



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2017 – 01:02 AM EDT

PDB ID : 3K8O  
Title : Crystal structure of human purine nucleoside phosphorylase in complex with DATMe-ImmH  
Authors : Ho, M.; Rinaldo-matthis, A.; Almo, S.C.; Schramm, V.L.  
Deposited on : unknown  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

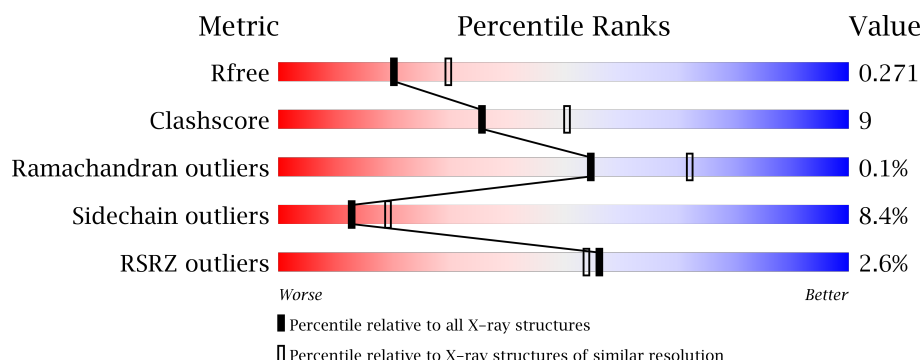
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	289	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>..</div> </div> </div>
1	Q	289	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>..</div> </div> </div>
1	S	289	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>..</div> </div> </div>
1	T	289	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>
1	U	289	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	Y	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	E	1006	-	-	-	X
2	SO4	Q	1005	-	-	-	X
2	SO4	S	1010	-	-	-	X
2	SO4	U	1009	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13632 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
1	E	283	Total	C	N	O	S	0	0	0
			2213	1408	388	402	15			
1	Q	284	Total	C	N	O	S	0	0	0
			2222	1413	389	405	15			
1	S	282	Total	C	N	O	S	0	0	0
			2205	1404	386	400	15			
1	T	282	Total	C	N	O	S	0	0	0
			2206	1403	387	401	15			
1	U	285	Total	C	N	O	S	0	0	0
			2230	1418	391	406	15			
1	Y	283	Total	C	N	O	S	0	0	0
			2212	1408	387	402	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	51	SER	GLY	ENGINEERED	UNP P00491
Q	51	SER	GLY	ENGINEERED	UNP P00491
S	51	SER	GLY	ENGINEERED	UNP P00491
T	51	SER	GLY	ENGINEERED	UNP P00491
U	51	SER	GLY	ENGINEERED	UNP P00491
Y	51	SER	GLY	ENGINEERED	UNP P00491

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



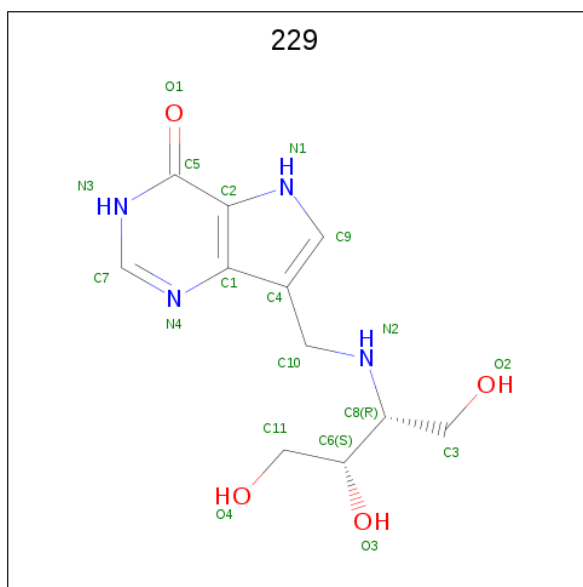
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	S	1	Total	O	S	0	0
			5	4	1		
2	S	1	Total	O	S	0	0
			5	4	1		
2	S	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		
2	U	1	Total	O	S	0	0
			5	4	1		
2	U	1	Total	O	S	0	0
			5	4	1		
2	U	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is 7-({[(1R,2S)-2,3-DIHYDROXY-1-(HYDROXYMETHYL)PROPYL]AMINO}METHYL)-3,5-DIHYDRO-4H-PYRROLO[3,2-D]PYRIMIDIN-4-ONE (three-letter code: 229) (formula: C<sub>11</sub>H<sub>16</sub>N<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			19	11	4	4		
3	Q	1	Total	C	N	O	0	0
			19	11	4	4		
3	S	1	Total	C	N	O	0	0
			19	11	4	4		
3	T	1	Total	C	N	O	0	0
			19	11	4	4		
3	U	1	Total	C	N	O	0	0
			19	11	4	4		
3	Y	1	Total	C	N	O	0	0
			19	11	4	4		

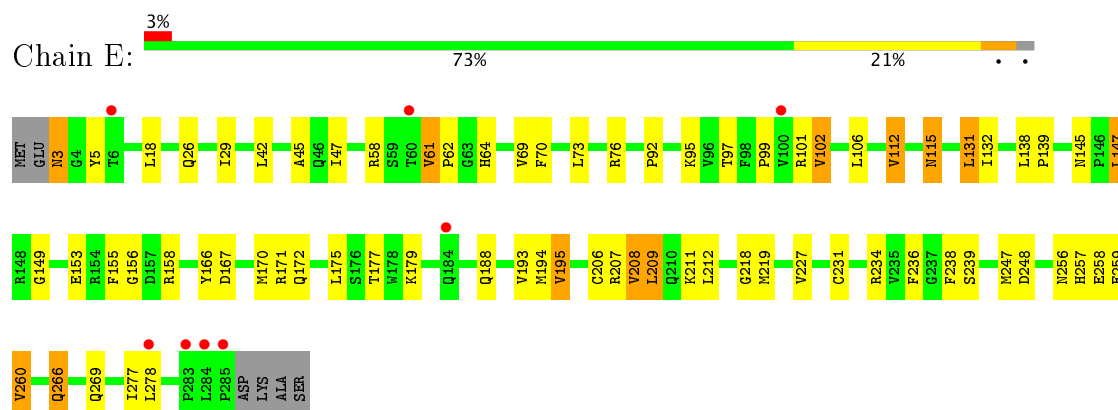
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	25	Total 25	O 25	0	0
4	Q	31	Total 31	O 31	0	0
4	S	28	Total 28	O 28	0	0
4	T	16	Total 16	O 16	0	0
4	U	16	Total 16	O 16	0	0
4	Y	34	Total 34	O 34	0	0

