



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 09:26 PM GMT

PDB ID : 5AB2  
Title : Crystal structure of aminopeptidase ERAP2 with ligand  
Authors : Mpakali, A.; Giastas, P.; Saridakis, E.; Mavridis, I.M.; Stratikos, E.  
Deposited on : 2015-07-31  
Resolution : 2.73 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

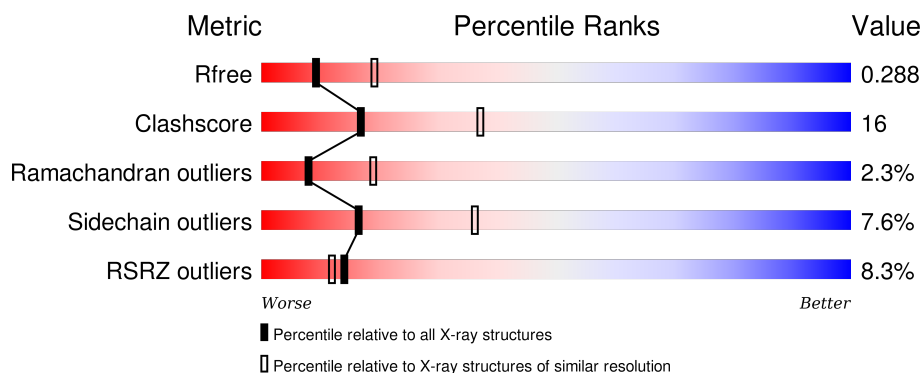
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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	967	<div> <div>2%</div> <div>69%</div> <div>22%</div> <div>7%</div> </div>
1	B	967	<div> <div>13%</div> <div>52%</div> <div>33%</div> <div>6%</div> <div>9%</div> </div>
2	C	6	<div> <div>33%</div> <div>50%</div> <div>33%</div> <div>17%</div> </div>
2	D	6	<div> <div>83%</div> <div>33%</div> <div>50%</div> <div>17%</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	NAG	B	1010	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15144 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 ENDOPLASMIC RETICULUM AMINOPEPTIDASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	897	Total	C	N	O	S	0	8	1
			7344	4737	1217	1361	29			
1	B	879	Total	C	N	O	S	0	0	1
			7156	4617	1188	1323	28			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	961	ARG	-	CLONING ARTIFACT	UNP Q6P179
A	962	HIS	-	EXPRESSION TAG	UNP Q6P179
A	963	HIS	-	EXPRESSION TAG	UNP Q6P179
A	964	HIS	-	EXPRESSION TAG	UNP Q6P179
A	965	HIS	-	EXPRESSION TAG	UNP Q6P179
A	966	HIS	-	EXPRESSION TAG	UNP Q6P179
A	967	HIS	-	EXPRESSION TAG	UNP Q6P179
B	961	ARG	-	EXPRESSION TAG	UNP Q6P179
B	962	HIS	-	EXPRESSION TAG	UNP Q6P179
B	963	HIS	-	EXPRESSION TAG	UNP Q6P179
B	964	HIS	-	EXPRESSION TAG	UNP Q6P179
B	965	HIS	-	EXPRESSION TAG	UNP Q6P179
B	966	HIS	-	EXPRESSION TAG	UNP Q6P179
B	967	HIS	-	EXPRESSION TAG	UNP Q6P179

- Molecule 2 is a protein called GPI.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	5	0
			80	52	17	11			
2	D	6	Total	C	N	O	0	0	0
			42	27	9	6			

