



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2020 – 10:28 AM EDT

PDB ID : 6OIU  
Title : X-ray crystal structure of the ectodomain of the Toxoplasma gondii ME49 Aminopeptidase N (TGME49\_224350)  
Authors : McGowan, S.; Drinkwater, N.  
Deposited on : 2019-04-09  
Resolution : 2.20 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
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) : 2.14.6

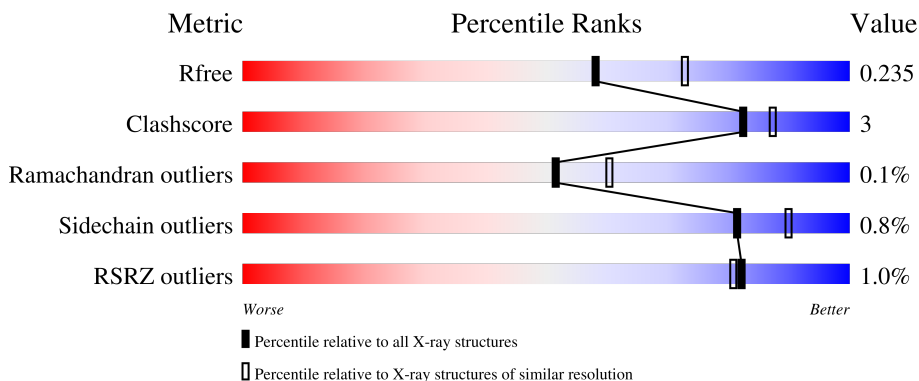
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	907	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>
1	B	907	<div> <div></div> <div>93%</div> <div>7%</div> <div>.</div> </div>
1	C	907	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div>.</div> </div> </div>
1	D	907	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30397 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	890	Total	C	N	O	S	0	0	0
			6951	4405	1212	1305	29			
1	B	899	Total	C	N	O	S	0	0	0
			6944	4403	1201	1311	29			
1	C	900	Total	C	N	O	S	0	0	0
			6998	4438	1212	1319	29			
1	D	886	Total	C	N	O	S	0	0	0
			6696	4244	1161	1262	29			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	519	MET	-	initiating methionine	UNP S8G5K8
A	840	GLN	ASN	conflict	UNP S8G5K8
A	1303	GLN	ASN	conflict	UNP S8G5K8
A	1420	HIS	-	expression tag	UNP S8G5K8
A	1421	HIS	-	expression tag	UNP S8G5K8
A	1422	HIS	-	expression tag	UNP S8G5K8
A	1423	HIS	-	expression tag	UNP S8G5K8
A	1424	HIS	-	expression tag	UNP S8G5K8
A	1425	HIS	-	expression tag	UNP S8G5K8
B	519	MET	-	initiating methionine	UNP S8G5K8
B	840	GLN	ASN	conflict	UNP S8G5K8
B	1303	GLN	ASN	conflict	UNP S8G5K8
B	1420	HIS	-	expression tag	UNP S8G5K8
B	1421	HIS	-	expression tag	UNP S8G5K8
B	1422	HIS	-	expression tag	UNP S8G5K8
B	1423	HIS	-	expression tag	UNP S8G5K8
B	1424	HIS	-	expression tag	UNP S8G5K8
B	1425	HIS	-	expression tag	UNP S8G5K8
C	519	MET	-	initiating methionine	UNP S8G5K8
C	840	GLN	ASN	conflict	UNP S8G5K8
C	1303	GLN	ASN	conflict	UNP S8G5K8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1420	HIS	-	expression tag	UNP S8G5K8
C	1421	HIS	-	expression tag	UNP S8G5K8
C	1422	HIS	-	expression tag	UNP S8G5K8
C	1423	HIS	-	expression tag	UNP S8G5K8
C	1424	HIS	-	expression tag	UNP S8G5K8
C	1425	HIS	-	expression tag	UNP S8G5K8
D	519	MET	-	initiating methionine	UNP S8G5K8
D	840	GLN	ASN	conflict	UNP S8G5K8
D	1303	GLN	ASN	conflict	UNP S8G5K8
D	1420	HIS	-	expression tag	UNP S8G5K8
D	1421	HIS	-	expression tag	UNP S8G5K8
D	1422	HIS	-	expression tag	UNP S8G5K8
D	1423	HIS	-	expression tag	UNP S8G5K8
D	1424	HIS	-	expression tag	UNP S8G5K8
D	1425	HIS	-	expression tag	UNP S8G5K8

