



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:02 pm BST

PDB ID : 3KED
Title : Crystal structure of Aminopeptidase N in complex with 2,4-diaminobutyric acid
Authors : Addlagatta, A.; Gumpena, R.
Deposited on : 2009-10-25
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

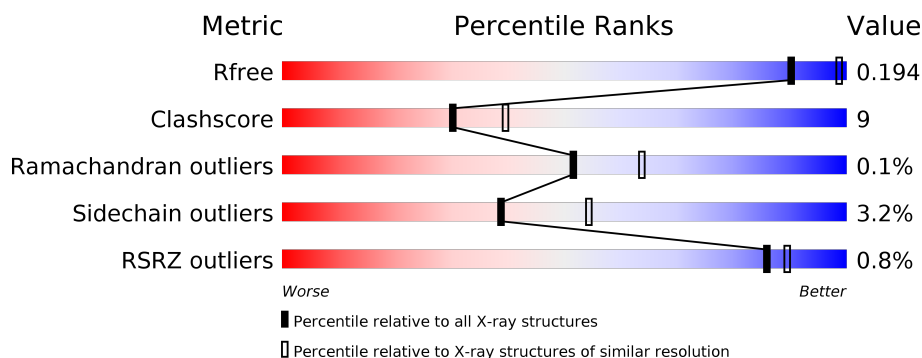
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	891	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -5px; left: 0;">%</div> <div style="position: absolute; top: 5px; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="position: absolute; top: 15px; left: 50%; transform: translate(-50%, -50%);">81%</div> <div style="position: absolute; top: 15px; right: 0; transform: translate(50%, -50%);">15%</div> <div style="position: absolute; top: 15px; right: 0;">..</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
5	GOL	A	978	-	-	X	-
6	MLA	A	992	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7580 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	7009	4434	1219	1328	28	0	7	0

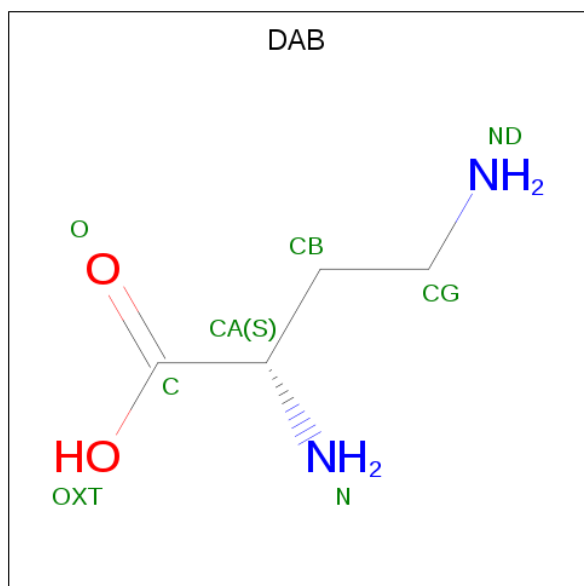
There are 21 discrepancies between the modelled and reference sequences:

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 2,4-DIAMINO BUTYRIC ACID (three-letter code: DAB) (formula: $C_4H_{10}N_2O_2$).

