



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 05:14 AM GMT

PDB ID : 3D67
Title : Crystal structure of Thrombin-Activatable Fibrinolysis Inhibitor (TAFI) in complex with 2-guanidino-ethyl-mercaptosuccinicacid (GEMSA)
Authors : Brondijk, T.H.C.; Huizinga, E.G.
Deposited on : 2008-05-19
Resolution : 3.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

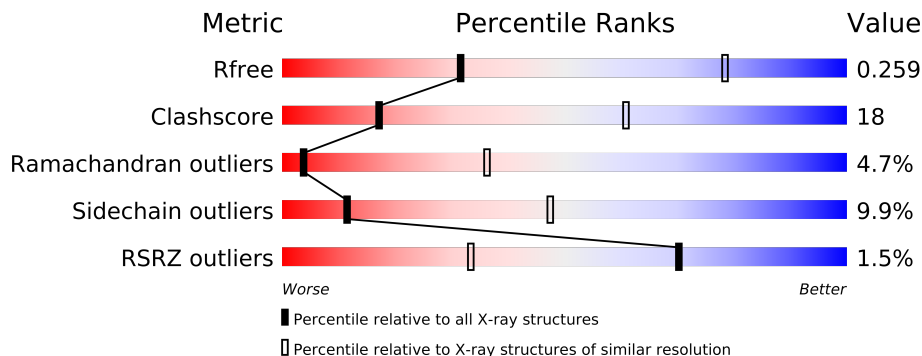
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.40 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}	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

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	A	601	-	X
2	NAG	A	603	-	X
2	NAG	A	604	-	X
2	NAG	B	603	-	X
2	NAG	C	601	-	X

2 Entry composition

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	C	N	O	S	0	0	0
			3246	2078	555	601	12			
1	B	401	Total	C	N	O	S	0	0	0
			3246	2078	555	601	12			
1	C	401	Total	C	N	O	S	0	0	0
			3246	2078	555	601	12			

There are 75 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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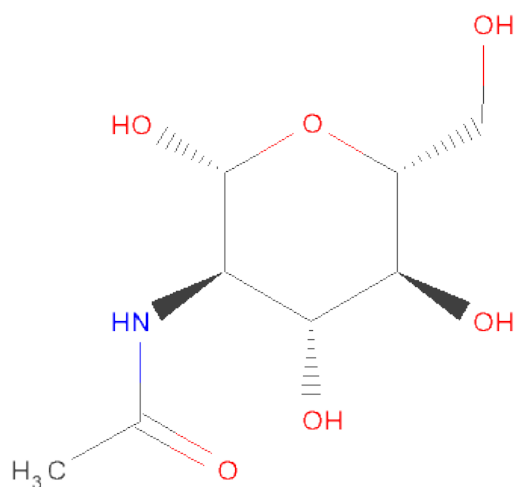
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	EXPRESSION TAG	UNP Q96IY4
A	147	THR	ALA	SEE REMARK 999	UNP Q96IY4
B	-22	GLY	-	EXPRESSION TAG	UNP Q96IY4
B	-21	SER	-	EXPRESSION TAG	UNP Q96IY4
B	-20	HIS	-	EXPRESSION TAG	UNP Q96IY4
B	-19	HIS	-	EXPRESSION TAG	UNP Q96IY4
B	-18	HIS	-	EXPRESSION TAG	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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- 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	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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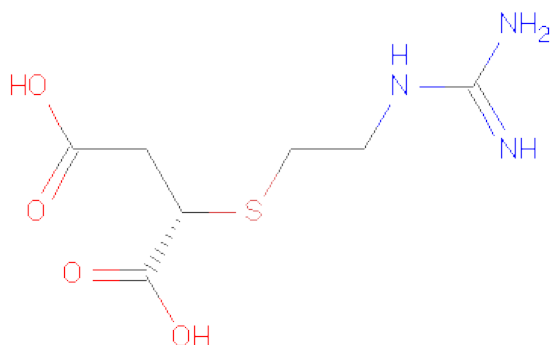
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

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

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

- Molecule 4 is (2-GUANIDINOETHYLMERCAPTO)SUCCINICACID (three-letter code: GEM) (formula: C₇H₁₃N₃O₄S).



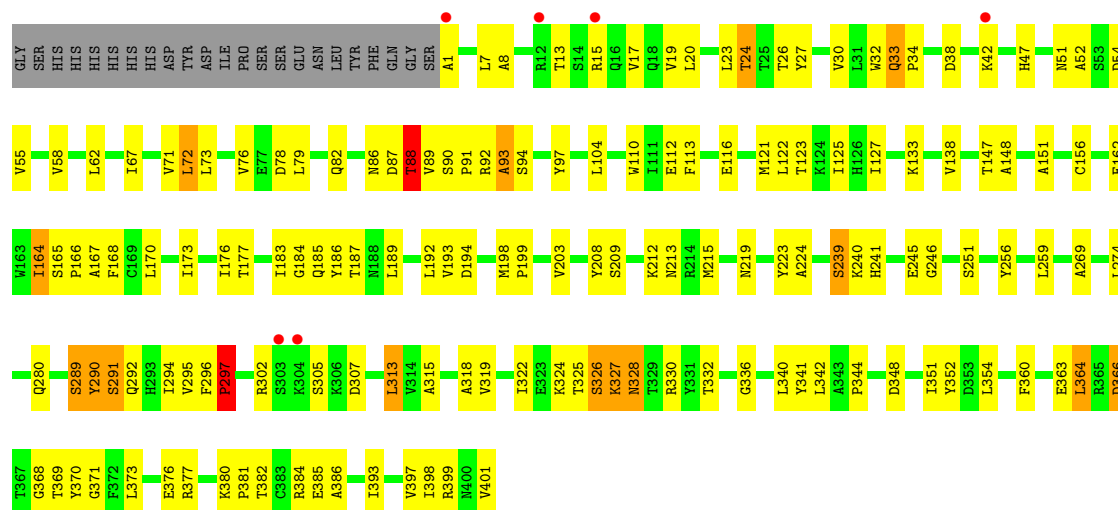
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	7	3	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			15	7	3	4	1		
4	C	1	Total	C	N	O	S	0	0
			15	7	3	4	1		

