



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:57 AM GMT

PDB ID : 3QJX  
Title : Crystal Structure of E. coli Aminopeptidase N in complex with L-Serine  
Authors : Addlagatta, A.; Gumpena, R.; Kishor, C.; Ganji, R.J.  
Deposited on : 2011-01-31  
Resolution : 1.45 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

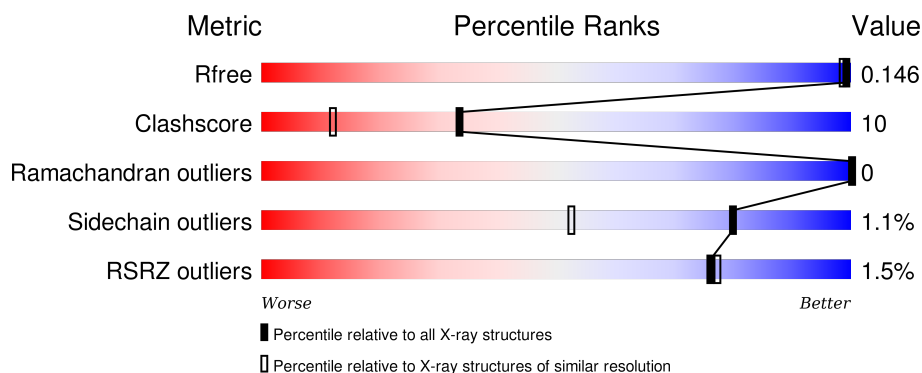
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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))
$R_{free}$	91344	1278 (1.48-1.44)
Clashscore	102246	1336 (1.48-1.44)
Ramachandran outliers	100387	1320 (1.48-1.44)
Sidechain outliers	100360	1320 (1.48-1.44)
RSRZ outliers	91569	1279 (1.48-1.44)

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	891	<div> <div></div> <div>77%</div> <div>16%</div> <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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	A	892	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MLI	A	950	-	-	-	X
6	GOL	A	970	-	-	-	X
6	GOL	A	972	-	-	-	X
6	GOL	A	973	-	-	-	X
6	GOL	A	975	-	-	-	X
6	GOL	A	976	-	-	-	X
6	GOL	A	977	-	-	X	X
6	GOL	A	978	-	-	-	X
6	GOL	A	979	-	-	-	X
6	GOL	A	982	-	-	X	X
6	GOL	A	983	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8314 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	866	7296	4638	1253	1377	28	0	62	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP P04825
A	-19	GLY	-	EXPRESSION TAG	UNP P04825
A	-18	SER	-	EXPRESSION TAG	UNP P04825
A	-17	SER	-	EXPRESSION TAG	UNP P04825
A	-16	HIS	-	EXPRESSION TAG	UNP P04825
A	-15	HIS	-	EXPRESSION TAG	UNP P04825
A	-14	HIS	-	EXPRESSION TAG	UNP P04825
A	-13	HIS	-	EXPRESSION TAG	UNP P04825
A	-12	HIS	-	EXPRESSION TAG	UNP P04825
A	-11	HIS	-	EXPRESSION TAG	UNP P04825
A	-10	SER	-	EXPRESSION TAG	UNP P04825
A	-9	SER	-	EXPRESSION TAG	UNP P04825
A	-8	GLY	-	EXPRESSION TAG	UNP P04825
A	-7	GLU	-	EXPRESSION TAG	UNP P04825
A	-6	ASN	-	EXPRESSION TAG	UNP P04825
A	-5	LEU	-	EXPRESSION TAG	UNP P04825
A	-4	TYR	-	EXPRESSION TAG	UNP P04825
A	-3	PHE	-	EXPRESSION TAG	UNP P04825
A	-2	GLN	-	EXPRESSION TAG	UNP P04825
A	-1	GLY	-	EXPRESSION TAG	UNP P04825
A	0	HIS	-	EXPRESSION TAG	UNP P04825

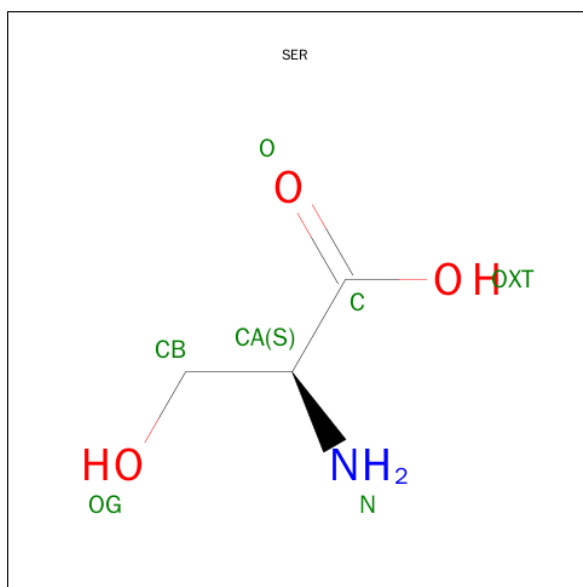
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Na	0	0
			3	3		

- Molecule 4 is SERINE (three-letter code: SER) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: C<sub>3</sub>H<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

