



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:03 AM GMT

PDB ID : 3D68  
Title : Crystal structure of a T325I/T329I/H333Y/H335Q mutant 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)

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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

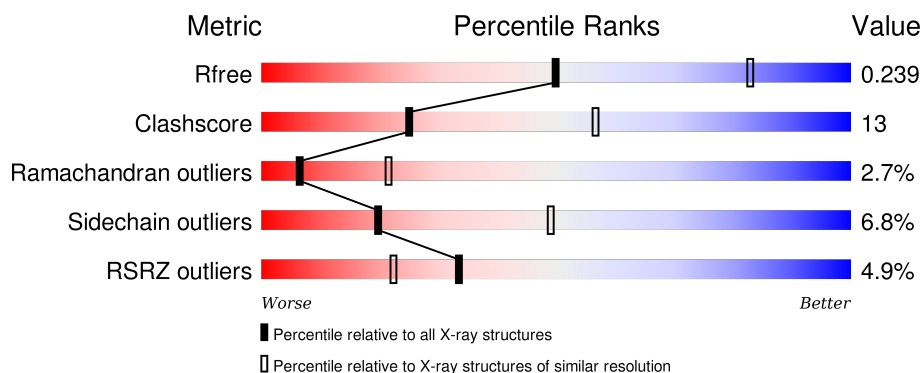
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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  $\geq 3$ , 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	424	<div> <div>3%</div> <div>71%</div> <div>21%</div> <div>• • 5%</div> </div>
1	B	424	<div> <div>2%</div> <div>68%</div> <div>21%</div> <div>• • 5%</div> </div>
1	C	424	<div> <div>9%</div> <div>67%</div> <div>24%</div> <div>• • 5%</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
2	NAG	A	603	X	-	-	-
2	NAG	B	602	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9940 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 Carboxypeptidase B2.

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

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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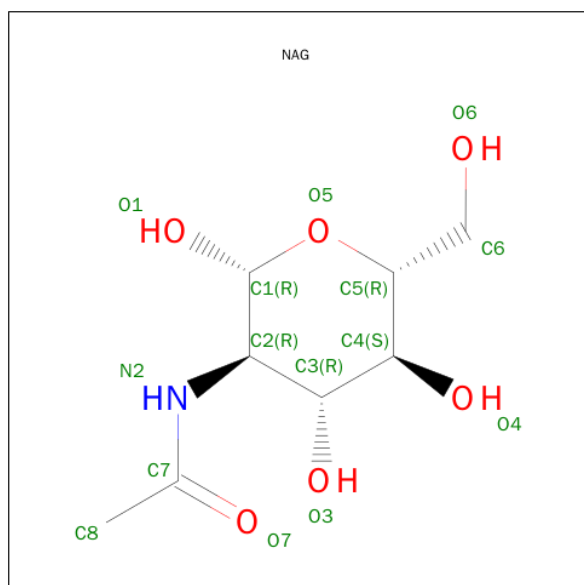
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	EXPRESSION TAG	UNP Q96IY4
A	147	THR	ALA	SEE REMARK 999	UNP Q96IY4
A	325	ILE	THR	ENGINEERED	UNP Q96IY4
A	329	ILE	THR	ENGINEERED	UNP Q96IY4
A	333	TYR	HIS	ENGINEERED	UNP Q96IY4
A	335	GLN	HIS	ENGINEERED	UNP Q96IY4
B	-22	GLY	-	EXPRESSION TAG	UNP Q96IY4
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:  $C_8H_{15}NO_6$ ).

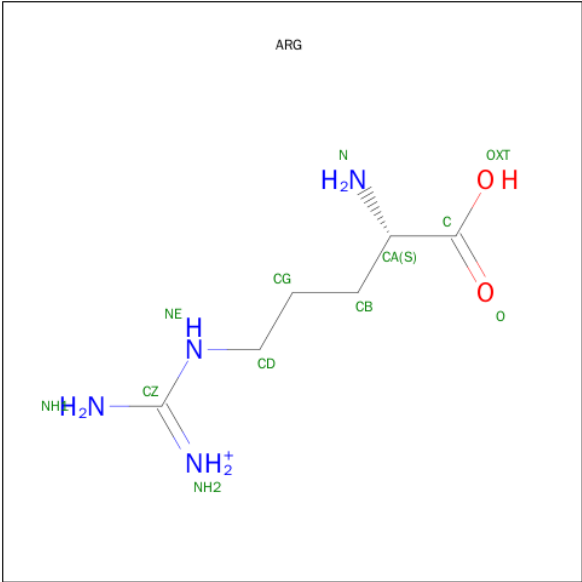


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	C	1	Total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

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

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

- Molecule 4 is ARGININE (three-letter code: ARG) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>4</sub>O<sub>2</sub>).



