



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:28 AM UTC

PDB ID : 1WS2 / pdb_00001ws2
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

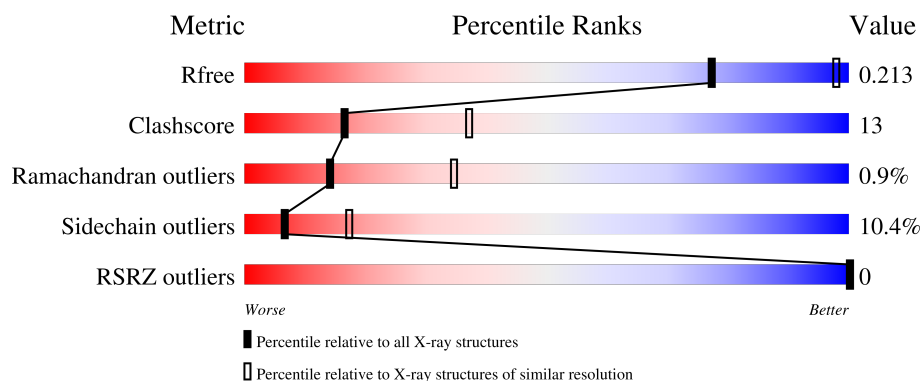
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	 60% 32% 6% •
1	B	301	 61% 29% 8% ••
1	C	301	 65% 26% 8% ••
1	D	301	 64% 28% 6% •

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	C	3900	-	-	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.

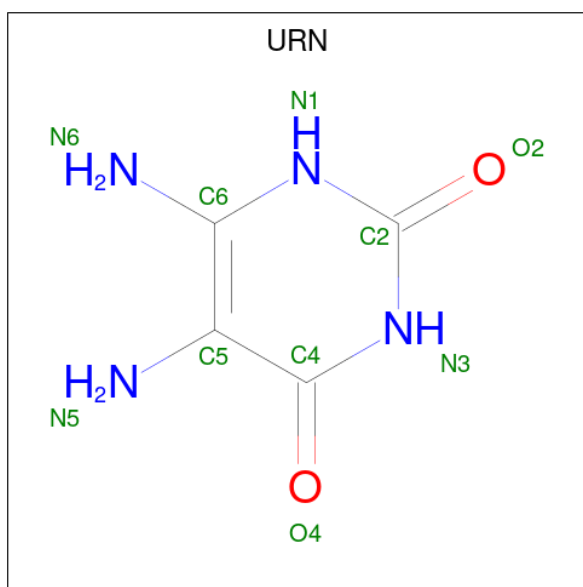
- Molecule 1 is a protein called Uricase.

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 (CCD ID: URN) (formula: C₄H₆N₄O₂).



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		

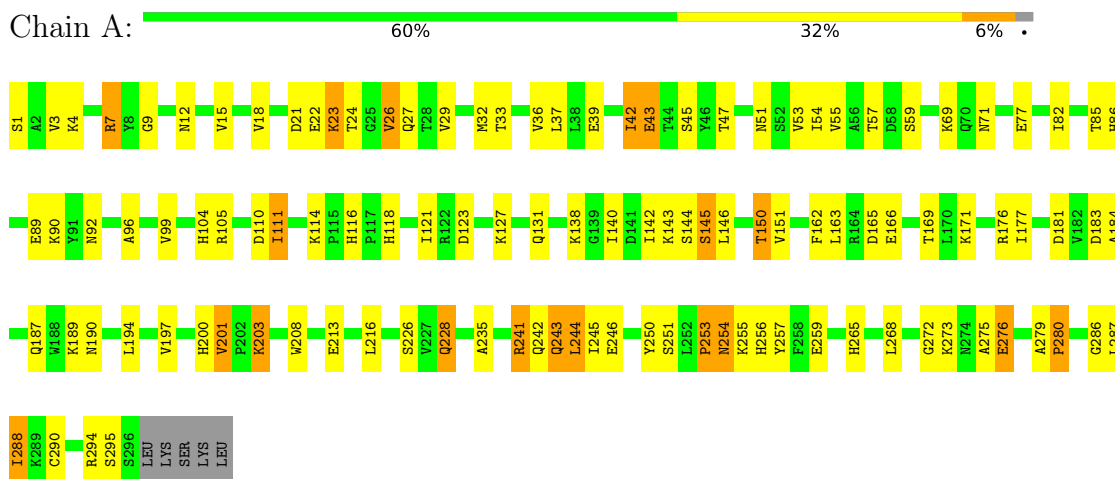
- Molecule 3 is water.

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		

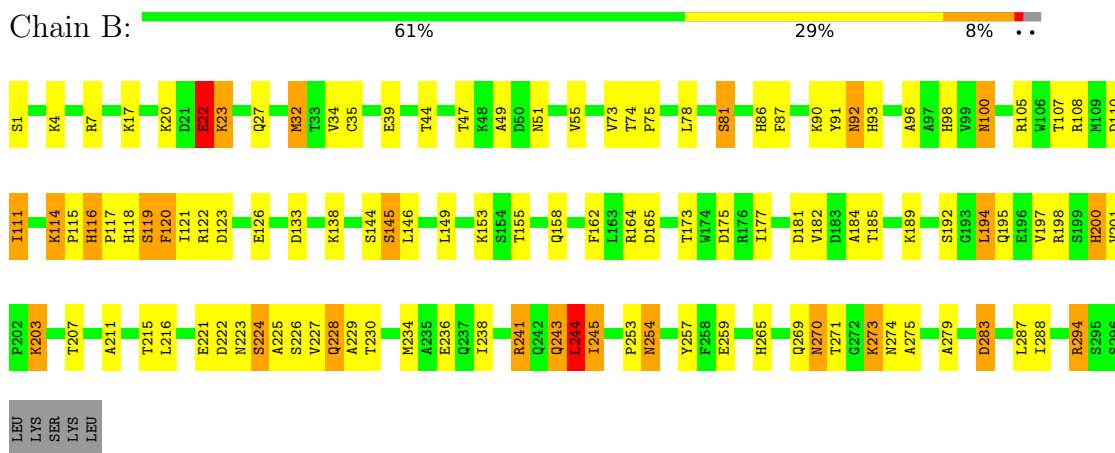
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