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.05Å 161.05Å 138.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.09 – 3.40 44.09 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.09-3.40) 99.6 (44.09-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.252 0.208 , 0.259	Depositor DCC
R_{free} test set	1472 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	112.6	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 138.5	EDS
Estimated twinning fraction	0.047 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 28898 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9940	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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, GEM

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	0.66	0/3334	0.73	0/4530
1	B	0.70	1/3334 (0.0%)	0.75	2/4530 (0.0%)
1	C	0.66	0/3334	0.72	0/4530
All	All	0.67	1/10002 (0.0%)	0.73	2/13590 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	4
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	377	ARG	CZ-NH1	9.69	1.45	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	ARG	NE-CZ-NH2	-9.97	115.32	120.30
1	B	290	TYR	N-CA-C	5.20	125.03	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	SER	Peptide
1	A	326	SER	Peptide
1	A	33	GLN	Peptide
1	B	289	SER	Peptide
1	B	33	GLN	Peptide
1	C	289	SER	Peptide
1	C	326	SER	Peptide
1	C	33	GLN	Peptide
1	C	364	LEU	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	3246	0	3155	122	0
1	B	3246	0	3155	107	0
1	C	3246	0	3156	115	0
2	A	56	0	52	2	0
2	B	56	0	52	2	0
2	C	42	0	39	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	15	0	10	1	0
4	B	15	0	10	1	0
4	C	15	0	10	1	0
All	All	9940	0	9639	344	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 18.

All (344) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:121:MET:HE2	1:C:177:THR:HG22	1.23	1.13
1:C:121:MET:CE	1:C:177:THR:HG22	1.99	0.93
1:C:164:ILE:HD11	1:C:382:THR:HG21	1.52	0.92

