



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:56 pm GMT

PDB ID : 3S19  
Title : Crystal Structure of the R262L mutant of 7-cyano-7-deazaguanine reductase, QueF from *Vibrio cholerae* complexed with preQ0  
Authors : Kim, Y.; Zhou, M.; Gu, M.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2011-05-14  
Resolution : 1.50 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	:	trunk28620
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)	:	recalc28949

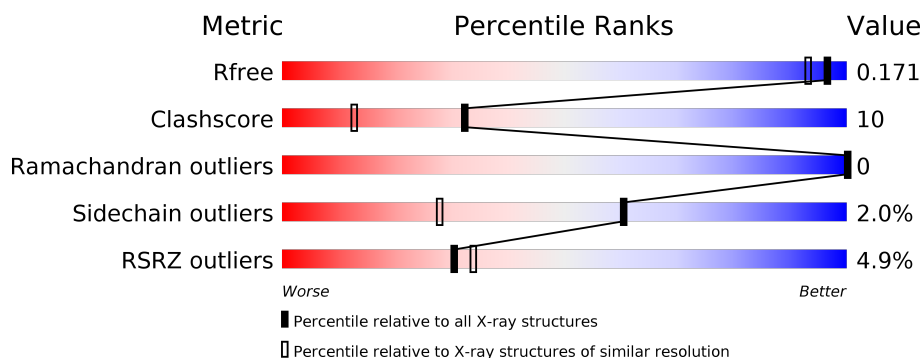
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2279 (1.50-1.50)
Clashscore	112137	2503 (1.50-1.50)
Ramachandran outliers	110173	2445 (1.50-1.50)
Sidechain outliers	110143	2443 (1.50-1.50)
RSRZ outliers	101464	2305 (1.50-1.50)

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

Mol	Chain	Length	Quality of chain
1	A	290	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>• 10%</div> </div> </div>
1	B	290	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>11%</div> </div> </div>
1	C	290	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>11%</div> </div> </div>
1	D	290	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>17%</div> <div>• 10%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	291	-	-	-	X
3	GOL	B	291	-	-	-	X
3	GOL	C	291	-	-	-	X
3	GOL	D	291	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10928 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 NADPH-dependent 7-cyano-7-deazaguanine reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	Se	0	33	0
			2372	1472	417	470	7	6			
1	B	259	Total	C	N	O	S	Se	0	38	0
			2402	1483	429	476	8	6			
1	C	259	Total	C	N	O	S	Se	0	38	0
			2391	1476	424	477	8	6			
1	D	261	Total	C	N	O	S	Se	0	42	0
			2456	1522	433	487	8	6			

There are 40 discrepancies between the modelled and reference sequences:

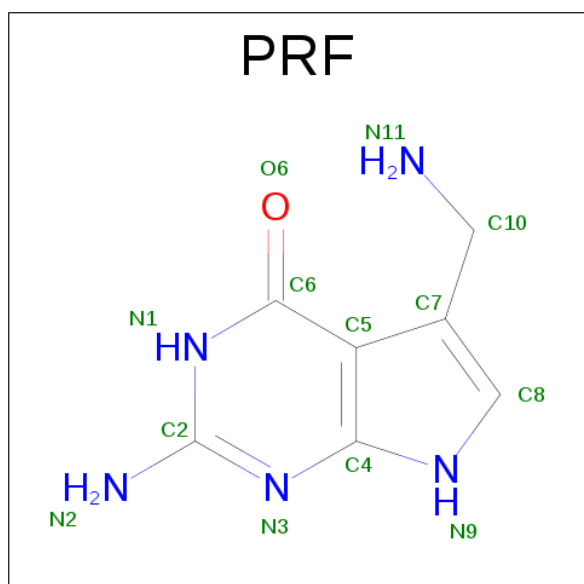
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q9KTK0
A	-1	ASN	-	EXPRESSION TAG	UNP Q9KTK0
A	0	ALA	-	EXPRESSION TAG	UNP Q9KTK0
A	1	MSE	-	EXPRESSION TAG	UNP Q9KTK0
A	2	ASN	-	EXPRESSION TAG	UNP Q9KTK0
A	3	ARG	-	EXPRESSION TAG	UNP Q9KTK0
A	4	LEU	-	EXPRESSION TAG	UNP Q9KTK0
A	5	LYS	-	EXPRESSION TAG	UNP Q9KTK0
A	6	ASN	-	EXPRESSION TAG	UNP Q9KTK0
A	262	LEU	ARG	ENGINEERED MUTATION	UNP Q9KTK0
B	-2	SER	-	EXPRESSION TAG	UNP Q9KTK0
B	-1	ASN	-	EXPRESSION TAG	UNP Q9KTK0
B	0	ALA	-	EXPRESSION TAG	UNP Q9KTK0
B	1	MSE	-	EXPRESSION TAG	UNP Q9KTK0
B	2	ASN	-	EXPRESSION TAG	UNP Q9KTK0
B	3	ARG	-	EXPRESSION TAG	UNP Q9KTK0
B	4	LEU	-	EXPRESSION TAG	UNP Q9KTK0
B	5	LYS	-	EXPRESSION TAG	UNP Q9KTK0
B	6	ASN	-	EXPRESSION TAG	UNP Q9KTK0
B	262	LEU	ARG	ENGINEERED MUTATION	UNP Q9KTK0
C	-2	SER	-	EXPRESSION TAG	UNP Q9KTK0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	ASN	-	EXPRESSION TAG	UNP Q9KTK0
C	0	ALA	-	EXPRESSION TAG	UNP Q9KTK0
C	1	MSE	-	EXPRESSION TAG	UNP Q9KTK0
C	2	ASN	-	EXPRESSION TAG	UNP Q9KTK0
C	3	ARG	-	EXPRESSION TAG	UNP Q9KTK0
C	4	LEU	-	EXPRESSION TAG	UNP Q9KTK0
C	5	LYS	-	EXPRESSION TAG	UNP Q9KTK0
C	6	ASN	-	EXPRESSION TAG	UNP Q9KTK0
C	262	LEU	ARG	ENGINEERED MUTATION	UNP Q9KTK0
D	-2	SER	-	EXPRESSION TAG	UNP Q9KTK0
D	-1	ASN	-	EXPRESSION TAG	UNP Q9KTK0
D	0	ALA	-	EXPRESSION TAG	UNP Q9KTK0
D	1	MSE	-	EXPRESSION TAG	UNP Q9KTK0
D	2	ASN	-	EXPRESSION TAG	UNP Q9KTK0
D	3	ARG	-	EXPRESSION TAG	UNP Q9KTK0
D	4	LEU	-	EXPRESSION TAG	UNP Q9KTK0
D	5	LYS	-	EXPRESSION TAG	UNP Q9KTK0
D	6	ASN	-	EXPRESSION TAG	UNP Q9KTK0
D	262	LEU	ARG	ENGINEERED MUTATION	UNP Q9KTK0

