



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:12 AM UTC

PDB ID : 1TYE / pdb_00001tye
Title : Structural basis for allostery in integrins and binding of ligand-mimetic therapeutics to the platelet receptor for fibrinogen
Authors : Xiao, T.; Takagi, J.; Collier, B.S.; Wang, J.-H.; Springer, T.A.
Deposited on : 2004-07-07
Resolution : 2.90 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

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

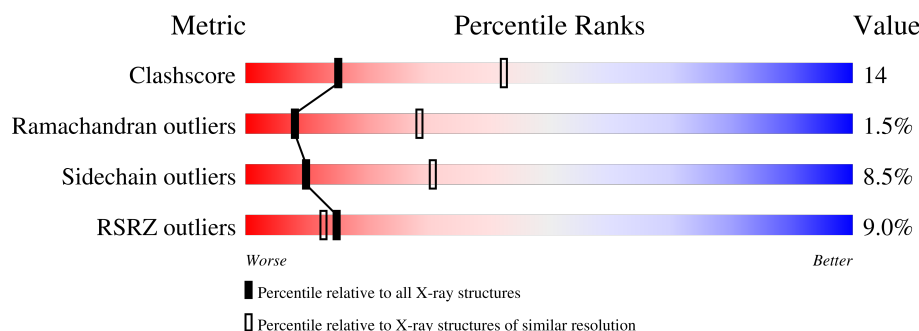
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	452	5% 72% 22% 5%
1	C	452	3% 70% 24% • •
1	E	452	2% 71% 23% 5%
2	B	440	12% 62% 32% 5%
2	D	440	12% 69% 25% 5%
2	F	440	20% 71% 24% • •

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Mol	Chain	Length	Quality of chain
3	G	4	
3	I	4	
4	H	5	

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
3	NAG	I	2	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 21019 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 Integrin alpha-IIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3468	2203	597	660	8			
1	C	452	Total	C	N	O	S	0	0	0
			3468	2203	597	660	8			
1	E	452	Total	C	N	O	S	0	0	0
			3468	2203	597	660	8			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	440	Total	C	N	O	S	0	0	0
			3400	2125	574	672	29			
2	D	440	Total	C	N	O	S	0	0	0
			3400	2125	574	672	29			
2	F	440	Total	C	N	O	S	0	0	0
			3400	2125	574	672	29			

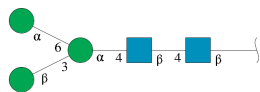
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	I	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose]

se-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

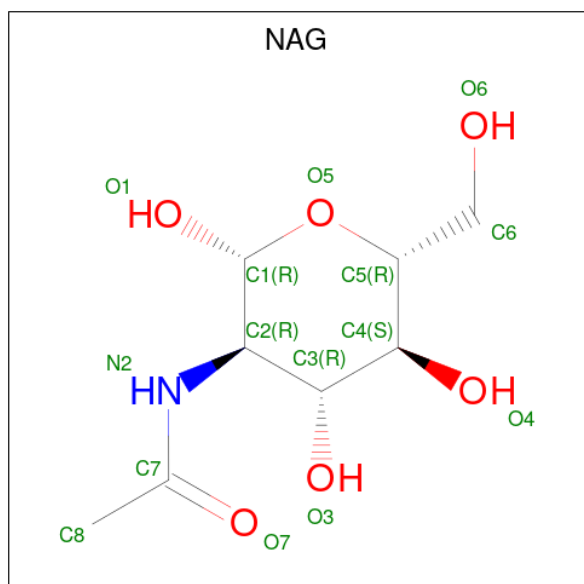


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

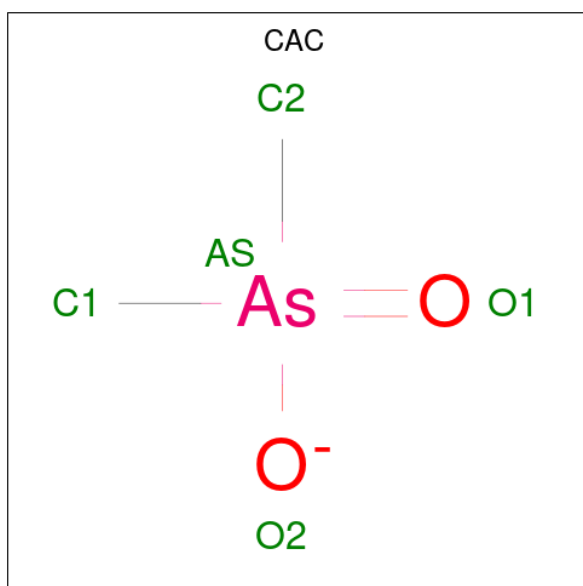
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Ca	0	0
			4	4		
5	B	2	Total	Ca	0	0
			2	2		
5	C	4	Total	Ca	0	0
			4	4		
5	D	2	Total	Ca	0	0
			2	2		
5	E	4	Total	Ca	0	0
			4	4		
5	F	2	Total	Ca	0	0
			2	2		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	As	C	O	0	0
			5	1	2	2		
7	D	1	Total	As	C	O	0	0
			5	1	2	2		
7	F	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total 1	Mg 1	0	0
8	D	1	Total 1	Mg 1	0	0
8	F	1	Total 1	Mg 1	0	0

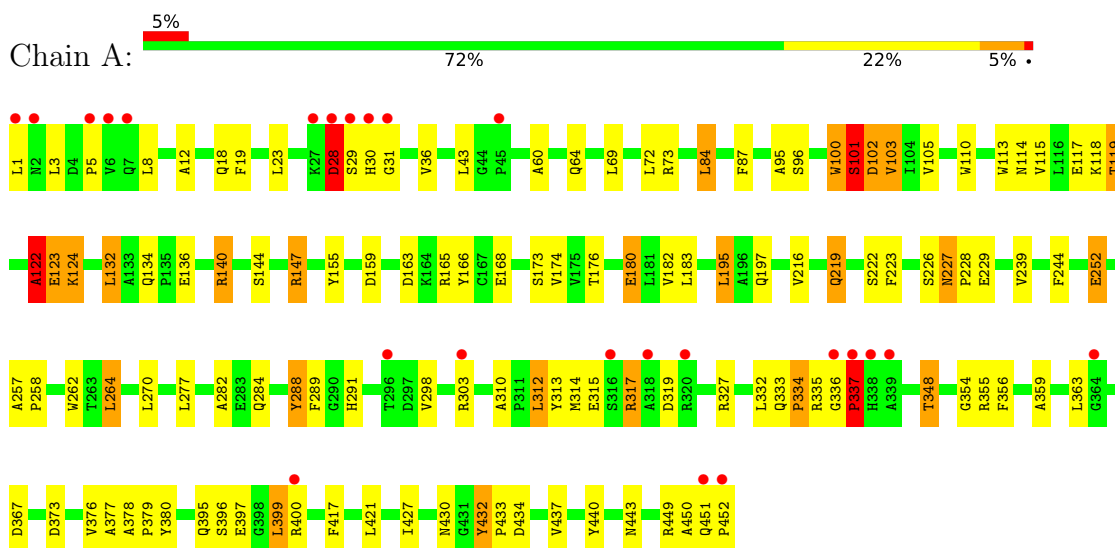
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	22	Total 22	O 22	0	0
9	B	16	Total 16	O 16	0	0
9	C	20	Total 20	O 20	0	0
9	D	19	Total 19	O 19	0	0
9	E	28	Total 28	O 28	0	0
9	F	15	Total 15	O 15	0	0

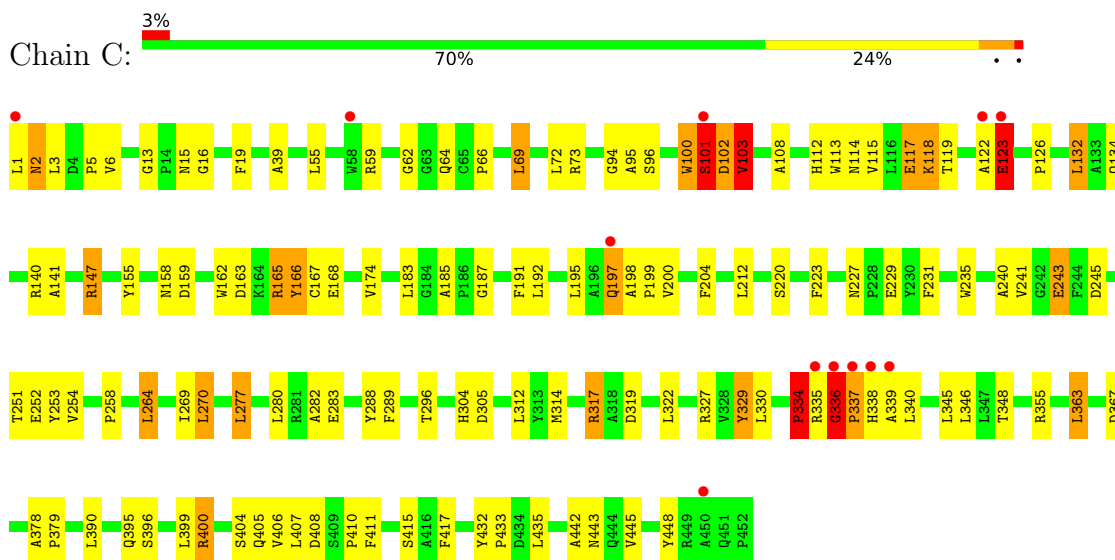
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Integrin alpha-IIb

