



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 02:36 am GMT

PDB ID : 5AB0
Title : Crystal structure of aminopeptidase ERAP2 with ligand
Authors : Mpakali, A.; Giastas, P.; Saridakis, E.; Stratikos, E.
Deposited on : 2015-07-31
Resolution : 2.50 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

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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

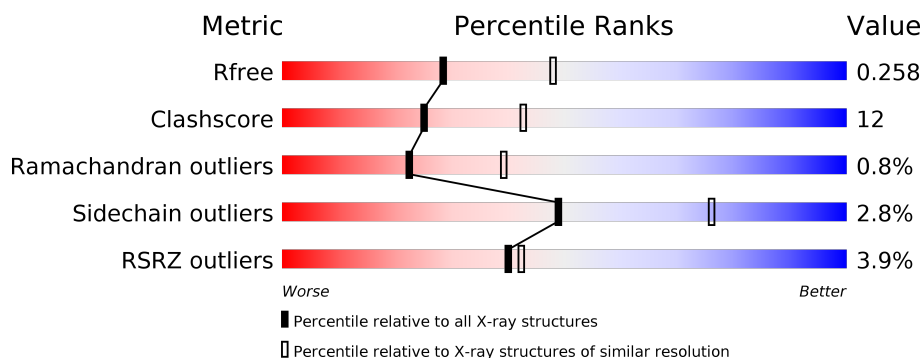
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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. 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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 72%, yellow 21%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 72% 21% • 6% </div> </div>
1	C	967	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, green 61%, yellow 29%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 6% 61% 29% • 9% </div> </div>
2	E	10	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 10%, yellow 60%, orange 30%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 10% 60% 30% </div> </div>
2	F	10	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 40%, green 40%, yellow 50%, orange 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 40% 40% 50% 10% </div> </div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15615 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 ENDOPLASMATIC RETICULUM AMINOPEPTIDASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	911	Total	C	N	O	S	0	4	1
			7425	4779	1236	1378	32			
1	C	882	Total	C	N	O	S	0	4	1
			7208	4646	1196	1338	28			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	961	ARG	-	EXPRESSION TAG	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
A	392	ASN	LYS	VARIANT	UNP Q6P179
C	961	ARG	-	EXPRESSION TAG	UNP Q6P179
C	962	HIS	-	EXPRESSION TAG	UNP Q6P179
C	963	HIS	-	EXPRESSION TAG	UNP Q6P179
C	964	HIS	-	EXPRESSION TAG	UNP Q6P179
C	965	HIS	-	EXPRESSION TAG	UNP Q6P179
C	966	HIS	-	EXPRESSION TAG	UNP Q6P179
C	967	HIS	-	EXPRESSION TAG	UNP Q6P179
C	392	ASN	LYS	VARIANT	UNP Q6P179

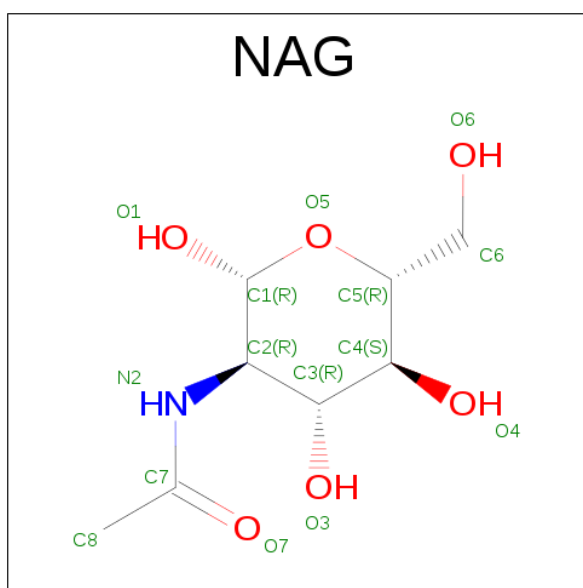
- Molecule 2 is a protein called DG025.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	10	Total	C	N	O	P	0	0	0
			93	64	16	12	1			
2	F	10	Total	C	N	O	P	0	0	0
			93	64	16	12	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