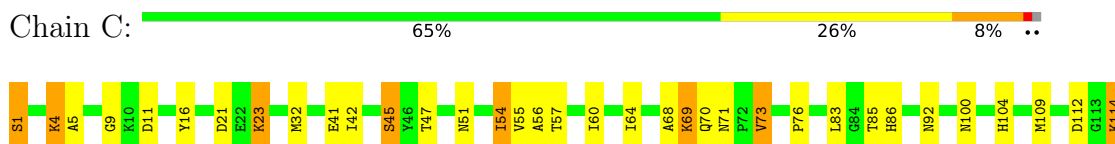
• Molecule 1: Uricase

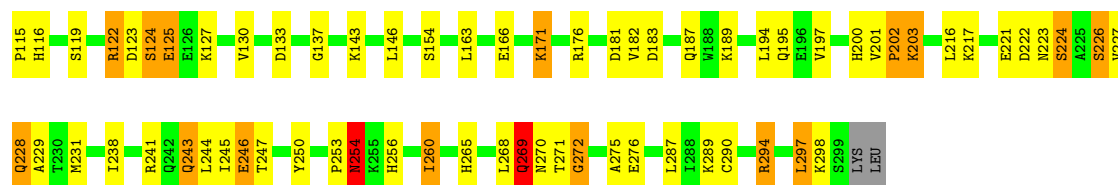


• Molecule 1: Uricase



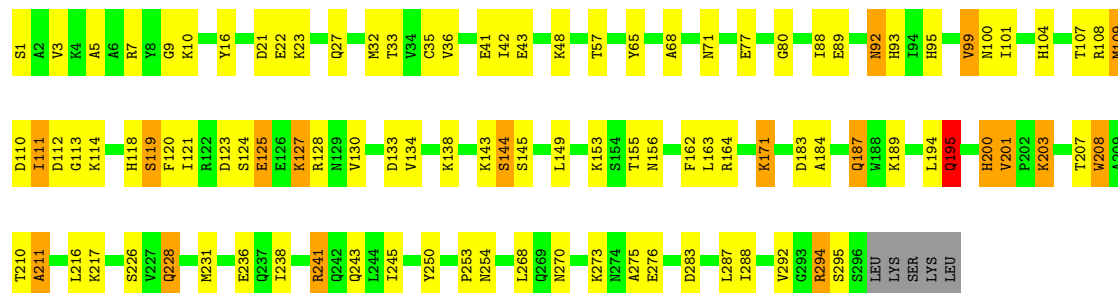
• Molecule 1: Uricase





• Molecule 1: Uricase

Chain D: 64% 28% 6% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.18Å 140.18Å 151.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.70) 99.3 (15.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 28.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9572	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: URN, SAC

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	1.70	27/2407 (1.1%)	1.56	26/3267 (0.8%)
1	B	1.75	26/2407 (1.1%)	1.58	30/3267 (0.9%)
1	C	1.68	19/2430 (0.8%)	1.63	29/3297 (0.9%)
1	D	1.74	25/2404 (1.0%)	1.51	22/3260 (0.7%)
All	All	1.71	97/9648 (1.0%)	1.57	107/13091 (0.8%)

