



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:14 PM GMT

PDB ID : 1WS2  
Title : urate oxidase from aspergillus flavus complexed with 5,6-diaminouracil  
Authors : Retailleau, P.; Colloc'h, N.; Vivares, D.; Bonnete, F.; Castro, B.; El Hajji, M.; Prange, T.  
Deposited on : 2004-10-29  
Resolution : 2.70 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.

---

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

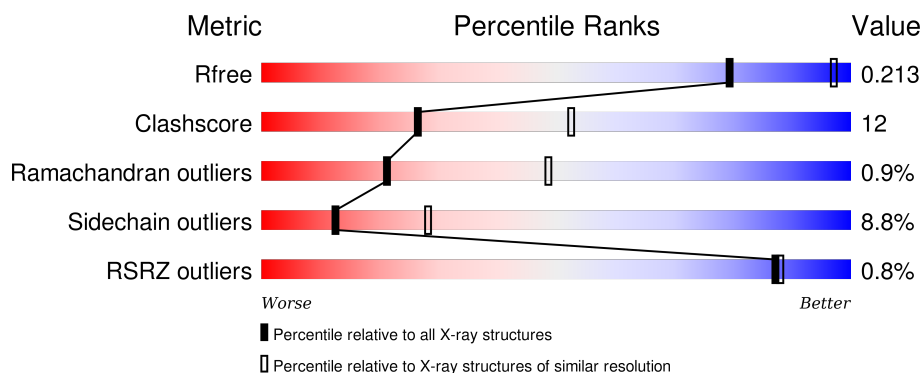
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	301	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>5%</div> <div>.</div> </div> </div>
1	B	301	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>.</div> <div>.</div> <div>.</div> </div> </div>
1	C	301	<div> <div></div> <div> <div></div> <div>74%</div> <div>20%</div> <div>5%</div> <div>.</div> </div> </div>
1	D	301	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>.</div> <div>.</div> </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	URN	A	900	-	-	-	X
2	URN	B	1900	-	-	-	X
2	URN	C	2900	-	-	-	X
2	URN	C	3900	-	-	X	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9572 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.

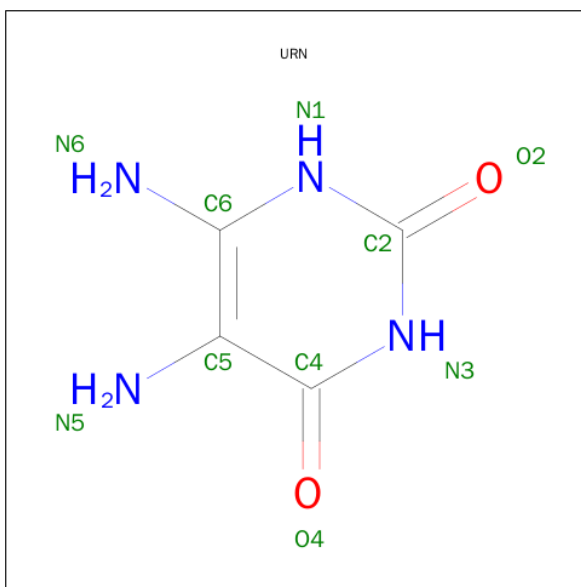
- Molecule 1 is a protein called Uricase.

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
			2362	1492	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 5,6-DIAMINOPYRIMIDINE-2,4(1H,3H)-DIONE (three-letter code: URN) (formula: C<sub>4</sub>H<sub>6</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	4	4	2		
2	B	1	Total	C	N	O	0	0
			10	4	4	2		
2	C	1	Total	C	N	O	0	0
			10	4	4	2		
2	C	1	Total	C	N	O	0	0
			10	4	4	2		

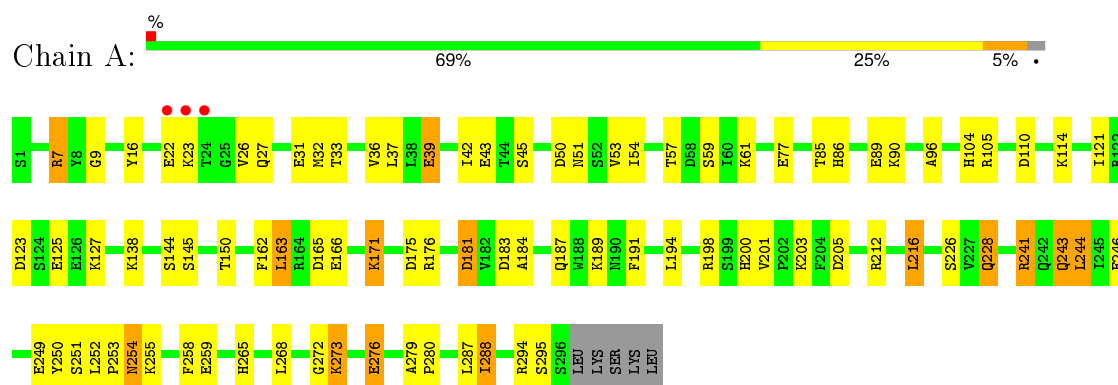
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	16	Total	O	0	0
			16	16		
3	C	13	Total	O	0	0
			13	13		
3	D	14	Total	O	0	0
			14	14		

