



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:21 PM UTC

PDB ID : 3D68 / pdb_00003d68
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

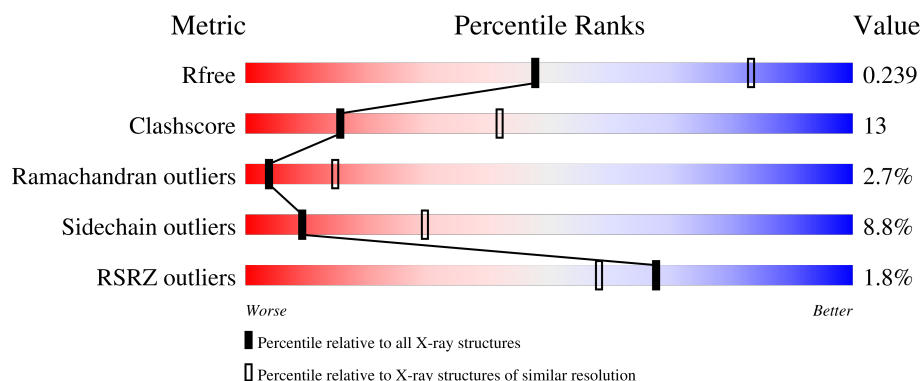
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

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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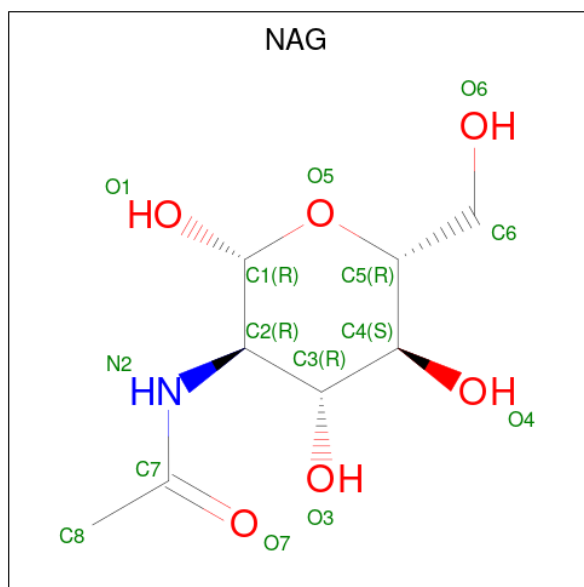
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP Q96IY4
A	147	THR	ALA	SEE REMARK 999	UNP Q96IY4
A	325	ILE	THR	engineered mutation	UNP Q96IY4
A	329	ILE	THR	engineered mutation	UNP Q96IY4
A	333	TYR	HIS	engineered mutation	UNP Q96IY4
A	335	GLN	HIS	engineered mutation	UNP Q96IY4
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 mutation	UNP Q96IY4
B	329	ILE	THR	engineered mutation	UNP Q96IY4
B	333	TYR	HIS	engineered mutation	UNP Q96IY4
B	335	GLN	HIS	engineered mutation	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 mutation	UNP Q96IY4
C	329	ILE	THR	engineered mutation	UNP Q96IY4
C	333	TYR	HIS	engineered mutation	UNP Q96IY4
C	335	GLN	HIS	engineered mutation	UNP Q96IY4

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

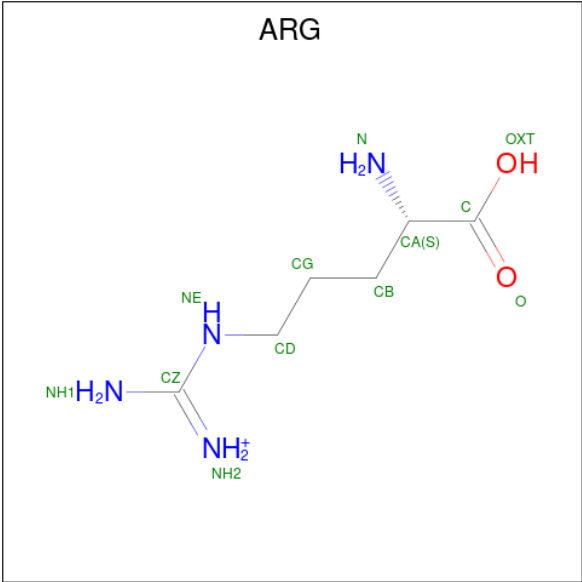


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	C	1	Total 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 (CCD ID: ZN) (formula: Zn).