- Molecule 2 is 7-DEAZA-7-AMINOMETHYL-GUANINE (three-letter code: PRF) (formula:  $C_7H_9N_5O$ ).



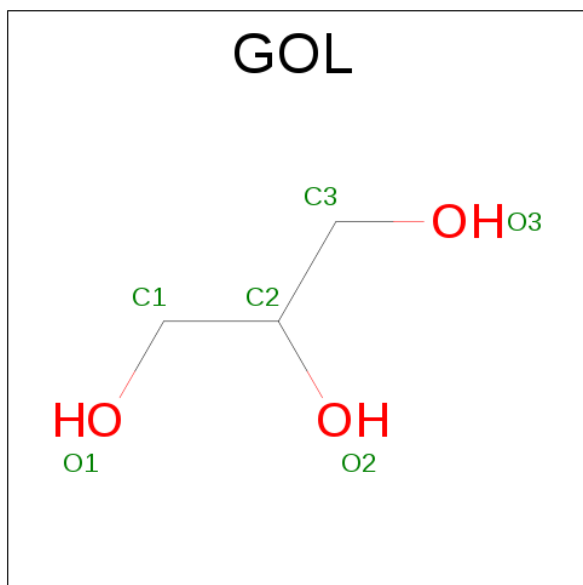
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	7	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	1
			26	14	10	2		
2	C	1	Total	C	N	O	0	1
			26	14	10	2		
2	D	1	Total	C	N	O	0	1
			26	14	10	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	296	Total	O	0	0
			296	296		
4	B	297	Total	O	0	0
			297	297		

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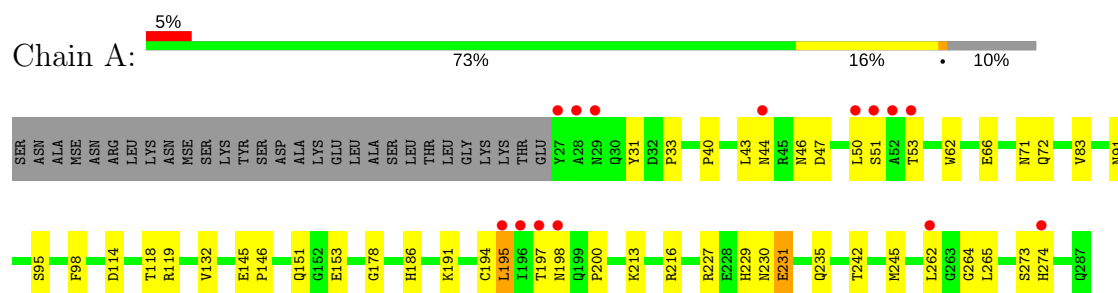
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	319	Total 319	O 319	0	0
4	D	280	Total 280	O 280	0	0

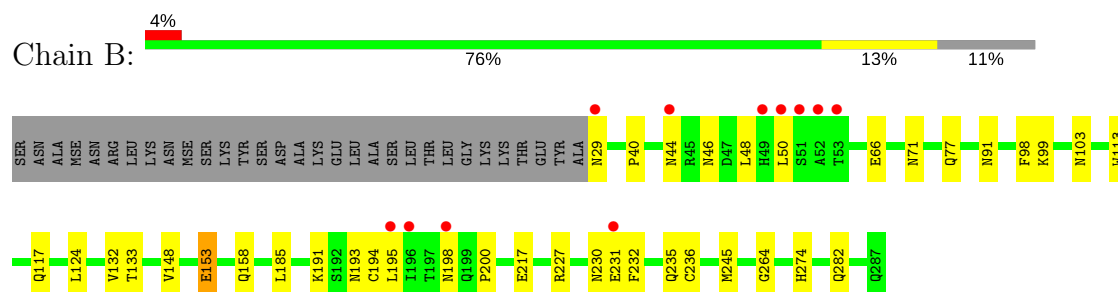
### 3 Residue-property plots [i](#)

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.

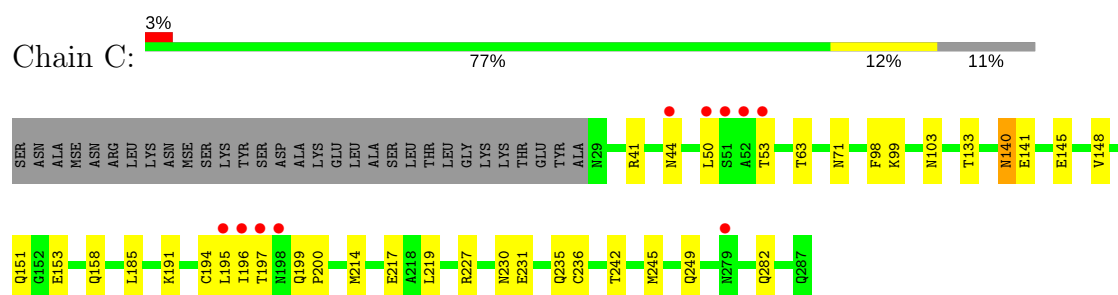
- Molecule 1: NADPH-dependent 7-cyano-7-deazaguanine reductase