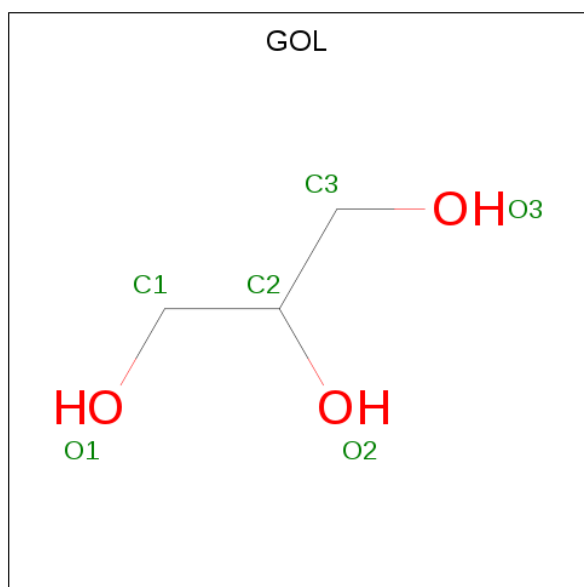


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

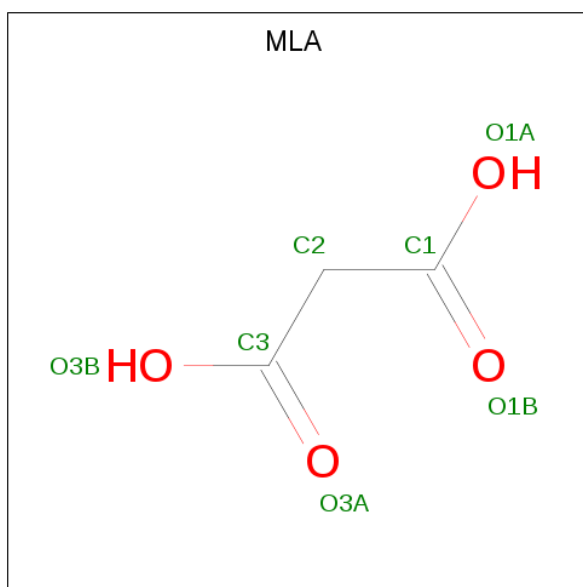
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		

- 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		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	1
			12	6	6		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is MALONIC ACID (three-letter code: MLA) (formula: C₃H₄O₄).



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

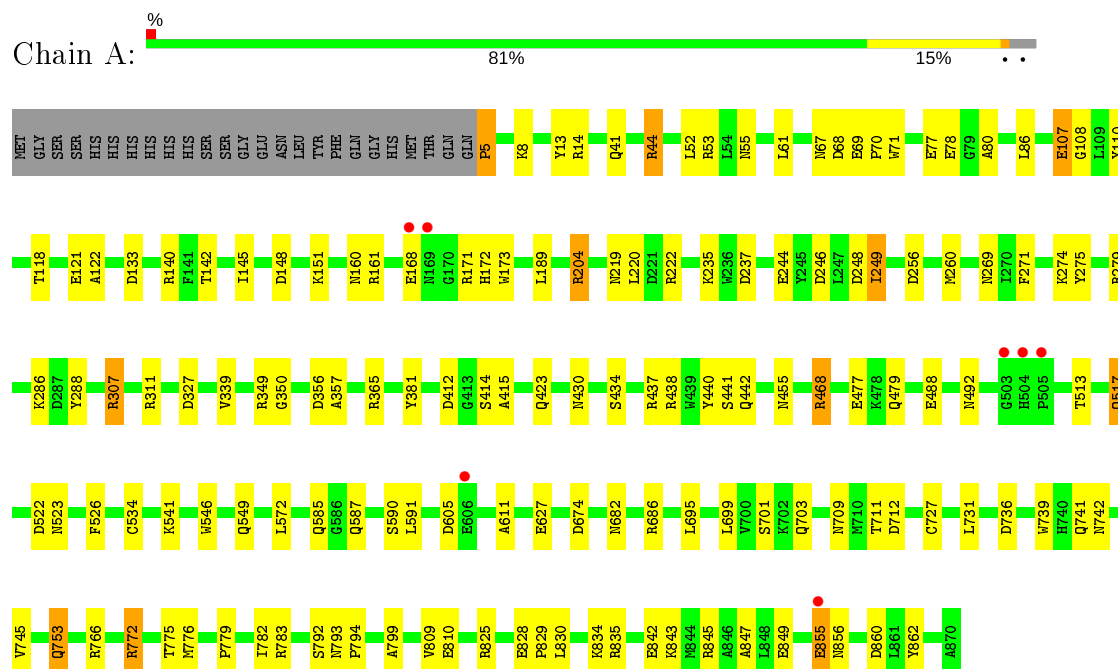
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	479	Total O 479 479	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: Aminopeptidase N