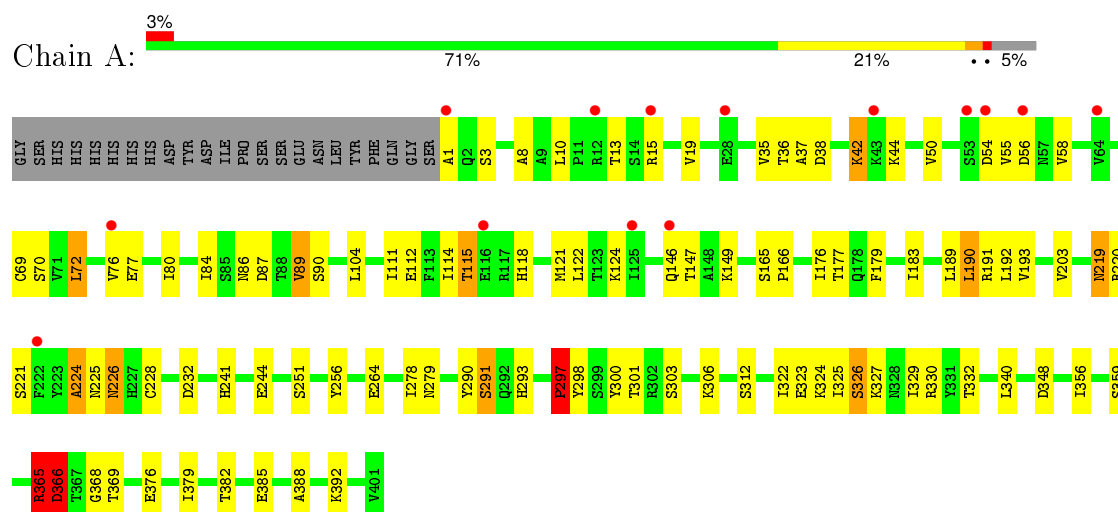
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	6	4	2		
4	B	1	Total	C	N	O	0	0
			12	6	4	2		
4	C	1	Total	C	N	O	0	0
			12	6	4	2		



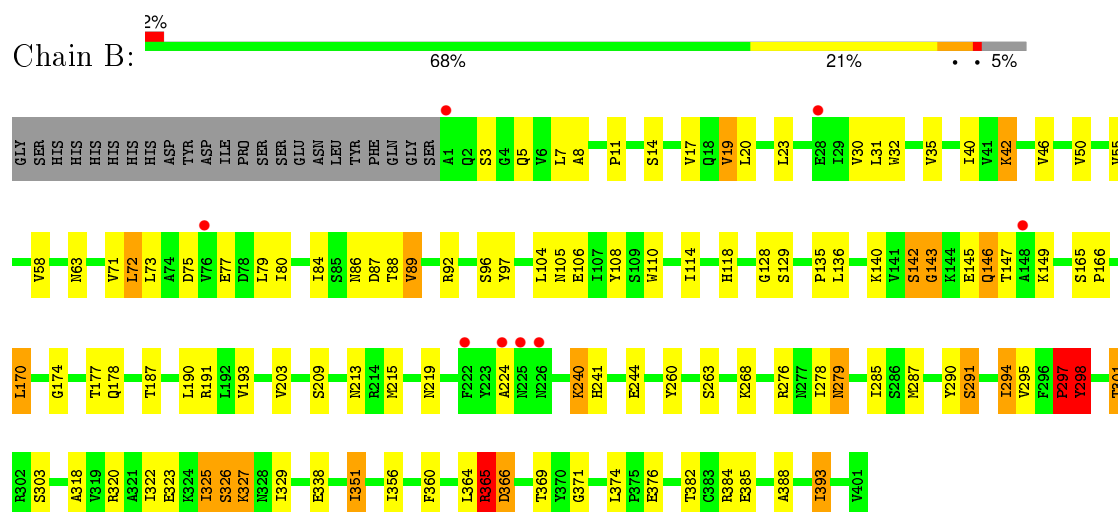
### 3 Residue-property plots [i](#)

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

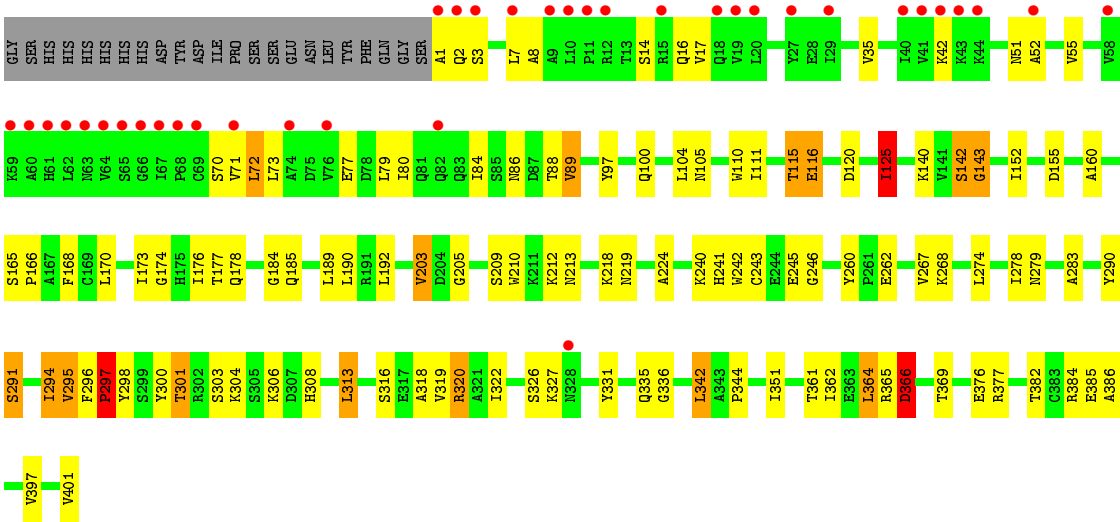


#### • Molecule 1: Carboxypeptidase B2



#### • Molecule 1: Carboxypeptidase B2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.188 , 0.232 0.194 , 0.239	Depositor DCC
$R_{free}$ test set	2582 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.9	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 71.6	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 50644 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9940	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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

### 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

All (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(°)	Ideal(°)
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
1	C	155	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	297	PRO	CA-C-N	-5.69	104.69	117.20
1	B	297	PRO	C-N-CA	5.58	135.65	121.70
1	B	366	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	B	276	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	276	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	298	TYR	CB-CA-C	5.29	120.99	110.40
1	B	365	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (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
1	B	326	SER	Peptide
1	C	218	LYS	Peptide
1	C	297	PRO	Mainchain,Peptide
1	C	326	SER	Peptide
1	C	364	LEU	Peptide