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:104:LEU:HD21	1:B:203:VAL:HG13	1.52	0.92
1:B:401:VAL:HG12	1:B:401:VAL:O	1.71	0.90
1:C:162:GLU:HG2	1:C:289:SER:OG	1.74	0.88
1:A:118:HIS:CE1	1:A:177:THR:HG23	2.10	0.86
1:C:110:TRP:CZ3	1:C:170:LEU:HD22	2.10	0.86
1:B:54:ASP:O	1:B:58:VAL:HG23	1.78	0.84
1:B:32:TRP:HE1	1:B:215:MET:HE2	1.39	0.83
1:A:233:LEU:HD22	1:A:267:VAL:HG23	1.58	0.83
1:C:121:MET:HE1	1:C:177:THR:HA	1.61	0.83
1:A:139:LEU:HD12	1:A:173:ILE:CD1	2.09	0.82
1:A:72:LEU:O	1:A:73:LEU:HD23	1.80	0.82
1:B:104:LEU:CD2	1:B:203:VAL:HG13	2.11	0.81
1:B:285:ILE:HD11	1:B:393:ILE:HD11	1.62	0.80
1:A:401:VAL:HG12	1:A:401:VAL:O	1.80	0.80
1:A:147:THR:HG23	1:A:149:LYS:HZ2	1.47	0.80
1:C:274:LEU:HD13	1:C:351:ILE:HD12	1.63	0.80
1:B:8:ALA:HB2	1:B:72:LEU:HD22	1.64	0.78
1:A:139:LEU:HD12	1:A:173:ILE:HD12	1.66	0.78
1:A:278:ILE:HG23	1:A:279:ASN:HD22	1.49	0.77
1:C:121:MET:HE2	1:C:177:THR:CG2	2.12	0.77
1:B:233:LEU:HD22	1:B:267:VAL:HG23	1.66	0.77
1:C:87:ASP:O	1:C:88:THR:HG22	1.86	0.75
2:A:604:NAG:H82	2:A:604:NAG:O3	1.86	0.74
1:C:322:ILE:HG23	1:C:385:GLU:HB2	1.71	0.73
1:A:313:LEU:HD11	1:C:324:LYS:CE	2.19	0.72
1:C:183:ILE:HD12	1:C:186:TYR:HE2	1.54	0.72
1:C:397:VAL:HG13	1:C:401:VAL:HG21	1.71	0.72
1:C:292:GLN:NE2	1:C:330:ARG:O	2.23	0.71
1:C:322:ILE:O	1:C:325:THR:HG22	1.90	0.71
1:C:1:ALA:HB2	2:C:602:NAG:H82	1.73	0.71
1:A:8:ALA:HB2	1:A:72:LEU:HD21	1.72	0.70
1:B:32:TRP:HE1	1:B:215:MET:CE	2.05	0.70
1:A:374:LEU:HD11	1:A:378:TYR:CD2	2.26	0.69
1:B:325:THR:HG21	1:B:385:GLU:HA	1.74	0.69
1:B:87:ASP:O	1:B:88:THR:HG22	1.92	0.69
1:B:401:VAL:CG1	1:B:401:VAL:O	2.40	0.68
1:C:110:TRP:CZ3	1:C:170:LEU:CD2	2.76	0.68
1:A:374:LEU:HD11	1:A:378:TYR:HD2	1.58	0.68
1:A:401:VAL:CG1	1:A:401:VAL:O	2.42	0.67
1:B:243:CYS:HA	1:B:247:ALA:HB3	1.76	0.67
1:C:62:LEU:HD23	1:C:67:ILE:HD12	1.76	0.66
1:C:104:LEU:HD21	1:C:203:VAL:HG13	1.78	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:54:ASP:O	1:A:58:VAL:HG23	1.96	0.66
1:B:285:ILE:CD1	1:B:393:ILE:HD11	2.26	0.65
1:B:23:LEU:HD11	1:B:61:HIS:ND1	2.11	0.65
1:B:104:LEU:HD21	1:B:203:VAL:CG1	2.26	0.65
1:A:76:VAL:CG1	1:A:80:ILE:HD11	2.27	0.64
1:A:278:ILE:CG2	1:A:279:ASN:HD22	2.11	0.64
1:C:307:ASP:OD2	1:C:352:TYR:OH	2.11	0.64
1:C:192:LEU:HD13	1:C:398:ILE:HG21	1.79	0.63
1:A:110:TRP:CZ3	1:A:170:LEU:CD2	2.82	0.63
1:A:278:ILE:CG2	1:A:279:ASN:ND2	2.62	0.62
1:B:76:VAL:O	1:B:79:LEU:N	2.33	0.61
1:C:7:LEU:HD22	1:C:71:VAL:HG22	1.83	0.61
1:A:110:TRP:CZ3	1:A:170:LEU:HD22	2.35	0.61
1:C:325:THR:HG21	1:C:385:GLU:CB	2.30	0.61
1:C:62:LEU:HD22	1:C:67:ILE:HG21	1.83	0.60
1:B:164:ILE:O	1:B:167:ALA:HB3	2.02	0.60
1:B:296:PHE:HB2	1:B:297:PRO:HD2	1.83	0.60
1:A:76:VAL:HG12	1:A:80:ILE:HD11	1.85	0.59
1:B:136:LEU:HB3	1:B:198:MET:HE3	1.83	0.59
1:B:322:ILE:HG23	1:B:385:GLU:HB2	1.85	0.59
1:A:189:LEU:O	1:A:189:LEU:HD12	2.03	0.59
1:A:251:SER:HA	1:A:256:TYR:CD1	2.37	0.59
1:B:1:ALA:CB	2:B:602:NAG:H83	2.33	0.59
1:B:165:SER:HB3	1:B:166:PRO:HD3	1.82	0.59
1:B:35:VAL:CG2	1:B:341:TYR:OH	2.50	0.58
1:C:1:ALA:CB	2:C:602:NAG:H82	2.33	0.58
1:A:340:LEU:HD11	1:A:363:GLU:OE1	2.03	0.58
1:A:294:ILE:CD1	1:A:318:ALA:HB3	2.33	0.58
1:B:73:LEU:HD13	1:B:373:LEU:HD12	1.85	0.58
1:A:7:LEU:HD22	1:A:71:VAL:HG22	1.86	0.58
1:A:87:ASP:O	1:A:88:THR:CG2	2.51	0.58
1:B:32:TRP:CZ2	1:B:215:MET:HE1	2.39	0.58
1:A:322:ILE:HG21	1:A:331:TYR:CE2	2.39	0.58
1:C:121:MET:CE	1:C:177:THR:HA	2.31	0.58
1:C:164:ILE:O	1:C:167:ALA:HB3	2.04	0.57
1:C:110:TRP:CE3	1:C:170:LEU:HD22	2.39	0.57
1:B:50:VAL:HG13	1:B:58:VAL:HG21	1.86	0.57
1:C:183:ILE:HD12	1:C:186:TYR:CE2	2.38	0.57
1:C:20:LEU:O	1:C:24:THR:HG23	2.04	0.57
1:A:114:ILE:HG23	1:A:122:LEU:HD13	1.86	0.57
1:B:335:HIS:O	1:B:335:HIS:CG	2.57	0.57
1:A:92:ARG:O	1:A:93:ALA:HB3	2.05	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:127:ILE:HD12	1:C:269:ALA:HB1	1.86	0.57
1:A:168:PHE:CE1	1:A:386:ALA:HB3	2.39	0.57
1:C:20:LEU:HA	1:C:23:LEU:HD12	1.86	0.57
1:A:121:MET:HE1	1:A:176:ILE:HG22	1.87	0.56
1:A:296:PHE:HB2	1:A:297:PRO:HD2	1.87	0.56
1:B:50:VAL:CG1	1:B:58:VAL:HG21	2.35	0.56
1:C:73:LEU:HD22	1:C:79:LEU:HD11	1.87	0.56
1:B:32:TRP:NE1	1:B:215:MET:CE	2.68	0.56
1:C:1:ALA:HB2	2:C:602:NAG:C8	2.34	0.56
1:B:163:TRP:CZ2	1:B:210:TRP:CD1	2.93	0.56
1:B:290:TYR:HB2	1:B:366:ASP:O	2.06	0.55
1:C:8:ALA:HB2	1:C:72:LEU:HD22	1.88	0.55
1:A:298:TYR:CE2	1:A:305:SER:HA	2.41	0.55
1:A:20:LEU:O	1:A:24:THR:HG23	2.05	0.55
1:B:229:ILE:HG22	1:B:230:GLY:N	2.22	0.55
1:B:374:LEU:HD11	1:B:378:TYR:HB2	1.88	0.55
1:C:7:LEU:CD2	1:C:71:VAL:HG22	2.37	0.55
1:B:164:ILE:HD11	1:B:382:THR:HG21	1.88	0.55
1:A:278:ILE:HG23	1:A:279:ASN:ND2	2.19	0.54
1:A:93:ALA:HB2	1:A:113:PHE:HE1	1.71	0.54
1:A:186:TYR:O	1:A:187:THR:C	2.44	0.54
1:A:51:ASN:O	1:A:55:VAL:HG23	2.08	0.54
1:B:108:TYR:OH	1:B:135:PRO:O	2.09	0.54
1:B:223:TYR:CE2	1:B:259:LEU:HD12	2.43	0.54
1:C:86:ASN:HA	1:C:89:VAL:HG23	1.88	0.54
1:C:382:THR:O	1:C:385:GLU:HG2	2.08	0.54
1:A:8:ALA:HB2	1:A:72:LEU:CD2	2.37	0.54
1:B:32:TRP:NE1	1:B:215:MET:HE2	2.15	0.54
1:A:147:THR:HG23	1:A:149:LYS:NZ	2.20	0.54
1:A:200:VAL:HG12	1:A:203:VAL:HG22	1.89	0.54
