



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:43 am BST

PDB ID : 1WS3  
Title : Urate oxidase from aspergillus flavus complexed with uracil  
Authors : Retailleau, P.; Colloc'h, N.; Vivares, D.; Bonnete, F.; Castro, B.; El Hajji, M.; Prange, T.  
Deposited on : 2004-10-29  
Resolution : 3.20 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

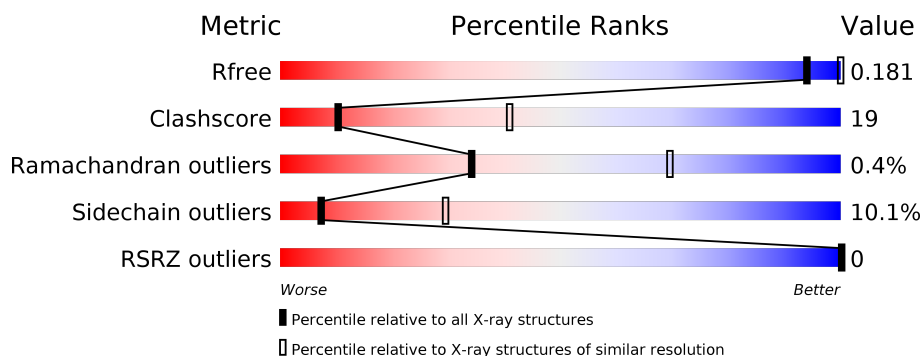
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	301	
1	B	301	
1	C	301	
1	D	301	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	URA	B	1900	-	-	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9507 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.

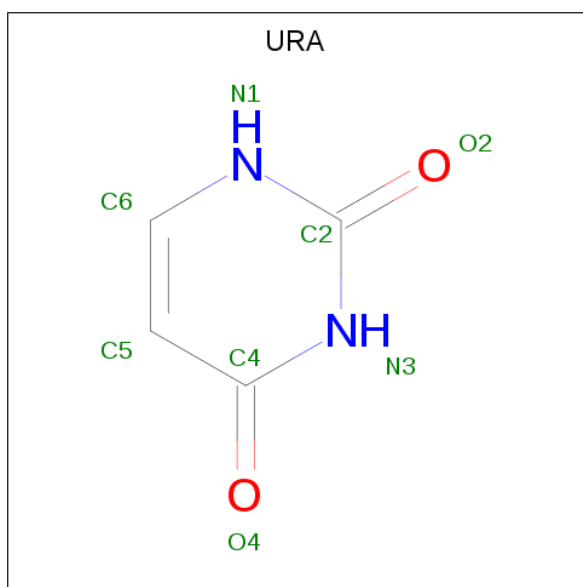
- Molecule 1 is a protein called Uricase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	1
			2363	1493	410	453	7			
1	B	296	Total	C	N	O	S	0	0	1
			2363	1493	410	453	7			
1	C	299	Total	C	N	O	S	0	0	1
			2386	1508	414	457	7			
1	D	296	Total	C	N	O	S	0	0	1
			2363	1493	410	453	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
B	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
C	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
D	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511

- Molecule 2 is URACIL (three-letter code: URA) (formula: C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>O<sub>2</sub>).

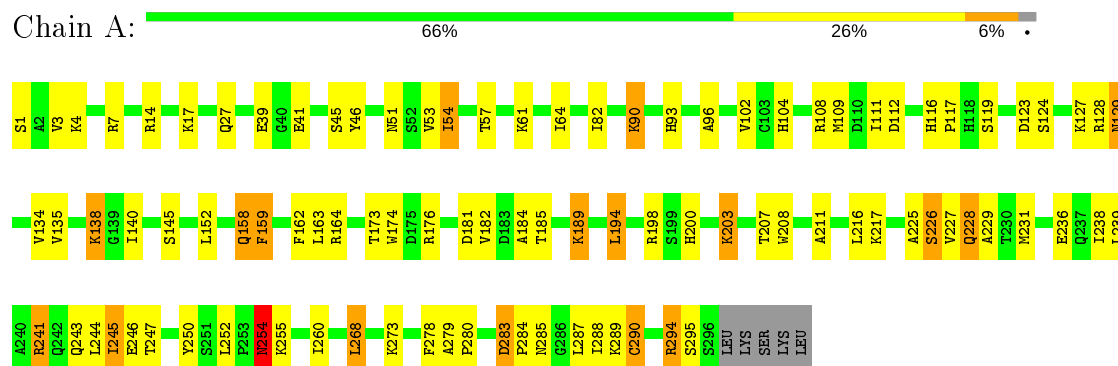


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	2	2		
2	B	1	Total	C	N	O	0	0
			8	4	2	2		
2	C	1	Total	C	N	O	0	0
			8	4	2	2		
2	D	1	Total	C	N	O	0	0
			8	4	2	2		