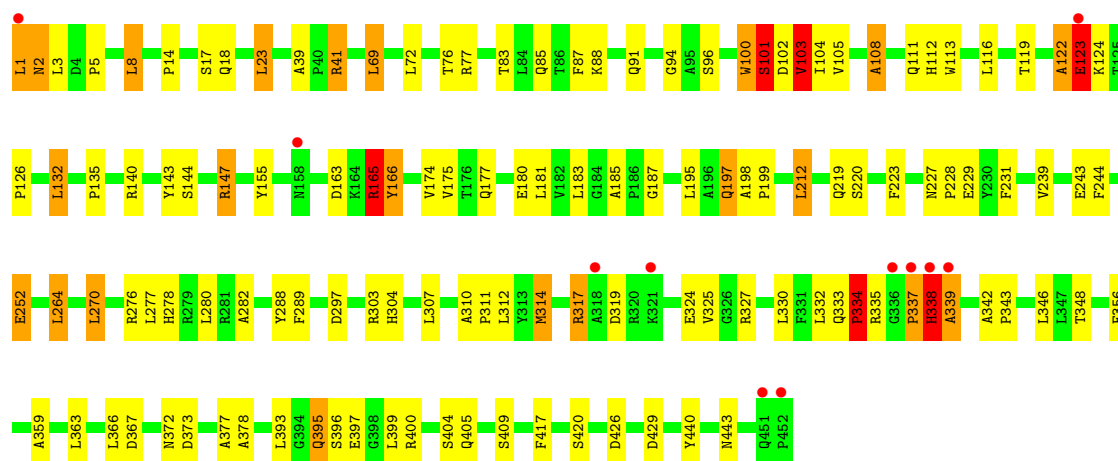


• Molecule 1: Integrin alpha-IIb

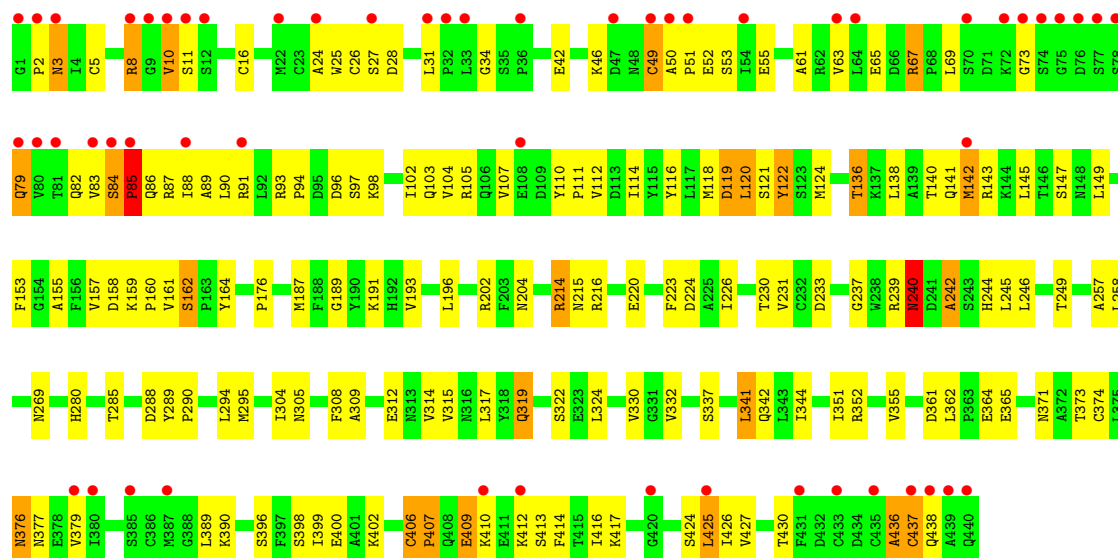


• Molecule 1: Integrin alpha-IIb

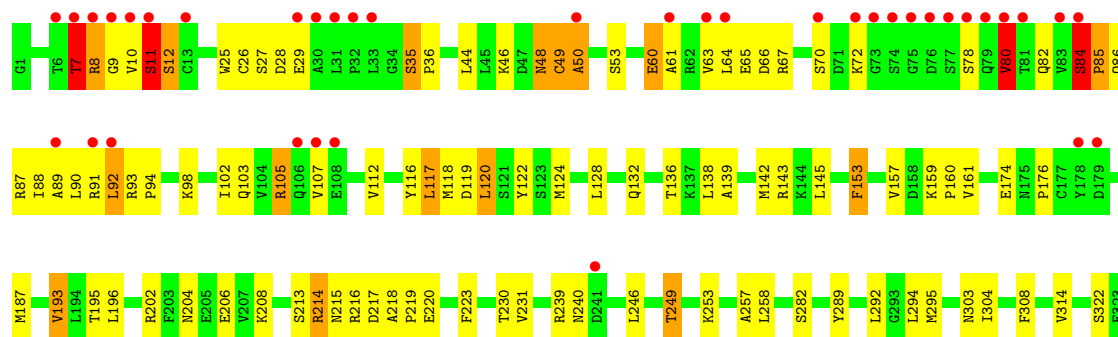


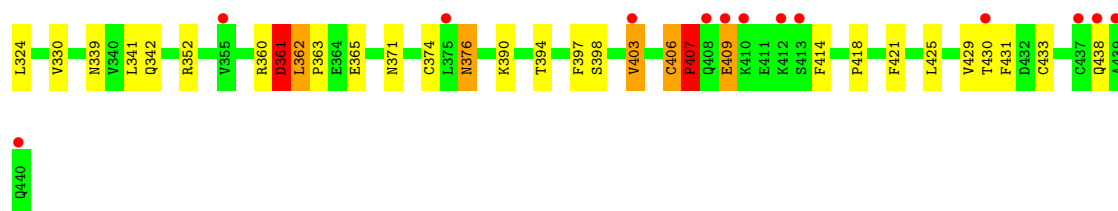


• Molecule 2: Integrin beta-3

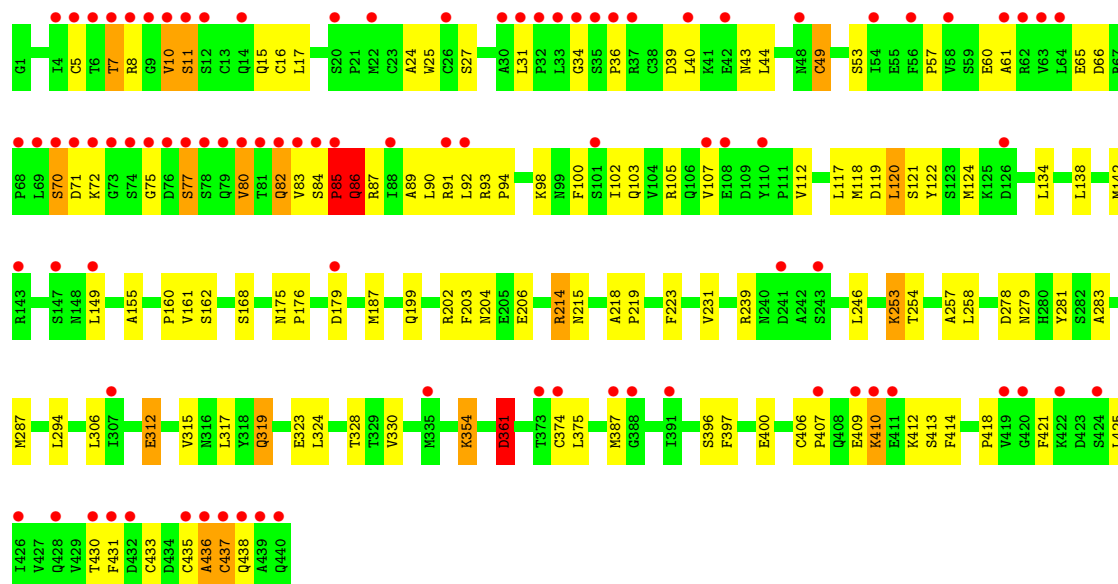


• Molecule 2: Integrin beta-3





• Molecule 2: Integrin beta-3



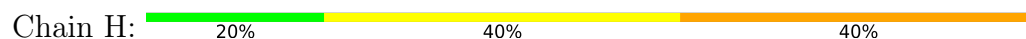
• Molecule 3: beta-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: beta-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 4: beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	332.09Å 332.09Å 88.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-2.90) 98.2 (50.00-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.254 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21019	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CAC, MAN, BMA, MG, 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	0.85	16/3564 (0.4%)	1.24	36/4857 (0.7%)
1	C	0.91	9/3564 (0.3%)	1.28	37/4857 (0.8%)
1	E	0.83	4/3564 (0.1%)	1.23	34/4857 (0.7%)
2	B	0.49	0/3461	1.04	22/4693 (0.5%)
2	D	0.76	8/3461 (0.2%)	1.21	29/4693 (0.6%)
2	F	0.50	0/3461	1.10	25/4693 (0.5%)
All	All	0.75	37/21075 (0.2%)	1.19	183/28650 (0.6%)

