



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:59 AM GMT

PDB ID : 2YZB  
Title : Crystal structure of uricase from *Arthrobacter globiformis* in complex with uric acid (substrate)  
Authors : Juan, E.C.M.; Hossain, M.T.; Hoque, M.M.; Suzuki, K.; Sekiguchi, T.; Takenaka, A.  
Deposited on : 2007-05-05  
Resolution : 1.90 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

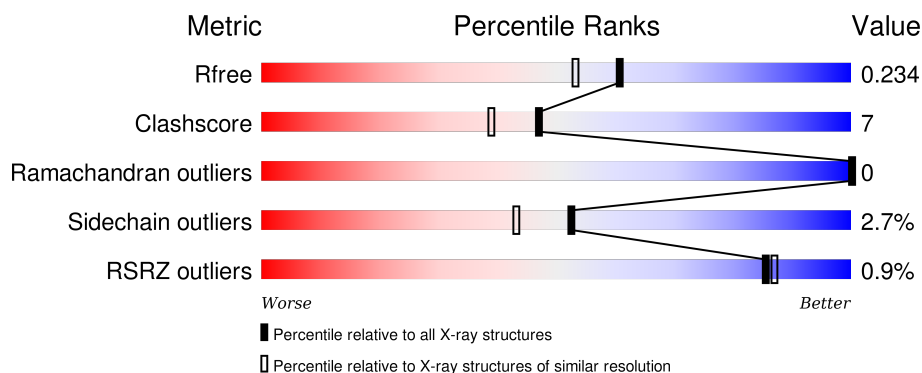
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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. 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	302	 87% 7% • 5%
1	B	302	 79% 15% • 5%
1	C	302	 81% 13% • 5%
1	D	302	 80% 14% • 5%
1	E	302	 76% 18% • 5%

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Mol	Chain	Length	Quality of chain
1	F	302	 % 81% 14% 5%
1	G	302	 2% 81% 13% • 5%
1	H	302	 % 79% 16% • 5%

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	URC	B	2303	-	-	-	X
2	URC	E	2308	-	-	X	X
2	URC	H	2305	-	-	-	X

## 2 Entry composition

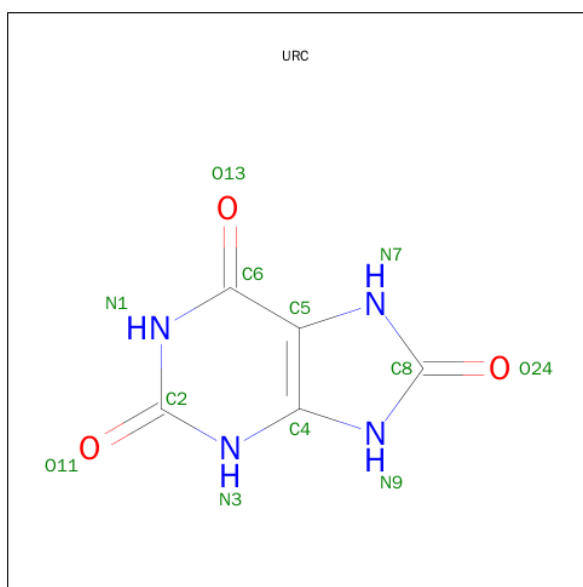
There are 3 unique types of molecules in this entry. The entry contains 19734 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uricase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2284	1436	408	437	3			
1	B	287	Total	C	N	O	S	0	0	0
			2287	1437	409	438	3			
1	C	287	Total	C	N	O	S	0	0	0
			2287	1437	409	438	3			
1	D	287	Total	C	N	O	S	0	0	0
			2284	1436	408	437	3			
1	E	286	Total	C	N	O	S	0	0	0
			2279	1433	407	436	3			
1	F	287	Total	C	N	O	S	0	0	0
			2288	1439	409	437	3			
1	G	287	Total	C	N	O	S	0	0	0
			2284	1436	408	437	3			
1	H	287	Total	C	N	O	S	0	0	0
			2284	1436	408	437	3			

- Molecule 2 is URIC ACID (three-letter code: URC) (formula: C<sub>5</sub>H<sub>4</sub>N<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	5	4	3		
2	B	1	Total	C	N	O	0	0
			12	5	4	3		
2	C	1	Total	C	N	O	0	0
			12	5	4	3		
2	D	1	Total	C	N	O	0	0
			12	5	4	3		
2	E	1	Total	C	N	O	0	0
			12	5	4	3		
2	F	1	Total	C	N	O	0	0
			12	5	4	3		
2	G	1	Total	C	N	O	0	0
			12	5	4	3		
2	H	1	Total	C	N	O	0	0
			12	5	4	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	204	Total	O	0	0
			204	204		
3	B	166	Total	O	0	0
			166	166		
3	C	160	Total	O	0	0
			160	160		
3	D	160	Total	O	0	0
			160	160		

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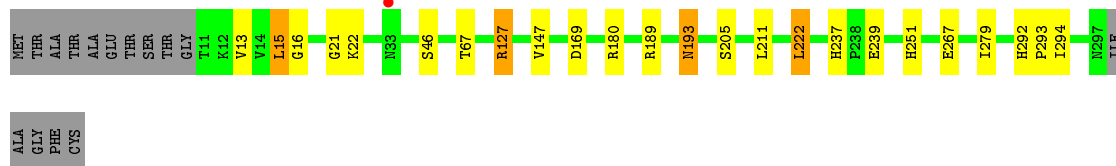
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	138	Total 138	O 138	0	0
3	F	182	Total 182	O 182	0	0
3	G	178	Total 178	O 178	0	0
3	H	173	Total 173	O 173	0	0

### 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.

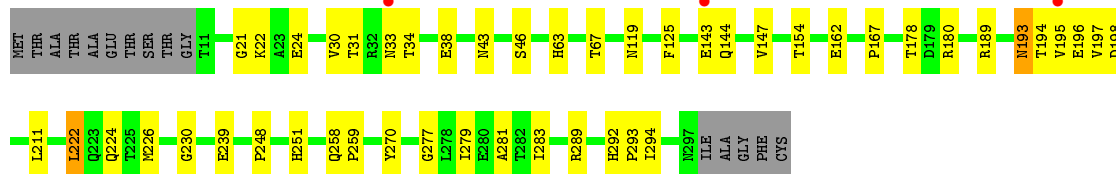
#### • Molecule 1: Uricase

Chain A: 