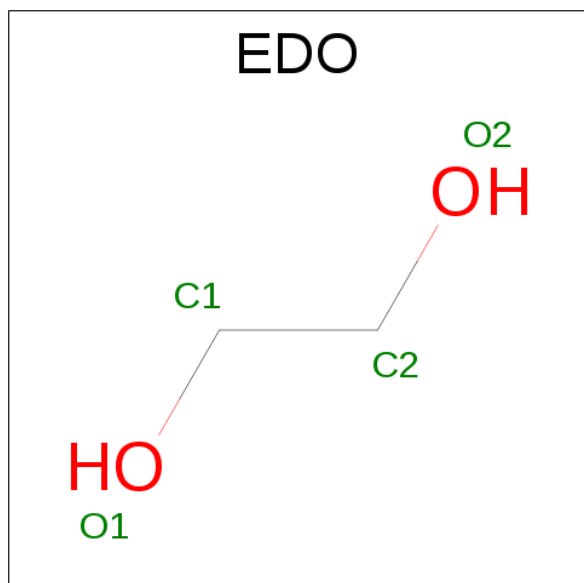
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

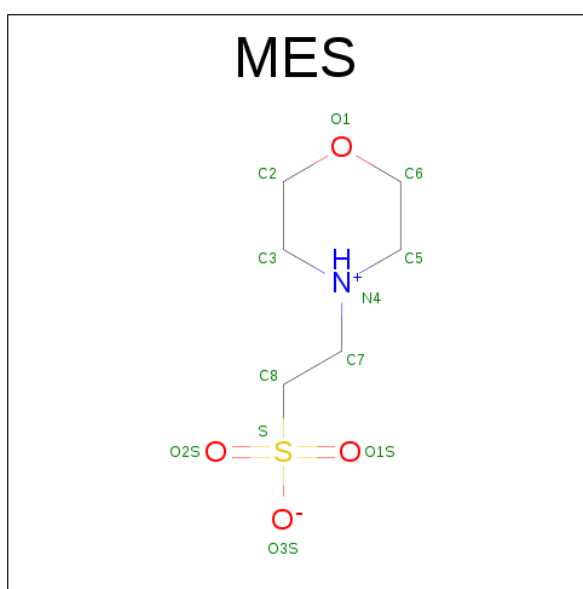
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			39	22	2	15		
6	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 9 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	278	Total	O	0	0
			278	278		

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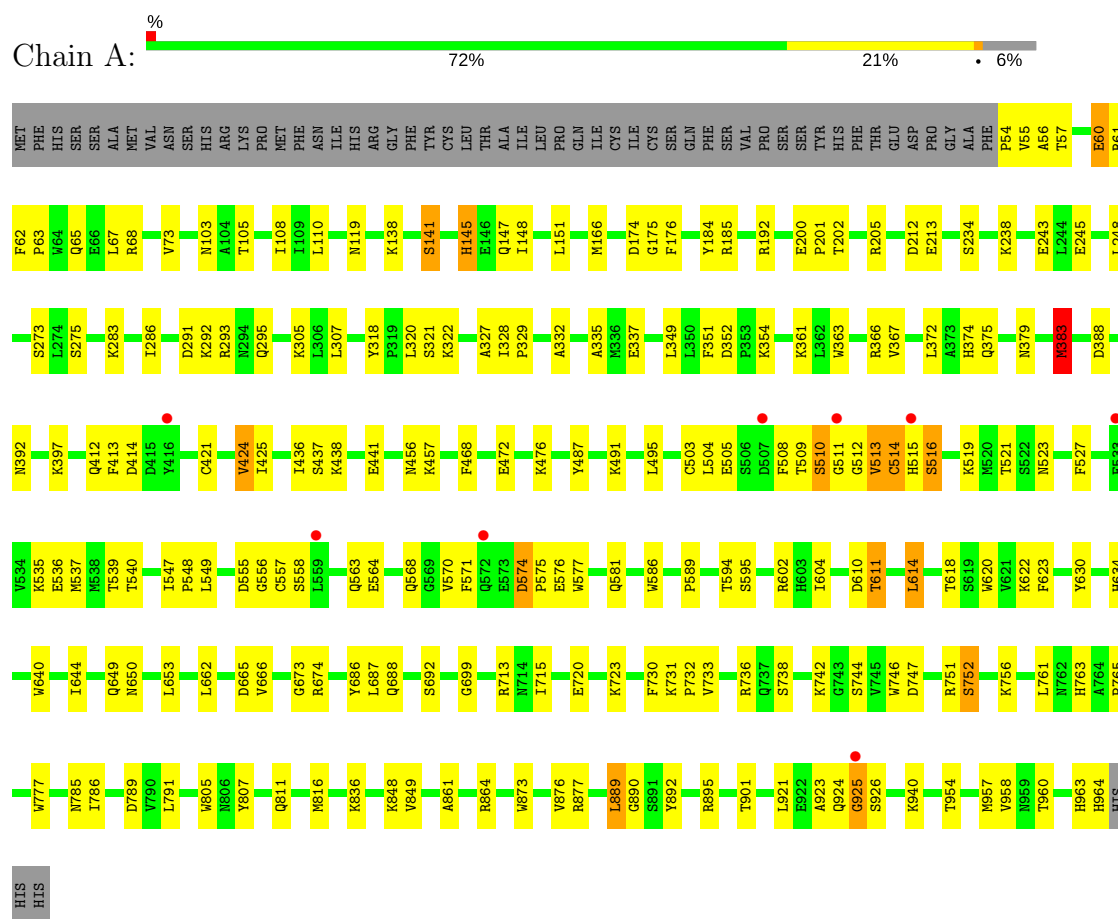
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	125	Total 125	O 125	0	0