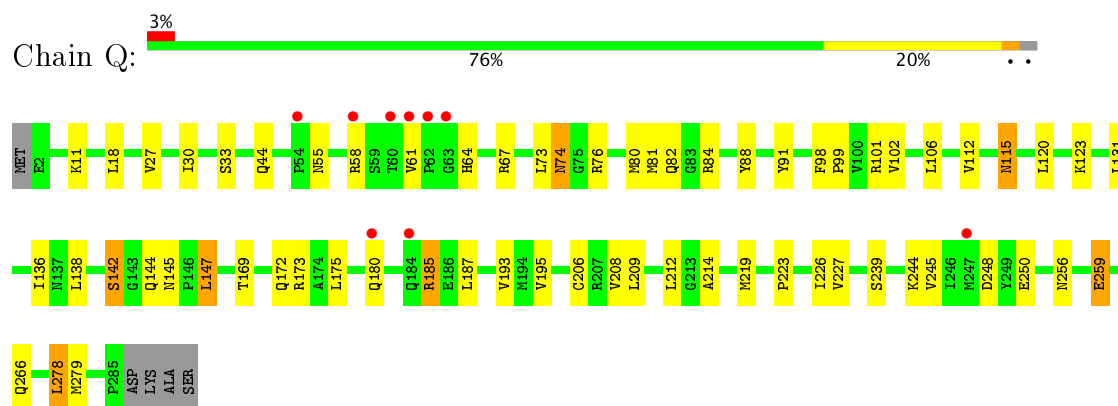
### 3 Residue-property plots

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

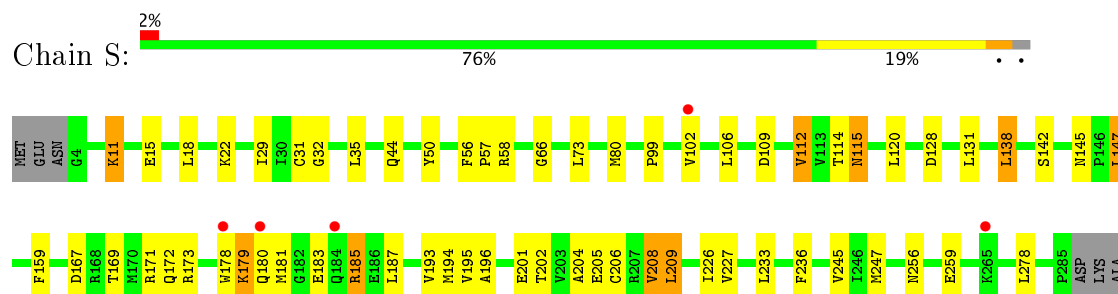
#### • Molecule 1: Purine nucleoside phosphorylase



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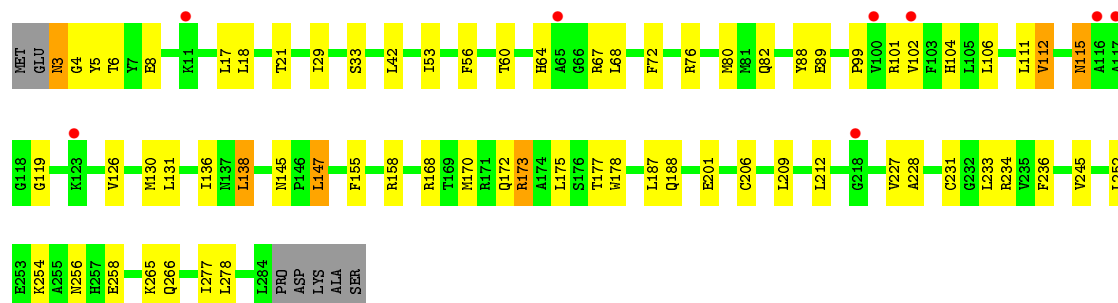
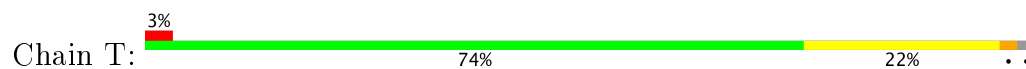
#### • Molecule 1: Purine nucleoside phosphorylase



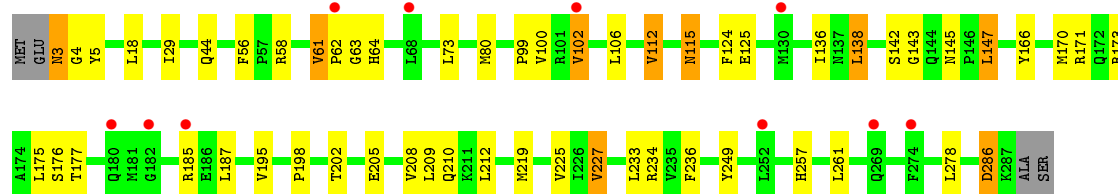
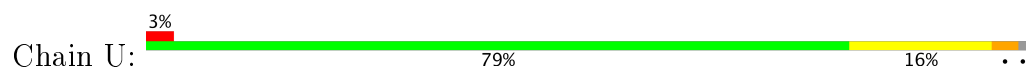


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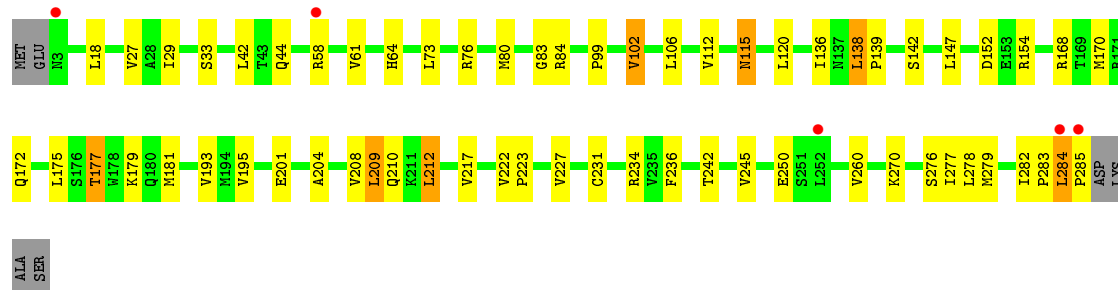
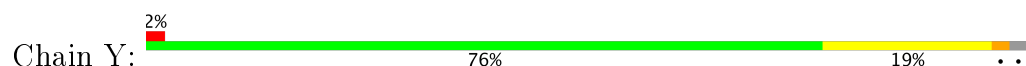
- Molecule 1: Purine nucleoside phosphorylase