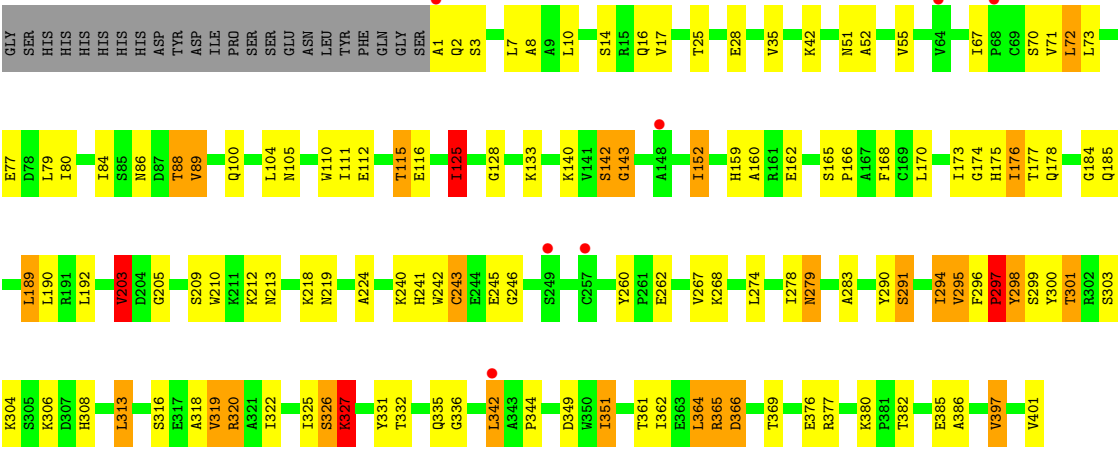
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

- Molecule 4 is ARGinine (CCD ID: ARG) (formula: C₆H₁₅N₄O₂).



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		

● Molecule 1: Carboxypeptidase B2



4 Data and refinement statistics

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 49.03 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.03-2.80) 100.0 (49.03-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.3.0008	Depositor
R, R_{free}	0.188 , 0.232 0.194 , 0.239	Depositor DCC
R_{free} test set	2582 reflections (5.10%)	wwPDB-VP
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 , 70.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	3/3336 (0.1%)	1.12	10/4532 (0.2%)
1	B	1.10	1/3336 (0.0%)	1.15	20/4532 (0.4%)
1	C	1.08	3/3336 (0.1%)	1.13	14/4532 (0.3%)
All	All	1.08	7/10008 (0.1%)	1.13	44/13596 (0.3%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	380	LYS	C-O	-6.07	1.19	1.24
1	C	88	THR	N-CA	5.78	1.53	1.46
1	B	88	THR	N-CA	5.76	1.53	1.46
1	A	343	ALA	CA-CB	-5.51	1.47	1.53
1	A	380	LYS	C-O	-5.49	1.19	1.24
1	C	152	ILE	C-O	-5.38	1.18	1.24
1	A	75	ASP	CA-C	-5.19	1.47	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	ASP	N-CA-C	-10.04	89.41	110.80
1	C	67	ILE	N-CA-C	7.43	115.27	107.76
1	B	297	PRO	CA-C-N	7.39	135.65	121.54
1	B	297	PRO	C-N-CA	7.39	135.65	121.54
1	B	243	CYS	N-CA-C	7.00	121.15	112.47
1	B	35	VAL	CB-CA-C	-6.43	103.45	112.14
1	C	176	ILE	CB-CA-C	-6.42	103.47	112.14
1	A	297	PRO	CA-C-N	6.22	133.43	121.54
1	A	297	PRO	C-N-CA	6.22	133.43	121.54
1	B	294	ILE	CB-CA-C	6.17	118.51	110.12
1	B	67	ILE	N-CA-C	6.15	114.75	107.73
1	A	48	PHE	N-CA-C	6.14	117.87	108.42
1	C	327	LYS	CB-CA-C	-5.99	107.95	116.34
1	B	297	PRO	N-CA-C	5.99	124.80	112.47
1	B	3	SER	N-CA-C	5.98	118.38	108.99
1	C	298	TYR	N-CA-C	5.96	123.49	110.80
1	B	368	GLY	N-CA-C	5.89	119.88	113.58
1	C	326	SER	N-CA-C	5.85	118.73	107.44
1	B	365	ARG	N-CA-C	5.79	117.99	110.53
1	C	365	ARG	O-C-N	5.70	129.46	122.84
1	A	297	PRO	O-C-N	5.67	130.30	122.64
1	B	176	ILE	CB-CA-C	-5.67	104.72	111.97
1	B	388	ALA	N-CA-C	-5.64	105.21	111.36
1	B	48	PHE	N-CA-C	5.63	117.82	108.99
1	A	175	HIS	N-CA-C	5.58	117.36	111.28
1	C	128	GLY	N-CA-C	5.54	117.65	110.45
1	B	297	PRO	O-C-N	5.52	130.09	122.64
1	C	243	CYS	N-CA-C	5.49	119.56	112.86
1	A	297	PRO	N-CA-C	5.49	123.78	112.47
1	B	298	TYR	CB-CA-C	5.31	120.99	110.42
1	A	194	ASP	N-CA-C	-5.30	102.20	110.42
1	C	112	GLU	N-CA-C	-5.28	105.44	111.14
1	B	182	ILE	CB-CA-C	-5.19	106.32	111.30
1	C	397	VAL	CB-CA-C	-5.14	105.39	111.97
1	C	349	ASP	CB-CA-C	-5.14	102.12	110.85
1	B	379	ILE	CB-CA-C	-5.08	105.38	111.88
1	C	203	VAL	CB-CA-C	5.07	118.67	112.02
1	C	125	ILE	CG1-CB-CG2	-5.06	95.52	110.70
1	B	365	ARG	CA-C-N	5.04	131.18	121.54
1	B	365	ARG	C-N-CA	5.04	131.18	121.54
1	B	329	ILE	N-CA-C	-5.02	100.89	108.12
1	C	189	LEU	N-CA-C	-5.02	105.46	111.03
1	A	118	HIS	CA-C-N	5.01	124.62	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	HIS	C-N-CA	5.01	124.62	119.56

