



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:13 PM UTC

PDB ID : 3INY / pdb_00003iny
Title : Crystal structure of human purine nucleoside phosphorylase in complex with 7-deazaguanine
Authors : de Azevedo Jr, W.F.; Santos, D.S.; Basso, L.A.
Deposited on : 2009-08-13
Resolution : 2.75 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

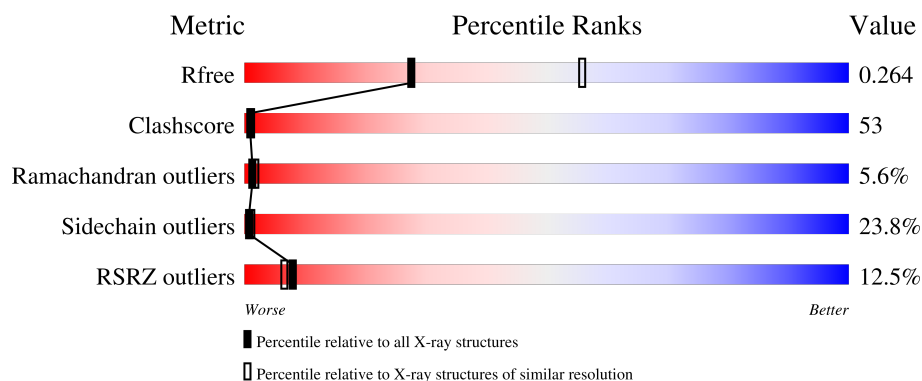
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	289	

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	SO4	A	292	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2301 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.

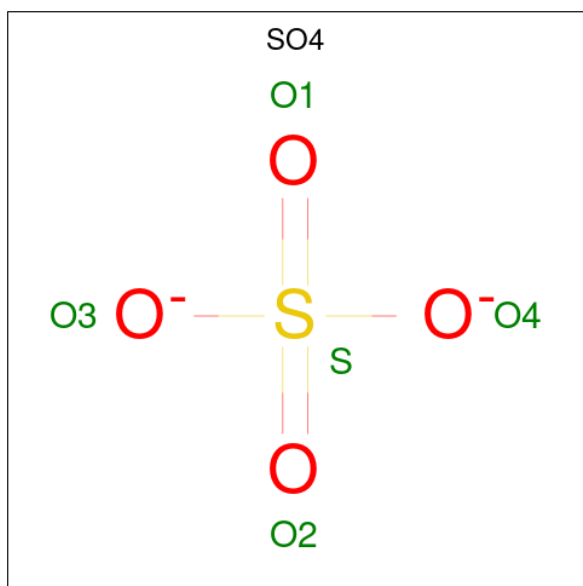
- Molecule 1 is a protein called Purine nucleoside phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2251	1429	394	413	15	0	0	0

There is a discrepancy between the modelled and reference sequences:

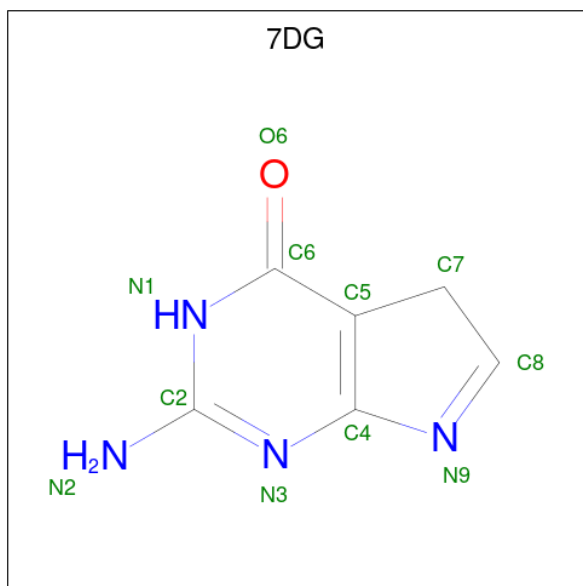
Chain	Residue	Modelled	Actual	Comment	Reference
A	51	SER	GLY	SEE REMARK 999	UNP P00491

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

- Molecule 3 is 7-DEAZAGUANINE (CCD ID: 7DG) (formula: $C_6H_6N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	6	4	1		

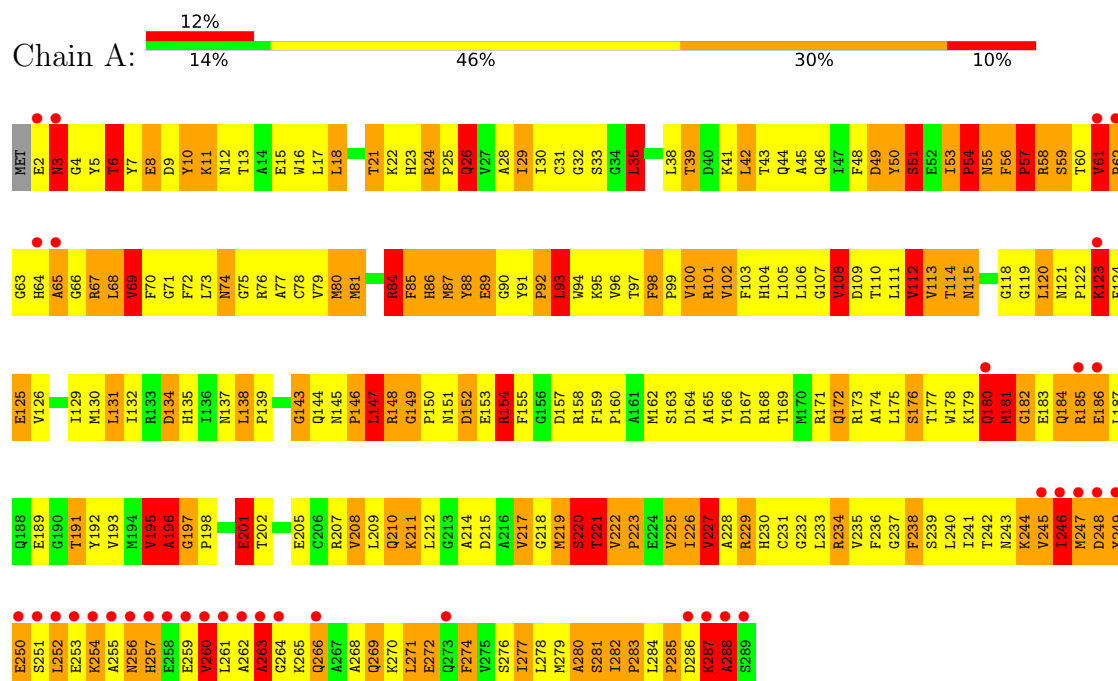
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		