- Molecule 1: Purine nucleoside phosphorylase



- Molecule 1: Purine nucleoside phosphorylase

ALA  
SER

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	269.21Å 51.88Å 129.07Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.98 – 2.39	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-2.40) 97.1 (19.98-2.39)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, $R_{free}$	0.223 , 0.272 0.219 , 0.271	Depositor DCC
$R_{free}$ test set	3473 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13632	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 229

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	E	0.55	0/2265	0.66	0/3066
1	Q	0.65	0/2274	0.76	2/3078 (0.1%)
1	S	0.62	0/2257	0.70	0/3055
1	T	0.58	0/2257	0.67	0/3054
1	U	0.54	0/2282	0.64	1/3088 (0.0%)
1	Y	0.67	1/2263 (0.0%)	0.72	1/3061 (0.0%)
All	All	0.60	1/13598 (0.0%)	0.69	4/18402 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	231	CYS	CB-SG	-5.15	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	278	LEU	CA-CB-CG	7.46	132.47	115.30
1	Q	84	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	U	233	LEU	CA-CB-CG	5.48	127.91	115.30
1	Y	212	LEU	CA-CB-CG	5.33	127.55	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	E	2213	0	2190	48	0
1	Q	2222	0	2196	42	0
1	S	2205	0	2184	45	0
1	T	2206	0	2183	37	0
1	U	2230	0	2207	38	0
1	Y	2212	0	2188	38	0
2	E	15	0	0	1	0
2	Q	15	0	0	0	0
2	S	15	0	0	1	0
2	T	10	0	0	1	0
2	U	15	0	0	1	0
2	Y	10	0	0	0	0
3	E	19	0	16	1	0
3	Q	19	0	16	1	0
3	S	19	0	16	2	0
3	T	19	0	16	1	0
3	U	19	0	16	2	0
3	Y	19	0	16	1	0
4	E	25	0	0	2	0
4	Q	31	0	0	1	0
4	S	28	0	0	0	0
4	T	16	0	0	0	0
4	U	16	0	0	0	0
4	Y	34	0	0	3	0
All	All	13632	0	13244	245	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 9.