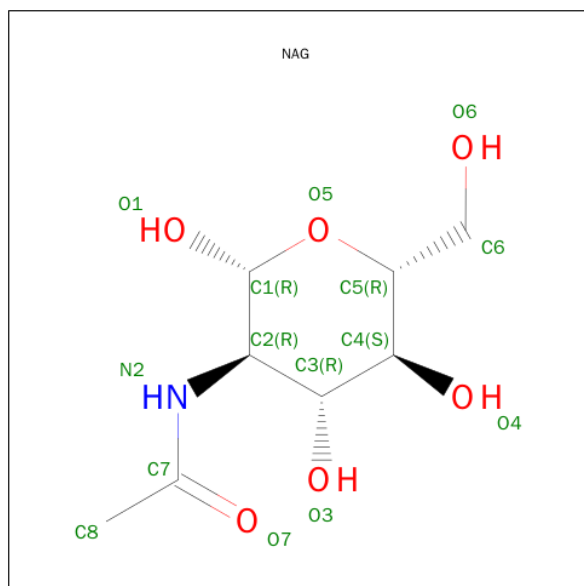
- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		
3	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

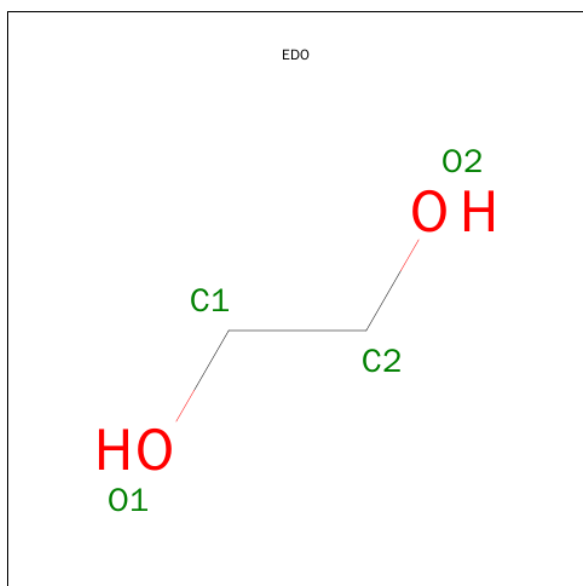


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Zn	0	0
			1	1		
6	A	1	Total	Zn	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	4	Total	C	N	O	0	0
			50	28	2	20		

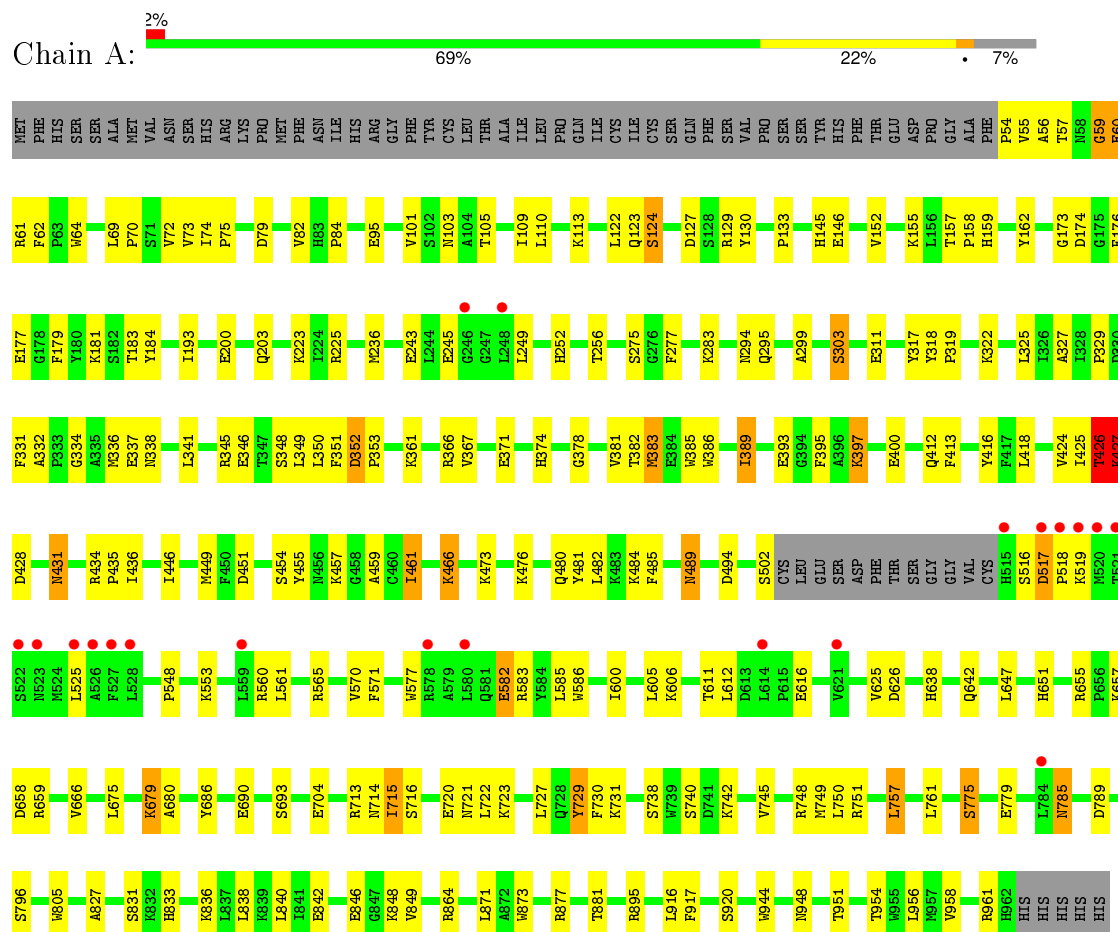
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	82	Total	O	0	0
			82	82		
9	B	20	Total	O	0	0
			20	20		