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 (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	184	ALA	CA-CB	-9.23	1.39	1.53
1	C	253	PRO	CA-C	-8.79	1.44	1.52
1	D	145	SER	CA-C	-7.85	1.42	1.52
1	C	70	GLN	CA-C	-7.59	1.42	1.52
1	D	22	GLU	N-CA	7.46	1.55	1.46
1	A	197	VAL	CA-CB	7.42	1.62	1.54
1	A	150	THR	N-CA	7.22	1.54	1.46
1	D	107	THR	CA-CB	-7.14	1.42	1.53
1	D	3	VAL	C-O	-7.00	1.17	1.23
1	B	165	ASP	CA-C	-6.98	1.47	1.53
1	D	5	ALA	N-CA	6.92	1.53	1.46
1	D	171	LYS	N-CA	6.88	1.54	1.45
1	C	47	THR	C-O	-6.88	1.15	1.24
1	A	24	THR	N-CA	6.77	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	ILE	CA-CB	6.69	1.62	1.54
1	D	183	ASP	CA-C	6.63	1.60	1.52
1	B	245	ILE	CA-CB	6.55	1.63	1.54
1	D	156	ASN	CA-C	-6.44	1.45	1.53
1	C	60	ILE	CA-CB	-6.38	1.46	1.54
1	B	236	GLU	CA-C	-6.33	1.44	1.52
1	A	15	VAL	CA-CB	6.32	1.63	1.54
1	A	3	VAL	CA-C	6.24	1.59	1.53
1	A	280	PRO	C-O	-6.24	1.16	1.23
1	C	125	GLU	CA-C	6.20	1.62	1.52
1	A	24	THR	CA-CB	6.20	1.63	1.53
1	D	210	THR	CA-CB	6.13	1.63	1.53
1	A	71	ASN	N-CA	-6.11	1.37	1.46
1	B	197	VAL	CA-CB	6.03	1.61	1.54
1	A	190	ASN	C-O	-6.02	1.16	1.23
1	C	197	VAL	CA-CB	6.02	1.62	1.54
1	C	253	PRO	C-O	-6.01	1.18	1.23
1	C	41	GLU	CA-C	-5.99	1.46	1.53
1	D	245	ILE	CA-CB	5.98	1.61	1.54
1	A	142	ILE	CA-CB	-5.96	1.46	1.54
1	D	68	ALA	N-CA	5.93	1.53	1.46
1	B	265	HIS	CA-C	-5.90	1.45	1.52
1	D	71	ASN	CA-C	-5.87	1.46	1.52
1	C	92	ASN	CA-C	-5.85	1.45	1.52
1	D	16	TYR	C-O	5.83	1.31	1.24
1	B	87	PHE	CA-C	-5.82	1.45	1.52
1	B	100	ASN	CA-CB	-5.82	1.44	1.53
1	B	115	PRO	CA-C	5.77	1.58	1.52
1	A	12	ASN	CA-C	-5.65	1.45	1.53
1	D	133	ASP	N-CA	5.65	1.53	1.46
1	A	22	GLU	CG-CD	5.62	1.66	1.52
1	D	99	VAL	N-CA	-5.58	1.39	1.46
1	C	5	ALA	N-CA	5.58	1.52	1.46
1	B	221	GLU	CA-C	-5.56	1.44	1.52
1	A	208	TRP	C-O	5.56	1.30	1.24
1	B	230	THR	C-O	5.52	1.30	1.24
1	B	121	ILE	N-CA	-5.51	1.39	1.46
1	C	183	ASP	N-CA	-5.47	1.39	1.46
1	C	73	VAL	C-O	-5.46	1.16	1.24
1	B	49	ALA	N-CA	5.45	1.54	1.46
1	D	292	VAL	CA-CB	-5.45	1.47	1.54
1	B	211	ALA	CA-C	5.45	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	ALA	CA-CB	-5.43	1.44	1.53
1	A	21	ASP	CA-C	5.41	1.59	1.53
1	B	92	ASN	CA-C	-5.40	1.45	1.52
1	A	23	LYS	CA-C	5.38	1.59	1.52
1	A	47	THR	CA-CB	5.37	1.61	1.53
1	D	287	LEU	CA-C	5.37	1.58	1.52
1	B	119	SER	CA-C	-5.36	1.46	1.52
1	C	245	ILE	CA-CB	5.36	1.60	1.54
1	A	213	GLU	CA-CB	-5.34	1.45	1.53
1	A	145	SER	N-CA	5.31	1.52	1.46
1	C	133	ASP	N-CA	5.29	1.53	1.46
1	B	182	VAL	N-CA	-5.27	1.40	1.46
1	A	105	ARG	N-CA	5.26	1.52	1.46
1	D	253	PRO	C-O	5.22	1.28	1.24
1	C	246	GLU	CA-CB	-5.21	1.45	1.53
1	B	279	ALA	CA-C	5.19	1.59	1.52
1	C	76	PRO	CA-C	5.19	1.61	1.52
1	B	185	THR	N-CA	5.18	1.52	1.46
1	B	175	ASP	N-CA	5.18	1.52	1.46
1	C	287	LEU	CA-C	5.15	1.58	1.52
1	D	113	GLY	C-O	-5.12	1.17	1.24
1	A	92	ASN	CA-C	-5.11	1.46	1.52
1	D	211	ALA	CA-C	5.10	1.59	1.52
1	B	269	GLN	CA-CB	5.09	1.59	1.53
1	B	257	TYR	C-O	-5.09	1.18	1.24
1	D	119	SER	C-O	5.08	1.29	1.23
1	A	99	VAL	N-CA	-5.07	1.40	1.46
1	D	120	PHE	CA-C	-5.07	1.46	1.52
1	A	151	VAL	CA-C	-5.06	1.47	1.52
1	C	202	PRO	CB-CG	5.06	1.75	1.49
1	A	275	ALA	CA-CB	-5.05	1.45	1.53
1	B	254	ASN	C-O	5.04	1.29	1.23
1	A	177	ILE	C-O	-5.04	1.18	1.24
1	A	18	VAL	C-O	-5.04	1.19	1.24
1	B	182	VAL	CA-CB	5.03	1.60	1.54
1	D	208	TRP	N-CA	-5.03	1.40	1.46
1	B	164	ARG	CA-C	-5.02	1.46	1.52
1	A	257	TYR	C-O	-5.02	1.18	1.24
1	D	125	GLU	CA-C	5.02	1.59	1.52
1	C	11	ASP	C-O	5.01	1.30	1.23
1	B	120	PHE	CA-C	-5.01	1.46	1.52