3 Residue-property plots [i](#)

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: Purine nucleoside phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	138.75Å 138.75Å 159.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.69 – 2.75 43.69 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.7 (43.69-2.75) 98.6 (43.69-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.209 , 0.269 0.207 , 0.264	Depositor DCC
R_{free} test set	765 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2301	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: SO4, 7DG

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	2.37	112/2303 (4.9%)	2.31	129/3115 (4.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	GLY	N-CA	20.02	1.72	1.44
1	A	93	LEU	CB-CG	12.05	1.77	1.53
1	A	93	LEU	CA-C	-10.97	1.37	1.52
1	A	245	VAL	N-CA	9.76	1.60	1.45
1	A	129	ILE	CA-CB	-9.72	1.42	1.54
1	A	65	ALA	CA-CB	9.71	1.69	1.53
1	A	148	ARG	CG-CD	9.60	1.81	1.52
1	A	260	VAL	CA-CB	9.60	1.67	1.54
1	A	55	ASN	N-CA	9.16	1.56	1.46
1	A	148	ARG	CA-C	-9.16	1.40	1.53
1	A	146	PRO	C-N	8.79	1.45	1.33
1	A	152	ASP	C-O	8.69	1.34	1.23
1	A	149	GLY	C-O	8.41	1.35	1.24
1	A	186	GLU	CA-C	8.29	1.62	1.52
1	A	197	GLY	N-CA	8.15	1.55	1.44
1	A	114	THR	C-O	-7.99	1.13	1.23
1	A	277	ILE	CA-CB	-7.97	1.45	1.54
1	A	65	ALA	CA-C	7.77	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	VAL	CA-CB	-7.68	1.44	1.54
1	A	91	TYR	C-N	-7.65	1.23	1.33
1	A	263	ALA	CA-C	7.59	1.62	1.52
1	A	288	ALA	N-CA	7.44	1.55	1.46
1	A	91	TYR	N-CA	7.39	1.54	1.45
1	A	87	MET	N-CA	-7.37	1.37	1.46
1	A	123	LYS	CG-CD	7.37	1.74	1.52
1	A	123	LYS	CB-CG	7.14	1.73	1.52
1	A	221	THR	C-O	7.09	1.32	1.24
1	A	54	PRO	N-CA	-7.06	1.38	1.47
1	A	33	SER	CA-C	-6.98	1.44	1.52
1	A	162	MET	C-O	6.93	1.32	1.24
1	A	6	THR	CA-C	-6.92	1.44	1.52
1	A	108	VAL	CA-CB	-6.91	1.47	1.54
1	A	240	LEU	N-CA	-6.84	1.37	1.46
1	A	180	GLN	CB-CG	6.75	1.72	1.52
1	A	57	PRO	C-O	-6.75	1.15	1.24
1	A	254	LYS	CA-C	6.72	1.61	1.53
1	A	93	LEU	C-O	6.67	1.32	1.24
1	A	239	SER	N-CA	-6.60	1.37	1.46
1	A	274	PHE	N-CA	-6.58	1.38	1.46
1	A	100	VAL	CA-CB	-6.51	1.46	1.54
1	A	220	SER	CA-C	-6.47	1.45	1.53
1	A	244	LYS	N-CA	6.43	1.53	1.45
1	A	195	VAL	CA-CB	-6.31	1.46	1.54
1	A	232	GLY	C-O	-6.22	1.17	1.24
1	A	246	ILE	CA-CB	6.22	1.62	1.54
1	A	8	GLU	CG-CD	6.20	1.67	1.52
1	A	96	VAL	CA-C	-6.14	1.45	1.52
1	A	55	ASN	CA-C	-6.14	1.45	1.52
1	A	260	VAL	CA-C	6.13	1.60	1.52
1	A	87	MET	C-O	-6.07	1.17	1.24
1	A	217	VAL	CA-CB	-6.06	1.47	1.54
1	A	195	VAL	CA-C	5.98	1.59	1.52
1	A	54	PRO	C-O	5.98	1.31	1.24
1	A	68	LEU	N-CA	-5.88	1.39	1.46
1	A	283	PRO	N-CA	-5.88	1.39	1.47
1	A	229	ARG	N-CA	-5.87	1.39	1.46
1	A	6	THR	CB-CG2	5.83	1.71	1.52
1	A	245	VAL	CA-CB	5.80	1.62	1.54
1	A	74	ASN	CA-C	-5.79	1.45	1.53
1	A	123	LYS	CA-CB	5.78	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	PRO	N-CA	5.77	1.53	1.47
1	A	88	TYR	N-CA	5.76	1.54	1.46
1	A	3	ASN	N-CA	5.75	1.53	1.46
1	A	98	PHE	C-O	-5.75	1.18	1.24
1	A	118	GLY	CA-C	-5.74	1.48	1.52
1	A	214	ALA	CA-CB	-5.74	1.44	1.53
1	A	96	VAL	C-O	-5.74	1.17	1.24
1	A	111	LEU	CA-C	-5.72	1.45	1.52
1	A	201	GLU	CB-CG	-5.70	1.35	1.52
1	A	81	MET	N-CA	-5.69	1.38	1.46
1	A	39	THR	CA-C	5.68	1.60	1.52
1	A	6	THR	CA-CB	-5.66	1.44	1.53
1	A	93	LEU	CG-CD1	5.64	1.71	1.52
1	A	148	ARG	CA-CB	-5.62	1.45	1.53
1	A	256	ASN	CA-C	5.54	1.60	1.52
1	A	163	SER	C-O	-5.54	1.17	1.24
1	A	201	GLU	CA-C	-5.49	1.45	1.53
1	A	112	VAL	C-O	5.48	1.29	1.24
1	A	256	ASN	N-CA	5.45	1.53	1.46
1	A	191	THR	CA-CB	-5.45	1.45	1.53
1	A	236	PHE	C-O	-5.44	1.17	1.23
1	A	195	VAL	N-CA	-5.43	1.39	1.46
1	A	134	ASP	C-O	5.42	1.30	1.23
1	A	48	PHE	CA-CB	-5.38	1.43	1.53
1	A	282	ILE	CA-C	-5.38	1.48	1.53
1	A	81	MET	CA-C	-5.36	1.46	1.52
1	A	280	ALA	CA-CB	-5.36	1.44	1.53
1	A	72	PHE	CA-C	-5.36	1.46	1.52
1	A	110	THR	N-CA	-5.33	1.39	1.45
1	A	59	SER	N-CA	5.33	1.52	1.45
1	A	181	MET	CG-SD	5.28	1.94	1.80
1	A	93	LEU	N-CA	-5.28	1.39	1.46
1	A	111	LEU	N-CA	-5.27	1.39	1.46
1	A	56	PHE	N-CA	-5.25	1.37	1.46
1	A	61	VAL	CA-CB	5.25	1.60	1.54
1	A	158	ARG	N-CA	-5.25	1.39	1.46
1	A	235	VAL	CA-C	-5.24	1.46	1.52
1	A	238	PHE	CA-C	-5.23	1.46	1.52
1	A	8	GLU	N-CA	-5.22	1.39	1.46
1	A	51	SER	N-CA	-5.21	1.39	1.46
1	A	105	LEU	C-O	-5.18	1.17	1.24
1	A	48	PHE	CA-C	-5.17	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	227	VAL	CA-C	-5.16	1.44	1.52
1	A	56	PHE	C-O	-5.15	1.17	1.24
1	A	147	LEU	CA-C	-5.15	1.45	1.52
1	A	260	VAL	N-CA	5.13	1.52	1.46
1	A	196	ALA	CA-C	-5.13	1.46	1.52
1	A	113	VAL	N-CA	-5.11	1.40	1.46
1	A	286	ASP	CA-CB	5.11	1.62	1.53
1	A	159	PHE	CD1-CE1	5.11	1.53	1.38
1	A	241	ILE	CA-CB	-5.08	1.48	1.54
1	A	246	ILE	N-CA	5.05	1.52	1.46

