



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2022 – 07:08 AM JST

PDB ID : 5YQB  
Title : Crystal structure of E.coli aminopeptidase N in complex with Puromycin  
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Deposited on : 2017-11-06  
Resolution : 1.56 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : ?? (??), CSD ??CSD?? (????)  
Xtriage (Phenix) : 1.13  
EDS : 2.29  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.29

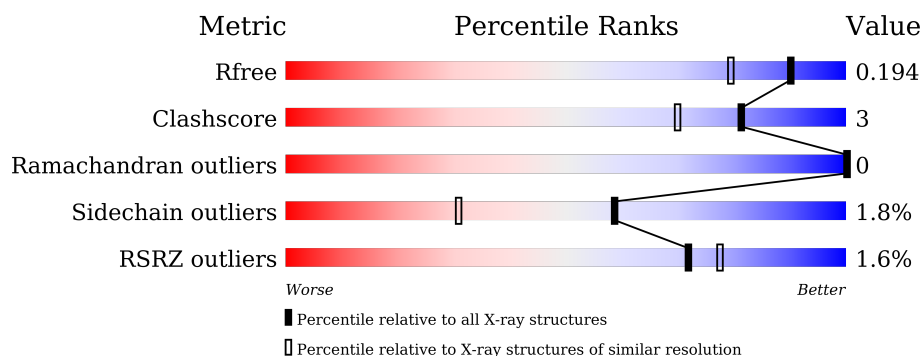
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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

Mol	Chain	Length	Quality of chain
1	A	891	<div> <div>2%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7949 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
1	A	866	Total	C	N	O	S	0	19	0
			7038	4460	1212	1337	29			

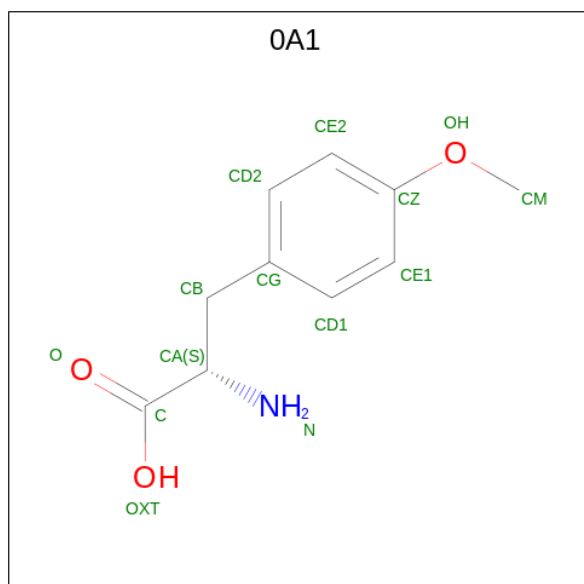
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	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	LEU	-	expression tag	UNP P04825
A	-6	VAL	-	expression tag	UNP P04825
A	-5	PRO	-	expression tag	UNP P04825
A	-4	ARG	-	expression tag	UNP P04825
A	-3	GLY	-	expression tag	UNP P04825
A	-2	SER	-	expression tag	UNP P04825
A	-1	HIS	-	expression tag	UNP P04825
A	0	MET	-	expression tag	UNP P04825

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

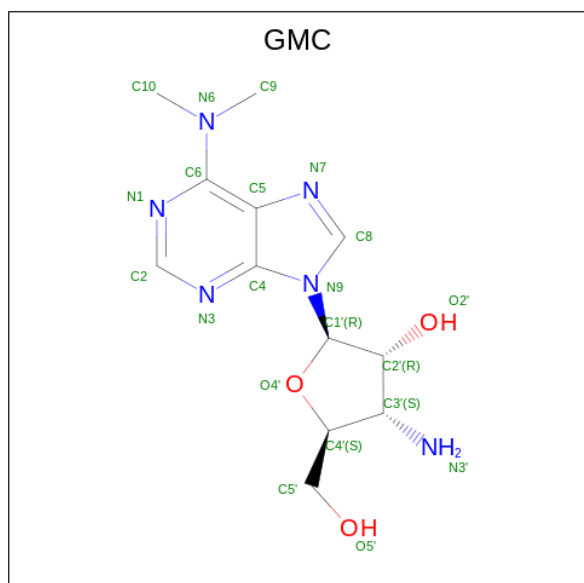
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is O-methyl-L-tyrosine (three-letter code: OA1) (formula:  $C_{10}H_{13}NO_3$ ).