1:C:104:LEU:CD2	1:C:203:VAL:HG13	2.38	0.54
1:B:182:ILE:HG22	1:B:183:ILE:N	2.22	0.54
1:B:54:ASP:O	1:B:58:VAL:CG2	2.52	0.54
1:C:8:ALA:HB2	1:C:72:LEU:CD2	2.38	0.54
1:A:165:SER:HB3	1:A:166:PRO:HD3	1.90	0.54
2:A:604:NAG:C8	2:A:604:NAG:O3	2.56	0.53
1:A:92:ARG:O	1:A:93:ALA:CB	2.55	0.53
1:B:374:LEU:HD11	1:B:378:TYR:CB	2.38	0.53
1:C:294:ILE:CD1	1:C:318:ALA:HB3	2.38	0.53
1:A:313:LEU:HD11	1:C:324:LYS:HE3	1.91	0.53
1:A:324:LYS:HD3	1:C:313:LEU:HD21	1.91	0.53
1:A:322:ILE:HG23	1:A:385:GLU:HB2	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:397:VAL:HG13	1:C:401:VAL:CG2	2.38	0.53
1:A:104:LEU:CD2	1:A:203:VAL:HG13	2.39	0.53
1:B:165:SER:CB	1:B:166:PRO:HD3	2.39	0.53
1:C:15:ARG:O	1:C:19:VAL:HG23	2.09	0.53
1:B:50:VAL:HG21	1:B:58:VAL:HG11	1.90	0.52
1:A:104:LEU:HD11	1:A:108:TYR:CE1	2.44	0.52
1:A:110:TRP:CE3	1:A:170:LEU:HD22	2.44	0.52
1:B:17:VAL:HG12	1:B:18:GLN:N	2.23	0.52
1:A:274:LEU:HD13	1:A:351:ILE:HD12	1.92	0.52
1:C:239:SER:OG	1:C:240:LYS:O	2.27	0.52
1:A:153:TRP:CD2	1:A:274:LEU:HD21	2.44	0.52
1:A:396:HIS:CE1	1:A:400:ASN:ND2	2.78	0.52
1:A:290:TYR:O	1:A:291:SER:HB2	2.11	0.51
1:A:87:ASP:O	1:A:88:THR:HG22	2.11	0.51
1:A:7:LEU:CD2	1:A:71:VAL:HG22	2.40	0.51
1:A:348:ASP:OD2	1:A:361:THR:OG1	2.29	0.51
1:C:93:ALA:HB2	1:C:113:PHE:HE1	1.75	0.51
1:C:32:TRP:HB3	1:C:290:TYR:OH	2.11	0.51
1:A:118:HIS:CE1	1:A:177:THR:CG2	2.90	0.50
1:A:322:ILE:HG21	1:A:331:TYR:CD2	2.46	0.50
1:C:241:HIS:O	1:C:344:PRO:HB2	2.11	0.50
1:C:165:SER:CB	1:C:166:PRO:HD3	2.42	0.50
1:C:325:THR:HG21	1:C:385:GLU:HA	1.92	0.50
1:C:87:ASP:O	1:C:88:THR:CG2	2.57	0.50
1:A:89:VAL:HG12	1:A:90:SER:N	2.26	0.50
1:C:223:TYR:CD1	1:C:259:LEU:HD11	2.46	0.50
1:A:121:MET:CE	1:A:176:ILE:HG22	2.42	0.50
1:A:198:MET:CE	1:A:201:VAL:HA	2.42	0.50
1:A:147:THR:CG2	1:A:149:LYS:HZ2	2.22	0.49
1:A:366:ASP:HB2	1:A:374:LEU:HD13	1.94	0.49
1:C:151:ALA:HA	1:C:194:ASP:O	2.12	0.49
1:C:93:ALA:HB2	1:C:113:PHE:CE1	2.47	0.49
1:C:76:VAL:HG13	1:C:373:LEU:HD11	1.93	0.49
1:B:54:ASP:HB3	1:B:58:VAL:HG23	1.95	0.49
1:A:198:MET:HE2	1:A:201:VAL:HA	1.94	0.49
1:C:168:PHE:CE1	1:C:386:ALA:HB3	2.47	0.49
1:A:369:THR:O	1:A:370:TYR:CG	2.66	0.49
1:B:73:LEU:HD22	1:B:79:LEU:HD11	1.94	0.49
1:A:12:ARG:O	1:A:42:LYS:HG2	2.12	0.49
1:A:147:THR:CG2	1:A:149:LYS:NZ	2.76	0.49
1:C:93:ALA:CB	1:C:113:PHE:HE1	2.25	0.49
2:C:604:NAG:H82	2:C:604:NAG:O3	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:289:SER:OG	1:B:290:TYR:N	2.46	0.49
1:A:311:LEU:HD21	1:A:357:LYS:O	2.13	0.49
1:C:54:ASP:O	1:C:58:VAL:HG23	2.13	0.49
1:C:138:VAL:HG22	1:C:198:MET:HB2	1.95	0.49
1:C:294:ILE:HD11	1:C:315:ALA:O	2.13	0.48
1:C:183:ILE:HB	1:C:186:TYR:CD2	2.48	0.48
1:A:176:ILE:HG21	1:A:190:LEU:HD11	1.95	0.48
1:A:108:TYR:OH	1:A:203:VAL:HG11	2.14	0.48
1:C:251:SER:HA	1:C:256:TYR:CG	2.48	0.48
1:C:183:ILE:HB	1:C:186:TYR:HD2	1.79	0.48
1:B:139:LEU:HD13	1:B:173:ILE:HD13	1.95	0.48
1:A:104:LEU:HD22	1:A:203:VAL:HG13	1.94	0.48
1:A:153:TRP:CE3	1:A:274:LEU:HD21	2.49	0.48
1:A:31:LEU:HD23	1:A:48:PHE:HB3	1.96	0.48
1:A:192:LEU:HD12	1:A:398:ILE:HD13	1.96	0.48
1:C:366:ASP:OD2	1:C:370:TYR:N	2.41	0.48
1:C:165:SER:HB3	1:C:166:PRO:HD3	1.95	0.48
1:B:278:ILE:HD11	1:B:354:LEU:HG	1.95	0.48
1:C:127:ILE:HD12	1:C:269:ALA:CB	2.43	0.48
1:A:313:LEU:HD11	1:C:324:LYS:HE2	1.94	0.48
1:C:122:LEU:HD21	1:C:173:ILE:HG23	1.96	0.48
1:B:73:LEU:HD22	1:B:79:LEU:CD1	2.44	0.48
1:B:213:ASN:OD1	1:B:213:ASN:C	2.52	0.47
1:B:1:ALA:HB2	2:B:602:NAG:H83	1.96	0.47
1:A:165:SER:O	1:A:166:PRO:C	2.52	0.47
1:A:318:ALA:O	1:A:321:ALA:HB3	2.14	0.47
1:A:37:ALA:O	1:A:40:ILE:HG13	2.15	0.47
1:B:209:SER:HA	1:B:213:ASN:O	2.14	0.47
1:B:389:ALA:O	1:B:393:ILE:HG23	2.15	0.47
1:B:76:VAL:O	1:B:77:GLU:C	2.53	0.47
4:B:660:GEM:HC52	4:B:660:GEM:C9	2.44	0.47
1:A:139:LEU:HD23	1:A:139:LEU:N	2.30	0.47
1:B:104:LEU:CD1	1:B:203:VAL:HG22	2.45	0.47
1:C:62:LEU:HD23	1:C:67:ILE:CD1	2.45	0.47
1:A:114:ILE:CG2	1:A:115:THR:N	2.77	0.47
1:C:73:LEU:HD22	1:C:79:LEU:CD1	2.44	0.47
1:C:348:ASP:OD2	4:C:660:GEM:N2	2.48	0.47
1:A:219:ASN:ND2	1:A:221:SER:OG	2.47	0.47
1:B:20:LEU:O	1:B:21:GLN:C	2.53	0.47
1:A:192:LEU:HD13	1:A:398:ILE:HG21	1.96	0.46
1:A:219:ASN:O	1:A:220:ARG:HG2	2.15	0.46
1:A:189:LEU:HD12	1:A:189:LEU:C	2.36	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:165:SER:O	1:C:168:PHE:N	2.44	0.46
1:C:30:VAL:HG11	1:C:215:MET:HB3	1.96	0.46
1:C:209:SER:HA	1:C:213:ASN:O	2.15	0.46
1:A:200:VAL:CG1	1:A:203:VAL:HG22	2.44	0.46
1:B:278:ILE:HG23	1:B:279:ASN:ND2	2.30	0.46
1:B:356:ILE:HD13	1:B:356:ILE:HA	1.75	0.46
1:B:7:LEU:N	1:B:7:LEU:HD23	2.31	0.46
1:C:164:ILE:HD11	1:C:382:THR:CG2	2.34	0.46
1:A:171:TRP:O	1:A:175:HIS:HB2	2.16	0.46
1:B:222:PHE:HB3	1:B:229:ILE:HG23	1.98	0.46
1:B:189:LEU:CD1	1:B:398:ILE:HD11	2.46	0.46
1:A:93:ALA:HB2	1:A:113:PHE:CE1	2.50	0.46
1:A:279:ASN:N	1:A:279:ASN:HD22	2.14	0.45
1:B:278:ILE:HG23	1:B:279:ASN:HD22	1.81	0.45
1:C:302:ARG:HG2	1:C:342:LEU:HD11	1.98	0.45
1:B:35:VAL:HG21	1:B:341:TYR:OH	2.15	0.45
1:A:200:VAL:HG12	1:A:203:VAL:CG2	2.46	0.45
1:B:278:ILE:CD1	1:B:354:LEU:HG	2.45	0.45
1:B:281:ILE:HG22	1:B:356:ILE:HG13	1.97	0.45
1:C:280:GLN:OE1	1:C:280:GLN:N	2.50	0.45