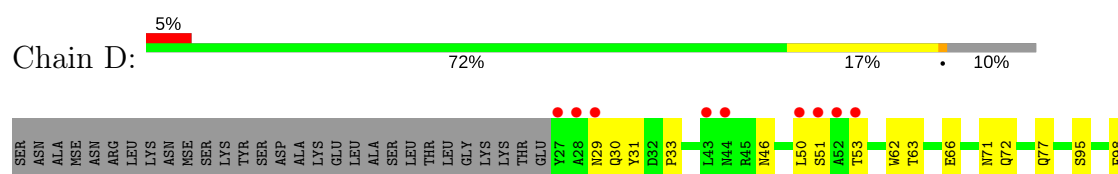
- Molecule 1: NADPH-dependent 7-cyano-7-deazaguanine reductase



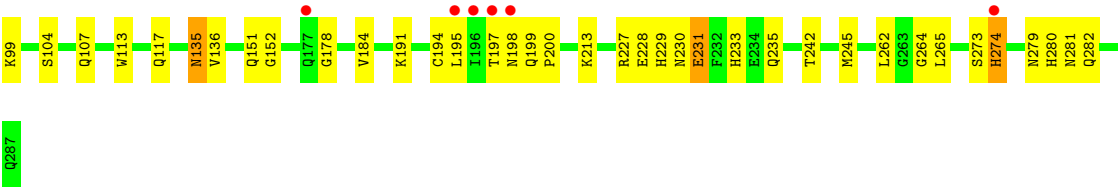
- Molecule 1: NADPH-dependent 7-cyano-7-deazaguanine reductase



- Molecule 1: NADPH-dependent 7-cyano-7-deazaguanine reductase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.33Å 71.33Å 71.33Å 109.98° 119.51° 99.50°	Depositor
Resolution (Å)	30.98 – 1.50 30.98 – 1.50	Depositor EDS
% Data completeness (in resolution range)	92.3 (30.98-1.50) 77.7 (30.98-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.03	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.68 (at 1.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_725)	Depositor
R, $R_{free}$	0.152 , 0.176 0.146 , 0.171	Depositor DCC
$R_{free}$ test set	7767 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.3	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.477 for l,-h-k-l,h 0.013 for -h-k-l,l,k 0.012 for k,h,-h-k-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10928	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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: GOL, PRF

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	0.39	0/2418	0.65	0/3283
1	B	0.40	0/2447	0.67	0/3320
1	C	0.40	0/2435	0.67	0/3304
1	D	0.38	0/2502	0.63	0/3397
All	All	0.39	0/9802	0.65	0/13304

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	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	71	ASN	Mainchain
1	B	71	ASN	Mainchain
1	C	71	ASN	Mainchain
1	D	71	ASN	Mainchain

## 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	2372	0	2232	49	0
1	B	2402	0	2250	37	0
1	C	2391	0	2239	52	0
1	D	2456	0	2309	64	0
2	A	13	0	7	0	0
2	B	26	0	15	0	0
2	C	26	0	15	1	0
2	D	26	0	14	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	1	0
3	D	6	0	8	3	0
4	A	296	0	0	9	0
4	B	297	0	0	5	0
4	C	319	0	0	8	0
4	D	280	0	0	7	0
All	All	10928	0	9113	191	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 10.