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	717	Total	O	0	0
			717	717		
4	B	750	Total	O	0	0
			750	750		
4	C	872	Total	O	0	0
			872	872		

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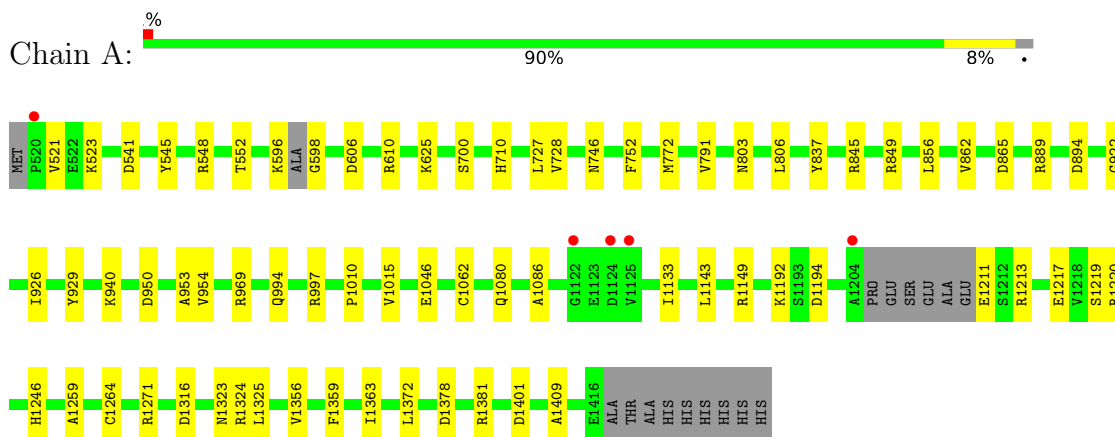
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	407	Total 407	O 407	0	0

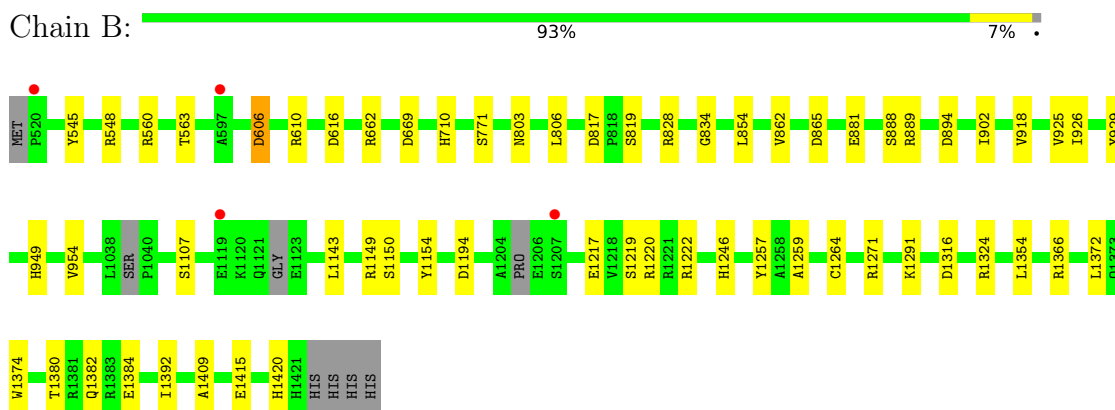
### 3 Residue-property plots

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.