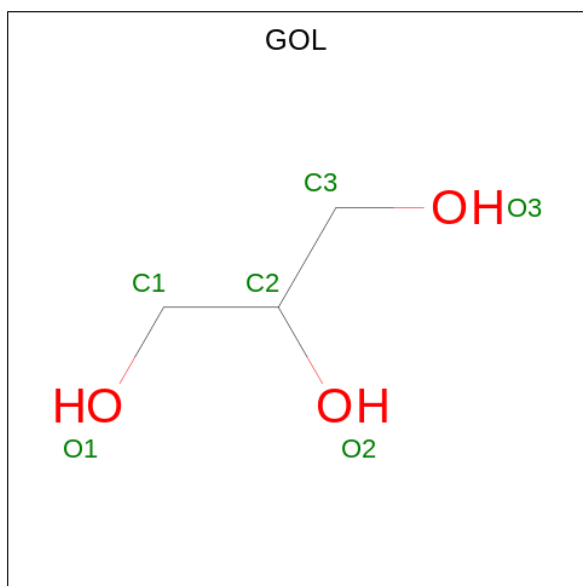
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	10	1	3		

- Molecule 4 is (2R,3R,4S,5S)-4-AMINO-2-[6-(DIMETHYLAMINO)-9H-PURIN-9-YL]-5-(HYDROXYMETHYL)TETRAHYDRO-3-FURANOL (three-letter code: GMC) (formula:  $C_{12}H_{18}N_6O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			21	12	6	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

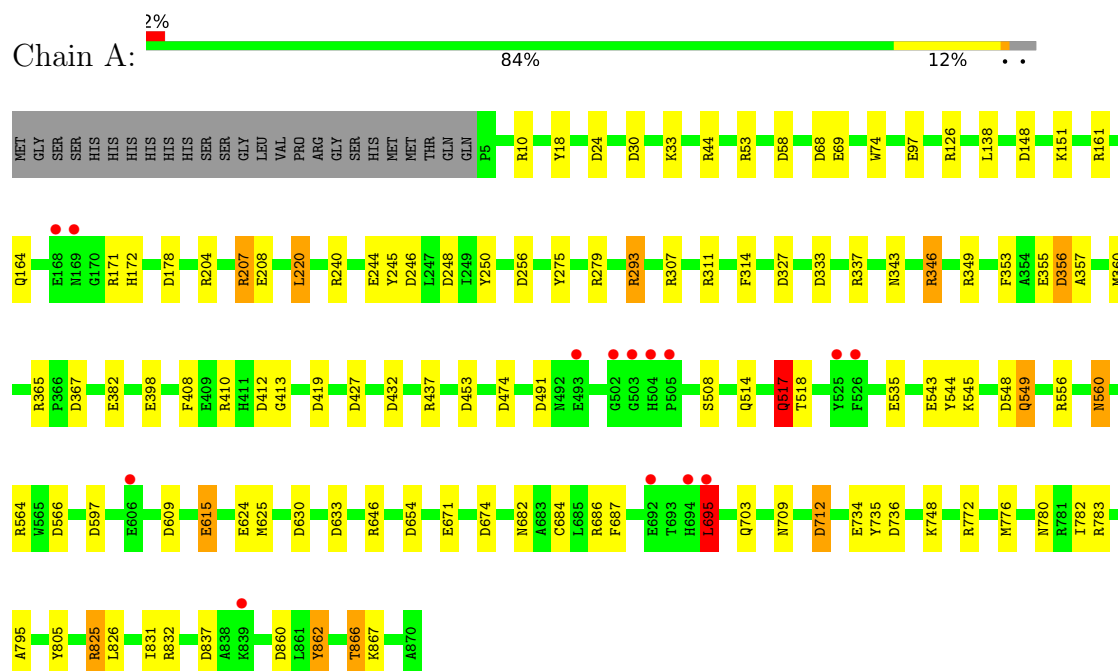
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	869	Total	O	0	0
			869	869		

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

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

- Molecule 1: Aminopeptidase N



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.29Å 120.29Å 170.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.56 34.73 – 1.56	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-1.56) 98.2 (34.73-1.56)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.76 (at 1.56Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.161 , 0.182 0.175 , 0.194	Depositor DCC
$R_{free}$ test set	9844 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GMC, ZN, GOL, 0A1