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	C	0	5
1	E	0	3
2	D	0	3
2	F	0	1
All	All	0	16

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	117	GLU	CA-C	29.25	1.84	1.53
2	D	85	PRO	N-CD	28.30	1.87	1.47
1	A	122	ALA	C-N	-23.32	1.04	1.33
1	E	123	GLU	C-N	-22.42	0.96	1.33
1	E	122	ALA	C-N	21.65	1.64	1.33
1	E	100	TRP	C-N	-19.14	1.06	1.33
1	C	101	SER	C-N	-19.07	1.06	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	100	TRP	C-N	-17.19	1.09	1.33
1	A	101	SER	CB-OG	14.38	1.71	1.42
1	C	118	LYS	N-CA	-12.44	1.30	1.46
1	A	123	GLU	C-N	11.41	1.49	1.33
1	A	123	GLU	CB-CG	10.70	1.84	1.52
1	C	122	ALA	C-O	-10.60	1.11	1.24
1	C	123	GLU	N-CA	10.14	1.59	1.46
2	D	7	THR	C-N	-9.57	1.19	1.33
1	A	122	ALA	N-CA	9.39	1.55	1.46
1	A	124	LYS	N-CA	-9.37	1.34	1.46
1	C	122	ALA	C-N	-8.57	1.21	1.33
1	A	123	GLU	C-O	8.12	1.33	1.23
2	D	84	SER	C-N	-7.20	1.17	1.33
1	A	123	GLU	N-CA	6.91	1.54	1.46
1	A	123	GLU	CA-C	-6.87	1.44	1.52
1	C	122	ALA	CA-C	6.76	1.61	1.52
1	C	123	GLU	C-N	-6.72	1.24	1.33
1	A	102	ASP	N-CA	6.49	1.54	1.46
2	D	8	ARG	CB-CG	-6.01	1.34	1.52
2	D	10	VAL	CA-C	-5.78	1.45	1.52
1	A	334	PRO	N-CD	5.55	1.55	1.47
2	D	85	PRO	CB-CG	5.40	1.76	1.49
1	A	28	ASP	CB-CG	-5.33	1.38	1.52
2	D	85	PRO	C-N	5.31	1.41	1.34
1	A	451	GLN	CB-CG	-5.22	1.36	1.52
1	A	101	SER	C-N	5.21	1.41	1.34
1	E	314	MET	SD-CE	5.18	1.92	1.79
1	A	122	ALA	C-O	5.17	1.30	1.23
1	A	451	GLN	C-N	-5.10	1.26	1.34
2	D	9	GLY	C-N	-5.03	1.26	1.33