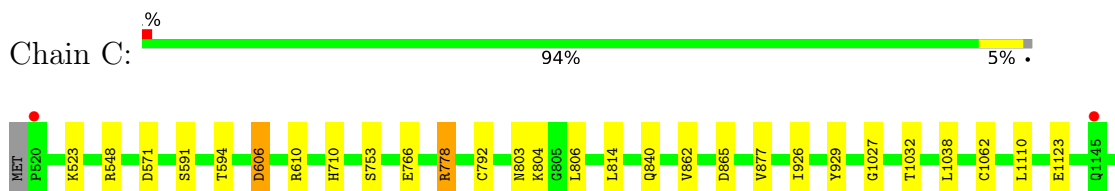
#### • Molecule 1: Aminopeptidase N



#### • Molecule 1: Aminopeptidase N

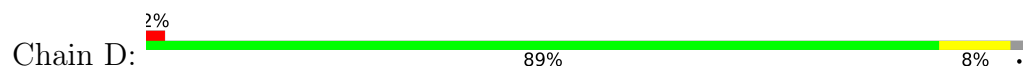


#### • Molecule 1: Aminopeptidase N





● Molecule 1: Aminopeptidase N





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.93Å 207.87Å 102.87Å 90.00° 94.34° 90.00°	Depositor
Resolution (Å)	38.54 – 2.20 38.54 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.54-2.20) 91.8 (38.54-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.190 , 0.236 0.190 , 0.235	Depositor DCC
$R_{free}$ test set	9637 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtriage
Anisotropy	0.717	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	30397	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: GOL, ZN

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	0.27	0/7091	0.41	0/9602
1	B	0.24	0/7085	0.40	0/9607
1	C	0.27	0/7142	0.41	0/9682
1	D	0.28	2/6833 (0.0%)	0.41	0/9289
All	All	0.26	2/28151 (0.0%)	0.40	0/38180

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1394	ASN	C-N	6.58	1.49	1.34
1	D	1393	ALA	C-N	-5.07	1.22	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	6951	0	6763	42	0
1	B	6944	0	6668	29	0
1	C	6998	0	6776	30	0
1	D	6696	0	6273	35	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	18	0	24	0	0
3	B	18	0	24	0	0
3	C	18	0	24	3	0
4	A	717	0	0	8	0
4	B	750	0	0	2	0
4	C	872	0	0	9	0
4	D	407	0	0	1	0
All	All	30397	0	26552	137	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 3.