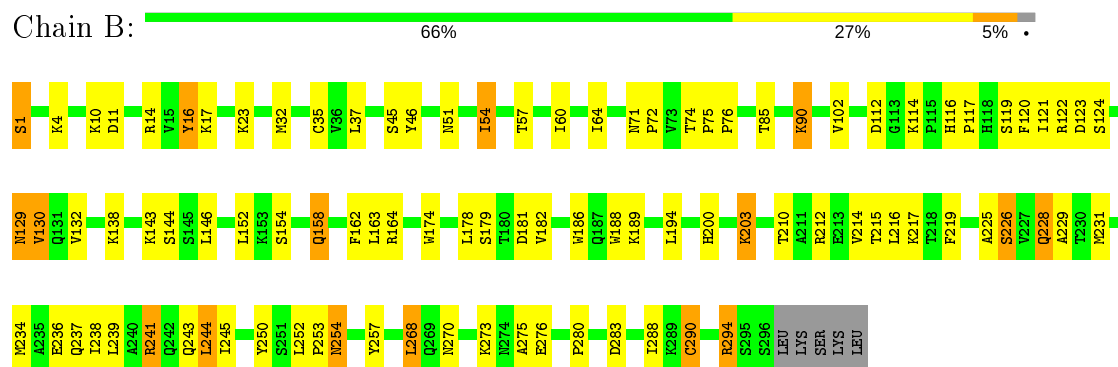
### 3 Residue-property plots

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

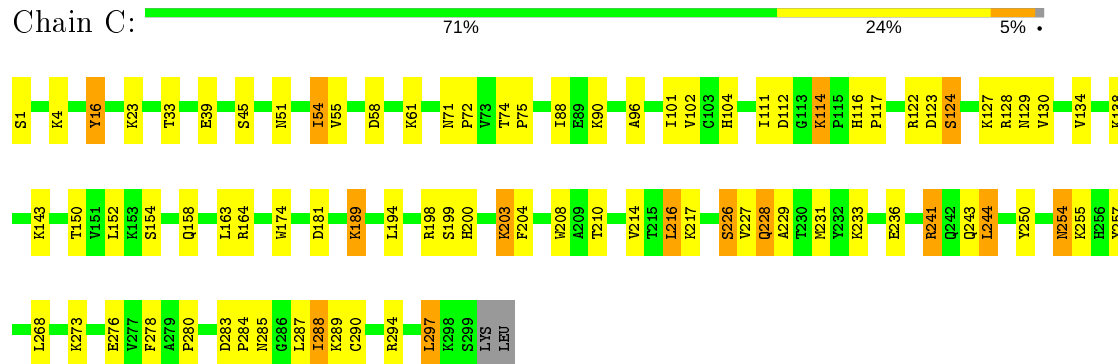
#### • Molecule 1: Uricase



#### • Molecule 1: Uricase



#### • Molecule 1: Uricase



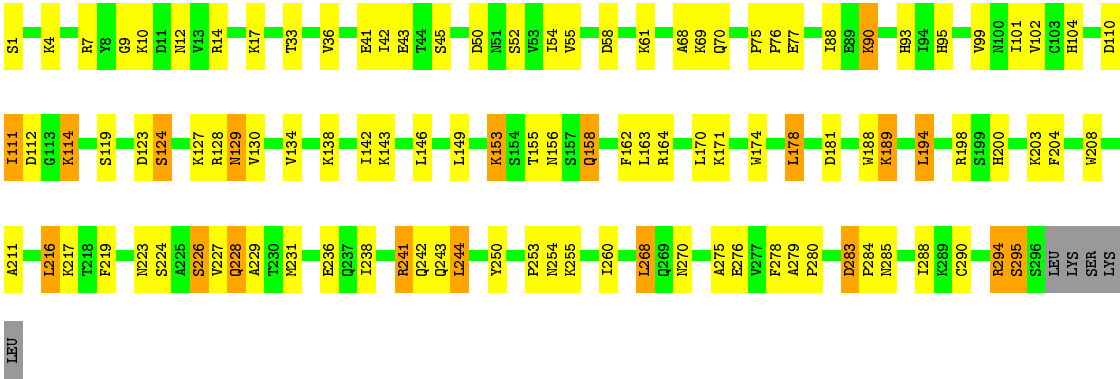
● Molecule 1: Uricase

Chain D: 

63%

29%

6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.60Å 140.60Å 151.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.20 36.07 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.00-3.20) 99.9 (36.07-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.89 (at 3.18Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, $R_{free}$	0.146 , 0.200 0.148 , 0.181	Depositor DCC
$R_{free}$ test set	2885 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.2	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9507	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 2.83% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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

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	0.64	1/2407 (0.0%)	0.81	1/3267 (0.0%)
1	B	0.63	0/2407	0.78	1/3267 (0.0%)
1	C	0.63	0/2430	0.79	1/3297 (0.0%)
1	D	0.62	0/2407	0.78	0/3267
All	All	0.63	1/9651 (0.0%)	0.79	3/13098 (0.0%)

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	A	1	0
1	B	0	1
All	All	1	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	PHE	CG-CD2	-5.16	1.31	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ASN	CB-CA-C	5.89	122.19	110.40
1	B	254	ASN	CB-CA-C	5.26	120.93	110.40
1	C	254	ASN	CB-CA-C	5.01	120.42	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	254	ASN	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1	SAC	Mainchain

## 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	2363	0	2324	91	0
1	B	2363	0	2324	87	0
1	C	2386	0	2353	88	0
1	D	2363	0	2324	113	0
2	A	8	0	3	0	0
2	B	8	0	3	1	0
2	C	8	0	3	1	0
2	D	8	0	3	1	0
All	All	9507	0	9337	352	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 19.