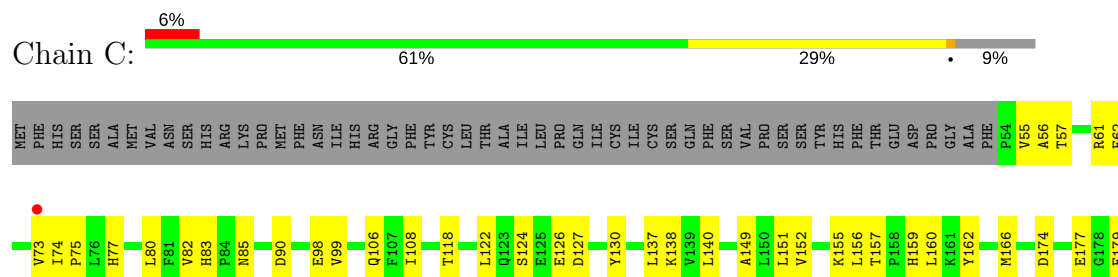
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: ENDOPLASMATIC RETICULUM AMINOPEPTIDASE 2



• Molecule 1: ENDOPLASMATIC RETICULUM AMINOPEPTIDASE 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.35Å 134.42Å 129.00Å 90.00° 90.49° 90.00°	Depositor
Resolution (Å)	65.73 – 2.50 67.21 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (65.73-2.50) 93.7 (67.21-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.198 , 0.258 0.198 , 0.258	Depositor DCC
R_{free} test set	4412 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,-l,-k 0.002 for -h,l,k 0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15615	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: ZN, BMA, 7GA, NAG, EDO, MES, 2X0, LYN

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	0.50	0/7620	0.62	1/10327 (0.0%)
1	C	0.41	0/7395	0.57	1/10021 (0.0%)
2	E	0.73	0/65	0.85	0/85
2	F	0.39	0/65	0.65	0/85
All	All	0.46	0/15145	0.60	2/20518 (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
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	MET	CG-SD-CE	-5.80	90.91	100.20
1	C	194	LEU	CA-CB-CG	5.38	127.67	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	889	LEU	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	7425	0	7350	149	0
1	C	7208	0	7148	198	0
2	E	93	0	91	14	0
2	F	93	0	92	12	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	56	0	52	1	0
4	C	84	0	78	0	0
5	A	56	0	50	0	0
5	C	28	0	25	0	0
6	A	78	0	68	1	0
7	A	8	0	12	3	0
7	C	8	0	12	1	0
8	A	12	0	12	0	0
9	C	61	0	52	3	0
10	A	278	0	0	28	0
10	C	125	0	0	23	0
All	All	15615	0	15042	366	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 12.