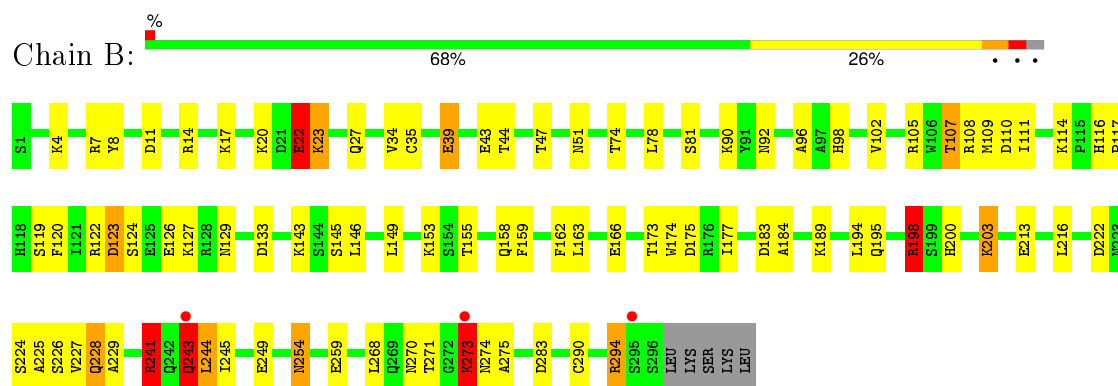
### 3 Residue-property plots [i](#)

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

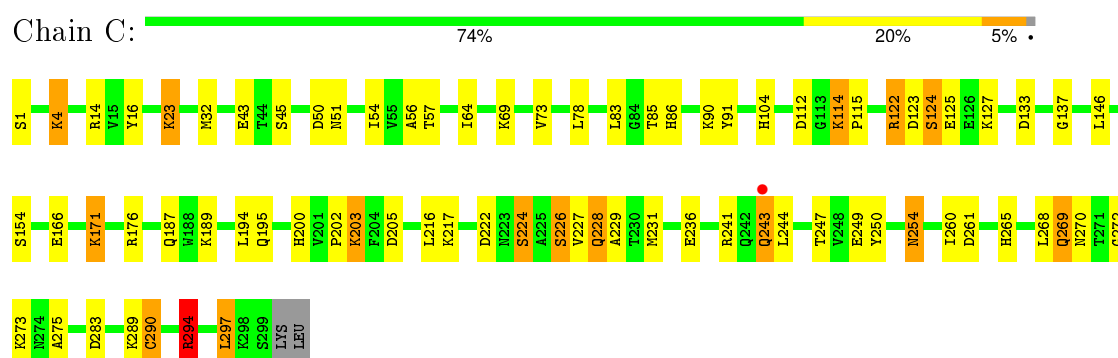
#### • Molecule 1: Uricase



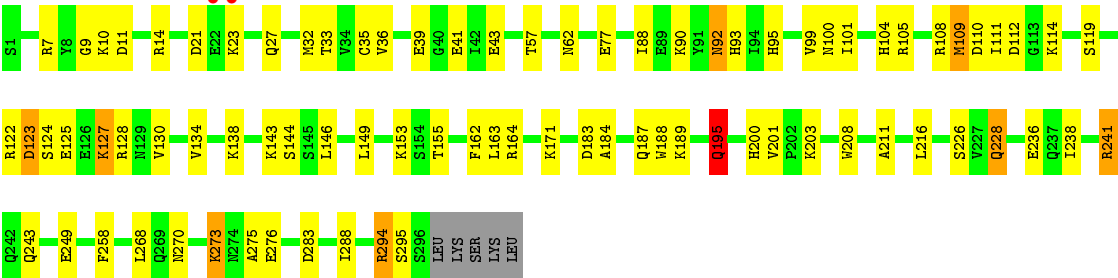
#### • Molecule 1: Uricase



#### • Molecule 1: Uricase



● Molecule 1: Uricase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.18Å 140.18Å 151.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.70 32.08 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.70) 100.0 (32.08-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.32 (at 2.68Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, $R_{free}$	0.163 , 0.212 0.152 , 0.213	Depositor DCC
$R_{free}$ test set	4746 reflections (11.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 32.8	EDS
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 47538 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: SAC, URN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.38	10/2407 (0.4%)	1.27	19/3267 (0.6%)
1	B	1.46	14/2407 (0.6%)	1.26	15/3267 (0.5%)
1	C	1.39	6/2430 (0.2%)	1.24	11/3297 (0.3%)
1	D	1.43	9/2404 (0.4%)	1.20	10/3260 (0.3%)
All	All	1.42	39/9648 (0.4%)	1.24	55/13091 (0.4%)

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	C	0	1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	GLU	CG-CD	9.43	1.66	1.51
1	D	249	GLU	CD-OE1	7.66	1.34	1.25
1	D	39	GLU	CB-CG	-7.25	1.38	1.52
1	A	249	GLU	CD-OE1	6.94	1.33	1.25
1	C	290	CYS	CB-SG	-6.83	1.70	1.82
1	B	290	CYS	CB-SG	-6.63	1.71	1.82
1	B	166	GLU	CG-CD	6.52	1.61	1.51
1	B	43	GLU	CG-CD	6.48	1.61	1.51
1	C	73	VAL	CB-CG2	6.41	1.66	1.52
1	D	184	ALA	CA-CB	-6.38	1.39	1.52
1	B	174	TRP	CB-CG	6.30	1.61	1.50
1	B	213	GLU	CG-CD	6.23	1.61	1.51
1	A	22	GLU	CB-CG	6.19	1.64	1.52
1	B	39	GLU	CB-CG	-6.16	1.40	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	127	LYS	CD-CE	6.02	1.66	1.51
1	C	249	GLU	CB-CG	-5.73	1.41	1.52
1	B	102	VAL	CB-CG1	5.59	1.64	1.52
1	D	62	ASN	CB-CG	5.54	1.63	1.51
1	A	31	GLU	CD-OE2	-5.53	1.19	1.25
1	D	258	PHE	CE1-CZ	5.49	1.47	1.37
1	B	8	TYR	CE2-CZ	5.48	1.45	1.38
1	A	39	GLU	CB-CG	-5.31	1.42	1.52
1	D	273	LYS	CB-CG	5.30	1.66	1.52
1	B	166	GLU	CB-CG	5.26	1.62	1.52
1	D	188	TRP	CB-CG	-5.25	1.40	1.50
1	B	243	GLN	CG-CD	5.21	1.63	1.51
1	B	159	PHE	CE2-CZ	5.20	1.47	1.37
1	B	273	LYS	CD-CE	5.20	1.64	1.51
1	A	273	LYS	CD-CE	5.20	1.64	1.51
1	D	105	ARG	CG-CD	-5.17	1.39	1.51
1	C	91	TYR	CD2-CE2	5.12	1.47	1.39
1	B	241	ARG	CG-CD	5.12	1.64	1.51
1	B	119	SER	CB-OG	-5.11	1.35	1.42
1	A	125	GLU	CB-CG	5.10	1.61	1.52
1	A	191	PHE	CD1-CE1	5.08	1.49	1.39
1	A	258	PHE	CE2-CZ	5.03	1.47	1.37
1	A	171	LYS	CD-CE	5.02	1.63	1.51
1	C	236	GLU	CG-CD	5.02	1.59	1.51
1	C	43	GLU	CG-CD	5.02	1.59	1.51