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.60Å 120.60Å 170.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.94 – 2.30 49.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.94-2.30) 97.6 (49.92-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.154 , 0.198 0.154 , 0.194	Depositor DCC
R_{free} test set	1908 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7580	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, MLA, DAB, 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	1.13	6/7164 (0.1%)	1.01	19/9724 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	842	GLU	CG-CD	5.55	1.60	1.51
1	A	107	GLU	CG-CD	5.55	1.60	1.51
1	A	440	TYR	CD2-CE2	-5.44	1.31	1.39
1	A	110	TYR	CE2-CZ	5.18	1.45	1.38
1	A	434	SER	CB-OG	-5.17	1.35	1.42
1	A	799	ALA	CA-CB	5.14	1.63	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	ARG	NE-CZ-NH2	-10.93	114.83	120.30
1	A	438	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	A	349	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	A	835	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	A	437	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	44	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	A	772	ARG	NE-CZ-NH1	-6.21	117.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ASP	CB-CG-OD1	-5.83	113.05	118.30
1	A	772	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	A	438	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	256	ASP	CB-CG-OD1	5.63	123.36	118.30
1	A	541	LYS	CD-CE-NZ	-5.44	99.19	111.70
1	A	736	ASP	CB-CG-OD1	5.42	123.17	118.30
1	A	830	LEU	CB-CG-CD2	-5.38	101.86	111.00
1	A	835	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	A	307	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	A	412	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	237	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	605	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	855[B]	GLU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7009	0	6842	130	2
2	A	1	0	0	0	0
3	A	8	0	9	0	0
4	A	2	0	0	0	0
5	A	60	0	80	11	0
6	A	21	0	6	4	1
7	A	479	0	0	44	2
All	All	7580	0	6937	131	4