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	PRO	CA-C-N	-17.09	95.66	122.49
1	A	54	PRO	C-N-CA	-17.09	95.66	122.49
1	A	212	LEU	N-CA-C	-15.83	89.55	114.09
1	A	91	TYR	CA-C-N	-15.01	105.66	120.52
1	A	91	TYR	C-N-CA	-15.01	105.66	120.52
1	A	281	SER	CA-C-N	-12.32	113.72	122.59
1	A	281	SER	C-N-CA	-12.32	113.72	122.59
1	A	92	PRO	CA-C-O	-11.23	107.33	122.15
1	A	147	LEU	N-CA-C	-10.31	99.48	113.30
1	A	118	GLY	N-CA-C	-10.07	92.79	110.71
1	A	148	ARG	NE-CZ-NH1	9.87	131.37	121.50
1	A	24	ARG	CA-C-N	-9.79	109.77	120.14
1	A	24	ARG	C-N-CA	-9.79	109.77	120.14
1	A	88	TYR	N-CA-C	-9.59	101.78	113.19
1	A	95	LYS	N-CA-C	-9.57	101.49	113.55
1	A	148	ARG	NH1-CZ-NH2	-9.34	107.15	119.30
1	A	91	TYR	N-CA-C	9.31	120.31	109.60
1	A	6	THR	CB-CA-C	-9.26	92.83	110.24
1	A	93	LEU	CA-C-O	8.75	130.08	119.49
1	A	245	VAL	N-CA-CB	8.69	122.18	112.45
1	A	69	VAL	N-CA-C	8.60	120.26	107.80
1	A	235	VAL	CB-CA-C	-8.32	98.23	110.62
1	A	219	MET	CA-C-O	-8.15	111.87	121.32
1	A	93	LEU	CA-C-N	-8.07	109.74	122.65
1	A	93	LEU	C-N-CA	-8.07	109.74	122.65
1	A	159	PHE	CA-C-N	-8.04	111.50	119.78
1	A	159	PHE	C-N-CA	-8.04	111.50	119.78
1	A	197	GLY	N-CA-C	-7.62	96.79	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	LYS	CA-C-O	-7.62	112.46	120.99
1	A	54	PRO	O-C-N	-7.57	112.43	122.64
1	A	185	ARG	N-CA-C	-7.55	97.64	109.72
1	A	149	GLY	CA-C-N	-7.50	113.01	120.21
1	A	149	GLY	C-N-CA	-7.50	113.01	120.21
1	A	149	GLY	O-C-N	-7.46	114.31	121.77
1	A	21	THR	N-CA-C	-7.41	97.75	109.23
1	A	29	ILE	CA-C-N	-7.30	114.14	123.19
1	A	29	ILE	C-N-CA	-7.30	114.14	123.19
1	A	93	LEU	O-C-N	-7.21	113.02	122.39
1	A	184	GLN	N-CA-C	7.21	122.88	107.67
1	A	256	ASN	N-CA-C	7.20	126.14	110.80
1	A	92	PRO	O-C-N	7.19	131.66	123.04
1	A	50	TYR	N-CA-C	-7.16	103.17	110.97
1	A	89	GLU	N-CA-C	-7.15	104.55	113.28
1	A	148	ARG	CB-CA-C	-7.10	95.46	111.30
1	A	225	VAL	N-CA-C	-7.10	103.86	110.53
1	A	245	VAL	CA-C-O	-7.02	113.43	121.44
1	A	67	ARG	N-CA-C	6.99	120.06	109.23
1	A	86	HIS	CA-C-N	-6.89	110.94	120.38
1	A	86	HIS	C-N-CA	-6.89	110.94	120.38
1	A	6	THR	OG1-CB-CG2	6.65	122.60	109.30
1	A	91	TYR	N-CA-CB	-6.63	100.00	109.75
1	A	261	LEU	CA-CB-CG	6.58	139.31	116.30
1	A	147	LEU	CA-C-O	6.55	127.12	119.32
1	A	131	LEU	N-CA-C	-6.54	99.86	110.20
1	A	233	LEU	N-CA-C	-6.49	101.97	110.53
1	A	154	ARG	N-CA-C	6.47	120.03	111.75
1	A	84	ARG	N-CA-C	-6.46	101.83	110.55
1	A	219	MET	N-CA-C	6.33	118.99	110.88
1	A	162	MET	CA-C-N	-6.33	111.13	120.38
1	A	162	MET	C-N-CA	-6.33	111.13	120.38
1	A	222	VAL	CA-C-N	-6.30	111.98	118.85
1	A	222	VAL	C-N-CA	-6.30	111.98	118.85
1	A	100	VAL	N-CA-C	-6.24	103.51	110.62
1	A	246	ILE	N-CA-C	6.23	122.30	109.34
1	A	87	MET	CB-CA-C	-6.21	100.12	110.68