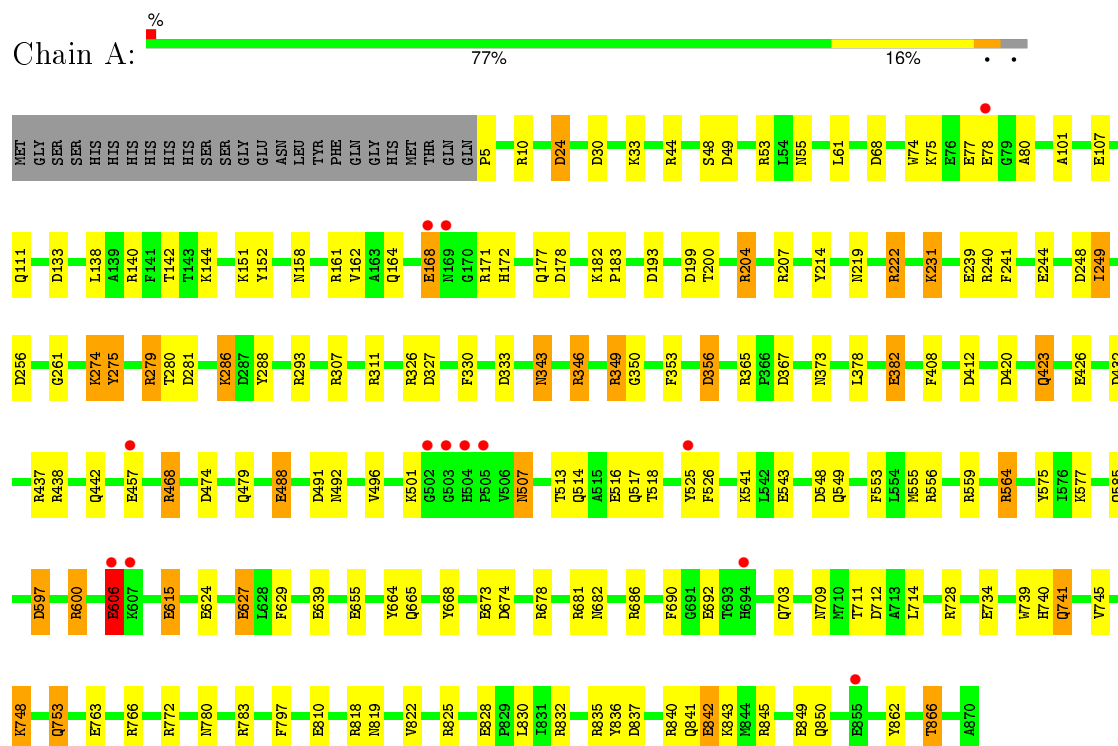
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	922	Total	O	0	0
			922	922		

### 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 errors 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: Aminopeptidase N





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.23Å 120.23Å 170.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.74 – 1.45 35.74 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.74-1.45) 99.9 (35.74-1.45)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.120 , 0.147 0.119 , 0.146	Depositor DCC
$R_{free}$ test set	7627 reflections (3.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.1	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 53.1	EDS
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 251676 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	8314	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, ZN, MLI, NA

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	1.54	73/7629 (1.0%)	1.42	99/10345 (1.0%)