All (352) 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:294:ARG:HG2	1:B:294:ARG:HH11	1.03	1.12
1:B:116:HIS:ND1	1:B:117:PRO:HD2	1.73	1.04
1:D:294:ARG:HH11	1:D:294:ARG:HG2	1.25	1.01
1:D:200:HIS:HD2	1:D:203:LYS:NZ	1.59	0.98
1:A:294:ARG:HH11	1:A:294:ARG:HG2	1.32	0.95
1:B:228:GLN:HE21	1:B:228:GLN:H	1.15	0.94
1:B:294:ARG:CG	1:B:294:ARG:HH11	1.82	0.93
1:D:104:HIS:HD2	1:D:127:LYS:NZ	1.68	0.92
1:A:228:GLN:HE21	1:A:228:GLN:H	1.17	0.91
1:B:294:ARG:HG2	1:B:294:ARG:NH1	1.85	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:THR:HA	1:B:234:MET:HE2	1.55	0.89
1:A:45:SER:CB	1:A:54:ILE:HD11	2.03	0.88
1:D:228:GLN:H	1:D:228:GLN:HE21	1.17	0.88
1:D:178:LEU:HD23	1:D:219:PHE:CE1	2.07	0.87
1:D:200:HIS:HD2	1:D:203:LYS:HZ3	1.20	0.87
1:A:200:HIS:HD2	1:A:203:LYS:NZ	1.73	0.87
1:A:45:SER:HB3	1:A:54:ILE:CD1	2.04	0.86
1:A:39:GLU:HB2	1:A:96:ALA:HB3	1.54	0.86
1:B:116:HIS:CG	1:B:117:PRO:HD2	2.10	0.85
1:C:227:VAL:O	1:C:231:MET:HG3	1.77	0.85
1:D:36:VAL:HG22	1:D:99:VAL:HG22	1.59	0.85
1:B:241:ARG:HH11	1:B:241:ARG:CG	1.89	0.84
1:B:241:ARG:HG3	1:B:241:ARG:HH11	1.42	0.84
1:A:45:SER:HB3	1:A:54:ILE:HD11	1.59	0.84
1:A:104:HIS:HD2	1:A:127:LYS:NZ	1.76	0.83
1:A:228:GLN:NE2	1:A:228:GLN:H	1.78	0.82
1:C:128:ARG:HD2	1:C:208:TRP:CD1	2.16	0.81
1:A:53:VAL:HG23	1:A:54:ILE:HD12	1.64	0.80
1:B:228:GLN:NE2	1:B:228:GLN:H	1.79	0.80
1:C:241:ARG:HH11	1:C:241:ARG:HG3	1.46	0.80
1:D:241:ARG:HH11	1:D:241:ARG:CG	1.95	0.80
1:A:227:VAL:O	1:A:231:MET:HG3	1.83	0.79
1:D:146:LEU:HD12	1:D:146:LEU:O	1.83	0.79
1:C:241:ARG:CG	1:C:241:ARG:HH11	1.96	0.79
1:D:227:VAL:O	1:D:231:MET:HG3	1.83	0.78
1:A:159:PHE:CE2	1:A:162:PHE:CD1	2.73	0.77
1:D:294:ARG:HH11	1:D:294:ARG:CG	1.95	0.77
1:C:294:ARG:HH11	1:C:294:ARG:HG2	1.49	0.77
1:A:128:ARG:HD2	1:A:208:TRP:CD1	2.21	0.76
1:A:241:ARG:HH11	1:A:241:ARG:CG	1.99	0.76
1:C:90:LYS:O	1:C:90:LYS:HG3	1.85	0.75
1:D:200:HIS:CD2	1:D:203:LYS:HZ3	2.04	0.75
1:D:146:LEU:HD12	1:D:146:LEU:C	2.08	0.74
1:C:228:GLN:HE21	1:C:228:GLN:H	1.33	0.73
1:B:268:LEU:HD21	1:D:70:GLN:NE2	2.03	0.73
1:A:241:ARG:HH11	1:A:241:ARG:HG3	1.52	0.73
1:B:231:MET:SD	1:B:288:ILE:HG22	2.29	0.73
1:B:215:THR:CA	1:B:234:MET:HE2	2.18	0.72
1:D:111:ILE:O	1:D:112:ASP:HB2	1.89	0.72
1:B:231:MET:SD	1:B:288:ILE:CG2	2.78	0.72
1:C:163:LEU:HD23	1:C:164:ARG:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:VAL:HG22	1:A:140:ILE:HG12	1.71	0.71
1:C:288:ILE:CD1	1:C:288:ILE:N	2.54	0.71
1:D:200:HIS:CD2	1:D:203:LYS:NZ	2.51	0.71
1:C:200:HIS:HD2	1:C:203:LYS:NZ	1.89	0.70
1:B:102:VAL:HG22	1:B:129:ASN:ND2	2.06	0.70
1:C:122:ARG:O	1:C:122:ARG:HG3	1.91	0.70
1:B:116:HIS:CE1	1:B:117:PRO:HD2	2.28	0.69
1:C:116:HIS:CG	1:C:117:PRO:HD2	2.28	0.69
1:A:45:SER:CB	1:A:54:ILE:CD1	2.68	0.68
1:B:241:ARG:NH1	1:B:241:ARG:HG3	2.08	0.68
1:C:71:ASN:HB3	1:C:72:PRO:HD2	1.75	0.68
1:B:90:LYS:HG3	1:B:90:LYS:O	1.93	0.68
1:D:88:ILE:HD13	1:D:134:VAL:HG12	1.74	0.67
1:C:297:LEU:HD23	1:C:297:LEU:N	2.09	0.67
1:B:257:TYR:CE2	1:B:280:PRO:HG3	2.30	0.67
1:D:178:LEU:HD23	1:D:219:PHE:HE1	1.57	0.66
1:B:226:SER:HB3	1:B:229:ALA:CB	2.26	0.66
1:A:108:ARG:HD3	1:A:116:HIS:O	1.96	0.66
1:D:104:HIS:HD2	1:D:127:LYS:HZ2	1.41	0.65
1:A:102:VAL:HG22	1:A:129:ASN:HD22	1.61	0.65
1:A:112:ASP:OD2	1:C:217:LYS:NZ	2.29	0.65
1:D:178:LEU:CD2	1:D:219:PHE:HE1	2.10	0.65
1:C:104:HIS:HD2	1:C:127:LYS:NZ	1.94	0.65
1:C:241:ARG:NH1	1:C:241:ARG:HG3	2.10	0.65
1:D:178:LEU:CD2	1:D:219:PHE:CE1	2.80	0.65
1:C:226:SER:HB3	1:C:229:ALA:CB	2.28	0.64
1:C:116:HIS:ND1	1:C:117:PRO:HD2	2.13	0.64
1:A:241:ARG:HG3	1:A:241:ARG:NH1	2.11	0.64
1:C:288:ILE:N	1:C:288:ILE:HD13	2.12	0.64
1:D:104:HIS:CD2	1:D:127:LYS:NZ	2.58	0.64
1:D:170:LEU:HD12	1:D:171:LYS:N	2.13	0.64
1:C:294:ARG:CG	1:C:294:ARG:HH11	2.10	0.64
1:B:210:THR:O	1:B:214:VAL:HG23	1.98	0.64
1:A:163:LEU:HD23	1:A:164:ARG:N	2.14	0.63
1:A:294:ARG:CG	1:A:294:ARG:HH11	2.09	0.63
1:D:90:LYS:O	1:D:90:LYS:HG3	1.97	0.63
1:A:228:GLN:HE21	1:A:228:GLN:N	1.93	0.63
