



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:55 am BST

PDB ID : 3INY
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

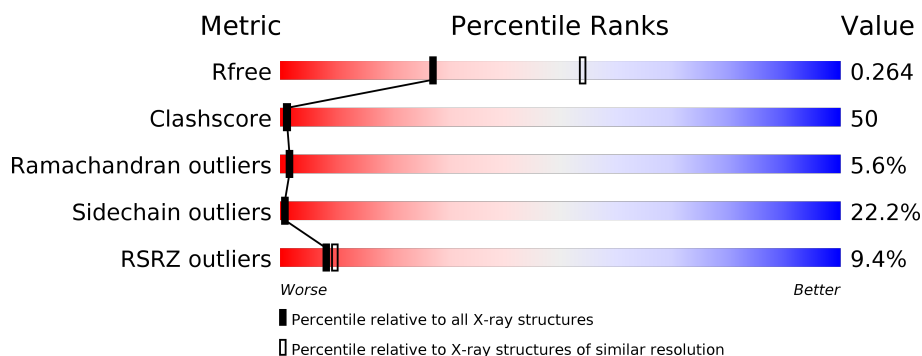
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 ≥ 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	<div> <div>9%</div> <div>25%</div> <div>48%</div> <div>20%</div> <div>6%</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	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:

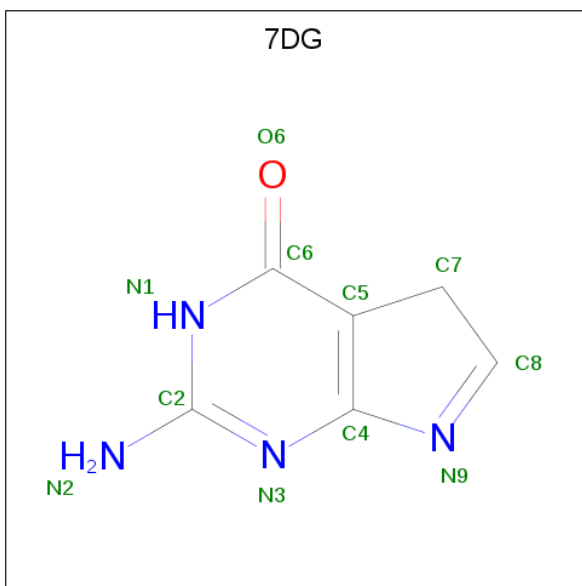
Chain	Residue	Modelled	Actual	Comment	Reference
A	51	SER	GLY	SEE REMARK 999	UNP P00491

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

• Molecule 1: 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 43.68 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.7 (43.69-2.75) 98.7 (43.68-2.75)	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 (4.99%)	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)	0.42 , 63.5	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	0.92	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	1.91	41/2303 (1.8%)	1.72	38/3115 (1.2%)

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 (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	GLY	N-CA	17.39	1.72	1.46
1	A	148	ARG	CG-CD	11.72	1.81	1.51
1	A	8	GLU	CG-CD	10.40	1.67	1.51
1	A	78	CYS	CB-SG	-9.28	1.66	1.82
1	A	201	GLU	CB-CG	-8.84	1.35	1.52
1	A	93	LEU	CB-CG	8.62	1.77	1.52
1	A	65	ALA	CA-CB	8.30	1.69	1.52
1	A	123	LYS	CB-CG	7.90	1.73	1.52
1	A	16	TRP	CB-CG	-7.79	1.36	1.50
1	A	125	GLU	CG-CD	7.53	1.63	1.51
1	A	2	GLU	CG-CD	7.51	1.63	1.51
1	A	180	GLN	CB-CG	7.47	1.72	1.52
1	A	166	TYR	CD1-CE1	-7.46	1.28	1.39
1	A	102	VAL	CB-CG2	-7.41	1.37	1.52
1	A	159	PHE	CD1-CE1	7.36	1.53	1.39
1	A	149	GLY	C-O	7.29	1.35	1.23
1	A	245	VAL	N-CA	7.05	1.60	1.46
1	A	94	TRP	CB-CG	6.90	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	GLY	N-CA	6.55	1.55	1.46
1	A	123	LYS	CG-CD	6.50	1.74	1.52
1	A	8	GLU	CB-CG	6.21	1.64	1.52
1	A	166	TYR	CD2-CE2	-6.14	1.30	1.39
1	A	260	VAL	CA-CB	6.08	1.67	1.54
1	A	93	LEU	CA-C	-6.06	1.37	1.52
1	A	152	ASP	C-O	6.00	1.34	1.23
1	A	6	THR	CB-CG2	5.90	1.71	1.52
1	A	195	VAL	CB-CG2	-5.72	1.40	1.52
1	A	91	TYR	C-N	-5.58	1.23	1.34
1	A	58	ARG	CG-CD	5.50	1.65	1.51
1	A	51	SER	CA-CB	5.44	1.61	1.52
1	A	159	PHE	CE2-CZ	5.29	1.47	1.37
1	A	54	PRO	N-CA	-5.28	1.38	1.47
1	A	93	LEU	CG-CD1	5.22	1.71	1.51
1	A	123	LYS	CD-CE	5.21	1.64	1.51
1	A	129	ILE	CA-CB	-5.21	1.42	1.54
1	A	55	ASN	N-CA	5.18	1.56	1.46
1	A	114	THR	C-O	-5.16	1.13	1.23
1	A	217	VAL	CB-CG2	-5.15	1.42	1.52
1	A	146	PRO	C-N	5.14	1.45	1.34
1	A	221	THR	C-O	5.04	1.32	1.23
1	A	98	PHE	CB-CG	-5.03	1.42	1.51