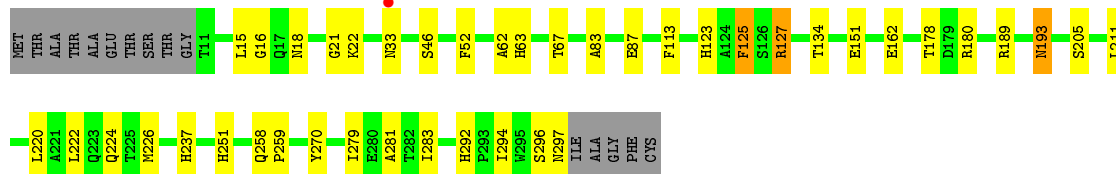
#### • Molecule 1: Uricase

Chain B: 




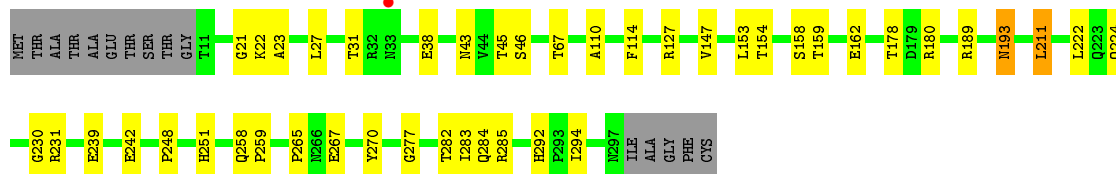
#### • Molecule 1: Uricase

Chain C: 

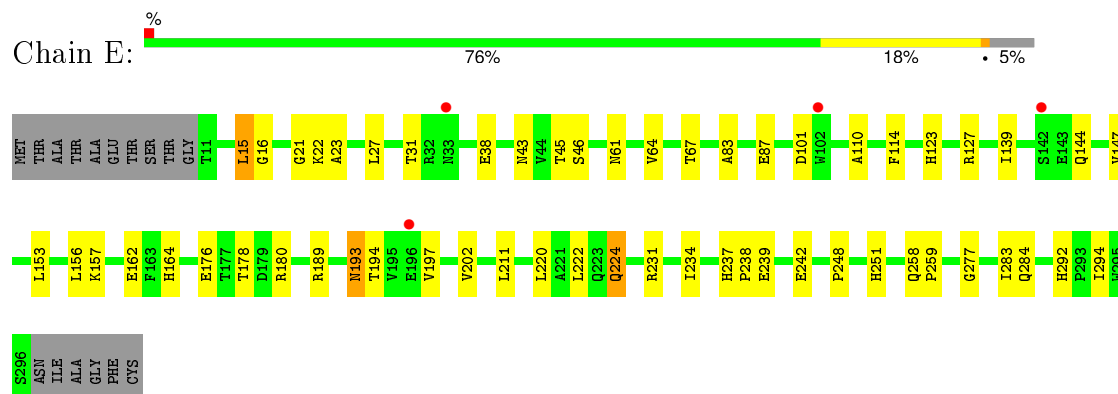


#### • Molecule 1: Uricase

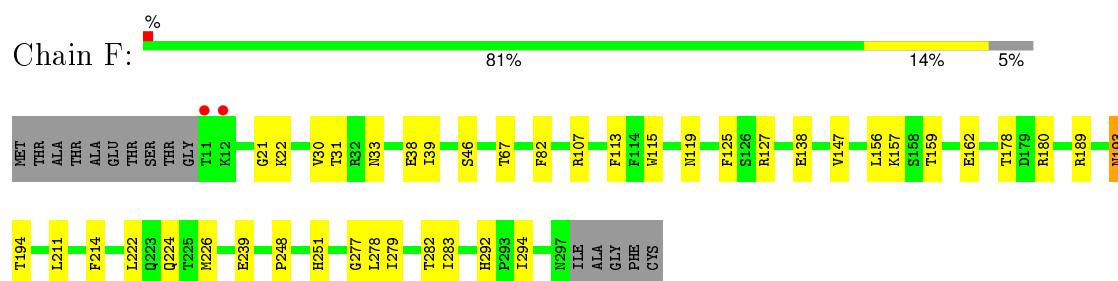
Chain D: 



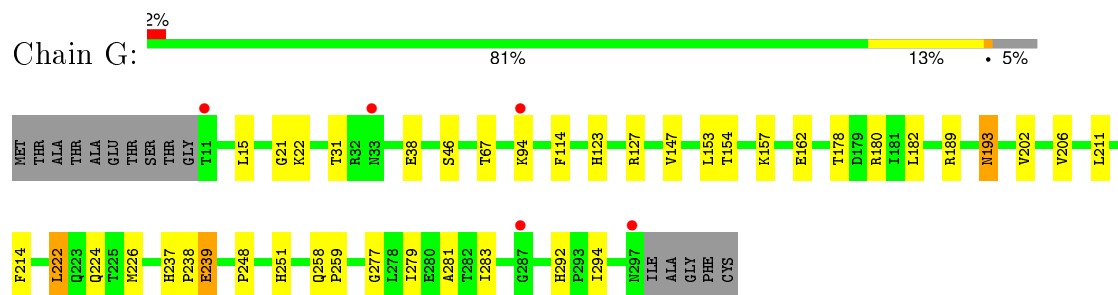
- Molecule 1: Uricase



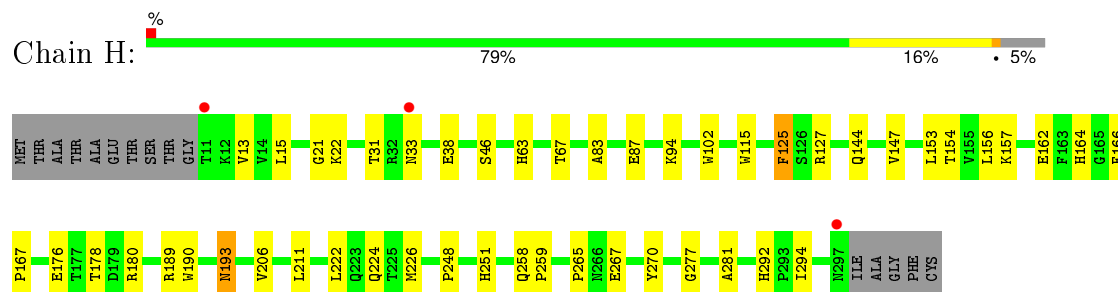
- Molecule 1: Uricase



- Molecule 1: Uricase



- Molecule 1: Uricase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.48Å 123.24Å 284.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 47.42 – 1.90	Depositor EDS
% Data completeness (in resolution range)	79.0 (20.00-1.90) 90.7 (47.42-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.07 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.190 , 0.223 0.204 , 0.234	Depositor DCC
$R_{free}$ test set	21132 reflections (9.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtriage
Anisotropy	1.123	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 213158 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19734	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.34	0/2336	0.62	0/3171
1	B	0.33	0/2339	0.60	0/3175
1	C	0.32	0/2339	0.60	0/3175
1	D	0.33	0/2336	0.62	0/3171
1	E	0.32	0/2331	0.59	0/3164
1	F	0.33	0/2340	0.62	0/3175
1	G	0.33	0/2336	0.61	0/3171
1	H	0.33	0/2336	0.62	0/3171
All	All	0.33	0/18693	0.61	0/25373