1:B:200:HIS:HD2	1:B:203:LYS:NZ	1.97	0.63
1:D:241:ARG:HG2	1:D:241:ARG:HH11	1.63	0.63
1:A:226:SER:HB3	1:A:229:ALA:CB	2.29	0.62
1:D:211:ALA:HA	1:D:238:ILE:CD1	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ILE:N	1:D:111:ILE:HD13	2.14	0.62
1:A:294:ARG:NH1	1:A:294:ARG:HG2	2.08	0.62
1:B:294:ARG:CG	1:B:294:ARG:NH1	2.50	0.62
1:A:104:HIS:HD2	1:A:127:LYS:HZ2	1.47	0.62
1:A:200:HIS:HD2	1:A:203:LYS:HZ3	1.48	0.62
1:A:288:ILE:N	1:A:288:ILE:HD12	2.13	0.62
1:B:146:LEU:O	1:B:146:LEU:HD12	2.00	0.62
1:C:112:ASP:HB2	1:C:114:LYS:CE	2.30	0.62
1:C:189:LYS:HD3	1:C:244:LEU:HD12	1.82	0.62
1:B:112:ASP:OD2	1:D:217:LYS:NZ	2.32	0.61
1:A:104:HIS:CD2	1:A:127:LYS:NZ	2.66	0.61
1:B:226:SER:HB3	1:B:229:ALA:HB3	1.81	0.61
1:A:200:HIS:HD2	1:A:203:LYS:CE	2.13	0.61
1:B:163:LEU:HD23	1:B:164:ARG:N	2.15	0.60
1:C:112:ASP:HB2	1:C:114:LYS:HE3	1.83	0.60
1:D:170:LEU:HD12	1:D:171:LYS:H	1.67	0.60
1:A:200:HIS:CD2	1:A:203:LYS:HE2	2.37	0.60
1:C:101:ILE:HB	1:C:130:VAL:HG22	1.83	0.60
1:A:152:LEU:C	1:A:152:LEU:HD23	2.21	0.60
1:D:241:ARG:CG	1:D:241:ARG:NH1	2.62	0.60
1:A:181:ASP:OD2	1:A:255:LYS:HE3	2.02	0.60
1:C:228:GLN:NE2	1:C:228:GLN:H	1.99	0.59
1:D:260:ILE:HD11	1:D:279:ALA:HB2	1.85	0.59
1:B:228:GLN:HE21	1:B:228:GLN:N	1.93	0.59
1:D:231:MET:HE3	1:D:250:TYR:HB3	1.84	0.59
1:C:226:SER:HB3	1:C:229:ALA:HB3	1.85	0.59
1:B:270:ASN:O	1:B:275:ALA:HA	2.02	0.59
1:C:45:SER:CB	1:C:54:ILE:HD11	2.32	0.59
1:C:189:LYS:HD3	1:C:244:LEU:CD1	2.32	0.59
1:C:200:HIS:HD2	1:C:203:LYS:HZ3	1.49	0.59
1:D:41:GLU:OE2	1:D:95:HIS:NE2	2.32	0.59
1:C:231:MET:HE3	1:C:250:TYR:HB3	1.85	0.58
1:D:17:LYS:HE3	1:D:68:ALA:O	2.02	0.58
1:D:211:ALA:HA	1:D:238:ILE:HD13	1.83	0.58
1:C:39:GLU:HB2	1:C:96:ALA:HB3	1.85	0.58
1:A:231:MET:HE3	1:A:250:TYR:HB3	1.87	0.57
1:D:110:ASP:C	1:D:111:ILE:HD13	2.25	0.57
1:A:287:LEU:HD23	1:B:37:LEU:HD21	1.86	0.57
1:D:76:PRO:HD2	1:D:77:GLU:OE1	2.04	0.57
1:D:128:ARG:HD2	1:D:208:TRP:CD1	2.39	0.57
1:D:104:HIS:CD2	1:D:127:LYS:HZ2	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:TYR:CE2	1:B:290:CYS:HB3	2.40	0.56
1:A:283:ASP:HB2	1:A:284:PRO:HA	1.86	0.56
1:C:210:THR:O	1:C:214:VAL:HG23	2.05	0.56
1:C:287:LEU:C	1:C:288:ILE:CD1	2.74	0.56
1:A:104:HIS:HD2	1:A:127:LYS:HZ1	1.54	0.56
1:A:61:LYS:HA	1:A:64:ILE:HD12	1.88	0.56
1:C:294:ARG:CG	1:C:294:ARG:NH1	2.68	0.56
1:A:3:VAL:HG12	1:A:3:VAL:O	2.06	0.56
1:C:287:LEU:C	1:C:288:ILE:HD12	2.26	0.56
1:D:200:HIS:HD2	1:D:203:LYS:HZ1	1.50	0.56
1:B:215:THR:CG2	1:B:234:MET:HE2	2.36	0.55
1:D:227:VAL:HG23	2:D:3900:URA:O2	2.06	0.55
1:D:75:PRO:HB2	1:D:76:PRO:HD2	1.89	0.55
1:A:104:HIS:CD2	1:A:127:LYS:HZ2	2.21	0.55
1:A:1:SAC:OG	1:B:236:GLU:HG2	2.06	0.55
1:A:57:THR:HG23	2:B:1900:URA:C5	2.42	0.55
1:D:104:HIS:HD2	1:D:127:LYS:HZ1	1.49	0.55
1:B:178:LEU:HD23	1:B:219:PHE:CE1	2.42	0.55
1:D:228:GLN:H	1:D:228:GLN:NE2	1.98	0.55
1:A:162:PHE:HA	1:B:51:ASN:O	2.06	0.55
1:A:211:ALA:HA	1:A:238:ILE:HD11	1.89	0.55
1:B:215:THR:HG23	1:B:234:MET:CE	2.37	0.55
1:A:200:HIS:CD2	1:A:203:LYS:NZ	2.65	0.55
1:B:158:GLN:O	1:B:225:ALA:HA	2.07	0.54
1:A:90:LYS:HG3	1:A:90:LYS:O	2.07	0.54
1:A:158:GLN:HG2	1:A:174:TRP:O	2.07	0.54
1:D:155:THR:O	1:D:156:ASN:HB2	2.08	0.54
1:B:215:THR:HG23	1:B:234:MET:HE2	1.90	0.53
1:C:287:LEU:O	1:C:288:ILE:HD12	2.07	0.53
1:A:182:VAL:HG22	1:A:252:LEU:HD22	1.91	0.53
1:B:102:VAL:HG22	1:B:129:ASN:HD22	1.74	0.53
1:D:45:SER:CB	1:D:54:ILE:HD11	2.37	0.53
1:D:123:ASP:O	1:D:124:SER:CB	2.55	0.53
1:D:101:ILE:HB	1:D:130:VAL:HG22	1.91	0.53
1:D:294:ARG:HG2	1:D:294:ARG:NH1	2.06	0.53
1:B:231:MET:HE3	1:B:250:TYR:HB3	1.91	0.53
1:B:71:ASN:HB3	1:B:72:PRO:HD2	1.90	0.53
1:C:123:ASP:O	1:C:124:SER:HB2	2.07	0.53
1:D:45:SER:CB	1:D:54:ILE:CD1	2.87	0.53
1:D:226:SER:HB3	1:D:229:ALA:CB	2.38	0.53
1:B:231:MET:O	1:B:234:MET:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:THR:OG1	1:D:104:HIS:HE1	1.92	0.52
1:C:1:SAC:OG	1:D:236:GLU:HG2	2.10	0.52
1:A:239:LEU:HD23	1:A:245:ILE:HG22	1.91	0.52