1	A	78	CYS	CA-CB-SG	-6.17	100.22	114.40
1	A	276	SER	CA-C-N	-6.13	112.83	120.56
1	A	276	SER	C-N-CA	-6.13	112.83	120.56
1	A	134	ASP	CA-C-N	-6.12	112.99	122.59
1	A	134	ASP	C-N-CA	-6.12	112.99	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	SER	N-CA-C	-6.07	104.36	110.97
1	A	90	GLY	CA-C-N	-5.99	111.82	120.51
1	A	90	GLY	C-N-CA	-5.99	111.82	120.51
1	A	26	GLN	N-CA-C	-5.96	106.14	113.41
1	A	75	GLY	N-CA-C	-5.94	106.53	115.32
1	A	158	ARG	CA-C-N	-5.87	115.77	123.34
1	A	158	ARG	C-N-CA	-5.87	115.77	123.34
1	A	22	LYS	N-CA-C	-5.83	105.67	112.89
1	A	192	TYR	CA-C-N	-5.82	114.87	122.37
1	A	192	TYR	C-N-CA	-5.82	114.87	122.37
1	A	139	PRO	CA-C-N	-5.80	112.89	120.14
1	A	139	PRO	C-N-CA	-5.80	112.89	120.14
1	A	151	ASN	CB-CA-C	-5.80	99.68	109.72
1	A	223	PRO	N-CA-C	-5.74	105.70	113.40
1	A	35	LEU	N-CA-C	-5.69	105.65	112.59
1	A	196	ALA	CB-CA-C	-5.68	102.14	110.95
1	A	147	LEU	O-C-N	-5.68	115.37	122.24
1	A	219	MET	N-CA-CB	-5.66	103.13	111.51
1	A	58	ARG	N-CA-C	-5.63	102.19	110.52
1	A	131	LEU	CA-C-N	-5.62	115.34	122.37
1	A	131	LEU	C-N-CA	-5.62	115.34	122.37
1	A	42	LEU	CA-C-N	-5.61	114.52	122.94
1	A	42	LEU	C-N-CA	-5.61	114.52	122.94
1	A	181	MET	N-CA-C	-5.59	106.05	112.92
1	A	148	ARG	O-C-N	-5.57	114.90	122.36
1	A	195	VAL	N-CA-CB	-5.57	100.91	111.21
1	A	257	HIS	N-CA-C	5.56	120.34	113.50
1	A	95	LYS	CD-CE-NZ	-5.48	94.38	111.90
1	A	220	SER	CA-C-O	-5.45	115.07	120.80
1	A	210	GLN	N-CA-CB	5.30	118.10	110.20
1	A	91	TYR	CA-C-O	-5.29	114.89	120.02
1	A	123	LYS	CA-CB-CG	5.28	124.66	114.10
1	A	56	PHE	CA-C-N	-5.25	113.28	119.84
1	A	56	PHE	C-N-CA	-5.25	113.28	119.84
1	A	53	ILE	N-CA-C	5.21	113.03	107.76
1	A	147	LEU	CA-C-N	-5.20	112.25	121.29
1	A	147	LEU	C-N-CA	-5.20	112.25	121.29
1	A	210	GLN	N-CA-C	-5.19	105.30	111.69
1	A	226	ILE	CA-C-N	-5.16	111.41	120.29
1	A	226	ILE	C-N-CA	-5.16	111.41	120.29
1	A	85	PHE	CB-CA-C	-5.15	101.31	109.80
1	A	230	HIS	CA-C-N	-5.13	114.52	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	HIS	C-N-CA	-5.13	114.52	122.67
1	A	10	TYR	N-CA-C	-5.12	105.70	111.28
1	A	91	TYR	CB-CA-C	-5.10	101.20	109.56
1	A	100	VAL	CA-C-N	-5.08	112.59	120.31
1	A	100	VAL	C-N-CA	-5.08	112.59	120.31
1	A	180	GLN	CB-CG-CD	5.08	121.24	112.60
1	A	234	ARG	CA-C-N	-5.06	116.08	123.06
1	A	234	ARG	C-N-CA	-5.06	116.08	123.06
1	A	143	GLY	N-CA-C	-5.05	101.21	113.18
1	A	164	ASP	CA-C-N	-5.05	113.76	120.63
1	A	164	ASP	C-N-CA	-5.05	113.76	120.63
1	A	197	GLY	CA-C-O	-5.04	114.31	121.52
1	A	274	PHE	N-CA-C	-5.03	105.69	111.07
1	A	210	GLN	CB-CA-C	5.02	119.88	110.70
1	A	3	ASN	CA-C-N	-5.00	111.60	121.41
1	A	3	ASN	C-N-CA	-5.00	111.60	121.41
1	A	202	THR	N-CA-C	-5.00	103.44	110.35

