W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 27, 2014 – 05:14 AM GMT

PDB ID : 3D68
Title : Crystal structure of a T325I/T329I/H333Y/H335Qmutant of Thrombin-Activatable Fibrinolysis Inhibitor (TAFI-IIYQ)
Authors : Brondijk, T.H.C.; Huizinga, E.G.
Deposited on : 2008-05-19
Resolution : 2.80 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Rfree		0.244
Clashscore		13
Ramachandran outliers		2.7%
Sidechain outliers		6.8%
RSRZ outliers		4.8%
	Worse / Better	

∎ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
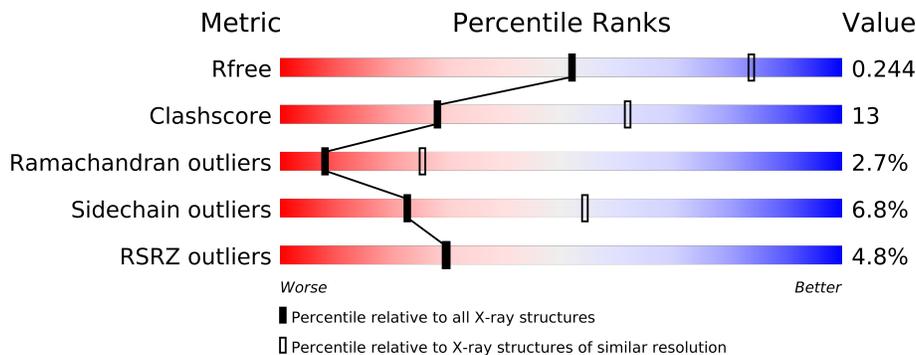
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	424	
1	B	424	
1	C	424	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	C	601	-	X
3	ZN	A	501	-	X
3	ZN	C	501	-	X
4	ARG	A	650	-	X

2   Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9940 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Carboxypeptidase B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total 3249	C 2084	N 552	O 601	S 12	0	0	0
1	B	401	Total 3249	C 2084	N 552	O 601	S 12	0	0	0
1	C	401	Total 3249	C 2084	N 552	O 601	S 12	0	0	0