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	Peptide,Mainchain
1	C	326	SER	Peptide
1	C	364	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	3249	0	3167	75	0
1	B	3249	0	3167	96	0
1	C	3249	0	3168	85	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	262	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 (262) 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:32:TRP:HE1	1:B:215:MET:HE2	1.12	1.09
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:OXT	1:C:401:VAL:HG12	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:32:TRP:NE1	1:B:215:MET:HE2	1.85	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:8:ALA:HB2	1:A:72:LEU:CD2	2.07	0.84
1:A:325:ILE:CD1	1:A:388:ALA:HB2	2.06	0.84
1:B:351:ILE:HD12	1:B:356:ILE:CG1	2.11	0.81
1:A:278:ILE:HD12	1:A:356:ILE:HD11	1.61	0.80
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:32:TRP:HE1	1:B:215:MET:CE	1.95	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:215:MET:HE3	1:B:215:MET:HA	1.70	0.72
1:B:285:ILE:CD1	1:B:393:ILE:HD11	2.18	0.72
1:A:325:ILE:HD12	1:A:388:ALA:CB	2.15	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:C:401:VAL:OXT	1:C:401:VAL:CG1	2.34	0.67
2:A:603:NAG:H83	2:A:603:NAG:O3	1.95	0.67
1:B:285:ILE:HD11	1:B:393:ILE:CD1	2.25	0.67
1:B:279:ASN:N	1:B:279:ASN:ND2	2.41	0.67
1:A:306:LYS:O	1:A:306:LYS:HG3	1.94	0.66
1:B:140:LYS:HZ1	1:B:146:GLN:NE2	1.94	0.66
1:C:300:TYR:CD1	1:C:301:THR:HG22	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:PRO:HD3	1:A:359:SER:O	1.96	0.65
1:B:75:ASP:O	1:B:79:LEU:HD12	1.96	0.65
1:B:294:ILE:HD11	1:B:318:ALA:HB3	1.79	0.65
1:C:176:ILE:CG2	1:C:190:LEU:CD1	2.75	0.65
1:A:121:MET:HE1	1:A:176:ILE:HG22	1.78	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:B:198:MET:HE2	1:B:201:VAL:HA	1.78	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:140:LYS:HZ3	1:B:146:GLN:HE22	1.48	0.62
1:B:142:SER:O	1:B:143:GLY:O	2.18	0.61
1:C:322:ILE:HG23	1:C:385:GLU:HB2	1.81	0.61
1:A:226:ASN:N	1:A:226:ASN:OD1	2.33	0.61
2:A:604:NAG:O3	2:A:604:NAG:H82	2.00	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
1:B:140:LYS:HZ3	1:B:146:GLN:NE2	1.99	0.60
2:A:603:NAG:O3	2:A:603:NAG:C8	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:108:TYR:OH	1:B:135:PRO:O	2.17	0.59
1:B:7:LEU:CD2	1:B:71:VAL:HG22	2.33	0.59
1:B:325:ILE:HD12	1:B:388:ALA:HB2	1.84	0.59
1:B:360:PHE:CD2	1:B:393:ILE:HD12	2.37	0.59
1:C:320:ARG:CG	1:C:320:ARG:HH11	2.16	0.59
1:C:320:ARG:HH11	1:C:320:ARG:HG2	1.68	0.59
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:B:128:GLY:C	1:B:136:LEU:HD12	2.29	0.58
1:C:84:ILE:HG22	1:C:84:ILE:O	2.03	0.58
1:A:179:PHE:CD1	1:A:183:ILE:HD12	2.38	0.58
1:C:209:SER:HA	1:C:213:ASN:O	2.04	0.58
1:A:147:THR:HG23	1:A:149:LYS:HZ1	1.64	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1:ALA:CB	2:C:602:NAG:H82	2.36	0.55
1:C:365:ARG:HD3	1:C:382:THR:OG1	2.07	0.55
1:A:89:VAL:HG12	1:A:90:SER:N	2.21	0.54
1:B:17:VAL:HG22	1:B:40:ILE:HG22	1.88	0.54
1:B:145:GLU:O	1:B:146:GLN:C	2.49	0.54
1:C:110:TRP:CZ3	1:C:170:LEU:HD22	2.41	0.54
1:A:111:ILE:O	1:A:115:THR:HB	2.08	0.54
1:A:112:GLU:OE2	1:A:124:LYS:NZ	2.38	0.54
1:C:397:VAL:HG13	1:C:401:VAL:CG2	2.37	0.54
4:A:650:ARG:O	4:A:650:ARG:HG2	2.08	0.54
1:B:32:TRP:NE1	1:B:215:MET:CE	2.62	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: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: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:241:HIS:HB3	1:B:244:GLU:OE1	2.11	0.51
1:B:366:ASP:OD2	1:B:371:GLY:N	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ARG:HB2	1:B:382:THR:HG23	1.92	0.51
2:C:601:NAG:H83	2:C:601:NAG:O3	2.11	0.51
1:B:165:SER:HB3	1:B:166:PRO:HD3	1.91	0.51
1:A:293:HIS:HA	1:A:332:THR:O	2.11	0.51
1:B:285:ILE:CD1	1:B:393:ILE:CD1	2.86	0.51
1:C:290:TYR:O	1:C:291:SER:CB	2.58	0.51
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:C:84:ILE:HG23	1:C:210:TRP:CZ3	2.47	0.49
1:C:7:LEU:CD2	1:C:71:VAL:HG22	2.39	0.49
1:A:35:VAL:HG13	1:A:36:THR:HG23	1.94	0.49
1:B:3:SER:CB	1:B:77:GLU:HB2	2.42	0.49
1:B:298:TYR:HB3	1:B:301:THR:HG23	1.94	0.49