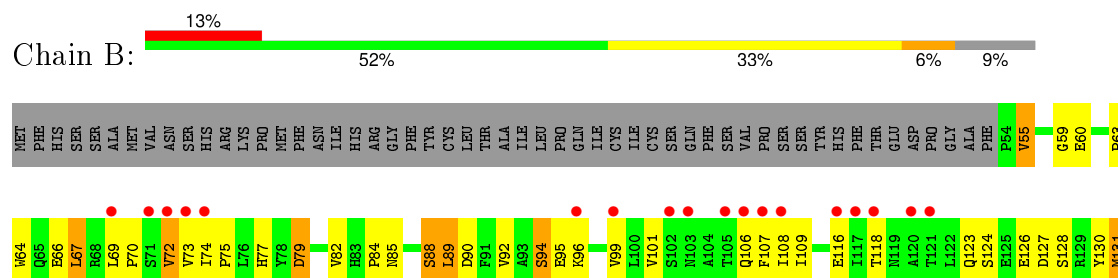
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

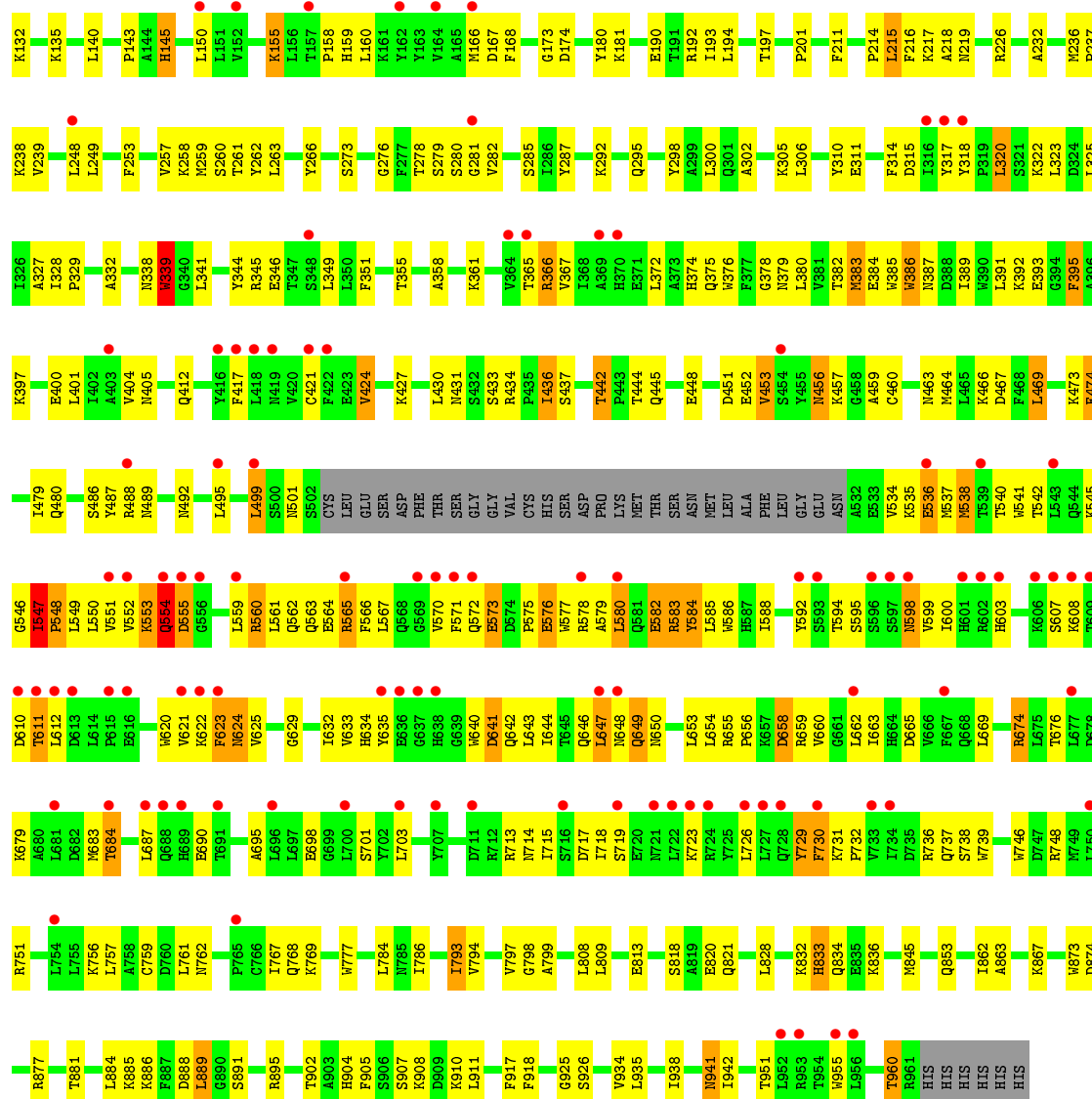
#### • Molecule 1: ENDOPLASMIC RETICULUM AMINOPEPTIDASE 2



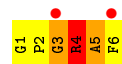
#### • Molecule 1: ENDOPLASMIC RETICULUM AMINOPEPTIDASE 2



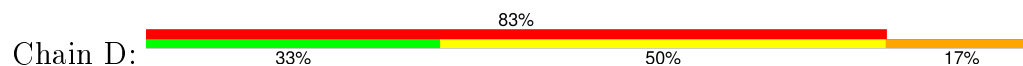




• Molecule 2: GPI



• Molecule 2: GPI



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.65Å 135.47Å 128.21Å 90.00° 90.24° 90.00°	Depositor
Resolution (Å)	49.01 – 2.73 49.01 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.01-2.73) 98.6 (49.01-2.73)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 2.73Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.223 , 0.286 0.231 , 0.288	Depositor DCC
$R_{free}$ test set	3395 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.7	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 52.1	EDS
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 67785 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15144	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, EDO

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	0.59	1/7550 (0.0%)	0.69	0/10229
1	B	0.40	1/7334 (0.0%)	0.59	1/9939 (0.0%)
2	C	0.84	0/82	1.64	0/106
2	D	0.59	0/43	1.16	0/56
All	All	0.51	2/15009 (0.0%)	0.65	1/20330 (0.0%)

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
2	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	GLY	C-N	-6.35	1.19	1.34
1	B	548	PRO	N-CD	5.19	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	547	ILE	C-N-CD	5.70	140.37	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	3[A]	GLY	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	7344	0	7297	146	0
1	B	7156	0	7112	330	0
2	C	80	0	79	11	0
2	D	42	0	42	6	0
3	A	78	0	68	0	0
4	A	140	0	125	3	0
4	B	56	0	50	2	0
5	A	28	0	26	0	0
5	B	42	0	39	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	12	0	18	0	0
7	B	12	0	18	0	0
8	B	50	0	43	6	0
9	A	82	0	0	10	0
9	B	20	0	0	7	0
All	All	15144	0	14917	490	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 16.