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2284	0	2179	28	0
1	B	2287	0	2183	35	0
1	C	2287	0	2183	41	0
1	D	2284	0	2179	41	0
1	E	2279	0	2177	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2288	0	2190	38	0
1	G	2284	0	2179	41	0
1	H	2284	0	2179	43	0
2	A	12	0	4	3	0
2	B	12	0	4	3	0
2	C	12	0	4	3	0
2	D	12	0	4	3	0
2	E	12	0	4	4	0
2	F	12	0	4	3	0
2	G	12	0	4	2	0
2	H	12	0	4	3	0
3	A	204	0	0	0	0
3	B	166	0	0	1	0
3	C	160	0	0	1	0
3	D	160	0	0	0	0
3	E	138	0	0	0	0
3	F	182	0	0	0	0
3	G	178	0	0	2	0
3	H	173	0	0	1	0
All	All	19734	0	17481	267	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (267) 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:B:67:THR:H	2:B:2303:URC:HN7	1.02	1.01
1:A:67:THR:H	2:A:2304:URC:HN7	0.99	0.99
1:G:67:THR:H	2:G:2306:URC:HN7	1.02	0.98
1:C:67:THR:H	2:C:2302:URC:HN7	0.95	0.95
1:D:67:THR:H	2:D:2301:URC:HN7	0.98	0.94
1:H:67:THR:H	2:H:2305:URC:HN7	0.95	0.91
1:E:67:THR:H	2:E:2308:URC:HN7	0.92	0.89
1:F:67:THR:H	2:F:2307:URC:HN7	0.92	0.88
1:A:292:HIS:HD2	1:A:294:ILE:H	1.25	0.84
1:E:231:ARG:HG3	1:H:13:VAL:HG21	1.60	0.83
1:C:292:HIS:HD2	1:C:294:ILE:H	1.24	0.81
1:E:67:THR:N	2:E:2308:URC:HN7	1.77	0.81
1:C:15:LEU:HD11	1:C:18:ASN:ND2	1.96	0.81
1:B:33:ASN:OD1	1:B:34:THR:HG23	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:THR:N	2:C:2302:URC:HN7	1.79	0.79
1:H:153:LEU:HD21	1:H:211:LEU:HD11	1.64	0.79
1:F:113:PHE:HB3	1:F:127:ARG:NH1	1.98	0.78
1:H:292:HIS:HD2	1:H:294:ILE:H	1.34	0.75
1:C:113:PHE:HB3	1:C:127:ARG:HE	1.50	0.75
2:E:2308:URC:HN3	1:H:180:ARG:HH12	1.33	0.74
1:F:67:THR:N	2:F:2307:URC:HN7	1.77	0.73
1:F:292:HIS:HD2	1:F:294:ILE:H	1.37	0.73
1:H:67:THR:N	2:H:2305:URC:HN7	1.80	0.72
1:G:153:LEU:HD21	1:G:211:LEU:HD11	1.71	0.72
1:D:67:THR:N	2:D:2301:URC:HN7	1.81	0.72
1:E:147:VAL:HG23	1:E:294:ILE:HD13	1.73	0.70
1:B:180:ARG:HH12	2:C:2302:URC:HN3	1.39	0.70
1:E:292:HIS:HD2	1:E:294:ILE:H	1.36	0.69
1:E:193:ASN:ND2	1:E:194:THR:HG22	2.08	0.68
1:G:292:HIS:HD2	1:G:294:ILE:H	1.40	0.68
1:E:193:ASN:HD22	1:E:194:THR:HG22	1.59	0.68
1:G:189:ARG:HH11	1:G:189:ARG:HG3	1.58	0.67
1:B:289:ARG:NH2	1:B:293:PRO:HD3	2.12	0.65
1:F:180:ARG:HH12	2:G:2306:URC:HN3	1.44	0.65
1:H:147:VAL:HG23	1:H:294:ILE:HD13	1.79	0.64
1:B:21:GLY:HA3	1:B:46:SER:O	1.96	0.64
1:E:180:ARG:HH12	2:H:2305:URC:HN3	1.44	0.64
1:D:31:THR:HB	1:D:38:GLU:HB2	1.80	0.63
1:A:180:ARG:HH12	2:D:2301:URC:HN3	1.47	0.63
1:E:234:ILE:HD12	1:E:283:ILE:HG22	1.81	0.63
1:E:83:ALA:HB3	1:E:87:GLU:OE2	1.99	0.62
1:H:21:GLY:HA3	1:H:46:SER:O	1.98	0.62
1:E:22:LYS:NZ	1:H:251:HIS:CE1	2.68	0.62
1:H:83:ALA:HB3	1:H:87:GLU:OE2	1.99	0.61
2:F:2307:URC:HN3	1:G:180:ARG:HH12	1.48	0.61
1:B:22:LYS:NZ	1:C:251:HIS:HE1	1.99	0.61
1:G:31:THR:HB	1:G:38:GLU:HB2	1.82	0.60
1:E:162:GLU:HG2	1:E:178:THR:O	2.01	0.60
2:B:2303:URC:HN3	1:C:180:ARG:HH12	1.48	0.60
1:E:251:HIS:CE1	1:H:22:LYS:NZ	2.69	0.60
1:D:189:ARG:HH11	1:D:189:ARG:HG3	1.67	0.60
1:E:189:ARG:HG3	1:E:189:ARG:HH11	1.66	0.60
1:H:94:LYS:HE2	1:H:144:GLN:HE22	1.68	0.59
1:E:156:LEU:HD23	1:E:156:LEU:C	2.23	0.59
1:D:242:GLU:HB3	1:D:284:GLN:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:THR:N	2:B:2303:URC:HN7	1.87	0.59
1:A:21:GLY:HA3	1:A:46:SER:O	2.03	0.59
1:D:114:PHE:O	1:D:127:ARG:HD2	2.03	0.59
1:H:189:ARG:HH11	1:H:189:ARG:HG3	1.67	0.59
1:F:21:GLY:HA3	1:F:46:SER:O	2.03	0.58
1:H:31:THR:HB	1:H:38:GLU:HB2	1.85	0.58
1:E:220:LEU:H	1:E:224:GLN:NE2	2.01	0.58
1:A:251:HIS:HE1	1:D:22:LYS:NZ	2.00	0.58
1:G:94:LYS:HG3	3:G:2476:HOH:O	2.04	0.57
1:G:226:MET:HE3	1:G:281:ALA:HB3	1.84	0.57
1:F:22:LYS:NZ	1:G:251:HIS:CE1	2.72	0.57
1:G:283:ILE:N	1:G:283:ILE:HD12	2.19	0.57
1:A:189:ARG:HH11	1:A:189:ARG:HG3	1.70	0.57
1:C:292:HIS:CD2	1:C:294:ILE:H	2.15	0.56
1:F:189:ARG:HH11	1:F:189:ARG:HG3	1.70	0.56
1:G:21:GLY:HA3	1:G:46:SER:O	2.04	0.56
1:D:21:GLY:HA3	1:D:46:SER:O	2.06	0.56
1:B:193:ASN:HD21	1:B:239:GLU:HA	1.71	0.56
1:D:153:LEU:HD21	1:D:211:LEU:HD11	1.87	0.56
1:A:67:THR:N	2:A:2304:URC:HN7	1.85	0.56
1:F:31:THR:HB	1:F:38:GLU:HB2	1.87	0.56
1:C:15:LEU:HD11	1:C:18:ASN:HD22	1.70	0.56
2:A:2304:URC:HN3	1:D:180:ARG:HH12	1.54	0.55
1:E:283:ILE:N	1:E:283:ILE:HD12	2.21	0.55
1:E:251:HIS:CE1	1:H:22:LYS:HZ3	2.24	0.55
1:F:292:HIS:CD2	1:F:294:ILE:H	2.22	0.55
1:E:27:LEU:C	1:E:27:LEU:HD13	2.27	0.55
1:B:189:ARG:HG3	1:B:189:ARG:HH11	1.73	0.54
1:E:193:ASN:HD22	1:E:193:ASN:C	2.10	0.54
1:D:147:VAL:HG23	1:D:294:ILE:HD13	1.90	0.54
1:C:189:ARG:HH11	1:C:189:ARG:HG3	1.71	0.54