All (191) 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:B:195[B]:LEU:H	1:B:195[B]:LEU:HD23	1.02	1.14
1:A:195:LEU:H	1:A:195:LEU:CD2	1.64	1.07
1:A:195:LEU:HD23	1:A:195:LEU:H	0.90	1.03
1:A:195:LEU:HD23	1:A:195:LEU:N	1.74	1.01
1:B:195[B]:LEU:CD2	1:B:195[B]:LEU:H	1.79	0.96
1:B:195[B]:LEU:HD21	1:B:232:PHE:HD1	1.30	0.95
1:C:196[A]:ILE:HD11	2:C:290[A]:PRF:H81	1.45	0.95
1:B:195[B]:LEU:HD23	1:B:195[B]:LEU:N	1.85	0.92
1:D:66[B]:GLU:HG3	4:D:985:HOH:O	1.69	0.90
1:B:148:VAL:HG12	1:C:151[B]:GLN:HE22	1.37	0.89
1:A:66[B]:GLU:HG3	4:A:294:HOH:O	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195[B]:LEU:HD21	1:B:232:PHE:CD1	2.09	0.87
1:B:193[B]:ASN:HD22	1:B:230:ASN:ND2	1.75	0.85
1:D:199[B]:GLN:HG3	1:D:200:PRO:HD2	1.58	0.84
1:D:77:GLN:HE21	1:D:113:TRP:HE1	1.28	0.81
1:B:77:GLN:HE21	1:B:113:TRP:HE1	1.28	0.80
1:A:62:TRP:CZ3	1:A:265[B]:LEU:HD13	2.18	0.78
1:A:62:TRP:HZ3	1:A:265[B]:LEU:HD13	1.47	0.77
1:C:194[B]:CYS:HB3	1:C:197[B]:THR:HG22	1.67	0.77
1:C:133[A]:THR:HG22	4:C:684:HOH:O	1.84	0.77
1:C:196[A]:ILE:HD12	1:C:197[A]:THR:N	1.99	0.77
1:D:72[B]:GLN:HG2	4:D:643:HOH:O	1.85	0.76
1:D:63:THR:HG21	3:D:291:GOL:H31	1.68	0.75
1:B:66[B]:GLU:HG3	4:B:372:HOH:O	1.87	0.75
1:A:153[B]:GLU:CD	1:A:216:ARG:HH12	1.93	0.72
1:D:95:SER:OG	1:D:265[B]:LEU:HD11	1.90	0.72
1:C:245[C]:MSE:HE3	4:C:584:HOH:O	1.87	0.72
1:C:145[A]:GLU:HG2	4:C:518:HOH:O	1.90	0.71
1:D:199[B]:GLN:HA	1:D:199[B]:GLN:HE21	1.56	0.71
1:C:195[B]:LEU:HB3	4:C:677:HOH:O	1.91	0.71
1:C:195[B]:LEU:HD23	1:C:230:ASN:HB3	1.73	0.70
1:C:231[B]:GLU:HG3	1:C:235:GLN:HB2	1.73	0.70
1:B:231[A]:GLU:HG3	1:B:235:GLN:HB2	1.74	0.69
1:B:117:GLN:HG3	4:B:1183:HOH:O	1.92	0.69
1:D:280[A]:HIS:HD2	1:D:282:GLN:H	1.39	0.69
1:A:194:CYS:O	1:A:198:ASN:N	2.27	0.68
1:C:158:GLN:HE22	1:C:217:GLU:HA	1.59	0.68
1:B:191:LYS:HE2	1:B:200:PRO:HB3	1.76	0.67
1:C:199:GLN:HE21	1:D:99:LYS:HZ1	1.39	0.67
1:B:158:GLN:HE22	1:B:217:GLU:HA	1.57	0.67
1:B:153[B]:GLU:HG2	1:B:185:LEU:HD23	1.77	0.67
1:D:199[A]:GLN:HG3	1:D:200:PRO:HD2	1.76	0.66
1:A:245[C]:MSE:HE2	4:A:649:HOH:O	1.95	0.66
1:C:191:LYS:HE2	1:C:200:PRO:HB3	1.77	0.66
1:B:148:VAL:CG1	1:C:151[B]:GLN:HE22	2.10	0.65
1:A:50[A]:LEU:HD21	1:A:242:THR:HG21	1.79	0.65
1:D:66[B]:GLU:HG2	1:D:264:GLY:HA3	1.79	0.64
1:C:148:VAL:HG21	1:C:282[B]:GLN:HG3	1.80	0.64
1:C:197[B]:THR:HG21	4:C:640:HOH:O	1.97	0.64
1:C:199:GLN:NE2	1:D:99:LYS:NZ	2.45	0.64
1:B:133[A]:THR:HG23	4:B:627:HOH:O	1.96	0.64
1:B:148:VAL:HG21	1:B:282[A]:GLN:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:LYS:HD3	1:D:227:ARG:HG3	1.80	0.63
1:A:191:LYS:HE2	1:A:200:PRO:HB3	1.80	0.63
1:D:245[A]:MSE:HE2	4:D:1033:HOH:O	1.98	0.63
1:A:195:LEU:N	1:A:195:LEU:CD2	2.43	0.63
1:D:62:TRP:HZ3	1:D:265[B]:LEU:HD13	1.64	0.63
1:D:63:THR:CG2	3:D:291:GOL:H31	2.29	0.62
1:D:151[C]:GLN:HG3	1:D:152:GLY:N	2.14	0.62
1:C:199:GLN:HE21	1:D:99:LYS:NZ	1.97	0.62
1:C:50[B]:LEU:HD11	1:C:242:THR:HG21	1.81	0.62
1:A:186:HIS:HE1	4:A:1078:HOH:O	1.81	0.61
1:B:133[A]:THR:HG22	4:B:996:HOH:O	1.99	0.61
1:A:95[B]:SER:HB2	1:A:265[B]:LEU:HD11	1.82	0.61
1:A:265[B]:LEU:HD12	4:A:369:HOH:O	1.99	0.61
1:C:191:LYS:HD3	1:C:227:ARG:HG3	1.83	0.61
1:B:193[B]:ASN:HD22	1:B:230:ASN:HD22	1.46	0.60
1:D:280[A]:HIS:CD2	1:D:282:GLN:H	2.20	0.59
1:A:66[B]:GLU:HG2	1:A:264:GLY:HA3	1.82	0.59
1:D:281:ASN:ND2	3:D:291:GOL:H32	2.17	0.59
1:A:245[C]:MSE:SE	4:A:831:HOH:O	2.71	0.59
1:D:229:HIS:NE2	1:D:231[B]:GLU:HG3	2.18	0.59
1:B:274[B]:HIS:ND1	1:B:274[B]:HIS:N	2.50	0.58
1:C:196[A]:ILE:CD1	1:C:197[A]:THR:HG23	2.33	0.58
1:C:63:THR:HG21	3:C:291:GOL:H32	1.84	0.58
1:B:153[B]:GLU:CG	1:B:185:LEU:HD23	2.33	0.58
1:A:274[B]:HIS:CD2	1:A:274[B]:HIS:N	2.72	0.58
1:A:191:LYS:HD3	1:A:227:ARG:HG3	1.86	0.58
1:C:196[A]:ILE:HD12	1:C:197[A]:THR:H	1.68	0.58
1:A:231[B]:GLU:OE2	1:A:235:GLN:NE2	2.37	0.57
1:A:178:GLY:HA3	1:A:213:LYS:HB3	1.86	0.57
1:D:245[A]:MSE:SE	4:D:1170:HOH:O	2.71	0.56
1:B:191:LYS:HD3	1:B:227:ARG:HG3	1.86	0.56
1:C:196[A]:ILE:HD13	4:C:1139:HOH:O	2.06	0.56
1:D:191:LYS:HE2	1:D:200:PRO:HB3	1.87	0.56
1:D:231[B]:GLU:OE2	1:D:235:GLN:NE2	2.40	0.55
1:A:151:GLN:O	1:A:186:HIS:HD2	1.88	0.55
1:A:230:ASN:O	1:A:231[B]:GLU:HG2	2.06	0.55
1:C:249[B]:GLN:HA	1:C:249[B]:GLN:HE21	1.73	0.54
1:D:194[B]:CYS:O	1:D:198[B]:ASN:N	2.40	0.54
1:D:62:TRP:CZ3	1:D:265[B]:LEU:HD13	2.42	0.54
1:D:50[A]:LEU:HD21	1:D:242:THR:HG21	1.89	0.54
1:D:51[B]:SER:OG	1:D:53[B]:THR:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279[B]:ASN:ND2	1:D:279[B]:ASN:O	2.42	0.53
1:C:199:GLN:NE2	1:D:99:LYS:HZ2	2.06	0.53
1:C:133[A]:THR:HG23	4:C:1173:HOH:O	2.08	0.52
1:D:178:GLY:HA3	1:D:213:LYS:HB3	1.90	0.52
1:A:51[B]:SER:HB2	1:A:53[B]:THR:HG22	1.91	0.52
1:A:274[B]:HIS:CD2	1:A:274[B]:HIS:H	2.28	0.52
1:B:231[B]:GLU:HB3	1:B:236[B]:CYS:SG	2.50	0.51
1:C:231[A]:GLU:HB3	1:C:236[A]:CYS:SG	2.51	0.51
1:B:44[A]:ASN:ND2	1:B:231[A]:GLU:OE1	2.44	0.51
1:D:195[B]:LEU:HD12	1:D:198[B]:ASN:ND2	2.27	0.51
1:D:66[B]:GLU:CG	1:D:264:GLY:HA3	2.40	0.51
1:A:114[B]:ASP:O	1:A:118[B]:THR:HG23	2.12	0.50
1:A:72[B]:GLN:H	1:A:72[B]:GLN:CD	2.14	0.50
1:B:274[B]:HIS:HD2	1:C:140[B]:ASN:O	1.95	0.50
1:D:230:ASN:O	1:D:231[B]:GLU:HG2	2.10	0.50
1:D:265[B]:LEU:O	1:D:265[B]:LEU:HD12	2.12	0.50
1:A:40:PRO:HA	1:A:91:ASN:HD22	1.77	0.49
1:B:194[A]:CYS:O	1:B:198[A]:ASN:N	2.45	0.49
1:B:245[A]:MSE:SE	4:B:1185:HOH:O	2.80	0.49
1:A:66[B]:GLU:CG	1:A:264:GLY:HA3	2.42	0.49
1:B:44[B]:ASN:O	1:B:48:LEU:HG	2.13	0.49
1:A:229:HIS:NE2	1:A:231[B]:GLU:HG3	2.27	0.49
1:D:273:SER:OG	1:D:274[B]:HIS:CD2	2.66	0.48
1:D:280[A]:HIS:HD2	1:D:282:GLN:N	2.09	0.48
1:D:273:SER:OG	1:D:274[B]:HIS:HD2	1.96	0.48
1:A:265[B]:LEU:HD12	1:A:265[B]:LEU:O	2.14	0.48
1:A:273:SER:OG	1:A:274[A]:HIS:HD2	1.96	0.47
1:B:99:LYS:NZ	1:B:103:ASN:HD21	2.13	0.47
1:D:279[B]:ASN:HD21	1:D:280[B]:HIS:CE1	2.32	0.47
1:A:229:HIS:CD2	4:A:1190:HOH:O	2.67	0.47
1:C:194[B]:CYS:CB	1:C:197[B]:THR:HG22	2.42	0.47
1:D:197[A]:THR:O	1:D:198[A]:ASN:CG	2.53	0.47
1:D:274[A]:HIS:CD2	1:D:274[A]:HIS:N	2.82	0.47
1:C:41:ARG:O	1:C:44[B]:ASN:OD1	2.32	0.47
1:D:77:GLN:NE2	1:D:113:TRP:HE1	2.06	0.47
1:B:195[B]:LEU:HD22	1:B:231[B]:GLU:CA	2.46	0.46
1:A:273:SER:OG	1:A:274[A]:HIS:CD2	2.68	0.46
1:C:140[A]:ASN:HD22	1:C:141:GLU:N	2.14	0.46
1:C:230:ASN:O	1:C:231[B]:GLU:HB2	2.16	0.46
1:C:153[B]:GLU:HG3	1:C:185:LEU:HD23	1.99	0.45
1:C:153[B]:GLU:H	1:C:153[B]:GLU:HG2	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46[B]:ASN:C	1:D:46[B]:ASN:OD1	2.54	0.45
1:A:145[B]:GLU:HG3	1:A:146:PRO:HD2	1.99	0.45
1:D:262[B]:LEU:HD23	4:D:893:HOH:O	2.17	0.45
1:A:119[B]:ARG:HG2	4:A:617:HOH:O	2.18	0.44
1:A:262[A]:LEU:HD23	4:A:794:HOH:O	2.17	0.44
1:C:227:ARG:HD3	1:D:107:GLN:HE22	1.81	0.44
1:A:44:ASN:ND2	1:A:235:GLN:HB3	2.31	0.44
1:C:197[B]:THR:HG23	1:C:199:GLN:N	2.17	0.44
1:C:196[A]:ILE:HD12	1:C:197[A]:THR:HG23	1.99	0.44
1:C:140[A]:ASN:HD22	1:C:140[A]:ASN:C	2.21	0.44
1:D:233:HIS:HD2	4:D:371:HOH:O	2.00	0.44
1:A:46[B]:ASN:OD1	1:A:47:ASP:N	2.51	0.43
1:C:153[B]:GLU:HG2	4:C:841:HOH:O	2.18	0.43
1:C:195[B]:LEU:HG	1:C:231[B]:GLU:HA	2.00	0.43
1:C:53[A]:THR:O	1:C:53[A]:THR:HG23	2.18	0.43
1:D:197[A]:THR:O	1:D:197[A]:THR:HG22	2.18	0.43
1:B:40:PRO:HA	1:B:91:ASN:HD22	1.82	0.43
1:D:274[A]:HIS:CD2	1:D:274[A]:HIS:H	2.36	0.43
1:B:195[B]:LEU:CD2	1:B:195[B]:LEU:N	2.57	0.43
1:A:231[A]:GLU:HG2	1:A:235:GLN:HE21	1.83	0.43
1:A:46[B]:ASN:OD1	1:A:46[B]:ASN:C	2.57	0.43
1:C:99:LYS:HZ3	1:C:103:ASN:HD21	1.67	0.43
1:D:31:TYR:CZ	1:D:33:PRO:HG3	2.54	0.43
1:C:158:GLN:HE22	1:C:217:GLU:CA	2.31	0.42
1:D:117[B]:GLN:NE2	4:D:952:HOH:O	2.52	0.42
1:A:53[B]:THR:O	1:A:53[B]:THR:HG23	2.20	0.42
1:D:66[B]:GLU:HG3	1:D:66[B]:GLU:H	1.63	0.42
1:A:44:ASN:OD1	1:A:231[A]:GLU:OE2	2.37	0.42
1:C:227:ARG:CD	1:D:107:GLN:HE22	2.32	0.42
1:C:50[B]:LEU:HD12	1:C:50[B]:LEU:HA	1.86	0.42
1:B:66[B]:GLU:HG2	1:B:264:GLY:HA3	2.02	0.42
1:D:151[C]:GLN:CG	1:D:184:VAL:HG11	2.50	0.42
1:D:197[B]:THR:C	1:D:199[B]:GLN:H	2.24	0.42
1:C:153[B]:GLU:HG3	1:C:185:LEU:CD2	2.50	0.42
1:D:195[A]:LEU:HD13	1:D:231[A]:GLU:HA	2.02	0.41
1:A:83:VAL:HG13	1:A:132[B]:VAL:CG1	2.50	0.41
1:C:214:MSE:HE1	1:C:219:LEU:HD13	2.02	0.41
1:A:31:TYR:CZ	1:A:33:PRO:HG3	2.55	0.41
1:D:30[B]:GLN:O	1:D:104:SER:HB2	2.21	0.41
1:B:124:LEU:HB2	1:B:132[B]:VAL:HG21	2.01	0.41
1:A:44:ASN:HB2	4:A:843:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151[C]:GLN:HG2	1:D:184:VAL:HG11	2.02	0.41
1:B:158:GLN:HE22	1:B:217:GLU:CA	2.31	0.41
1:A:66[B]:GLU:H	1:A:66[B]:GLU:HG3	1.61	0.41
1:B:195[B]:LEU:HD22	1:B:231[B]:GLU:C	2.40	0.41
1:C:231[B]:GLU:HG3	1:C:235:GLN:CB	2.48	0.41
1:D:135[A]:ASN:HD22	1:D:136:VAL:N	2.19	0.41
1:B:274[B]:HIS:CD2	1:C:140[B]:ASN:O	2.73	0.41
1:D:53[B]:THR:O	1:D:53[B]:THR:HG23	2.21	0.40
1:D:117[B]:GLN:HE21	1:D:117[B]:GLN:HB3	1.72	0.40
1:D:229:HIS:NE2	1:D:231[B]:GLU:CG	2.84	0.40
1:C:227:ARG:HE	1:D:107:GLN:NE2	2.19	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	293/290 (101%)	289 (99%)	4 (1%)	0	100	100
1	B	296/290 (102%)	292 (99%)	4 (1%)	0	100	100
1	C	296/290 (102%)	292 (99%)	4 (1%)	0	100	100
1	D	303/290 (104%)	298 (98%)	5 (2%)	0	100	100
All	All	1188/1160 (102%)	1171 (99%)	17 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	264/250 (106%)	258 (98%)	6 (2%)	56	23
1	B	268/250 (107%)	260 (97%)	8 (3%)	46	14
1	C	268/250 (107%)	265 (99%)	3 (1%)	78	56
1	D	274/250 (110%)	265 (97%)	9 (3%)	43	11
All	All	1074/1000 (107%)	1048 (98%)	26 (2%)	60	21