1:C:110:TRP:CH2	1:C:170:LEU:HD22	2.49	0.45
1:C:184:GLY:HA2	1:C:187:THR:HB	1.98	0.45
1:A:391:SER:HB3	1:C:399:ARG:NH2	2.31	0.45
1:B:104:LEU:HD11	1:B:203:VAL:HG22	1.98	0.45
1:B:200:VAL:O	1:B:203:VAL:HG23	2.16	0.45
1:B:205:GLY:O	1:B:206:TYR:C	2.54	0.45
1:A:300:TYR:O	1:A:342:LEU:HD21	2.17	0.45
1:B:165:SER:CB	1:B:166:PRO:CD	2.94	0.45
1:B:351:ILE:CD1	1:B:356:ILE:HB	2.47	0.45
1:B:294:ILE:HD13	1:B:318:ALA:HB3	1.99	0.45
1:B:32:TRP:CE2	1:B:215:MET:HE1	2.52	0.45
1:B:7:LEU:HD22	1:B:71:VAL:HG22	1.97	0.45
1:B:72:LEU:HD12	1:B:72:LEU:HA	1.78	0.45
1:B:173:ILE:HD11	1:B:197:VAL:HB	1.98	0.45
1:A:240:LYS:HB2	1:A:300:TYR:CE1	2.52	0.45
1:C:295:VAL:HG21	1:C:340:LEU:HD12	1.99	0.45
1:C:173:ILE:O	1:C:177:THR:HG23	2.17	0.45
1:A:380:LYS:HB3	1:A:381:PRO:HD3	1.99	0.45
1:B:52:ALA:HA	1:B:55:VAL:HG23	1.98	0.44
1:B:51:ASN:O	1:B:55:VAL:HG23	2.17	0.44
1:C:87:ASP:O	1:C:88:THR:CB	2.65	0.44
1:C:296:PHE:HB2	1:C:297:PRO:CD	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:296:PHE:HB2	1:C:297:PRO:HD2	1.98	0.44
1:C:380:LYS:HB3	1:C:381:PRO:CD	2.47	0.44
1:C:90:SER:HB2	1:C:91:PRO:HD2	1.98	0.44
1:A:108:TYR:CZ	1:A:135:PRO:HD2	2.53	0.44
1:B:385:GLU:O	1:B:388:ALA:N	2.51	0.44
1:A:199:PRO:O	1:A:200:VAL:HG23	2.18	0.44
1:A:90:SER:HB2	1:A:91:PRO:CD	2.48	0.44
1:B:395:TRP:HA	1:B:398:ILE:HD12	1.99	0.44
1:C:94:SER:OG	1:C:97:TYR:HB2	2.18	0.44
1:C:92:ARG:O	1:C:93:ALA:HB3	2.17	0.44
1:B:94:SER:O	1:B:95:ALA:C	2.56	0.44
1:B:73:LEU:CD1	1:B:373:LEU:HD12	2.48	0.43
1:B:161:ARG:O	1:B:163:TRP:N	2.51	0.43
1:C:52:ALA:HA	1:C:55:VAL:HG23	2.00	0.43
1:B:165:SER:HB3	1:B:166:PRO:CD	2.46	0.43
1:C:208:TYR:CE1	1:C:212:LYS:HB2	2.53	0.43
1:B:17:VAL:HG22	1:B:40:ILE:HG22	2.00	0.43
1:C:156:CYS:HB2	1:C:199:PRO:O	2.18	0.43
1:C:340:LEU:HD11	1:C:363:GLU:OE1	2.18	0.43
1:C:274:LEU:HD13	1:C:351:ILE:CD1	2.42	0.43
1:C:76:VAL:HG13	1:C:373:LEU:CD1	2.48	0.43
1:C:295:VAL:HG13	1:C:336:GLY:CA	2.49	0.43
1:B:334:GLY:HA3	1:B:339:THR:OG1	2.19	0.43
1:B:287:MET:SD	1:B:362:ILE:HD12	2.58	0.43
1:A:348:ASP:OD1	1:A:349:ASP:N	2.52	0.43
1:C:251:SER:HA	1:C:256:TYR:CD1	2.54	0.43
1:B:329:THR:HG21	1:B:365:ARG:NH2	2.34	0.43
1:A:170:LEU:O	1:A:171:TRP:C	2.57	0.43
1:A:104:LEU:CD2	1:A:203:VAL:CG1	2.97	0.43
1:C:33:GLN:NE2	1:C:47:HIS:CE1	2.87	0.42
1:B:215:MET:HE3	1:B:215:MET:HA	1.99	0.42
1:A:87:ASP:C	1:A:88:THR:HG22	2.39	0.42
1:C:348:ASP:N	1:C:348:ASP:OD1	2.51	0.42
1:A:278:ILE:CG2	1:A:279:ASN:N	2.81	0.42
1:C:294:ILE:HD11	1:C:318:ALA:HB3	2.01	0.42
1:B:6:VAL:C	1:B:7:LEU:HD23	2.39	0.42
1:A:33:GLN:C	1:A:34:PRO:O	2.57	0.42
1:A:271:ALA:HB1	1:A:275:ARG:HH12	1.83	0.42
1:A:190:LEU:HA	1:A:190:LEU:HD23	1.87	0.42
1:C:184:GLY:O	1:C:185:GLN:C	2.58	0.42
1:C:360:PHE:CD2	1:C:393:ILE:HD13	2.55	0.42
1:C:319:VAL:O	1:C:319:VAL:CG1	2.68	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:112:GLU:HB3	1:C:116:GLU:OE2	2.19	0.42
1:A:110:TRP:CE3	1:A:170:LEU:CD2	3.03	0.42
1:B:168:PHE:HA	1:B:383:CYS:SG	2.59	0.42
1:C:322:ILE:HA	1:C:325:THR:HG22	2.02	0.42
1:A:184:GLY:O	1:A:186:TYR:N	2.53	0.41
1:A:348:ASP:CG	4:A:660:GEM:HN42	2.24	0.41
1:C:360:PHE:CD2	1:C:360:PHE:N	2.87	0.41
1:A:131:PHE:C	1:A:133:LYS:H	2.24	0.41
1:A:75:ASP:OD1	1:A:75:ASP:C	2.59	0.41
1:A:328:ASN:N	1:A:328:ASN:OD1	2.53	0.41
1:C:354:LEU:HD23	1:C:354:LEU:O	2.20	0.41
1:B:313:LEU:HD23	1:B:317:GLU:OE1	2.20	0.41
1:C:380:LYS:HB3	1:C:381:PRO:HD3	2.02	0.41
1:B:325:THR:HG21	1:B:385:GLU:CA	2.47	0.41
1:C:295:VAL:HG13	1:C:336:GLY:HA2	2.03	0.41
1:B:206:TYR:O	1:B:209:SER:OG	2.19	0.41
1:A:114:ILE:CG2	1:A:122:LEU:HD13	2.51	0.41
1:B:177:THR:HG22	1:B:178:GLN:N	2.36	0.41
1:B:213:ASN:OD1	1:B:215:MET:N	2.48	0.41
1:B:238:ALA:HB2	1:B:261:PRO:HB3	2.03	0.41
1:B:244:GLU:O	1:B:245:GLU:C	2.59	0.41
1:A:202:ASN:HB2	1:A:233:LEU:HD12	2.03	0.41
1:B:138:VAL:HG22	1:B:198:MET:HB2	2.03	0.41
1:C:246:GLY:HA3	1:C:344:PRO:HD3	2.02	0.41
1:C:27:TYR:CD2	1:C:58:VAL:HG22	2.55	0.41
1:B:351:ILE:HD12	1:B:356:ILE:HB	2.02	0.41
1:B:78:ASP:OD1	1:B:82:GLN:NE2	2.47	0.41
1:B:305:SER:O	1:B:308:HIS:N	2.54	0.41
1:A:3:SER:HB2	1:A:77:GLU:HB2	2.03	0.41
1:A:169:CYS:HB3	1:A:199:PRO:HB3	2.02	0.41
1:A:139:LEU:HD12	1:A:173:ILE:HD13	2.00	0.40
1:A:112:GLU:O	1:A:115:THR:HG22	2.21	0.40
1:A:183:ILE:HB	1:A:186:TYR:CD2	2.55	0.40
1:A:153:TRP:C	1:A:153:TRP:CD1	2.93	0.40
1:A:156:CYS:N	1:A:198:MET:O	2.53	0.40
1:B:6:VAL:HB	1:B:73:LEU:HB2	2.03	0.40
1:C:168:PHE:CD2	1:C:168:PHE:C	2.94	0.40
1:A:293:HIS:HA	1:A:332:THR:O	2.21	0.40
1:C:78:ASP:O	1:C:82:GLN:N	2.42	0.40
1:A:223:TYR:CG	1:A:259:LEU:HD11	2.56	0.40
1:A:176:ILE:CG2	1:A:190:LEU:HD11	2.51	0.40
1:B:218:LYS:HE3	1:B:230:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:121:MET:HE3	1:B:176:ILE:CG2	2.51	0.40
2:C:601:NAG:O3	2:C:601:NAG:H83	2.21	0.40
1:B:295:VAL:HG12	1:B:296:PHE:N	2.36	0.40
1:B:223:TYR:CG	1:B:259:LEU:HD11	2.56	0.40
1:C:360:PHE:CE2	1:C:393:ILE:HD13	2.57	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%)	337 (84%)	45 (11%)	17 (4%)	4	40
1	B	399/424 (94%)	338 (85%)	42 (10%)	19 (5%)	4	36
1	C	399/424 (94%)	337 (84%)	42 (10%)	20 (5%)	3	34
All	All	1197/1272 (94%)	1012 (84%)	129 (11%)	56 (5%)	4	36