1:B:104:LEU:HD21	1:B:203:VAL:HG13	1.94	0.49
1:B:278:ILE:HG22	1:B:279:ASN:ND2	2.28	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:142:SER:C	1:C:143:GLY:O	2.55	0.49
1:A:224:ALA:HB1	1:A:225:ASN:OD1	2.13	0.48
1:C:320:ARG:HG2	1:C:320:ARG:NH1	2.28	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:A:192:LEU:HD22	1:C:192:LEU:HD21	1.96	0.48
1:C:104:LEU:HD11	1:C:203:VAL:HG22	1.96	0.48
1:B:209:SER:HA	1:B:213:ASN:O	2.13	0.48
1:B:376:GLU:CD	2:B:604:NAG:H83	2.38	0.48
1:A:326:SER:OG	1:A:385:GLU:OE1	2.29	0.48
1:B:110:TRP:CZ3	1:B:170:LEU:HD22	2.49	0.47
1:B:356:ILE:HD13	1:B:356:ILE:N	2.28	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:HD22	1:A:279:ASN:H	1.61	0.47
1:C:16:GLN:O	1:C:17:VAL:C	2.57	0.47
1:C:304:LYS:HD3	1:C:308:HIS:CD2	2.50	0.47
1:A:348:ASP:CG	4:A:650:ARG:HH12	2.23	0.47
1:B:92:ARG:NH1	1:B:106:GLU:OE2	2.48	0.47
1:C:184:GLY:O	1:C:185:GLN:C	2.56	0.47
1:A:76:VAL:O	1:A:77:GLU:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ASP:C	1:A:232:ASP:OD1	2.56	0.47
1:B:142:SER:C	1:B:143:GLY:O	2.57	0.47
1:C:86:ASN:CG	1:C:89:VAL:HG21	2.40	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:A:368:GLY:O	1:A:369:THR:C	2.58	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:A:87:ASP:OD1	1:A:87:ASP:C	2.59	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:O3	2:B:604:NAG:H82	2.17	0.45
1:B:298:TYR:OH	1:B:353:ASP:OD1	2.31	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:B:326:SER:OG	1:B:385:GLU:OE1	2.35	0.45
1:C:159:HIS:HB2	1:C:162:GLU:CD	2.42	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:A:121:MET:HE3	1:A:190:LEU:CD1	2.48	0.44
1:B:174:GLY:O	1:B:178:GLN:HB2	2.18	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:A:189:LEU:O	1:A:193:VAL:HG12	2.18	0.44
1:A:3:SER:HB3	1:A:77:GLU:HB2	2.00	0.43
1:C:1:ALA:HB2	2:C:602:NAG:C8	2.48	0.43
1:B:187:THR:O	1:B:191:ARG:HB2	2.18	0.43
1:C:168:PHE:CE1	1:C:386:ALA:HB3	2.54	0.43
1:B:322:ILE:HG23	1:B:385:GLU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ASN:O	1:C:55:VAL:CG2	2.67	0.43
1:C:80:ILE:HG22	1:C:84:ILE:HD11	2.01	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:B:5:GLN:NE2	1:B:55:VAL:HG11	2.34	0.43
1:B:147:THR:H	1:B:149:LYS:HZ3	1.66	0.43
1:C:1:ALA:CB	2:C:602:NAG:C8	2.97	0.43
1:C:10:LEU:C	1:C:10:LEU:CD2	2.92	0.43
1:C:241:HIS:O	1:C:242:TRP:C	2.59	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:A:86:ASN:O	1:A:87:ASP:C	2.63	0.42
1:A:147:THR:CG2	1:A:149:LYS:HZ1	2.29	0.42
1:A:268:LYS:O	1:A:269:ALA:C	2.63	0.42
1:C:165:SER:HB3	1:C:166:PRO:HD3	2.00	0.42
1:A:114:ILE:HG23	1:A:122:LEU:HD12	2.01	0.42
1:A:226:ASN:HB2	1:A:251:SER:CB	2.50	0.42
1:B:20:LEU:HD23	1:B:20:LEU:HA	1.78	0.42
1:B:88:THR:O	1:B:88:THR:CG2	2.66	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:40:ILE:HG12	1:B:46:VAL:HG21	2.02	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:A:184:GLY:O	1:A:185:GLN:C	2.62	0.42
2:A:604:NAG:O3	2:A:604:NAG:C7	2.68	0.42
1:C:125:ILE:HD11	1:C:140:LYS:HB2	2.02	0.42
1:C:279:ASN:N	1:C:279:ASN:ND2	2.68	0.42
1:C:10:LEU:C	1:C:10:LEU:HD23	2.46	0.41
1:A:190:LEU:HD23	1:A:190:LEU:HA	1.88	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:219:ASN:ND2	1:A:264:GLU:OE1	2.54	0.41
1:A:376:GLU:HA	1:A:379:ILE:HG13	2.03	0.41
1:A:86:ASN:HA	1:A:89:VAL:HG23	2.03	0.41
1:A:290:TYR:O	1:A:291:SER:HB2	2.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ILE:HG21	1:B:393:ILE:HD13	1.68	0.41
1:A:121:MET:HE3	1:A:190:LEU:HD11	2.02	0.41
1:A:324:LYS:HE2	1:C:313:LEU:HD11	2.02	0.41
1:C:320:ARG:HH11	1:C:320:ARG:HB3	1.85	0.41
1:A:15:ARG:O	1:A:19:VAL:HG23	2.21	0.41
1:A:366:ASP:OD2	1:A:369:THR:N	2.54	0.41
1:B:244:GLU:O	1:B:245:GLU:C	2.63	0.41
1:C:80:ILE:HG22	1:C:84:ILE:CD1	2.51	0.41
1:C:2:GLN:O	1:C:77:GLU:HB2	2.21	0.40
1:C:296:PHE:HB2	1:C:297:PRO:HD2	2.03	0.40
1:A:205:GLY:O	1:A:206:TYR:C	2.64	0.40
1:B:7:LEU:HD22	1:B:71:VAL:HG22	2.01	0.40
1:B:184:GLY:O	1:B:185:GLN:C	2.62	0.40
1:C:142:SER:O	1:C:143:GLY:C	2.65	0.40
1:A:50:VAL:HG11	1:A:55:VAL:HA	2.03	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