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ARG	NE-CZ-NH1	22.13	131.37	120.30
1	A	148	ARG	NH1-CZ-NH2	-11.13	107.15	119.40
1	A	261	LEU	CA-CB-CG	10.44	139.31	115.30
1	A	54	PRO	C-N-CA	-10.42	95.66	121.70
1	A	118	GLY	N-CA-C	-8.12	92.79	113.10
1	A	212	LEU	N-CA-C	-7.94	89.55	111.00
1	A	78	CYS	CA-CB-SG	-7.66	100.22	114.00
1	A	95	LYS	CD-CE-NZ	-7.53	94.38	111.70
1	A	148	ARG	CB-CA-C	-7.47	95.46	110.40
1	A	6	THR	CB-CA-C	-6.95	92.83	111.60
1	A	235	VAL	CB-CA-C	-6.93	98.23	111.40
1	A	212	LEU	CA-CB-CG	6.84	131.03	115.30
1	A	93	LEU	CB-CG-CD2	-6.83	99.39	111.00
1	A	219	MET	CG-SD-CE	6.81	111.10	100.20
1	A	197	GLY	N-CA-C	-6.52	96.79	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	PRO	O-C-N	-6.42	112.43	122.70
1	A	134	ASP	CB-CG-OD1	-6.24	112.69	118.30
1	A	93	LEU	O-C-N	-6.05	113.02	122.70
1	A	252	LEU	CA-CB-CG	6.00	129.10	115.30
1	A	185	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	91	TYR	N-CA-CB	-5.89	100.00	110.60
1	A	131	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	49	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	120	LEU	CB-CG-CD2	-5.66	101.38	111.00
1	A	256	ASN	N-CA-C	5.61	126.14	111.00
1	A	92	PRO	O-C-N	5.60	131.66	122.70
1	A	6	THR	OG1-CB-CG2	5.48	122.60	110.00
1	A	96	VAL	CG1-CB-CG2	-5.46	102.16	110.90
1	A	92	PRO	CA-C-O	-5.36	107.33	120.20
1	A	151	ASN	CB-CA-C	-5.36	99.68	110.40
1	A	196	ALA	CB-CA-C	-5.30	102.14	110.10
1	A	206	CYS	CA-CB-SG	-5.26	104.54	114.00
1	A	149	GLY	C-N-CD	5.20	139.31	128.40
1	A	138	LEU	CB-CA-C	5.17	120.02	110.20
1	A	101	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	87	MET	CB-CA-C	-5.14	100.12	110.40
1	A	123	LYS	CA-CB-CG	5.12	124.66	113.40
1	A	3	ASN	C-N-CA	-5.09	111.60	122.30

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	224	0
2	A	15	0	0	3	0
3	A	11	0	6	3	0
4	A	24	0	0	12	0
All	All	2301	0	2229	224	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 50.