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	1.42	35/7247 (0.5%)	1.49	96/9835 (1.0%)

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	1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	615	GLU	CD-OE2	9.96	1.36	1.25
1	A	382	GLU	CG-CD	-9.57	1.37	1.51
1	A	543	GLU	CD-OE1	8.56	1.35	1.25
1	A	866	THR	CB-OG1	-7.69	1.27	1.43
1	A	207	ARG	CD-NE	7.36	1.58	1.46
1	A	349	ARG	CD-NE	-7.23	1.34	1.46
1	A	69	GLU	CD-OE2	-7.21	1.17	1.25
1	A	564	ARG	CD-NE	-7.05	1.34	1.46
1	A	349	ARG	CG-CD	6.79	1.69	1.51
1	A	862	TYR	CE1-CZ	-6.75	1.29	1.38
1	A	624	GLU	CG-CD	6.17	1.61	1.51
1	A	518	THR	C-O	6.13	1.34	1.23
1	A	560	ASN	CG-OD1	5.83	1.36	1.24
1	A	508	SER	CA-CB	-5.69	1.44	1.52
1	A	10	ARG	CZ-NH2	5.67	1.40	1.33
1	A	508	SER	CB-OG	-5.66	1.34	1.42
1	A	346[A]	ARG	CZ-NH2	-5.62	1.25	1.33
1	A	346[B]	ARG	CZ-NH2	-5.62	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	GLU	CG-CD	5.56	1.60	1.51
1	A	517[A]	GLN	CD-OE1	5.53	1.36	1.24
1	A	517[B]	GLN	CD-OE1	5.53	1.36	1.24
1	A	560	ASN	CB-CG	5.52	1.63	1.51
1	A	349	ARG	CZ-NH2	-5.32	1.26	1.33
1	A	74	TRP	CZ3-CH2	5.30	1.48	1.40
1	A	250	TYR	CG-CD1	-5.28	1.32	1.39
1	A	18	TYR	CE2-CZ	-5.27	1.31	1.38
1	A	244	GLU	CD-OE1	-5.21	1.20	1.25
1	A	624	GLU	CB-CG	5.21	1.62	1.52
1	A	275	TYR	CE1-CZ	-5.18	1.31	1.38
1	A	398	GLU	CG-CD	5.14	1.59	1.51
1	A	357	ALA	N-CA	5.12	1.56	1.46
1	A	349	ARG	NE-CZ	5.08	1.39	1.33
1	A	684	CYS	CB-SG	-5.07	1.73	1.81
1	A	734	GLU	CD-OE2	5.07	1.31	1.25
1	A	671	GLU	CD-OE1	5.03	1.31	1.25