The worst 5 of 490 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:PHE:CE1	1:B:567:LEU:O	1.72	1.40
1:B:554:GLN:CG	1:B:560:ARG:HD2	1.59	1.31
1:B:566:PHE:CD1	1:B:567:LEU:N	2.10	1.18
1:B:554:GLN:HG2	1:B:560:ARG:HD2	1.32	1.12
1:B:554:GLN:HG2	1:B:560:ARG:CD	1.88	1.03

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	901/967 (93%)	814 (90%)	75 (8%)	12 (1%)	15	36
1	B	875/967 (90%)	732 (84%)	117 (13%)	26 (3%)	5	12
2	C	8/6 (133%)	4 (50%)	0	4 (50%)	0	0
2	D	4/6 (67%)	4 (100%)	0	0	100	100
All	All	1788/1946 (92%)	1554 (87%)	192 (11%)	42 (2%)	8	19

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	THR
1	A	60	GLU
1	A	245	GLU
1	A	582	GLU
1	A	616	GLU

### 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	813/870 (93%)	768 (94%)	45 (6%)	27	54
1	B	790/870 (91%)	715 (90%)	75 (10%)	11	24
2	C	6/3 (200%)	4 (67%)	2 (33%)	0	0
2	D	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	1612/1746 (92%)	1489 (92%)	123 (8%)	16	36

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	145	HIS
1	B	424	VAL
1	B	833	HIS
1	B	193	ILE
1	B	339	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	562	GLN
1	B	581	GLN
1	B	624	ASN
1	B	634	HIS
1	B	959	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 ⓘ