All (137) 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:C:1032:THR:HG23	4:C:2296:HOH:O	1.68	0.92
1:D:1149:ARG:HB2	1:D:1219:SER:HB3	1.67	0.74
1:A:596:LYS:HA	1:A:598:GLY:N	2.06	0.70
1:A:889:ARG:NH1	4:A:2102:HOH:O	2.25	0.70
1:C:1316:ASP:O	1:C:1324:ARG:NH1	2.25	0.69
1:B:828:ARG:NH1	4:B:1605:HOH:O	2.30	0.63
1:D:606:ASP:OD1	1:D:610:ARG:N	2.31	0.62
1:D:1022:ILE:HB	1:D:1047:LEU:HB3	1.81	0.62
1:C:1366:ARG:NH2	4:C:1609:HOH:O	2.32	0.62
1:C:1149:ARG:HB2	1:C:1219:SER:HB3	1.81	0.62
1:D:1316:ASP:O	1:D:1324:ARG:NH1	2.34	0.61
1:B:1316:ASP:O	1:B:1324:ARG:NH1	2.34	0.60
1:C:1334:ARG:NH2	4:C:1615:HOH:O	2.34	0.60
1:A:548:ARG:NH1	4:A:2121:HOH:O	2.35	0.59
1:C:571:ASP:HA	1:C:610:ARG:HG2	1.84	0.59
1:C:1372:LEU:HD23	1:C:1409:ALA:HB2	1.83	0.59
1:D:1135:VAL:HG13	1:D:1191:LEU:HD11	1.85	0.59
1:A:1149:ARG:HB2	1:A:1219:SER:HB3	1.85	0.58
1:A:746:ASN:ND2	4:A:2122:HOH:O	2.35	0.58
1:A:1372:LEU:HD23	1:A:1409:ALA:HB2	1.85	0.58
1:C:591:SER:H	1:C:594:THR:HG22	1.68	0.58
1:C:1370:ALA:HB2	3:C:1505:GOL:H32	1.85	0.58
1:A:1149:ARG:NH1	4:A:2119:HOH:O	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:ASP:OD1	1:C:610:ARG:N	2.37	0.56
1:C:1366:ARG:O	3:C:1505:GOL:O3	2.21	0.56
1:A:1211:GLU:HG2	1:A:1213:ARG:HH21	1.71	0.56
1:D:1372:LEU:HD23	1:D:1409:ALA:HB2	1.88	0.56
1:A:1192:LYS:NZ	4:A:2131:HOH:O	2.38	0.55
1:A:596:LYS:CA	1:A:598:GLY:N	2.69	0.55
1:A:772:MET:HG2	1:A:837:TYR:CZ	2.41	0.55
1:C:1390:ARG:NH2	1:C:1414:PRO:O	2.40	0.54
1:D:1143:LEU:HD21	1:D:1194:ASP:HB3	1.90	0.54
1:D:728:VAL:HG11	1:D:791:VAL:HG11	1.90	0.54
1:D:560:ARG:O	1:D:622:ALA:HB1	2.08	0.53
1:D:559:ARG:HD2	1:D:563:THR:HG23	1.90	0.53
1:A:625:LYS:NZ	4:A:2140:HOH:O	2.41	0.53
1:B:606:ASP:OD1	1:B:610:ARG:N	2.28	0.53
1:A:994:GLN:OE1	1:A:997:ARG:NH2	2.43	0.51
1:B:1143:LEU:HD21	1:B:1194:ASP:HB3	1.92	0.51
1:C:877:VAL:HG21	1:C:1150:SER:HB3	1.92	0.51
1:A:1323:ASN:ND2	4:A:2147:HOH:O	2.44	0.50
1:C:778:ARG:NH1	4:C:1636:HOH:O	2.42	0.50
1:A:727:LEU:C	1:A:727:LEU:HD12	2.30	0.50
1:A:606:ASP:OD1	1:A:610:ARG:N	2.40	0.50
1:D:1264:CYS:HA	1:D:1271:ARG:HG3	1.94	0.50
1:D:902:ILE:HD13	1:D:925:VAL:HG21	1.94	0.50
1:A:1316:ASP:O	1:A:1324:ARG:NH1	2.45	0.50