1:A:226:SER:HB3	1:A:229:ALA:HB3	1.92	0.52
1:C:33:THR:OG1	1:C:104:HIS:HE1	1.91	0.52
1:C:229:ALA:O	1:C:233:LYS:HG3	2.10	0.52
1:A:211:ALA:HA	1:A:238:ILE:CD1	2.39	0.51
1:B:45:SER:HB2	1:B:54:ILE:CD1	2.40	0.51
1:D:283:ASP:HB2	1:D:284:PRO:HA	1.92	0.51
1:D:142:ILE:HG22	1:D:188:TRP:HD1	1.75	0.51
1:A:260:ILE:HD11	1:A:279:ALA:HB2	1.92	0.51
1:B:182:VAL:HG22	1:B:252:LEU:HD22	1.93	0.51
1:B:146:LEU:C	1:B:146:LEU:HD12	2.31	0.51
1:B:158:GLN:HB3	1:B:174:TRP:HA	1.91	0.51
1:A:46:TYR:HE2	1:B:290:CYS:HB3	1.76	0.51
1:C:45:SER:CB	1:C:54:ILE:CD1	2.88	0.51
1:A:158:GLN:HB3	1:A:174:TRP:HA	1.93	0.51
1:D:226:SER:HB3	1:D:229:ALA:H	1.75	0.51
1:A:290:CYS:HB3	1:B:46:TYR:CE2	2.46	0.51
1:A:236:GLU:HG2	1:B:1:SAC:OG	2.11	0.50
1:D:254:ASN:O	1:D:285:ASN:HB2	2.11	0.50
1:D:189:LYS:HD3	1:D:244:LEU:HD12	1.92	0.50
1:C:289:LYS:O	1:C:290:CYS:HB3	2.11	0.50
1:D:178:LEU:HD23	1:D:219:PHE:CZ	2.45	0.50
1:C:111:ILE:O	1:C:112:ASP:HB2	2.11	0.50
1:C:58:ASP:O	1:C:61:LYS:HB3	2.11	0.50
1:A:194:LEU:O	1:A:198:ARG:HG3	2.12	0.50
1:B:200:HIS:CD2	1:B:203:LYS:HE2	2.45	0.50
1:D:104:HIS:CD2	1:D:127:LYS:HZ1	2.27	0.50
1:D:102:VAL:HG13	1:D:129:ASN:ND2	2.27	0.50
1:D:45:SER:HB2	1:D:54:ILE:CD1	2.42	0.49
1:A:109:MET:HE1	1:C:216:LEU:HD12	1.93	0.49
1:C:181:ASP:OD2	1:C:255:LYS:HE3	2.12	0.49
1:C:51:ASN:O	1:D:162:PHE:HA	2.12	0.49
1:D:294:ARG:NH1	1:D:294:ARG:CG	2.60	0.49
1:A:51:ASN:O	1:B:162:PHE:HA	2.11	0.49
1:A:254:ASN:O	1:A:285:ASN:HB2	2.12	0.49
1:B:74:THR:HA	1:B:75:PRO:C	2.31	0.49
1:B:120:PHE:N	1:B:120:PHE:CD1	2.81	0.49
1:B:130:VAL:HG23	1:B:132:VAL:HG23	1.95	0.49
1:B:231:MET:SD	1:B:288:ILE:HG21	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:LEU:HD23	1:D:164:ARG:N	2.28	0.49
1:A:159:PHE:CD2	1:A:162:PHE:CD1	3.01	0.49
1:C:284:PRO:HB3	1:D:12:ASN:O	2.13	0.49
1:C:88:ILE:HD13	1:C:134:VAL:HG12	1.95	0.49
1:A:27:GLN:NE2	1:C:154:SER:OG	2.45	0.48
1:A:41:GLU:HB2	1:A:93:HIS:HB2	1.95	0.48
1:D:241:ARG:HH11	1:D:241:ARG:HG3	1.77	0.48
1:B:121:ILE:HD11	1:D:149:LEU:CD1	2.42	0.48
1:C:203:LYS:HE2	1:C:244:LEU:HD23	1.95	0.48
1:C:257:TYR:CE2	1:C:280:PRO:HG3	2.48	0.48
1:D:242:GLN:OE1	1:D:244:LEU:HB2	2.14	0.48
1:B:152:LEU:HD12	1:B:179:SER:HB2	1.94	0.48
1:C:241:ARG:CG	1:C:241:ARG:NH1	2.65	0.48
1:B:123:ASP:O	1:B:124:SER:HB2	2.12	0.48
1:B:200:HIS:HD2	1:B:203:LYS:CE	2.26	0.48
1:B:257:TYR:CD2	1:B:280:PRO:HG3	2.47	0.48
1:D:112:ASP:HB2	1:D:114:LYS:CE	2.44	0.48
1:A:111:ILE:O	1:A:112:ASP:HB2	2.13	0.48
1:A:268:LEU:HD12	1:A:268:LEU:HA	1.63	0.48
1:D:158:GLN:NE2	1:D:223:ASN:OD1	2.47	0.48
1:C:163:LEU:C	1:C:163:LEU:HD23	2.34	0.48
1:C:150:THR:OG1	1:C:181:ASP:OD1	2.23	0.48
1:C:231:MET:CE	1:C:250:TYR:HB3	2.43	0.47
1:D:270:ASN:O	1:D:275:ALA:HA	2.14	0.47
1:B:102:VAL:HA	1:B:129:ASN:HD22	1.80	0.47
1:D:142:ILE:HG22	1:D:188:TRP:CD1	2.49	0.47
1:D:278:PHE:O	1:D:280:PRO:HD3	2.14	0.47
1:A:231:MET:HE3	1:A:250:TYR:CB	2.45	0.47
1:B:60:ILE:O	1:B:64:ILE:HG13	2.14	0.47
1:C:45:SER:HB2	1:C:54:ILE:HD11	1.96	0.47
1:C:236:GLU:HG3	1:D:1:SAC:OG	2.15	0.47
1:B:226:SER:HB3	1:B:229:ALA:H	1.80	0.47
1:B:215:THR:O	1:B:234:MET:CE	2.63	0.47
1:A:158:GLN:O	1:A:225:ALA:HA	2.15	0.47
1:B:116:HIS:CG	1:B:117:PRO:CD	2.92	0.47
1:D:58:ASP:O	1:D:61:LYS:HB3	2.14	0.47
1:A:53:VAL:CG2	1:A:54:ILE:HD12	2.41	0.46
1:A:200:HIS:CD2	1:A:203:LYS:HZ3	2.28	0.46
1:B:45:SER:CB	1:B:54:ILE:CD1	2.94	0.46
1:C:158:GLN:HG2	1:C:174:TRP:O	2.16	0.46
1:C:45:SER:HB2	1:C:54:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:LEU:HA	1:D:194:LEU:HD23	1.57	0.46
1:C:112:ASP:O	1:C:114:LYS:HE2	2.16	0.46
1:D:211:ALA:HA	1:D:238:ILE:HD11	1.97	0.46
1:D:200:HIS:CD2	1:D:203:LYS:HZ1	2.28	0.46
1:D:41:GLU:HB2	1:D:93:HIS:HB2	1.97	0.46
1:B:244:LEU:HD12	1:B:244:LEU:HA	1.67	0.46
1:B:181:ASP:O	1:B:253:PRO:HD2	2.16	0.46
1:D:231:MET:CE	1:D:250:TYR:HB3	2.45	0.46
1:B:215:THR:CG2	1:B:234:MET:CE	2.94	0.45
1:D:241:ARG:HG3	1:D:241:ARG:NH1	2.30	0.45
1:B:245:ILE:HD13	1:B:245:ILE:N	2.31	0.45
1:C:216:LEU:HA	1:C:216:LEU:HD12	1.74	0.45