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLY	-	EXPRESSION TAG	UNP Q96IY4
A	-21	SER	-	EXPRESSION TAG	UNP Q96IY4
A	-20	HIS	-	EXPRESSION TAG	UNP Q96IY4
A	-19	HIS	-	EXPRESSION TAG	UNP Q96IY4
A	-18	HIS	-	EXPRESSION TAG	UNP Q96IY4
A	-17	HIS	-	EXPRESSION TAG	UNP Q96IY4
A	-16	HIS	-	EXPRESSION TAG	UNP Q96IY4
A	-15	HIS	-	EXPRESSION TAG	UNP Q96IY4
A	-14	ASP	-	EXPRESSION TAG	UNP Q96IY4
A	-13	TYR	-	EXPRESSION TAG	UNP Q96IY4
A	-12	ASP	-	EXPRESSION TAG	UNP Q96IY4
A	-11	ILE	-	EXPRESSION TAG	UNP Q96IY4
A	-10	PRO	-	EXPRESSION TAG	UNP Q96IY4
A	-9	SER	-	EXPRESSION TAG	UNP Q96IY4
A	-8	SER	-	EXPRESSION TAG	UNP Q96IY4
A	-7	GLU	-	EXPRESSION TAG	UNP Q96IY4
A	-6	ASN	-	EXPRESSION TAG	UNP Q96IY4
A	-5	LEU	-	EXPRESSION TAG	UNP Q96IY4
A	-4	TYR	-	EXPRESSION TAG	UNP Q96IY4
A	-3	PHE	-	EXPRESSION TAG	UNP Q96IY4
A	-2	GLN	-	EXPRESSION TAG	UNP Q96IY4
A	-1	GLY	-	EXPRESSION TAG	UNP Q96IY4
A	0	SER	-	EXPRESSION TAG	UNP Q96IY4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	EXPRESSION TAG	UNP Q96IY4
A	147	THR	ALA	SEE REMARK 999	UNP Q96IY4
A	325	ILE	THR	ENGINEERED	UNP Q96IY4
A	329	ILE	THR	ENGINEERED	UNP Q96IY4
A	333	TYR	HIS	ENGINEERED	UNP Q96IY4
A	335	GLN	HIS	ENGINEERED	UNP Q96IY4
B	-22	GLY	-	EXPRESSION TAG	UNP Q96IY4
B	-21	SER	-	EXPRESSION TAG	UNP Q96IY4
B	-20	HIS	-	EXPRESSION TAG	UNP Q96IY4
B	-19	HIS	-	EXPRESSION TAG	UNP Q96IY4
B	-18	HIS	-	EXPRESSION TAG	UNP Q96IY4
B	-17	HIS	-	EXPRESSION TAG	UNP Q96IY4
B	-16	HIS	-	EXPRESSION TAG	UNP Q96IY4
B	-15	HIS	-	EXPRESSION TAG	UNP Q96IY4
B	-14	ASP	-	EXPRESSION TAG	UNP Q96IY4
B	-13	TYR	-	EXPRESSION TAG	UNP Q96IY4
B	-12	ASP	-	EXPRESSION TAG	UNP Q96IY4
B	-11	ILE	-	EXPRESSION TAG	UNP Q96IY4
B	-10	PRO	-	EXPRESSION TAG	UNP Q96IY4
B	-9	SER	-	EXPRESSION TAG	UNP Q96IY4
B	-8	SER	-	EXPRESSION TAG	UNP Q96IY4
B	-7	GLU	-	EXPRESSION TAG	UNP Q96IY4
B	-6	ASN	-	EXPRESSION TAG	UNP Q96IY4
B	-5	LEU	-	EXPRESSION TAG	UNP Q96IY4
B	-4	TYR	-	EXPRESSION TAG	UNP Q96IY4
B	-3	PHE	-	EXPRESSION TAG	UNP Q96IY4
B	-2	GLN	-	EXPRESSION TAG	UNP Q96IY4
B	-1	GLY	-	EXPRESSION TAG	UNP Q96IY4
B	0	SER	-	EXPRESSION TAG	UNP Q96IY4
B	1	ALA	-	EXPRESSION TAG	UNP Q96IY4
B	147	THR	ALA	SEE REMARK 999	UNP Q96IY4
B	325	ILE	THR	ENGINEERED	UNP Q96IY4
B	329	ILE	THR	ENGINEERED	UNP Q96IY4
B	333	TYR	HIS	ENGINEERED	UNP Q96IY4
B	335	GLN	HIS	ENGINEERED	UNP Q96IY4
C	-22	GLY	-	EXPRESSION TAG	UNP Q96IY4
C	-21	SER	-	EXPRESSION TAG	UNP Q96IY4
C	-20	HIS	-	EXPRESSION TAG	UNP Q96IY4
C	-19	HIS	-	EXPRESSION TAG	UNP Q96IY4
C	-18	HIS	-	EXPRESSION TAG	UNP Q96IY4
C	-17	HIS	-	EXPRESSION TAG	UNP Q96IY4
C	-16	HIS	-	EXPRESSION TAG	UNP Q96IY4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	HIS	-	EXPRESSION TAG	UNP Q96IY4
C	-14	ASP	-	EXPRESSION TAG	UNP Q96IY4
C	-13	TYR	-	EXPRESSION TAG	UNP Q96IY4
C	-12	ASP	-	EXPRESSION TAG	UNP Q96IY4
C	-11	ILE	-	EXPRESSION TAG	UNP Q96IY4
C	-10	PRO	-	EXPRESSION TAG	UNP Q96IY4
C	-9	SER	-	EXPRESSION TAG	UNP Q96IY4
C	-8	SER	-	EXPRESSION TAG	UNP Q96IY4
C	-7	GLU	-	EXPRESSION TAG	UNP Q96IY4
C	-6	ASN	-	EXPRESSION TAG	UNP Q96IY4
C	-5	LEU	-	EXPRESSION TAG	UNP Q96IY4
C	-4	TYR	-	EXPRESSION TAG	UNP Q96IY4
C	-3	PHE	-	EXPRESSION TAG	UNP Q96IY4
C	-2	GLN	-	EXPRESSION TAG	UNP Q96IY4
C	-1	GLY	-	EXPRESSION TAG	UNP Q96IY4
C	0	SER	-	EXPRESSION TAG	UNP Q96IY4
C	1	ALA	-	EXPRESSION TAG	UNP Q96IY4
C	147	THR	ALA	SEE REMARK 999	UNP Q96IY4
C	325	ILE	THR	ENGINEERED	UNP Q96IY4
C	329	ILE	THR	ENGINEERED	UNP Q96IY4
C	333	TYR	HIS	ENGINEERED	UNP Q96IY4
C	335	GLN	HIS	ENGINEERED	UNP Q96IY4