1:A:752:PHE:HB2	1:A:791:VAL:HG22	1.94	0.50
1:C:862:VAL:HA	1:C:865:ASP:OD1	2.12	0.49
1:D:1111:LYS:O	1:D:1115:GLU:HG3	2.12	0.49
1:D:743:SER:HB3	1:D:782:GLU:OE2	2.13	0.49
1:A:1378:ASP:OD2	1:A:1381:ARG:NH1	2.44	0.49
1:C:804:LYS:HE2	1:C:840:GLN:HE22	1.78	0.49
1:A:969:ARG:NH2	1:A:1046:GLU:OE2	2.45	0.49
1:C:548:ARG:NH1	4:C:1629:HOH:O	2.41	0.49
1:A:1143:LEU:HD21	1:A:1194:ASP:HB3	1.95	0.49
1:A:1086:ALA:HB2	1:A:1133:ILE:HG23	1.94	0.48
1:A:1217:GLU:OE1	1:A:1220:ARG:NH2	2.38	0.48
1:B:1354:LEU:HD21	1:B:1392:ILE:HA	1.96	0.48
1:D:926:ILE:HA	1:D:929:TYR:HD2	1.78	0.48
1:D:1246:HIS:CD2	1:D:1259:ALA:HB2	2.48	0.48
1:C:926:ILE:HA	1:C:929:TYR:HD2	1.77	0.48
1:D:1024:ILE:HG22	1:D:1026:VAL:HG13	1.95	0.48
1:D:1395:ALA:HB3	1:D:1398:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:862:VAL:HA	1:D:865:ASP:OD1	2.13	0.48
1:B:662:ARG:HH21	1:B:669:ASP:HB3	1.78	0.48
1:A:926:ILE:HA	1:A:929:TYR:HD2	1.78	0.47
1:B:862:VAL:HA	1:B:865:ASP:OD1	2.14	0.47
1:B:926:ILE:HA	1:B:929:TYR:HD2	1.79	0.47
1:A:845:ARG:NH2	1:A:950:ASP:OD2	2.48	0.47
1:A:1010:PRO:HB3	1:A:1015:VAL:HA	1.96	0.47
1:B:1372:LEU:HD23	1:B:1409:ALA:HB2	1.96	0.47
1:B:1380:THR:O	1:B:1384:GLU:HG3	2.15	0.47
1:A:862:VAL:HA	1:A:865:ASP:OD1	2.14	0.46
3:C:1505:GOL:O3	3:C:1505:GOL:O1	2.26	0.46
1:D:1010:PRO:HB3	1:D:1015:VAL:HA	1.98	0.46
1:D:1301:VAL:O	1:D:1337:GLN:NE2	2.40	0.46
1:B:902:ILE:HD13	1:B:925:VAL:HG21	1.98	0.46
1:C:1394:ASN:ND2	4:C:1643:HOH:O	2.44	0.46
1:B:1150:SER:OG	1:B:1222:ARG:NH1	2.47	0.46
1:B:1217:GLU:OE1	1:B:1220:ARG:NH2	2.41	0.46
1:C:1027:GLY:HA2	1:C:1038:LEU:HD12	1.98	0.46
1:A:521:VAL:O	1:A:523:LYS:HD2	2.15	0.46
1:A:856:LEU:HD21	1:A:954:VAL:HG23	1.98	0.46
1:C:523:LYS:NZ	4:C:1659:HOH:O	2.47	0.45
1:B:1415:GLU:OE1	1:B:1420:HIS:NE2	2.50	0.45
1:B:1246:HIS:CD2	1:B:1259:ALA:HB2	2.51	0.45
1:C:877:VAL:HG13	1:C:1154:TYR:CE1	2.52	0.45
1:B:771:SER:OG	1:B:834:GLY:HA2	2.16	0.45
1:D:803:ASN:HB2	1:D:806:LEU:O	2.17	0.45
1:B:545:TYR:HB2	1:B:548:ARG:O	2.17	0.44
1:A:803:ASN:HB2	1:A:806:LEU:O	2.17	0.44
1:B:1264:CYS:HA	1:B:1271:ARG:HG3	1.99	0.44
1:D:823:ASP:OD1	1:D:1213:ARG:NH1	2.44	0.44
1:D:792:CYS:HB2	1:D:814:LEU:HD23	2.00	0.44
1:A:545:TYR:HB2	1:A:548:ARG:O	2.17	0.44