1:B:11:ASP:OD1	1:B:35:CYS:HB2	2.16	0.45
1:A:189:LYS:HA	1:A:246:GLU:OE2	2.17	0.45
1:B:144:SER:HB2	1:B:186:TRP:NE1	2.32	0.45
1:B:45:SER:CB	1:B:54:ILE:HD12	2.47	0.45
1:C:1:SAC:C1A	1:D:295:SER:HB2	2.46	0.45
1:B:234:MET:O	1:B:238:ILE:HD12	2.16	0.45
1:A:184:ALA:HB2	1:A:250:TYR:CE1	2.52	0.45
1:D:181:ASP:O	1:D:253:PRO:HD2	2.17	0.45
1:D:75:PRO:HB2	1:D:76:PRO:CD	2.47	0.44
1:A:159:PHE:CD2	1:A:162:PHE:CE1	3.06	0.44
1:A:226:SER:HB3	1:A:229:ALA:HB2	1.98	0.44
1:B:276:GLU:OE1	1:D:69:LYS:NZ	2.40	0.44
1:C:104:HIS:HD2	1:C:127:LYS:HZ2	1.65	0.44
1:C:181:ASP:CG	1:C:255:LYS:HE3	2.38	0.44
1:D:216:LEU:HA	1:D:216:LEU:HD12	1.55	0.44
1:D:203:LYS:HE2	1:D:244:LEU:HD23	2.00	0.44
1:C:152:LEU:HD23	1:C:152:LEU:C	2.38	0.44
1:D:194:LEU:O	1:D:198:ARG:HG3	2.18	0.44
1:D:228:GLN:N	1:D:228:GLN:HE21	1.98	0.44
1:D:76:PRO:HB2	1:D:130:VAL:HG11	1.99	0.44
1:C:194:LEU:HD23	1:C:194:LEU:HA	1.81	0.44
1:D:254:ASN:HD22	1:D:254:ASN:N	2.16	0.44
1:B:200:HIS:HD2	1:B:203:LYS:HZ3	1.64	0.43
1:B:268:LEU:HA	1:B:268:LEU:HD13	1.65	0.43
1:C:283:ASP:HB2	1:C:284:PRO:HA	2.00	0.43
1:C:102:VAL:HA	1:C:129:ASN:HD22	1.83	0.43
1:C:163:LEU:HD13	1:D:55:VAL:HG22	2.00	0.43
1:C:278:PHE:O	1:C:280:PRO:HD3	2.18	0.43
1:C:123:ASP:O	1:C:124:SER:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:TRP:CZ2	1:D:204:PHE:HD1	2.36	0.43
1:C:74:THR:HA	1:C:75:PRO:C	2.39	0.43
1:C:287:LEU:C	1:C:288:ILE:HD13	2.38	0.43
1:D:153:LYS:HB2	1:D:153:LYS:HE2	1.83	0.43
1:D:9:GLY:HA3	1:D:36:VAL:O	2.18	0.43
1:D:102:VAL:HG22	1:D:129:ASN:HD22	1.84	0.43
1:C:194:LEU:O	1:C:198:ARG:HG3	2.18	0.43
1:A:200:HIS:CD2	1:A:203:LYS:CE	2.95	0.43
1:B:217:LYS:NZ	1:D:112:ASP:OD2	2.48	0.43
1:D:146:LEU:C	1:D:146:LEU:CD1	2.81	0.43
1:A:102:VAL:HG22	1:A:129:ASN:ND2	2.33	0.42
1:A:173:THR:HG23	1:A:173:THR:O	2.18	0.42
1:B:188:TRP:CE3	1:B:245:ILE:CD1	3.01	0.42
1:A:116:HIS:HA	1:A:117:PRO:HD2	1.83	0.42
1:B:122:ARG:HG3	1:B:122:ARG:O	2.19	0.42
1:A:17:LYS:HA	1:C:276:GLU:O	2.19	0.42
1:A:289:LYS:O	1:A:290:CYS:HB3	2.18	0.42
1:C:55:VAL:HG22	1:D:163:LEU:HD13	2.01	0.42
1:A:283:ASP:CB	1:A:284:PRO:HA	2.48	0.42
1:A:82:ILE:HD13	1:A:82:ILE:HG21	1.80	0.42
1:C:71:ASN:HB3	1:C:72:PRO:CD	2.48	0.42
1:D:268:LEU:HA	1:D:268:LEU:HD12	1.54	0.42
1:C:16:TYR:C	1:C:16:TYR:CD1	2.93	0.42
1:B:17:LYS:HA	1:D:276:GLU:O	2.20	0.42
1:A:123:ASP:O	1:A:124:SER:HB2	2.20	0.42
1:B:237:GLN:O	1:B:241:ARG:HG3	2.20	0.42
1:C:128:ARG:HD2	1:C:208:TRP:CG	2.55	0.42
1:C:227:VAL:HG23	2:C:2900:URA:O2	2.20	0.42
1:A:294:ARG:NH1	1:A:294:ARG:CG	2.72	0.41
1:D:76:PRO:HB2	1:D:130:VAL:CG1	2.50	0.41
1:D:181:ASP:OD1	1:D:255:LYS:HE3	2.20	0.41
1:A:158:GLN:HB3	1:A:173:THR:O	2.20	0.41
1:C:226:SER:HB3	1:C:229:ALA:H	1.86	0.41
1:D:111:ILE:O	1:D:112:ASP:CB	2.63	0.41
1:A:217:LYS:NZ	1:C:112:ASP:OD2	2.47	0.41
1:C:45:SER:HB3	1:C:54:ILE:CD1	2.50	0.41
1:B:16:TYR:CD1	1:B:16:TYR:C	2.94	0.41
1:C:285:ASN:C	1:D:10:LYS:HD2	2.41	0.41
1:A:203:LYS:O	1:A:207:THR:OG1	2.25	0.41
1:D:226:SER:HB3	1:D:229:ALA:HB3	2.02	0.41
1:A:135:VAL:HG12	1:A:138:LYS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:SER:HB3	1:A:185:THR:HG23	2.03	0.41
1:B:212:ARG:HG2	1:B:212:ARG:HH11	1.85	0.41
1:C:200:HIS:CD2	1:C:203:LYS:HZ3	2.35	0.41
1:D:42:ILE:O	1:D:43:GLU:C	2.58	0.41
1:C:297:LEU:HD22	1:C:297:LEU:HA	1.69	0.41
1:D:227:VAL:HB	1:D:288:ILE:HD13	2.03	0.41
1:B:76:PRO:HG2	1:B:130:VAL:HG11	2.03	0.40
1:D:50:ASP:OD1	1:D:52:SER:OG	2.31	0.40
1:B:10:LYS:HD3	1:B:57:THR:HB	2.03	0.40
1:D:45:SER:HB2	1:D:54:ILE:HD11	2.03	0.40
1:A:278:PHE:O	1:A:280:PRO:HD3	2.22	0.40
1:D:75:PRO:CB	1:D:76:PRO:CD	2.99	0.40
1:B:239:LEU:HA	1:B:239:LEU:HD23	1.86	0.40
1:D:158:GLN:HB3	1:D:174:TRP:HA	2.04	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	294/301 (98%)	279 (95%)	15 (5%)	0	100	100
1	B	294/301 (98%)	276 (94%)	17 (6%)	1 (0%)	41	74
1	C	297/301 (99%)	283 (95%)	11 (4%)	3 (1%)	15	54
1	D	294/301 (98%)	277 (94%)	16 (5%)	1 (0%)	41	74
All	All	1179/1204 (98%)	1115 (95%)	59 (5%)	5 (0%)	34	69

