10	6.69	1.55	1.41
5	B	302	MTE	C7-C6	10.31	1.61	1.53
5	A	301	MTE	C7-C6	11.51	1.62	1.53
5	E	305	MTE	C7-C6	11.60	1.62	1.53
5	C	303	MTE	C7-C6	12.49	1.62	1.53
5	D	304	MTE	C7-C6	14.16	1.64	1.53

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	301	MTE	O3'-C7-C6	-23.93	92.61	108.96
5	B	302	MTE	O3'-C7-C6	-23.84	92.67	108.96
5	E	305	MTE	O3'-C7-C6	-23.46	92.93	108.96
5	D	304	MTE	O3'-C7-C6	-22.78	93.39	108.96
5	C	303	MTE	O3'-C7-C6	-22.32	93.71	108.96
5	E	305	MTE	C9-C10-N8	-3.85	114.31	118.34
5	A	301	MTE	C9-C10-N8	-3.56	114.62	118.34
5	C	303	MTE	C9-C10-N8	-3.56	114.62	118.34
5	B	302	MTE	C9-C10-N8	-3.53	114.65	118.34
5	D	304	MTE	C9-C10-N8	-3.12	115.08	118.34
5	B	302	MTE	N3-C2-N1	-2.74	121.04	125.53
5	E	305	MTE	N3-C2-N1	-2.65	121.20	125.53
5	C	303	MTE	N3-C2-N1	-2.61	121.26	125.53
5	A	301	MTE	N3-C2-N1	-2.57	121.32	125.53
5	D	304	MTE	N3-C2-N1	-2.56	121.34	125.53
5	E	305	MTE	O2P-P-O1P	-2.44	102.73	110.58
5	B	302	MTE	C9-C10-N1	-2.41	113.77	118.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	304	MTE	C9-C10-N1	-2.38	113.83	118.76
2	A	401	URE	O-C-N2	-2.33	114.91	121.03
2	E	405	URE	O-C-N2	-2.30	115.00	121.03
2	C	403	URE	O-C-N2	-2.29	115.01	121.03
5	B	302	MTE	O2P-P-O1P	-2.28	103.22	110.58
5	E	305	MTE	C9-C10-N1	-2.28	114.03	118.76
2	B	402	URE	O-C-N2	-2.26	115.10	121.03
5	C	303	MTE	C9-C10-N1	-2.24	114.12	118.76
5	A	301	MTE	C9-C10-N1	-2.23	114.14	118.76
2	D	404	URE	O-C-N2	-2.21	115.24	121.03
5	C	303	MTE	O2P-P-O1P	-2.20	103.49	110.58
5	D	304	MTE	O2P-P-O1P	-2.13	103.73	110.58
5	E	305	MTE	N2-C2-N1	2.18	120.81	117.20
5	E	305	MTE	O3P-P-O2P	2.19	115.70	107.38
5	C	303	MTE	N2-C2-N1	2.29	121.00	117.20
5	A	301	MTE	N2-C2-N1	2.31	121.03	117.20
5	B	302	MTE	N2-C2-N1	2.54	121.41	117.20
5	A	301	MTE	C4-C9-C10	2.85	117.14	114.56
5	C	303	MTE	C9-N5-C6	3.18	127.20	118.65
5	B	302	MTE	C9-N5-C6	3.22	127.31	118.65
5	D	304	MTE	C9-N5-C6	3.31	127.54	118.65
5	A	301	MTE	C9-N5-C6	3.32	127.57	118.65
5	C	303	MTE	C4-C9-C10	3.33	117.58	114.56
5	E	305	MTE	C9-N5-C6	3.43	127.86	118.65
5	D	304	MTE	C4-C9-C10	3.50	117.73	114.56
5	B	302	MTE	C4-C9-C10	3.60	117.82	114.56
5	E	305	MTE	C4-C9-C10	3.67	117.89	114.56
5	D	304	MTE	C10-N8-C7	3.77	131.07	123.67
5	B	302	MTE	C10-N8-C7	4.00	131.52	123.67
5	E	305	MTE	C10-N8-C7	4.17	131.83	123.67
5	B	302	MTE	C4-N3-C2	4.25	121.84	115.94
5	C	303	MTE	C10-N8-C7	4.36	132.22	123.67
5	E	305	MTE	C4-N3-C2	4.40	122.04	115.94
5	A	301	MTE	C10-N8-C7	4.48	132.45	123.67
5	C	303	MTE	C4-N3-C2	4.48	122.16	115.94
5	A	301	MTE	C4-N3-C2	4.65	122.39	115.94
5	D	304	MTE	C4-N3-C2	4.66	122.40	115.94
5	C	303	MTE	C2-N1-C10	4.97	125.72	114.54
5	A	301	MTE	C2-N1-C10	4.98	125.74	114.54
5	E	305	MTE	C2-N1-C10	5.02	125.83	114.54
5	B	302	MTE	C2-N1-C10	5.07	125.94	114.54
5	D	304	MTE	C2-N1-C10	5.23	126.30	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	303	MTE	O4'-P-O1P	5.26	120.54	107.14
5	B	302	MTE	O4'-P-O1P	5.32	120.70	107.14
5	D	304	MTE	O4'-P-O1P	5.42	120.94	107.14
5	A	301	MTE	O4'-P-O1P	5.45	121.01	107.14
5	E	305	MTE	O4'-P-O1P	5.84	122.01	107.14
5	D	304	MTE	N8-C10-N1	9.09	131.09	116.62
5	A	301	MTE	N8-C10-N1	9.19	131.25	116.62
5	C	303	MTE	N8-C10-N1	9.20	131.26	116.62
5	B	302	MTE	N8-C10-N1	9.40	131.58	116.62
5	E	305	MTE	N8-C10-N1	9.45	131.66	116.62