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	LYS	CE-NZ	9.03	1.71	1.49
1	A	606	GLU	CG-CD	9.01	1.65	1.51
1	A	207	ARG	CD-NE	8.47	1.60	1.46
1	A	585	GLN	CG-CD	8.47	1.70	1.51
1	A	763	GLU	CG-CD	8.22	1.64	1.51
1	A	828	GLU	CG-CD	8.20	1.64	1.51
1	A	525	TYR	CG-CD2	7.89	1.49	1.39
1	A	673	GLU	CD-OE1	7.83	1.34	1.25
1	A	828	GLU	CD-OE2	-7.77	1.17	1.25
1	A	161	ARG	CB-CG	-7.70	1.31	1.52
1	A	207	ARG	CG-CD	7.64	1.71	1.51
1	A	161	ARG	CG-CD	7.32	1.70	1.51
1	A	766	ARG	CG-CD	7.32	1.70	1.51
1	A	692	GLU	CD-OE1	7.30	1.33	1.25
1	A	549	GLN	CG-CD	7.08	1.67	1.51
1	A	144	LYS	CD-CE	-7.06	1.33	1.51
1	A	525	TYR	CE1-CZ	6.98	1.47	1.38
1	A	231	LYS	CD-CE	-6.95	1.33	1.51
1	A	140	ARG	CZ-NH1	6.89	1.42	1.33
1	A	161	ARG	CZ-NH2	6.74	1.41	1.33
1	A	168	GLU	CG-CD	6.68	1.61	1.51
1	A	164	GLN	CB-CG	-6.61	1.34	1.52
1	A	161	ARG	CZ-NH1	6.50	1.41	1.33
1	A	615	GLU	CD-OE2	6.27	1.32	1.25
1	A	553	PHE	CD1-CE1	6.12	1.51	1.39
1	A	346[A]	ARG	NE-CZ	6.09	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346[B]	ARG	NE-CZ	6.09	1.41	1.33
1	A	842[A]	GLU	CD-OE2	6.06	1.32	1.25
1	A	842[B]	GLU	CD-OE2	6.06	1.32	1.25
1	A	841	GLN	CB-CG	-6.00	1.36	1.52
1	A	279	ARG	CG-CD	5.89	1.66	1.51
1	A	797	PHE	CE2-CZ	5.89	1.48	1.37
1	A	457	GLU	CD-OE2	5.83	1.32	1.25
1	A	78[A]	GLU	CG-CD	5.83	1.60	1.51
1	A	78[B]	GLU	CG-CD	5.83	1.60	1.51
1	A	564[A]	ARG	CZ-NH1	5.82	1.40	1.33
1	A	564[B]	ARG	CZ-NH1	5.82	1.40	1.33
1	A	624	GLU	CB-CG	5.76	1.63	1.52
1	A	286	LYS	CD-CE	5.67	1.65	1.51
1	A	426	GLU	CD-OE2	5.60	1.31	1.25
1	A	577	LYS	CD-CE	-5.57	1.37	1.51
1	A	627[A]	GLU	CG-CD	5.55	1.60	1.51
1	A	627[B]	GLU	CG-CD	5.55	1.60	1.51
1	A	468[A]	ARG	CB-CG	-5.54	1.37	1.52
1	A	468[B]	ARG	CB-CG	-5.54	1.37	1.52
1	A	343	ASN	CG-OD1	5.50	1.36	1.24
1	A	629	PHE	CG-CD1	5.43	1.46	1.38
1	A	810[A]	GLU	CG-CD	5.43	1.60	1.51
1	A	810[B]	GLU	CG-CD	5.43	1.60	1.51
1	A	274[A]	LYS	CE-NZ	5.39	1.62	1.49
1	A	274[B]	LYS	CE-NZ	5.39	1.62	1.49
1	A	606	GLU	CD-OE2	5.39	1.31	1.25
1	A	161	ARG	NE-CZ	5.36	1.40	1.33
1	A	244	GLU	CG-CD	5.36	1.59	1.51
1	A	835	ARG	CZ-NH2	5.35	1.40	1.33
1	A	639[A]	GLU	CB-CG	5.29	1.62	1.52
1	A	639[B]	GLU	CB-CG	5.29	1.62	1.52
1	A	330	PHE	CG-CD1	5.23	1.46	1.38
1	A	766	ARG	CZ-NH1	5.23	1.39	1.33
1	A	501	LYS	CE-NZ	5.21	1.62	1.49
1	A	543[A]	GLU	CD-OE1	5.21	1.31	1.25
1	A	543[B]	GLU	CD-OE1	5.21	1.31	1.25
1	A	772	ARG	CD-NE	5.19	1.55	1.46
1	A	488[A]	GLU	CG-CD	5.16	1.59	1.51
1	A	488[B]	GLU	CG-CD	5.16	1.59	1.51
1	A	488[A]	GLU	CD-OE1	5.15	1.31	1.25
1	A	488[B]	GLU	CD-OE1	5.15	1.31	1.25
1	A	516	GLU	CD-OE1	-5.14	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	690	PHE	CG-CD1	5.10	1.46	1.38
1	A	152	TYR	CD2-CE2	5.09	1.47	1.39
1	A	748	LYS	CE-NZ	5.03	1.61	1.49
1	A	734	GLU	CD-OE2	5.03	1.31	1.25
1	A	866	THR	CB-OG1	-5.00	1.33	1.43