24 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	1001	3	14,14,15	1.29	1 (7%)	15,19,21	1.71	1 (6%)
3	NAG	A	1002	1,3	14,14,15	0.51	0	15,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BMA	A	1003	3	11,11,12	1.16	2 (18%)	15,15,17	1.44	3 (20%)
4	NAG	A	1004	1,4	14,14,15	0.65	0	15,19,21	0.58	0
4	NAG	A	1005	4	14,14,15	0.43	0	15,19,21	0.39	0
3	NAG	A	1006	1,3	14,14,15	1.09	1 (7%)	15,19,21	0.44	0
3	NAG	A	1007	3	14,14,15	0.53	0	15,19,21	0.59	0
3	BMA	A	1008	3	11,11,12	2.00	4 (36%)	15,15,17	2.21	6 (40%)
4	NAG	A	1010	1,4	14,14,15	0.30	0	15,19,21	0.71	0
4	NAG	A	1011	4	14,14,15	0.39	0	15,19,21	0.26	0
4	NAG	A	1012	1,4	14,14,15	0.67	1 (7%)	15,19,21	0.70	1 (6%)
4	NAG	A	1013	4	14,14,15	0.88	1 (7%)	15,19,21	0.78	1 (6%)
4	NAG	A	1014	1,4	14,14,15	0.30	0	15,19,21	1.32	1 (6%)
4	NAG	A	1015	4	14,14,15	0.29	0	15,19,21	0.32	0
4	NAG	A	1016	1,4	14,14,15	0.96	1 (7%)	15,19,21	1.02	1 (6%)
4	NAG	A	1017	4	14,14,15	0.44	0	15,19,21	0.27	0
8	NAG	B	1001	1,8	14,14,15	0.77	0	15,19,21	1.55	2 (13%)
8	NAG	B	1002	8	14,14,15	0.62	0	15,19,21	1.39	1 (6%)
8	BMA	B	1003	8	11,11,12	1.67	1 (9%)	15,15,17	1.21	2 (13%)
8	BMA	B	1004	8	11,11,12	1.01	0	15,15,17	1.46	2 (13%)
4	NAG	B	1006	1,4	14,14,15	0.38	0	15,19,21	0.48	0
4	NAG	B	1007	4	14,14,15	0.49	0	15,19,21	0.45	0
4	NAG	B	1008	1,4	14,14,15	0.32	0	15,19,21	0.86	0
4	NAG	B	1009	4	14,14,15	0.68	1 (7%)	15,19,21	0.70	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	NAG	A	1001	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1002	1,3	-	0/6/23/26	0/1/1/1
3	BMA	A	1003	3	-	0/2/19/22	0/1/1/1
4	NAG	A	1004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1005	4	-	0/6/23/26	0/1/1/1
3	NAG	A	1006	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1007	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1008	3	-	0/2/19/22	0/1/1/1
4	NAG	A	1010	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1011	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1012	1,4	-	0/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1013	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1014	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1015	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1016	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1017	4	-	0/6/23/26	0/1/1/1
8	NAG	B	1001	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	1002	8	-	0/6/23/26	0/1/1/1
8	BMA	B	1003	8	-	0/2/19/22	0/1/1/1
8	BMA	B	1004	8	-	0/2/19/22	0/1/1/1
4	NAG	B	1006	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1007	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1008	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1009	4	-	0/6/23/26	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1006	NAG	O5-C1	-3.66	1.37	1.43
4	A	1016	NAG	O5-C1	-3.33	1.38	1.43
4	A	1012	NAG	O5-C1	-2.40	1.39	1.43
3	A	1003	BMA	O5-C5	2.21	1.48	1.43
4	B	1009	NAG	C1-C2	2.35	1.55	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1001	NAG	O4-C4-C3	-4.22	100.85	110.36
3	A	1008	BMA	C3-C4-C5	-2.26	106.20	110.23
4	A	1012	NAG	O4-C4-C3	-2.15	105.50	110.36
3	A	1008	BMA	O2-C2-C3	-2.11	105.94	110.19
8	B	1004	BMA	O2-C2-C3	-2.09	105.98	110.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1014	NAG	2	0
4	A	1015	NAG	1	0
4	A	1016	NAG	1	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1001	NAG	5	0
8	B	1002	NAG	1	0
8	B	1003	BMA	1	0
8	B	1004	BMA	1	0
4	B	1006	NAG	1	0
4	B	1007	NAG	1	0
4	B	1009	NAG	1	0

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	NAG	A	1009	1	14,14,15	0.32	0	15,19,21	0.78	1 (6%)
5	NAG	A	1018	1	14,14,15	0.48	0	15,19,21	0.48	0
7	EDO	A	1962	-	3,3,3	0.65	0	2,2,2	0.15	0
7	EDO	A	1963	-	3,3,3	0.45	0	2,2,2	0.44	0
7	EDO	A	1964	-	3,3,3	0.53	0	2,2,2	0.25	0
5	NAG	B	1005	1	14,14,15	0.51	0	15,19,21	0.57	0
5	NAG	B	1010	1	14,14,15	0.34	0	15,19,21	0.31	0
5	NAG	B	1011	1	14,14,15	0.50	0	15,19,21	0.31	0
7	EDO	B	1961	-	3,3,3	0.49	0	2,2,2	0.20	0
7	EDO	B	1962	-	3,3,3	0.46	0	2,2,2	0.39	0
7	EDO	B	1963	-	3,3,3	0.43	0	2,2,2	0.42	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
5	NAG	A	1009	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1018	1	-	0/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	1962	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1963	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1964	-	-	0/1/1/1	0/0/0/0
5	NAG	B	1005	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1010	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1011	1	-	0/6/23/26	0/1/1/1
7	EDO	B	1961	-	-	0/1/1/1	0/0/0/0
7	EDO	B	1962	-	-	0/1/1/1	0/0/0/0
7	EDO	B	1963	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1009	NAG	C1-O5-C5	2.14	115.28	112.14