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 (131) 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:279:ARG:HD2	7:A:1191:HOH:O	1.48	1.13
1:A:591:LEU:N	5:A:978:GOL:H12	1.68	1.09
1:A:591:LEU:H	5:A:978:GOL:C1	1.65	1.08
1:A:855[B]:GLU:O	7:A:1174:HOH:O	1.72	1.07
1:A:549:GLN:HG3	7:A:932:HOH:O	1.56	1.04
1:A:590:SER:HA	5:A:978:GOL:H11	1.39	1.04
1:A:591:LEU:H	5:A:978:GOL:H12	0.89	1.02
1:A:8:LYS:HG3	7:A:1238:HOH:O	1.61	1.00
1:A:53[B]:ARG:HH22	1:A:77[B]:GLU:CD	1.65	0.99
1:A:53[B]:ARG:NH2	1:A:77[B]:GLU:OE2	1.98	0.97
1:A:517:GLN:HB2	7:A:884:HOH:O	1.64	0.96
1:A:148:ASP:CG	7:A:1304:HOH:O	2.05	0.93
1:A:140:ARG:CD	7:A:1084:HOH:O	2.16	0.92
1:A:779:PRO:O	1:A:783:ARG:HG3	1.70	0.90
1:A:249:ILE:HD12	1:A:249:ILE:H	1.36	0.90
1:A:140:ARG:HD3	7:A:1084:HOH:O	1.73	0.84
1:A:357:ALA:C	7:A:1175:HOH:O	2.14	0.84
1:A:709:ASN:ND2	1:A:712:ASP:H	1.76	0.83
1:A:488:GLU:CD	7:A:1270:HOH:O	2.17	0.83
1:A:219:ASN:HD22	1:A:222[B]:ARG:HH21	1.27	0.81
1:A:219:ASN:HD22	1:A:222[B]:ARG:NH2	1.77	0.81
1:A:468:ARG:HD2	7:A:1138:HOH:O	1.83	0.79
1:A:55:ASN:HD22	1:A:133:ASP:H	1.34	0.74
1:A:709:ASN:HD21	1:A:712:ASP:H	1.35	0.74
1:A:442:GLN:HE22	1:A:479:GLN:H	1.32	0.74
1:A:772:ARG:HG2	7:A:1035:HOH:O	1.86	0.74
1:A:219:ASN:ND2	1:A:222[B]:ARG:NH2	2.36	0.73
1:A:357:ALA:CA	7:A:1175:HOH:O	2.37	0.73
1:A:357:ALA:HA	7:A:1175:HOH:O	1.88	0.73
1:A:148:ASP:OD2	7:A:1304:HOH:O	2.06	0.72
1:A:53[B]:ARG:NH2	1:A:77[B]:GLU:CD	2.42	0.72
1:A:67:ASN:O	1:A:68:ASP:HB2	1.89	0.71
1:A:546:TRP:CZ2	5:A:970:GOL:H31	2.27	0.69
1:A:742:ASN:OD1	7:A:1063:HOH:O	2.11	0.69
1:A:168:GLU:HG2	7:A:1119:HOH:O	1.92	0.68
1:A:249:ILE:HD12	1:A:249:ILE:N	2.07	0.68
1:A:792:SER:C	1:A:794:PRO:HD3	2.14	0.68
1:A:171:ARG:NE	7:A:988:HOH:O	1.81	0.67
1:A:585[A]:GLN:CB	1:A:587:GLN:HE21	2.09	0.66
1:A:161:ARG:HD3	7:A:1042:HOH:O	1.95	0.65
1:A:219:ASN:ND2	1:A:222[B]:ARG:HH21	1.96	0.64
1:A:53[B]:ARG:NH1	1:A:77[B]:GLU:OE2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53[B]:ARG:CZ	1:A:77[B]:GLU:OE2	2.46	0.64
1:A:522:ASP:HB2	7:A:1145:HOH:O	1.97	0.64
1:A:828:GLU:HB3	1:A:829:PRO:HD3	1.80	0.63
1:A:753:GLN:HE21	1:A:753:GLN:HA	1.64	0.63
1:A:140:ARG:HD2	7:A:1084:HOH:O	1.90	0.62
1:A:546:TRP:CH2	5:A:970:GOL:H31	2.35	0.61
1:A:13:TYR:O	1:A:14:ARG:HD2	2.01	0.61
1:A:71:TRP:O	5:A:971:GOL:H2	2.00	0.60
1:A:279:ARG:CD	7:A:1191:HOH:O	2.26	0.60
1:A:585[A]:GLN:HB2	1:A:587:GLN:HE21	1.67	0.58
1:A:591:LEU:N	5:A:978:GOL:C1	2.45	0.58
1:A:160:ASN:OD1	1:A:249:ILE:HD11	2.04	0.57
1:A:513:THR:H	1:A:517:GLN:HE22	1.51	0.57
1:A:219:ASN:HD22	1:A:222[B]:ARG:CZ	2.18	0.57
1:A:845:ARG:NH1	7:A:1311:HOH:O	2.28	0.56
1:A:55:ASN:ND2	1:A:133:ASP:H	2.03	0.56
1:A:522:ASP:HB3	1:A:523:ASN:HD22	1.72	0.55
1:A:77[B]:GLU:HG3	1:A:78:GLU:N	2.21	0.55
1:A:585[B]:GLN:HB2	1:A:587:GLN:HE21	1.72	0.54
1:A:219:ASN:ND2	1:A:222[B]:ARG:CZ	2.71	0.54
1:A:8:LYS:CG	7:A:1238:HOH:O	2.38	0.53
1:A:709:ASN:ND2	1:A:711:THR:HB	2.24	0.53