The worst 5 of 366 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:922:GLU:HA	1:C:926:SER:HB3	1.46	0.97
1:C:424:VAL:HG22	1:C:452:GLU:HB3	1.50	0.94
1:A:720:GLU:OE2	10:A:3217:HOH:O	1.86	0.93
1:C:424:VAL:HG21	1:C:456:ASN:HB2	1.48	0.93
1:A:508:PHE:H	1:A:509:THR:HA	1.36	0.88

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	913/967 (94%)	851 (93%)	56 (6%)	6 (1%)	25	43
1	C	882/967 (91%)	815 (92%)	61 (7%)	6 (1%)	25	43
2	E	7/10 (70%)	3 (43%)	2 (29%)	2 (29%)	0	0
2	F	7/10 (70%)	3 (43%)	3 (43%)	1 (14%)	0	0
All	All	1809/1954 (93%)	1672 (92%)	122 (7%)	15 (1%)	22	39

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	510	SER
1	A	516	SER
2	E	4	HIS
2	F	4	HIS
1	A	730	PHE

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	822/870 (94%)	801 (97%)	21 (3%)	51	78
1	C	796/870 (92%)	775 (97%)	21 (3%)	51	78
2	E	6/6 (100%)	4 (67%)	2 (33%)	0	0
2	F	6/6 (100%)	5 (83%)	1 (17%)	2	4
All	All	1630/1752 (93%)	1585 (97%)	45 (3%)	49	76

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	963	HIS
1	C	194	LEU
1	C	961	ARG
1	C	159	HIS
1	C	257	VAL

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 ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
2	LYN	E	10	2	9,9,9	1.83	1 (11%)	8,10,10	0.95	0
2	LYN	F	10	2	9,9,9	1.79	1 (11%)	8,10,10	0.80	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
2	LYN	E	10	2	-	0/8/9/9	0/0/0/0
2	LYN	F	10	2	-	0/8/9/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	10	LYN	C-NT	5.28	1.43	1.32
2	E	10	LYN	C-NT	5.34	1.43	1.32

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	10	LYN	1	0

5.5 Carbohydrates [i](#)

17 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
5	NAG	A	1071	1,5	14,14,15	0.55	0	15,19,21	0.50	0
5	NAG	A	1072	5	14,14,15	0.46	0	15,19,21	0.56	0
6	NAG	A	1073	1,6	14,14,15	0.62	0	15,19,21	0.72	1 (6%)
6	NAG	A	1074	6	14,14,15	0.65	1 (7%)	15,19,21	0.57	0
6	BMA	A	1075	6	11,11,12	0.79	0	13,15,17	1.48	2 (15%)
6	NAG	A	1076	1,6	14,14,15	0.31	0	15,19,21	1.12	2 (13%)
6	NAG	A	1077	6	14,14,15	1.12	1 (7%)	15,19,21	1.32	1 (6%)
6	BMA	A	1078	6	11,11,12	1.59	2 (18%)	13,15,17	2.39	5 (38%)
5	NAG	A	1079	1,5	14,14,15	1.51	1 (7%)	15,19,21	1.29	3 (20%)
5	NAG	A	1080	5	14,14,15	0.25	0	15,19,21	0.41	0
9	BMA	C	1001	9	11,11,12	2.05	2 (18%)	13,15,17	1.35	2 (15%)
9	BMA	C	1002	9	11,11,12	1.36	2 (18%)	13,15,17	1.52	2 (15%)
9	NAG	C	1003	1,9	14,14,15	0.42	0	15,19,21	0.65	0
9	NAG	C	1004	9	14,14,15	1.12	1 (7%)	15,19,21	1.49	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BMA	C	1005	9	11,11,12	1.20	1 (9%)	13,15,17	1.26	2 (15%)
5	NAG	C	1007	1,5	14,14,15	0.69	1 (7%)	15,19,21	0.58	0
5	NAG	C	1008	5	14,14,15	0.30	0	15,19,21	0.73	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	1071	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1072	5	-	0/6/23/26	0/1/1/1
6	NAG	A	1073	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1074	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1075	6	-	0/2/19/22	0/1/1/1
6	NAG	A	1076	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1077	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1078	6	-	0/2/19/22	0/1/1/1
5	NAG	A	1079	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1080	5	-	0/6/23/26	0/1/1/1
9	BMA	C	1001	9	-	0/2/19/22	0/1/1/1
9	BMA	C	1002	9	-	0/2/19/22	0/1/1/1
9	NAG	C	1003	1,9	-	0/6/23/26	0/1/1/1
9	NAG	C	1004	9	-	0/6/23/26	0/1/1/1
9	BMA	C	1005	9	-	0/2/19/22	0/1/1/1
5	NAG	C	1007	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1008	5	-	0/6/23/26	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1079	NAG	O5-C1	-5.35	1.35	1.43
9	C	1001	BMA	C2-C3	-5.19	1.45	1.52
9	C	1004	NAG	O5-C1	-4.11	1.37	1.43
9	C	1001	BMA	C1-C2	-3.06	1.44	1.52
6	A	1074	NAG	O5-C1	-2.33	1.39	1.43