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ASP	CB-CG-OD1	10.94	128.15	118.30
1	A	198	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	C	122	ARG	NE-CZ-NH1	-8.46	116.07	120.30
1	C	14	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	212	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	B	11	ASP	CB-CG-OD1	7.49	125.04	118.30
1	D	146	LEU	CB-CG-CD2	-7.47	98.30	111.00
1	A	212	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	D	122	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	A	252	LEU	CB-CG-CD1	-7.31	98.57	111.00
1	B	254	ASN	CB-CA-C	7.31	125.02	110.40
1	A	198	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	A	255	LYS	CD-CE-NZ	-7.24	95.05	111.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	A	105	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	175	ASP	CB-CG-OD1	7.09	124.68	118.30
1	C	205	ASP	CB-CG-OD1	6.95	124.56	118.30
1	C	217	LYS	CD-CE-NZ	-6.95	95.71	111.70
1	D	35	CYS	CA-CB-SG	-6.88	101.61	114.00
1	C	50	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	B	268	LEU	CA-CB-CG	6.80	130.93	115.30
1	A	288	ILE	CG1-CB-CG2	-6.79	96.46	111.40
1	D	183	ASP	CB-CG-OD2	-6.74	112.24	118.30
1	B	14	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	C	78	LEU	CB-CG-CD2	-6.57	99.84	111.00
1	B	123	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	D	14	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	D	288	ILE	CG1-CB-CG2	-6.30	97.53	111.40
1	A	50	ASP	CB-CG-OD1	6.22	123.90	118.30
1	B	198	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	283	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	163	LEU	CB-CG-CD1	-5.86	101.03	111.00
1	C	294	ARG	NE-CZ-NH1	-5.81	117.40	120.30
1	C	261	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	C	133	ASP	CB-CG-OD2	5.66	123.40	118.30
1	B	109	MET	CG-SD-CE	-5.66	91.14	100.20
1	B	183	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	61	LYS	CD-CE-NZ	-5.59	98.85	111.70
1	D	183	ASP	N-CA-CB	-5.57	100.57	110.60
1	D	149	LEU	N-CA-C	-5.57	95.97	111.00
1	A	181	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	B	123	ASP	CB-CG-OD1	5.44	123.20	118.30
1	C	261	ASP	CB-CG-OD1	5.38	123.14	118.30
1	D	11	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	B	249	GLU	OE1-CD-OE2	5.24	129.59	123.30
1	B	163	LEU	CB-CG-CD1	-5.22	102.13	111.00
1	A	183	ASP	N-CA-CB	-5.19	101.26	110.60
1	A	205	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	107	THR	CA-CB-CG2	-5.16	105.18	112.40
1	D	123	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	B	105	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	127	LYS	CD-CE-NZ	-5.06	100.06	111.70
1	A	187	GLN	CA-CB-CG	-5.06	102.27	113.40
1	A	110	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	216	LEU	CB-CG-CD1	5.03	119.55	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	137	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2363	0	2324	56	0
1	B	2363	0	2324	60	0
1	C	2386	0	2353	62	0
1	D	2362	0	2320	62	0
2	A	10	0	6	1	0
2	B	10	0	6	3	0
2	C	20	0	12	8	0
3	A	15	0	0	1	0
3	B	16	0	0	1	0
3	C	13	0	0	0	0
3	D	14	0	0	0	0
All	All	9572	0	9345	230	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 12.

All (230) 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:C:202:PRO:CG	1:C:202:PRO:CB	1.74	1.46
1:B:294:ARG:HG2	1:B:294:ARG:HH11	1.07	1.12
1:B:294:ARG:CG	1:B:294:ARG:HH11	1.64	1.10
1:B:241:ARG:HH11	1:B:241:ARG:CG	1.65	1.10
1:B:241:ARG:HG3	1:B:241:ARG:HH11	0.98	1.09
1:D:241:ARG:HH11	1:D:241:ARG:HG3	0.97	1.06
1:B:241:ARG:NH1	1:B:241:ARG:HG3	1.70	1.02
1:A:228:GLN:NE2	1:A:228:GLN:H	1.58	1.00
1:B:243:GLN:HA	1:B:243:GLN:HE21	1.25	0.99