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	101	SER	O-C-N	-29.89	82.84	122.59
1	A	122	ALA	O-C-N	-24.58	97.70	121.79
2	D	84	SER	CA-C-N	23.94	149.76	119.84
2	D	84	SER	C-N-CA	23.94	149.76	119.84
1	E	123	GLU	O-C-N	-22.16	93.12	122.59
2	D	84	SER	O-C-N	-17.81	100.84	121.32
1	E	100	TRP	O-C-N	-17.15	102.43	123.36
1	A	102	ASP	N-CA-C	16.91	131.16	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	334	PRO	CA-N-CD	-16.48	88.93	112.00
1	C	100	TRP	O-C-N	-16.07	103.66	123.27
1	E	100	TRP	CA-C-N	16.04	152.18	121.54
1	E	100	TRP	C-N-CA	16.04	152.18	121.54
2	B	84	SER	C-N-CD	-15.07	63.23	125.00
2	D	85	PRO	CA-N-CD	-14.56	91.61	112.00
2	F	436	ALA	N-CA-C	-14.22	91.35	110.55
1	A	122	ALA	CA-C-N	13.91	147.07	121.62
1	A	122	ALA	C-N-CA	13.91	147.07	121.62
1	C	100	TRP	CA-C-N	13.20	146.76	121.54
1	C	100	TRP	C-N-CA	13.20	146.76	121.54
1	C	101	SER	CA-C-N	12.90	146.18	121.54
1	C	101	SER	C-N-CA	12.90	146.18	121.54
1	A	122	ALA	N-CA-C	-12.45	92.78	111.34
1	C	117	GLU	O-C-N	12.18	138.73	123.14
1	A	337	PRO	CA-N-CD	-11.39	96.06	112.00
2	B	409	GLU	N-CA-C	-11.24	93.10	109.96
1	A	122	ALA	CA-C-O	-11.01	107.29	119.40
2	F	77	SER	N-CA-C	-11.00	93.43	109.59
2	F	72	LYS	N-CA-C	10.82	126.52	110.30
2	F	85	PRO	CB-CA-C	10.73	129.27	111.56
2	F	7	THR	N-CA-C	10.55	124.28	111.40
2	F	82	GLN	OE1-CD-NE2	-10.09	112.51	122.60
2	D	409	GLU	N-CA-C	-10.08	95.09	110.10
1	E	334	PRO	CA-N-CD	-9.84	98.22	112.00
1	E	333	GLN	OE1-CD-NE2	-9.79	112.81	122.60
2	F	86	GLN	OE1-CD-NE2	-9.55	113.05	122.60
1	E	122	ALA	O-C-N	9.52	132.37	122.09
1	C	337	PRO	CA-N-CD	-9.43	98.80	112.00
1	A	28	ASP	CA-CB-CG	9.31	121.91	112.60
1	C	102	ASP	N-CA-C	9.28	130.57	110.80
1	C	122	ALA	CA-C-N	9.21	139.12	121.54
1	C	122	ALA	C-N-CA	9.21	139.12	121.54
2	F	409	GLU	N-CA-C	-8.97	96.74	110.10
2	B	2	PRO	N-CA-C	-8.95	97.14	111.19
1	A	123	GLU	CA-C-N	-8.89	108.83	121.72
1	A	123	GLU	C-N-CA	-8.89	108.83	121.72
2	F	11	SER	N-CA-C	8.74	129.43	110.80
2	D	85	PRO	N-CA-CB	8.68	112.36	103.25
1	A	334	PRO	N-CA-CB	8.57	111.33	103.19
1	C	122	ALA	O-C-N	8.53	132.50	122.17
1	C	123	GLU	O-C-N	-8.51	111.27	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	85	PRO	N-CA-CB	-8.47	94.35	103.25
1	C	122	ALA	CB-CA-C	8.39	124.88	110.79
1	C	69	LEU	N-CA-C	8.29	122.25	110.23
1	C	103	VAL	N-CA-C	8.13	121.67	108.99
1	A	102	ASP	N-CA-CB	-8.12	97.72	110.22
1	E	103	VAL	N-CA-C	8.10	121.52	108.97
2	B	84	SER	CB-CA-C	7.97	120.90	108.63
1	E	123	GLU	CA-C-N	7.87	133.78	122.85
1	E	123	GLU	C-N-CA	7.87	133.78	122.85
2	B	79	GLN	N-CA-C	-7.83	94.13	110.80
2	D	85	PRO	N-CD-CG	-7.79	91.52	103.20
1	E	101	SER	N-CA-CB	-7.75	97.39	110.49
2	D	406	CYS	CA-C-N	7.72	127.76	119.89
2	D	406	CYS	C-N-CA	7.72	127.76	119.89
2	D	11	SER	N-CA-C	7.58	121.38	110.24
1	E	165	ARG	N-CA-C	7.38	119.33	111.28
1	E	378	ALA	CA-C-N	7.37	129.05	119.84
1	E	378	ALA	C-N-CA	7.37	129.05	119.84
1	E	339	ALA	N-CA-C	7.36	119.62	109.18
2	F	410	LYS	N-CA-C	-7.29	103.99	114.12
2	F	82	GLN	CG-CD-NE2	7.24	127.25	116.40
1	E	337	PRO	CA-N-CD	-7.14	102.00	112.00
1	C	223	PHE	N-CA-C	7.07	120.53	110.14
1	A	95	ALA	N-CA-C	-7.01	104.72	113.20
1	E	223	PHE	N-CA-C	6.99	120.41	110.14
2	D	78	SER	N-CA-C	6.87	119.79	111.82
2	F	86	GLN	CG-CD-NE2	6.83	126.64	116.40
1	E	333	GLN	CG-CD-NE2	6.81	126.61	116.40
1	C	117	GLU	CA-C-O	-6.78	111.32	120.47
1	A	101	SER	CA-C-N	-6.71	110.62	120.28
1	A	101	SER	C-N-CA	-6.71	110.62	120.28
2	D	85	PRO	N-CA-C	-6.68	98.71	112.47
1	A	123	GLU	O-C-N	6.66	130.54	123.42
1	A	103	VAL	N-CA-C	6.65	118.99	108.89
1	C	39	ALA	CA-C-N	6.64	128.14	119.84
1	C	39	ALA	C-N-CA	6.64	128.14	119.84
2	F	80	VAL	N-CA-C	6.59	117.59	108.89
1	E	123	GLU	CA-CB-CG	6.54	127.19	114.10
1	A	100	TRP	O-C-N	-6.53	115.39	123.36
2	D	60	GLU	N-CA-C	6.50	121.03	111.34
2	D	240	ASN	N-CA-C	6.49	118.89	111.11
2	D	8	ARG	CA-C-N	6.48	126.25	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	8	ARG	C-N-CA	6.48	126.25	120.10
1	E	338	HIS	N-CA-C	6.43	120.72	109.80
2	D	231	VAL	N-CA-C	6.41	119.18	112.83
2	F	231	VAL	N-CA-C	6.31	118.95	112.90
1	A	378	ALA	CA-C-N	6.25	127.66	119.84
1	A	378	ALA	C-N-CA	6.25	127.66	119.84
1	A	134	GLN	CA-C-N	6.15	127.53	119.84
1	A	134	GLN	C-N-CA	6.15	127.53	119.84
1	E	185	ALA	CA-C-N	6.15	126.61	119.47
1	E	185	ALA	C-N-CA	6.15	126.61	119.47
2	F	175	ASN	CA-C-N	6.13	125.83	119.82
2	F	175	ASN	C-N-CA	6.13	125.83	119.82
1	C	108	ALA	CA-C-N	6.12	125.81	119.56
1	C	108	ALA	C-N-CA	6.12	125.81	119.56
2	B	319	GLN	N-CA-C	-6.05	104.60	111.14
1	A	144	SER	CA-C-N	5.99	125.69	119.82
1	A	144	SER	C-N-CA	5.99	125.69	119.82
1	E	310	ALA	CA-C-N	5.95	127.27	119.84
1	E	310	ALA	C-N-CA	5.95	127.27	119.84
2	F	85	PRO	CA-C-N	5.86	129.97	120.60
2	F	85	PRO	C-N-CA	5.86	129.97	120.60
1	E	363	LEU	N-CA-C	-5.83	103.01	110.53
1	A	310	ALA	CA-C-N	5.83	127.12	119.84
1	A	310	ALA	C-N-CA	5.83	127.12	119.84
2	D	80	VAL	N-CA-C	5.82	117.54	109.45
2	D	282	SER	N-CA-C	5.80	119.53	112.23
2	B	118	MET	N-CA-C	5.78	118.15	108.96
2	B	406	CYS	CA-C-N	5.70	125.65	119.78
2	B	406	CYS	C-N-CA	5.70	125.65	119.78
2	D	217	ASP	N-CA-C	5.68	118.74	109.59
1	E	69	LEU	N-CA-C	5.68	118.52	110.50
2	B	84	SER	N-CA-C	-5.64	102.33	110.40
2	F	361	ASP	N-CA-C	5.63	122.78	110.80
1	C	159	ASP	N-CA-C	-5.62	104.38	111.92
1	C	192	LEU	N-CA-C	-5.62	104.78	111.69
1	A	168	GLU	N-CA-C	-5.61	104.40	111.92
2	B	85	PRO	O-C-N	-5.60	115.08	122.64
1	A	110	TRP	N-CA-C	5.55	119.75	112.92
1	E	108	ALA	CA-C-N	5.55	125.23	119.56
1	E	108	ALA	C-N-CA	5.55	125.23	119.56
2	D	193	VAL	N-CA-C	5.53	116.92	111.67
2	D	85	PRO	O-C-N	-5.52	115.18	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	LEU	N-CA-C	-5.51	102.75	110.35
2	B	410	LYS	N-CA-C	-5.48	106.59	113.72
1	C	191	PHE	N-CA-C	5.48	121.46	113.40
1	A	257	ALA	CA-C-N	5.45	126.65	119.84
1	A	257	ALA	C-N-CA	5.45	126.65	119.84
2	B	162	SER	N-CA-C	-5.45	102.72	109.64
1	C	334	PRO	N-CD-CG	5.43	111.34	103.20
2	F	118	MET	N-CA-C	5.41	118.44	109.46
2	B	8	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	C	378	ALA	CA-C-N	5.38	126.56	119.84
1	C	378	ALA	C-N-CA	5.38	126.56	119.84
1	C	336	GLY	C-N-CD	-5.37	102.98	125.00
1	A	432	TYR	CA-C-N	5.36	125.28	119.76
1	A	432	TYR	C-N-CA	5.36	125.28	119.76
2	D	85	PRO	CA-CB-CG	-5.34	94.34	104.50
1	C	378	ALA	N-CA-C	-5.34	101.07	108.76
1	C	134	GLN	CA-C-N	5.34	126.51	119.84
1	C	134	GLN	C-N-CA	5.34	126.51	119.84
1	E	144	SER	CA-C-N	5.30	125.01	119.82
1	E	144	SER	C-N-CA	5.30	125.01	119.82
1	A	12	ALA	N-CA-C	5.25	117.17	109.24
2	B	10	VAL	N-CA-C	5.24	120.24	109.34
1	E	119	THR	N-CA-C	5.23	119.29	113.01
1	A	173	SER	N-CA-C	5.22	116.78	108.79
2	B	231	VAL	N-CA-C	5.22	118.80	112.80
2	D	407	PRO	N-CA-C	5.22	119.41	111.11
1	C	119	THR	N-CA-C	5.21	120.56	113.37
2	F	312	GLU	N-CA-C	5.21	117.63	111.33
2	B	242	ALA	N-CA-C	5.19	118.14	110.46
2	D	153	PHE	N-CA-C	5.16	116.14	108.60
2	B	224	ASP	N-CA-C	-5.15	105.75	111.36
2	F	83	VAL	CA-C-N	5.13	129.88	121.57
2	F	83	VAL	C-N-CA	5.13	129.88	121.57
1	A	223	PHE	N-CA-C	5.13	117.95	109.85
2	B	244	HIS	N-CA-C	5.11	117.04	107.99
2	D	48	ASN	N-CA-C	5.07	118.61	111.52
2	D	35	SER	CA-C-N	5.06	124.82	119.76
2	D	35	SER	C-N-CA	5.06	124.82	119.76
2	B	85	PRO	N-CA-C	5.04	122.86	112.47
1	C	168	GLU	N-CA-C	-5.04	104.36	111.56
1	E	39	ALA	CA-C-N	5.03	126.13	119.84
1	E	39	ALA	C-N-CA	5.03	126.13	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	44	LEU	N-CA-C	-5.03	107.09	113.43
1	E	85	GLN	N-CA-C	5.03	117.60	109.06
1	C	95	ALA	N-CA-C	-5.02	107.21	113.19
2	D	118	MET	N-CA-C	5.01	117.40	109.24
2	B	119	ASP	N-CA-C	-5.00	100.92	108.67
2	B	122	TYR	N-CA-C	5.00	116.73	111.28
1	C	363	LEU	N-CA-C	-5.00	103.33	110.59

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	TRP	Mainchain
1	A	122	ALA	Mainchain,Peptide
1	A	28	ASP	Mainchain
1	C	100	TRP	Mainchain,Peptide
1	C	101	SER	Mainchain,Peptide
1	C	123	GLU	Mainchain
2	D	11	SER	Mainchain
2	D	84	SER	Mainchain,Peptide
1	E	100	TRP	Mainchain,Peptide
1	E	123	GLU	Mainchain
2	F	361	ASP	Mainchain

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	3468	0	3300	86	0
1	C	3468	0	3299	80	0
1	E	3468	0	3297	84	0
2	B	3400	0	3350	117	0
2	D	3400	0	3350	96	0
2	F	3400	0	3350	88	0
3	G	50	0	43	6	0
3	I	50	0	43	9	0
4	H	61	0	52	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	0	0	0
5	B	2	0	0	0	0
5	C	4	0	0	0	0
5	D	2	0	0	0	0
5	E	4	0	0	0	0
5	F	2	0	0	0	0
6	B	28	0	26	2	0
6	D	28	0	26	0	0
6	E	14	0	13	0	0
6	F	28	0	26	3	0
7	B	5	0	0	1	0
7	D	5	0	0	1	0
7	F	5	0	0	1	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
9	A	22	0	0	1	0
9	B	16	0	0	0	0
9	C	20	0	0	1	0
9	D	19	0	0	0	0
9	E	28	0	0	1	0
9	F	15	0	0	0	0
All	All	21019	0	20175	559	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 14.