1:A:590:SER:CA	5:A:978:GOL:H11	2.26	0.53
1:A:274[B]:LYS:CD	7:A:1069:HOH:O	2.57	0.52
1:A:709:ASN:HD21	1:A:712:ASP:N	2.05	0.52
1:A:585[A]:GLN:HB3	1:A:587:GLN:HE21	1.73	0.52
1:A:350:GLY:C	7:A:938:HOH:O	2.48	0.51
1:A:430:ASN:ND2	7:A:1284:HOH:O	2.41	0.51
1:A:279:ARG:CG	7:A:1191:HOH:O	2.55	0.51
1:A:682:ASN:ND2	1:A:703:GLN:HE22	2.08	0.51
1:A:249:ILE:CD1	1:A:249:ILE:N	2.74	0.51
1:A:534:CYS:HA	7:A:947:HOH:O	2.10	0.51
1:A:709:ASN:HD22	1:A:711:THR:H	1.59	0.50
1:A:845:ARG:O	1:A:849:GLU:HG2	2.11	0.50
1:A:269:ASN:HB3	1:A:271:PHE:HE1	1.77	0.50
1:A:274[B]:LYS:HD3	7:A:1069:HOH:O	2.11	0.50
1:A:339:VAL:HG21	1:A:611:ALA:HB1	1.93	0.49
1:A:220:LEU:HB2	7:A:1096:HOH:O	2.12	0.49
1:A:442:GLN:NE2	1:A:479:GLN:H	2.07	0.49
1:A:709:ASN:HD22	1:A:711:THR:N	2.10	0.49
1:A:274[A]:LYS:HE3	1:A:275:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:MET:O	1:A:782:ILE:HD11	2.13	0.48
1:A:204:ARG:HD3	1:A:244:GLU:OE2	2.12	0.48
1:A:783:ARG:NH2	1:A:825:ARG:HE	2.12	0.47
1:A:414:SER:HB2	7:A:1199:HOH:O	2.15	0.47
1:A:44:ARG:NH1	1:A:86:LEU:O	2.39	0.47
1:A:219:ASN:HD22	1:A:222[B]:ARG:NE	2.12	0.47
1:A:794:PRO:HD2	7:A:1094:HOH:O	2.14	0.47
1:A:142:THR:HG23	7:A:915:HOH:O	2.15	0.46
1:A:70:PRO:O	6:A:992:MLA:HC22	2.16	0.46
1:A:627:GLU:CG	7:A:938:HOH:O	2.63	0.46
1:A:77[B]:GLU:HG2	1:A:80:ALA:HB3	1.98	0.46
1:A:5:PRO:HG2	1:A:862:TYR:CD2	2.51	0.46
1:A:121:GLU:HG3	1:A:122:ALA:HA	1.97	0.46
1:A:488:GLU:CG	7:A:1270:HOH:O	2.58	0.45
1:A:151:LYS:HB2	1:A:151:LYS:HE3	1.49	0.45
1:A:107:GLU:HG3	7:A:945:HOH:O	2.17	0.44
1:A:219:ASN:ND2	1:A:222[B]:ARG:NE	2.65	0.44
1:A:455:ASN:OD1	1:A:455:ASN:C	2.54	0.44
1:A:766[A]:ARG:HH22	1:A:810:GLU:CD	2.21	0.44
1:A:168:GLU:HG2	1:A:168:GLU:H	1.61	0.44
1:A:220:LEU:HA	1:A:220:LEU:HD12	1.74	0.44
1:A:53[B]:ARG:NH2	1:A:77[B]:GLU:OE1	2.50	0.44
1:A:682:ASN:HD21	1:A:703:GLN:HE22	1.66	0.43
1:A:809:VAL:CG2	1:A:847:ALA:HB1	2.49	0.43
1:A:492:ASN:HB3	1:A:526:PHE:CE2	2.53	0.43
1:A:727:CYS:O	1:A:731:LEU:HG	2.17	0.43
1:A:739:TRP:CG	1:A:745:VAL:HG11	2.52	0.43
1:A:189:LEU:C	1:A:189:LEU:HD23	2.39	0.43
1:A:246:ASP:OD2	1:A:307:ARG:HD3	2.19	0.43
1:A:41:GLN:NE2	7:A:1023:HOH:O	2.45	0.43
1:A:145:ILE:O	1:A:173:TRP:HA	2.19	0.43
1:A:108:GLY:O	1:A:118:THR:HA	2.19	0.42
1:A:845:ARG:NE	7:A:1130:HOH:O	2.51	0.42
1:A:627:GLU:HG3	7:A:938:HOH:O	2.20	0.42
6:A:991:MLA:O3A	6:A:991:MLA:O1B	2.37	0.42
1:A:69:GLU:OE2	6:A:992:MLA:HC21	2.19	0.42
1:A:843:LYS:HE2	7:A:1080:HOH:O	2.18	0.42
1:A:69:GLU:CG	6:A:992:MLA:HC21	2.49	0.42
1:A:627:GLU:HG2	7:A:1047:HOH:O	2.20	0.41
1:A:381:TYR:CE2	5:A:973[A]:GOL:H31	2.55	0.41
1:A:513:THR:N	1:A:517:GLN:HE22	2.15	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:ARG:HD3	7:A:1049:HOH:O	2.20	0.41
1:A:793:ASN:N	1:A:794:PRO:HD3	2.36	0.41
1:A:834:LYS:HE2	7:A:1115:HOH:O	2.21	0.41
1:A:311:ARG:HA	1:A:415:ALA:HB1	2.03	0.41
1:A:590:SER:HA	5:A:978:GOL:C1	2.29	0.41
1:A:44:ARG:HH11	1:A:44:ARG:HD3	1.58	0.40
1:A:365:ARG:HH21	1:A:441:SER:HB3	1.86	0.40