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	PRO
1	A	219	ASN
1	A	224	ALA
1	A	243	CYS
1	A	291	SER
1	A	297	PRO
1	A	370	TYR
1	B	34	PRO
1	B	94	SER
1	B	219	ASN
1	B	224	ALA
1	B	290	TYR
1	B	297	PRO
1	B	336	GLY

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Mol	Chain	Res	Type
1	C	34	PRO
1	C	219	ASN
1	C	224	ALA
1	C	290	TYR
1	C	366	ASP
1	A	93	ALA
1	A	185	GLN
1	A	336	GLY
1	B	42	LYS
1	B	291	SER
1	B	327	LYS
1	C	245	GLU
1	C	291	SER
1	C	297	PRO
1	A	42	LYS
1	A	148	ALA
1	A	371	GLY
1	B	77	GLU
1	B	89	VAL
1	B	95	ALA
1	B	162	GLU
1	C	38	ASP
1	C	42	LYS
1	C	93	ALA
1	C	328	ASN
1	C	364	LEU
1	C	368	GLY
1	A	366	ASP
1	B	146	GLN
1	B	376	GLU
1	C	88	THR
1	C	371	GLY
1	A	191	ARG
1	C	148	ALA
1	C	327	LYS
1	C	377	ARG
1	A	290	TYR
1	B	306	LYS
1	B	350	TRP
1	B	366	ASP
1	A	200	VAL
1	C	17	VAL