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349[A]	ARG	NE-CZ-NH2	-12.18	114.21	120.30
1	A	349[C]	ARG	NE-CZ-NH2	-12.18	114.21	120.30
1	A	681	ARG	NE-CZ-NH2	11.82	126.21	120.30
1	A	279	ARG	NE-CZ-NH1	-10.73	114.94	120.30
1	A	832	ARG	NE-CZ-NH2	-10.45	115.07	120.30
1	A	432	ASP	CB-CG-OD1	10.26	127.54	118.30
1	A	207	ARG	NE-CZ-NH1	-10.18	115.21	120.30
1	A	837	ASP	CB-CG-OD2	9.34	126.70	118.30
1	A	279	ARG	NE-CZ-NH2	9.12	124.86	120.30
1	A	204[A]	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	A	204[B]	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	A	240	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	600[A]	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	600[B]	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	437	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	A	214	TYR	CB-CG-CD1	-8.33	116.00	121.00
1	A	627[A]	GLU	OE1-CD-OE2	8.11	133.03	123.30
1	A	627[B]	GLU	OE1-CD-OE2	8.11	133.03	123.30
1	A	365	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	311	ARG	NE-CZ-NH1	-8.02	116.29	120.30
1	A	835	ARG	NE-CZ-NH1	-7.75	116.43	120.30
1	A	204[A]	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	A	204[B]	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	A	835	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	A	828	GLU	OE1-CD-OE2	-7.29	114.55	123.30
1	A	597	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	A	68	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	A	556	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	A	349[A]	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	A	349[C]	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	A	564[A]	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	564[B]	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	367	ASP	CB-CG-OD1	7.06	124.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	A	678	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	A	548	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	420	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	A	600[A]	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	A	600[B]	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	A	681	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	A	49	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	178	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	426	GLU	OE1-CD-OE2	-6.42	115.59	123.30
1	A	241	PHE	CB-CG-CD1	-6.42	116.30	120.80
1	A	240	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	686	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	256	ASP	CB-CG-OD1	6.17	123.86	118.30
1	A	356	ASP	O-C-N	6.12	132.49	122.70
1	A	548	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	161	ARG	NE-CZ-NH1	-6.09	117.26	120.30
1	A	346[A]	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	A	346[B]	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	A	239	GLU	OE1-CD-OE2	-6.04	116.05	123.30
1	A	222	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	333	ASP	CB-CG-OD1	5.96	123.67	118.30
1	A	432	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	A	193	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	866	THR	OG1-CB-CG2	-5.82	96.61	110.00
1	A	420	ASP	CB-CG-OD1	5.78	123.51	118.30
1	A	818	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	A	474	ASP	CB-CG-OD1	-5.75	113.12	118.30
1	A	200[A]	THR	OG1-CB-CG2	-5.74	96.81	110.00
1	A	200[B]	THR	OG1-CB-CG2	-5.74	96.81	110.00
1	A	24[A]	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	24[B]	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	275	TYR	CB-CG-CD2	-5.59	117.65	121.00
1	A	44	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	A	728	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	843	LYS	CD-CE-NZ	-5.54	98.95	111.70
1	A	836	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	A	248	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	A	286	LYS	CD-CE-NZ	-5.51	99.03	111.70
1	A	48	SER	CA-CB-OG	-5.49	96.37	111.20
1	A	353	PHE	CB-CG-CD1	5.49	124.64	120.80
1	A	326	ARG	NE-CZ-NH2	-5.46	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	830	LEU	CB-CG-CD1	5.45	120.27	111.00
1	A	311	ARG	NH1-CZ-NH2	5.40	125.34	119.40
1	A	828	GLU	CG-CD-OE1	5.40	129.10	118.30
1	A	353	PHE	CB-CG-CD2	-5.36	117.05	120.80
1	A	207	ARG	CD-NE-CZ	5.33	131.07	123.60
1	A	664	TYR	CD1-CE1-CZ	-5.30	115.03	119.80
1	A	346[A]	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	346[B]	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	10	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	373	ASN	CB-CG-ND2	-5.22	104.17	116.70
1	A	423[A]	GLN	CA-CB-CG	-5.22	101.92	113.40
1	A	423[B]	GLN	CA-CB-CG	-5.22	101.92	113.40
1	A	438	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	161	ARG	CD-NE-CZ	5.17	130.84	123.60
1	A	346[A]	ARG	NH1-CZ-NH2	-5.15	113.74	119.40
1	A	346[B]	ARG	NH1-CZ-NH2	-5.15	113.74	119.40
1	A	161	ARG	NE-CZ-NH2	5.13	122.86	120.30
1	A	629	PHE	CB-CG-CD1	5.12	124.38	120.80
1	A	491	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	288	TYR	CB-CG-CD1	5.06	124.04	121.00
1	A	575	TYR	CG-CD2-CE2	5.04	125.33	121.30
1	A	307	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	A	382[A]	GLU	OE1-CD-OE2	-5.02	117.28	123.30
1	A	382[B]	GLU	OE1-CD-OE2	-5.02	117.28	123.30

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	A	7296	0	7277	143	1
2	A	1	0	0	0	0
3	A	3	0	0	0	0
4	A	7	0	4	0	0
5	A	7	0	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	78	0	76	31	0
7	A	922	0	0	44	1
All	All	8314	0	7359	151	1