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	98	PHE
1	A	195	LEU
1	A	197	THR
1	A	231[A]	GLU
1	A	231[B]	GLU
1	B	29	ASN
1	B	46[A]	ASN
1	B	46[B]	ASN
1	B	50[A]	LEU
1	B	50[B]	LEU
1	B	98	PHE
1	B	153[A]	GLU
1	B	153[B]	GLU
1	C	98	PHE
1	C	140[A]	ASN
1	C	140[B]	ASN
1	D	29	ASN
1	D	98	PHE
1	D	135[A]	ASN
1	D	135[B]	ASN
1	D	228	GLU
1	D	231[A]	GLU
1	D	231[B]	GLU
1	D	274[A]	HIS
1	D	274[B]	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	91	ASN
1	A	186	HIS
1	A	235	GLN
1	A	275	GLN
1	A	279	ASN
1	B	57	GLN
1	B	77	GLN
1	B	91	ASN
1	B	103	ASN
1	B	106	ASN
1	B	151	GLN
1	B	158	GLN
1	B	230	ASN
1	B	233	HIS
1	B	275	GLN
1	C	103	ASN
1	C	106	ASN
1	C	158	GLN
1	C	199	GLN
1	C	233	HIS
1	D	77	GLN
1	D	107	GLN
1	D	233	HIS
1	D	235	GLN
1	D	275	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