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:GLN:HE21	1:B:228:GLN:H	1.05	0.99
1:D:228:GLN:H	1:D:228:GLN:HE21	1.03	0.99
1:C:228:GLN:NE2	1:C:228:GLN:H	1.62	0.96
1:D:241:ARG:HG3	1:D:241:ARG:NH1	1.78	0.94
1:B:243:GLN:HA	1:B:243:GLN:NE2	1.82	0.94
1:B:228:GLN:NE2	1:B:228:GLN:H	1.65	0.93
1:C:57:THR:N	2:C:3900:URN:HN52	1.66	0.92
1:A:228:GLN:HE21	1:A:228:GLN:N	1.67	0.91
1:C:228:GLN:N	1:C:228:GLN:HE21	1.67	0.91
1:D:92:ASN:HD22	1:D:92:ASN:H	1.19	0.90
1:A:104:HIS:HD2	1:A:127:LYS:NZ	1.69	0.90
1:C:57:THR:H	2:C:3900:URN:HN52	0.92	0.90
1:B:294:ARG:HG2	1:B:294:ARG:NH1	1.88	0.88
1:C:112:ASP:HB2	1:C:114:LYS:NZ	1.90	0.86
1:A:200:HIS:HD2	1:A:203:LYS:NZ	1.73	0.85
1:D:104:HIS:HD2	1:D:127:LYS:NZ	1.72	0.85
1:D:228:GLN:H	1:D:228:GLN:NE2	1.74	0.85
1:D:92:ASN:H	1:D:92:ASN:ND2	1.75	0.85
1:C:104:HIS:HD2	1:C:127:LYS:NZ	1.75	0.84
1:A:200:HIS:HD2	1:A:203:LYS:HZ3	1.26	0.82
1:D:241:ARG:HH11	1:D:241:ARG:CG	1.89	0.82
1:D:112:ASP:CB	1:D:112:ASP:C	2.48	0.81
1:B:200:HIS:HD2	1:B:203:LYS:NZ	1.79	0.81
1:A:57:THR:H	2:B:1900:URN:HN52	1.30	0.80
1:A:104:HIS:HD2	1:A:127:LYS:HZ2	1.27	0.80
1:C:176:ARG:HH12	2:C:2900:URN:HN1	1.27	0.80
1:B:243:GLN:CA	1:B:243:GLN:HE21	1.94	0.79
1:A:57:THR:HG23	2:B:1900:URN:N5	1.97	0.79
1:D:294:ARG:HH11	1:D:294:ARG:CG	1.95	0.79
1:A:228:GLN:HE21	1:A:228:GLN:H	0.83	0.77
1:B:228:GLN:HE21	1:B:228:GLN:N	1.83	0.76
1:C:227:VAL:O	1:C:231:MET:HG3	1.86	0.76
1:B:22:GLU:OE2	1:B:22:GLU:HA	1.85	0.75
1:D:294:ARG:HH11	1:D:294:ARG:HG2	1.50	0.75
1:B:195:GLN:HA	1:B:195:GLN:OE1	1.86	0.75
1:C:104:HIS:HD2	1:C:127:LYS:HZ1	1.31	0.74
1:C:228:GLN:HE21	1:C:228:GLN:H	0.82	0.74
1:D:112:ASP:CB	1:D:112:ASP:N	2.50	0.74
1:B:227:VAL:HG23	2:B:1900:URN:O2	1.88	0.73
1:B:226:SER:HB3	1:B:229:ALA:HB3	1.70	0.72
1:C:112:ASP:HB2	1:C:114:LYS:HZ3	1.55	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:SER:HB3	1:B:229:ALA:CB	2.21	0.70
1:D:104:HIS:HD2	1:D:127:LYS:HZ3	1.38	0.70
1:D:111:ILE:N	1:D:111:ILE:HD13	2.07	0.70
1:B:294:ARG:CG	1:B:294:ARG:NH1	2.39	0.69
1:D:195:GLN:OE1	1:D:195:GLN:HA	1.92	0.69
1:D:200:HIS:HD2	1:D:203:LYS:NZ	1.91	0.68
1:A:162:PHE:HA	1:B:51:ASN:O	1.94	0.68
1:D:92:ASN:N	1:D:92:ASN:ND2	2.41	0.67
1:C:200:HIS:HD2	1:C:203:LYS:NZ	1.92	0.67
1:A:254:ASN:H	1:A:254:ASN:HD22	1.44	0.66
1:B:200:HIS:CD2	1:B:203:LYS:NZ	2.62	0.65
1:D:112:ASP:C	1:D:112:ASP:N	2.52	0.64
1:B:222:ASP:OD2	1:B:224:SER:HB2	1.97	0.64
1:B:200:HIS:HD2	1:B:203:LYS:HZ1	1.44	0.63
1:A:45:SER:HB2	1:A:54:ILE:HD11	1.81	0.63
1:C:171:LYS:HE3	1:C:171:LYS:HA	1.79	0.63
1:C:45:SER:HB3	1:C:54:ILE:HD11	1.80	0.62
1:B:146:LEU:O	1:B:146:LEU:HD12	1.99	0.62
1:C:45:SER:CB	1:C:54:ILE:HD11	2.30	0.62
1:A:7:ARG:HD3	1:A:37:LEU:HD13	1.80	0.62
1:C:294:ARG:CG	1:C:294:ARG:HH11	2.12	0.62
1:D:110:ASP:C	1:D:111:ILE:HD13	2.20	0.62
1:A:45:SER:CB	1:A:54:ILE:HD11	2.30	0.61
1:B:122:ARG:O	1:B:122:ARG:HG3	1.99	0.61
1:D:228:GLN:N	1:D:228:GLN:HE21	1.86	0.61
1:A:104:HIS:CD2	1:A:127:LYS:HZ2	2.16	0.61
1:A:203:LYS:HE2	1:A:244:LEU:HD23	1.81	0.61
1:B:110:ASP:O	1:B:111:ILE:HD13	2.01	0.60
1:A:45:SER:HB2	1:A:54:ILE:CD1	2.32	0.60
1:D:104:HIS:HD2	1:D:127:LYS:HZ2	1.47	0.60
1:B:200:HIS:HD2	1:B:203:LYS:HZ3	1.50	0.60
1:C:294:ARG:HH11	1:C:294:ARG:HG2	1.67	0.60
1:A:200:HIS:CD2	1:A:203:LYS:NZ	2.62	0.59
1:A:181:ASP:O	1:A:253:PRO:HD2	2.01	0.59