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 (151) 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:231:LYS:NZ	1:A:231:LYS:CE	1.71	1.48
1:A:825[B]:ARG:NH2	7:A:1776:HOH:O	1.58	1.31
1:A:627[A]:GLU:HG3	7:A:1384:HOH:O	1.23	1.27
1:A:783[B]:ARG:NH2	1:A:825[B]:ARG:HD2	1.49	1.26
1:A:783[B]:ARG:HH21	1:A:825[B]:ARG:CD	1.52	1.23
1:A:107[A]:GLU:OE2	7:A:1270:HOH:O	1.58	1.19
1:A:350[A]:GLY:O	7:A:1384:HOH:O	1.59	1.18
1:A:825[B]:ARG:CZ	7:A:1362:HOH:O	1.90	1.17
1:A:343:ASN:OD1	1:A:346[A]:ARG:NH1	1.76	1.16
1:A:346[A]:ARG:NH2	1:A:615:GLU:OE1	1.81	1.12
6:A:979:GOL:H32	6:A:983:GOL:O2	1.35	1.11
1:A:204[B]:ARG:HG3	1:A:204[B]:ARG:HH11	1.00	1.11
1:A:627[A]:GLU:HG2	7:A:1796:HOH:O	1.49	1.11
1:A:783[B]:ARG:HG2	1:A:783[B]:ARG:HH11	1.08	1.10
1:A:783[A]:ARG:NH1	6:A:977:GOL:O3	1.85	1.10
1:A:783[B]:ARG:NH2	1:A:825[B]:ARG:CD	2.11	1.09
1:A:5:PRO:N	7:A:1167:HOH:O	1.84	1.08
1:A:488[B]:GLU:OE1	1:A:559:ARG:NH2	1.86	1.06
1:A:507[A]:ASN:OD1	7:A:1331:HOH:O	1.69	1.06
6:A:979:GOL:C3	6:A:983:GOL:O2	2.00	1.06
1:A:783[B]:ARG:HH21	1:A:825[B]:ARG:HD2	0.90	1.04
1:A:825[B]:ARG:HG3	1:A:825[B]:ARG:HH11	1.23	1.01
1:A:825[B]:ARG:NH1	7:A:1362:HOH:O	1.93	0.97
1:A:346[B]:ARG:NH1	7:A:1801:HOH:O	1.98	0.96
1:A:281[A]:ASP:OD1	7:A:943:HOH:O	1.84	0.95
1:A:346[A]:ARG:NH1	7:A:1075:HOH:O	2.00	0.95
1:A:783[B]:ARG:NH2	1:A:825[B]:ARG:NE	2.15	0.95
1:A:249[A]:ILE:HG22	7:A:1526:HOH:O	1.69	0.93
1:A:249[A]:ILE:CG2	7:A:1526:HOH:O	2.15	0.93
1:A:204[B]:ARG:CG	1:A:204[B]:ARG:HH11	1.81	0.93
1:A:279:ARG:NH1	1:A:281[A]:ASP:OD1	2.03	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845[B]:ARG:NH2	7:A:1666:HOH:O	2.04	0.91
1:A:627[B]:GLU:HG3	7:A:1367:HOH:O	1.68	0.91
1:A:279:ARG:NH1	1:A:281[A]:ASP:OD2	2.05	0.90
1:A:783[A]:ARG:CZ	7:A:1776:HOH:O	2.20	0.89
1:A:783[B]:ARG:HG2	1:A:783[B]:ARG:NH1	1.78	0.88
1:A:514:GLN:H	1:A:517[B]:GLN:HE22	1.17	0.88
1:A:349[C]:ARG:NH2	7:A:1285:HOH:O	2.06	0.87
1:A:825[B]:ARG:HG3	1:A:825[B]:ARG:NH1	1.83	0.87
1:A:274[B]:LYS:NZ	6:A:977:GOL:H32	1.90	0.86
1:A:204[B]:ARG:HG3	1:A:204[B]:ARG:NH1	1.80	0.85
1:A:468[B]:ARG:HB2	6:A:974:GOL:H11	1.58	0.85
1:A:783[A]:ARG:HH12	6:A:977:GOL:C3	1.90	0.83
1:A:286:LYS:HE3	6:A:978:GOL:O2	1.78	0.83
1:A:274[A]:LYS:NZ	6:A:982:GOL:O3	2.10	0.83
1:A:279:ARG:NH1	1:A:281[A]:ASP:CG	2.34	0.81
1:A:107[A]:GLU:CD	7:A:1270:HOH:O	2.03	0.80
1:A:541:LYS:HE2	1:A:627[B]:GLU:OE1	1.82	0.80