11 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	PRF	A	290	1	13,14,14	2.59	6 (46%)	10,20,20	2.84	7 (70%)
3	GOL	A	291	-	5,5,5	0.38	0	5,5,5	0.23	0
2	PRF	B	290[A]	1	13,14,14	2.71	7 (53%)	10,20,20	2.88	7 (70%)
2	PRF	B	290[B]	1	13,14,14	2.80	7 (53%)	10,20,20	2.89	6 (60%)
3	GOL	B	291	-	5,5,5	0.36	0	5,5,5	0.11	0
2	PRF	C	290[A]	1	13,14,14	2.74	6 (46%)	10,20,20	2.88	7 (70%)
2	PRF	C	290[B]	1	13,14,14	2.75	7 (53%)	10,20,20	3.07	7 (70%)
3	GOL	C	291	-	5,5,5	0.32	0	5,5,5	0.33	0
2	PRF	D	290[A]	1	13,14,14	2.78	7 (53%)	10,20,20	2.93	7 (70%)
2	PRF	D	290[B]	1	13,14,14	2.81	7 (53%)	10,20,20	3.00	7 (70%)
3	GOL	D	291	-	5,5,5	0.36	0	5,5,5	0.18	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
2	PRF	A	290	1	-	0/0/2/2	0/2/2/2
3	GOL	A	291	-	-	0/4/4/4	0/0/0/0
2	PRF	B	290[A]	1	-	0/0/2/2	0/2/2/2
2	PRF	B	290[B]	1	-	0/0/2/2	0/2/2/2
3	GOL	B	291	-	-	0/4/4/4	0/0/0/0
2	PRF	C	290[A]	1	-	0/0/2/2	0/2/2/2
2	PRF	C	290[B]	1	-	0/0/2/2	0/2/2/2
3	GOL	C	291	-	-	0/4/4/4	0/0/0/0
2	PRF	D	290[A]	1	-	0/0/2/2	0/2/2/2
2	PRF	D	290[B]	1	-	0/0/2/2	0/2/2/2
3	GOL	D	291	-	-	0/4/4/4	0/0/0/0