All (224) 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:CG	1:A:123:LYS:CD	1.74	1.60
1:A:93:LEU:CB	1:A:93:LEU:CG	1.77	1.60
1:A:148:ARG:CD	1:A:148:ARG:CG	1.81	1.59
1:A:149:GLY:N	1:A:149:GLY:CA	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: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:210:GLN:CD	1:A:246:ILE:HG21	1.96	0.85
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: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: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:201:GLU:CD	3:A:293:7DG:HN21	1.89	0.75
1:A:61:VAL:H	1:A:62:PRO:HD3	1.51	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: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:81:MET:HE2	1:A:84:ARG:HA	1.71	0.72
1:A:61:VAL:N	1:A:62:PRO:HD3	2.04	0.72
1:A:87:MET:HE1	1:A:196:ALA:HB2	1.71	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:181:MET:CE	1:A:183:GLU:OE2	2.40	0.69
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: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:255:ALA:HB3	4:A:303:HOH:O	1.93	0.67
1:A:58:ARG:HD3	4:A:314:HOH:O	1.93	0.67
1:A:167:ASP:HB2	4:A:308:HOH:O	1.93	0.67
1:A:81:MET:HE1	1:A:84:ARG:HA	1.77	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:87:MET:HE1	1:A:196:ALA:CB	2.27	0.64
1:A:2:GLU:HG3	1:A:150:PRO:O	1.97	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: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
1:A:166:TYR:CD2	1:A:166:TYR:N	2.68	0.60
1:A:153:GLU:CB	4:A:347:HOH:O	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ARG:HH11	1:A:101:ARG:HG2	1.66	0.60
1:A:84:ARG:NH1	2:A:290:SO4:O1	2.35	0.60
1:A:263:ALA:CB	1:A:266:GLN:HE22	2.09	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:248:ASP:O	1:A:249:TYR:C	2.40	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:79:VAL:O	1:A:79:VAL:CG1	2.50	0.59
1:A:87:MET:HG3	1:A:93:LEU:CD1	2.33	0.59
1:A:181:MET:HE1	1:A:183:GLU:OE2	2.03	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:134:ASP:O	1:A:191:THR:HA	2.03	0.58
1:A:31:CYS:SG	1:A:80:MET:HE3	2.44	0.58
1:A:99:PRO:O	1:A:100:VAL:C	2.42	0.58
1:A:251:SER:C	1:A:253:GLU:H	2.07	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:181:MET:HE2	1:A:183:GLU:OE2	2.04	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: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:23:HIS:C	1:A:24:ARG:HD3	2.26	0.55
1:A:201:GLU:OE2	3:A:293:7DG:N2	2.39	0.55
1:A:120:LEU:HD12	1:A:215:ASP:C	2.26	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:172:GLN:O	1:A:173:ARG:C	2.43	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:147:LEU:HD22	1:A:226:ILE:HG22	1.89	0.54
1:A:24:ARG:N	1:A:24:ARG:HD3	2.21	0.54
1:A:193:VAL:HG13	1:A:193:VAL:O	2.07	0.54
1:A:74:ASN:CG	1:A:74:ASN:O	2.41	0.54
1:A:103:PHE:O	1:A:104:HIS:C	2.46	0.54
1:A:76:ARG:NH2	1:A:282:ILE:O	2.38	0.54
1:A:93:LEU:HD21	1:A:144:GLN:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ALA:C	1:A:264:GLY:H	2.11	0.54
1:A:255:ALA:CB	4:A:341:HOH:O	2.56	0.54
1:A:265:LYS:O	1:A:269:GLN:HB2	2.08	0.54
1:A:84:ARG:HG2	1:A:84:ARG:HH11	1.73	0.54
1:A:86:HIS:O	1:A:87:MET:C	2.44	0.54
1:A:157:ASP:O	1:A:160:PRO:HD3	2.08	0.53
1:A:180:GLN:HG2	1:A:181:MET:HG3	1.91	0.53
1:A:86:HIS:CD2	1:A:88:TYR:CE1	2.97	0.53
1:A:171:ARG:HG3	1:A:171:ARG:HH11	1.73	0.53
1:A:92:PRO:HB3	2:A:292:SO4:O2	2.09	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:93:LEU:CD1	1:A:93:LEU:CB	2.82	0.51