1:B:39:GLU:HB2	1:B:96:ALA:HB3	1.84	0.59
1:B:194:LEU:HD13	1:B:198:ARG:HH21	1.67	0.59
1:A:104:HIS:HD2	1:A:127:LYS:HZ1	1.50	0.59
1:A:39:GLU:HB2	1:A:96:ALA:HB3	1.84	0.59
1:D:109:MET:CE	1:D:119:SER:HB3	2.32	0.59
2:C:2900:URN:HN51	1:D:57:THR:H	1.51	0.58
1:D:294:ARG:NH1	1:D:294:ARG:CG	2.63	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ASN:O	1:D:162:PHE:HA	2.02	0.58
1:A:166:GLU:OE1	1:A:166:GLU:N	2.32	0.58
1:D:200:HIS:HD2	1:D:203:LYS:HZ3	1.50	0.58
1:D:27:GLN:O	1:D:108:ARG:NH2	2.28	0.58
1:A:104:HIS:CD2	1:A:127:LYS:NZ	2.61	0.57
1:A:9:GLY:HA3	1:A:36:VAL:O	2.03	0.57
1:D:33:THR:OG1	1:D:104:HIS:HE1	1.88	0.57
1:B:200:HIS:CD2	1:B:203:LYS:HZ3	2.23	0.57
1:B:259:GLU:HA	3:B:1035:HOH:O	2.04	0.56
1:A:243:GLN:HA	1:A:243:GLN:NE2	2.19	0.56
1:B:241:ARG:NH1	1:B:241:ARG:CG	2.39	0.56
1:C:104:HIS:CD2	1:C:127:LYS:HZ1	2.19	0.56
1:D:211:ALA:HA	1:D:238:ILE:CD1	2.35	0.56
1:A:228:GLN:NE2	1:A:228:GLN:N	2.38	0.56
1:D:104:HIS:CD2	1:D:127:LYS:NZ	2.65	0.56
1:D:153:LYS:HD3	1:D:155:THR:O	2.06	0.56
1:D:163:LEU:HD23	1:D:164:ARG:N	2.21	0.56
1:A:243:GLN:CA	1:A:243:GLN:HE21	2.19	0.55
1:A:243:GLN:CA	1:A:243:GLN:NE2	2.69	0.55
1:A:189:LYS:HA	1:A:246:GLU:OE2	2.06	0.54
1:B:145:SER:HB2	1:B:184:ALA:O	2.08	0.54
1:D:41:GLU:HB2	1:D:93:HIS:HB2	1.90	0.53
1:C:297:LEU:HD23	1:C:297:LEU:N	2.24	0.53
1:D:104:HIS:CD2	1:D:127:LYS:HZ2	2.26	0.53
1:D:211:ALA:HA	1:D:238:ILE:HD13	1.91	0.53
1:C:57:THR:N	2:C:3900:URN:N5	2.40	0.53
1:D:88:ILE:HD13	1:D:134:VAL:HG12	1.91	0.53
1:C:226:SER:HB3	1:C:229:ALA:CB	2.39	0.52
1:A:200:HIS:CD2	1:A:203:LYS:HZ3	2.17	0.52
1:C:195:GLN:HA	1:C:195:GLN:OE1	2.10	0.52
1:D:125:GLU:O	1:D:127:LYS:HE2	2.10	0.52
1:C:227:VAL:HG23	2:C:2900:URN:O2	2.10	0.52
1:D:243:GLN:HE21	1:D:243:GLN:HA	1.75	0.52
1:D:200:HIS:CD2	1:D:203:LYS:HZ3	2.27	0.51
1:D:36:VAL:HG22	1:D:99:VAL:HG22	1.93	0.51
1:D:41:GLU:OE2	1:D:95:HIS:NE2	2.39	0.51
1:C:200:HIS:CD2	1:C:203:LYS:NZ	2.76	0.51
1:A:27:GLN:NE2	1:C:154:SER:OG	2.44	0.51
1:C:112:ASP:HB2	1:C:114:LYS:HZ2	1.71	0.50
1:D:163:LEU:C	1:D:163:LEU:HD23	2.31	0.50
1:C:254:ASN:HD22	1:C:254:ASN:H	1.59	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:SER:OG	1:B:225:ALA:N	2.45	0.49
1:D:9:GLY:HA3	1:D:36:VAL:O	2.12	0.49
1:B:22:GLU:OE2	1:B:22:GLU:CA	2.58	0.49
1:C:289:LYS:O	1:C:290:CYS:HB3	2.13	0.49
1:C:104:HIS:CD2	1:C:127:LYS:NZ	2.68	0.49
1:A:276:GLU:HG3	1:C:69:LYS:NZ	2.27	0.49
1:C:57:THR:HG23	2:C:3900:URN:N5	2.28	0.49
1:B:271:THR:O	1:B:274:ASN:HB2	2.13	0.48
1:C:226:SER:HB3	1:C:229:ALA:H	1.78	0.48
1:D:111:ILE:O	1:D:112:ASP:CB	2.61	0.48
1:D:109:MET:HE3	1:D:119:SER:HB3	1.93	0.48
1:A:51:ASN:O	1:B:162:PHE:HA	2.13	0.48
1:D:104:HIS:CD2	1:D:127:LYS:HZ3	2.26	0.47
1:C:294:ARG:CG	1:C:294:ARG:NH1	2.75	0.47
1:A:176:ARG:HH12	2:A:900:URN:HN62	1.62	0.47
1:A:104:HIS:CD2	1:A:127:LYS:HZ1	2.29	0.47
1:C:104:HIS:HD2	1:C:127:LYS:HZ2	1.61	0.47
1:C:123:ASP:O	1:C:124:SER:HB2	2.15	0.47
1:A:287:LEU:C	1:A:288:ILE:HD12	2.35	0.47
1:C:268:LEU:HD12	1:C:269:GLN:H	1.80	0.47
1:A:33:THR:OG1	1:A:104:HIS:HE1	1.97	0.47
1:D:111:ILE:C	1:D:112:ASP:CB	2.83	0.47
1:D:270:ASN:O	1:D:275:ALA:HA	2.15	0.47
1:B:200:HIS:CD2	1:B:203:LYS:HZ1	2.27	0.46
1:C:222:ASP:OD2	1:C:224:SER:HB2	2.15	0.46
1:D:10:LYS:HD3	1:D:57:THR:HB	1.97	0.46
1:A:241:ARG:HG3	1:A:241:ARG:NH1	2.29	0.46
1:C:166:GLU:N	1:C:166:GLU:OE1	2.37	0.46