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	124	SER

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Mol	Chain	Res	Type
1	B	23	LYS
1	C	124	SER
1	C	23	LYS
1	C	204	PHE

### 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	260/266 (98%)	232 (89%)	28 (11%)	6	27
1	B	260/266 (98%)	230 (88%)	30 (12%)	5	24
1	C	263/266 (99%)	243 (92%)	20 (8%)	13	45
1	D	260/266 (98%)	233 (90%)	27 (10%)	7	28
All	All	1043/1064 (98%)	938 (90%)	105 (10%)	7	29

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

Mol	Chain	Res	Type
1	A	4	LYS
1	A	7	ARG
1	A	14	ARG
1	A	54	ILE
1	A	90	LYS
1	A	119	SER
1	A	129	ASN
1	A	138	LYS
1	A	158	GLN
1	A	176	ARG
1	A	189	LYS
1	A	194	LEU
1	A	203	LYS
1	A	216	LEU
1	A	226	SER
1	A	228	GLN
1	A	241	ARG

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Mol	Chain	Res	Type
1	A	243	GLN
1	A	244	LEU
1	A	245	ILE
1	A	247	THR
1	A	254	ASN
1	A	268	LEU
1	A	273	LYS
1	A	283	ASP
1	A	290	CYS
1	A	294	ARG
1	A	295	SER
1	B	4	LYS
1	B	14	ARG
1	B	16	TYR
1	B	32	MET
1	B	54	ILE
1	B	85	THR
1	B	90	LYS
1	B	114	LYS
1	B	119	SER
1	B	129	ASN
1	B	130	VAL
1	B	138	LYS
1	B	143	LYS
1	B	154	SER
1	B	158	GLN
1	B	189	LYS
1	B	194	LEU
1	B	203	LYS
1	B	216	LEU
1	B	226	SER
1	B	228	GLN
1	B	241	ARG
1	B	243	GLN
1	B	244	LEU
1	B	254	ASN
1	B	268	LEU
1	B	273	LYS
1	B	283	ASP
1	B	290	CYS
1	B	294	ARG
1	C	4	LYS