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1004	NAG	O4-C4-C3	-4.09	101.46	110.36
6	A	1078	BMA	O2-C2-C3	-3.63	103.04	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1001	BMA	O2-C2-C3	-3.10	104.09	110.17
6	A	1075	BMA	O2-C2-C3	-2.88	104.52	110.17
9	C	1005	BMA	O2-C2-C3	-2.46	105.34	110.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1077	NAG	1	0
6	A	1078	BMA	1	0
9	C	1001	BMA	1	0
9	C	1003	NAG	2	0

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1069	1	14,14,15	0.90	1 (7%)	15,19,21	1.09	1 (6%)
4	NAG	A	1070	1	14,14,15	0.51	0	15,19,21	0.64	0
4	NAG	A	1081	1	14,14,15	0.57	0	15,19,21	0.88	1 (6%)
4	NAG	A	1082	1	14,14,15	0.35	0	15,19,21	0.57	0
7	EDO	A	1964	-	3,3,3	0.54	0	2,2,2	0.23	0
7	EDO	A	1965	-	3,3,3	0.33	0	2,2,2	0.47	0
8	MES	A	2002	-	12,12,12	2.13	1 (8%)	14,16,16	2.46	7 (50%)
4	NAG	C	1006	1	14,14,15	0.68	0	15,19,21	0.67	0
4	NAG	C	1009	1	14,14,15	1.07	2 (14%)	15,19,21	0.93	1 (6%)
4	NAG	C	1010	1	14,14,15	0.21	0	15,19,21	0.55	0
4	NAG	C	1011	1	14,14,15	0.66	1 (7%)	15,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1012	1	14,14,15	0.30	0	15,19,21	0.53	0
4	NAG	C	1013	1	14,14,15	0.75	1 (7%)	15,19,21	0.78	1 (6%)
7	EDO	C	1962	-	3,3,3	0.48	0	2,2,2	0.28	0
7	EDO	C	1963	-	3,3,3	0.52	0	2,2,2	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1069	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1070	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1081	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1082	1	-	0/6/23/26	0/1/1/1
7	EDO	A	1964	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1965	-	-	0/1/1/1	0/0/0/0
8	MES	A	2002	-	-	0/6/14/14	0/1/1/1
4	NAG	C	1006	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1009	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1010	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1011	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1012	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1013	1	-	0/6/23/26	0/1/1/1
7	EDO	C	1962	-	-	0/1/1/1	0/0/0/0
7	EDO	C	1963	-	-	0/1/1/1	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2002	MES	C8-S	-6.98	1.67	1.77
4	C	1009	NAG	O5-C1	-2.87	1.39	1.43
4	C	1011	NAG	O5-C1	-2.30	1.39	1.43
4	C	1013	NAG	C1-C2	2.24	1.55	1.52
4	C	1009	NAG	C1-C2	2.34	1.55	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2002	MES	C2-C3-N4	-2.38	106.77	110.11
4	C	1009	NAG	C4-C3-C2	2.50	114.69	111.02
4	C	1013	NAG	C1-O5-C5	2.60	115.76	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2002	MES	C7-N4-C3	2.84	118.53	111.26
8	A	2002	MES	O1S-S-C8	3.04	109.40	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1069	NAG	1	0
7	A	1965	EDO	3	0
7	C	1962	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	911/967 (94%)	0.04	8 (0%) 84 85	22, 44, 77, 103	0
1	C	882/967 (91%)	0.37	59 (6%) 19 19	28, 68, 107, 125	0
2	E	7/10 (70%)	1.05	0 100 100	61, 66, 81, 84	0
2	F	7/10 (70%)	2.52	4 (57%) 0 0	75, 81, 95, 98	0
All	All	1807/1954 (92%)	0.22	71 (3%) 40 42	22, 54, 100, 125	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	580	LEU	5.6
2	F	9	PHE	4.5
2	F	7	PHE	4.5
1	C	746	TRP	4.4
1	C	559	LEU	4.1