## 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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 13.

All (250) 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: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
1:C:401:VAL:HG12	1:C:401:VAL:OXT	1.66	0.94
1:C:176:ILE:CG2	1:C:190:LEU:HD11	2.01	0.91
1:A:147:THR:HG23	1:A:149:LYS:HZ3	1.37	0.90
1:B:285:ILE:HD11	1:B:393:ILE:HD11	1.57	0.86
1:B:279:ASN:N	1:B:279:ASN:HD22	1.67	0.86
1:A:8:ALA:HB2	1:A:72:LEU:HD22	1.58	0.86
1:A:290:TYR:O	1:A:291:SER:CB	2.23	0.86
1:A:290:TYR:O	1:A:291:SER:HB3	1.74	0.85
1:C:86:ASN:HA	1:C:89:VAL:HG23	1.57	0.84
1:A:325:ILE:CD1	1:A:388:ALA:HB2	2.06	0.84
1:A:8:ALA:HB2	1:A:72:LEU:CD2	2.07	0.84
1:B:351:ILE:HD12	1:B:356:ILE:CG1	2.11	0.81
1:B:32:TRP:HE1	1:B:215:MET:CE	1.95	0.80
1:A:278:ILE:HD12	1:A:356:ILE:HD11	1.61	0.80
1:B:32:TRP:HE1	1:B:215:MET:HE2	1.48	0.79
1:B:140:LYS:NZ	1:B:146:GLN:NE2	2.31	0.79
1:C:142:SER:O	1:C:143:GLY:O	2.03	0.77
1:B:118:HIS:CE1	1:B:177:THR:HG23	2.20	0.75
1:C:7:LEU:HD22	1:C:71:VAL:HG22	1.69	0.75
1:A:80:ILE:HG22	1:A:84:ILE:HD12	1.70	0.73
1:B:326:SER:O	1:B:329:ILE:HG22	1.89	0.72
1:B:285:ILE:CD1	1:B:393:ILE:HD11	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:HD12	1:A:388:ALA:CB	2.15	0.71
1:B:140:LYS:HZ1	1:B:146:GLN:NE2	1.86	0.71
1:A:165:SER:HB3	1:A:166:PRO:HD3	1.73	0.70
1:A:278:ILE:CD1	1:A:356:ILE:HD11	2.22	0.69
1:C:86:ASN:HA	1:C:89:VAL:CG2	2.23	0.68
1:B:279:ASN:N	1:B:279:ASN:ND2	2.41	0.68
1:C:401:VAL:OXT	1:C:401:VAL:CG1	2.34	0.67
1:B:285:ILE:HD11	1:B:393:ILE:CD1	2.25	0.67
2:A:603:NAG:O3	2:A:603:NAG:H83	1.95	0.67
1:A:306:LYS:HG3	1:A:306:LYS:O	1.94	0.66
1:C:300:TYR:CD1	1:C:301:THR:HG22	2.31	0.65
1:A:297:PRO:HD3	1:A:359:SER:O	1.96	0.65
1:B:294:ILE:HD11	1:B:318:ALA:HB3	1.79	0.65
1:B:75:ASP:O	1:B:79:LEU:HD12	1.96	0.65
1:C:176:ILE:CG2	1:C:190:LEU:CD1	2.75	0.65
1:A:118:HIS:CE1	1:A:177:THR:HG23	2.32	0.65
1:A:300:TYR:CD2	1:A:301:THR:HG23	2.32	0.65
1:B:351:ILE:CD1	1:B:356:ILE:HG12	2.23	0.64
1:B:118:HIS:NE2	1:B:177:THR:HG23	2.13	0.64
1:C:397:VAL:HG13	1:C:401:VAL:HG21	1.79	0.62
1:C:295:VAL:HG12	1:C:361:THR:HB	1.81	0.62
1:A:80:ILE:CG2	1:A:84:ILE:HD12	2.29	0.62
1:B:32:TRP:NE1	1:B:215:MET:CE	2.62	0.62
1:C:322:ILE:HG23	1:C:385:GLU:HB2	1.81	0.61
1:B:142:SER:O	1:B:143:GLY:O	2.18	0.61
2:A:604:NAG:H82	2:A:604:NAG:O3	2.00	0.61
1:A:226:ASN:OD1	1:A:226:ASN:N	2.33	0.61
1:C:88:THR:O	1:C:88:THR:HG22	2.01	0.61
1:C:111:ILE:O	1:C:115:THR:HB	2.00	0.61
1:A:300:TYR:HD2	1:A:301:THR:HG23	1.66	0.60
1:C:262:GLU:HG2	1:C:267:VAL:HG12	1.83	0.60
1:B:63:ASN:HA	2:B:603:NAG:H82	1.82	0.60
1:B:8:ALA:HB2	1:B:72:LEU:CD2	2.27	0.60
2:A:603:NAG:C8	2:A:603:NAG:O3	2.50	0.60
1:C:176:ILE:HG21	1:C:190:LEU:CD1	2.21	0.60
1:C:274:LEU:HD13	1:C:351:ILE:HD12	1.82	0.60
1:B:7:LEU:CD2	1:B:71:VAL:HG22	2.33	0.59
1:B:360:PHE:CD2	1:B:393:ILE:HD12	2.37	0.59
1:B:325:ILE:HD12	1:B:388:ALA:HB2	1.84	0.59
1:C:320:ARG:CG	1:C:320:ARG:HH11	2.16	0.59
1:C:320:ARG:HG2	1:C:320:ARG:HH11	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ALA:HB2	1:A:72:LEU:HD21	1.84	0.58
1:B:140:LYS:NZ	1:B:146:GLN:HE22	1.99	0.58
1:C:84:ILE:O	1:C:84:ILE:HG22	2.03	0.58
1:C:209:SER:HA	1:C:213:ASN:O	2.04	0.58
1:A:179:PHE:CD1	1:A:183:ILE:HD12	2.38	0.58
1:A:147:THR:HG23	1:A:149:LYS:HZ1	1.64	0.57
1:B:23:LEU:HD21	1:B:58:VAL:HG13	1.85	0.57
1:B:290:TYR:O	1:B:291:SER:OG	2.21	0.57
1:B:278:ILE:CG2	1:B:279:ASN:ND2	2.67	0.57
1:A:149:LYS:HE3	1:A:191:ARG:O	2.04	0.56
1:B:11:PRO:O	1:B:42:LYS:O	2.23	0.56
1:B:279:ASN:HD22	1:B:279:ASN:H	1.53	0.56
1:B:215:MET:HE3	1:B:215:MET:HA	1.88	0.56
1:B:290:TYR:O	1:B:291:SER:CB	2.54	0.56
1:C:86:ASN:ND2	1:C:89:VAL:HG21	2.21	0.56
1:C:294:ILE:HG22	1:C:362:ILE:HG23	1.87	0.56