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Mol	Chain	Res	Type
1	C	16	TYR
1	C	54	ILE
1	C	114	LYS
1	C	138	LYS
1	C	143	LYS
1	C	189	LYS
1	C	199	SER
1	C	203	LYS
1	C	216	LEU
1	C	226	SER
1	C	228	GLN
1	C	241	ARG
1	C	243	GLN
1	C	244	LEU
1	C	254	ASN
1	C	268	LEU
1	C	273	LYS
1	C	288	ILE
1	C	297	LEU
1	D	4	LYS
1	D	7	ARG
1	D	14	ARG
1	D	90	LYS
1	D	111	ILE
1	D	114	LYS
1	D	119	SER
1	D	129	ASN
1	D	138	LYS
1	D	143	LYS
1	D	153	LYS
1	D	158	GLN
1	D	178	LEU
1	D	189	LYS
1	D	194	LEU
1	D	216	LEU
1	D	224	SER
1	D	226	SER
1	D	228	GLN
1	D	241	ARG
1	D	243	GLN
1	D	244	LEU
1	D	268	LEU

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Mol	Chain	Res	Type
1	D	283	ASP
1	D	290	CYS
1	D	294	ARG
1	D	295	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS
1	A	129	ASN
1	A	200	HIS
1	A	228	GLN
1	B	86	HIS
1	B	129	ASN
1	B	200	HIS
1	B	228	GLN
1	B	243	GLN
1	C	86	HIS
1	C	104	HIS
1	C	129	ASN
1	C	200	HIS
1	C	228	GLN
1	D	70	GLN
1	D	104	HIS
1	D	129	ASN
1	D	200	HIS
1	D	228	GLN
1	D	243	GLN
1	D	254	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	SAC	C	1	1	7,8,9	1.34	2 (28%)	8,9,11	1.84	2 (25%)
1	SAC	A	1	1	7,8,9	2.16	2 (28%)	8,9,11	2.09	2 (25%)
1	SAC	D	1	1	7,8,9	0.99	0	8,9,11	2.06	3 (37%)
1	SAC	B	1	1	7,8,9	1.05	0	8,9,11	1.47	2 (25%)

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
1	SAC	C	1	1	-	1/7/8/10	-
1	SAC	A	1	1	-	2/7/8/10	-
1	SAC	D	1	1	-	2/7/8/10	-
1	SAC	B	1	1	-	0/7/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	SAC	OAC-C1A	3.73	1.31	1.23
1	A	1	SAC	C1A-N	2.85	1.44	1.34
1	C	1	SAC	OAC-C1A	2.30	1.28	1.23
1	C	1	SAC	O-C	2.11	1.28	1.19

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	SAC	OAC-C1A-N	-4.41	113.84	121.95
1	D	1	SAC	CA-N-C1A	-3.83	116.08	123.15
1	C	1	SAC	C-CA-N	3.47	115.99	109.73
1	C	1	SAC	CA-N-C1A	-3.19	117.27	123.15
1	B	1	SAC	O-C-CA	-2.61	117.95	124.78
1	A	1	SAC	C2A-C1A-N	2.59	120.49	116.10
1	D	1	SAC	O-C-CA	-2.58	118.02	124.78
1	D	1	SAC	OAC-C1A-N	-2.37	117.60	121.95
1	B	1	SAC	C-CA-N	2.30	113.88	109.73



There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	SAC	C-CA-CB-OG
1	A	1	SAC	N-CA-CB-OG
1	C	1	SAC	C-CA-CB-OG
1	D	1	SAC	C-CA-CB-OG
1	D	1	SAC	N-CA-CB-OG

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	1	SAC	2	0
1	A	1	SAC	1	0
1	D	1	SAC	1	0
1	B	1	SAC	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	URA	B	1900	-	6,8,8	2.87	2 (33%)	4,10,10	12.43	2 (50%)
2	URA	D	3900	-	6,8,8	2.87	2 (33%)	4,10,10	12.76	2 (50%)
2	URA	C	2900	-	6,8,8	2.56	2 (33%)	4,10,10	12.58	2 (50%)
2	URA	A	900	-	6,8,8	2.83	2 (33%)	4,10,10	12.86	2 (50%)

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	URA	B	1900	-	-	-	0/1/1/1
2	URA	D	3900	-	-	-	0/1/1/1
2	URA	C	2900	-	-	-	0/1/1/1
2	URA	A	900	-	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3900	URA	C4-N3	4.62	1.41	1.33
2	A	900	URA	C4-N3	4.55	1.41	1.33
2	B	1900	URA	C4-N3	4.39	1.40	1.33
2	B	1900	URA	C2-N1	4.27	1.46	1.38
2	D	3900	URA	C2-N1	4.26	1.46	1.38
2	A	900	URA	C2-N1	4.13	1.46	1.38
2	C	2900	URA	C4-N3	3.98	1.40	1.33
2	C	2900	URA	C2-N1	3.75	1.45	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3900	URA	N1-C2-N3	-20.68	111.99	128.43
2	C	2900	URA	N1-C2-N3	-20.52	112.11	128.43
2	B	1900	URA	N1-C2-N3	-20.27	112.32	128.43
2	A	900	URA	N1-C2-N3	-20.25	112.33	128.43
2	A	900	URA	C6-N1-C2	15.69	122.16	114.42
2	D	3900	URA	C6-N1-C2	14.81	121.73	114.42
2	C	2900	URA	C6-N1-C2	14.43	121.54	114.42
2	B	1900	URA	C6-N1-C2	14.31	121.48	114.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1900	URA	1	0
2	D	3900	URA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2900	URA	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	295/301 (98%)	-0.80	0 100 100	12, 31, 56, 76	0
1	B	295/301 (98%)	-0.72	0 100 100	16, 30, 55, 77	0
1	C	298/301 (99%)	-0.76	0 100 100	12, 31, 56, 75	0
1	D	295/301 (98%)	-0.82	0 100 100	13, 31, 54, 80	0
All	All	1183/1204 (98%)	-0.77	0 100 100	12, 31, 55, 80	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	SAC	A	1	9/10	0.92	0.19	46,59,63,79	0
1	SAC	C	1	9/10	0.94	0.19	47,58,65,78	0
1	SAC	D	1	9/10	0.94	0.16	43,49,60,71	0
1	SAC	B	1	9/10	0.94	0.28	42,57,69,71	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	URA	B	1900	8/8	0.57	0.59	45,46,47,47	8
2	URA	D	3900	8/8	0.74	0.35	41,42,43,43	8
2	URA	C	2900	8/8	0.80	0.39	44,45,47,47	8
2	URA	A	900	8/8	0.81	0.31	42,43,44,44	8

## 6.5 Other polymers [i](#)

There are no such residues in this entry.