All (245) 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:S:179:LYS:H	1:S:179:LYS:HE2	1.12	1.08
1:S:185:ARG:CG	1:S:185:ARG:HH11	1.71	1.00
1:S:185:ARG:HH11	1:S:185:ARG:HG2	1.33	0.92
1:Y:73:LEU:HD22	1:Y:80:MET:HE2	1.57	0.87
1:Y:276:SER:C	1:Y:277:ILE:CA	2.45	0.84
1:E:3:ASN:HD22	1:E:5:TYR:H	1.25	0.81
1:U:170:MET:CE	1:U:236:PHE:HB2	2.09	0.81
1:S:179:LYS:N	1:S:179:LYS:HE2	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:170:MET:HE3	1:U:236:PHE:HB2	1.61	0.80
1:E:3:ASN:ND2	1:E:5:TYR:H	1.80	0.79
1:Y:64:HIS:HD2	1:Y:84:ARG:H	1.33	0.76
1:E:171:ARG:NH2	4:E:310:HOH:O	2.20	0.75
1:U:29:ILE:HG23	1:U:112:VAL:HG22	1.69	0.75
1:Q:74:ASN:HD22	1:Q:74:ASN:N	1.84	0.75
1:S:185:ARG:HG3	1:S:185:ARG:HH11	1.51	0.74
1:Q:44:GLN:HE22	1:S:180:GLN:HA	1.53	0.73
1:U:3:ASN:ND2	1:U:5:TYR:H	1.86	0.73
1:Y:73:LEU:HD22	1:Y:80:MET:CE	2.18	0.72
1:S:185:ARG:NH1	1:S:185:ARG:CG	2.43	0.72
1:Q:195:VAL:O	1:Q:219:MET:HA	1.91	0.71
1:Y:177:THR:CG2	4:Y:303:HOH:O	2.38	0.71
1:Q:248:ASP:OD1	1:Q:250:GLU:HG2	1.92	0.70
1:E:177:THR:CG2	1:E:277:ILE:HG21	2.22	0.69
1:U:125:GLU:CG	1:U:185:ARG:HH12	2.06	0.69
1:E:166:TYR:O	1:E:171:ARG:NH1	2.26	0.68
1:Q:33:SER:OG	1:Q:64:HIS:HE1	1.76	0.68
1:S:185:ARG:NH1	1:S:185:ARG:HG2	2.06	0.68
1:S:11:LYS:HE2	1:S:15:GLU:OE1	1.95	0.67
1:Y:177:THR:HG22	4:Y:303:HOH:O	1.94	0.67
1:Q:58:ARG:HG2	1:Q:91:TYR:OH	1.95	0.67
1:Y:42:LEU:HD21	1:Y:80:MET:HE3	1.76	0.66
1:Y:61:VAL:HG23	1:Y:64:HIS:ND1	2.10	0.66
1:S:29:ILE:HG23	1:S:112:VAL:HG22	1.77	0.66
1:E:257:HIS:HA	1:E:260:VAL:HG13	1.76	0.65
1:T:177:THR:HG21	1:T:277:ILE:HG23	1.78	0.64
1:E:29:ILE:HG23	1:E:112:VAL:HG22	1.81	0.63
1:U:62:PRO:O	1:U:257:HIS:NE2	2.30	0.63
1:Q:58:ARG:CG	1:Q:91:TYR:OH	2.47	0.62
1:Q:44:GLN:NE2	1:S:180:GLN:HA	2.13	0.62
1:E:47:ILE:HG12	1:E:69:VAL:HG22	1.82	0.62
1:S:206:CYS:HB3	1:S:247:MET:SD	2.40	0.62
1:Y:64:HIS:CD2	1:Y:84:ARG:H	2.15	0.61
1:U:99:PRO:HA	1:U:102:VAL:HG13	1.81	0.61
1:U:136:ILE:HG22	1:U:138:LEU:HD13	1.82	0.60
1:Q:67:ARG:NH2	1:Q:82:GLN:OE1	2.33	0.60
1:Y:99:PRO:HA	1:Y:102:VAL:HG13	1.83	0.60
1:S:32:GLY:H	1:S:35:LEU:HD12	1.67	0.59
1:S:131:LEU:HD21	1:S:236:PHE:CE1	2.37	0.59
1:Q:115:ASN:ND2	1:Q:239:SER:OG	2.24	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:166:TYR:O	1:U:171:ARG:NH1	2.36	0.59
1:Q:120:LEU:HD23	1:Q:245:VAL:HG21	1.84	0.58
1:S:167:ASP:O	1:S:171:ARG:HG3	2.03	0.58
1:U:205:GLU:O	1:U:208:VAL:HG22	2.03	0.58
1:Y:61:VAL:CG2	1:Y:64:HIS:ND1	2.67	0.58
1:E:257:HIS:HA	1:E:260:VAL:CG1	2.34	0.57
1:U:170:MET:HE1	1:U:236:PHE:HB2	1.85	0.57
1:T:112:VAL:HA	1:T:236:PHE:O	2.05	0.57
1:S:73:LEU:HD22	1:S:80:MET:CE	2.34	0.57
2:E:1003:SO4:O4	3:E:9006:229:H31	2.05	0.56
1:U:63:GLY:H	1:U:261:LEU:HD21	1.69	0.56
1:Y:27:VAL:HG11	1:Y:279:MET:HE1	1.88	0.56
1:E:139:PRO:HA	1:Y:142:SER:HB2	1.88	0.56
1:Y:193:VAL:HG11	1:Y:209:LEU:HG	1.88	0.55
1:E:177:THR:HG23	1:E:277:ILE:HG21	1.89	0.55
1:Q:193:VAL:HB	1:Q:214:ALA:CB	2.37	0.55
1:U:145:ASN:OD1	1:U:147:LEU:HB2	2.07	0.55
1:Q:55:ASN:HB2	1:Q:98:PHE:CZ	2.41	0.55
1:U:219:MET:HB2	3:U:9003:229:H32	1.88	0.55
1:T:170:MET:CE	1:T:234:ARG:HG2	2.38	0.54
1:Y:115:ASN:HD22	1:Y:115:ASN:C	2.11	0.54
1:S:120:LEU:HD23	1:S:245:VAL:HG21	1.88	0.54
1:U:125:GLU:HG3	1:U:185:ARG:HH12	1.71	0.54
1:S:201:GLU:H	1:S:201:GLU:CD	2.11	0.54
1:E:266:GLN:HE21	1:E:266:GLN:HA	1.72	0.54
1:Y:177:THR:HG23	4:Y:303:HOH:O	2.06	0.54
1:E:97:THR:HB	1:E:227:VAL:HG21	1.90	0.54
1:U:170:MET:HE2	1:U:234:ARG:HG2	1.90	0.54
1:S:202:THR:OG1	1:S:205:GLU:HG3	2.07	0.53
1:E:207:ARG:O	1:E:211:LYS:HG2	2.09	0.53
2:T:5001:SO4:O2	3:T:9004:229:H31	2.08	0.53
1:E:3:ASN:C	1:E:3:ASN:HD22	2.12	0.53
1:Q:33:SER:HA	1:Q:64:HIS:CE1	2.44	0.53
1:T:99:PRO:HA	1:T:102:VAL:HG22	1.91	0.53
1:T:17:LEU:O	1:T:21:THR:HG22	2.10	0.52
1:U:3:ASN:HD22	1:U:4:GLY:N	2.07	0.52
3:Y:9001:229:O4	3:Y:9001:229:N2	2.42	0.52
1:Q:74:ASN:N	1:Q:74:ASN:ND2	2.55	0.52
1:S:99:PRO:HA	1:S:102:VAL:HG13	1.92	0.52
1:U:61:VAL:HG22	1:U:64:HIS:CD2	2.44	0.52
1:Q:142:SER:HB2	1:Y:139:PRO:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:256:ASN:ND2	1:S:259:GLU:H	2.08	0.52
1:Y:181:MET:CE	1:Y:270:LYS:HG3	2.39	0.52
1:E:115:ASN:HD22	1:E:115:ASN:C	2.13	0.52
1:U:195:VAL:O	1:U:219:MET:HA	2.10	0.52
1:E:62:PRO:O	1:E:257:HIS:NE2	2.34	0.52
1:Y:201:GLU:CD	1:Y:201:GLU:H	2.13	0.52
1:E:42:LEU:HD23	1:E:73:LEU:HB2	1.92	0.51
1:Q:136:ILE:HG22	1:Q:138:LEU:CD1	2.40	0.51
3:S:9005:229:N2	3:S:9005:229:O4	2.44	0.51
1:Y:170:MET:HE2	1:Y:234:ARG:HG2	1.93	0.51
1:Q:99:PRO:HA	1:Q:102:VAL:HG13	1.92	0.50
1:S:185:ARG:HG3	1:S:185:ARG:NH1	2.18	0.50
1:E:112:VAL:HA	1:E:236:PHE:O	2.12	0.50
1:T:155:PHE:O	1:T:231:CYS:HA	2.12	0.50
1:E:208:VAL:HA	1:E:211:LYS:HE2	1.93	0.49
1:Q:73:LEU:HD22	1:Q:80:MET:HE1	1.94	0.49
1:Y:170:MET:CE	1:Y:234:ARG:HG2	2.42	0.49
1:S:159:PHE:HZ	1:T:88:TYR:HH	1.61	0.49
1:E:145:ASN:OD1	1:E:147:LEU:HB2	2.12	0.49
1:E:155:PHE:O	1:E:231:CYS:HA	2.13	0.49
1:S:29:ILE:HG12	1:S:112:VAL:HG13	1.93	0.49
1:U:286:ASP:OD1	1:U:286:ASP:N	2.45	0.49
1:T:177:THR:HG21	1:T:277:ILE:CG2	2.43	0.49
1:S:178:TRP:CD2	1:S:187:LEU:HB2	2.48	0.48
1:T:158:ARG:HH21	1:U:198:PRO:HG3	1.78	0.48
1:Q:67:ARG:NE	1:Q:82:GLN:OE1	2.47	0.48
1:Y:136:ILE:HG22	1:Y:138:LEU:HD13	1.94	0.48
1:T:119:GLY:O	1:T:245:VAL:HG22	2.13	0.48
1:T:67:ARG:NE	1:T:82:GLN:OE1	2.40	0.48
1:U:61:VAL:HG22	1:U:64:HIS:HD2	1.79	0.48
1:E:99:PRO:HA	1:E:102:VAL:HG13	1.96	0.48
1:T:29:ILE:HG23	1:T:112:VAL:HG22	1.95	0.48
1:E:45:ALA:HA	1:E:70:PHE:O	2.13	0.48
1:U:115:ASN:HD22	1:U:115:ASN:C	2.17	0.48
1:U:124:PHE:N	1:U:124:PHE:CD1	2.81	0.48
1:Y:152:ASP:OD1	1:Y:154:ARG:HB2	2.14	0.48
1:Q:145:ASN:OD1	1:Q:147:LEU:HB2	2.14	0.47