1:B:87:ASP:O	1:B:88:THR:HB	2.07	0.55
1:B:97:TYR:OH	1:B:106:GLU:HG3	2.06	0.55
1:A:147:THR:CG2	1:A:149:LYS:NZ	2.65	0.55
1:C:365:ARG:HD3	1:C:382:THR:OG1	2.07	0.55
1:C:1:ALA:CB	2:C:602:NAG:H82	2.36	0.55
1:A:121:MET:HE1	1:A:176:ILE:HG22	1.89	0.55
1:A:89:VAL:HG12	1:A:90:SER:N	2.21	0.54
1:C:110:TRP:CZ3	1:C:170:LEU:HD22	2.41	0.54
1:B:17:VAL:HG22	1:B:40:ILE:HG22	1.88	0.54
1:A:112:GLU:OE2	1:A:124:LYS:NZ	2.38	0.54
1:A:111:ILE:O	1:A:115:THR:HB	2.08	0.54
1:C:397:VAL:HG13	1:C:401:VAL:CG2	2.37	0.54
4:A:650:ARG:HG2	4:A:650:ARG:O	2.08	0.54
1:B:128:GLY:C	1:B:136:LEU:HD12	2.29	0.54
1:C:174:GLY:O	1:C:178:GLN:HG3	2.08	0.53
1:B:50:VAL:HG11	1:B:55:VAL:HA	1.90	0.53
1:C:173:ILE:O	1:C:177:THR:HG23	2.08	0.53
1:B:366:ASP:HB2	1:B:374:LEU:HD13	1.90	0.53
1:C:295:VAL:HG21	1:C:336:GLY:HA2	1.91	0.53
1:B:32:TRP:NE1	1:B:215:MET:HE1	2.23	0.53
1:B:351:ILE:HG23	1:B:356:ILE:HB	1.90	0.52
1:C:365:ARG:CG	1:C:366:ASP:H	2.22	0.52
1:C:1:ALA:HB2	2:C:602:NAG:H82	1.91	0.52
1:B:278:ILE:HG23	1:B:279:ASN:ND2	2.24	0.52
1:B:146:GLN:HA	1:B:149:LYS:HZ3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ALA:O	1:C:55:VAL:HG23	2.09	0.52
1:C:8:ALA:HB2	1:C:72:LEU:HD22	1.92	0.52
1:C:51:ASN:O	1:C:55:VAL:HG23	2.09	0.52
1:C:242:TRP:CH2	1:C:260:TYR:HA	2.44	0.52
1:B:118:HIS:NE2	1:B:177:THR:CG2	2.73	0.52
1:B:129:SER:N	1:B:136:LEU:HD12	2.25	0.52
1:A:54:ASP:O	1:A:58:VAL:HG23	2.09	0.51
1:B:366:ASP:OD2	1:B:371:GLY:N	2.39	0.51
1:B:241:HIS:HB3	1:B:244:GLU:OE1	2.11	0.51
1:B:32:TRP:NE1	1:B:215:MET:HE2	2.19	0.51
1:B:365:ARG:HB2	1:B:382:THR:HG23	1.92	0.51
2:C:601:NAG:O3	2:C:601:NAG:H83	2.11	0.51
1:B:165:SER:HB3	1:B:166:PRO:HD3	1.91	0.51
1:B:285:ILE:CD1	1:B:393:ILE:CD1	2.86	0.51
1:A:293:HIS:HA	1:A:332:THR:O	2.11	0.51
1:C:290:TYR:O	1:C:291:SER:CB	2.58	0.51
1:B:108:TYR:OH	1:B:135:PRO:O	2.17	0.50
1:C:295:VAL:CG2	1:C:336:GLY:HA2	2.40	0.50
1:A:291:SER:OG	1:A:293:HIS:CD2	2.65	0.50
1:B:72:LEU:O	1:B:73:LEU:HD23	2.12	0.50
1:B:145:GLU:O	1:B:146:GLN:C	2.49	0.49
1:C:84:ILE:HG23	1:C:210:TRP:CZ3	2.47	0.49
1:B:140:LYS:HZ3	1:B:146:GLN:HE22	1.60	0.49
1:C:7:LEU:CD2	1:C:71:VAL:HG22	2.39	0.49
1:B:3:SER:CB	1:B:77:GLU:HB2	2.42	0.49
1:A:35:VAL:HG13	1:A:36:THR:HG23	1.94	0.49
1:B:140:LYS:HZ3	1:B:146:GLN:NE2	2.09	0.49
1:B:298:TYR:HB3	1:B:301:THR:HG23	1.94	0.49
1:B:278:ILE:HG22	1:B:279:ASN:ND2	2.28	0.49
1:B:104:LEU:HD21	1:B:203:VAL:HG13	1.94	0.49
2:C:604:NAG:H82	2:C:604:NAG:O3	2.13	0.49
1:B:3:SER:HB2	1:B:77:GLU:HB2	1.95	0.49
1:C:320:ARG:HG2	1:C:320:ARG:NH1	2.28	0.48
1:A:224:ALA:HB1	1:A:225:ASN:OD1	2.13	0.48
1:A:118:HIS:NE2	1:A:177:THR:CG2	2.77	0.48
1:C:72:LEU:O	1:C:73:LEU:HD23	2.13	0.48
1:C:104:LEU:HD11	1:C:203:VAL:HG22	1.96	0.48
1:A:192:LEU:HD22	1:C:192:LEU:HD21	1.96	0.48
1:B:209:SER:HA	1:B:213:ASN:O	2.13	0.48
1:A:326:SER:OG	1:A:385:GLU:OE1	2.29	0.48
1:B:356:ILE:N	1:B:356:ILE:HD13	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:TRP:CZ3	1:B:170:LEU:HD22	2.49	0.47
1:B:382:THR:O	1:B:385:GLU:HG2	2.14	0.47
1:C:246:GLY:HA3	1:C:342:LEU:O	2.14	0.47
1:B:63:ASN:HA	2:B:603:NAG:C8	2.45	0.47
1:C:279:ASN:N	1:C:279:ASN:HD22	2.12	0.47
1:A:279:ASN:H	1:A:279:ASN:HD22	1.61	0.47
1:C:304:LYS:HD3	1:C:308:HIS:CD2	2.50	0.47
1:B:92:ARG:NH1	1:B:106:GLU:OE2	2.48	0.47
1:A:322:ILE:HG23	1:A:385:GLU:HB2	1.96	0.46
1:C:290:TYR:O	1:C:291:SER:HB2	2.15	0.46
1:A:42:LYS:O	1:A:44:LYS:N	2.45	0.46
1:A:104:LEU:CD2	1:A:203:VAL:HG13	2.46	0.46
1:C:240:LYS:O	1:C:241:HIS:HB2	2.16	0.46
1:B:240:LYS:O	1:B:241:HIS:CG	2.69	0.46
1:C:160:ALA:HB1	1:C:205:GLY:O	2.16	0.46
1:B:142:SER:O	1:B:190:LEU:HD13	2.16	0.46
1:C:278:ILE:HG23	1:C:279:ASN:ND2	2.31	0.46
1:A:118:HIS:CE1	1:A:177:THR:CG2	2.99	0.45
1:C:319:VAL:HG22	1:C:331:TYR:HB2	1.98	0.45
1:B:294:ILE:HD13	1:B:294:ILE:HG21	1.56	0.45