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	71	ASN	CA-C-N	-11.96	107.77	119.85
1	C	71	ASN	C-N-CA	-11.96	107.77	119.85
1	B	181	ASP	CA-C-N	-8.45	112.71	123.19
1	B	181	ASP	C-N-CA	-8.45	112.71	123.19
1	B	81	SER	N-CA-C	-8.36	101.40	111.69
1	C	45	SER	N-CA-C	-8.23	102.27	111.82
1	B	254	ASN	CB-CA-C	8.02	125.02	111.22
1	D	254	ASN	N-CA-C	7.84	121.01	110.35
1	C	201	VAL	CA-C-N	-7.74	111.67	119.56
1	C	201	VAL	C-N-CA	-7.74	111.67	119.56
1	D	149	LEU	N-CA-C	-7.70	95.97	108.52
1	A	4	LYS	N-CA-C	7.17	120.00	111.33
1	B	253	PRO	CA-C-N	-7.05	112.70	123.14
1	B	253	PRO	C-N-CA	-7.05	112.70	123.14
1	A	290	CYS	N-CA-C	7.05	119.58	108.79
1	D	201	VAL	CA-C-N	-7.01	112.41	119.56
1	D	201	VAL	C-N-CA	-7.01	112.41	119.56
1	C	253	PRO	CA-C-N	-6.98	113.76	122.84
1	C	253	PRO	C-N-CA	-6.98	113.76	122.84
1	C	254	ASN	N-CA-C	6.98	120.13	108.20
1	C	68	ALA	N-CA-C	-6.85	103.88	111.82
1	B	200	HIS	N-CA-C	6.82	120.57	112.93
1	C	9	GLY	N-CA-C	6.80	119.29	110.45
1	A	253	PRO	CA-C-N	-6.73	111.20	122.64
1	A	253	PRO	C-N-CA	-6.73	111.20	122.64
1	A	24	THR	N-CA-C	6.67	120.28	111.75
1	C	181	ASP	CA-C-N	-6.64	114.96	123.19
1	C	181	ASP	C-N-CA	-6.64	114.96	123.19
1	B	224	SER	N-CA-C	6.62	120.40	110.14
1	A	145	SER	N-CA-C	6.57	118.19	108.60
1	A	116	HIS	N-CA-C	6.51	117.86	109.72
1	D	183	ASP	N-CA-CB	-6.46	100.57	110.65
1	B	201	VAL	CA-C-N	-6.28	113.22	119.56
1	B	201	VAL	C-N-CA	-6.28	113.22	119.56
1	D	71	ASN	CA-C-N	-6.27	113.32	119.78
1	D	71	ASN	C-N-CA	-6.27	113.32	119.78
1	B	283	ASP	N-CA-C	-6.25	102.60	108.22
1	C	238	ILE	N-CA-C	-6.20	104.46	110.72
1	C	69	LYS	CA-C-N	-6.17	112.86	122.67
1	C	69	LYS	C-N-CA	-6.17	112.86	122.67
1	B	144	SER	CA-C-N	-6.11	111.84	121.87
1	B	144	SER	C-N-CA	-6.11	111.84	121.87
1	D	194	LEU	N-CA-C	6.10	118.46	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	HIS	N-CA-C	6.08	120.18	109.96
1	B	145	SER	N-CA-C	6.02	117.93	108.96
1	A	183	ASP	N-CA-CB	-6.02	101.26	110.65
1	D	145	SER	N-CA-C	6.01	118.26	108.76
1	A	92	ASN	CB-CA-C	-5.98	101.49	110.88
1	B	194	LEU	CA-C-N	5.97	129.09	120.79
1	B	194	LEU	C-N-CA	5.97	129.09	120.79
1	D	118	HIS	N-CA-C	5.97	119.85	112.03
1	A	140	ILE	N-CA-C	5.97	116.77	107.28
1	B	118	HIS	N-CA-C	5.95	117.44	110.41
1	B	223	ASN	CA-C-N	-5.94	112.46	122.92
1	B	223	ASN	C-N-CA	-5.94	112.46	122.92
1	A	187	GLN	CA-CB-CG	-5.91	102.27	114.10
1	C	116	HIS	CA-C-N	-5.89	113.55	119.56
1	C	116	HIS	C-N-CA	-5.89	113.55	119.56
1	A	242	GLN	CA-C-N	5.87	129.62	120.82
1	A	242	GLN	C-N-CA	5.87	129.62	120.82
1	D	283	ASP	N-CA-C	-5.87	102.85	108.13
1	C	55	VAL	N-CA-C	-5.82	101.16	108.84
1	D	207	THR	N-CA-C	5.80	117.68	111.36
1	B	116	HIS	N-CA-C	5.79	118.00	109.50
1	B	165	ASP	N-CA-C	-5.78	101.84	108.49
1	D	144	SER	N-CA-C	-5.71	100.58	109.72
1	D	3	VAL	N-CA-C	5.70	115.76	108.12
1	D	65	TYR	N-CA-C	-5.68	105.00	111.14
1	B	75	PRO	CA-C-N	-5.62	113.10	119.28
1	B	75	PRO	C-N-CA	-5.62	113.10	119.28
1	D	22	GLU	N-CA-C	5.59	118.30	111.82
1	B	55	VAL	N-CA-C	-5.57	101.53	108.89
1	D	35	CYS	CA-CB-SG	-5.56	101.61	114.40
1	C	260	ILE	CB-CA-C	-5.54	102.90	110.77
1	D	89	GLU	N-CA-C	5.53	118.49	111.69
1	A	26	VAL	N-CA-C	5.52	120.82	109.34
1	C	122	ARG	NE-CZ-NH1	-5.43	116.07	121.50
1	C	269	GLN	N-CA-C	5.40	118.12	107.98
1	A	55	VAL	N-CA-C	-5.39	99.84	107.98
1	B	93	HIS	CA-C-N	-5.34	115.70	122.37
1	B	93	HIS	C-N-CA	-5.34	115.70	122.37
1	D	288	ILE	CB-CA-C	-5.32	102.76	110.63
1	B	105	ARG	N-CA-C	5.32	117.40	109.59
1	C	221	GLU	N-CA-C	5.31	119.48	112.89
1	B	244	LEU	N-CA-C	5.30	122.09	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ILE	CB-CA-C	-5.28	105.12	112.04
1	C	256	HIS	N-CA-C	5.28	118.55	110.20
1	A	255	LYS	CD-CE-NZ	-5.27	95.05	111.90
1	A	286	GLY	N-CA-C	-5.26	105.80	112.54
1	B	192	SER	N-CA-C	5.18	117.00	111.36
1	D	80	GLY	N-CA-C	-5.18	106.52	112.73
1	C	223	ASN	CA-C-N	-5.15	111.72	122.07
1	C	223	ASN	C-N-CA	-5.15	111.72	122.07
1	B	270	ASN	N-CA-C	5.15	120.31	112.54
1	A	118	HIS	N-CA-C	5.14	118.76	112.03
1	A	29	VAL	N-CA-C	5.11	116.97	108.99
1	C	182	VAL	CA-C-N	-5.08	115.82	122.99
1	C	182	VAL	C-N-CA	-5.08	115.82	122.99
1	A	201	VAL	CA-C-N	-5.06	114.60	119.87
1	A	201	VAL	C-N-CA	-5.06	114.60	119.87
1	C	217	LYS	CD-CE-NZ	-5.06	95.71	111.90
1	D	187	GLN	N-CA-C	5.06	116.98	108.73
1	A	169	THR	N-CA-C	-5.05	106.96	114.64
1	A	71	ASN	CA-C-N	-5.04	114.58	119.78
1	A	71	ASN	C-N-CA	-5.04	114.58	119.78
1	D	200	HIS	N-CA-C	5.04	119.52	113.17
1	C	125	GLU	CB-CG-CD	5.02	121.13	112.60