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%)	4	16
1	B	399/424 (94%)	359 (90%)	29 (7%)	11 (3%)	4	14
1	C	399/424 (94%)	366 (92%)	22 (6%)	11 (3%)	4	14
All	All	1197/1272 (94%)	1083 (90%)	82 (7%)	32 (3%)	4	15

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%)	330 (93%)	24 (7%)	14	42
1	B	354/375 (94%)	321 (91%)	33 (9%)	8	27
1	C	354/375 (94%)	317 (90%)	37 (10%)	6	22
All	All	1062/1125 (94%)	968 (91%)	94 (9%)	9	29

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	13	THR
1	A	25	THR
1	A	56	ASP
1	A	64	VAL
1	A	69	CYS
1	A	70	SER
1	A	72	LEU
1	A	115	THR
1	A	185	GLN
1	A	190	LEU
1	A	221	SER
1	A	226	ASN
1	A	279	ASN
1	A	297	PRO
1	A	303	SER
1	A	312	SER
1	A	323	GLU
1	A	325	ILE
1	A	329	ILE
1	A	330	ARG
1	A	351	ILE
1	A	365	ARG
1	A	392	LYS
1	B	14	SER
1	B	17	VAL
1	B	19	VAL
1	B	35	VAL
1	B	64	VAL
1	B	72	LEU
1	B	96	SER
1	B	105	ASN
1	B	114	ILE
1	B	123	THR