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	ARG	NE-CZ-NH2	-18.49	111.05	120.30
1	A	686	ARG	NE-CZ-NH2	15.88	128.24	120.30
1	A	686	ARG	NE-CZ-NH1	-14.45	113.08	120.30
1	A	564	ARG	NE-CZ-NH2	-13.75	113.43	120.30
1	A	10	ARG	NE-CZ-NH1	13.17	126.88	120.30
1	A	624	GLU	OE1-CD-OE2	13.14	139.07	123.30
1	A	491	ASP	CB-CG-OD1	12.61	129.65	118.30
1	A	825	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	A	825	ARG	NE-CZ-NH1	10.71	125.66	120.30
1	A	432	ASP	CB-CG-OD1	10.04	127.34	118.30
1	A	53	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	A	279	ARG	NE-CZ-NH2	-9.65	115.47	120.30
1	A	367	ASP	CB-CG-OD1	9.62	126.95	118.30
1	A	837	ASP	CB-CG-OD1	9.60	126.94	118.30
1	A	866	THR	OG1-CB-CG2	-9.30	88.60	110.00
1	A	437	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	474	ASP	CB-CG-OD1	-9.04	110.16	118.30
1	A	633	ASP	CB-CG-OD1	8.82	126.24	118.30
1	A	349	ARG	NH1-CZ-NH2	8.73	129.00	119.40
1	A	256	ASP	CB-CG-OD1	8.53	125.98	118.30
1	A	566	ASP	CB-CG-OD2	-8.53	110.62	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	A	44	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	A	138	LEU	CB-CG-CD1	-8.34	96.82	111.00
1	A	609	ASP	CB-CG-OD2	-8.24	110.88	118.30
1	A	307	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	A	712	ASP	CB-CG-OD1	8.12	125.61	118.30
1	A	410	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	A	597	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	A	333	ASP	CB-CG-OD1	7.44	125.00	118.30
1	A	58	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	A	772	ARG	NE-CZ-NH1	-7.35	116.62	120.30
1	A	419	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	A	353	PHE	CB-CG-CD1	7.27	125.89	120.80
1	A	609	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	246	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	832	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	A	204[A]	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	A	204[B]	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	A	453	ASP	CB-CG-OD1	-7.04	111.96	118.30
1	A	356	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	248	ASP	CB-CG-OD1	-6.97	112.02	118.30
1	A	355	GLU	OE1-CD-OE2	6.84	131.51	123.30
1	A	695	LEU	CB-CG-CD2	-6.83	99.39	111.00
1	A	126	ARG	NE-CZ-NH2	6.69	123.64	120.30
1	A	307	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	68	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	A	220	LEU	CB-CG-CD1	6.36	121.82	111.00
1	A	244	GLU	OE1-CD-OE2	6.15	130.68	123.30
1	A	275	TYR	CB-CG-CD2	-6.14	117.31	121.00
1	A	654	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	A	204[A]	ARG	NE-CZ-NH1	-6.09	117.25	120.30
1	A	204[B]	ARG	NE-CZ-NH1	-6.09	117.25	120.30
1	A	735	TYR	CZ-CE2-CD2	-6.08	114.33	119.80
1	A	356	ASP	O-C-N	6.07	132.41	122.70
1	A	148	ASP	CB-CG-OD1	-6.05	112.85	118.30
1	A	687	PHE	CB-CG-CD1	6.03	125.02	120.80
1	A	625	MET	CG-SD-CE	6.02	109.83	100.20
1	A	783	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	311	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	A	783	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	10	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	474	ASP	OD1-CG-OD2	5.81	134.33	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ASP	CB-CG-OD2	5.78	123.51	118.30
1	A	630	ASP	CB-CG-OD2	-5.78	113.09	118.30
1	A	256	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	240	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	736	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	279	ARG	CD-NE-CZ	5.59	131.43	123.60
1	A	674	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	633	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	A	805	TYR	CB-CG-CD1	5.54	124.32	121.00
1	A	337	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	245	TYR	CB-CG-CD1	5.42	124.25	121.00
1	A	408	PHE	CG-CD2-CE2	5.39	126.73	120.80
1	A	178	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	548	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	365	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	826	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	A	556	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	A	427	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	543	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	A	560	ASN	CB-CG-OD1	5.25	132.09	121.60
1	A	314	PHE	CB-CG-CD1	5.24	124.47	120.80
1	A	356	ASP	OD1-CG-OD2	-5.22	113.37	123.30
1	A	544	TYR	CB-CG-CD1	5.18	124.11	121.00
1	A	413	GLY	O-C-N	-5.16	114.44	122.70
1	A	646	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	A	543	GLU	CG-CD-OE1	5.11	128.51	118.30
1	A	293	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	248	ASP	N-CA-CB	-5.08	101.45	110.60
1	A	365	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	654	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	97	GLU	OE1-CD-OE2	5.04	129.35	123.30
1	A	564	ARG	NH1-CZ-NH2	5.02	124.92	119.40
1	A	862	TYR	CB-CG-CD1	-5.01	117.99	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	412	ASP	Sidechain

## 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	7038	0	6911	32	1
2	A	1	0	0	0	0
3	A	14	0	12	1	0
4	A	21	0	18	3	0
5	A	6	0	8	0	0
6	A	869	0	0	15	1
All	All	7949	0	6949	36	2

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 3.