1:B:949:HIS:CG	1:B:954:VAL:HG11	2.52	0.43
1:D:662:ARG:HH21	1:D:669:ASP:HB3	1.82	0.43
1:A:1080:GLN:NE2	4:A:2123:HOH:O	2.36	0.43
1:B:1149:ARG:HB2	1:B:1219:SER:HB3	2.01	0.43
1:A:940:LYS:HE3	1:A:940:LYS:HB2	1.86	0.43
1:A:596:LYS:O	1:A:598:GLY:N	2.51	0.43
1:A:541:ASP:HB3	1:A:552:THR:HB	2.00	0.43
1:C:1217:GLU:OE1	1:C:1220:ARG:NH2	2.38	0.43
1:D:1403:LEU:HA	1:D:1406:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:792:CYS:HB2	1:C:814:LEU:HD23	2.01	0.42
1:D:1105:LEU:O	1:D:1109:LEU:HD12	2.19	0.42
1:D:931:THR:HG23	1:D:1025:LYS:HE3	2.01	0.42
1:A:922:GLY:O	1:A:926:ILE:HG12	2.19	0.42
1:A:1246:HIS:CD2	1:A:1259:ALA:HB2	2.54	0.42
1:B:803:ASN:HB2	1:B:806:LEU:O	2.20	0.42
1:B:881:GLU:HG3	1:B:1154:TYR:HE1	1.84	0.42
1:D:849:ARG:HA	1:D:953:ALA:HB1	2.01	0.42
1:D:1176:LEU:HA	1:D:1176:LEU:HD12	1.86	0.42
1:A:849:ARG:HA	1:A:953:ALA:HB1	2.02	0.42
1:C:1326:ARG:O	1:C:1330:PHE:HB2	2.20	0.42
1:B:1257:TYR:CE2	1:B:1291:LYS:HB3	2.54	0.42
1:D:796:PHE:HB3	1:D:810:ASN:HD22	1.84	0.42
1:C:1290:ASP:OD1	1:C:1324:ARG:NE	2.40	0.42
1:C:766:GLU:HG2	4:C:2029:HOH:O	2.20	0.42
1:A:1264:CYS:HA	1:A:1271:ARG:HG3	2.00	0.41
1:A:1356:VAL:HA	1:A:1359:PHE:CE2	2.54	0.41
1:D:774:TRP:CE2	1:D:778:ARG:HG3	2.56	0.41
1:D:840:GLN:O	1:D:844:ASN:HB2	2.21	0.41
1:B:560:ARG:O	1:B:563:THR:OG1	2.32	0.41
1:D:1391:ARG:NH1	4:D:1653:HOH:O	2.53	0.41
1:B:854:LEU:HD23	1:B:918:VAL:HG11	2.03	0.41
1:C:1110:LEU:HD23	1:C:1110:LEU:HA	1.93	0.41
1:C:610:ARG:NH1	4:C:1658:HOH:O	2.54	0.41
1:C:803:ASN:HB2	1:C:806:LEU:O	2.21	0.41
1:A:728:VAL:HG11	1:A:791:VAL:HG11	2.03	0.40
1:B:1366:ARG:NH1	4:B:1622:HOH:O	2.38	0.40
1:B:888:SER:OG	1:B:889:ARG:N	2.54	0.40
1:A:1325:LEU:HD23	1:A:1363:ILE:HG21	2.04	0.40
1:B:1374:TRP:O	1:B:1382:GLN:HG2	2.22	0.40
1:D:1257:TYR:CE2	1:D:1291:LYS:HB3	2.56	0.40
1:B:817:ASP:OD2	1:B:819:SER:OG	2.30	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	884/907 (98%)	864 (98%)	20 (2%)	0	100	100
1	B	891/907 (98%)	869 (98%)	22 (2%)	0	100	100
1	C	896/907 (99%)	875 (98%)	19 (2%)	2 (0%)	47	55
1	D	878/907 (97%)	851 (97%)	27 (3%)	0	100	100
All	All	3549/3628 (98%)	3459 (98%)	88 (2%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1123	GLU
1	C	1205	PRO