1:B:270:ASN:O	1:B:275:ALA:HA	2.15	0.46
1:C:200:HIS:HD2	1:C:203:LYS:HZ3	1.62	0.46
1:B:273:LYS:HB2	1:B:273:LYS:HE3	1.70	0.46
1:A:150:THR:HB	1:C:122:ARG:HB3	1.97	0.46
1:A:200:HIS:O	1:A:201:VAL:C	2.55	0.45
1:D:77:GLU:N	1:D:77:GLU:OE1	2.44	0.45
1:D:143:LYS:HG3	1:D:187:GLN:HG3	1.97	0.45
1:B:114:LYS:HE2	1:B:114:LYS:HB2	1.75	0.45
1:C:56:ALA:HA	2:C:3900:URN:N5	2.31	0.45
1:C:231:MET:HE3	1:C:250:TYR:HB3	1.99	0.45
1:C:200:HIS:CD2	1:C:203:LYS:HZ3	2.35	0.45
1:A:123:ASP:O	1:C:123:ASP:O	2.35	0.45
1:A:145:SER:HB2	1:A:184:ALA:O	2.17	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:HIS:O	1:C:268:LEU:HB2	2.16	0.45
1:C:146:LEU:C	1:C:146:LEU:HD12	2.37	0.45
1:C:4:LYS:HE2	1:C:4:LYS:HB3	1.75	0.45
1:A:163:LEU:C	1:A:163:LEU:HD23	2.36	0.45
1:B:23:LYS:HG2	1:B:23:LYS:H	1.37	0.44
1:B:74:THR:O	1:B:74:THR:HG23	2.17	0.44
1:A:254:ASN:N	1:A:254:ASN:HD22	2.09	0.44
1:A:45:SER:CB	1:A:54:ILE:CD1	2.93	0.44
1:A:184:ALA:HB2	1:A:250:TYR:CE1	2.53	0.44
1:C:254:ASN:N	1:C:254:ASN:HD22	2.15	0.44
1:B:20:LYS:HG2	1:B:27:GLN:NE2	2.32	0.44
1:B:98:HIS:ND1	1:B:133:ASP:OD1	2.39	0.43
1:C:243:GLN:HA	1:C:243:GLN:NE2	2.32	0.43
1:C:187:GLN:HB3	1:C:247:THR:OG1	2.18	0.43
1:C:226:SER:HB3	1:C:229:ALA:HB3	2.00	0.43
1:A:241:ARG:HH11	1:A:241:ARG:CG	2.32	0.43
1:A:200:HIS:HD2	1:A:203:LYS:HZ1	1.62	0.43
1:D:200:HIS:O	1:D:201:VAL:C	2.56	0.43
1:D:101:ILE:HB	1:D:130:VAL:HG22	2.00	0.43
1:D:21:ASP:OD2	1:D:21:ASP:C	2.56	0.43
1:B:203:LYS:HE2	1:B:244:LEU:HD22	2.00	0.43
1:A:259:GLU:HA	3:A:1028:HOH:O	2.18	0.43
1:B:120:PHE:N	1:B:120:PHE:CD1	2.86	0.43
1:B:107:THR:HG22	1:B:108:ARG:N	2.34	0.43
1:C:114:LYS:HA	1:C:115:PRO:HD2	1.87	0.43
1:C:85:THR:O	1:C:86:HIS:C	2.55	0.42
1:D:123:ASP:O	1:D:124:SER:CB	2.67	0.42
1:C:228:GLN:N	1:C:228:GLN:NE2	2.44	0.42
1:C:270:ASN:O	1:C:275:ALA:HA	2.19	0.42
1:A:85:THR:O	1:A:86:HIS:C	2.55	0.42
1:B:146:LEU:C	1:B:146:LEU:HD12	2.39	0.42
1:B:126:GLU:OE1	1:B:149:LEU:HD13	2.19	0.42
1:B:78:LEU:O	1:B:81:SER:HB2	2.20	0.42
1:A:279:ALA:HA	1:A:280:PRO:HD3	1.84	0.42
1:A:121:ILE:HD13	1:A:121:ILE:HG21	1.74	0.42
1:B:244:LEU:HD12	1:B:244:LEU:HA	1.82	0.42
1:B:17:LYS:HA	1:D:276:GLU:O	2.20	0.41
1:D:128:ARG:HD2	1:D:208:TRP:CD1	2.54	0.41
1:C:231:MET:HE3	1:C:250:TYR:CB	2.50	0.41
1:B:228:GLN:NE2	1:B:228:GLN:N	2.49	0.41
1:B:34:VAL:HG12	1:B:35:CYS:N	2.36	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:SAC:OG	1:D:236:GLU:HG2	2.20	0.41
1:C:112:ASP:CB	1:C:114:LYS:NZ	2.73	0.41
1:B:153:LYS:HE2	1:B:155:THR:O	2.20	0.41
1:D:241:ARG:CG	1:D:241:ARG:NH1	2.61	0.41
1:A:243:GLN:N	1:A:243:GLN:HE21	2.18	0.41
1:B:116:HIS:CG	1:B:117:PRO:HD2	2.56	0.41
1:D:187:GLN:HB3	1:D:187:GLN:HE21	1.61	0.41
1:B:44:THR:HA	1:B:47:THR:OG1	2.20	0.41
1:A:165:ASP:HB2	1:A:166:GLU:OE1	2.21	0.41
1:B:123:ASP:O	1:D:123:ASP:O	2.38	0.41
1:B:123:ASP:O	1:B:124:SER:HB2	2.21	0.41
1:C:64:ILE:HG12	1:C:83:LEU:HD21	2.02	0.41
1:C:194:LEU:HD23	1:C:194:LEU:HA	1.84	0.41
1:A:265:HIS:O	1:A:268:LEU:HB2	2.21	0.41
1:D:195:GLN:CA	1:D:195:GLN:OE1	2.65	0.40
1:A:77:GLU:OE2	1:A:144:SER:OG	2.33	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%)	273 (93%)	17 (6%)	4 (1%)	14	35
1	B	294/301 (98%)	279 (95%)	14 (5%)	1 (0%)	46	75
1	C	297/301 (99%)	282 (95%)	12 (4%)	3 (1%)	19	45
1	D	293/301 (97%)	277 (94%)	13 (4%)	3 (1%)	19	45
All	All	1178/1204 (98%)	1111 (94%)	56 (5%)	11 (1%)	21	49