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	GLN	Peptide
1	A	196	ALA	Peptide
1	A	50	TYR	Peptide
1	A	62	PRO	Peptide
1	A	64	HIS	Peptide
1	A	65	ALA	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	2251	0	2223	239	0
2	A	15	0	0	3	0
3	A	11	0	6	3	0
4	A	24	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2301	0	2229	239	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 53.

All (239) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LYS:CD	1:A:123:LYS:CG	1.74	1.60
1:A:93:LEU:CG	1:A:93:LEU:CB	1.77	1.60
1:A:148:ARG:CG	1:A:148:ARG:CD	1.81	1.59
1:A:149:GLY:CA	1:A:149:GLY:N	1.72	1.50
1:A:49:ASP:HB3	1:A:51:SER:HB2	1.24	1.18
1:A:210:GLN:OE1	1:A:246:ILE:HG21	1.46	1.12
1:A:49:ASP:HB3	1:A:51:SER:CB	1.87	1.05
1:A:284:LEU:HB2	1:A:288:ALA:HB2	1.36	1.04
1:A:148:ARG:CG	1:A:149:GLY:H	1.75	0.99
1:A:121:ASN:HD21	1:A:123:LYS:HD3	1.25	0.98
1:A:207:ARG:O	1:A:211:LYS:HG3	1.66	0.96
1:A:181:MET:HE2	1:A:183:GLU:OE2	1.68	0.93
1:A:210:GLN:CD	1:A:246:ILE:HG21	1.96	0.90
1:A:93:LEU:CB	1:A:93:LEU:CD2	2.51	0.89
1:A:148:ARG:CG	1:A:149:GLY:N	2.33	0.88
1:A:263:ALA:HB3	1:A:266:GLN:NE2	1.87	0.88
1:A:148:ARG:HG2	1:A:149:GLY:N	1.88	0.87
1:A:179:LYS:O	1:A:182:GLY:N	2.08	0.87
1:A:148:ARG:HG2	1:A:149:GLY:H	1.40	0.86
1:A:152:ASP:OD1	1:A:154:ARG:HB2	1.79	0.83
1:A:81:MET:CE	1:A:84:ARG:HA	2.09	0.83
1:A:153:GLU:HB2	4:A:347:HOH:O	1.80	0.82
1:A:88:TYR:HB2	1:A:198:PRO:HB3	1.62	0.81
1:A:201:GLU:CD	3:A:293:7DG:HN21	1.89	0.80
1:A:268:ALA:O	1:A:272:GLU:HG3	1.83	0.79
1:A:263:ALA:HB3	1:A:266:GLN:HE22	1.48	0.78
1:A:87:MET:HE1	1:A:196:ALA:HB2	1.64	0.78
1:A:2:GLU:N	4:A:319:HOH:O	2.16	0.76
1:A:42:LEU:HD12	1:A:69:VAL:HG22	1.65	0.76
1:A:263:ALA:CB	1:A:266:GLN:NE2	2.50	0.75
1:A:61:VAL:H	1:A:62:PRO:HD3	1.51	0.74
1:A:87:MET:HE1	1:A:196:ALA:CB	2.17	0.74
1:A:208:VAL:HA	1:A:211:LYS:HD2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:MET:HE2	1:A:84:ARG:HA	1.69	0.74
1:A:148:ARG:HG3	1:A:149:GLY:H	1.50	0.74
1:A:210:GLN:HE22	1:A:246:ILE:CG2	2.01	0.74
1:A:243:ASN:ND2	3:A:293:7DG:O6	2.22	0.72
1:A:79:VAL:O	1:A:79:VAL:HG13	1.88	0.72
1:A:61:VAL:H	1:A:62:PRO:CD	2.02	0.72
1:A:61:VAL:N	1:A:62:PRO:HD3	2.04	0.72
1:A:39:THR:CG2	1:A:80:MET:HE2	2.20	0.71
1:A:146:PRO:HG3	1:A:223:PRO:HB3	1.72	0.71
1:A:121:ASN:OD1	1:A:123:LYS:HB2	1.90	0.70
1:A:210:GLN:NE2	1:A:246:ILE:HG21	2.06	0.69
1:A:242:THR:HB	1:A:260:VAL:HA	1.74	0.69
1:A:35:LEU:CD1	1:A:114:THR:HB	2.22	0.69
1:A:121:ASN:ND2	1:A:123:LYS:HD3	2.05	0.69
1:A:181:MET:CE	1:A:183:GLU:OE2	2.40	0.69
1:A:284:LEU:CB	1:A:288:ALA:HB2	2.21	0.69
1:A:99:PRO:O	1:A:102:VAL:N	2.26	0.69
1:A:2:GLU:O	1:A:3:ASN:O	2.11	0.69
1:A:245:VAL:HG22	1:A:246:ILE:H	1.58	0.68
1:A:58:ARG:HD3	4:A:314:HOH:O	1.93	0.67
1:A:255:ALA:HB3	4:A:303:HOH:O	1.93	0.67
1:A:167:ASP:HB2	4:A:308:HOH:O	1.93	0.67
1:A:284:LEU:HB2	1:A:288:ALA:CB	2.21	0.66
1:A:210:GLN:NE2	1:A:246:ILE:CG2	2.59	0.66
1:A:268:ALA:O	1:A:272:GLU:CG	2.44	0.65
1:A:49:ASP:HB3	1:A:51:SER:OG	1.97	0.65
1:A:49:ASP:CB	1:A:51:SER:HB2	2.15	0.65
1:A:2:GLU:HG3	1:A:150:PRO:O	1.97	0.64
1:A:81:MET:HE1	1:A:84:ARG:HA	1.79	0.64
1:A:248:ASP:O	1:A:249:TYR:C	2.40	0.64
1:A:4:GLY:HA3	1:A:94:TRP:CZ3	2.32	0.64
1:A:263:ALA:O	1:A:266:GLN:OE1	2.17	0.63
1:A:42:LEU:CD1	1:A:69:VAL:HG22	2.29	0.63
1:A:4:GLY:HA3	1:A:94:TRP:CH2	2.33	0.62
1:A:99:PRO:O	1:A:100:VAL:C	2.42	0.62
1:A:251:SER:C	1:A:253:GLU:H	2.07	0.62
1:A:178:TRP:CD1	1:A:187:LEU:HB2	2.34	0.62
1:A:84:ARG:NE	1:A:220:SER:HB2	2.14	0.62
1:A:178:TRP:CG	1:A:187:LEU:HB2	2.34	0.62
1:A:173:ARG:HD2	1:A:281:SER:HB3	1.82	0.61