All (559) 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)
2:D:85:PRO:CB	2:D:85:PRO:CG	1.76	1.59
1:A:123:GLU:CG	1:A:123:GLU:CB	1.84	1.52
1:C:117:GLU:C	1:C:117:GLU:CA	1.84	1.50
1:A:101:SER:CB	1:A:101:SER:OG	1.70	1.38
2:D:85:PRO:CD	2:D:85:PRO:N	1.87	1.37
1:E:91:GLN:HG2	1:E:108:ALA:HB1	1.32	1.11
2:F:66:ASP:HA	2:F:86:GLN:HE22	1.16	1.07
2:F:84:SER:HB2	2:F:103:GLN:H	1.19	1.05
1:A:303:ARG:HD2	1:A:335:ARG:HE	1.21	1.02
2:D:85:PRO:CD	2:D:85:PRO:CA	2.37	1.02
2:F:84:SER:HB3	2:F:85:PRO:HD2	1.41	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:25:TRP:HE1	2:D:27:SER:HB2	1.30	0.96
2:D:85:PRO:CG	2:D:85:PRO:CA	2.44	0.95
2:F:84:SER:HB3	2:F:85:PRO:CD	2.00	0.91
2:B:61:ALA:HB2	2:B:90:LEU:HD12	1.52	0.89
1:E:395:GLN:HG2	1:E:397:GLU:H	1.41	0.85
2:D:61:ALA:HB2	2:D:90:LEU:HD12	1.59	0.85
2:B:67:ARG:H	2:B:67:ARG:HD2	1.41	0.85
2:D:91:ARG:HG2	2:D:430:THR:HB	1.59	0.84
2:F:66:ASP:HA	2:F:86:GLN:NE2	1.91	0.84
1:A:303:ARG:HB2	1:A:335:ARG:HH21	1.43	0.83
2:F:412:LYS:HE2	2:F:413:SER:H	1.43	0.81
2:D:84:SER:C	2:D:85:PRO:CD	2.52	0.81
3:G:1:NAG:H61	3:G:2:NAG:H82	1.63	0.80
2:D:84:SER:HB2	2:D:103:GLN:H	1.44	0.80
1:E:278:HIS:CE1	1:E:339:ALA:HB1	2.17	0.80
2:D:376:ASN:H	2:D:376:ASN:HD22	1.28	0.80
1:A:101:SER:OG	1:A:102:ASP:N	2.15	0.79
2:D:63:VAL:HA	2:D:88:ILE:HG22	1.63	0.79
1:A:264:LEU:O	1:A:282:ALA:HB3	1.84	0.78
2:D:361:ASP:O	2:D:414:PHE:HB3	1.83	0.78
2:D:27:SER:HB3	2:D:438:GLN:HB3	1.66	0.77
1:E:1:LEU:HA	1:E:367:ASP:HB3	1.67	0.77
2:F:84:SER:CB	2:F:85:PRO:CD	2.60	0.77
1:E:264:LEU:O	1:E:282:ALA:HB3	1.85	0.76
2:D:85:PRO:O	2:D:425:LEU:HD13	1.85	0.76
1:C:227:ASN:HD21	1:C:229:GLU:HG3	1.51	0.76
1:C:245:ASP:HA	1:C:338:HIS:HE1	1.48	0.76
2:D:112:VAL:HG11	2:D:142:MET:HE2	1.68	0.75
2:B:365:GLU:HG3	2:B:407:PRO:HG3	1.69	0.75
2:F:112:VAL:HG11	2:F:142:MET:HE2	1.69	0.75
1:A:163:ASP:OD1	1:A:165:ARG:HD3	1.86	0.74
2:B:85:PRO:O	2:B:425:LEU:HD13	1.86	0.74
2:B:412:LYS:HE2	2:B:413:SER:H	1.52	0.74
2:B:361:ASP:OD2	2:B:414:PHE:HA	1.88	0.74
2:D:85:PRO:CG	2:D:85:PRO:N	2.45	0.73
2:B:91:ARG:HG3	2:B:430:THR:HB	1.68	0.73
1:E:122:ALA:O	1:E:123:GLU:HB2	1.87	0.73
2:B:373:THR:HG22	2:B:379:VAL:HG22	1.71	0.73
1:C:16:GLY:H	1:C:443:ASN:HD21	1.37	0.73
2:F:375:LEU:HD12	2:F:375:LEU:H	1.54	0.73
2:B:84:SER:OG	2:B:103:GLN:HG3	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:HG22	1:A:132:LEU:HD13	1.71	0.72
2:F:436:ALA:HB3	2:F:438:GLN:NE2	2.03	0.72
2:D:26:CYS:HB2	2:D:44:LEU:HD13	1.72	0.72
2:B:3:ASN:HD21	2:B:5:CYS:HB2	1.54	0.71
2:F:85:PRO:O	2:F:425:LEU:HD13	1.90	0.71
1:A:303:ARG:HD2	1:A:335:ARG:NE	2.02	0.71
2:F:93:ARG:HB2	2:F:94:PRO:HD2	1.72	0.70
2:F:134:LEU:O	2:F:138:LEU:HB2	1.92	0.70
1:E:359:ALA:HB3	1:E:377:ALA:HB3	1.74	0.69
1:A:303:ARG:HB2	1:A:335:ARG:NH2	2.07	0.69
2:D:136:THR:HA	2:D:204:ASN:HD21	1.58	0.69
1:E:91:GLN:HG2	1:E:108:ALA:CB	2.19	0.69
3:I:3:MAN:H3	3:I:4:BMA:O2	1.91	0.69
1:A:114:ASN:HD22	1:A:115:VAL:H	1.41	0.68
2:F:119:ASP:HB3	2:F:124:MET:HE2	1.75	0.68
1:A:119:THR:CG2	1:A:119:THR:O	2.40	0.68
2:D:25:TRP:NE1	2:D:27:SER:HB2	2.08	0.68
2:D:215:ASN:HB3	7:D:1302:CAC:C1	2.22	0.68
1:C:395:GLN:HG2	1:C:396:SER:N	2.08	0.68
2:D:8:ARG:CZ	2:D:8:ARG:HB2	2.23	0.68
2:F:160:PRO:HA	2:F:187:MET:HE2	1.75	0.68
1:A:1:LEU:HD13	1:A:367:ASP:HB3	1.73	0.68
1:A:312:LEU:HD22	2:B:258:LEU:HD12	1.75	0.68
2:D:93:ARG:HB2	2:D:94:PRO:HD2	1.76	0.68
3:I:1:NAG:H61	3:I:2:NAG:C8	2.24	0.67
2:B:104:VAL:HG21	2:B:355:VAL:HG11	1.76	0.67
2:B:337:SER:O	2:B:341:LEU:HD23	1.95	0.67
4:H:1:NAG:C6	4:H:2:NAG:H82	2.24	0.67
1:A:303:ARG:CD	1:A:335:ARG:HE	2.02	0.67
2:B:82:GLN:NE2	2:B:107:VAL:HG12	2.10	0.66
1:A:332:LEU:O	1:A:334:PRO:HD3	1.95	0.66
2:B:83:VAL:HG22	2:B:104:VAL:HG12	1.78	0.66
2:D:376:ASN:HD22	2:D:376:ASN:N	1.92	0.66
2:B:111:PRO:HB2	2:B:242:ALA:HB2	1.77	0.66
1:E:278:HIS:CE1	1:E:339:ALA:CB	2.78	0.66
1:C:163:ASP:OD1	1:C:165:ARG:HD3	1.96	0.66
2:D:176:PRO:HB2	2:D:214:ARG:HB2	1.78	0.65
1:A:122:ALA:O	1:A:123:GLU:HG3	1.97	0.65
2:B:365:GLU:HG3	2:B:407:PRO:CG	2.25	0.65
2:F:400:GLU:HB2	6:F:1020:NAG:H81	1.78	0.65
2:D:11:SER:O	2:D:12:SER:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:PRO:CB	2:D:85:PRO:CD	2.66	0.64
2:D:218:ALA:HB3	2:D:219:PRO:HD3	1.80	0.64
2:B:63:VAL:HA	2:B:88:ILE:HG22	1.79	0.64
2:D:92:LEU:HD13	2:D:403:VAL:HG11	1.78	0.64
2:F:66:ASP:CG	2:F:85:PRO:HG3	2.23	0.63
1:E:105:VAL:HG22	1:E:132:LEU:HD13	1.81	0.63
2:F:306:LEU:HB3	2:F:328:THR:HG22	1.81	0.63
2:F:84:SER:HB2	2:F:103:GLN:N	2.02	0.63
1:A:227:ASN:C	1:A:227:ASN:HD22	2.05	0.63
2:B:376:ASN:HD22	2:B:376:ASN:N	1.96	0.63
2:F:61:ALA:HA	2:F:89:ALA:O	1.99	0.63