2:B:604:NAG:H82	2:B:604:NAG:O3	2.17	0.45
1:B:32:TRP:CZ2	1:B:215:MET:HE1	2.52	0.45
1:C:152:ILE:HG23	1:C:283:ALA:HB3	1.97	0.45
1:C:262:GLU:HB3	1:C:268:LYS:HD2	1.98	0.45
1:C:300:TYR:CE1	1:C:301:THR:HG22	2.51	0.45
1:B:285:ILE:CG1	1:B:393:ILE:HD11	2.46	0.45
1:A:8:ALA:CB	1:A:72:LEU:HD22	2.37	0.44
1:B:31:LEU:HD23	1:B:31:LEU:HA	1.66	0.44
1:A:241:HIS:HB3	1:A:244:GLU:OE1	2.17	0.44
1:C:303:SER:O	1:C:335:GLN:NE2	2.44	0.44
1:B:40:ILE:HG12	1:B:46:VAL:CG2	2.47	0.44
1:C:245:GLU:O	1:C:344:PRO:HD3	2.17	0.44
1:B:174:GLY:O	1:B:178:GLN:HB2	2.18	0.44
1:C:142:SER:C	1:C:143:GLY:O	2.55	0.44
1:B:19:VAL:HG12	1:B:20:LEU:N	2.33	0.44
1:B:80:ILE:HG22	1:B:84:ILE:HD12	1.99	0.44
1:B:32:TRP:CE2	1:B:215:MET:HE1	2.52	0.44
1:A:189:LEU:O	1:A:193:VAL:HG12	2.18	0.44
1:C:1:ALA:HB2	2:C:602:NAG:C8	2.48	0.43
1:A:3:SER:HB3	1:A:77:GLU:HB2	2.00	0.43
1:C:168:PHE:CE1	1:C:386:ALA:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:THR:O	1:B:191:ARG:HB2	2.18	0.43
1:B:322:ILE:HG23	1:B:385:GLU:HB2	1.99	0.43
1:C:80:ILE:HG22	1:C:84:ILE:HD11	2.01	0.43
1:C:51:ASN:O	1:C:55:VAL:CG2	2.67	0.43
1:B:376:GLU:CD	2:B:604:NAG:H83	2.38	0.43
1:A:232:ASP:C	1:A:232:ASP:OD1	2.56	0.43
1:B:287:MET:CE	1:B:364:LEU:HD21	2.48	0.43
1:A:365:ARG:HD2	1:A:385:GLU:OE2	2.19	0.43
1:B:30:VAL:HG11	1:B:215:MET:HB3	2.01	0.43
1:C:278:ILE:CG2	1:C:279:ASN:ND2	2.82	0.43
1:C:294:ILE:HD11	1:C:318:ALA:HB3	2.00	0.43
1:C:327:LYS:NZ	1:C:365:ARG:HH22	2.16	0.43
1:C:1:ALA:CB	2:C:602:NAG:C8	2.97	0.43
1:B:5:GLN:NE2	1:B:55:VAL:HG11	2.34	0.43
1:B:86:ASN:HA	1:B:89:VAL:HG23	2.01	0.42
1:A:165:SER:CB	1:A:166:PRO:HD3	2.47	0.42
1:B:260:TYR:O	1:B:263:SER:HB3	2.19	0.42
1:C:16:GLN:O	1:C:17:VAL:C	2.57	0.42
1:A:147:THR:CG2	1:A:149:LYS:HZ1	2.29	0.42
1:C:165:SER:HB3	1:C:166:PRO:HD3	2.00	0.42
1:A:226:ASN:HB2	1:A:251:SER:CB	2.50	0.42
1:B:88:THR:O	1:B:88:THR:CG2	2.66	0.42
1:A:348:ASP:CG	4:A:650:ARG:HH12	2.23	0.42
1:B:20:LEU:HA	1:B:20:LEU:HD23	1.78	0.42
1:C:184:GLY:O	1:C:185:GLN:C	2.56	0.42
1:A:114:ILE:HG23	1:A:122:LEU:HD12	2.01	0.42
1:B:142:SER:C	1:B:143:GLY:O	2.57	0.42
1:A:228:CYS:HB2	1:A:251:SER:OG	2.19	0.42
1:A:365:ARG:HD3	1:A:382:THR:OG1	2.19	0.42
1:B:325:ILE:HG21	1:B:385:GLU:HA	2.02	0.42
1:C:84:ILE:O	1:C:84:ILE:CG2	2.65	0.42
1:B:40:ILE:HG12	1:B:46:VAL:HG21	2.02	0.42
1:A:76:VAL:O	1:A:77:GLU:C	2.57	0.42
2:A:604:NAG:C7	2:A:604:NAG:O3	2.68	0.42
1:C:279:ASN:N	1:C:279:ASN:ND2	2.68	0.42
1:C:125:ILE:HD11	1:C:140:LYS:HB2	2.02	0.42
1:C:86:ASN:CG	1:C:89:VAL:HG21	2.40	0.41
1:B:365:ARG:CG	1:B:366:ASP:H	2.33	0.41
1:C:376:GLU:OE1	2:C:604:NAG:H83	2.19	0.41
1:A:190:LEU:HA	1:A:190:LEU:HD23	1.88	0.41
1:A:219:ASN:ND2	1:A:264:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:GLY:O	1:A:369:THR:C	2.58	0.41
1:A:376:GLU:HA	1:A:379:ILE:HG13	2.03	0.41
1:B:393:ILE:HD13	1:B:393:ILE:HG21	1.68	0.41
1:A:290:TYR:O	1:A:291:SER:HB2	2.14	0.41
1:A:86:ASN:HA	1:A:89:VAL:HG23	2.03	0.41
1:C:320:ARG:HH11	1:C:320:ARG:HB3	1.85	0.41
1:A:324:LYS:HE2	1:C:313:LEU:HD11	2.02	0.41
1:A:87:ASP:OD1	1:A:87:ASP:C	2.59	0.41
1:A:366:ASP:OD2	1:A:369:THR:N	2.54	0.41
1:A:15:ARG:O	1:A:19:VAL:HG23	2.21	0.41
1:B:326:SER:OG	1:B:385:GLU:OE1	2.35	0.41
1:C:80:ILE:HG22	1:C:84:ILE:CD1	2.51	0.41
1:C:296:PHE:HB2	1:C:297:PRO:HD2	2.03	0.40
1:C:2:GLN:O	1:C:77:GLU:HB2	2.21	0.40
1:B:7:LEU:HD22	1:B:71:VAL:HG22	2.01	0.40
1:A:251:SER:HA	1:A:256:TYR:CG	2.56	0.40
1:A:340:LEU:HD13	4:A:650:ARG:HD3	2.04	0.40
1:A:50:VAL:HG11	1:A:55:VAL:HA	2.03	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	399/424 (94%)	358 (90%)	31 (8%)	10 (2%)	7	24
1	B	399/424 (94%)	359 (90%)	29 (7%)	11 (3%)	6	21
1	C	399/424 (94%)	366 (92%)	22 (6%)	11 (3%)	6	21
All	All	1197/1272 (94%)	1083 (90%)	82 (7%)	32 (3%)	6	21