1:A:42:LEU:HD13	1:A:71:GLY:HA3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:TYR:N	1:A:166:TYR:CD2	2.68	0.60
1:A:153:GLU:CB	4:A:347:HOH:O	2.44	0.60
1:A:101:ARG:HG2	1:A:101:ARG:HH11	1.66	0.60
1:A:84:ARG:NH1	2:A:290:SO4:O1	2.35	0.60
1:A:23:HIS:C	1:A:24:ARG:HD3	2.26	0.60
1:A:263:ALA:CB	1:A:266:GLN:HE22	2.09	0.60
1:A:120:LEU:HD12	1:A:215:ASP:C	2.26	0.60
1:A:135:HIS:CE1	1:A:222:VAL:HG13	2.36	0.60
1:A:30:ILE:HG23	1:A:84:ARG:HB3	1.83	0.60
1:A:39:THR:HG23	1:A:80:MET:HE2	1.83	0.59
1:A:31:CYS:HA	1:A:114:THR:OG1	2.03	0.59
1:A:58:ARG:CG	4:A:314:HOH:O	2.50	0.59
1:A:74:ASN:CG	1:A:74:ASN:O	2.41	0.59
1:A:79:VAL:O	1:A:79:VAL:CG1	2.50	0.59
1:A:103:PHE:O	1:A:104:HIS:C	2.46	0.59
1:A:87:MET:HG3	1:A:93:LEU:CD1	2.33	0.59
1:A:262:ALA:C	1:A:264:GLY:H	2.11	0.59
1:A:87:MET:HG3	1:A:93:LEU:HD11	1.85	0.58
1:A:87:MET:CE	1:A:196:ALA:CB	2.81	0.58
1:A:172:GLN:O	1:A:173:ARG:C	2.43	0.58
1:A:134:ASP:O	1:A:191:THR:HA	2.03	0.58
1:A:39:THR:HG22	1:A:80:MET:HE2	1.83	0.58
1:A:84:ARG:CZ	1:A:220:SER:HB2	2.34	0.57
1:A:29:ILE:HG12	1:A:112:VAL:HG13	1.86	0.57
1:A:243:ASN:HB3	1:A:259:GLU:HB2	1.87	0.57
1:A:35:LEU:HD13	1:A:114:THR:HB	1.87	0.56
1:A:32:GLY:H	1:A:35:LEU:HD12	1.71	0.56
1:A:57:PRO:HB2	1:A:85:PHE:CZ	2.41	0.56
1:A:122:PRO:C	1:A:124:PHE:H	2.13	0.56
1:A:168:ARG:HA	1:A:171:ARG:NH1	2.21	0.56
1:A:87:MET:CG	1:A:93:LEU:CD1	2.84	0.56
1:A:201:GLU:OE2	3:A:293:7DG:N2	2.39	0.55
1:A:49:ASP:OD1	1:A:51:SER:OG	2.21	0.55
1:A:208:VAL:HA	1:A:211:LYS:CD	2.37	0.55
1:A:122:PRO:O	1:A:124:PHE:N	2.40	0.55
1:A:167:ASP:O	1:A:171:ARG:HG3	2.07	0.55
1:A:24:ARG:HD3	1:A:24:ARG:N	2.21	0.54
1:A:147:LEU:HD22	1:A:226:ILE:HG22	1.89	0.54
1:A:193:VAL:HG13	1:A:193:VAL:O	2.07	0.54
1:A:86:HIS:O	1:A:87:MET:C	2.44	0.54
1:A:76:ARG:NH2	1:A:282:ILE:O	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:HD21	1:A:144:GLN:O	2.07	0.54
1:A:11:LYS:O	1:A:12:ASN:C	2.50	0.54
1:A:255:ALA:CB	4:A:341:HOH:O	2.56	0.54
1:A:84:ARG:HG2	1:A:84:ARG:HH11	1.73	0.54
1:A:222:VAL:O	1:A:223:PRO:C	2.50	0.54
1:A:265:LYS:O	1:A:269:GLN:HB2	2.08	0.54
1:A:157:ASP:O	1:A:160:PRO:HD3	2.08	0.53
1:A:86:HIS:CD2	1:A:88:TYR:CE1	2.97	0.53
1:A:180:GLN:HG2	1:A:181:MET:HG3	1.91	0.53
1:A:92:PRO:HB3	2:A:292:SO4:O2	2.09	0.53
1:A:171:ARG:HG3	1:A:171:ARG:HH11	1.73	0.53
1:A:207:ARG:HH21	1:A:247:MET:HA	1.74	0.52
1:A:61:VAL:N	1:A:62:PRO:CD	2.69	0.52
1:A:26:GLN:HG3	1:A:285:PRO:HG3	1.91	0.52
1:A:125:GLU:CD	1:A:185:ARG:HD2	2.36	0.51
1:A:93:LEU:CB	1:A:93:LEU:CD1	2.82	0.51
1:A:217:VAL:HG22	1:A:218:GLY:N	2.24	0.51
1:A:201:GLU:CD	1:A:201:GLU:N	2.69	0.51
1:A:169:THR:HG22	1:A:173:ARG:HE	1.76	0.51
1:A:146:PRO:HB2	1:A:227:VAL:HG12	1.92	0.51
1:A:56:PHE:O	1:A:57:PRO:C	2.47	0.51
1:A:155:PHE:O	1:A:231:CYS:HA	2.11	0.51
1:A:196:ALA:O	1:A:197:GLY:O	2.29	0.51
1:A:10:TYR:CZ	1:A:101:ARG:HD2	2.46	0.50
1:A:93:LEU:HB3	1:A:146:PRO:HA	1.92	0.50
1:A:113:VAL:HG23	1:A:113:VAL:O	2.11	0.50
1:A:31:CYS:SG	1:A:80:MET:HE3	2.51	0.50
1:A:134:ASP:HB3	1:A:191:THR:HG23	1.94	0.50
1:A:274:PHE:CE1	1:A:278:LEU:HD11	2.47	0.49
1:A:17:LEU:O	1:A:21:THR:HG22	2.13	0.49
1:A:101:ARG:HH11	1:A:101:ARG:CG	2.24	0.48
1:A:93:LEU:CG	1:A:93:LEU:CA	2.81	0.48
1:A:130:MET:O	1:A:238:PHE:HA	2.13	0.48
1:A:113:VAL:HB	1:A:221:THR:HG23	1.96	0.48
1:A:278:LEU:O	1:A:279:MET:C	2.56	0.48
1:A:122:PRO:C	1:A:124:PHE:N	2.70	0.48
1:A:87:MET:C	1:A:89:GLU:N	2.69	0.48
1:A:87:MET:C	1:A:89:GLU:H	2.21	0.48
1:A:23:HIS:O	1:A:24:ARG:HD3	2.14	0.47
1:A:119:GLY:O	1:A:244:LYS:HB3	2.13	0.47
1:A:249:TYR:O	1:A:250:GLU:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:CYS:SG	1:A:80:MET:CE	3.03	0.47