2:D:84:SER:CB	2:D:85:PRO:HD2	2.29	0.63
1:E:338:HIS:ND1	1:E:338:HIS:N	2.47	0.62
2:F:218:ALA:HB3	2:F:219:PRO:HD3	1.80	0.62
2:D:8:ARG:HB2	2:D:8:ARG:NH1	2.14	0.62
1:A:69:LEU:O	1:A:140:ARG:NH1	2.32	0.62
1:E:227:ASN:ND2	1:E:229:GLU:H	1.98	0.62
2:B:230:THR:HG23	2:B:304:ILE:HD12	1.82	0.61
1:C:243:GLU:H	1:C:304:HIS:CD2	2.18	0.61
1:C:317:ARG:HG2	1:C:317:ARG:HH11	1.64	0.61
2:D:61:ALA:HA	2:D:89:ALA:O	2.00	0.61
2:B:122:TYR:HB2	2:B:214:ARG:HG2	1.83	0.61
1:C:16:GLY:H	1:C:443:ASN:ND2	1.98	0.61
4:H:1:NAG:H62	4:H:2:NAG:H82	1.80	0.61
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.81	0.61
1:E:180:GLU:HB3	1:E:197:GLN:HE22	1.66	0.61
2:F:215:ASN:HB3	7:F:1303:CAC:C1	2.31	0.61
2:D:28:ASP:CG	2:D:29:GLU:H	2.09	0.60
1:E:227:ASN:C	1:E:227:ASN:HD22	2.08	0.60
2:B:436:ALA:HB3	2:B:438:GLN:NE2	2.15	0.60
2:D:94:PRO:HB3	2:D:406:CYS:HB2	1.82	0.60
2:B:31:LEU:HD11	2:B:49:CYS:SG	2.42	0.60
2:B:61:ALA:HA	2:B:89:ALA:O	2.01	0.60
1:C:55:LEU:O	1:C:66:PRO:HD2	2.02	0.60
3:I:2:NAG:H3	3:I:3:MAN:O5	2.00	0.60
1:E:69:LEU:O	1:E:140:ARG:NH1	2.35	0.59
2:F:8:ARG:HH11	2:F:8:ARG:HG3	1.67	0.59
1:A:114:ASN:ND2	1:A:115:VAL:H	2.00	0.59
1:A:155:TYR:CE2	1:A:165:ARG:HD2	2.37	0.59
2:B:65:GLU:HG2	2:B:87:ARG:HB3	1.84	0.59
2:B:436:ALA:C	2:B:438:GLN:HE21	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:176:PRO:HB2	2:F:214:ARG:HB2	1.83	0.59
2:F:437:CYS:O	2:F:437:CYS:SG	2.60	0.59
2:D:361:ASP:O	2:D:414:PHE:CB	2.51	0.59
2:F:436:ALA:HB3	2:F:438:GLN:HE21	1.66	0.59
1:A:317:ARG:HH11	1:A:317:ARG:HG2	1.67	0.59
1:A:119:THR:O	1:A:119:THR:HG22	2.00	0.59
2:B:371:ASN:HB2	2:B:398:SER:HB3	1.85	0.58
1:C:117:GLU:CA	1:C:118:LYS:N	2.61	0.58
2:B:337:SER:HB2	2:B:341:LEU:HD23	1.85	0.58
1:C:117:GLU:C	1:C:117:GLU:N	2.58	0.58
1:E:303:ARG:HD2	1:E:334:PRO:O	2.03	0.58
2:F:31:LEU:HD21	2:F:49:CYS:SG	2.43	0.58
2:F:354:LYS:HB3	2:F:387:MET:HG2	1.86	0.58
1:A:113:TRP:CE3	1:A:147:ARG:HD2	2.37	0.58
1:E:88:LYS:O	1:E:91:GLN:HB2	2.03	0.58
1:E:155:TYR:CE2	1:E:165:ARG:HD2	2.39	0.58
1:A:227:ASN:ND2	1:A:229:GLU:H	2.01	0.58
2:F:5:CYS:HB2	2:F:39:ASP:HA	1.84	0.58
1:E:41:ARG:HG2	1:E:41:ARG:HH11	1.69	0.58
1:E:426:ASP:CG	1:E:429:ASP:HA	2.28	0.58
1:A:30:HIS:HB3	1:E:429:ASP:OD2	2.04	0.57
1:A:101:SER:OG	1:A:101:SER:CA	2.50	0.57
2:D:418:PRO:HG2	2:D:421:PHE:HB2	1.87	0.57
1:A:395:GLN:CD	1:A:396:SER:H	2.13	0.57
2:F:61:ALA:HB2	2:F:90:LEU:HD12	1.87	0.57
1:E:3:LEU:O	1:E:5:PRO:HD3	2.03	0.57
1:C:330:LEU:HD22	1:C:399:LEU:HD12	1.85	0.57
1:C:334:PRO:HB2	1:C:338:HIS:HA	1.87	0.57
1:E:317:ARG:HG2	1:E:317:ARG:HH11	1.69	0.57
2:F:17:LEU:HD13	2:F:57:PRO:HG2	1.87	0.57
1:C:245:ASP:HA	1:C:338:HIS:CE1	2.36	0.57
2:D:219:PRO:HG3	2:D:253:LYS:HG3	1.86	0.57
2:F:27:SER:O	2:F:53:SER:HB2	2.05	0.57
2:F:122:TYR:HB2	2:F:214:ARG:HG2	1.87	0.57
3:G:2:NAG:O3	3:G:3:MAN:H5	2.03	0.57
1:E:180:GLU:HB3	1:E:197:GLN:NE2	2.20	0.57
1:E:41:ARG:HH11	1:E:41:ARG:CG	2.18	0.56
2:D:407:PRO:HB2	2:D:431:PHE:CE2	2.40	0.56
1:C:19:PHE:CE1	1:C:445:VAL:HG23	2.41	0.56
2:B:84:SER:HB2	2:B:103:GLN:H	1.69	0.56
2:D:136:THR:HA	2:D:204:ASN:ND2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:3:MAN:H3	3:G:4:BMA:O2	2.05	0.56
3:I:2:NAG:C3	3:I:3:MAN:O5	2.54	0.56
2:B:82:GLN:HB2	2:B:105:ARG:O	2.05	0.56
2:F:10:VAL:HB	2:F:15:GLN:NE2	2.21	0.56
2:B:8:ARG:O	2:B:10:VAL:HG23	2.06	0.56
2:B:223:PHE:CD2	2:B:295:MET:HE1	2.41	0.56
1:C:264:LEU:O	1:C:282:ALA:HB3	2.07	0.55
2:B:161:VAL:HG23	2:B:285:THR:HG22	1.88	0.55
1:A:216:VAL:O	1:A:219:GLN:HB3	2.05	0.55
2:B:400:GLU:HB2	6:B:1006:NAG:H83	1.87	0.55
1:C:340:LEU:HD12	1:C:340:LEU:H	1.71	0.55
1:C:13:GLY:HA3	1:C:19:PHE:CD2	2.40	0.55
1:C:404:SER:O	1:C:405:GLN:HB2	2.05	0.55
2:D:82:GLN:NE2	2:D:107:VAL:HG12	2.20	0.55
1:E:166:TYR:O	1:E:187:GLY:HA3	2.05	0.55
4:H:3:MAN:H3	4:H:4:BMA:O2	2.07	0.55
1:E:2:ASN:N	1:E:2:ASN:HD22	2.05	0.55
1:C:243:GLU:H	1:C:304:HIS:HD2	1.55	0.55
2:B:158:ASP:O	2:B:189:GLY:HA2	2.06	0.55
1:C:114:ASN:ND2	1:C:115:VAL:H	2.05	0.55
1:C:243:GLU:HB2	1:C:304:HIS:HD2	1.72	0.55
2:D:102:ILE:HG22	2:D:397:PHE:HB2	1.89	0.55
1:A:18:GLN:H	1:A:443:ASN:HD21	1.54	0.54
1:C:197:GLN:NE2	1:C:220:SER:HB3	2.20	0.54
2:D:70:SER:OG	2:D:80:VAL:HG22	2.07	0.54
2:B:390:LYS:H	2:B:390:LYS:HD2	1.73	0.54
1:C:69:LEU:O	1:C:140:ARG:NH1	2.39	0.54
1:C:390:LEU:HG	1:C:406:VAL:HG22	1.90	0.54
2:B:161:VAL:CG2	2:B:285:THR:HG22	2.38	0.54
1:E:2:ASN:HD22	1:E:2:ASN:H	1.56	0.54
1:E:395:GLN:HG2	1:E:397:GLU:N	2.19	0.54
1:A:303:ARG:CB	1:A:335:ARG:HH21	2.18	0.54
1:E:124:LYS:N	2:F:168:SER:HG	2.05	0.54
1:E:244:PHE:HB2	1:E:252:GLU:HG3	1.90	0.54
2:F:10:VAL:HB	2:F:15:GLN:HE22	1.71	0.54