All (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
1	B	89	VAL
1	B	143	GLY
1	B	219	ASN
1	B	291	SER
1	C	143	GLY
1	C	219	ASN
1	C	291	SER
1	C	297	PRO
1	A	224	ALA
1	B	42	LYS
1	B	146	GLN
1	B	224	ALA
1	C	42	LYS
1	C	89	VAL
1	C	224	ALA
1	C	298	TYR
1	B	327	LYS
1	A	146	GLN
1	A	327	LYS
1	C	142	SER
1	A	366	ASP
1	B	142	SER
1	B	298	TYR
1	C	364	LEU
1	C	366	ASP
1	A	298	TYR
1	B	297	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	354/375 (94%)	336 (95%)	18 (5%)	29	63
1	B	354/375 (94%)	327 (92%)	27 (8%)	16	42
1	C	354/375 (94%)	327 (92%)	27 (8%)	16	42
All	All	1062/1125 (94%)	990 (93%)	72 (7%)	20	49

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	13	THR
1	A	56	ASP
1	A	69	CYS
1	A	70	SER
1	A	72	LEU
1	A	115	THR
1	A	190	LEU
1	A	220	ARG
1	A	221	SER
1	A	226	ASN
1	A	303	SER
1	A	312	SER
1	A	323	GLU
1	A	329	ILE
1	A	330	ARG
1	A	365	ARG
1	A	392	LYS
1	B	14	SER
1	B	19	VAL
1	B	35	VAL
1	B	72	LEU
1	B	96	SER
1	B	105	ASN
1	B	114	ILE
1	B	147	THR
1	B	170	LEU
1	B	193	VAL
1	B	240	LYS
1	B	268	LYS
1	B	279	ASN
1	B	294	ILE
1	B	295	VAL
1	B	297	PRO