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%)	318 (90%)	36 (10%)	11	46
1	B	354/375 (94%)	312 (88%)	42 (12%)	8	36
1	C	354/375 (94%)	327 (92%)	27 (8%)	19	64
All	All	1062/1125 (94%)	957 (90%)	105 (10%)	11	47

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	24	THR
1	A	45	GLN
1	A	61	HIS
1	A	69	CYS
1	A	72	LEU
1	A	96	SER
1	A	105	ASN
1	A	109	SER
1	A	115	THR
1	A	125	ILE
1	A	145	GLU
1	A	147	THR
1	A	149	LYS
1	A	185	GLN
1	A	189	LEU
1	A	191	ARG
1	A	221	SER
1	A	239	SER
1	A	243	CYS
1	A	250	SER
1	A	264	GLU
1	A	291	SER
1	A	297	PRO
1	A	300	TYR
1	A	301	THR
1	A	305	SER

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Mol	Chain	Res	Type
1	A	307	ASP
1	A	328	ASN
1	A	329	THR
1	A	332	THR
1	A	335	HIS
1	A	366	ASP
1	A	369	THR
1	A	384	ARG
1	A	401	VAL
1	B	14	SER
1	B	17	VAL
1	B	25	THR
1	B	36	THR
1	B	69	CYS
1	B	70	SER
1	B	72	LEU
1	B	79	LEU
1	B	88	THR
1	B	105	ASN
1	B	109	SER
1	B	123	THR
1	B	125	ILE
1	B	145	GLU
1	B	147	THR
1	B	158	ILE
1	B	170	LEU
1	B	176	ILE
1	B	177	THR
1	B	222	PHE
1	B	236	ASN
1	B	240	LYS
1	B	257	CYS
1	B	259	LEU
1	B	278	ILE
1	B	289	SER
1	B	294	ILE
1	B	297	PRO
1	B	302	ARG
1	B	313	LEU
1	B	317	GLU
1	B	327	LYS
1	B	329	THR

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Mol	Chain	Res	Type
1	B	332	THR
1	B	335	HIS
1	B	351	ILE
1	B	359	SER
1	B	366	ASP
1	B	369	THR
1	B	384	ARG
1	B	393	ILE
1	B	399	ARG
1	C	13	THR
1	C	24	THR
1	C	26	THR
1	C	51	ASN
1	C	72	LEU
1	C	88	THR
1	C	123	THR
1	C	125	ILE
1	C	133	LYS
1	C	147	THR
1	C	164	ILE
1	C	176	ILE
1	C	189	LEU
1	C	193	VAL
1	C	239	SER
1	C	291	SER
1	C	297	PRO
1	C	305	SER
1	C	313	LEU
1	C	326	SER
1	C	327	LYS
1	C	328	ASN
1	C	332	THR
1	C	341	TYR
1	C	369	THR
1	C	376	GLU
1	C	384	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	57	ASN

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Mol	Chain	Res	Type
1	A	100	GLN
1	A	118	HIS
1	A	185	GLN
1	A	279	ASN
1	A	292	GLN
1	A	308	HIS
1	A	396	HIS
1	A	400	ASN
1	B	279	ASN
1	B	308	HIS
1	C	33	GLN
1	C	45	GLN
1	C	100	GLN
1	C	188	ASN
1	C	226	ASN
1	C	292	GLN
1	C	308	HIS
1	C	400	ASN