2:D:82:GLN:HB2	2:D:105:ARG:O	2.08	0.54
1:E:2:ASN:HB2	1:E:405:GLN:OE1	2.08	0.54
2:F:361:ASP:O	2:F:414:PHE:HB3	2.08	0.53
2:B:257:ALA:O	2:B:258:LEU:HB2	2.09	0.53
1:C:3:LEU:H	1:C:405:GLN:HE22	1.56	0.53
1:C:379:PRO:HA	1:C:417:PHE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:CYS:SG	2:B:24:ALA:O	2.66	0.53
2:D:66:ASP:HB2	2:D:85:PRO:HD3	1.90	0.53
1:E:227:ASN:HD22	1:E:228:PRO:N	2.06	0.53
2:B:161:VAL:HG12	2:B:162:SER:O	2.09	0.53
2:F:7:THR:HG22	2:F:8:ARG:HG3	1.91	0.53
1:A:262:TRP:CD1	2:B:317:LEU:HD12	2.44	0.53
2:D:223:PHE:CE2	2:D:295:MET:HE1	2.44	0.53
2:D:122:TYR:HB2	2:D:213:SER:O	2.09	0.52
2:D:157:VAL:O	2:D:220:GLU:HB3	2.10	0.52
1:E:174:VAL:HG23	1:E:239:VAL:HG23	1.92	0.52
1:C:166:TYR:O	1:C:187:GLY:HA3	2.09	0.52
2:D:27:SER:CB	2:D:438:GLN:HB3	2.39	0.52
2:D:84:SER:O	2:D:85:PRO:C	2.52	0.52
3:I:1:NAG:H61	3:I:2:NAG:H82	1.91	0.52
2:B:157:VAL:O	2:B:220:GLU:HB3	2.09	0.52
2:B:191:LYS:HD3	2:B:280:HIS:NE2	2.25	0.52
1:E:143:TYR:OH	1:E:219:GLN:HG3	2.09	0.52
2:B:69:LEU:HB2	2:B:105:ARG:NH1	2.24	0.52
2:D:376:ASN:H	2:D:376:ASN:ND2	2.04	0.52
2:B:50:ALA:C	2:B:52:GLU:H	2.18	0.52
1:E:332:LEU:O	1:E:334:PRO:HD3	2.10	0.52
1:C:3:LEU:O	1:C:5:PRO:HD3	2.10	0.52
1:E:227:ASN:HD21	1:E:229:GLU:HG3	1.74	0.52
2:D:84:SER:HB3	2:D:85:PRO:HD2	1.91	0.51
2:F:82:GLN:HB2	2:F:105:ARG:O	2.10	0.51
2:B:111:PRO:HB2	2:B:242:ALA:CB	2.39	0.51
1:C:15:ASN:HA	1:C:443:ASN:ND2	2.25	0.51
2:D:60:GLU:O	2:D:98:LYS:HE2	2.09	0.51
1:E:177:GLN:HA	1:E:177:GLN:NE2	2.24	0.51
1:E:342:ALA:HB1	1:E:343:PRO:HD2	1.91	0.51
1:E:282:ALA:HB2	1:E:289:PHE:CG	2.45	0.51
2:F:25:TRP:HE1	2:F:27:SER:HB2	1.76	0.51
2:F:103:GLN:HG2	2:F:396:SER:HB3	1.91	0.51
2:D:371:ASN:HB2	2:D:398:SER:HB3	1.92	0.51
1:A:227:ASN:HD21	1:A:229:GLU:HG3	1.76	0.51
2:B:28:ASP:HB2	2:B:53:SER:OG	2.10	0.51
1:E:163:ASP:OD1	1:E:165:ARG:HD3	2.11	0.51
1:A:395:GLN:CD	1:A:397:GLU:H	2.18	0.51
2:B:119:ASP:O	2:B:124:MET:HG3	2.10	0.51
2:F:5:CYS:CB	2:F:39:ASP:HA	2.41	0.51
4:H:2:NAG:C3	4:H:3:MAN:O5	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:TRP:CE3	1:C:147:ARG:HD2	2.45	0.50
2:F:100:PHE:HA	6:F:1015:NAG:H83	1.94	0.50
1:A:262:TRP:HD1	2:B:317:LEU:HD12	1.75	0.50
2:F:16:CYS:SG	2:F:24:ALA:O	2.69	0.50
1:A:395:GLN:OE1	1:A:397:GLU:HB2	2.11	0.50
2:F:86:GLN:CD	2:F:86:GLN:H	2.19	0.50
1:C:114:ASN:HD22	1:C:115:VAL:H	1.58	0.50
2:D:374:CYS:HB2	2:D:376:ASN:ND2	2.27	0.50
2:F:66:ASP:CB	2:F:85:PRO:HG3	2.42	0.50
2:F:278:ASP:O	2:F:279:ASN:HB2	2.12	0.50
2:B:143:ARG:NH1	2:B:147:SER:HA	2.27	0.50
2:F:39:ASP:OD2	2:F:43:ASN:HB2	2.12	0.50
3:G:2:NAG:O3	3:G:3:MAN:C5	2.59	0.49
1:C:395:GLN:HG2	1:C:396:SER:H	1.75	0.49
2:D:7:THR:HG22	2:D:8:ARG:HG3	1.94	0.49
2:D:132:GLN:HE21	2:D:208:LYS:HA	1.77	0.49
1:C:2:ASN:N	1:C:2:ASN:HD22	2.10	0.49
2:D:67:ARG:HG2	2:D:86:GLN:HE22	1.77	0.49
1:E:282:ALA:HB2	1:E:289:PHE:CB	2.42	0.49
1:C:167:CYS:HB3	1:C:185:ALA:HB1	1.94	0.49
2:D:50:ALA:HB3	2:D:53:SER:OG	2.11	0.49
2:D:195:THR:HG22	2:D:196:LEU:N	2.28	0.49
1:E:8:LEU:H	1:E:8:LEU:HD23	1.78	0.49
2:F:203:PHE:HD2	2:F:204:ASN:ND2	2.10	0.49
2:D:230:THR:HG23	2:D:304:ILE:HD12	1.94	0.49
1:E:87:PHE:CD1	1:E:124:LYS:HE3	2.47	0.49
1:E:282:ALA:HB2	1:E:289:PHE:HB3	1.95	0.49
2:F:92:LEU:HD12	2:F:92:LEU:O	2.13	0.49
1:E:113:TRP:CE3	1:E:147:ARG:HD2	2.47	0.49
2:B:376:ASN:N	2:B:376:ASN:ND2	2.61	0.48
1:E:101:SER:OG	1:E:102:ASP:N	2.44	0.48
1:E:330:LEU:HD22	1:E:399:LEU:HD12	1.96	0.48
1:A:354:GLY:HA2	1:A:380:TYR:C	2.38	0.48
2:B:3:ASN:ND2	2:B:5:CYS:H	2.11	0.48
1:A:105:VAL:HG22	1:A:132:LEU:CD1	2.42	0.48
1:A:227:ASN:HD22	1:A:228:PRO:N	2.12	0.48
2:B:114:ILE:HD11	2:B:142:MET:HG3	1.96	0.48
2:B:119:ASP:HB3	2:B:124:MET:HE2	1.93	0.48
1:C:282:ALA:HB2	1:C:289:PHE:HB3	1.96	0.48
1:A:427:ILE:HG22	1:A:434:ASP:OD2	2.14	0.48
2:F:120:LEU:HD22	2:F:155:ALA:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:LEU:HA	1:C:367:ASP:HB3	1.94	0.48
2:F:361:ASP:O	2:F:414:PHE:CB	2.61	0.48
3:I:1:NAG:H61	3:I:2:NAG:H81	1.93	0.48
1:C:227:ASN:ND2	1:C:229:GLU:H	2.11	0.48
2:F:119:ASP:O	2:F:124:MET:HG3	2.14	0.48
2:F:418:PRO:HG2	2:F:421:PHE:HB2	1.95	0.48
3:I:1:NAG:C6	3:I:2:NAG:H82	2.44	0.48
1:A:359:ALA:HB3	1:A:377:ALA:HB3	1.95	0.48
2:B:376:ASN:ND2	2:B:376:ASN:H	2.12	0.48
1:C:317:ARG:HG2	1:C:317:ARG:NH1	2.28	0.48
2:D:257:ALA:O	2:D:258:LEU:HB2	2.14	0.47
1:A:19:PHE:O	1:A:440:TYR:HA	2.15	0.47
1:A:195:LEU:HD11	1:A:239:VAL:HG11	1.96	0.47
2:B:3:ASN:HD21	2:B:5:CYS:CB	2.25	0.47
2:B:116:TYR:HB3	2:B:153:PHE:HB2	1.95	0.47
1:C:395:GLN:NE2	1:C:400:ARG:HH12	2.13	0.47
1:E:23:LEU:HG	1:E:420:SER:OG	2.14	0.47