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
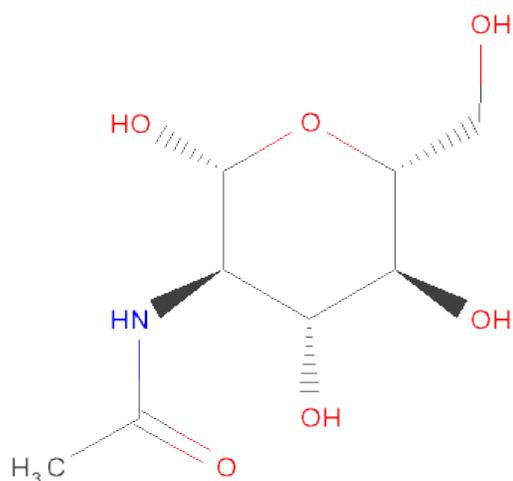
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	C	1	Total 14	C 8	N 1	O 5	0	0
2	C	1	Total 14	C 8	N 1	O 5	0	0
2	C	1	Total 14	C 8	N 1	O 5	0	0

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

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

- Molecule 4 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).
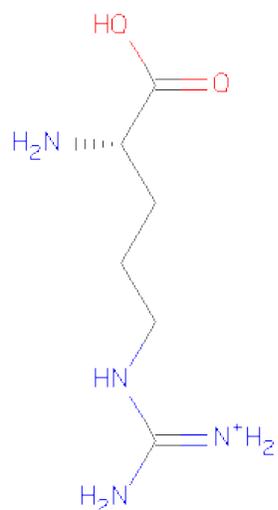
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	6	4	2		
4	B	1	Total	C	N	O	0	0
			12	6	4	2		
4	C	1	Total	C	N	O	0	0
			12	6	4	2		

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: Carboxypeptidase B2

Chain A:
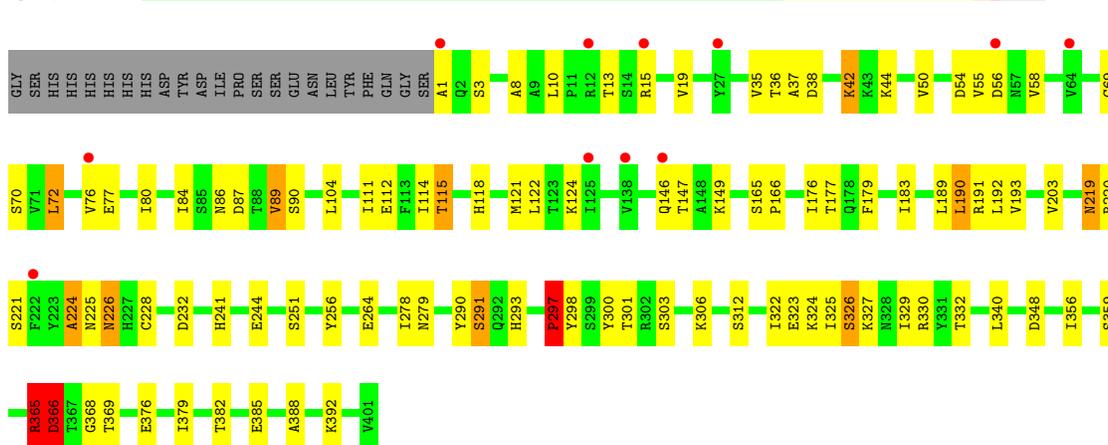
- Molecule 1: Carboxypeptidase B2