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Mol	Chain	Res	Type
1	B	301	THR
1	B	303	SER
1	B	320	ARG
1	B	323	GLU
1	B	325	ILE
1	B	327	LYS
1	B	351	ILE
1	B	365	ARG
1	B	369	THR
1	B	384	ARG
1	B	393	ILE
1	C	3	SER
1	C	14	SER
1	C	35	VAL
1	C	70	SER
1	C	72	LEU
1	C	79	LEU
1	C	100	GLN
1	C	105	ASN
1	C	115	THR
1	C	116	GLU
1	C	125	ILE
1	C	189	LEU
1	C	203	VAL
1	C	212	LYS
1	C	243	CYS
1	C	294	ILE
1	C	295	VAL
1	C	297	PRO
1	C	301	THR
1	C	306	LYS
1	C	313	LEU
1	C	316	SER
1	C	320	ARG
1	C	342	LEU
1	C	369	THR
1	C	377	ARG
1	C	384	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	100	GLN
1	A	185	GLN
1	A	279	ASN
1	A	293	HIS
1	B	45	GLN
1	B	57	ASN
1	B	100	GLN
1	B	146	GLN
1	B	279	ASN
1	B	280	GLN
1	B	293	HIS
1	B	400	ASN
1	C	100	GLN
1	C	175	HIS
1	C	226	ASN
1	C	279	ASN
1	C	400	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 for Mogul analysis.

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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	601	1	14,14,15	0.95	1 (7%)	15,19,21	2.63	2 (13%)
2	NAG	A	602	1	14,14,15	0.64	0	15,19,21	1.09	1 (6%)
2	NAG	A	603	1	14,14,15	1.58	2 (14%)	15,19,21	1.68	4 (26%)
2	NAG	A	604	1	14,14,15	0.79	0	15,19,21	2.19	6 (40%)
4	ARG	A	650	-	5,11,11	1.07	0	3,13,13	1.08	0
2	NAG	B	601	1	14,14,15	0.66	0	15,19,21	1.92	1 (6%)
2	NAG	B	602	1	14,14,15	0.71	0	15,19,21	1.97	4 (26%)
2	NAG	B	603	1	14,14,15	0.63	0	15,19,21	2.12	2 (13%)
2	NAG	B	604	1	14,14,15	0.76	0	15,19,21	2.05	4 (26%)
4	ARG	B	650	-	5,11,11	0.67	0	3,13,13	0.68	0
2	NAG	C	601	1	14,14,15	0.92	1 (7%)	15,19,21	3.16	2 (13%)
2	NAG	C	602	1	14,14,15	1.48	2 (14%)	15,19,21	2.52	3 (20%)
2	NAG	C	604	1	14,14,15	0.71	0	15,19,21	1.74	4 (26%)
4	ARG	C	650	-	5,11,11	0.68	0	3,13,13	0.91	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	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	-	-	0/5/11/11	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	-	-	0/5/11/11	0/0/0/0
2	NAG	C	601	1	-	1/6/23/26	0/1/1/1
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	-	-	0/5/11/11	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	NAG	C3-C2	2.09	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAG	C1-C2	2.42	1.55	1.52
2	C	602	NAG	C2-N2	2.45	1.50	1.46
2	A	601	NAG	C1-C2	3.17	1.56	1.52
2	C	602	NAG	C1-C2	4.21	1.58	1.52
2	A	603	NAG	C1-C2	4.74	1.59	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	604	NAG	C3-C4-C5	-3.80	103.57	110.20
2	A	604	NAG	C4-C3-C2	-3.77	105.37	111.23
2	B	604	NAG	C3-C4-C5	-3.64	103.86	110.20
2	C	602	NAG	O7-C7-C8	-3.19	116.21	122.06
2	A	603	NAG	O7-C7-C8	-3.13	116.33	122.06
2	C	604	NAG	C3-C4-C5	-2.92	105.10	110.20
2	B	602	NAG	O7-C7-N2	-2.77	116.23	121.86
2	B	602	NAG	C3-C4-C5	-2.76	105.39	110.20
2	A	604	NAG	C2-N2-C7	-2.22	120.18	123.04
2	C	601	NAG	O3-C3-C2	2.01	113.10	109.11
2	C	604	NAG	C8-C7-N2	2.23	120.36	116.11
2	A	603	NAG	C4-C3-C2	2.25	114.72	111.23
2	B	603	NAG	C8-C7-N2	2.34	120.59	116.11
2	A	604	NAG	O5-C5-C6	2.35	112.45	107.35
2	A	603	NAG	O3-C3-C2	2.45	113.97	109.11
2	B	604	NAG	O4-C4-C5	2.47	115.79	109.24
2	A	604	NAG	O4-C4-C5	2.47	115.80	109.24
2	A	601	NAG	C2-N2-C7	2.57	126.34	123.04
2	A	603	NAG	C8-C7-N2	3.03	121.90	116.11
2	C	604	NAG	C1-O5-C5	3.06	116.13	112.25
2	B	604	NAG	O4-C4-C3	3.11	117.33	110.34
2	C	604	NAG	O4-C4-C3	3.14	117.40	110.34
2	A	602	NAG	C1-O5-C5	3.19	116.30	112.25
2	B	602	NAG	C8-C7-N2	3.43	122.67	116.11
2	B	604	NAG	C1-O5-C5	4.02	117.34	112.25
2	A	604	NAG	C1-O5-C5	4.24	117.63	112.25
2	C	602	NAG	C2-N2-C7	4.58	128.92	123.04
2	B	602	NAG	C1-O5-C5	4.72	118.24	112.25
2	B	601	NAG	C1-O5-C5	5.63	119.39	112.25
2	B	603	NAG	C1-O5-C5	7.04	121.19	112.25
2	C	602	NAG	C1-O5-C5	7.39	121.62	112.25
2	A	601	NAG	C1-O5-C5	9.29	124.04	112.25
2	C	601	NAG	C1-O5-C5	11.31	126.61	112.25