1:A:217:VAL:HG22	1:A:218:GLY:N	2.24	0.51
1:A:122:PRO:C	1:A:124:PHE:H	2.13	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:196:ALA:O	1:A:197:GLY:O	2.29	0.51
1:A:155:PHE:O	1:A:231:CYS:HA	2.11	0.51
1:A:113:VAL:O	1:A:113:VAL:HG23	2.11	0.50
1:A:39:THR:CG2	1:A:80:MET:HE2	2.41	0.50
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:134:ASP:HB3	1:A:191:THR:HG23	1.94	0.50
1:A:87:MET:HE3	1:A:196:ALA:HB1	1.93	0.50
1:A:274:PHE:CE1	1:A:278:LEU:HD11	2.47	0.49
1:A:11:LYS:O	1:A:12:ASN:C	2.50	0.49
1:A:17:LEU:O	1:A:21:THR:HG22	2.13	0.49
1:A:222:VAL:O	1:A:223:PRO:C	2.50	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:119:GLY:O	1:A:244:LYS:HB3	2.13	0.47
1:A:23:HIS:O	1:A:24:ARG:HD3	2.14	0.47
1:A:249:TYR:O	1:A:250:GLU:HB2	2.13	0.47
1:A:56:PHE:O	1:A:57:PRO:C	2.47	0.47
1:A:175:LEU:HD11	1:A:189:GLU:OE1	2.15	0.47
1:A:148:ARG:CB	1:A:148:ARG:CD	2.79	0.47
1:A:196:ALA:C	1:A:197:GLY:O	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:31:CYS:SG	1:A:80:MET:CE	3.03	0.46
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:242:THR:HA	1:A:262:ALA:HB2	1.97	0.46
1:A:43:THR:O	1:A:44:GLN:HB2	2.16	0.46
1:A:201:GLU:N	1:A:201:GLU:CD	2.69	0.46
1:A:137:ASN:ND2	1:A:226:ILE:HD11	2.31	0.46
1:A:58:ARG:CD	4:A:314:HOH:O	2.55	0.46
1:A:125:GLU:CD	1:A:185:ARG:HD2	2.36	0.46
1:A:220:SER:HA	4:A:295:HOH:O	2.15	0.46
1:A:122:PRO:C	1:A:124:PHE:N	2.70	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:87:MET:C	1:A:89:GLU:N	2.69	0.45
1:A:18:LEU:HA	1:A:18:LEU:HD12	1.88	0.45
1:A:277:ILE:O	1:A:279:MET:N	2.50	0.45
1:A:45:ALA:HA	1:A:70:PHE:O	2.17	0.45
1:A:81:MET:HE2	1:A:81:MET:HB3	1.90	0.45
1:A:39:THR:HG22	1:A:80:MET:HE2	1.99	0.45
1:A:32:GLY:HA3	1:A:115:ASN:HA	1.99	0.44
1:A:195:VAL:O	1:A:219:MET:HG2	2.17	0.44
1:A:92:PRO:HB3	2:A:292:SO4:S	2.57	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:92:PRO:C	1:A:94:TRP:N	2.70	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:278:LEU:O	1:A:279:MET:C	2.56	0.43
1:A:87:MET:C	1:A:89:GLU:H	2.21	0.43
1:A:35:LEU:HD12	1:A:114:THR:CB	2.48	0.43
1:A:177:THR:HA	1:A:180:GLN:HB3	2.00	0.43
1:A:93:LEU:HB2	1:A:93:LEU:CD2	2.46	0.43
1:A:257:HIS:HA	1:A:260:VAL:CG1	2.49	0.43
1:A:147:LEU:HA	1:A:147:LEU:HD12	1.44	0.43
1:A:221:THR:O	1:A:222:VAL:C	2.57	0.43
1:A:6:THR:O	1:A:9:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:170:MET:HE2	1:A:170:MET:HB3	1.91	0.43
1:A:21:THR:OG1	1:A:23:HIS:HD2	2.02	0.43
1:A:145:ASN:HA	1:A:146:PRO:HD3	1.71	0.43
1:A:86:HIS:CD2	1:A:88:TYR:CZ	3.07	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:35:LEU:HD12	1:A:114:THR:OG1	2.18	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: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:245:VAL:HG13	1:A:246:ILE:N	2.35	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:HG22	1:A:177:THR:O	2.20	0.41
1:A:87:MET:CE	1:A:196:ALA:HB1	2.48	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:179:LYS:O	1:A:180:GLN:C	2.59	0.41
1:A:138:LEU:HA	1:A:138:LEU:HD12	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:282:ILE:O	1:A:283:PRO:C	2.60	0.40
1:A:285:PRO:O	1:A:287:LYS:N	2.54	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	286/289 (99%)	239 (84%)	31 (11%)	16 (6%)	2 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%)	186 (78%)	53 (22%)	1 1