All (4) 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)
7:A:1342:HOH:O	7:A:1354:HOH:O[4_455]	1.94	0.26
7:A:1341:HOH:O	7:A:1352:HOH:O[4_565]	1.95	0.25
1:A:204:ARG:NH2	1:A:585[A]:GLN:OE1[4_455]	2.02	0.18
1:A:288:TYR:OH	6:A:992:MLA:O3A[3_454]	2.19	0.01

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	871/891 (98%)	853 (98%)	17 (2%)	1 (0%)	51 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	856	ASN

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	748/763 (98%)	724 (97%)	24 (3%)	39 54

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	52	LEU
1	A	61	LEU
1	A	172	HIS
1	A	204	ARG
1	A	235	LYS
1	A	249	ILE
1	A	260	MET
1	A	286	LYS
1	A	327	ASP
1	A	356	ASP
1	A	423	GLN
1	A	468	ARG
1	A	477	GLU
1	A	517	GLN
1	A	572	LEU
1	A	674	ASP
1	A	695	LEU
1	A	699	LEU
1	A	701	SER
1	A	741	GLN
1	A	753	GLN
1	A	775	THR
1	A	860	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN

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Mol	Chain	Res	Type
1	A	55	ASN
1	A	219	ASN
1	A	442	GLN
1	A	517	GLN
1	A	523	ASN
1	A	569	GLN
1	A	587	GLN
1	A	661	ASN
1	A	665	GLN
1	A	682	ASN
1	A	709	ASN
1	A	753	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	$\# Z > 2$
5	GOL	A	972	-	5,5,5	0.74	0	5,5,5	0.85	0
3	DAB	A	880	2	3,7,7	1.52	1 (33%)	1,8,8	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	976	-	5,5,5	0.40	0	5,5,5	0.63	0
5	GOL	A	971	-	5,5,5	0.32	0	5,5,5	1.58	2 (40%)
5	GOL	A	973[B]	-	5,5,5	0.50	0	5,5,5	0.70	0
5	GOL	A	978	-	5,5,5	0.47	0	5,5,5	0.46	0
5	GOL	A	975	-	5,5,5	0.44	0	5,5,5	0.51	0
6	MLA	A	990	-	0,6,6	0.00	-	0,7,7	0.00	-
6	MLA	A	991	-	0,6,6	0.00	-	0,7,7	0.00	-
5	GOL	A	970	-	5,5,5	0.58	0	5,5,5	1.52	1 (20%)
5	GOL	A	974	-	5,5,5	0.46	0	5,5,5	0.89	0
5	GOL	A	977	-	5,5,5	0.44	0	5,5,5	0.71	0
5	GOL	A	973[A]	-	5,5,5	0.59	0	5,5,5	0.57	0
6	MLA	A	992	-	0,6,6	0.00	-	0,7,7	0.00	-