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	61	0
1	B	2363	0	2324	66	0
1	C	2386	0	2353	69	0
1	D	2362	0	2320	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	243	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 13.

All (243) 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:HH11	1:B:294:ARG:CG	1.64	1.10
1:B:241:ARG:CG	1:B:241:ARG:HH11	1.65	1.10
1:B:241:ARG:HH11	1:B:241:ARG:HG3	0.98	1.09
1:D:241:ARG:HG3	1:D:241:ARG:HH11	0.97	1.06
1:D:109:MET:HE3	1:D:119:SER:HB3	1.36	1.05
1:B:241:ARG:HG3	1:B:241:ARG:NH1	1.70	1.02
1:A:228:GLN:H	1:A:228:GLN:NE2	1.58	1.00
1:B:243:GLN:HA	1:B:243:GLN:HE21	1.25	0.99
1:B:228:GLN:H	1:B:228:GLN:HE21	1.05	0.99
1:D:228:GLN:H	1:D:228:GLN:HE21	1.03	0.99
1:C:228:GLN:H	1:C:228:GLN:NE2	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:H	1:B:228:GLN:NE2	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:HE21	1:C:228:GLN:N	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:D:112:ASP:CB	1:D:112:ASP:C	2.48	0.86
1:A:200:HIS:HD2	1:A:203:LYS:NZ	1.73	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:HIS:HD2	1:A:127:LYS:HZ1	1.24	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:104:HIS:HD2	1:D:127:LYS:HZ2	1.20	0.84
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: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:C:176:ARG:HH12	2:C:2900:URN:HN1	1.27	0.80
1:B:243:GLN:HE21	1:B:243:GLN:CA	1.94	0.79
1:A:57:THR:HG23	2:B:1900:URN:N5	1.97	0.79
1:D:294:ARG:CG	1:D:294:ARG:HH11	1.95	0.79
1:A:228:GLN:H	1:A:228:GLN:HE21	0.83	0.77
1:D:92:ASN:H	1:D:92:ASN:ND2	1.75	0.76
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:B:195:GLN:OE1	1:B:195:GLN:HA	1.86	0.75
1:D:294:ARG:HH11	1:D:294:ARG:HG2	1.50	0.75
1:C:104:HIS:HD2	1:C:127:LYS:HZ1	1.31	0.74
1:C:228:GLN:H	1:C:228:GLN:HE21	0.82	0.74
1:D:112:ASP:CB	1:D:112:ASP:N	2.50	0.74
1:A:104:HIS:CD2	1:A:127:LYS:HZ1	2.05	0.74
1:C:112:ASP:HB2	1:C:114:LYS:HZ3	1.51	0.73
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:B:226:SER:HB3	1:B:229:ALA:CB	2.21	0.70
1:D:111:ILE:HD13	1:D:111:ILE:N	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:112:ASP:C	1:D:112:ASP:N	2.52	0.68
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:ND2	1:D:92:ASN:N	2.41	0.67
1:C:200:HIS:HD2	1:C:203:LYS:NZ	1.92	0.67
1:D:110:ASP:C	1:D:111:ILE:HD13	2.20	0.67
1:B:32:MET:HE1	1:B:73:VAL:HB	1.77	0.66
1:A:254:ASN:HD22	1:A:254:ASN:H	1.44	0.66
1:D:104:HIS:CD2	1:D:127:LYS:HZ2	2.09	0.66
1:B:200:HIS:CD2	1:B:203:LYS:NZ	2.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:146:LEU:HD12	1:B:146:LEU:O	1.99	0.62
1:C:45:SER:HB3	1:C:54:ILE:HD11	1.80	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:HH11	1:C:294:ARG:CG	2.12	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:HE21	1:D:228:GLN:N	1.86	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: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:181:ASP:O	1:A:253:PRO:HD2	2.01	0.59
1:A:200:HIS:CD2	1:A:203:LYS:NZ	2.62	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:39:GLU:HB2	1:A:96:ALA:HB3	1.84	0.59
1:A:166:GLU:N	1:A:166:GLU:OE1	2.32	0.58
1:C:51:ASN:O	1:D:162:PHE:HA	2.02	0.58
2:C:2900:URN:HN51	1:D:57:THR:H	1.51	0.58
1:D:294:ARG:CG	1:D:294:ARG:NH1	2.63	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: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:CG	1:B:241:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLN:NE2	1:A:243:GLN:CA	2.69	0.55
1:D:163:LEU:HD23	1:D:163:LEU:C	2.31	0.55
1:C:109:MET:HE3	1:C:119:SER:HB3	1.88	0.54
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:N	1:C:297:LEU:HD23	2.24	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:A:104:HIS:HD2	1:A:127:LYS:HZ2	1.52	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:OE1	1:C:195:GLN:HA	2.10	0.52
1:C:227:VAL:HG23	2:C:2900:URN:O2	2.10	0.52
1:D:125:GLU:O	1:D:127:LYS:HE2	2.10	0.52
1:D:243:GLN:HE21	1:D:243:GLN:HA	1.75	0.52
1:A:287:LEU:C	1:A:288:ILE:HD12	2.35	0.51
1:D:200:HIS:CD2	1:D:203:LYS:HZ3	2.27	0.51
1:D:111:ILE:C	1:D:112:ASP:CB	2.83	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:A:104:HIS:CD2	1:A:127:LYS:NZ	2.61	0.51
1:A:200:HIS:O	1:A:201:VAL:C	2.55	0.50
1:C:146:LEU:C	1:C:146:LEU:HD12	2.37	0.49
1:C:254:ASN:HD22	1:C:254:ASN:H	1.59	0.49