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Mol	Chain	Res	Type
1	B	147	THR
1	B	170	LEU
1	B	173	ILE
1	B	193	VAL
1	B	268	LYS
1	B	279	ASN
1	B	294	ILE
1	B	295	VAL
1	B	297	PRO
1	B	301	THR
1	B	303	SER
1	B	320	ARG
1	B	323	GLU
1	B	324	LYS
1	B	325	ILE
1	B	326	SER
1	B	327	LYS
1	B	351	ILE
1	B	356	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	25	THR
1	C	28	GLU
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	133	LYS
1	C	175	HIS
1	C	189	LEU
1	C	203	VAL
1	C	212	LYS
1	C	243	CYS

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Mol	Chain	Res	Type
1	C	279	ASN
1	C	294	ILE
1	C	295	VAL
1	C	297	PRO
1	C	299	SER
1	C	301	THR
1	C	306	LYS
1	C	313	LEU
1	C	316	SER
1	C	319	VAL
1	C	320	ARG
1	C	325	ILE
1	C	327	LYS
1	C	332	THR
1	C	342	LEU
1	C	351	ILE
1	C	369	THR
1	C	377	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	175	HIS
1	A	185	GLN
1	A	236	ASN
1	A	279	ASN
1	A	292	GLN
1	A	293	HIS
1	A	328	ASN
1	B	45	GLN
1	B	57	ASN
1	B	100	GLN
1	B	126	HIS
1	B	146	GLN
1	B	225	ASN
1	B	279	ASN
1	B	280	GLN
1	B	335	GLN
1	B	400	ASN
1	C	5	GLN
1	C	100	GLN

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Mol	Chain	Res	Type
1	C	175	HIS
1	C	226	ASN
1	C	279	ASN
1	C	292	GLN
1	C	308	HIS

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 oligosaccharides 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	603	1	14,14,15	1.65	2 (14%)	17,19,21	2.49	7 (41%)
2	NAG	A	601	1	14,14,15	1.00	1 (7%)	17,19,21	2.52	3 (17%)
2	NAG	C	604	1	14,14,15	0.73	0	17,19,21	1.97	7 (41%)
2	NAG	B	601	1	14,14,15	0.69	0	17,19,21	1.75	2 (11%)
2	NAG	B	603	1	14,14,15	0.66	0	17,19,21	2.05	2 (11%)
2	NAG	A	602	1	14,14,15	0.66	0	17,19,21	1.28	3 (17%)
2	NAG	C	601	1	14,14,15	0.97	1 (7%)	17,19,21	2.95	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	604	1	14,14,15	0.81	0	17,19,21	2.32	8 (47%)
2	NAG	B	602	1	14,14,15	0.73	0	17,19,21	2.01	5 (29%)
2	NAG	B	604	1	14,14,15	0.79	0	17,19,21	1.93	6 (35%)
2	NAG	C	602	1	14,14,15	1.56	2 (14%)	17,19,21	2.69	7 (41%)
4	ARG	A	650	-	10,11,11	1.09	1 (10%)	9,13,13	1.77	2 (22%)
4	ARG	B	650	-	10,11,11	0.85	0	9,13,13	1.56	2 (22%)
4	ARG	C	650	-	10,11,11	0.89	0	9,13,13	1.59	2 (22%)