All (36) 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:346[B]:ARG:NH1	1:A:615:GLU:OE1	1.71	1.23
1:A:514:GLN:H	1:A:517[A]:GLN:HE22	1.34	0.73
1:A:862:TYR:O	1:A:866:THR:HG23	1.89	0.71
1:A:24[B]:ASP:OD2	6:A:1001:HOH:O	2.07	0.70
1:A:24[B]:ASP:CG	6:A:1001:HOH:O	2.29	0.69
1:A:346[B]:ARG:CZ	1:A:615:GLU:OE1	2.43	0.67
4:A:903:GMC:N7	4:A:903:GMC:H101	2.09	0.66
1:A:517[B]:GLN:HG2	6:A:1542:HOH:O	1.97	0.64
4:A:903:GMC:H2'	4:A:903:GMC:N3	2.14	0.61
1:A:360[B]:MET:HG2	1:A:831:ILE:CD1	2.32	0.60
1:A:171:ARG:NH1	6:A:1003:HOH:O	2.28	0.59
1:A:24[B]:ASP:OD1	6:A:1001:HOH:O	2.17	0.58
1:A:709:ASN:ND2	1:A:712:ASP:H	2.03	0.56
4:A:903:GMC:N3	4:A:903:GMC:C2'	2.69	0.55
1:A:360[B]:MET:HG2	1:A:831:ILE:HD11	1.91	0.52
3:A:902:OA1:HE1	6:A:1223:HOH:O	2.08	0.52
1:A:535[B]:GLU:OE2	1:A:560:ASN:CG	2.50	0.50
1:A:780:ASN:ND2	6:A:1014:HOH:O	2.45	0.49
1:A:709:ASN:HD21	1:A:712:ASP:H	1.58	0.49
1:A:360[B]:MET:CG	1:A:831:ILE:CD1	2.92	0.47
1:A:695:LEU:CD2	6:A:1868:HOH:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360[B]:MET:CE	1:A:867:LYS:HD2	2.44	0.46
1:A:549:GLN:HG2	6:A:1594:HOH:O	2.15	0.46
1:A:695:LEU:HD21	6:A:1859:HOH:O	2.15	0.45
1:A:535[B]:GLU:OE1	6:A:1002:HOH:O	2.21	0.44
1:A:795:ALA:HB3	6:A:1061:HOH:O	2.17	0.44
1:A:682:ASN:HD21	1:A:703:GLN:HE22	1.66	0.43
1:A:30:ASP:HB3	1:A:33:LYS:O	2.19	0.43
1:A:695:LEU:HD22	6:A:1868:HOH:O	2.17	0.43
1:A:360[B]:MET:HG2	1:A:831:ILE:HD12	1.99	0.42
1:A:535[B]:GLU:OE2	1:A:560:ASN:ND2	2.52	0.42
1:A:682:ASN:ND2	1:A:703:GLN:HE22	2.17	0.42
1:A:545[B]:LYS:NZ	6:A:1034:HOH:O	2.52	0.41
1:A:748:LYS:HG3	6:A:1019:HOH:O	2.21	0.40
1:A:776:MET:O	1:A:782:ILE:HD11	2.22	0.40
1:A:343:ASN:OD1	1:A:346[B]:ARG:NH2	2.55	0.40

All (2) 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)
6:A:1297:HOH:O	6:A:1297:HOH:O[6_554]	1.07	1.13
1:A:208:GLU:OE1	1:A:545[B]:LYS:NZ[5_544]	2.16	0.04

## 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	883/891 (99%)	870 (98%)	13 (2%)	0	<a href="#">100</a> <a href="#">100</a>

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	760/763 (100%)	746 (98%)	14 (2%)	59 31

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	LYS
1	A	164	GLN
1	A	172	HIS
1	A	207	ARG
1	A	220	LEU
1	A	293	ARG
1	A	327	ASP
1	A	356	ASP
1	A	517[A]	GLN
1	A	517[B]	GLN
1	A	549	GLN
1	A	695	LEU
1	A	825	ARG
1	A	860	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	682	ASN
1	A	709	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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%)	-0.21	14 (1%) 72 77	15, 22, 34, 57	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	694	HIS	4.5
1	A	504	HIS	4.0
1	A	525	TYR	3.6
1	A	695	LEU	3.3
1	A	606	GLU	3.2
1	A	503	GLY	3.1
1	A	169	ASN	2.8
1	A	168	GLU	2.8
1	A	526	PHE	2.8
1	A	505	PRO	2.2
1	A	493	GLU	2.2
1	A	692	GLU	2.2
1	A	502	GLY	2.1
1	A	839	LYS	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	A	904	6/6	0.61	0.18	46,52,57,60	0
4	GMC	A	903	21/21	0.83	0.14	25,32,47,57	21
3	0A1	A	902	14/14	0.93	0.08	16,20,25,25	0
2	ZN	A	901	1/1	1.00	0.03	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.