1:A:783[B]:ARG:NH2	1:A:825[B]:ARG:HE	1.78	0.80
1:A:231:LYS:NZ	1:A:231:LYS:CD	2.42	0.80
1:A:442:GLN:HE22	1:A:479:GLN:H	1.30	0.78
1:A:286:LYS:HE3	6:A:978:GOL:HO2	1.48	0.78
1:A:597:ASP:OD1	1:A:600[B]:ARG:NH1	2.18	0.76
1:A:842[B]:GLU:HG2	7:A:886:HOH:O	1.87	0.75
1:A:204[B]:ARG:CG	1:A:204[B]:ARG:NH1	2.44	0.75
1:A:783[A]:ARG:NE	7:A:1776:HOH:O	2.19	0.75
1:A:783[B]:ARG:CG	1:A:783[B]:ARG:HH11	1.93	0.74
1:A:286:LYS:CE	6:A:978:GOL:O2	2.35	0.73
6:A:979:GOL:H32	6:A:983:GOL:HO2	1.54	0.71
1:A:24[B]:ASP:CG	7:A:1125:HOH:O	2.29	0.69
1:A:513:THR:H	1:A:517[A]:GLN:HE22	1.38	0.69
1:A:627[B]:GLU:OE2	7:A:1797:HOH:O	2.09	0.69
1:A:24[B]:ASP:OD1	7:A:1125:HOH:O	2.11	0.68
1:A:55:ASN:HD22	1:A:133:ASP:H	1.43	0.67
1:A:274[B]:LYS:HZ3	6:A:977:GOL:H32	1.57	0.67
1:A:171[A]:ARG:HD3	7:A:946:HOH:O	1.95	0.65
1:A:783[B]:ARG:CG	1:A:783[B]:ARG:NH1	2.55	0.65
1:A:24[B]:ASP:OD2	7:A:1125:HOH:O	2.14	0.65
1:A:783[B]:ARG:CZ	1:A:825[B]:ARG:HE	2.12	0.63
1:A:219:ASN:ND2	1:A:222:ARG:HH21	1.99	0.61
1:A:274[B]:LYS:HZ1	6:A:977:GOL:H32	1.64	0.61
1:A:77[B]:GLU:HG2	1:A:80:ALA:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:TRP:HE1	6:A:972:GOL:H11	1.66	0.60
1:A:349[A]:ARG:NH2	7:A:889:HOH:O	2.07	0.59
1:A:627[A]:GLU:CG	7:A:1796:HOH:O	2.23	0.59
1:A:274[B]:LYS:HD3	7:A:1597:HOH:O	2.02	0.59
1:A:274[A]:LYS:HZ3	6:A:977:GOL:H32	1.66	0.59
1:A:158:ASN:ND2	1:A:182[B]:LYS:HZ1	2.01	0.58
1:A:783[B]:ARG:CZ	1:A:825[B]:ARG:NE	2.67	0.58
1:A:555:MET:O	1:A:564[B]:ARG:HD3	2.04	0.57
1:A:714:LEU:HD22	1:A:748:LYS:HD3	1.85	0.57
1:A:274[A]:LYS:HZ3	6:A:982:GOL:HO3	1.47	0.57
1:A:514:GLN:H	1:A:517[B]:GLN:NE2	1.95	0.57
1:A:600[B]:ARG:HD3	1:A:655:GLU:OE2	2.05	0.56
1:A:249[A]:ILE:HG23	7:A:1526:HOH:O	1.92	0.56
1:A:53[B]:ARG:HH22	1:A:77[B]:GLU:CD	2.09	0.56
1:A:783[A]:ARG:CZ	6:A:977:GOL:O3	2.52	0.56
1:A:275:TYR:OH	6:A:977:GOL:H11	2.04	0.56
1:A:850:GLN:OE1	7:A:1273:HOH:O	2.18	0.56
1:A:709:ASN:ND2	1:A:712:ASP:H	2.04	0.55
1:A:261:GLY:HA2	6:A:977:GOL:H31	1.88	0.55
1:A:75:LYS:HE3	1:A:77[A]:GLU:OE2	2.06	0.55
1:A:442:GLN:NE2	1:A:479:GLN:H	2.02	0.54
1:A:77[B]:GLU:CG	1:A:80:ALA:HB3	2.38	0.54
6:A:977:GOL:HO2	6:A:982:GOL:HO1	0.60	0.54
6:A:977:GOL:O2	6:A:982:GOL:O1	1.80	0.53
1:A:274[B]:LYS:HZ1	6:A:977:GOL:C3	2.22	0.52
1:A:741[A]:GLN:NE2	1:A:741[A]:GLN:H	2.08	0.52
1:A:138[B]:LEU:HD12	1:A:183:PRO:HD3	1.92	0.52
1:A:168:GLU:HG2	7:A:908:HOH:O	2.10	0.51