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:A:163:LEU:HD23	1:A:163:LEU:C	2.36	0.49
1:C:289:LYS:O	1:C:290:CYS:HB3	2.13	0.49
1:A:276:GLU:HG3	1:C:69:LYS:NZ	2.27	0.49
1:C:104:HIS:CD2	1:C:127:LYS:NZ	2.68	0.49
1:C:57:THR:HG23	2:C:3900:URN:N5	2.28	0.49
1:C:112:ASP:HB2	1:C:114:LYS:HZ2	1.75	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:21:ASP:OD2	1:D:21:ASP:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:HIS:O	1:D:201:VAL:C	2.56	0.48
1:A:51:ASN:O	1:B:162:PHE:HA	2.13	0.48
1:A:176:ARG:HH12	2:A:900:URN:HN62	1.62	0.47
1:C:294:ARG:CG	1:C:294:ARG:NH1	2.75	0.47
1:B:203:LYS:O	1:B:207:THR:OG1	2.25	0.47
1:C:85:THR:O	1:C:86:HIS:C	2.55	0.47
1:A:85:THR:O	1:A:86:HIS:C	2.55	0.47
1:A:165:ASP:OD2	1:B:91:TYR:OH	2.28	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: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:B:146:LEU:HD12	1:B:146:LEU:C	2.39	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:NH1	1:A:241:ARG:HG3	2.29	0.46
1:C:166:GLU:OE1	1:C:166:GLU:N	2.37	0.46
1:B:270:ASN:O	1:B:275:ALA:HA	2.15	0.46
1:B:273:LYS:HE3	1:B:273:LYS:HB2	1.70	0.46
1:C:200:HIS:HD2	1:C:203:LYS:HZ3	1.62	0.46
1:A:150:THR:HB	1:C:122:ARG:HB3	1.97	0.46
1:D:77:GLU:OE1	1:D:77:GLU:N	2.44	0.45
1:D:143:LYS:HG3	1:D:187:GLN:HG3	1.97	0.45
1:B:114:LYS:HB2	1:B:114:LYS:HE2	1.75	0.45
1:C:56:ALA:HA	2:C:3900:URN:N5	2.31	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
1:C:4:LYS:HE2	1:C:4:LYS:HB3	1.75	0.45
1:C:265:HIS:O	1:C:268:LEU:HB2	2.16	0.45
1:B:23:LYS:H	1:B:23:LYS:HG2	1.37	0.44
1:B:215:THR:O	1:B:234:MET:HE2	2.17	0.44
1:A:110:ASP:C	1:A:111:ILE:HD13	2.41	0.44
1:B:74:THR:O	1:B:74:THR:HG23	2.17	0.44
1:A:254:ASN:HD22	1:A:254:ASN:N	2.09	0.44
1:C:21:ASP:OD2	1:C:21:ASP:C	2.59	0.44
1:A:45:SER:CB	1:A:54:ILE:CD1	2.93	0.44
1:A:69:LYS:NZ	1:C:276:GLU:OE1	2.44	0.44
1:A:184:ALA:HB2	1:A:250:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:LYS:HG2	1:B:27:GLN:NE2	2.32	0.44
1:C:254:ASN:HD22	1:C:254:ASN:N	2.15	0.44
1:A:276:GLU:HG3	1:C:69:LYS:HZ2	1.83	0.43
1:B:98:HIS:ND1	1:B:133:ASP:OD1	2.39	0.43
1:B:119:SER:C	1:B:120:PHE:CD1	2.95	0.43
1:C:187:GLN:HB3	1:C:247:THR:OG1	2.18	0.43
1:C:231:MET:HE3	1:C:250:TYR:HB3	2.00	0.43
1:C:243:GLN:NE2	1:C:243:GLN:HA	2.32	0.43
1:A:241:ARG:HH11	1:A:241:ARG:CG	2.32	0.43
1:C:226:SER:HB3	1:C:229:ALA:HB3	2.00	0.43
1:A:200:HIS:HD2	1:A:203:LYS:HZ1	1.62	0.43
1:D:101:ILE:HB	1:D:130:VAL:HG22	2.00	0.43
1:A:259:GLU:HA	3:A:1028:HOH:O	2.18	0.43
1:B:203:LYS:HE2	1:B:244:LEU:HD22	2.00	0.43
1:D:231:MET:HE3	1:D:250:TYR:HB3	2.01	0.43
1:B:120:PHE:CD1	1:B:120:PHE:N	2.86	0.43
1:A:146:LEU:HD12	1:A:146:LEU:C	2.43	0.43
1:C:114:LYS:HA	1:C:115:PRO:HD2	1.87	0.43
1:C:231:MET:HE3	1:C:250:TYR:CB	2.48	0.43
1:B:107:THR:HG22	1:B:108:ARG:N	2.34	0.42
1:B:86:HIS:CD2	1:B:86:HIS:C	2.97	0.42
1:C:228:GLN:NE2	1:C:228:GLN:N	2.44	0.42
1:C:270:ASN:O	1:C:275:ALA:HA	2.19	0.42
1:A:121:ILE:HG21	1:A:121:ILE:HD13	1.74	0.42
1:A:279:ALA:HA	1:A:280:PRO:HD3	1.84	0.42
1:B:78:LEU:O	1:B:81:SER:HB2	2.20	0.42
1:B:126:GLU:OE1	1:B:149:LEU:HD13	2.19	0.42
1:B:244:LEU:HD12	1:B:244:LEU:HA	1.82	0.42
1:C:163:LEU:C	1:C:163:LEU:HD23	2.45	0.42
1:B:17:LYS:HA	1:D:276:GLU:O	2.20	0.41
1:D:123:ASP:O	1:D:124:SER:CB	2.67	0.41
1:D:128:ARG:HD2	1:D:208:TRP:CD1	2.54	0.41
1:C:32:MET:HE1	1:C:73:VAL:HB	2.00	0.41
1:B:34:VAL:HG12	1:B:35:CYS:N	2.36	0.41
1:B:228:GLN:NE2	1:B:228:GLN:N	2.49	0.41
1:C:1:SAC:OG	1:D:236:GLU:HG2	2.20	0.41
1:B:153:LYS:HE2	1:B:155:THR:O	2.20	0.41
1:C:112:ASP:CB	1:C:114:LYS:NZ	2.73	0.41
1:A:243:GLN:HE21	1:A:243:GLN:N	2.18	0.41
1:B:116:HIS:CG	1:B:117:PRO:HD2	2.56	0.41
1:D:241:ARG:NH1	1:D:241:ARG:CG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ILE:O	1:A:43:GLU:C	2.64	0.41
1:B:44:THR:HA	1:B:47:THR:OG1	2.20	0.41
1:D:187:GLN:HE21	1:D:187:GLN:HB3	1.61	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: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:C:271:THR:O	1:C:272:GLY:C	2.63	0.41
1:A:265:HIS:O	1:A:268:LEU:HB2	2.21	0.41
1:B:287:LEU:C	1:B:288:ILE:HD12	2.46	0.40
1:D:195:GLN:OE1	1:D:195:GLN:CA	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/301 (98%)	273 (93%)	17 (6%)	4 (1%)	9	23
1	B	294/301 (98%)	279 (95%)	14 (5%)	1 (0%)	36	60
1	C	297/301 (99%)	282 (95%)	12 (4%)	3 (1%)	12	32
1	D	293/301 (97%)	277 (94%)	13 (4%)	3 (1%)	12	32
All	All	1178/1204 (98%)	1111 (94%)	56 (5%)	11 (1%)	14	35