1:A:175:LEU:HD11	1:A:189:GLU:OE1	2.15	0.47
1:A:148:ARG:CD	1:A:148:ARG:CB	2.79	0.47
1:A:255:ALA:HB1	4:A:341:HOH:O	2.15	0.47
1:A:143:GLY:O	1:A:145:ASN:N	2.47	0.47
1:A:86:HIS:CD2	1:A:88:TYR:OH	2.68	0.46
1:A:121:ASN:O	1:A:124:PHE:HB2	2.16	0.46
1:A:174:ALA:HA	1:A:278:LEU:HD21	1.97	0.46
1:A:221:THR:O	1:A:222:VAL:C	2.57	0.46
1:A:242:THR:HA	1:A:262:ALA:HB2	1.97	0.46
1:A:58:ARG:CD	4:A:314:HOH:O	2.55	0.46
1:A:137:ASN:ND2	1:A:226:ILE:HD11	2.31	0.46
1:A:92:PRO:C	1:A:94:TRP:N	2.70	0.46
1:A:220:SER:HA	4:A:295:HOH:O	2.15	0.46
1:A:196:ALA:C	1:A:197:GLY:O	2.52	0.45
1:A:179:LYS:O	1:A:180:GLN:C	2.59	0.45
1:A:132:ILE:CG2	1:A:166:TYR:CE1	2.99	0.45
1:A:205:GLU:O	1:A:208:VAL:HG13	2.16	0.45
1:A:18:LEU:HD12	1:A:18:LEU:HA	1.88	0.45
1:A:38:LEU:HB3	1:A:80:MET:HE1	1.98	0.45
1:A:45:ALA:HA	1:A:70:PHE:O	2.17	0.45
1:A:277:ILE:O	1:A:279:MET:N	2.50	0.45
1:A:282:ILE:O	1:A:283:PRO:C	2.60	0.45
1:A:43:THR:O	1:A:44:GLN:HB2	2.16	0.44
1:A:251:SER:C	1:A:253:GLU:N	2.75	0.44
1:A:32:GLY:HA3	1:A:115:ASN:HA	1.99	0.44
1:A:92:PRO:HB3	2:A:292:SO4:S	2.57	0.44
1:A:195:VAL:O	1:A:219:MET:HG2	2.17	0.44
1:A:165:ALA:O	1:A:229:ARG:HD3	2.17	0.44
1:A:21:THR:HA	1:A:46:GLN:HE22	1.82	0.44
1:A:257:HIS:HA	1:A:260:VAL:HG12	1.98	0.44
1:A:60:THR:O	1:A:61:VAL:HG23	2.17	0.44
1:A:87:MET:CE	1:A:196:ALA:HB1	2.48	0.44
1:A:42:LEU:HD12	1:A:69:VAL:CG2	2.41	0.44
1:A:25:PRO:HG2	1:A:108:VAL:HG23	1.99	0.43
1:A:285:PRO:C	1:A:287:LYS:H	2.26	0.43
1:A:6:THR:O	1:A:7:TYR:C	2.61	0.43
1:A:15:GLU:O	1:A:16:TRP:C	2.61	0.43
1:A:35:LEU:HD12	1:A:114:THR:CB	2.48	0.43
1:A:277:ILE:C	1:A:279:MET:N	2.75	0.43
1:A:93:LEU:CD2	1:A:93:LEU:HB2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:THR:HA	1:A:180:GLN:HB3	2.00	0.43
1:A:81:MET:HE2	1:A:81:MET:HB3	1.92	0.43
1:A:257:HIS:HA	1:A:260:VAL:CG1	2.49	0.43
1:A:6:THR:O	1:A:9:ASP:HB2	2.18	0.43
1:A:147:LEU:HD12	1:A:147:LEU:HA	1.44	0.43
1:A:121:ASN:HA	1:A:122:PRO:HD3	1.73	0.43
1:A:63:GLY:O	1:A:66:GLY:N	2.51	0.43
1:A:266:GLN:CD	1:A:266:GLN:H	2.27	0.43
1:A:21:THR:OG1	1:A:23:HIS:HD2	2.02	0.43
1:A:86:HIS:CD2	1:A:88:TYR:CZ	3.07	0.43
1:A:145:ASN:HA	1:A:146:PRO:HD3	1.71	0.43
1:A:146:PRO:HG2	1:A:223:PRO:HA	2.00	0.42
1:A:3:ASN:O	1:A:5:TYR:N	2.50	0.42
1:A:109:ASP:OD2	1:A:109:ASP:C	2.62	0.42
1:A:201:GLU:CD	1:A:201:GLU:H	2.27	0.42
1:A:53:ILE:O	1:A:54:PRO:C	2.60	0.42
1:A:35:LEU:HD12	1:A:114:THR:OG1	2.18	0.42
1:A:181:MET:O	1:A:182:GLY:C	2.62	0.42
1:A:113:VAL:O	1:A:237:GLY:HA3	2.20	0.42
1:A:171:ARG:NH1	4:A:345:HOH:O	2.37	0.42
1:A:68:LEU:HA	1:A:68:LEU:HD12	1.71	0.42
1:A:121:ASN:OD1	1:A:123:LYS:CB	2.63	0.41
1:A:225:VAL:O	1:A:228:ALA:HB3	2.20	0.41
1:A:278:LEU:C	1:A:280:ALA:N	2.74	0.41
1:A:28:ALA:HA	1:A:79:VAL:O	2.20	0.41
1:A:17:LEU:HD23	1:A:17:LEU:HA	1.89	0.41
1:A:24:ARG:HD2	1:A:24:ARG:HA	1.88	0.41
1:A:59:SER:HB3	1:A:62:PRO:HD2	2.02	0.41
1:A:177:THR:O	1:A:177:THR:HG22	2.20	0.41
1:A:277:ILE:C	1:A:279:MET:H	2.29	0.41
1:A:102:VAL:O	1:A:103:PHE:C	2.63	0.41
1:A:13:THR:OG1	1:A:55:ASN:ND2	2.53	0.41
1:A:63:GLY:O	1:A:66:GLY:HA3	2.21	0.41
1:A:73:LEU:HD12	1:A:73:LEU:HA	1.99	0.41
1:A:97:THR:O	1:A:98:PHE:C	2.63	0.41
1:A:107:GLY:O	1:A:108:VAL:C	2.64	0.41
1:A:138:LEU:HD12	1:A:138:LEU:HA	1.70	0.40
1:A:271:LEU:O	1:A:271:LEU:HD22	2.21	0.40
1:A:154:ARG:HB2	1:A:154:ARG:HE	1.65	0.40
1:A:245:VAL:HG13	1:A:246:ILE:N	2.35	0.40
1:A:88:TYR:CD2	1:A:88:TYR:C	3.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:PRO:O	1:A:287:LYS:N	2.54	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	286/289 (99%)	239 (84%)	31 (11%)	16 (6%)	1 2