1:T:170:MET:HG2	1:T:173:ARG:HH21	1.79	0.47
1:T:136:ILE:HG22	1:T:138:LEU:HD13	1.97	0.47
1:Y:120:LEU:HD23	1:Y:245:VAL:HG21	1.95	0.47
1:E:153:GLU:HA	1:E:156:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:256:ASN:HD22	1:E:258:GLU:HB2	1.80	0.47
1:E:170:MET:CE	1:E:236:PHE:HB2	2.45	0.47
1:E:177:THR:CG2	1:E:277:ILE:CG2	2.93	0.46
1:U:73:LEU:HD22	1:U:80:MET:CE	2.44	0.46
1:Q:74:ASN:HD22	1:Q:74:ASN:H	1.60	0.46
1:Q:144:GLN:OE1	1:Q:144:GLN:HA	2.15	0.46
1:E:167:ASP:O	1:E:171:ARG:HG3	2.15	0.46
1:S:169:THR:HA	1:S:172:GLN:HE21	1.80	0.46
3:Q:9002:229:N2	3:Q:9002:229:O4	2.49	0.46
1:T:256:ASN:ND2	1:T:258:GLU:HB3	2.31	0.46
1:U:29:ILE:HG12	1:U:112:VAL:HG13	1.98	0.46
1:Q:61:VAL:HG11	1:Q:88:TYR:OH	2.16	0.45
1:S:181:MET:HB3	1:S:183:GLU:HG2	1.99	0.45
1:Y:282:ILE:HA	1:Y:283:PRO:HD3	1.75	0.45
1:Y:222:VAL:HB	1:Y:223:PRO:HD3	1.98	0.45
1:S:147:LEU:HD22	1:S:226:ILE:CG2	2.47	0.45
1:S:73:LEU:HD22	1:S:80:MET:HE3	1.99	0.45
1:T:145:ASN:OD1	1:T:147:LEU:HB2	2.17	0.45
1:S:193:VAL:HG11	1:S:209:LEU:HG	1.98	0.45
1:E:170:MET:HE2	1:E:234:ARG:HG2	1.99	0.45
1:E:193:VAL:HG11	1:E:209:LEU:HG	1.98	0.45
1:E:61:VAL:HG22	1:E:64:HIS:CD2	2.52	0.45
1:T:33:SER:OG	1:T:64:HIS:NE2	2.46	0.45
1:U:73:LEU:HD22	1:U:80:MET:HE1	1.97	0.45
1:Y:284:LEU:HB3	1:Y:285:PRO:HD2	1.99	0.45
1:Q:136:ILE:HG22	1:Q:138:LEU:HD13	1.99	0.44
1:Q:244:LYS:HD2	4:Q:299:HOH:O	2.16	0.44
1:Q:58:ARG:HG3	1:Q:91:TYR:OH	2.16	0.44
1:T:6:THR:HB	1:T:8:GLU:OE2	2.17	0.44
1:U:166:TYR:OH	1:U:225:VAL:HG21	2.16	0.44
1:Y:112:VAL:HA	1:Y:236:PHE:O	2.17	0.44
1:E:256:ASN:ND2	1:E:259:GLU:H	2.14	0.44
1:S:109:ASP:HA	1:S:233:LEU:HD22	2.00	0.44
1:T:72:PHE:HA	1:T:76:ARG:O	2.17	0.44
1:Y:33:SER:OG	1:Y:64:HIS:HE1	2.00	0.44
1:T:256:ASN:HD22	1:T:258:GLU:HB3	1.82	0.44
1:T:60:THR:OG1	1:T:89:GLU:OE2	2.31	0.44
1:T:201:GLU:CD	1:T:201:GLU:H	2.21	0.44
1:T:3:ASN:HD22	1:T:4:GLY:N	2.16	0.44
1:U:112:VAL:HA	1:U:236:PHE:O	2.17	0.44
1:U:124:PHE:N	1:U:124:PHE:HD1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:74:ASN:HD21	1:Q:279:MET:HB2	1.83	0.44
1:S:196:ALA:CB	1:U:143:GLY:HA2	2.48	0.44
1:Q:131:LEU:HD21	1:Q:187:LEU:HD21	2.00	0.44
1:T:111:LEU:HD23	1:T:228:ALA:HB2	2.00	0.44
1:Q:147:LEU:HD22	1:Q:226:ILE:CG2	2.48	0.43
1:E:206:CYS:HB3	1:E:247:MET:SD	2.58	0.43
1:U:100:VAL:HB	1:U:227:VAL:CG2	2.48	0.43
1:Y:115:ASN:ND2	1:Y:115:ASN:C	2.71	0.43
1:E:76:ARG:HA	1:E:76:ARG:HD3	1.75	0.43
1:Y:242:THR:OG1	1:Y:260:VAL:HG13	2.18	0.43
1:E:194:MET:HG2	1:E:195:VAL:N	2.32	0.43
1:E:177:THR:HG21	1:E:277:ILE:CG2	2.48	0.43
1:Q:33:SER:OG	1:Q:64:HIS:CE1	2.63	0.43
1:S:145:ASN:OD1	1:S:147:LEU:HB2	2.18	0.43
1:T:104:HIS:HB2	1:T:233:LEU:HD21	1.99	0.43
1:S:50:TYR:CD2	1:S:66:GLY:HA2	2.53	0.43
1:T:178:TRP:CD2	1:T:187:LEU:HB2	2.54	0.43
1:Y:120:LEU:HD11	1:Y:217:VAL:HB	1.99	0.43
1:E:92:PRO:HD2	1:E:95:LYS:HD2	2.01	0.42
1:T:168:ARG:O	1:T:172:GLN:HG3	2.18	0.42
1:Q:30:ILE:HG12	1:Q:81:MET:SD	2.59	0.42
1:U:202:THR:OG1	1:U:205:GLU:HG3	2.19	0.42
1:Q:67:ARG:CZ	1:Q:82:GLN:OE1	2.66	0.42
2:S:3001:SO4:O3	3:S:9005:229:H31	2.19	0.42
1:S:56:PHE:HA	1:S:57:PRO:HD3	1.94	0.42
1:T:206:CYS:SG	1:T:245:VAL:HB	2.59	0.42
1:Y:64:HIS:HD2	1:Y:84:ARG:N	2.09	0.42
1:E:149:GLY:O	1:E:158:ARG:NH1	2.44	0.42
1:T:170:MET:HE2	1:T:234:ARG:HG2	2.01	0.42
1:T:42:LEU:HG	1:T:80:MET:HE3	2.01	0.42
1:E:170:MET:HE1	1:E:236:PHE:HB2	2.00	0.42
1:Y:201:GLU:N	1:Y:201:GLU:CD	2.73	0.42
1:E:26:GLN:OE1	1:E:76:ARG:HD2	2.20	0.42
1:S:195:VAL:HG21	1:S:209:LEU:HD21	2.02	0.42
1:E:177:THR:HG21	1:E:277:ILE:HG21	2.01	0.42
1:S:115:ASN:HD22	1:S:115:ASN:C	2.22	0.42
1:E:195:VAL:O	1:E:219:MET:HA	2.19	0.42
1:Q:169:THR:HA	1:Q:172:GLN:NE2	2.35	0.42
1:T:130:MET:HA	1:T:188:GLN:O	2.20	0.42
1:T:168:ARG:NH2	1:U:249:TYR:O	2.53	0.42
2:U:4001:SO4:O3	3:U:9003:229:O2	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:115:ASN:HD22	1:T:115:ASN:C	2.23	0.42
1:Y:204:ALA:O	1:Y:208:VAL:HG13	2.19	0.42
1:Q:11:LYS:HB3	1:Q:11:LYS:HE2	1.93	0.41
1:S:180:GLN:HB3	1:S:180:GLN:HE21	1.71	0.41
1:S:194:MET:HG2	1:S:195:VAL:N	2.35	0.41
1:Y:64:HIS:CD2	1:Y:83:GLY:HA2	2.55	0.41
1:S:31:CYS:HA	1:S:114:THR:OG1	2.20	0.41
1:S:204:ALA:O	1:S:208:VAL:HG13	2.20	0.41
1:U:125:GLU:HG3	1:U:185:ARG:NH1	2.36	0.41
1:Q:180:GLN:HA	1:S:44:GLN:HE22	1.86	0.41
1:E:218:GLY:HA3	4:E:290:HOH:O	2.20	0.41
1:S:138:LEU:HD12	1:S:138:LEU:HA	1.92	0.41
1:Y:29:ILE:HG23	1:Y:112:VAL:HG22	2.03	0.41
1:T:53:ILE:HG21	1:T:56:PHE:CD1	2.56	0.41
1:U:175:LEU:HD12	1:U:187:LEU:HD23	2.03	0.41
1:E:115:ASN:HD21	1:E:239:SER:CB	2.35	0.41
1:Q:185:ARG:HD2	1:Q:185:ARG:HA	1.76	0.41
1:Q:256:ASN:ND2	1:Q:259:GLU:H	2.19	0.41
1:Q:76:ARG:HA	1:Q:76:ARG:HD3	1.86	0.41
1:S:128:ASP:OD1	1:S:185:ARG:HG2	2.20	0.41
1:E:132:ILE:HG13	1:E:238:PHE:HA	2.03	0.40
1:E:131:LEU:N	1:E:188:GLN:O	2.48	0.40
1:Q:223:PRO:O	1:Q:227:VAL:HG13	2.22	0.40
1:T:3:ASN:ND2	1:T:5:TYR:H	2.19	0.40
1:T:68:LEU:HD12	1:T:68:LEU:HA	1.91	0.40
1:T:131:LEU:HD23	1:T:131:LEU:HA	1.94	0.40
1:Y:168:ARG:O	1:Y:172:GLN:HG3	2.22	0.40
1:E:147:LEU:O	1:E:158:ARG:NH2	2.55	0.40
1:S:196:ALA:HB3	1:U:143:GLY:HA2	2.04	0.40
1:U:3:ASN:HD22	1:U:5:TYR:H	1.66	0.40
1:Q:193:VAL:HG11	1:Q:209:LEU:HG	2.04	0.40
1:Q:27:VAL:HG11	1:Q:279:MET:HE1	2.02	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	E	281/289 (97%)	273 (97%)	8 (3%)	0	100	100
1	Q	282/289 (98%)	273 (97%)	9 (3%)	0	100	100
1	S	280/289 (97%)	269 (96%)	11 (4%)	0	100	100
1	T	280/289 (97%)	273 (98%)	7 (2%)	0	100	100
1	U	283/289 (98%)	275 (97%)	8 (3%)	0	100	100
1	Y	279/289 (96%)	273 (98%)	5 (2%)	1 (0%)	38	54
All	All	1685/1734 (97%)	1636 (97%)	48 (3%)	1 (0%)	55	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	44	GLN