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	B	22	GLU
1	C	23	LYS
1	A	43	GLU
1	C	272	GLY
1	D	23	LYS
1	D	195	GLN
1	D	43	GLU
1	C	124	SER
1	A	272	GLY
1	A	26	VAL

### 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%)	236 (91%)	24 (9%)	11	25
1	B	260/266 (98%)	236 (91%)	24 (9%)	11	25
1	C	263/266 (99%)	240 (91%)	23 (9%)	13	29
1	D	259/266 (97%)	238 (92%)	21 (8%)	15	33
All	All	1042/1064 (98%)	950 (91%)	92 (9%)	12	28

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	16	TYR
1	A	32	MET
1	A	42	ILE
1	A	53	VAL
1	A	59	SER
1	A	89	GLU
1	A	90	LYS
1	A	114	LYS
1	A	138	LYS
1	A	171	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	194	LEU
1	A	216	LEU
1	A	226	SER
1	A	228	GLN
1	A	241	ARG
1	A	243	GLN
1	A	244	LEU
1	A	251	SER
1	A	254	ASN
1	A	273	LYS
1	A	276	GLU
1	A	294	ARG
1	A	295	SER
1	B	4	LYS
1	B	7	ARG
1	B	22	GLU
1	B	23	LYS
1	B	90	LYS
1	B	92	ASN
1	B	129	ASN
1	B	143	LYS
1	B	158	GLN
1	B	173	THR
1	B	177	ILE
1	B	189	LYS
1	B	198	ARG
1	B	203	LYS
1	B	216	LEU
1	B	228	GLN
1	B	241	ARG
1	B	243	GLN
1	B	244	LEU
1	B	245	ILE
1	B	254	ASN
1	B	273	LYS
1	B	283	ASP
1	B	294	ARG
1	C	4	LYS
1	C	16	TYR
1	C	23	LYS
1	C	32	MET
1	C	90	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	114	LYS
1	C	125	GLU
1	C	171	LYS
1	C	189	LYS
1	C	203	LYS
1	C	216	LEU
1	C	224	SER
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	260	ILE
1	C	269	GLN
1	C	273	LYS
1	C	294	ARG
1	C	297	LEU
1	D	7	ARG
1	D	32	MET
1	D	90	LYS
1	D	92	ASN
1	D	100	ASN
1	D	109	MET
1	D	114	LYS
1	D	138	LYS
1	D	144	SER
1	D	171	LYS
1	D	189	LYS
1	D	195	GLN
1	D	216	LEU
1	D	226	SER
1	D	228	GLN
1	D	241	ARG
1	D	268	LEU
1	D	273	LYS
1	D	283	ASP
1	D	294	ARG
1	D	295	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	86	HIS
1	A	104	HIS
1	A	129	ASN
1	A	200	HIS
1	A	228	GLN
1	A	243	GLN
1	A	254	ASN
1	A	285	ASN
1	B	12	ASN
1	B	118	HIS
1	B	129	ASN
1	B	200	HIS
1	B	228	GLN
1	B	243	GLN
1	B	274	ASN
1	C	86	HIS
1	C	104	HIS
1	C	129	ASN
1	C	200	HIS
1	C	228	GLN
1	C	243	GLN
1	C	254	ASN
1	D	86	HIS
1	D	92	ASN
1	D	104	HIS
1	D	129	ASN
1	D	187	GLN
1	D	200	HIS
1	D	228	GLN
1	D	243	GLN