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	302	MTE	C6
5	E	305	MTE	C6
5	A	301	MTE	C6
5	D	304	MTE	C6
5	C	303	MTE	C6

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	301	MTE	1	0
5	B	302	MTE	3	0
5	C	303	MTE	3	0
5	D	304	MTE	2	0
5	E	305	MTE	2	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, 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	262/298 (87%)	-0.07	4 (1%) 76 80	29, 50, 74, 105	0
1	B	263/298 (88%)	0.13	13 (4%) 33 39	34, 55, 80, 99	0
1	C	264/298 (88%)	0.19	8 (3%) 54 60	36, 56, 80, 102	0
1	D	262/298 (87%)	0.20	8 (3%) 52 58	36, 56, 81, 98	0
1	E	262/298 (87%)	0.25	13 (4%) 32 38	38, 58, 82, 101	0
All	All	1313/1490 (88%)	0.14	46 (3%) 48 54	29, 55, 81, 105	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	31	ASN	3.7
1	B	31	ASN	3.7
1	D	89	ARG	3.6
1	A	150	ARG	3.3
1	E	27	ALA	3.2
1	B	150	ARG	3.1
1	E	20	LEU	3.1
1	C	150	ARG	3.1
1	B	22	PHE	3.0
1	B	257	GLY	2.9
1	E	263	GLN	2.9
1	D	263	GLN	2.9
1	E	151	PHE	2.9
1	B	256	SER	2.8
1	E	150	ARG	2.8
1	D	256	SER	2.7
1	B	21	GLU	2.7
1	C	18	LYS	2.7
1	C	64	LYS	2.6
1	E	244	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	255	GLY	2.6
1	B	151	PHE	2.6
1	B	263	GLN	2.5
1	C	263	GLN	2.5
1	B	63	LEU	2.4
1	E	66	ASP	2.4
1	A	151	PHE	2.4
1	B	24	LYS	2.4
1	D	61	GLY	2.4
1	E	26	ALA	2.3
1	C	21	GLU	2.3
1	D	87	LEU	2.3
1	D	31	ASN	2.3
1	D	64	LYS	2.3
1	D	205	GLY	2.3
1	B	89	ARG	2.2
1	C	26	ALA	2.2
1	E	87	LEU	2.2
1	B	23	SER	2.1
1	C	19	ALA	2.1
1	E	22	PHE	2.1
1	A	263	GLN	2.0
1	B	25	PRO	2.0
1	A	264	ARG	2.0
1	E	89	ARG	2.0
1	C	151	PHE	2.0

## 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	URE	D	404	4/4	0.83	0.44	12.04	40,43,53,55	0
2	URE	C	403	4/4	0.84	0.34	6.13	49,56,62,64	0
2	URE	E	405	4/4	0.74	0.39	4.36	51,53,61,63	0
2	URE	B	402	4/4	0.84	0.21	3.57	52,58,63,63	0
2	URE	A	401	4/4	0.74	0.26	2.83	49,62,62,66	0
5	MTE	E	305	24/24	0.97	0.19	0.63	42,48,54,57	0
5	MTE	C	303	24/24	0.97	0.18	0.54	41,45,51,54	0
5	MTE	B	302	24/24	0.96	0.16	0.47	26,43,50,55	0
5	MTE	D	304	24/24	0.97	0.18	0.16	37,47,52,54	0
5	MTE	A	301	24/24	0.98	0.15	0.14	34,41,44,51	0
4	O	E	605	1/1	1.00	0.15	-0.52	32,32,32,32	0
4	O	B	602	1/1	1.00	0.14	-0.64	32,32,32,32	0
3	MO	E	505	1/1	0.99	0.14	-0.66	49,49,49,49	0
4	O	D	604	1/1	1.00	0.16	-0.89	31,31,31,31	0
3	MO	B	502	1/1	1.00	0.13	-0.91	41,41,41,41	0
3	MO	D	504	1/1	0.99	0.15	-1.38	41,41,41,41	0
3	MO	A	501	1/1	1.00	0.13	-1.54	40,40,40,40	0
3	MO	C	503	1/1	1.00	0.14	-2.03	41,41,41,41	0
4	O	C	603	1/1	1.00	0.14	-2.45	42,42,42,42	0
4	O	A	601	1/1	1.00	0.12	-3.51	35,35,35,35	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.