### 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	E	235/240 (98%)	211 (90%)	24 (10%)	8	12
1	Q	236/240 (98%)	218 (92%)	18 (8%)	15	24
1	S	234/240 (98%)	217 (93%)	17 (7%)	16	26
1	T	234/240 (98%)	215 (92%)	19 (8%)	14	21
1	U	237/240 (99%)	215 (91%)	22 (9%)	10	15
1	Y	234/240 (98%)	215 (92%)	19 (8%)	14	21
All	All	1410/1440 (98%)	1291 (92%)	119 (8%)	13	19

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	3	ASN
1	E	18	LEU
1	E	58	ARG
1	E	61	VAL
1	E	101	ARG
1	E	102	VAL
1	E	106	LEU
1	E	112	VAL
1	E	115	ASN
1	E	131	LEU
1	E	138	LEU
1	E	147	LEU
1	E	172	GLN
1	E	175	LEU
1	E	179	LYS
1	E	195	VAL
1	E	208	VAL
1	E	209	LEU
1	E	212	LEU
1	E	248	ASP
1	E	260	VAL
1	E	266	GLN
1	E	269	GLN
1	E	278	LEU
1	Q	18	LEU
1	Q	74	ASN
1	Q	101	ARG
1	Q	106	LEU
1	Q	112	VAL
1	Q	115	ASN
1	Q	123	LYS
1	Q	142	SER
1	Q	147	LEU
1	Q	173	ARG
1	Q	175	LEU
1	Q	185	ARG
1	Q	206	CYS
1	Q	208	VAL
1	Q	212	LEU
1	Q	259	GLU
1	Q	266	GLN
1	Q	278	LEU
1	S	11	LYS

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Mol	Chain	Res	Type
1	S	18	LEU
1	S	22	LYS
1	S	58	ARG
1	S	106	LEU
1	S	112	VAL
1	S	115	ASN
1	S	138	LEU
1	S	142	SER
1	S	147	LEU
1	S	173	ARG
1	S	179	LYS
1	S	185	ARG
1	S	208	VAL
1	S	209	LEU
1	S	227	VAL
1	S	278	LEU
1	T	3	ASN
1	T	18	LEU
1	T	101	ARG
1	T	106	LEU
1	T	112	VAL
1	T	115	ASN
1	T	126	VAL
1	T	138	LEU
1	T	147	LEU
1	T	173	ARG
1	T	175	LEU
1	T	209	LEU
1	T	212	LEU
1	T	227	VAL
1	T	252	LEU
1	T	254	LYS
1	T	265	LYS
1	T	266	GLN
1	T	278	LEU
1	U	3	ASN
1	U	18	LEU
1	U	44	GLN
1	U	56	PHE
1	U	58	ARG
1	U	61	VAL
1	U	102	VAL