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	290	PRF	C5-C4	-3.23	1.34	1.43
2	D	290[B]	PRF	C5-C4	-3.04	1.34	1.43
2	B	290[B]	PRF	C5-C4	-3.03	1.34	1.43
2	B	290[A]	PRF	C5-C4	-2.97	1.35	1.43
2	D	290[A]	PRF	C5-C4	-2.93	1.35	1.43
2	C	290[A]	PRF	C5-C4	-2.88	1.35	1.43
2	C	290[B]	PRF	C5-C4	-2.87	1.35	1.43
2	A	290	PRF	C10-C7	-2.76	1.42	1.51
2	D	290[B]	PRF	C10-C7	-2.34	1.43	1.51
2	B	290[A]	PRF	C10-C7	-2.24	1.43	1.51
2	D	290[A]	PRF	C10-C7	-2.21	1.43	1.51
2	B	290[B]	PRF	C10-C7	-2.07	1.44	1.51
2	C	290[B]	PRF	C10-C7	-2.05	1.44	1.51
2	D	290[B]	PRF	C6-N1	2.23	1.37	1.33
2	D	290[A]	PRF	C6-N1	2.26	1.37	1.33
2	C	290[A]	PRF	C6-N1	2.34	1.37	1.33
2	C	290[B]	PRF	C6-N1	2.38	1.37	1.33
2	B	290[A]	PRF	C6-N1	2.41	1.37	1.33
2	B	290[B]	PRF	C6-N1	2.45	1.37	1.33
2	A	290	PRF	O6-C6	2.69	1.31	1.24
2	C	290[A]	PRF	O6-C6	2.86	1.31	1.24
2	B	290[A]	PRF	O6-C6	2.90	1.31	1.24
2	D	290[A]	PRF	O6-C6	2.96	1.32	1.24
2	C	290[B]	PRF	O6-C6	2.97	1.32	1.24
2	D	290[B]	PRF	O6-C6	2.99	1.32	1.24
2	B	290[B]	PRF	O6-C6	3.01	1.32	1.24
2	A	290	PRF	C7-C5	3.24	1.45	1.41
2	D	290[B]	PRF	C7-C5	3.58	1.46	1.41
2	C	290[B]	PRF	C7-C5	3.58	1.46	1.41
2	B	290[A]	PRF	C7-C5	3.75	1.46	1.41
2	B	290[B]	PRF	C7-C5	3.78	1.46	1.41
2	D	290[A]	PRF	C7-C5	3.78	1.46	1.41
2	C	290[A]	PRF	C7-C5	3.87	1.46	1.41
2	A	290	PRF	C4-N9	3.92	1.42	1.34
2	C	290[A]	PRF	C4-N9	3.93	1.42	1.34
2	B	290[A]	PRF	C4-N9	3.98	1.42	1.34
2	C	290[B]	PRF	C4-N9	4.12	1.42	1.34
2	D	290[A]	PRF	C4-N9	4.23	1.42	1.34
2	D	290[B]	PRF	C4-N9	4.29	1.42	1.34
2	B	290[B]	PRF	C4-N9	4.29	1.42	1.34
2	A	290	PRF	C2-N2	5.08	1.44	1.34
2	B	290[A]	PRF	C2-N2	5.65	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	290[A]	PRF	C2-N2	5.72	1.45	1.34
2	B	290[B]	PRF	C2-N2	5.81	1.46	1.34
2	C	290[B]	PRF	C2-N2	5.85	1.46	1.34
2	C	290[A]	PRF	C2-N2	5.87	1.46	1.34
2	D	290[B]	PRF	C2-N2	5.92	1.46	1.34