1:F:251:HIS:CE1	1:G:22:LYS:NZ	2.75	0.54
1:B:289:ARG:HH21	1:B:292:HIS:HA	1.72	0.54
1:B:22:LYS:NZ	1:C:251:HIS:CE1	2.76	0.54
1:D:193:ASN:HD22	1:D:193:ASN:C	2.11	0.53
1:F:283:ILE:HD12	1:F:283:ILE:N	2.23	0.53
1:E:22:LYS:HZ2	1:H:251:HIS:CE1	2.26	0.53
1:E:31:THR:HB	1:E:38:GLU:HB2	1.89	0.53
1:F:193:ASN:HD22	1:F:193:ASN:C	2.11	0.53
1:D:127:ARG:HH11	1:D:127:ARG:HG2	1.73	0.52
1:G:154:THR:HB	1:H:127:ARG:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:251:HIS:HE1	1:G:22:LYS:NZ	2.08	0.52
1:D:265:PRO:HG2	1:D:267:GLU:HG3	1.92	0.52
1:F:22:LYS:HZ2	1:G:251:HIS:CE1	2.27	0.52
1:G:153:LEU:CD2	1:G:211:LEU:HD11	2.39	0.51
1:H:162:GLU:HG2	1:H:178:THR:HA	1.92	0.51
1:B:147:VAL:HG23	1:B:294:ILE:HD13	1.92	0.51
1:D:282:THR:HG22	1:D:284:GLN:HG3	1.93	0.51
1:G:202:VAL:O	1:G:206:VAL:HG23	2.11	0.51
1:H:226:MET:HE3	1:H:281:ALA:HB3	1.92	0.51
1:C:52:PHE:HA	3:C:2341:HOH:O	2.11	0.51
1:G:189:ARG:NH1	1:G:189:ARG:HG3	2.26	0.50
1:E:21:GLY:HA3	1:E:46:SER:O	2.11	0.50
1:A:13:VAL:HG21	1:D:231:ARG:HG3	1.92	0.50
1:D:162:GLU:HG2	1:D:178:THR:O	2.11	0.50
1:A:22:LYS:NZ	1:D:251:HIS:CE1	2.79	0.50
1:A:22:LYS:NZ	1:D:251:HIS:HE1	2.08	0.50
1:A:147:VAL:HG23	1:A:294:ILE:HD13	1.94	0.50
1:G:226:MET:CE	1:G:279:ILE:HG22	2.42	0.50
1:E:251:HIS:HE1	1:H:22:LYS:HZ3	1.57	0.50
1:C:189:ARG:NH1	1:C:189:ARG:HG3	2.26	0.50
1:B:226:MET:HE3	1:B:281:ALA:HB3	1.93	0.50
1:E:164:HIS:HB3	1:E:176:GLU:HB3	1.94	0.50
1:A:193:ASN:C	1:A:193:ASN:HD22	2.16	0.49
1:G:94:LYS:HE3	3:G:2476:HOH:O	2.12	0.49
1:G:114:PHE:O	1:G:127:ARG:HD2	2.13	0.49
1:G:193:ASN:C	1:G:193:ASN:HD22	2.14	0.49
1:B:251:HIS:CE1	1:C:22:LYS:NZ	2.81	0.49
1:C:283:ILE:N	1:C:283:ILE:HD12	2.28	0.49
1:B:143:GLU:HG2	1:B:144:GLN:N	2.27	0.49
1:D:258:GLN:HA	1:D:258:GLN:HE21	1.77	0.49
1:A:251:HIS:CE1	1:D:22:LYS:NZ	2.81	0.48
1:G:147:VAL:HG23	1:G:294:ILE:HD13	1.95	0.48
1:C:193:ASN:HD22	1:C:193:ASN:C	2.16	0.48
1:E:251:HIS:HE1	1:H:22:LYS:NZ	2.08	0.48
1:E:242:GLU:HB3	1:E:284:GLN:HB3	1.95	0.48
1:B:193:ASN:HD22	1:B:193:ASN:C	2.17	0.48
1:C:83:ALA:N	1:C:87:GLU:OE2	2.41	0.48
1:E:153:LEU:HD21	1:E:211:LEU:HD21	1.95	0.48
1:G:193:ASN:HD21	1:G:239:GLU:HA	1.78	0.48
1:B:248:PRO:HA	1:B:277:GLY:O	2.13	0.48
1:D:258:GLN:HA	1:D:258:GLN:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:GLN:N	1:C:259:PRO:CD	2.77	0.48
1:A:22:LYS:HZ2	1:D:251:HIS:CE1	2.32	0.48
1:E:156:LEU:HD23	1:E:157:LYS:N	2.29	0.48
1:G:157:LYS:HG3	1:G:214:PHE:CE2	2.49	0.48
1:E:22:LYS:NZ	1:H:251:HIS:HE1	2.10	0.47
1:G:127:ARG:HB3	1:H:154:THR:HB	1.96	0.47
1:B:222:LEU:HD13	1:B:279:ILE:HB	1.96	0.47
1:F:248:PRO:HA	1:F:277:GLY:O	2.14	0.47
1:E:15:LEU:HD22	1:E:16:GLY:O	2.14	0.47
1:A:205:SER:OG	1:A:237:HIS:HE1	1.97	0.47
1:E:239:GLU:H	1:E:239:GLU:CD	2.18	0.47
1:A:239:GLU:CD	1:A:239:GLU:H	2.18	0.47
1:B:22:LYS:HZ3	1:C:251:HIS:HE1	1.62	0.47
1:E:123:HIS:CG	1:F:159:THR:HG22	2.49	0.47
1:C:15:LEU:HD13	1:C:16:GLY:O	2.15	0.47
1:F:115:TRP:CH2	1:F:127:ARG:HG2	2.49	0.47
1:F:22:LYS:NZ	1:G:251:HIS:HE1	2.10	0.47
1:C:123:HIS:HB2	1:D:158:SER:OG	2.15	0.47
1:C:205:SER:OG	1:C:237:HIS:CE1	2.67	0.47
1:F:282:THR:C	1:F:283:ILE:HD12	2.35	0.47
1:C:21:GLY:HA3	1:C:46:SER:O	2.14	0.47
1:C:226:MET:HE3	1:C:281:ALA:HB3	1.96	0.47
1:A:267:GLU:HG2	1:B:30:VAL:O	2.14	0.47
1:E:139:ILE:HG12	1:E:144:GLN:HB3	1.96	0.46
1:F:156:LEU:HD23	1:F:156:LEU:C	2.35	0.46
1:C:151:GLU:OE2	1:C:189:ARG:NH2	2.49	0.46
1:B:24:GLU:HA	1:B:43:ASN:ND2	2.31	0.46
1:H:193:ASN:C	1:H:193:ASN:HD22	2.18	0.46
1:D:292:HIS:HD2	1:D:294:ILE:HG22	1.79	0.46
1:G:292:HIS:CD2	1:G:294:ILE:H	2.27	0.46
1:D:22:LYS:HE2	1:D:67:THR:O	2.15	0.46
1:A:205:SER:OG	1:A:237:HIS:CE1	2.68	0.46
1:D:193:ASN:HD21	1:D:239:GLU:HA	1.80	0.46
1:B:31:THR:HB	1:B:38:GLU:HB2	1.98	0.45
1:C:127:ARG:HG3	1:C:127:ARG:NH2	2.31	0.45
1:D:189:ARG:HG3	1:D:189:ARG:NH1	2.28	0.45
1:F:193:ASN:ND2	1:F:194:THR:HG22	2.32	0.45
1:H:156:LEU:C	1:H:156:LEU:HD23	2.37	0.45
1:F:162:GLU:HG2	1:F:178:THR:HA	1.98	0.45
1:C:127:ARG:HB2	1:D:154:THR:HB	1.98	0.45
1:E:22:LYS:HZ3	1:H:251:HIS:CE1	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:HIS:HB3	1:G:239:GLU:OE2	2.17	0.45
1:A:251:HIS:HE1	1:D:22:LYS:HZ2	1.65	0.45
1:D:127:ARG:NH1	1:D:127:ARG:HG2	2.32	0.44
1:B:144:GLN:NE2	1:B:195:VAL:HG11	2.32	0.44
1:H:125:PHE:N	1:H:125:PHE:CD1	2.85	0.44
1:E:61:ASN:O	1:H:166:PHE:HA	2.17	0.44
1:A:189:ARG:HG3	1:A:189:ARG:NH1	2.31	0.44
1:E:197:VAL:CG1	1:E:202:VAL:HG21	2.47	0.44
1:B:22:LYS:HZ2	1:C:251:HIS:CE1	2.36	0.44