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Mol	Chain	Res	Type
1	U	106	LEU
1	U	112	VAL
1	U	115	ASN
1	U	138	LEU
1	U	142	SER
1	U	147	LEU
1	U	173	ARG
1	U	176	SER
1	U	177	THR
1	U	209	LEU
1	U	210	GLN
1	U	212	LEU
1	U	227	VAL
1	U	278	LEU
1	U	286	ASP
1	Y	18	LEU
1	Y	58	ARG
1	Y	76	ARG
1	Y	102	VAL
1	Y	106	LEU
1	Y	115	ASN
1	Y	138	LEU
1	Y	147	LEU
1	Y	175	LEU
1	Y	177	THR
1	Y	179	LYS
1	Y	195	VAL
1	Y	209	LEU
1	Y	210	GLN
1	Y	212	LEU
1	Y	227	VAL
1	Y	250	GLU
1	Y	278	LEU
1	Y	284	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	3	ASN
1	E	115	ASN
1	E	172	GLN
1	E	256	ASN

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Mol	Chain	Res	Type
1	E	266	GLN
1	Q	23	HIS
1	Q	64	HIS
1	Q	74	ASN
1	Q	115	ASN
1	Q	172	GLN
1	Q	256	ASN
1	Q	266	GLN
1	Q	273	GLN
1	S	115	ASN
1	S	151	ASN
1	S	172	GLN
1	S	180	GLN
1	S	256	ASN
1	S	266	GLN
1	T	3	ASN
1	T	115	ASN
1	T	172	GLN
1	T	210	GLN
1	T	266	GLN
1	T	273	GLN
1	U	3	ASN
1	U	115	ASN
1	U	172	GLN
1	U	180	GLN
1	U	210	GLN
1	U	256	ASN
1	U	266	GLN
1	Y	64	HIS
1	Y	115	ASN
1	Y	172	GLN
1	Y	273	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

22 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	E	1002	-	4,4,4	0.25	0	6,6,6	0.17	0
2	SO4	E	1003	-	4,4,4	0.11	0	6,6,6	0.44	0
2	SO4	E	1006	-	4,4,4	0.21	0	6,6,6	0.18	0
3	229	E	9006	-	19,20,20	1.23	1 (5%)	13,27,27	3.19	4 (30%)
2	SO4	Q	1005	-	4,4,4	0.17	0	6,6,6	0.24	0
2	SO4	Q	1012	-	4,4,4	0.22	0	6,6,6	0.30	0
2	SO4	Q	2001	-	4,4,4	0.07	0	6,6,6	0.38	0
3	229	Q	9002	-	19,20,20	1.08	1 (5%)	13,27,27	3.18	4 (30%)
2	SO4	S	1010	-	4,4,4	0.17	0	6,6,6	0.22	0
2	SO4	S	1013	-	4,4,4	0.18	0	6,6,6	0.15	0
2	SO4	S	3001	-	4,4,4	0.38	0	6,6,6	0.28	0
3	229	S	9005	-	19,20,20	1.21	2 (10%)	13,27,27	3.14	4 (30%)
2	SO4	T	1007	-	4,4,4	0.15	0	6,6,6	0.27	0
2	SO4	T	5001	-	4,4,4	0.23	0	6,6,6	0.16	0
3	229	T	9004	-	19,20,20	1.19	1 (5%)	13,27,27	2.91	6 (46%)
2	SO4	U	1008	-	4,4,4	0.18	0	6,6,6	0.33	0
2	SO4	U	1009	-	4,4,4	0.15	0	6,6,6	0.33	0
2	SO4	U	4001	-	4,4,4	0.43	0	6,6,6	0.30	0
3	229	U	9003	-	19,20,20	1.17	1 (5%)	13,27,27	2.84	5 (38%)
2	SO4	Y	1001	-	4,4,4	0.16	0	6,6,6	0.23	0
2	SO4	Y	1004	-	4,4,4	0.17	0	6,6,6	0.33	0
3	229	Y	9001	-	19,20,20	1.16	2 (10%)	13,27,27	2.81	5 (38%)