### 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	717/775 (92%)	712 (99%)	5 (1%)	84	91
1	B	705/775 (91%)	700 (99%)	5 (1%)	84	91
1	C	719/775 (93%)	713 (99%)	6 (1%)	81	90
1	D	653/775 (84%)	647 (99%)	6 (1%)	78	88
All	All	2794/3100 (90%)	2772 (99%)	22 (1%)	81	90

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	700	SER
1	A	710	HIS
1	A	894	ASP
1	A	1062	CYS

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Mol	Chain	Res	Type
1	A	1401	ASP
1	B	606	ASP
1	B	616	ASP
1	B	710	HIS
1	B	894	ASP
1	B	1107	SER
1	C	606	ASP
1	C	710	HIS
1	C	753	SER
1	C	778	ARG
1	C	1062	CYS
1	C	1401	ASP
1	D	710	HIS
1	D	743	SER
1	D	894	ASP
1	D	1055	GLU
1	D	1079	GLU
1	D	1366	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 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	$\# Z  > 2$
3	GOL	C	1504	-	5,5,5	0.89	0	5,5,5	1.01	0
3	GOL	B	1504	-	5,5,5	0.90	0	5,5,5	0.99	0
3	GOL	A	2005	-	5,5,5	0.89	0	5,5,5	1.02	0
3	GOL	B	1503	-	5,5,5	0.92	0	5,5,5	1.05	0
3	GOL	C	1505	-	5,5,5	0.91	0	5,5,5	0.97	0
3	GOL	B	1505	-	5,5,5	0.89	0	5,5,5	1.02	0
3	GOL	C	1503	-	5,5,5	0.91	0	5,5,5	1.02	0
3	GOL	A	2004	-	5,5,5	0.91	0	5,5,5	1.00	0
3	GOL	A	2003	-	5,5,5	0.90	0	5,5,5	1.00	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
3	GOL	C	1504	-	-	2/4/4/4	-
3	GOL	B	1504	-	-	2/4/4/4	-
3	GOL	A	2005	-	-	1/4/4/4	-
3	GOL	B	1503	-	-	2/4/4/4	-
3	GOL	C	1505	-	-	1/4/4/4	-
3	GOL	B	1505	-	-	0/4/4/4	-
3	GOL	C	1503	-	-	0/4/4/4	-
3	GOL	A	2004	-	-	2/4/4/4	-
3	GOL	A	2003	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1504	GOL	C1-C2-C3-O3
3	B	1503	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	1503	GOL	O2-C2-C3-O3
3	A	2003	GOL	C1-C2-C3-O3
3	C	1504	GOL	C1-C2-C3-O3
3	A	2004	GOL	O1-C1-C2-C3
3	B	1504	GOL	O2-C2-C3-O3
3	A	2003	GOL	O2-C2-C3-O3
3	C	1505	GOL	C1-C2-C3-O3
3	C	1504	GOL	O2-C2-C3-O3
3	A	2004	GOL	O1-C1-C2-O2
3	A	2005	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1505	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	890/907 (98%)	-0.39	5 (0%)	89 88	12, 25, 42, 68	1 (0%)
1	B	899/907 (99%)	-0.37	4 (0%)	92 91	14, 26, 42, 70	2 (0%)
1	C	900/907 (99%)	-0.49	6 (0%)	87 86	11, 21, 41, 76	0
1	D	886/907 (97%)	0.07	22 (2%)	57 55	22, 39, 59, 76	0
All	All	3575/3628 (98%)	-0.30	37 (1%)	82 81	11, 27, 50, 76	3 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1059	ALA	4.3
1	D	596	LYS	3.9
1	D	1128	ALA	3.5
1	C	520	PRO	3.5
1	D	561	GLU	3.4
1	C	1145	GLN	3.3
1	D	1029	ILE	3.3
1	A	520	PRO	3.2
1	D	1204	ALA	3.1
1	D	1146	GLY	3.0
1	D	1122	GLY	2.8
1	D	622	ALA	2.8
1	A	1125	VAL	2.7
1	D	996	ASP	2.6
1	D	1145	GLN	2.6
1	D	1396	PRO	2.6
1	D	744	GLY	2.6
1	A	1124	ASP	2.6
1	D	1397	GLY	2.5
1	C	1207	SER	2.5
1	B	1207	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	1200	ALA	2.5
1	C	1205	PRO	2.5
1	D	993	PHE	2.5
1	D	1030	GLY	2.5
1	A	1204	ALA	2.4
1	A	1122	GLY	2.3
1	B	520	PRO	2.2
1	B	1119	GLU	2.2
1	D	1203	SER	2.2
1	D	1199	TYR	2.1
1	D	597	ALA	2.1
1	C	1204	ALA	2.1
1	C	1206	GLU	2.0
1	D	1202	LEU	2.0
1	B	597	ALA	2.0
1	D	1002	LEU	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
3	GOL	A	2005	6/6	0.84	0.21	37,39,41,48	0
3	GOL	B	1503	6/6	0.84	0.23	37,38,43,45	0
3	GOL	C	1505	6/6	0.85	0.18	32,33,39,44	0
2	ZN	A	2002	1/1	0.87	0.10	56,56,56,56	0
3	GOL	C	1503	6/6	0.87	0.17	31,32,38,45	0
3	GOL	C	1504	6/6	0.88	0.20	25,34,39,42	0
3	GOL	A	2004	6/6	0.88	0.17	34,36,42,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	2003	6/6	0.88	0.20	34,35,36,38	0
3	GOL	B	1504	6/6	0.89	0.24	38,44,51,54	0
3	GOL	B	1505	6/6	0.92	0.22	36,39,44,49	0
2	ZN	D	1502	1/1	0.96	0.04	78,78,78,78	0
2	ZN	C	1502	1/1	0.97	0.07	51,51,51,51	0
2	ZN	B	1502	1/1	0.97	0.07	62,62,62,62	0
2	ZN	D	1501	1/1	0.98	0.11	32,32,32,32	0
2	ZN	C	1501	1/1	0.99	0.09	16,16,16,16	0
2	ZN	A	2001	1/1	0.99	0.07	16,16,16,16	0
2	ZN	B	1501	1/1	0.99	0.06	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.