1:H:87:GLU:HB2	3:H:2308:HOH:O	2.17	0.44
1:G:279:ILE:N	1:G:279:ILE:HD12	2.32	0.44
1:C:134:THR:HG21	1:C:189:ARG:NH2	2.32	0.44
1:H:258:GLN:N	1:H:259:PRO:CD	2.80	0.44
1:F:193:ASN:HD21	1:F:239:GLU:HA	1.83	0.44
1:C:125:PHE:CD1	1:C:125:PHE:N	2.86	0.44
1:A:222:LEU:HD13	1:A:279:ILE:HB	1.99	0.44
1:D:43:ASN:O	1:D:110:ALA:HA	2.18	0.44
1:C:205:SER:OG	1:C:237:HIS:HE1	2.01	0.44
1:C:258:GLN:NE2	1:C:258:GLN:HA	2.33	0.43
1:F:226:MET:CE	1:F:279:ILE:HG22	2.48	0.43
1:F:147:VAL:HG23	1:F:294:ILE:HD13	1.99	0.43
1:B:22:LYS:HE2	1:B:67:THR:O	2.18	0.43
1:F:157:LYS:HG3	1:F:214:PHE:CE2	2.54	0.43
1:G:123:HIS:O	1:H:157:LYS:HA	2.18	0.43
1:B:167:PRO:HD3	1:C:62:ALA:O	2.18	0.43
1:F:22:LYS:HZ2	1:G:251:HIS:HE1	1.65	0.43
1:E:43:ASN:O	1:E:110:ALA:HA	2.19	0.43
1:B:258:GLN:N	1:B:259:PRO:CD	2.81	0.43
1:F:125:PHE:CD1	1:F:125:PHE:N	2.87	0.43
1:H:63:HIS:HB3	1:H:102:TRP:CD1	2.53	0.43
1:H:265:PRO:HG2	1:H:267:GLU:HG3	2.01	0.43
1:E:258:GLN:N	1:E:259:PRO:CD	2.82	0.43
1:C:127:ARG:HH21	1:C:127:ARG:HG3	1.84	0.42
1:H:189:ARG:HH11	1:H:189:ARG:CG	2.32	0.42
1:A:22:LYS:HZ2	1:D:251:HIS:HE1	1.66	0.42
1:B:251:HIS:HD2	3:B:2399:HOH:O	2.01	0.42
1:A:251:HIS:HE1	1:D:22:LYS:HZ3	1.66	0.42
1:G:258:GLN:N	1:G:259:PRO:CD	2.81	0.42
1:E:64:VAL:O	1:H:167:PRO:HD2	2.18	0.42
1:E:292:HIS:CD2	1:E:294:ILE:H	2.26	0.42
1:G:162:GLU:HG2	1:G:178:THR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:GLU:HG2	1:B:178:THR:HA	2.02	0.42
1:G:226:MET:HE2	1:G:279:ILE:HG22	2.01	0.42
1:C:279:ILE:HD12	1:C:279:ILE:N	2.34	0.42
1:F:278:LEU:C	1:F:279:ILE:HD12	2.40	0.42
1:F:189:ARG:HG3	1:F:189:ARG:NH1	2.33	0.42
1:E:251:HIS:CE1	1:H:22:LYS:HZ2	2.37	0.42
1:C:226:MET:CE	1:C:279:ILE:HG22	2.49	0.42
1:B:22:LYS:HZ2	1:C:251:HIS:HE1	1.67	0.41
1:H:190:TRP:CZ3	1:H:206:VAL:HG11	2.55	0.41
1:A:292:HIS:CD2	1:A:293:PRO:HD2	2.55	0.41
1:B:193:ASN:HD22	1:B:194:THR:HG22	1.86	0.41
1:F:251:HIS:CE1	1:G:22:LYS:HZ2	2.37	0.41
1:B:125:PHE:N	1:B:125:PHE:CD1	2.87	0.41
1:G:248:PRO:HA	1:G:277:GLY:O	2.20	0.41
1:A:127:ARG:HB2	1:B:154:THR:HB	2.02	0.41
1:A:15:LEU:HD22	1:A:16:GLY:O	2.20	0.41
1:C:220:LEU:H	1:C:224:GLN:NE2	2.18	0.41
1:H:248:PRO:HA	1:H:277:GLY:O	2.20	0.41
1:F:251:HIS:CE1	1:G:22:LYS:HZ3	2.38	0.41
1:D:248:PRO:HA	1:D:277:GLY:O	2.20	0.41
1:F:251:HIS:HE1	1:G:22:LYS:HZ3	1.68	0.41
1:G:237:HIS:HA	1:G:238:PRO:HD3	1.84	0.41
1:E:237:HIS:HA	1:E:238:PRO:HD3	1.93	0.41
1:C:296:SER:O	1:C:297:ASN:HB3	2.21	0.41
1:H:292:HIS:CD2	1:H:294:ILE:H	2.23	0.41
1:H:164:HIS:HB3	1:H:176:GLU:HB3	2.01	0.41
1:H:115:TRP:CH2	1:H:127:ARG:HG2	2.55	0.41
1:D:23:ALA:HA	1:D:45:THR:HG23	2.02	0.41
1:F:30:VAL:HG22	1:F:39:ILE:CD1	2.51	0.41
1:A:292:HIS:HA	1:A:293:PRO:HD3	1.91	0.41
1:D:258:GLN:N	1:D:259:PRO:CD	2.84	0.41
1:B:197:VAL:HG12	1:B:198:ASP:N	2.36	0.41
1:F:82:PHE:N	1:F:82:PHE:CD1	2.88	0.40
1:C:123:HIS:CG	1:D:159:THR:HG22	2.57	0.40
1:E:23:ALA:HA	1:E:45:THR:HG23	2.01	0.40
1:D:285:ARG:HG3	1:D:285:ARG:HH11	1.86	0.40
1:F:107:ARG:HG3	1:F:138:GLU:HG2	2.02	0.40
1:C:162:GLU:HG2	1:C:178:THR:O	2.22	0.40
1:A:251:HIS:CE1	1:D:22:LYS:HZ2	2.40	0.40
2:E:2308:URC:HN3	1:H:180:ARG:NH1	2.10	0.40
1:H:153:LEU:CD2	1:H:211:LEU:HD11	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:ILE:HD11	1:E:283:ILE:O	2.21	0.40
1:F:279:ILE:N	1:F:279:ILE:HD12	2.36	0.40
1:E:248:PRO:HA	1:E:277:GLY:O	2.21	0.40
1:B:230:GLY:HA3	1:B:283:ILE:HG13	2.03	0.40
1:G:182:LEU:HD11	1:G:222:LEU:HG	2.04	0.40
1:E:114:PHE:O	1:E:127:ARG:HD2	2.22	0.40
1:D:230:GLY:HA3	1:D:283:ILE:HG13	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/302 (94%)	279 (98%)	6 (2%)	0	100	100
1	B	285/302 (94%)	279 (98%)	6 (2%)	0	100	100
1	C	285/302 (94%)	279 (98%)	6 (2%)	0	100	100
1	D	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
1	E	284/302 (94%)	280 (99%)	4 (1%)	0	100	100
1	F	285/302 (94%)	279 (98%)	6 (2%)	0	100	100
1	G	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
1	H	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
All	All	2279/2416 (94%)	2234 (98%)	45 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/250 (95%)	231 (98%)	6 (2%)	55	47
1	B	238/250 (95%)	230 (97%)	8 (3%)	44	33
1	C	238/250 (95%)	230 (97%)	8 (3%)	44	33
1	D	237/250 (95%)	231 (98%)	6 (2%)	55	47
1	E	237/250 (95%)	232 (98%)	5 (2%)	61	55
1	F	238/250 (95%)	232 (98%)	6 (2%)	55	47
1	G	237/250 (95%)	232 (98%)	5 (2%)	61	55
1	H	237/250 (95%)	230 (97%)	7 (3%)	48	38
All	All	1899/2000 (95%)	1848 (97%)	51 (3%)	52	43