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	897/967 (92%)	-0.04	20 (2%) 65 66	24, 47, 86, 151	0
1	B	879/967 (90%)	0.82	121 (13%) 4 3	30, 100, 150, 170	0
2	C	6/6 (100%)	1.90	2 (33%) 0 0	42, 47, 52, 54	0
2	D	6/6 (100%)	5.31	5 (83%) 0 0	74, 77, 84, 90	6 (100%)
All	All	1788/1946 (91%)	0.41	148 (8%) 14 12	24, 66, 137, 170	6 (0%)

The worst 5 of 148 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	580	LEU	8.6
1	A	520	MET	8.1
1	B	602	ARG	7.6
2	D	6	PHE	7.6
1	B	72	VAL	7.5

### 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](#)

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( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	1002	14/15	0.95	0.25	0.80	43,68,77,77	0
3	NAG	A	1006	14/15	0.96	0.13	-0.04	41,46,56,62	0
3	NAG	A	1001	14/15	0.91	0.21	-0.17	79,90,107,113	0
4	NAG	B	1008	14/15	0.83	0.16	-0.26	91,115,128,134	0
3	BMA	A	1008	11/12	0.76	0.15	-	90,97,105,107	0
4	NAG	A	1013	14/15	0.69	0.25	-	112,122,130,132	0
4	NAG	B	1007	14/15	0.77	0.23	-	131,158,162,163	0
4	NAG	A	1005	14/15	0.66	0.39	-	142,155,160,161	0
8	NAG	B	1002	14/15	0.87	0.14	-	50,77,88,88	0
8	BMA	B	1004	11/12	0.82	0.18	-	73,100,109,113	0
8	NAG	B	1001	14/15	0.89	0.23	-	57,67,76,79	0
4	NAG	A	1004	14/15	0.83	0.25	-	91,119,136,146	0
8	BMA	B	1003	11/12	0.79	0.13	-	73,98,104,104	0
4	NAG	A	1014	14/15	0.80	0.19	-	106,127,136,138	0
4	NAG	A	1015	14/15	0.67	0.26	-	119,132,141,141	0
4	NAG	A	1011	14/15	0.80	0.23	-	103,114,118,119	0
4	NAG	A	1010	14/15	0.89	0.12	-	76,84,97,106	0
4	NAG	A	1016	14/15	0.81	0.18	-	57,92,108,122	0
4	NAG	A	1012	14/15	0.87	0.17	-	95,103,114,117	0
4	NAG	B	1009	14/15	0.76	0.25	-	121,133,137,140	0
4	NAG	B	1006	14/15	0.70	0.20	-	138,153,159,164	0
4	NAG	A	1017	14/15	0.77	0.30	-	115,128,133,139	0
3	NAG	A	1007	14/15	0.91	0.12	-	46,66,84,88	0
3	BMA	A	1003	11/12	0.83	0.23	-	109,117,121,122	0

## 6.4 Ligands

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( $\text{\AA}^2$ )	Q<0.9
5	NAG	B	1010	14/15	0.40	0.46	6.13	112,136,147,147	0
5	NAG	A	1009	14/15	0.91	0.17	0.39	60,84,88,89	0
6	ZN	A	1119	1/1	0.99	0.21	-0.93	28,28,28,28	0
6	ZN	B	1119	1/1	0.97	0.22	-1.17	60,60,60,60	0
7	EDO	A	1962	4/4	0.87	0.11	-1.65	51,56,57,65	0
7	EDO	B	1962	4/4	0.78	0.38	-	96,99,103,116	0
5	NAG	B	1005	14/15	0.69	0.29	-	143,151,154,154	0
7	EDO	B	1963	4/4	0.84	0.27	-	99,99,104,120	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	B	1961	4/4	0.77	0.29	-	81,93,96,97	0
5	NAG	A	1018	14/15	0.80	0.23	-	97,110,122,129	0
7	EDO	A	1964	4/4	0.69	0.31	-	74,80,84,88	0
7	EDO	A	1963	4/4	0.91	0.10	-	83,89,90,96	0
5	NAG	B	1011	14/15	0.66	0.27	-	132,143,148,150	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.