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	B	22	GLU
1	C	23	LYS

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Mol	Chain	Res	Type
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 [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	260/266 (98%)	231 (89%)	29 (11%)	6	15
1	B	260/266 (98%)	234 (90%)	26 (10%)	7	19
1	C	263/266 (99%)	236 (90%)	27 (10%)	7	18
1	D	259/266 (97%)	233 (90%)	26 (10%)	7	19
All	All	1042/1064 (98%)	934 (90%)	108 (10%)	7	17

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
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	111	ILE
1	A	114	LYS
1	A	131	GLN
1	A	138	LYS
1	A	143	LYS
1	A	171	LYS

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Mol	Chain	Res	Type
1	A	194	LEU
1	A	203	LYS
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	245	ILE
1	A	251	SER
1	A	254	ASN
1	A	273	LYS
1	A	276	GLU
1	A	288	ILE
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	32	MET
1	B	90	LYS
1	B	92	ASN
1	B	100	ASN
1	B	111	ILE
1	B	114	LYS
1	B	138	LYS
1	B	158	GLN
1	B	173	THR
1	B	177	ILE
1	B	189	LYS
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

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Mol	Chain	Res	Type
1	C	4	LYS
1	C	16	TYR
1	C	23	LYS
1	C	42	ILE
1	C	54	ILE
1	C	100	ASN
1	C	114	LYS
1	C	125	GLU
1	C	130	VAL
1	C	143	LYS
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	246	GLU
1	C	254	ASN
1	C	260	ILE
1	C	269	GLN
1	C	294	ARG
1	C	297	LEU
1	C	298	LYS
1	D	7	ARG
1	D	32	MET
1	D	42	ILE
1	D	48	LYS
1	D	92	ASN
1	D	100	ASN
1	D	109	MET
1	D	111	ILE
1	D	114	LYS
1	D	121	ILE
1	D	127	LYS
1	D	138	LYS
1	D	144	SER
1	D	171	LYS
1	D	189	LYS

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Mol	Chain	Res	Type
1	D	195	GLN
1	D	203	LYS
1	D	216	LEU
1	D	217	LYS
1	D	226	SER
1	D	228	GLN
1	D	241	ARG
1	D	268	LEU
1	D	273	LYS
1	D	294	ARG
1	D	295	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	27	GLN
1	A	86	HIS
1	A	104	HIS
1	A	129	ASN
1	A	158	GLN
1	A	200	HIS
1	A	228	GLN
1	A	243	GLN
1	A	254	ASN
1	B	19	HIS
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	B	281	GLN
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	27	GLN
1	D	62	ASN

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Mol	Chain	Res	Type
1	D	92	ASN
1	D	104	HIS
1	D	129	ASN
1	D	158	GLN
1	D	187	GLN
1	D	200	HIS
1	D	228	GLN
1	D	243	GLN
1	D	269	GLN
1	D	281	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	2.35	1 (14%)	7,9,11	3.16	2 (28%)
1	SAC	B	1	1	7,8,9	2.00	2 (28%)	7,9,11	2.30	1 (14%)
1	SAC	C	1	1	7,8,9	1.95	1 (14%)	7,9,11	2.97	2 (28%)
1	SAC	D	1	1	7,8,9	1.41	1 (14%)	7,9,11	2.85	4 (57%)