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	290[B]	PRF	C5-C6-N1	-5.45	118.89	124.12
2	C	290[A]	PRF	C5-C6-N1	-5.19	119.14	124.12
2	D	290[B]	PRF	C5-C6-N1	-5.07	119.25	124.12
2	D	290[A]	PRF	C5-C6-N1	-5.02	119.30	124.12
2	B	290[B]	PRF	C5-C6-N1	-4.87	119.44	124.12
2	B	290[A]	PRF	C5-C6-N1	-4.82	119.50	124.12
2	A	290	PRF	C5-C6-N1	-4.63	119.67	124.12
2	A	290	PRF	C7-C5-C4	-3.52	104.32	110.22
2	D	290[B]	PRF	N3-C2-N1	-3.42	122.46	127.46
2	D	290[A]	PRF	C7-C5-C4	-3.28	104.73	110.22
2	D	290[A]	PRF	N3-C2-N1	-3.18	122.82	127.46
2	C	290[A]	PRF	N3-C2-N1	-3.10	122.93	127.46
2	D	290[B]	PRF	C7-C5-C4	-3.05	105.11	110.22
2	A	290	PRF	C10-C7-C8	-3.04	120.83	126.96
2	B	290[A]	PRF	C7-C5-C4	-3.01	105.18	110.22
2	B	290[A]	PRF	C10-C7-C8	-3.00	120.92	126.96
2	D	290[A]	PRF	C10-C7-C8	-2.97	120.98	126.96
2	C	290[B]	PRF	C7-C5-C4	-2.91	105.35	110.22
2	C	290[A]	PRF	C7-C5-C4	-2.90	105.36	110.22
2	B	290[B]	PRF	C7-C5-C4	-2.85	105.44	110.22
2	B	290[B]	PRF	N3-C2-N1	-2.79	123.38	127.46
2	A	290	PRF	N3-C2-N1	-2.76	123.42	127.46
2	C	290[B]	PRF	N3-C2-N1	-2.66	123.58	127.46
2	B	290[A]	PRF	N3-C2-N1	-2.63	123.62	127.46
2	C	290[A]	PRF	C10-C7-C8	-2.54	121.84	126.96
2	D	290[B]	PRF	C10-C7-C8	-2.49	121.95	126.96
2	C	290[B]	PRF	C10-C7-C8	-2.35	122.22	126.96
2	C	290[B]	PRF	C2-N3-C4	2.29	117.83	115.16
2	A	290	PRF	C2-N3-C4	2.33	117.88	115.16
2	B	290[A]	PRF	C6-N1-C2	2.36	119.45	116.06
2	B	290[A]	PRF	C2-N3-C4	2.36	117.91	115.16
2	C	290[A]	PRF	C2-N3-C4	2.42	117.99	115.16
2	B	290[B]	PRF	C6-N1-C2	2.51	119.67	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	290	PRF	C6-N1-C2	2.55	119.72	116.06
2	B	290[B]	PRF	C2-N3-C4	2.77	118.40	115.16
2	D	290[A]	PRF	C2-N3-C4	2.82	118.46	115.16
2	C	290[B]	PRF	C6-N1-C2	2.83	120.12	116.06
2	D	290[B]	PRF	C2-N3-C4	2.95	118.60	115.16
2	D	290[A]	PRF	C6-N1-C2	3.08	120.49	116.06
2	C	290[A]	PRF	C6-N1-C2	3.14	120.58	116.06
2	D	290[B]	PRF	C6-N1-C2	3.18	120.63	116.06
2	D	290[A]	PRF	C6-C5-C4	3.40	116.93	115.02
2	C	290[A]	PRF	C6-C5-C4	3.69	117.10	115.02
2	A	290	PRF	C6-C5-C4	3.98	117.26	115.02
2	D	290[B]	PRF	C6-C5-C4	4.01	117.28	115.02
2	B	290[A]	PRF	C6-C5-C4	4.71	117.67	115.02
2	B	290[B]	PRF	C6-C5-C4	4.97	117.82	115.02
2	C	290[B]	PRF	C6-C5-C4	5.31	118.01	115.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	290[A]	PRF	1	0
3	C	291	GOL	1	0
3	D	291	GOL	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	A	257/290 (88%)	0.02	14 (5%)	26 30	9, 15, 37, 69	1 (0%)
1	B	255/290 (87%)	-0.08	11 (4%)	36 41	8, 13, 27, 51	2 (0%)
1	C	255/290 (87%)	-0.09	10 (3%)	40 45	8, 12, 26, 42	2 (0%)
1	D	257/290 (88%)	-0.00	15 (5%)	24 27	9, 15, 37, 56	2 (0%)
All	All	1024/1160 (88%)	-0.04	50 (4%)	30 34	8, 14, 32, 69	7 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	ILE	12.5
1	D	195[A]	LEU	7.4
1	C	196[A]	ILE	7.3
1	D	196[A]	ILE	6.8
1	A	195	LEU	5.6
1	A	53[A]	THR	5.3
1	A	197	THR	5.2
1	D	197[A]	THR	5.0
1	B	53[A]	THR	4.7
1	C	53[A]	THR	4.5
1	B	52[A]	ALA	4.4
1	A	51[A]	SER	4.3
1	A	27	TYR	4.2
1	D	53[A]	THR	4.1
1	B	51[A]	SER	4.0
1	D	198[A]	ASN	4.0
1	D	28	ALA	3.8
1	A	29[A]	ASN	3.7
1	A	50[A]	LEU	3.7
1	B	195[A]	LEU	3.7
1	C	198[A]	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	198	ASN	3.6
1	B	196[A]	ILE	3.4
1	C	195[A]	LEU	3.4
1	A	52[A]	ALA	3.4
1	B	29	ASN	3.2
1	C	51[A]	SER	3.2
1	D	51[A]	SER	3.1
1	B	50[A]	LEU	3.0
1	C	52[A]	ALA	3.0
1	A	28	ALA	2.9
1	C	44[A]	ASN	2.5
1	D	27	TYR	2.5
1	C	50[A]	LEU	2.5
1	D	29	ASN	2.5
1	D	43[A]	LEU	2.5
1	B	44[A]	ASN	2.4
1	A	44	ASN	2.4
1	D	274[A]	HIS	2.4
1	A	274[A]	HIS	2.4
1	C	197[A]	THR	2.4
1	C	279[A]	ASN	2.3
1	B	198[A]	ASN	2.3
1	D	44	ASN	2.3
1	B	231[A]	GLU	2.2
1	D	50[A]	LEU	2.1
1	D	52[A]	ALA	2.1
1	A	262[A]	LEU	2.1
1	D	177	GLN	2.1
1	B	49[A]	HIS	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

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(Å <sup>2</sup> )	Q<0.9
3	GOL	A	291	6/6	0.60	0.41	39.40	39,42,46,51	0
3	GOL	B	291	6/6	0.69	0.36	17.36	24,37,42,46	0
3	GOL	C	291	6/6	0.80	0.28	9.86	23,28,36,39	0
3	GOL	D	291	6/6	0.90	0.20	6.87	17,20,33,41	0
2	PRF	A	290	13/13	0.97	0.08	-0.52	9,12,16,17	0
2	PRF	C	290[A]	13/13	0.97	0.08	-0.61	6,8,14,16	13
2	PRF	C	290[B]	13/13	0.97	0.08	-0.61	7,9,13,15	13
2	PRF	B	290[B]	13/13	0.98	0.07	-0.67	5,8,11,11	13
2	PRF	B	290[A]	13/13	0.98	0.07	-0.72	6,8,13,14	13
2	PRF	D	290[A]	13/13	0.98	0.07	-0.77	8,11,15,16	13
2	PRF	D	290[B]	13/13	0.98	0.07	-0.81	8,13,15,16	13

## 6.5 Other polymers [i](#)

There are no such residues in this entry.