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	127	ARG
1	A	169	ASP
1	A	193	ASN
1	A	211	LEU
1	A	222	LEU
1	B	63	HIS
1	B	119	ASN
1	B	193	ASN
1	B	196	GLU
1	B	211	LEU
1	B	222	LEU
1	B	224	GLN
1	B	270	TYR
1	C	33	ASN
1	C	63	HIS
1	C	125	PHE
1	C	127	ARG
1	C	193	ASN
1	C	211	LEU
1	C	222	LEU
1	C	270	TYR
1	D	27	LEU

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Mol	Chain	Res	Type
1	D	193	ASN
1	D	211	LEU
1	D	222	LEU
1	D	224	GLN
1	D	270	TYR
1	E	15	LEU
1	E	101	ASP
1	E	193	ASN
1	E	222	LEU
1	E	224	GLN
1	F	33	ASN
1	F	119	ASN
1	F	193	ASN
1	F	211	LEU
1	F	222	LEU
1	F	224	GLN
1	G	15	LEU
1	G	193	ASN
1	G	222	LEU
1	G	224	GLN
1	G	239	GLU
1	H	15	LEU
1	H	33	ASN
1	H	125	PHE
1	H	193	ASN
1	H	222	LEU
1	H	224	GLN
1	H	270	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	43	ASN
1	A	47	GLN
1	A	111	GLN
1	A	193	ASN
1	A	237	HIS
1	A	251	HIS
1	A	258	GLN
1	A	262	GLN
1	A	292	HIS