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	-	1/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SAC	B	1	1	-	0/7/8/10	-
1	SAC	C	1	1	-	2/7/8/10	-
1	SAC	D	1	1	-	0/7/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	SAC	C2A-C1A	5.31	1.61	1.50
1	C	1	SAC	C2A-C1A	4.40	1.59	1.50
1	B	1	SAC	C2A-C1A	3.78	1.58	1.50
1	D	1	SAC	C2A-C1A	3.06	1.56	1.50
1	B	1	SAC	CA-N	2.05	1.49	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	SAC	C-CA-N	7.74	124.44	109.50
1	C	1	SAC	C-CA-N	7.30	123.58	109.50
1	B	1	SAC	C-CA-N	5.60	120.31	109.50
1	D	1	SAC	OAC-C1A-C2A	4.49	130.06	122.05
1	D	1	SAC	C2A-C1A-N	-3.83	109.76	116.12
1	D	1	SAC	O-C-CA	-3.23	116.45	124.77
1	C	1	SAC	OG-CB-CA	2.80	118.84	111.13
1	D	1	SAC	CB-CA-C	2.53	116.91	111.35
1	A	1	SAC	C2A-C1A-N	-2.45	112.06	116.12

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	1	SAC	N-CA-CB-OG
1	C	1	SAC	C-CA-CB-OG
1	A	1	SAC	OAC-C1A-N-CA

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 oligosaccharides 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	-	8,10,10	1.38	1 (12%)	9,14,14	3.74	5 (55%)
2	URN	C	2900	-	8,10,10	1.53	2 (25%)	9,14,14	3.30	6 (66%)
2	URN	C	3900	-	8,10,10	2.23	3 (37%)	9,14,14	3.88	6 (66%)
2	URN	B	1900	-	8,10,10	1.64	2 (25%)	9,14,14	4.11	6 (66%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3900	URN	C6-N6	3.92	1.42	1.34
2	C	3900	URN	C2-N1	3.06	1.42	1.37
2	B	1900	URN	C4-N3	-3.04	1.33	1.38
2	C	3900	URN	C4-N3	-2.96	1.33	1.38
2	C	2900	URN	C2-N3	-2.31	1.33	1.37
2	A	900	URN	C2-N3	2.30	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2900	URN	C4-N3	-2.25	1.34	1.38
2	B	1900	URN	C2-N1	2.21	1.41	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1900	URN	O2-C2-N3	-6.83	109.73	121.86
2	A	900	URN	C5-C4-N3	6.58	123.67	111.10
2	C	3900	URN	O2-C2-N3	-6.41	110.47	121.86
2	C	3900	URN	N1-C2-N3	6.28	125.61	115.74
2	B	1900	URN	N1-C2-N3	5.88	124.98	115.74
2	C	2900	URN	C5-C4-N3	5.66	121.91	111.10
2	A	900	URN	C4-N3-C2	-5.60	118.65	126.37
2	A	900	URN	O4-C4-C5	-5.07	114.70	127.48
2	C	3900	URN	C4-N3-C2	-4.97	119.53	126.37
2	B	1900	URN	C4-N3-C2	-4.89	119.63	126.37
2	B	1900	URN	C5-C4-N3	4.75	120.18	111.10
2	C	2900	URN	O2-C2-N3	-4.03	114.70	121.86
2	C	2900	URN	C4-N3-C2	-3.91	120.99	126.37
2	C	2900	URN	O4-C4-C5	-3.60	118.39	127.48
2	C	2900	URN	N1-C2-N3	3.59	121.39	115.74
2	A	900	URN	O2-C2-N1	-3.59	115.49	121.86
2	C	3900	URN	C5-C4-N3	3.54	117.87	111.10
2	B	1900	URN	N6-C6-N1	3.54	127.34	117.16
2	C	3900	URN	N6-C6-N1	3.22	126.41	117.16
2	A	900	URN	N1-C2-N3	2.90	120.30	115.74
2	C	2900	URN	N6-C6-N1	2.65	124.79	117.16
2	B	1900	URN	O4-C4-C5	-2.45	121.31	127.48
2	C	3900	URN	O4-C4-C5	-2.28	121.73	127.48

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
2	C	2900	URN	3	0
2	C	3900	URN	5	0
2	B	1900	URN	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 [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, 95th 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 ²)	Q<0.9
1	A	295/301 (98%)	-1.01	0 100 100	22, 40, 59, 80	0
1	B	295/301 (98%)	-0.91	0 100 100	24, 41, 60, 79	0
1	C	298/301 (99%)	-0.99	0 100 100	22, 40, 62, 73	0
1	D	295/301 (98%)	-0.97	0 100 100	24, 40, 61, 84	0
All	All	1183/1204 (98%)	-0.97	0 100 100	22, 40, 60, 84	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, 95th 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 ²)	Q<0.9
1	SAC	A	1	9/10	0.87	0.09	60,62,67,68	0
1	SAC	B	1	9/10	0.88	0.11	57,59,63,65	0
1	SAC	C	1	9/10	0.89	0.09	58,59,62,62	0
1	SAC	D	1	9/10	0.91	0.08	54,55,56,56	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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	URN	A	900	10/10	0.67	0.18	29,33,35,36	10
2	URN	C	3900	10/10	0.74	0.14	27,31,36,36	10
2	URN	C	2900	10/10	0.80	0.16	37,42,44,46	10
2	URN	B	1900	10/10	0.81	0.13	26,32,34,35	10

6.5 Other polymers [i](#)

There are no such residues in this entry.