Chain B:
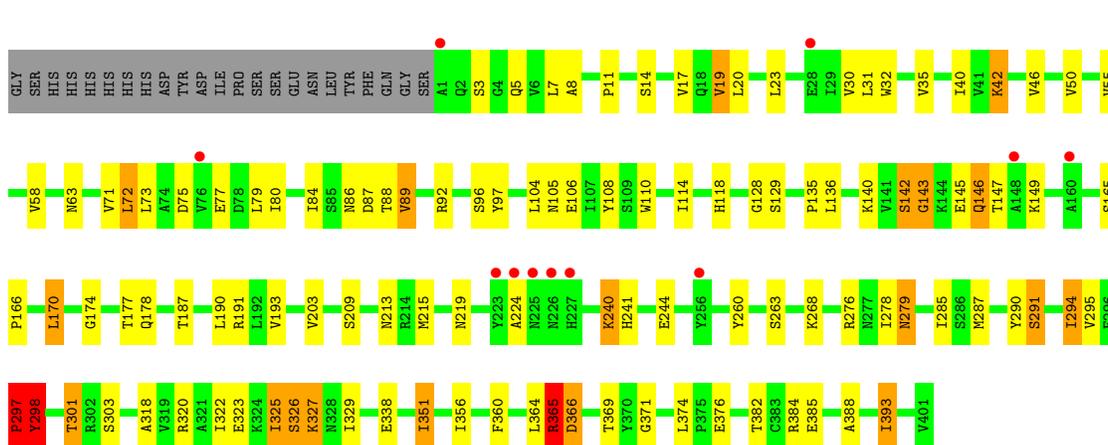
- Molecule 1: Carboxypeptidase B2

Chain C:
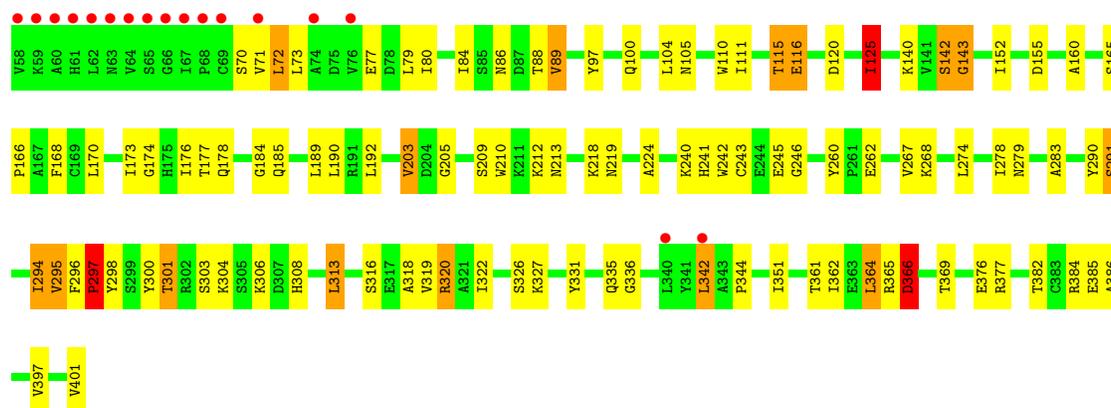
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	159.46Å 159.46Å 139.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.03 – 2.80 49.01 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.03-2.80) 100.0 (49.01-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.232 0.201 , 0.244	Depositor DCC
R_{free} test set	2582 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	69.9	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 71.9	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 50644 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9940	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.87	1/3336 (0.0%)	0.86	2/4532 (0.0%)
1	B	0.92	2/3336 (0.1%)	0.89	7/4532 (0.2%)
1	C	0.88	2/3336 (0.1%)	0.89	4/4532 (0.1%)
All	All	0.89	5/10008 (0.0%)	0.88	13/13596 (0.1%)