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Mol	Chain	Res	Type
1	B	43	ASN
1	B	111	GLN
1	B	144	GLN
1	B	193	ASN
1	B	237	HIS
1	B	251	HIS
1	B	258	GLN
1	B	262	GLN
1	B	292	HIS
1	C	43	ASN
1	C	47	GLN
1	C	63	HIS
1	C	111	GLN
1	C	193	ASN
1	C	224	GLN
1	C	237	HIS
1	C	251	HIS
1	C	258	GLN
1	C	284	GLN
1	C	292	HIS
1	D	43	ASN
1	D	47	GLN
1	D	63	HIS
1	D	111	GLN
1	D	144	GLN
1	D	193	ASN
1	D	237	HIS
1	D	251	HIS
1	D	258	GLN
1	D	262	GLN
1	D	284	GLN
1	D	292	HIS
1	E	33	ASN
1	E	40	GLN
1	E	43	ASN
1	E	47	GLN
1	E	111	GLN
1	E	119	ASN
1	E	193	ASN
1	E	224	GLN
1	E	237	HIS
1	E	251	HIS

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Mol	Chain	Res	Type
1	E	258	GLN
1	E	292	HIS
1	F	43	ASN
1	F	63	HIS
1	F	111	GLN
1	F	193	ASN
1	F	237	HIS
1	F	251	HIS
1	F	262	GLN
1	F	292	HIS
1	G	33	ASN
1	G	43	ASN
1	G	111	GLN
1	G	193	ASN
1	G	237	HIS
1	G	251	HIS
1	G	258	GLN
1	G	262	GLN
1	G	292	HIS
1	H	43	ASN
1	H	47	GLN
1	H	111	GLN
1	H	144	GLN
1	H	193	ASN
1	H	237	HIS
1	H	251	HIS
1	H	262	GLN
1	H	292	HIS

### 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

8 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	URC	A	2304	-	12,13,13	4.59	4 (33%)	10,19,19	7.55	7 (70%)
2	URC	B	2303	-	12,13,13	4.37	4 (33%)	10,19,19	7.39	7 (70%)
2	URC	C	2302	-	12,13,13	4.47	4 (33%)	10,19,19	7.47	7 (70%)
2	URC	D	2301	-	12,13,13	4.43	4 (33%)	10,19,19	7.46	7 (70%)
2	URC	E	2308	-	12,13,13	4.53	4 (33%)	10,19,19	7.51	7 (70%)
2	URC	F	2307	-	12,13,13	4.60	4 (33%)	10,19,19	7.52	7 (70%)
2	URC	G	2306	-	12,13,13	4.48	4 (33%)	10,19,19	7.53	7 (70%)
2	URC	H	2305	-	12,13,13	4.48	4 (33%)	10,19,19	7.49	7 (70%)

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	URC	A	2304	-	-	0/0/24/24	0/2/2/2
2	URC	B	2303	-	-	0/0/24/24	0/2/2/2
2	URC	C	2302	-	-	0/0/24/24	0/2/2/2
2	URC	D	2301	-	-	0/0/24/24	0/2/2/2
2	URC	E	2308	-	-	0/0/24/24	0/2/2/2
2	URC	F	2307	-	-	0/0/24/24	0/2/2/2
2	URC	G	2306	-	-	0/0/24/24	0/2/2/2
2	URC	H	2305	-	-	0/0/24/24	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2307	URC	C4-N3	-10.43	1.33	1.46
2	A	2304	URC	C4-N3	-10.37	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2306	URC	C4-N3	-10.35	1.34	1.46
2	E	2308	URC	C4-N3	-10.10	1.34	1.46
2	C	2302	URC	C4-N3	-10.01	1.34	1.46
2	H	2305	URC	C4-N3	-9.93	1.34	1.46
2	D	2301	URC	C4-N3	-9.91	1.34	1.46
2	F	2307	URC	C4-N9	-9.83	1.33	1.44
2	E	2308	URC	C4-N9	-9.70	1.33	1.44
2	H	2305	URC	C4-N9	-9.62	1.33	1.44
2	B	2303	URC	C4-N3	-9.61	1.34	1.46
2	A	2304	URC	C4-N9	-9.55	1.33	1.44
2	C	2302	URC	C4-N9	-9.50	1.33	1.44
2	B	2303	URC	C4-N9	-9.45	1.33	1.44
2	G	2306	URC	C4-N9	-9.42	1.33	1.44
2	D	2301	URC	C4-N9	-9.32	1.33	1.44
2	A	2304	URC	C5-N7	-5.85	1.32	1.45
2	D	2301	URC	C5-N7	-5.85	1.32	1.45
2	E	2308	URC	C5-N7	-5.77	1.33	1.45
2	H	2305	URC	C5-N7	-5.76	1.33	1.45
2	C	2302	URC	C5-N7	-5.72	1.33	1.45
2	F	2307	URC	C5-N7	-5.66	1.33	1.45
2	B	2303	URC	C5-N7	-5.60	1.33	1.45
2	G	2306	URC	C5-N7	-5.51	1.33	1.45
2	D	2301	URC	C5-C6	-2.83	1.48	1.53
2	F	2307	URC	C5-C6	-2.77	1.48	1.53
2	B	2303	URC	C5-C6	-2.75	1.48	1.53
2	C	2302	URC	C5-C6	-2.65	1.48	1.53
2	A	2304	URC	C5-C6	-2.64	1.48	1.53
2	E	2308	URC	C5-C6	-2.60	1.48	1.53
2	H	2305	URC	C5-C6	-2.50	1.48	1.53
2	G	2306	URC	C5-C6	-2.39	1.48	1.53