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	LYN	E	10	10/10	0.62	0.67	-	64,83,107,109	0
2	LYN	F	10	10/10	0.09	0.60	-	87,102,106,122	0

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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	A	1071	14/15	0.94	0.15	-0.35	44,52,76,76	0
5	NAG	C	1007	14/15	0.91	0.13	-0.56	42,55,65,65	0
9	NAG	C	1003	14/15	0.96	0.13	-0.71	32,38,42,47	0
6	NAG	A	1073	14/15	0.97	0.13	-0.79	33,37,48,55	0
6	NAG	A	1076	14/15	0.93	0.14	-1.13	55,68,81,96	0
5	NAG	A	1072	14/15	0.90	0.15	-	69,82,88,88	0
9	BMA	C	1002	11/12	0.83	0.19	-	81,93,99,100	0
9	BMA	C	1001	11/12	0.89	0.17	-	64,70,84,85	0
6	BMA	A	1078	11/12	0.68	0.20	-	116,118,123,125	0
9	NAG	C	1004	14/15	0.90	0.17	-	35,47,60,62	0
5	NAG	C	1008	14/15	0.83	0.22	-	57,71,82,87	0
9	BMA	C	1005	11/12	0.87	0.12	-	61,69,74,76	0
6	NAG	A	1077	14/15	0.82	0.23	-	87,99,117,117	0
5	NAG	A	1080	14/15	0.69	0.26	-	105,117,121,122	0
6	NAG	A	1074	14/15	0.93	0.13	-	52,61,70,88	0
5	NAG	A	1079	14/15	0.81	0.20	-	89,102,111,118	0
6	BMA	A	1075	11/12	0.80	0.17	-	87,95,100,102	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	C	1011	14/15	0.88	0.25	1.23	88,100,105,111	0
4	NAG	C	1009	14/15	0.80	0.20	0.06	87,94,99,104	0
3	ZN	A	1008	1/1	0.99	0.15	-0.88	23,23,23,23	0
7	EDO	C	1962	4/4	0.91	0.12	-1.30	57,61,62,71	0
3	ZN	C	1020	1/1	0.99	0.12	-1.46	39,39,39,39	0
4	NAG	C	1012	14/15	0.62	0.25	-	101,111,116,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	1081	14/15	0.79	0.18	-	88,103,108,112	0
7	EDO	A	1965	4/4	0.91	0.17	-	56,59,61,74	0
4	NAG	A	1070	14/15	0.90	0.13	-	72,85,96,97	0
4	NAG	A	1082	14/15	0.55	0.33	-	83,98,105,106	0
7	EDO	A	1964	4/4	0.72	0.30	-	57,61,62,62	0
4	NAG	C	1006	14/15	0.74	0.20	-	96,107,113,123	0
4	NAG	A	1069	14/15	0.71	0.21	-	84,98,99,101	0
4	NAG	C	1013	14/15	0.57	0.32	-	108,122,126,127	0
4	NAG	C	1010	14/15	0.78	0.29	-	105,115,120,122	0
7	EDO	C	1963	4/4	0.81	0.20	-	89,91,96,99	0
8	MES	A	2002	12/12	0.78	0.14	-	87,98,123,140	0

6.5 Other polymers [i](#)

There are no such residues in this entry.