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	4
1	B	0	2
1	C	0	5
All	All	0	11

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	338	GLU	CG-CD	8.09	1.64	1.51
1	B	338	GLU	CB-CG	6.94	1.65	1.52
1	C	116	GLU	CG-CD	6.46	1.61	1.51
1	C	97	TYR	CD1-CE1	-5.57	1.30	1.39
1	A	1	ALA	CA-CB	5.33	1.63	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	ASP	N-CA-C	-8.00	89.41	111.00
1	B	297	PRO	CA-C-N	-7.35	101.03	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	125	ILE	CG1-CB-CG2	-7.22	95.52	111.40
1	C	120	ASP	CB-CG-OD1	6.52	124.17	118.30
1	C	366	ASP	CB-CG-OD2	-5.94	112.95	118.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	PRO	Peptide
1	A	326	SER	Peptide
1	A	365	ARG	Peptide
1	A	37	ALA	Peptide
1	B	297	PRO	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3249	0	3167	69	0
1	B	3249	0	3167	95	0
1	C	3249	0	3168	80	0
2	A	56	0	52	4	0
2	B	56	0	52	4	0
2	C	42	0	39	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	12	0	12	3	0
4	B	12	0	12	0	0
4	C	12	0	12	0	0
All	All	9940	0	9681	250	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

The worst 5 of 250 close contacts within the same asymmetric unit are listed below:

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:176:ILE:HG21	1:C:190:LEU:HD11	1.35	1.02
1:A:325:ILE:HD12	1:A:388:ALA:HB2	1.36	1.01
1:B:351:ILE:HD12	1:B:356:ILE:HG12	1.43	0.99
1:B:8:ALA:HB2	1:B:72:LEU:HD21	1.46	0.97
1:A:147:THR:HG23	1:A:149:LYS:NZ	1.82	0.94

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	399/424 (94%)	358 (90%)	31 (8%)	10 (2%)	9	28
1	B	399/424 (94%)	359 (90%)	29 (7%)	11 (3%)	8	24
1	C	399/424 (94%)	366 (92%)	22 (6%)	11 (3%)	8	24
All	All	1197/1272 (94%)	1083 (90%)	82 (7%)	32 (3%)	8	25

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	42	LYS
1	A	89	VAL
1	A	219	ASN
1	A	291	SER

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	354/375 (94%)	336 (95%)	18 (5%)	33	69
1	B	354/375 (94%)	327 (92%)	27 (8%)	19	46
1	C	354/375 (94%)	327 (92%)	27 (8%)	19	46
All	All	1062/1125 (94%)	990 (93%)	72 (7%)	22	54

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	295	VAL
1	B	351	ILE
1	C	316	SER
1	B	297	PRO
1	B	320	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	146	GLN
1	B	279	ASN
1	C	175	HIS
1	B	57	ASN
1	B	100	GLN

5.3.3   RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6   Ligand geometry ⓘ

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
2	NAG	A	601	1	12,14,15	0.70	0	15,19,21	1.45	2 (13%)
2	NAG	A	602	1	12,14,15	0.76	0	15,19,21	0.83	0
2	NAG	A	603	1	12,14,15	1.20	3 (25%)	15,19,21	2.61	6 (40%)
2	NAG	A	604	1	12,14,15	0.68	0	15,19,21	2.21	5 (33%)
4	ARG	A	650	-	11,11,11	0.96	0	13,13,13	2.97	4 (30%)
2	NAG	B	601	1	12,14,15	0.87	1 (8%)	15,19,21	1.20	0
2	NAG	B	602	1	12,14,15	0.81	0	15,19,21	1.65	4 (26%)
2	NAG	B	603	1	12,14,15	0.60	0	15,19,21	1.36	2 (13%)
2	NAG	B	604	1	12,14,15	0.67	0	15,19,21	1.87	5 (33%)
4	ARG	B	650	-	11,11,11	0.77	0	13,13,13	2.51	4 (30%)
2	NAG	C	601	1	12,14,15	0.80	0	15,19,21	1.98	2 (13%)
2	NAG	C	602	1	12,14,15	1.40	2 (16%)	15,19,21	1.77	3 (20%)
2	NAG	C	604	1	12,14,15	0.81	0	15,19,21	1.57	3 (20%)
4	ARG	C	650	-	11,11,11	0.80	0	13,13,13	2.53	4 (30%)