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2306	URC	O24-C8-N9	-3.07	122.34	125.90
2	A	2304	URC	O24-C8-N9	-3.05	122.36	125.90
2	D	2301	URC	O24-C8-N7	-3.02	122.40	125.90
2	F	2307	URC	O24-C8-N7	-3.00	122.42	125.90
2	A	2304	URC	O24-C8-N7	-2.99	122.43	125.90
2	B	2303	URC	O24-C8-N7	-2.97	122.45	125.90
2	E	2308	URC	O24-C8-N9	-2.97	122.45	125.90
2	H	2305	URC	O24-C8-N9	-2.97	122.46	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2307	URC	O24-C8-N9	-2.96	122.47	125.90
2	E	2308	URC	O24-C8-N7	-2.91	122.52	125.90
2	H	2305	URC	O24-C8-N7	-2.91	122.53	125.90
2	C	2302	URC	O24-C8-N9	-2.88	122.56	125.90
2	C	2302	URC	O24-C8-N7	-2.87	122.57	125.90
2	G	2306	URC	O24-C8-N7	-2.85	122.60	125.90
2	B	2303	URC	O24-C8-N9	-2.85	122.60	125.90
2	D	2301	URC	O24-C8-N9	-2.78	122.68	125.90
2	B	2303	URC	N1-C2-N3	2.10	118.44	116.14
2	D	2301	URC	N1-C2-N3	2.23	118.58	116.14
2	F	2307	URC	N1-C2-N3	2.26	118.61	116.14
2	E	2308	URC	N1-C2-N3	2.27	118.63	116.14
2	G	2306	URC	N1-C2-N3	2.30	118.65	116.14
2	C	2302	URC	N1-C2-N3	2.30	118.66	116.14
2	H	2305	URC	N1-C2-N3	2.35	118.71	116.14
2	A	2304	URC	N1-C2-N3	2.37	118.74	116.14
2	D	2301	URC	O13-C6-C5	4.96	127.48	119.47
2	B	2303	URC	O13-C6-C5	5.00	127.55	119.47
2	A	2304	URC	O13-C6-C5	5.06	127.64	119.47
2	E	2308	URC	O13-C6-C5	5.13	127.76	119.47
2	C	2302	URC	O13-C6-C5	5.17	127.82	119.47
2	H	2305	URC	O13-C6-C5	5.18	127.84	119.47
2	G	2306	URC	O13-C6-C5	5.18	127.84	119.47
2	F	2307	URC	O13-C6-C5	5.26	127.97	119.47
2	A	2304	URC	N9-C4-N3	7.34	126.39	112.36
2	F	2307	URC	N9-C4-N3	7.36	126.44	112.36
2	E	2308	URC	N9-C4-N3	7.37	126.45	112.36
2	H	2305	URC	N9-C4-N3	7.40	126.51	112.36
2	C	2302	URC	N9-C4-N3	7.40	126.52	112.36
2	G	2306	URC	N9-C4-N3	7.40	126.52	112.36
2	D	2301	URC	N9-C4-N3	7.46	126.64	112.36
2	B	2303	URC	N9-C4-N3	7.53	126.77	112.36
2	C	2302	URC	N7-C8-N9	8.68	114.88	108.88
2	D	2301	URC	N7-C8-N9	8.75	114.93	108.88
2	B	2303	URC	N7-C8-N9	8.78	114.95	108.88
2	H	2305	URC	N7-C8-N9	8.88	115.01	108.88
2	E	2308	URC	N7-C8-N9	8.90	115.03	108.88
2	G	2306	URC	N7-C8-N9	8.96	115.07	108.88
2	F	2307	URC	N7-C8-N9	9.02	115.11	108.88
2	A	2304	URC	N7-C8-N9	9.16	115.21	108.88
2	B	2303	URC	C5-C4-N9	19.06	111.15	102.69
2	H	2305	URC	C5-C4-N9	19.36	111.28	102.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2301	URC	C5-C4-N9	19.36	111.28	102.69
2	C	2302	URC	C5-C4-N9	19.41	111.31	102.69
2	F	2307	URC	C5-C4-N9	19.41	111.31	102.69
2	E	2308	URC	C5-C4-N9	19.48	111.33	102.69
2	A	2304	URC	C5-C4-N9	19.51	111.35	102.69
2	G	2306	URC	C5-C4-N9	19.51	111.35	102.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2304	URC	3	0
2	B	2303	URC	3	0
2	C	2302	URC	3	0
2	D	2301	URC	3	0
2	E	2308	URC	4	0
2	F	2307	URC	3	0
2	G	2306	URC	2	0
2	H	2305	URC	3	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	287/302 (95%)	-0.17	1 (0%) 94 94	22, 29, 40, 53	0
1	B	287/302 (95%)	-0.16	3 (1%) 84 86	24, 31, 47, 65	0
1	C	287/302 (95%)	-0.13	1 (0%) 94 94	24, 32, 41, 67	0
1	D	287/302 (95%)	-0.14	1 (0%) 94 94	23, 30, 44, 63	0
1	E	286/302 (94%)	-0.06	4 (1%) 78 80	25, 35, 49, 63	0
1	F	287/302 (95%)	-0.19	2 (0%) 89 90	23, 30, 42, 58	0
1	G	287/302 (95%)	-0.10	5 (1%) 73 76	21, 31, 47, 63	0
1	H	287/302 (95%)	-0.15	3 (1%) 84 86	23, 32, 43, 62	0
All	All	2295/2416 (94%)	-0.14	20 (0%) 85 87	21, 31, 46, 67	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	33	ASN	3.4
1	H	11	THR	3.1
1	F	11	THR	2.9
1	H	33	ASN	2.9
1	G	287	GLY	2.7
1	C	33	ASN	2.6
1	G	297	ASN	2.6
1	B	143	GLU	2.6
1	B	33	ASN	2.5
1	G	11	THR	2.5
1	E	196	GLU	2.4
1	G	33	ASN	2.4
1	F	12	LYS	2.4
1	A	33	ASN	2.4
1	E	142	SER	2.3
1	E	33	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	297	ASN	2.1
1	B	195	VAL	2.1
1	G	94	LYS	2.1
1	E	102	TRP	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( $\text{\AA}^2$ )	Q<0.9
2	URC	H	2305	12/12	0.86	0.14	2.81	39,41,44,45	0
2	URC	E	2308	12/12	0.89	0.14	2.71	35,38,45,46	0
2	URC	B	2303	12/12	0.88	0.14	2.58	42,45,48,48	0
2	URC	G	2306	12/12	0.93	0.14	1.92	32,35,41,41	0
2	URC	A	2304	12/12	0.91	0.14	1.80	32,38,42,44	0
2	URC	D	2301	12/12	0.89	0.15	1.69	32,35,41,42	0
2	URC	C	2302	12/12	0.92	0.12	1.08	35,37,43,43	0
2	URC	F	2307	12/12	0.90	0.13	1.04	30,35,42,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.