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	51	SER
1	A	123	LYS
1	A	180	GLN
1	A	246	ILE
1	A	263	ALA
1	A	61	VAL
1	A	77	ALA
1	A	182	GLY
1	A	285	PRO
1	A	287	LYS
1	A	288	ALA
1	A	250	GLU
1	A	256	ASN
1	A	252	LEU
1	A	260	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	239/240 (100%)	182 (76%)	57 (24%)	1 1

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	6	THR
1	A	8	GLU
1	A	11	LYS
1	A	18	LEU
1	A	26	GLN
1	A	35	LEU
1	A	41	LYS
1	A	49	ASP
1	A	54	PRO
1	A	57	PRO
1	A	61	VAL
1	A	67	ARG
1	A	69	VAL
1	A	80	MET
1	A	84	ARG
1	A	93	LEU
1	A	101	ARG
1	A	102	VAL
1	A	106	LEU
1	A	108	VAL
1	A	112	VAL
1	A	115	ASN
1	A	120	LEU
1	A	123	LYS
1	A	125	GLU
1	A	126	VAL
1	A	131	LEU
1	A	138	LEU
1	A	147	LEU

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Mol	Chain	Res	Type
1	A	154	ARG
1	A	172	GLN
1	A	176	SER
1	A	180	GLN
1	A	181	MET
1	A	186	GLU
1	A	195	VAL
1	A	201	GLU
1	A	208	VAL
1	A	209	LEU
1	A	211	LYS
1	A	220	SER
1	A	221	THR
1	A	227	VAL
1	A	234	ARG
1	A	247	MET
1	A	248	ASP
1	A	249	TYR
1	A	252	LEU
1	A	254	LYS
1	A	260	VAL
1	A	266	GLN
1	A	269	GLN
1	A	270	LYS
1	A	271	LEU
1	A	272	GLU
1	A	287	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	23	HIS
1	A	46	GLN
1	A	55	ASN
1	A	180	GLN
1	A	210	GLN
1	A	256	ASN
1	A	266	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

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	SO4	A	290	-	4,4,4	0.59	0	6,6,6	1.05	0
2	SO4	A	291	-	4,4,4	0.37	0	6,6,6	1.53	1 (16%)
3	7DG	A	293	-	9,12,12	1.61	2 (22%)	10,17,17	3.63	6 (60%)
2	SO4	A	292	-	4,4,4	0.28	0	6,6,6	1.94	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	7DG	A	293	-	-	-	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	293	7DG	C8-N9	3.07	1.38	1.29
3	A	293	7DG	C6-C5	2.52	1.48	1.44

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	293	7DG	C8-N9-C4	6.40	111.84	103.02
3	A	293	7DG	N9-C4-N3	6.26	133.37	125.45
3	A	293	7DG	N2-C2-N3	-4.74	110.41	119.67
2	A	292	SO4	O4-S-O1	-3.20	92.84	109.56
3	A	293	7DG	C5-C6-N1	-2.63	113.71	115.70
2	A	291	SO4	O3-S-O1	-2.48	96.57	109.56
3	A	293	7DG	N2-C2-N1	2.45	121.94	116.76
3	A	293	7DG	N1-C2-N3	2.36	127.65	123.32
2	A	292	SO4	O3-S-O1	-2.11	98.54	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	290	SO4	1	0
3	A	293	7DG	3	0
2	A	292	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	288/289 (99%)	0.48	36 (12%) 8 6	14, 38, 95, 123	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	LEU	10.5
1	A	261	LEU	9.1
1	A	65	ALA	7.5
1	A	255	ALA	6.7
1	A	288	ALA	6.5
1	A	260	VAL	5.8
1	A	263	ALA	5.8
1	A	245	VAL	5.7
1	A	249	TYR	5.5
1	A	256	ASN	5.5
1	A	257	HIS	5.3
1	A	62	PRO	5.1
1	A	264	GLY	5.1
1	A	286	ASP	4.9
1	A	254	LYS	4.4
1	A	259	GLU	4.4
1	A	246	ILE	4.2
1	A	287	LYS	4.1
1	A	64	HIS	4.1
1	A	262	ALA	3.9
1	A	180	GLN	3.7
1	A	61	VAL	3.6
1	A	258	GLU	3.5
1	A	2	GLU	3.4
1	A	253	GLU	3.4
1	A	251	SER	2.9
1	A	250	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	247	MET	2.8
1	A	289	SER	2.7
1	A	185	ARG	2.7
1	A	123	LYS	2.3
1	A	266	GLN	2.1
1	A	248	ASP	2.1
1	A	273	GLN	2.1
1	A	186	GLU	2.0
1	A	3	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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
3	7DG	A	293	11/11	0.95	0.09	20,25,27,29	2
2	SO4	A	291	5/5	0.97	0.08	39,42,45,47	0
2	SO4	A	292	5/5	0.99	0.07	23,26,29,31	0
2	SO4	A	290	5/5	0.99	0.04	23,24,29,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.