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.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	NAG	2	0
2	A	604	NAG	2	0
4	A	650	ARG	3	0
2	B	603	NAG	2	0
2	B	604	NAG	2	0
2	C	601	NAG	1	0
2	C	602	NAG	4	0
2	C	604	NAG	2	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	401/424 (94%)	0.25	14 (3%) 48 35	50, 67, 77, 95	0
1	B	401/424 (94%)	0.20	8 (1%) 68 58	51, 67, 81, 96	0
1	C	401/424 (94%)	0.57	37 (9%) 11 5	43, 67, 75, 97	0
All	All	1203/1272 (94%)	0.34	59 (4%) 33 22	43, 67, 77, 97	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	ALA	8.6
1	C	11	PRO	6.4
1	B	225	ASN	5.6
1	C	64	VAL	5.4
1	C	68	PRO	5.3
1	C	67	ILE	5.2
1	C	9	ALA	4.9
1	A	1	ALA	4.2
1	C	12	ARG	4.0
1	C	10	LEU	3.9
1	A	222	PHE	3.7
1	C	2	GLN	3.7
1	B	1	ALA	3.7
1	C	43	LYS	3.7
1	B	224	ALA	3.6
1	C	19	VAL	3.5
1	C	58	VAL	3.5
1	C	62	LEU	3.4
1	C	76	VAL	3.3
1	C	65	SER	3.2
1	B	226	ASN	3.2
1	A	15	ARG	3.1
1	C	61	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	60	ALA	3.0
1	C	63	ASN	2.9
1	C	74	ALA	2.9
1	C	44	LYS	2.9
1	C	66	GLY	2.8
1	B	148	ALA	2.8
1	C	15	ARG	2.8
1	C	41	VAL	2.7
1	B	76	VAL	2.7
1	C	27	TYR	2.7
1	C	40	ILE	2.7
1	C	3	SER	2.7
1	C	18	GLN	2.6
1	C	20	LEU	2.5
1	A	12	ARG	2.5
1	C	42	LYS	2.5
1	C	7	LEU	2.5
1	A	56	ASP	2.5
1	C	328	ASN	2.4
1	A	43	LYS	2.4
1	C	52	ALA	2.4
1	A	116	GLU	2.3
1	A	76	VAL	2.3
1	C	71	VAL	2.3
1	C	69	CYS	2.3
1	B	28	GLU	2.3
1	B	222	PHE	2.2
1	A	146	GLN	2.2
1	C	29	ILE	2.2
1	A	54	ASP	2.2
1	A	53	SER	2.1
1	A	28	GLU	2.1
1	C	59	LYS	2.1
1	A	125	ILE	2.1
1	A	64	VAL	2.1
1	C	82	GLN	2.1

## 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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å <sup>2</sup> )	Q<0.9
4	ARG	B	650	12/12	0.87	0.25	1.24	72,74,77,78	0
4	ARG	C	650	12/12	0.82	0.23	0.61	65,69,77,80	0
2	NAG	B	601	14/15	0.87	0.21	0.32	58,63,65,66	0
2	NAG	A	602	14/15	0.93	0.37	0.29	84,86,88,88	0
2	NAG	C	602	14/15	0.80	0.39	0.02	79,82,84,84	0
2	NAG	C	604	14/15	0.87	0.25	-0.04	57,60,64,66	0
2	NAG	B	602	14/15	0.87	0.27	-0.16	73,75,78,79	0
4	ARG	A	650	12/12	0.85	0.19	-0.74	67,70,74,75	0
2	NAG	B	604	14/15	0.89	0.16	-	68,72,74,74	0
2	NAG	B	603	14/15	0.85	0.14	-	66,67,70,71	0
3	ZN	C	501	1/1	0.98	0.21	-	69,69,69,69	0
2	NAG	C	601	14/15	0.62	0.44	-	75,76,79,80	0
2	NAG	A	601	14/15	0.84	0.41	-	75,76,77,78	0
2	NAG	A	603	14/15	0.82	0.29	-	57,67,69,69	0
3	ZN	A	501	1/1	0.98	0.20	-	71,71,71,71	0
3	ZN	B	501	1/1	0.98	0.18	-	73,73,73,73	0
2	NAG	A	604	14/15	0.87	0.17	-	58,62,63,63	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.