### 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	A	1	1	7,8,9	2.42	1 (14%)	7,9,11	3.16	3 (42%)
1	SAC	B	1	1	7,8,9	2.10	3 (42%)	7,9,11	1.84	2 (28%)
1	SAC	C	1	1	7,8,9	2.04	1 (14%)	7,9,11	1.73	2 (28%)
1	SAC	D	1	1	7,8,9	1.52	1 (14%)	7,9,11	2.92	5 (71%)

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	A	1	1	-	0/6/8/10	0/0/0/0
1	SAC	B	1	1	-	0/6/8/10	0/0/0/0
1	SAC	C	1	1	-	0/6/8/10	0/0/0/0
1	SAC	D	1	1	-	0/6/8/10	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	SAC	CB-CA	2.16	1.57	1.52
1	B	1	SAC	CA-N	2.29	1.49	1.46
1	D	1	SAC	C2A-C1A	3.16	1.56	1.50
1	B	1	SAC	C2A-C1A	3.90	1.58	1.50
1	C	1	SAC	C2A-C1A	4.54	1.59	1.50
1	A	1	SAC	C2A-C1A	5.49	1.61	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	SAC	CB-CA-N	-6.20	97.02	110.60
1	B	1	SAC	CB-CA-N	-3.86	102.14	110.60
1	D	1	SAC	CB-CA-N	-3.45	103.05	110.60
1	D	1	SAC	O-C-CA	-3.40	116.45	125.44
1	D	1	SAC	C2A-C1A-N	-3.32	109.76	116.11
1	C	1	SAC	CB-CA-N	-2.92	104.20	110.60
1	D	1	SAC	OG-CB-CA	-2.28	105.85	111.04

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	SAC	C2A-C1A-N	-2.12	112.06	116.11
1	B	1	SAC	OG-CB-CA	-2.05	106.37	111.04
1	C	1	SAC	OG-CB-CA	3.43	118.84	111.04
1	D	1	SAC	OAC-C1A-C2A	4.36	130.06	122.06
1	A	1	SAC	CA-N-C1A	4.70	137.32	121.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	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	URN	A	900	-	5,10,10	2.02	2 (40%)	5,14,14	2.40	3 (60%)
2	URN	B	1900	-	5,10,10	1.39	1 (20%)	5,14,14	4.78	4 (80%)
2	URN	C	2900	-	5,10,10	1.19	1 (20%)	5,14,14	4.25	4 (80%)
2	URN	C	3900	-	5,10,10	2.18	2 (40%)	5,14,14	5.78	3 (60%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	URN	C6-N1	2.12	1.38	1.35
2	C	2900	URN	C6-N1	2.20	1.38	1.35
2	B	1900	URN	C6-N1	2.58	1.39	1.35
2	C	3900	URN	C6-N1	3.17	1.39	1.35
2	A	900	URN	C4-N3	3.34	1.39	1.33
2	C	3900	URN	C6-N6	3.34	1.42	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1900	URN	C5-C6-N6	-3.61	116.72	124.14
2	C	2900	URN	C5-C6-N6	-2.82	118.35	124.14
2	A	900	URN	C6-C5-N5	2.02	122.76	119.58
2	A	900	URN	N6-C6-N1	2.52	120.60	116.95
2	C	2900	URN	C6-C5-N5	2.75	123.91	119.58
2	A	900	URN	C4-N3-C2	3.94	118.65	115.25
2	B	1900	URN	C4-C5-C6	4.85	119.18	114.58
2	C	3900	URN	C4-N3-C2	4.95	119.53	115.25
2	B	1900	URN	C4-N3-C2	5.07	119.63	115.25
2	C	2900	URN	N6-C6-N1	5.41	124.79	116.95
2	C	3900	URN	N6-C6-N1	6.52	126.41	116.95
2	C	2900	URN	C4-N3-C2	6.64	120.99	115.25
2	B	1900	URN	N6-C6-N1	7.17	127.34	116.95
2	C	3900	URN	C4-C5-C6	9.81	123.91	114.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	URN	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1900	URN	3	0
2	C	2900	URN	3	0
2	C	3900	URN	5	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%)	-0.71	3 (1%) 84 85	22, 40, 59, 80	0
1	B	295/301 (98%)	-0.63	3 (1%) 84 85	24, 41, 60, 79	0
1	C	298/301 (99%)	-0.67	1 (0%) 94 95	22, 40, 62, 73	0
1	D	295/301 (98%)	-0.77	2 (0%) 89 90	24, 40, 61, 84	0
All	All	1183/1204 (98%)	-0.69	9 (0%) 87 88	22, 40, 60, 84	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	GLU	3.8
1	B	295	SER	2.7
1	B	243	GLN	2.6
1	A	23	LYS	2.4
1	D	23	LYS	2.4
1	C	243	GLN	2.4
1	B	273	LYS	2.3
1	D	22	GLU	2.2
1	A	24	THR	2.0

### 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. 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
1	SAC	D	1	9/10	0.94	0.18	-	54,55,56,56	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	SAC	C	1	9/10	0.95	0.23	-	58,59,62,62	0
1	SAC	B	1	9/10	0.92	0.28	-	57,59,63,65	0
1	SAC	A	1	9/10	0.92	0.29	-	60,62,67,68	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. 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	URN	C	3900	10/10	0.77	0.34	11.26	27,31,36,36	10
2	URN	C	2900	10/10	0.81	0.37	11.01	37,42,44,46	10
2	URN	A	900	10/10	0.78	0.37	7.30	29,33,35,36	10
2	URN	B	1900	10/10	0.87	0.27	5.01	26,32,34,35	10

### 6.5 Other polymers [i](#)

There are no such residues in this entry.