1:A:849[A]:GLU:OE1	7:A:1156:HOH:O	2.19	0.51
1:A:274[A]:LYS:NZ	6:A:982:GOL:HO3	2.07	0.51
1:A:753:GLN:HE21	1:A:753:GLN:HA	1.76	0.51
1:A:142[B]:THR:HG23	1:A:177[B]:GLN:HG2	1.93	0.50
1:A:783[A]:ARG:HH12	6:A:977:GOL:H32	1.73	0.50
1:A:492:ASN:HB3	1:A:526:PHE:CE2	2.47	0.50
1:A:274[B]:LYS:NZ	6:A:977:GOL:C3	2.69	0.50
1:A:682:ASN:ND2	1:A:703:GLN:HE22	2.10	0.49
1:A:518[B]:THR:HG23	7:A:1278:HOH:O	2.13	0.49
1:A:274[A]:LYS:NZ	6:A:977:GOL:H32	2.29	0.48
1:A:849[A]:GLU:CD	7:A:1156:HOH:O	2.52	0.47
1:A:423[B]:GLN:NE2	7:A:902:HOH:O	2.36	0.47
1:A:249[A]:ILE:HD11	7:A:1519:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:GLN:HE22	1:A:674:ASP:HA	1.80	0.47
1:A:343:ASN:OD1	1:A:346[B]:ARG:HD2	2.14	0.47
1:A:488[B]:GLU:HG3	1:A:496:VAL:HG13	1.97	0.47
1:A:468[B]:ARG:HH11	1:A:468[B]:ARG:HG3	1.80	0.47
1:A:158:ASN:CG	1:A:182[B]:LYS:HZ1	2.17	0.47
1:A:709:ASN:HD21	1:A:712:ASP:H	1.61	0.47
1:A:279:ARG:HG3	1:A:281[A]:ASP:OD1	2.15	0.46
1:A:682:ASN:HD21	1:A:703:GLN:HE22	1.64	0.46
1:A:101:ALA:HA	1:A:111[B]:GLN:OE1	2.15	0.46
1:A:862:TYR:O	1:A:866:THR:HG23	2.16	0.46
1:A:74:TRP:NE1	6:A:972:GOL:H11	2.32	0.45
1:A:825[A]:ARG:NH1	7:A:885:HOH:O	2.50	0.45
1:A:61:LEU:O	6:A:973:GOL:H31	2.17	0.45
1:A:378:LEU:O	1:A:382[B]:GLU:HB2	2.18	0.44
1:A:53[B]:ARG:HG3	1:A:53[B]:ARG:NH1	2.33	0.44
1:A:627[B]:GLU:CD	7:A:1797:HOH:O	2.53	0.44
1:A:293[B]:ARG:NH1	7:A:1636:HOH:O	2.48	0.44
1:A:151:LYS:HE2	1:A:151:LYS:HB2	1.47	0.44
1:A:274[B]:LYS:HB3	1:A:274[B]:LYS:HE3	1.58	0.43
1:A:468[B]:ARG:NH1	1:A:468[B]:ARG:HG3	2.34	0.43
1:A:739:TRP:CG	1:A:745:VAL:HG11	2.53	0.43
1:A:274[B]:LYS:HE3	1:A:780[B]:ASN:HD21	1.83	0.43
6:A:972:GOL:H32	7:A:1515:HOH:O	2.18	0.43
1:A:30:ASP:HB3	1:A:33:LYS:O	2.19	0.43
1:A:408:PHE:O	1:A:412[A]:ASP:HB2	2.18	0.43
1:A:840:ARG:HG2	7:A:934:HOH:O	2.18	0.42
6:A:977:GOL:O2	6:A:982:GOL:C1	2.66	0.42
1:A:783[B]:ARG:HG3	7:A:1245:HOH:O	2.18	0.42
1:A:53[B]:ARG:HG3	1:A:53[B]:ARG:HH11	1.85	0.42
1:A:819:ASN:HB3	1:A:822[B]:VAL:HG22	2.03	0.41
6:A:976:GOL:H31	7:A:1467:HOH:O	2.19	0.41
1:A:162:VAL:HG21	1:A:177[B]:GLN:HG3	2.03	0.41
1:A:740:HIS:CE1	1:A:741[B]:GLN:HG3	2.56	0.40
1:A:606:GLU:H	1:A:606:GLU:CD	2.23	0.40
1:A:709:ASN:HD22	1:A:711:THR:H	1.69	0.40
1:A:280[B]:THR:HG23	1:A:668:TYR:CD2	2.56	0.40
1:A:488[B]:GLU:OE1	1:A:559:ARG:CZ	2.64	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204[B]:ARG:NE	7:A:963:HOH:O[4_565]	2.17	0.03