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	NAG	A	601	1	-	0/6/23/26	0/1/1/1
2	NAG	A	602	1	-	0/6/23/26	0/1/1/1
2	NAG	A	603	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	604	1	-	0/6/23/26	0/1/1/1
4	ARG	A	650	-	-	0/11/11/11	0/0/0/0
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1
2	NAG	B	602	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	603	1	-	0/6/23/26	0/1/1/1
2	NAG	B	604	1	-	0/6/23/26	0/1/1/1
4	ARG	B	650	-	-	0/11/11/11	0/0/0/0
2	NAG	C	601	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	602	1	-	0/6/23/26	0/1/1/1
2	NAG	C	604	1	-	0/6/23/26	0/1/1/1
4	ARG	C	650	-	-	0/11/11/11	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)
2	C	602	NAG	C2-N2	3.70	1.50	1.46
2	A	603	NAG	C3-C2	2.26	1.57	1.52
2	A	603	NAG	O5-C5	-2.20	1.41	1.45
2	C	602	NAG	O5-C5	-2.17	1.41	1.45
2	B	601	NAG	O5-C5	-2.11	1.41	1.45

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	650	ARG	C-CA-N	8.45	123.36	109.36
2	A	603	NAG	O5-C5-C4	-7.30	101.39	110.65
4	C	650	ARG	C-CA-N	6.80	120.63	109.36
4	B	650	ARG	C-CA-N	6.69	120.44	109.36
2	A	604	NAG	O5-C5-C6	5.21	112.45	106.98

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	602	NAG	C1
2	A	603	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	NAG	O7-C7-N2-C2

There are no ring outliers.

5.7 Other polymers (i)

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 ⓘ

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, 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	401/424 (94%)	0.15	11 (2%)	52	52	50, 67, 77, 95	0
1	B	401/424 (94%)	0.16	11 (2%)	52	52	51, 67, 81, 96	0
1	C	401/424 (94%)	0.50	36 (8%)	10	8	43, 67, 75, 97	0
All	All	1203/1272 (94%)	0.27	58 (4%)	29	30	43, 67, 77, 97	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	ALA	9.3
1	C	11	PRO	7.5
1	C	64	VAL	6.6
1	A	1	ALA	6.4
1	B	225	ASN	6.0

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3   Carbohydrates ⓘ

There are no carbohydrates in this entry.

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, 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	A	501	1/1	0.27	5.41	71,71,71,71	0
4	ARG	A	650	12/12	0.26	4.13	67,70,74,75	0
3	ZN	C	501	1/1	0.25	2.98	69,69,69,69	0
2	NAG	C	601	14/15	0.45	2.52	75,76,79,80	0
2	NAG	A	603	14/15	0.34	1.77	57,67,69,69	0
2	NAG	B	601	14/15	0.25	1.36	58,63,65,66	0
4	ARG	B	650	12/12	0.26	1.33	72,74,77,78	0
3	ZN	B	501	1/1	0.23	1.26	73,73,73,73	0
2	NAG	A	601	14/15	0.43	1.15	75,76,77,78	0
4	ARG	C	650	12/12	0.27	1.09	65,69,77,80	0
2	NAG	C	604	14/15	0.28	1.03	57,60,64,66	0
2	NAG	B	604	14/15	0.20	0.48	68,72,74,74	0
2	NAG	A	604	14/15	0.19	0.41	58,62,63,63	0
2	NAG	C	602	14/15	0.41	0.24	79,82,84,84	0
2	NAG	A	602	14/15	0.35	0.13	84,86,88,88	0
2	NAG	B	602	14/15	0.26	0.06	73,75,78,79	0
2	NAG	B	603	14/15	0.16	-0.35	66,67,70,71	0

6.5   Other polymers ⓘ

There are no such residues in this entry.