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	6	THR
1	A	11	LYS

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Mol	Chain	Res	Type
1	A	18	LEU
1	A	24	ARG
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	106	LEU
1	A	112	VAL
1	A	115	ASN
1	A	120	LEU
1	A	123	LYS
1	A	125	GLU
1	A	131	LEU
1	A	133	ARG
1	A	138	LEU
1	A	147	LEU
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	244	LYS
1	A	247	MET
1	A	248	ASP
1	A	249	TYR
1	A	252	LEU

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Mol	Chain	Res	Type
1	A	254	LYS
1	A	260	VAL
1	A	261	LEU
1	A	266	GLN
1	A	269	GLN
1	A	270	LYS
1	A	271	LEU
1	A	287	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	55	ASN
1	A	115	ASN
1	A	210	GLN
1	A	256	ASN
1	A	266	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	292	-	4,4,4	0.30	0	6,6,6	2.01	3 (50%)
2	SO4	A	291	-	4,4,4	0.35	0	6,6,6	1.62	2 (33%)
3	7DG	A	293	-	10,12,12	1.65	2 (20%)	8,17,17	6.06	7 (87%)
2	SO4	A	290	-	4,4,4	0.51	0	6,6,6	1.13	0

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	C6-C5	3.38	1.48	1.41
3	A	293	7DG	C4-N9	2.24	1.39	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	293	7DG	C4-N9-C8	12.19	111.84	103.85
3	A	293	7DG	C6-C5-C4	7.59	119.37	115.00
3	A	293	7DG	C5-C4-N9	-4.89	105.66	110.40
3	A	293	7DG	N2-C2-N3	-4.40	110.41	117.25
3	A	293	7DG	C5-C7-C8	4.15	106.70	102.54
3	A	293	7DG	C6-N1-C2	4.04	122.35	115.93
2	A	292	SO4	O4-S-O1	-3.16	92.84	109.31
3	A	293	7DG	N2-C2-N1	3.01	121.94	117.25
2	A	291	SO4	O3-S-O1	-2.44	96.57	109.31
2	A	291	SO4	O4-S-O3	2.41	119.37	109.06
2	A	292	SO4	O4-S-O3	2.35	119.09	109.06
2	A	292	SO4	O3-S-O1	-2.06	98.54	109.31

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	292	SO4	2	0
3	A	293	7DG	3	0
2	A	290	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	0.36	27 (9%) 8 10	14, 38, 95, 123	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	ALA	9.8
1	A	260	VAL	7.7
1	A	252	LEU	7.2
1	A	256	ASN	6.4
1	A	249	TYR	6.3
1	A	262	ALA	6.2
1	A	258	GLU	5.3
1	A	263	ALA	5.0
1	A	286	ASP	4.8
1	A	253	GLU	4.8
1	A	259	GLU	4.7
1	A	65	ALA	4.7
1	A	254	LYS	4.6
1	A	257	HIS	4.3
1	A	288	ALA	4.2
1	A	184	GLN	4.0
1	A	185	ARG	3.7
1	A	250	GLU	3.6
1	A	64	HIS	2.9
1	A	265	LYS	2.7
1	A	261	LEU	2.7
1	A	251	SER	2.6
1	A	247	MET	2.6
1	A	289	SER	2.3
1	A	2	GLU	2.2
1	A	180	GLN	2.1
1	A	61	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
3	7DG	A	293	11/11	0.96	0.17	20,25,27,29	2
2	SO4	A	291	5/5	0.97	0.10	39,42,45,47	0
2	SO4	A	292	5/5	0.98	0.20	23,26,29,31	0
2	SO4	A	290	5/5	0.98	0.14	23,24,29,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.