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	SO4	E	1002	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1006	-	-	0/0/0/0	0/0/0/0
3	229	E	9006	-	-	0/11/13/13	0/2/2/2
2	SO4	Q	1005	-	-	0/0/0/0	0/0/0/0
2	SO4	Q	1012	-	-	0/0/0/0	0/0/0/0
2	SO4	Q	2001	-	-	0/0/0/0	0/0/0/0
3	229	Q	9002	-	-	0/11/13/13	0/2/2/2
2	SO4	S	1010	-	-	0/0/0/0	0/0/0/0
2	SO4	S	1013	-	-	0/0/0/0	0/0/0/0
2	SO4	S	3001	-	-	0/0/0/0	0/0/0/0
3	229	S	9005	-	-	0/11/13/13	0/2/2/2
2	SO4	T	1007	-	-	0/0/0/0	0/0/0/0
2	SO4	T	5001	-	-	0/0/0/0	0/0/0/0
3	229	T	9004	-	-	0/11/13/13	0/2/2/2
2	SO4	U	1008	-	-	0/0/0/0	0/0/0/0
2	SO4	U	1009	-	-	0/0/0/0	0/0/0/0
2	SO4	U	4001	-	-	0/0/0/0	0/0/0/0
3	229	U	9003	-	-	0/11/13/13	0/2/2/2
2	SO4	Y	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	Y	1004	-	-	0/0/0/0	0/0/0/0
3	229	Y	9001	-	-	0/11/13/13	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	9005	229	C7-N4	2.02	1.35	1.32
3	Y	9001	229	C7-N4	2.61	1.36	1.32
3	Y	9001	229	C5-C2	2.87	1.46	1.41
3	Q	9002	229	C5-C2	3.31	1.47	1.41
3	S	9005	229	C5-C2	3.53	1.48	1.41
3	U	9003	229	C5-C2	3.63	1.48	1.41
3	T	9004	229	C5-C2	3.91	1.48	1.41
3	E	9006	229	C5-C2	4.16	1.49	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	9006	229	N4-C7-N3	-7.63	122.22	128.86
3	S	9005	229	N4-C7-N3	-7.30	122.50	128.86
3	Q	9002	229	N4-C7-N3	-6.93	122.83	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	9005	229	C5-C2-C1	-6.27	114.61	120.84
3	E	9006	229	C5-C2-C1	-6.17	114.70	120.84
3	Q	9002	229	C5-C2-C1	-6.13	114.75	120.84
3	T	9004	229	N4-C7-N3	-6.09	123.56	128.86
3	Y	9001	229	N4-C7-N3	-6.06	123.58	128.86
3	U	9003	229	N4-C7-N3	-5.96	123.67	128.86
3	U	9003	229	C5-C2-C1	-5.67	115.20	120.84
3	T	9004	229	C5-C2-C1	-5.48	115.40	120.84
3	Y	9001	229	C5-C2-C1	-4.99	115.88	120.84
3	Y	9001	229	C4-C10-N2	-3.00	103.94	112.83
3	Y	9001	229	C2-C1-N4	-2.32	122.23	124.92
3	T	9004	229	C2-C1-N4	-2.25	122.30	124.92
3	T	9004	229	C4-C10-N2	-2.08	106.66	112.83
3	U	9003	229	C3-C8-N2	2.10	113.21	109.33
3	S	9005	229	C10-N2-C8	2.25	119.73	114.95
3	U	9003	229	C10-N2-C8	2.65	120.56	114.95
3	E	9006	229	C10-N2-C8	2.71	120.69	114.95
3	T	9004	229	C10-N2-C8	3.26	121.86	114.95
3	Y	9001	229	C7-N3-C5	3.64	121.99	115.91
3	Q	9002	229	C10-N2-C8	3.83	123.08	114.95
3	T	9004	229	C7-N3-C5	3.95	122.51	115.91
3	U	9003	229	C7-N3-C5	4.27	123.03	115.91
3	S	9005	229	C7-N3-C5	4.45	123.33	115.91
3	Q	9002	229	C7-N3-C5	4.59	123.57	115.91
3	E	9006	229	C7-N3-C5	4.74	123.82	115.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1003	SO4	1	0
3	E	9006	229	1	0
3	Q	9002	229	1	0
2	S	3001	SO4	1	0
3	S	9005	229	2	0
2	T	5001	SO4	1	0
3	T	9004	229	1	0
2	U	4001	SO4	1	0
3	U	9003	229	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Y	9001	229	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	E	283/289 (97%)	0.12	8 (2%) 53 51	37, 46, 60, 67	0
1	Q	284/289 (98%)	-0.03	9 (3%) 48 46	35, 44, 56, 65	0
1	S	282/289 (97%)	-0.03	5 (1%) 69 66	36, 44, 55, 64	0
1	T	282/289 (97%)	0.22	8 (2%) 53 51	35, 46, 54, 63	0
1	U	285/289 (98%)	0.22	10 (3%) 44 43	37, 46, 58, 64	0
1	Y	283/289 (97%)	-0.10	5 (1%) 69 66	34, 45, 53, 65	0
All	All	1699/1734 (97%)	0.07	45 (2%) 56 54	34, 45, 58, 67	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	184	GLN	5.8
1	Q	60	THR	5.5
1	Q	184	GLN	3.8
1	T	123	LYS	3.7
1	U	102	VAL	3.6
1	Q	247	MET	3.6
1	U	252	LEU	3.5
1	T	65	ALA	3.4
1	T	116	ALA	3.4
1	U	182	GLY	3.2
1	Y	284	LEU	3.0
1	S	178	TRP	3.0
1	Q	61	VAL	3.0
1	E	285	PRO	3.0
1	S	102	VAL	2.8
1	Q	62	PRO	2.8
1	U	62	PRO	2.7
1	Y	252	LEU	2.6
1	T	218	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	Y	58	ARG	2.5
1	E	284	LEU	2.4
1	E	100	VAL	2.4
1	E	184	GLN	2.4
1	T	102	VAL	2.4
1	T	117	ALA	2.4
1	U	274	PHE	2.3
1	E	60	THR	2.3
1	U	68	LEU	2.3
1	T	100	VAL	2.3
1	Y	3	ASN	2.3
1	S	180	GLN	2.2
1	Q	54	PRO	2.2
1	U	269	GLN	2.2
1	U	180	GLN	2.2
1	U	130	MET	2.2
1	E	278	LEU	2.2
1	E	283	PRO	2.2
1	Y	285	PRO	2.2
1	Q	58	ARG	2.2
1	Q	63	GLY	2.2
1	S	265	LYS	2.1
1	T	11	LYS	2.1
1	Q	180	GLN	2.1
1	U	185	ARG	2.1
1	E	6	THR	2.1

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	U	1009	5/5	0.98	0.23	4.94	42,44,46,48	0
2	SO4	S	1010	5/5	0.98	0.28	4.21	47,47,49,50	0
2	SO4	E	1006	5/5	0.98	0.19	3.38	48,49,51,51	0
2	SO4	Q	1005	5/5	0.98	0.25	2.71	47,47,48,49	0
3	229	Y	9001	19/19	0.92	0.14	0.14	38,39,43,46	0
3	229	S	9005	19/19	0.94	0.14	-0.45	38,40,42,45	0
2	SO4	Y	1004	5/5	0.98	0.13	-0.52	47,47,50,51	0
3	229	T	9004	19/19	0.93	0.14	-0.69	45,47,48,51	0
2	SO4	U	4001	5/5	0.97	0.12	-0.71	45,46,48,50	0
3	229	E	9006	19/19	0.91	0.14	-0.78	40,44,49,50	0
2	SO4	T	5001	5/5	0.99	0.10	-1.00	47,48,50,51	0
3	229	U	9003	19/19	0.94	0.12	-1.26	48,49,50,53	0
3	229	Q	9002	19/19	0.96	0.09	-1.26	35,39,44,45	0
2	SO4	Y	1001	5/5	0.99	0.10	-1.27	39,40,41,43	0
2	SO4	S	3001	5/5	0.98	0.11	-1.33	41,41,45,45	0
2	SO4	Q	2001	5/5	0.99	0.07	-1.88	39,40,44,44	0
2	SO4	E	1003	5/5	0.99	0.07	-2.88	35,39,40,43	0
2	SO4	T	1007	5/5	0.97	0.34	-	69,70,70,72	0
2	SO4	U	1008	5/5	0.98	0.17	-	50,51,53,54	0
2	SO4	E	1002	5/5	0.96	0.28	-	68,69,69,70	0
2	SO4	Q	1012	5/5	0.97	0.43	-	65,65,66,67	0
2	SO4	S	1013	5/5	0.93	0.35	-	76,76,77,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.