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
5	GOL	A	972	-	-	0/4/4/4	-
3	DAB	A	880	2	-	0/3/7/7	-
5	GOL	A	976	-	-	4/4/4/4	-
5	GOL	A	971	-	-	3/4/4/4	-
5	GOL	A	973[B]	-	-	2/4/4/4	-
5	GOL	A	978	-	-	3/4/4/4	-
5	GOL	A	975	-	-	1/4/4/4	-
6	MLA	A	990	-	-	0/0/4/4	-
6	MLA	A	991	-	-	0/0/4/4	-
5	GOL	A	970	-	-	2/4/4/4	-
5	GOL	A	974	-	-	2/4/4/4	-
5	GOL	A	977	-	-	2/4/4/4	-
5	GOL	A	973[A]	-	-	4/4/4/4	-
6	MLA	A	992	-	-	0/0/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	880	DAB	CA-N	2.09	1.51	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	971	GOL	O2-C2-C1	2.83	121.61	109.12
5	A	971	GOL	O1-C1-C2	2.09	120.20	110.20
5	A	970	GOL	C3-C2-C1	-2.02	103.87	111.70

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	976	GOL	C1-C2-C3-O3
5	A	971	GOL	O1-C1-C2-C3
5	A	973[B]	GOL	O1-C1-C2-C3
5	A	978	GOL	C1-C2-C3-O3
5	A	978	GOL	O2-C2-C3-O3
5	A	970	GOL	O1-C1-C2-C3
5	A	974	GOL	O1-C1-C2-C3
5	A	977	GOL	C1-C2-C3-O3
5	A	973[B]	GOL	O1-C1-C2-O2
5	A	976	GOL	O1-C1-C2-C3
5	A	978	GOL	O1-C1-C2-C3
5	A	973[A]	GOL	C1-C2-C3-O3
5	A	970	GOL	O1-C1-C2-O2
5	A	976	GOL	O1-C1-C2-O2
5	A	976	GOL	O2-C2-C3-O3
5	A	971	GOL	O1-C1-C2-O2
5	A	971	GOL	O2-C2-C3-O3
5	A	977	GOL	O2-C2-C3-O3
5	A	973[A]	GOL	O1-C1-C2-O2
5	A	973[A]	GOL	O2-C2-C3-O3
5	A	974	GOL	O1-C1-C2-O2
5	A	975	GOL	O1-C1-C2-O2
5	A	973[A]	GOL	O1-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	971	GOL	1	0
5	A	978	GOL	7	0
6	A	991	MLA	1	0
5	A	970	GOL	2	0
5	A	973[A]	GOL	1	0
6	A	992	MLA	3	1

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	866/891 (97%)	-0.40	7 (0%) 86 89	18, 28, 42, 65	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	HIS	5.1
1	A	855[A]	GLU	3.4
1	A	169	ASN	3.0
1	A	503	GLY	2.8
1	A	168	GLU	2.8
1	A	606	GLU	2.4
1	A	505	PRO	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MLA	A	991	7/7	0.81	0.42	75,77,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MLA	A	990	7/7	0.88	0.24	54,55,57,59	0
5	GOL	A	973[B]	6/6	0.88	0.53	38,42,42,43	6
5	GOL	A	973[A]	6/6	0.88	0.53	26,33,33,36	6
5	GOL	A	976	6/6	0.89	0.21	58,59,62,62	0
5	GOL	A	978	6/6	0.90	0.15	41,42,43,43	6
4	NA	A	952	1/1	0.92	0.14	40,40,40,40	0
5	GOL	A	975	6/6	0.93	0.10	41,46,54,54	0
5	GOL	A	970	6/6	0.93	0.13	39,46,49,53	0
5	GOL	A	972	6/6	0.93	0.15	48,49,53,57	0
5	GOL	A	977	6/6	0.94	0.12	31,45,46,52	0
4	NA	A	951	1/1	0.94	0.10	40,40,40,40	0
6	MLA	A	992	7/7	0.95	0.15	62,64,65,65	0
5	GOL	A	974	6/6	0.96	0.14	47,54,55,56	0
3	DAB	A	880	8/8	0.97	0.17	22,31,33,33	0
5	GOL	A	971	6/6	0.99	0.09	32,36,39,41	0
2	ZN	A	875	1/1	1.00	0.11	22,22,22,22	0

6.5 Other polymers

There are no such residues in this entry.