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	0.83	1 (8%)	15,19,21	1.06	1 (6%)
2	NAG	A	602	1	12,14,15	0.59	0	15,19,21	1.73	2 (13%)
2	NAG	A	603	1	12,14,15	0.90	1 (8%)	15,19,21	2.02	4 (26%)
2	NAG	A	604	1	12,14,15	0.53	0	15,19,21	1.53	2 (13%)
4	GEM	A	660	3	14,14,14	0.76	0	17,17,17	0.84	0
2	NAG	B	601	1	12,14,15	0.89	1 (8%)	15,19,21	1.34	2 (13%)
2	NAG	B	602	1	12,14,15	1.06	1 (8%)	15,19,21	1.52	1 (6%)
2	NAG	B	603	1	12,14,15	0.51	0	15,19,21	1.09	1 (6%)
2	NAG	B	604	1	12,14,15	0.56	0	15,19,21	1.11	1 (6%)
4	GEM	B	660	3	14,14,14	0.78	0	17,17,17	1.25	2 (11%)
2	NAG	C	601	1	12,14,15	0.53	0	15,19,21	1.25	1 (6%)
2	NAG	C	602	1	12,14,15	0.90	1 (8%)	15,19,21	1.89	5 (33%)
2	NAG	C	604	1	12,14,15	0.51	0	15,19,21	1.34	2 (13%)
4	GEM	C	660	3	14,14,14	0.78	0	17,17,17	0.87	1 (5%)

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	-	2/6/23/26	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	GEM	A	660	3	-	0/15/15/15	0/0/0/0
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1
2	NAG	B	602	1	-	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	GEM	B	660	3	-	0/15/15/15	0/0/0/0
2	NAG	C	601	1	1/1/5/7	2/6/23/26	1/1/1/1
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	GEM	C	660	3	-	0/15/15/15	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	NAG	O5-C5	-2.54	1.40	1.45
2	B	601	NAG	C2-N2	2.17	1.48	1.46
2	C	602	NAG	C2-N2	2.12	1.48	1.46
2	A	601	NAG	O5-C5	-2.06	1.41	1.45
2	A	603	NAG	O5-C5	-2.06	1.41	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	NAG	O5-C5-C4	-5.81	103.28	110.65
2	A	604	NAG	O5-C5-C6	4.80	112.01	106.98
2	B	602	NAG	O5-C5-C4	-4.69	104.70	110.65
2	C	602	NAG	O5-C5-C6	4.56	111.76	106.98
2	A	602	NAG	O5-C5-C6	4.52	111.72	106.98
2	A	602	NAG	C3-C2-N2	-4.30	105.21	111.76
2	C	601	NAG	O5-C5-C6	4.06	111.24	106.98
2	C	602	NAG	C2-N2-C7	3.45	128.88	123.09
2	C	604	NAG	O5-C5-C6	3.24	110.38	106.98
2	B	604	NAG	O5-C5-C4	3.06	114.54	110.65
4	B	660	GEM	C9-C8-S7	2.99	117.67	109.04
2	B	603	NAG	O5-C5-C6	2.88	110.00	106.98
4	B	660	GEM	C10-C8-C9	-2.87	106.04	111.85
2	B	601	NAG	O5-C5-C4	2.61	113.97	110.65
2	A	603	NAG	O5-C5-C6	2.50	109.60	106.98
2	C	602	NAG	O7-C7-C8	-2.49	117.19	122.04
2	B	601	NAG	O5-C5-C6	2.44	109.54	106.98
2	A	603	NAG	O3-C3-C2	2.40	114.12	109.09
2	A	604	NAG	C3-C2-N2	-2.36	108.17	111.76
2	C	602	NAG	O5-C5-C4	-2.29	107.75	110.65
2	A	603	NAG	O4-C4-C5	2.25	115.22	109.28
4	C	660	GEM	C10-C8-S7	2.22	114.69	107.92
2	A	601	NAG	O5-C5-C4	-2.15	107.92	110.65
2	C	602	NAG	O7-C7-N2	2.14	126.37	121.90
2	C	604	NAG	O5-C5-C4	2.04	113.25	110.65

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	603	NAG	C1
2	C	601	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	NAG	C8-C7-N2-C2
2	A	601	NAG	O7-C7-N2-C2
2	C	601	NAG	O7-C7-N2-C2
2	A	601	NAG	C8-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	NAG	C1-C2-C3-C4-C5-O5

5.7 Other polymers ⓘ

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%)	0.04	4 (0%)	79 44	94, 116, 129, 138	0
1	B	401/424 (94%)	0.08	7 (1%)	67 31	97, 115, 142, 153	0
1	C	401/424 (94%)	0.08	6 (1%)	70 33	90, 119, 139, 148	0
All	All	1203/1272 (94%)	0.07	17 (1%)	70 35	90, 117, 137, 153	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	342	LEU	3.6
1	B	2	GLN	2.7
1	C	12	ARG	2.5
1	B	338	GLU	2.4
1	A	137	TYR	2.4
1	C	1	ALA	2.3
1	B	148	ALA	2.3
1	C	15	ARG	2.3
1	B	302	ARG	2.2
1	B	5	GLN	2.2
1	A	300	TYR	2.1
1	C	304	LYS	2.1
1	C	303	SER	2.1
1	B	341	TYR	2.1
1	A	5	GLN	2.0
1	C	42	LYS	2.0
1	A	298	TYR	2.0

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
2	NAG	A	603	14/15	0.38	50.11	116,121,122,122	0
2	NAG	A	601	14/15	0.61	6.03	129,130,131,131	0
2	NAG	A	604	14/15	0.48	2.98	97,99,100,101	0
2	NAG	B	603	14/15	0.31	2.79	122,122,123,124	0
2	NAG	C	601	14/15	0.46	2.14	133,134,134,134	0
2	NAG	C	604	14/15	0.40	1.95	87,91,92,93	0
2	NAG	C	602	14/15	0.40	0.87	133,135,136,136	0
4	GEM	C	660	15/15	0.27	0.54	116,122,124,125	0
3	ZN	A	501	1/1	0.28	0.46	117,117,117,117	0
2	NAG	B	601	14/15	0.24	0.30	106,110,112,113	0
4	GEM	A	660	15/15	0.25	0.25	102,107,112,112	0
3	ZN	B	501	1/1	0.28	0.01	120,120,120,120	0
2	NAG	A	602	14/15	0.25	-0.16	127,129,131,131	0
4	GEM	B	660	15/15	0.23	-0.17	121,124,126,126	0
3	ZN	C	501	1/1	0.25	-0.59	126,126,126,126	0
2	NAG	B	602	14/15	0.25	-0.62	122,123,126,127	0
2	NAG	B	604	14/15	0.34	-0.77	111,112,114,114	0

6.5 Other polymers ⓘ

There are no such residues in this entry.