## 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	926/891 (104%)	912 (98%)	14 (2%)	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	802/763 (105%)	791 (99%)	11 (1%)	74	42

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	HIS
1	A	249[A]	ILE
1	A	249[B]	ILE
1	A	327	ASP
1	A	356	ASP
1	A	507[A]	ASN
1	A	507[B]	ASN
1	A	606	GLU

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Mol	Chain	Res	Type
1	A	741[A]	GLN
1	A	741[B]	GLN
1	A	753	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	219	ASN
1	A	442	GLN
1	A	514	GLN
1	A	569	GLN
1	A	623	ASN
1	A	665	GLN
1	A	682	ASN
1	A	709	ASN
1	A	753	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 ⓘ

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 for Mogul analysis.

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	$\# Z  > 2$
4	SER	A	900	2	3,6,6	0.75	0	1,7,7	2.73	1 (100%)
5	MLI	A	950	-	0,6,6	0.00	-	0,7,7	0.00	-
6	GOL	A	970	-	5,5,5	2.22	3 (60%)	5,5,5	2.17	2 (40%)
6	GOL	A	971	-	5,5,5	0.80	0	5,5,5	0.79	0
6	GOL	A	972	-	5,5,5	3.11	3 (60%)	5,5,5	2.31	2 (40%)
6	GOL	A	973	-	5,5,5	1.00	0	5,5,5	1.58	1 (20%)
6	GOL	A	974	-	5,5,5	1.68	2 (40%)	5,5,5	1.31	1 (20%)
6	GOL	A	975	-	5,5,5	1.25	0	5,5,5	1.26	0
6	GOL	A	976	-	5,5,5	1.24	1 (20%)	5,5,5	1.64	1 (20%)
6	GOL	A	977	-	5,5,5	0.73	0	5,5,5	2.23	2 (40%)
6	GOL	A	978	-	5,5,5	1.22	0	5,5,5	2.18	3 (60%)
6	GOL	A	979	-	5,5,5	0.93	0	5,5,5	1.75	2 (40%)
6	GOL	A	981	-	5,5,5	0.58	0	5,5,5	1.52	1 (20%)
6	GOL	A	982	-	5,5,5	0.83	0	5,5,5	1.71	1 (20%)
6	GOL	A	983	-	5,5,5	0.91	0	5,5,5	1.16	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
4	SER	A	900	2	-	0/2/6/6	0/0/0/0
5	MLI	A	950	-	-	0/0/4/4	0/0/0/0
6	GOL	A	970	-	-	0/4/4/4	0/0/0/0
6	GOL	A	971	-	-	0/4/4/4	0/0/0/0
6	GOL	A	972	-	-	0/4/4/4	0/0/0/0
6	GOL	A	973	-	-	0/4/4/4	0/0/0/0
6	GOL	A	974	-	-	0/4/4/4	0/0/0/0
6	GOL	A	975	-	-	0/4/4/4	0/0/0/0
6	GOL	A	976	-	-	0/4/4/4	0/0/0/0
6	GOL	A	977	-	-	0/4/4/4	0/0/0/0
6	GOL	A	978	-	-	0/4/4/4	0/0/0/0
6	GOL	A	979	-	-	0/4/4/4	0/0/0/0
6	GOL	A	981	-	-	0/4/4/4	0/0/0/0
6	GOL	A	982	-	-	0/4/4/4	0/0/0/0
6	GOL	A	983	-	-	0/4/4/4	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	972	GOL	O2-C2	-5.23	1.27	1.43
6	A	976	GOL	O2-C2	-2.65	1.35	1.43
6	A	974	GOL	O2-C2	-2.29	1.36	1.43
6	A	970	GOL	C3-C2	-2.06	1.44	1.52
6	A	974	GOL	C1-C2	2.12	1.60	1.52
6	A	970	GOL	C1-C2	2.77	1.62	1.52
6	A	972	GOL	O3-C3	2.82	1.54	1.42
6	A	970	GOL	O2-C2	3.12	1.52	1.43
6	A	972	GOL	C3-C2	3.58	1.66	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	972	GOL	O1-C1-C2	-4.01	90.73	110.18
6	A	970	GOL	C3-C2-C1	-3.58	97.08	111.12
6	A	978	GOL	O2-C2-C1	-3.38	93.14	108.65
4	A	900	SER	OG-CB-CA	-2.73	105.34	111.16
6	A	976	GOL	O2-C2-C3	-2.64	96.55	108.65
6	A	979	GOL	O2-C2-C1	-2.18	98.65	108.65
6	A	970	GOL	O3-C3-C2	-2.14	99.81	110.18
6	A	978	GOL	O1-C1-C2	2.27	121.20	110.18
6	A	977	GOL	O2-C2-C3	2.35	119.42	108.65
6	A	974	GOL	O1-C1-C2	2.46	122.12	110.18
6	A	979	GOL	O3-C3-C2	2.49	122.26	110.18
6	A	978	GOL	O3-C3-C2	2.64	122.97	110.18
6	A	981	GOL	O2-C2-C1	2.75	121.25	108.65
6	A	973	GOL	C3-C2-C1	2.87	122.38	111.12
6	A	972	GOL	O2-C2-C3	3.19	123.29	108.65
6	A	982	GOL	O2-C2-C3	3.26	123.60	108.65
6	A	977	GOL	O2-C2-C1	3.56	124.96	108.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	972	GOL	3	0
6	A	973	GOL	1	0
6	A	974	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	976	GOL	1	0
6	A	977	GOL	16	0
6	A	978	GOL	3	0
6	A	979	GOL	3	0
6	A	982	GOL	6	0
6	A	983	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	866/891 (97%)	-0.27	13 (1%) 76 77	6, 12, 25, 46	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	HIS	5.5
1	A	503	GLY	5.1
1	A	169	ASN	4.2
1	A	168	GLU	3.7
1	A	502	GLY	3.5
1	A	694	HIS	3.4
1	A	606	GLU	3.3
1	A	505	PRO	3.2
1	A	855	GLU	2.9
1	A	607	LYS	2.7
1	A	457	GLU	2.7
1	A	525	TYR	2.3
1	A	78[A]	GLU	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(Å <sup>2</sup> )	Q<0.9
6	GOL	A	972	6/6	0.94	0.23	31.69	21,25,30,30	0
6	GOL	A	976	6/6	0.94	0.55	26.50	12,23,30,31	6
5	MLI	A	950	7/7	0.93	0.22	21.28	20,26,31,32	0
6	GOL	A	975	6/6	0.98	0.15	14.75	9,13,15,18	6
6	GOL	A	982	6/6	0.76	0.48	12.03	31,34,35,35	6
3	NA	A	892	1/1	0.99	0.15	9.83	21,21,21,21	1
6	GOL	A	973	6/6	0.96	0.12	8.68	17,36,49,58	0
6	GOL	A	977	6/6	0.92	0.29	5.72	27,29,30,35	6
6	GOL	A	970	6/6	0.95	0.12	4.52	17,25,26,28	0
6	GOL	A	983	6/6	0.90	0.18	3.74	27,33,35,35	6
6	GOL	A	979	6/6	0.91	0.17	3.65	21,26,27,27	6
6	GOL	A	978	6/6	0.94	0.14	3.62	11,21,25,33	6
3	NA	A	890	1/1	1.00	0.07	1.72	15,15,15,15	0
6	GOL	A	974	6/6	0.97	0.14	1.28	16,17,22,26	6
6	GOL	A	971	6/6	0.97	0.09	0.17	19,27,31,37	0
4	SER	A	900	7/7	0.99	0.08	-0.48	7,7,9,10	0
2	ZN	A	880	1/1	1.00	0.05	-4.16	6,6,6,6	0
6	GOL	A	981	6/6	0.93	0.15	-	24,27,32,34	6
3	NA	A	891	1/1	0.99	0.15	-	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.