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	603	1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	A	601	1	-	4/6/23/26	0/1/1/1
2	NAG	C	604	1	-	4/6/23/26	0/1/1/1
2	NAG	B	601	1	-	4/6/23/26	0/1/1/1
2	NAG	B	603	1	-	4/6/23/26	0/1/1/1
2	NAG	A	602	1	-	0/6/23/26	0/1/1/1
2	NAG	C	601	1	-	4/6/23/26	0/1/1/1
2	NAG	A	604	1	-	4/6/23/26	0/1/1/1
2	NAG	B	602	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	604	1	-	2/6/23/26	0/1/1/1
2	NAG	C	602	1	-	4/6/23/26	0/1/1/1
4	ARG	A	650	-	-	2/11/11/11	-
4	ARG	B	650	-	-	2/11/11/11	-
4	ARG	C	650	-	-	3/11/11/11	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	NAG	C1-C2	4.91	1.59	1.52
2	C	602	NAG	C1-C2	4.37	1.58	1.52
2	A	601	NAG	C1-C2	3.31	1.56	1.52
2	C	602	NAG	C2-N2	2.66	1.50	1.46
2	C	601	NAG	C1-C2	2.54	1.55	1.52
2	A	603	NAG	C3-C2	2.26	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	650	ARG	CG-CB	2.09	1.60	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	NAG	C1-O5-C5	10.76	126.61	112.19
2	A	601	NAG	C1-O5-C5	8.85	124.04	112.19
2	C	602	NAG	C1-O5-C5	7.04	121.62	112.19
2	B	603	NAG	C1-O5-C5	6.72	121.19	112.19
2	A	603	NAG	O5-C1-C2	-5.64	102.56	111.29
2	B	601	NAG	C1-O5-C5	5.38	119.39	112.19
2	B	602	NAG	C1-O5-C5	4.52	118.24	112.19
2	C	602	NAG	C2-N2-C7	4.49	128.92	122.90
2	C	602	NAG	O5-C1-C2	4.41	118.12	111.29
2	A	604	NAG	C1-C2-N2	4.19	117.04	110.43
2	A	604	NAG	C1-O5-C5	4.06	117.63	112.19
2	B	602	NAG	C8-C7-N2	3.95	122.67	116.12
2	A	603	NAG	C1-C2-N2	3.90	116.58	110.43
2	A	603	NAG	O5-C5-C4	-3.88	101.39	110.83
4	B	650	ARG	OXT-C-O	-3.86	115.33	124.08
2	A	604	NAG	C4-C3-C2	-3.86	105.37	111.02
2	C	604	NAG	O5-C1-C2	-3.85	105.33	111.29
2	B	604	NAG	C1-O5-C5	3.85	117.34	112.19
2	A	604	NAG	C3-C4-C5	-3.67	103.57	110.23
2	B	604	NAG	C3-C4-C5	-3.52	103.86	110.23
4	C	650	ARG	OXT-C-O	-3.50	116.14	124.08
2	A	603	NAG	C8-C7-N2	3.49	121.90	116.12
4	A	650	ARG	OXT-C-O	-3.40	116.38	124.08
2	A	601	NAG	O5-C1-C2	3.33	116.44	111.29
4	A	650	ARG	CB-CA-C	-3.29	101.72	110.45
2	C	602	NAG	O7-C7-C8	-3.28	116.21	122.05
2	B	602	NAG	O7-C7-N2	-3.26	116.23	121.98
2	A	603	NAG	O7-C7-C8	-3.22	116.33	122.05
2	A	602	NAG	C1-O5-C5	3.07	116.30	112.19
2	C	604	NAG	O4-C4-C3	2.98	117.40	110.38
2	B	604	NAG	O4-C4-C3	2.95	117.33	110.38
2	C	604	NAG	C1-O5-C5	2.94	116.13	112.19
2	C	604	NAG	C3-C4-C5	-2.83	105.10	110.23
2	B	603	NAG	C8-C7-N2	2.70	120.59	116.12
2	B	602	NAG	C3-C4-C5	-2.67	105.39	110.23
2	C	602	NAG	C1-C2-N2	2.65	114.61	110.43
2	A	604	NAG	O4-C4-C5	2.63	115.80	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	604	NAG	O4-C4-C5	2.63	115.79	109.32
2	C	601	NAG	O5-C5-C4	2.58	117.10	110.83
2	A	601	NAG	C2-N2-C7	2.56	126.34	122.90
2	C	604	NAG	C8-C7-N2	2.56	120.36	116.12
2	A	603	NAG	C4-C3-C2	2.53	114.72	111.02
4	C	650	ARG	CB-CA-C	-2.53	103.75	110.45
2	A	604	NAG	O5-C5-C6	2.46	112.45	107.66
2	A	602	NAG	C1-C2-N2	-2.40	106.66	110.43
2	C	604	NAG	C1-C2-N2	2.39	114.20	110.43
2	B	602	NAG	O5-C1-C2	2.38	114.97	111.29
4	B	650	ARG	CB-CA-C	-2.24	104.52	110.45
2	C	601	NAG	C8-C7-N2	2.22	119.81	116.12
2	A	603	NAG	O3-C3-C2	2.20	113.97	109.40
2	A	604	NAG	O5-C1-C2	-2.19	107.90	111.29
2	C	602	NAG	O5-C5-C4	-2.12	105.68	110.83
2	A	602	NAG	O5-C1-C2	2.10	114.54	111.29
2	B	604	NAG	C8-C7-N2	2.09	119.58	116.12
2	C	602	NAG	C4-C3-C2	2.08	114.07	111.02
2	A	604	NAG	C2-N2-C7	-2.03	120.18	122.90
2	C	604	NAG	O4-C4-C5	2.01	114.28	109.32
2	B	601	NAG	O7-C7-C8	-2.01	118.48	122.05
2	B	604	NAG	O7-C7-C8	-2.00	118.49	122.05

All (2) chirality outliers are listed below:

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

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAG	C8-C7-N2-C2
2	A	601	NAG	O7-C7-N2-C2
2	A	603	NAG	C8-C7-N2-C2
2	A	603	NAG	O7-C7-N2-C2
2	B	601	NAG	C8-C7-N2-C2
2	B	601	NAG	O7-C7-N2-C2
2	B	602	NAG	C8-C7-N2-C2
2	B	602	NAG	O7-C7-N2-C2
2	B	603	NAG	C8-C7-N2-C2
2	B	603	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	C	601	NAG	C8-C7-N2-C2
2	C	601	NAG	O7-C7-N2-C2
2	C	602	NAG	O5-C5-C6-O6
2	C	601	NAG	O5-C5-C6-O6
2	C	602	NAG	C4-C5-C6-O6
2	C	601	NAG	C4-C5-C6-O6
2	A	601	NAG	O5-C5-C6-O6
4	A	650	ARG	NE-CD-CG-CB
2	A	604	NAG	C4-C5-C6-O6
2	A	604	NAG	O5-C5-C6-O6
2	A	604	NAG	C8-C7-N2-C2
2	A	604	NAG	O7-C7-N2-C2
2	B	604	NAG	C8-C7-N2-C2
2	B	604	NAG	O7-C7-N2-C2
2	C	604	NAG	C8-C7-N2-C2
2	C	604	NAG	O7-C7-N2-C2
2	C	604	NAG	O5-C5-C6-O6
2	C	602	NAG	C8-C7-N2-C2
4	A	650	ARG	OXT-C-CA-N
4	C	650	ARG	NE-CD-CG-CB
2	C	604	NAG	C4-C5-C6-O6
2	B	603	NAG	C4-C5-C6-O6
2	C	602	NAG	O7-C7-N2-C2
2	A	603	NAG	O5-C5-C6-O6
2	A	601	NAG	C4-C5-C6-O6
4	B	650	ARG	OXT-C-CA-N
4	C	650	ARG	O-C-CA-N
4	B	650	ARG	NE-CD-CG-CB
4	C	650	ARG	OXT-C-CA-N
2	B	601	NAG	C4-C5-C6-O6
2	A	603	NAG	C4-C5-C6-O6
2	B	601	NAG	O5-C5-C6-O6
2	B	603	NAG	O5-C5-C6-O6

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	C	604	NAG	2	0
2	B	603	NAG	2	0
2	C	601	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	NAG	2	0
2	B	604	NAG	2	0
2	C	602	NAG	4	0
4	A	650	ARG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.32	7 (1%) 69 60	50, 67, 77, 95	0
1	B	401/424 (94%)	0.19	8 (1%) 65 56	51, 67, 81, 96	0
1	C	401/424 (94%)	0.25	7 (1%) 69 60	43, 67, 75, 97	0
All	All	1203/1272 (94%)	0.26	22 (1%) 67 58	43, 67, 77, 97	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	ALA	6.0
1	B	1	ALA	4.2
1	A	91	PRO	4.1
1	A	1	ALA	4.0
1	B	148	ALA	3.8
1	B	224	ALA	3.7
1	B	147	THR	3.1
1	B	93	ALA	2.8
1	C	249	SER	2.8
1	A	249	SER	2.7
1	B	226	ASN	2.6
1	A	222	PHE	2.6
1	C	64	VAL	2.5
1	C	68	PRO	2.5
1	B	256	TYR	2.5
1	C	342	LEU	2.4
1	A	309	GLU	2.3
1	C	148	ALA	2.2
1	C	257	CYS	2.2
1	A	221	SER	2.2
1	A	341	TYR	2.2
1	B	225	ASN	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å ²)	Q<0.9
2	NAG	C	602	14/15	0.47	0.15	79,82,84,84	0
2	NAG	B	602	14/15	0.56	0.15	73,75,78,79	0
2	NAG	A	603	14/15	0.59	0.13	57,67,69,69	0
2	NAG	C	601	14/15	0.64	0.15	75,76,79,80	0
2	NAG	B	603	14/15	0.74	0.12	66,67,70,71	0
2	NAG	A	604	14/15	0.77	0.15	58,62,63,63	0
2	NAG	A	601	14/15	0.79	0.11	75,76,77,78	0
2	NAG	B	604	14/15	0.81	0.11	68,72,74,74	0
2	NAG	A	602	14/15	0.82	0.11	84,86,88,88	0
2	NAG	C	604	14/15	0.84	0.09	57,60,64,66	0
4	ARG	A	650	12/12	0.85	0.19	67,70,74,75	0
4	ARG	C	650	12/12	0.85	0.18	65,69,77,80	0
4	ARG	B	650	12/12	0.86	0.17	72,74,77,78	0
2	NAG	B	601	14/15	0.87	0.11	58,63,65,66	0
3	ZN	B	501	1/1	0.98	0.05	73,73,73,73	0
3	ZN	C	501	1/1	0.99	0.05	69,69,69,69	0
3	ZN	A	501	1/1	0.99	0.05	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.