2:F:435:CYS:HB2	2:F:436:ALA:O	2.15	0.47
1:A:18:GLN:H	1:A:443:ASN:ND2	2.13	0.47
1:A:123:GLU:CD	1:A:165:ARG:NH2	2.72	0.47
2:B:120:LEU:HD22	2:B:155:ALA:HB1	1.97	0.47
2:B:319:GLN:O	2:B:322:SER:HB3	2.14	0.47
1:C:174:VAL:HG11	1:C:240:ALA:HA	1.96	0.47
1:C:94:GLY:C	1:C:96:SER:H	2.22	0.47
1:C:227:ASN:HD22	1:C:227:ASN:C	2.21	0.47
2:D:7:THR:HG22	2:D:8:ARG:N	2.30	0.47
2:B:82:GLN:HB3	2:B:107:VAL:HG12	1.97	0.47
1:C:166:TYR:CE1	2:D:216:ARG:HD2	2.49	0.47
9:C:1434:HOH:O	2:D:216:ARG:HD3	2.13	0.47
1:A:303:ARG:CZ	1:A:336:GLY:H	2.27	0.47
1:C:314:MET:HE1	2:D:324:LEU:HB3	1.97	0.47
1:A:395:GLN:CG	1:A:396:SER:H	2.28	0.47
2:D:376:ASN:N	2:D:376:ASN:ND2	2.63	0.47
2:B:102:ILE:HD12	2:B:425:LEU:HD23	1.97	0.46
2:D:90:LEU:HD23	2:D:429:VAL:HG12	1.97	0.46
1:A:421:LEU:CD2	1:A:437:VAL:HG22	2.45	0.46
2:B:337:SER:HB2	2:B:341:LEU:CD2	2.45	0.46
1:E:94:GLY:C	1:E:96:SER:H	2.22	0.46
1:E:227:ASN:ND2	1:E:227:ASN:C	2.71	0.46
1:A:73:ARG:NH1	1:C:73:ARG:HB2	2.31	0.46
1:A:117:GLU:O	1:A:118:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:GLU:HA	2:B:315:VAL:HG23	1.97	0.46
1:C:155:TYR:CZ	1:C:165:ARG:HD2	2.51	0.46
2:B:223:PHE:HD1	2:B:226:ILE:HD12	1.81	0.46
1:A:84:LEU:HD12	1:A:115:VAL:HG13	1.98	0.46
1:A:101:SER:CB	1:A:101:SER:HG	2.14	0.46
1:A:327:ARG:HH21	1:A:348:THR:HG21	1.80	0.46
2:B:361:ASP:O	2:B:414:PHE:HB3	2.15	0.46
1:E:393:LEU:HG	1:E:404:SER:HB3	1.98	0.46
1:C:283:GLU:HG2	1:C:329:TYR:OH	2.15	0.46
2:D:105:ARG:HB3	2:D:394:THR:HG23	1.98	0.46
1:E:395:GLN:HB2	1:E:400:ARG:HH11	1.81	0.46
1:A:114:ASN:HD22	1:A:115:VAL:N	2.11	0.46
1:C:103:VAL:HG21	1:C:200:VAL:HG11	1.98	0.46
1:C:235:TRP:HZ2	1:C:270:LEU:HD21	1.80	0.46
1:E:243:GLU:H	1:E:304:HIS:CD2	2.34	0.46
1:A:258:PRO:HB2	1:A:288:TYR:CD2	2.50	0.46
1:A:432:TYR:HA	1:A:433:PRO:HD3	1.82	0.46
2:B:121:SER:O	2:B:124:MET:HB2	2.15	0.46
2:B:351:ILE:C	2:B:352:ARG:HD2	2.40	0.46
1:C:132:LEU:N	1:C:132:LEU:HD22	2.31	0.46
2:D:132:GLN:NE2	2:D:208:LYS:HA	2.31	0.46
2:F:102:ILE:HD12	2:F:425:LEU:CD2	2.46	0.45
1:E:440:TYR:CD1	1:E:440:TYR:C	2.94	0.45
2:B:389:LEU:HD23	2:B:389:LEU:H	1.81	0.45
2:D:407:PRO:HB2	2:D:431:PHE:HE2	1.81	0.45
1:E:332:LEU:O	1:E:334:PRO:CD	2.65	0.45
1:C:19:PHE:HE1	1:C:445:VAL:HG23	1.79	0.45
2:D:67:ARG:H	2:D:86:GLN:HE22	1.62	0.45
1:A:227:ASN:C	1:A:227:ASN:ND2	2.71	0.45
2:D:362:LEU:O	2:D:363:PRO:C	2.60	0.45
2:F:98:LYS:HA	2:F:98:LYS:HD2	1.78	0.45
1:A:282:ALA:HB2	1:A:289:PHE:CG	2.50	0.45
1:C:132:LEU:HB2	1:C:141:ALA:HB3	1.98	0.45
1:E:314:MET:HE1	2:F:324:LEU:HB3	1.97	0.45
2:F:319:GLN:HA	2:F:330:VAL:HG21	1.98	0.45
1:A:291:HIS:HD2	2:B:258:LEU:HD13	1.81	0.45
1:E:317:ARG:HG2	1:E:317:ARG:NH1	2.32	0.45
1:E:395:GLN:HG2	1:E:396:SER:N	2.30	0.45
2:B:42:GLU:CD	2:B:42:GLU:H	2.23	0.45
1:C:254:VAL:HG22	1:C:269:ILE:CD1	2.47	0.45
1:A:313:TYR:HE1	1:A:315:GLU:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:ARG:HG2	1:C:329:TYR:CE1	2.52	0.45
1:C:329:TYR:CD1	1:C:329:TYR:N	2.85	0.45
2:B:376:ASN:HD22	2:B:376:ASN:H	1.62	0.45
1:C:264:LEU:HD22	1:C:282:ALA:HB3	1.97	0.45
1:E:270:LEU:HD13	1:E:276:ARG:HA	1.98	0.45
1:A:3:LEU:O	1:A:5:PRO:HD3	2.17	0.44
1:A:176:THR:OG1	1:A:180:GLU:HG2	2.17	0.44
2:B:176:PRO:HB2	2:B:214:ARG:HB2	1.99	0.44
2:D:92:LEU:CD1	2:D:403:VAL:HG11	2.44	0.44
1:E:14:PRO:HG2	1:E:17:SER:HB3	1.98	0.44
2:F:94:PRO:HB3	2:F:406:CYS:HB2	1.98	0.44
1:A:29:SER:HB3	1:A:102:ASP:OD1	2.17	0.44
2:B:308:PHE:HB2	2:B:330:VAL:HG22	1.99	0.44
2:D:35:SER:HA	2:D:36:PRO:HD3	1.84	0.44
2:D:160:PRO:HA	2:D:187:MET:HE2	1.99	0.44
2:D:360:ARG:HH11	2:D:360:ARG:HG2	1.83	0.44
2:F:71:ASP:O	2:F:107:VAL:HG22	2.17	0.44
2:F:84:SER:OG	2:F:103:GLN:HB2	2.18	0.44
2:F:317:LEU:HA	3:I:1:NAG:H81	2.00	0.44
2:B:112:VAL:O	2:B:149:LEU:HD12	2.17	0.44
1:C:59:ARG:HG3	1:C:62:GLY:H	1.82	0.44
2:B:88:ILE:HG13	2:B:427:VAL:HG13	2.00	0.44
2:B:249:THR:HG22	2:B:309:ALA:HB3	2.00	0.44
1:C:241:VAL:HG12	1:C:253:TYR:HD1	1.81	0.44
1:E:338:HIS:HB2	1:E:339:ALA:H	1.43	0.44
1:A:317:ARG:HG2	1:A:317:ARG:NH1	2.31	0.44
2:D:119:ASP:O	2:D:124:MET:HG3	2.18	0.44
2:B:25:TRP:CG	2:B:26:CYS:H	2.36	0.44
1:A:284:GLN:OE1	1:A:314:MET:HB2	2.18	0.44
2:B:196:LEU:HD12	2:B:237:GLY:C	2.42	0.44
1:C:227:ASN:ND2	1:C:227:ASN:C	2.75	0.44
1:C:296:THR:O	1:C:305:ASP:HB2	2.17	0.44
1:A:379:PRO:HA	1:A:417:PHE:O	2.18	0.43
1:A:400:ARG:NH1	1:A:400:ARG:HG3	2.33	0.43
2:B:220:GLU:OE1	7:B:1301:CAC:C1	2.66	0.43
1:C:155:TYR:CE2	1:C:165:ARG:HD2	2.53	0.43
2:B:240:ASN:ND2	2:B:240:ASN:N	2.66	0.43
2:D:159:LYS:HE2	2:D:289:TYR:CE1	2.53	0.43
2:F:57:PRO:O	2:F:93:ARG:HD2	2.17	0.43
1:E:231:PHE:N	1:E:231:PHE:CD1	2.85	0.43
1:A:195:LEU:HD11	1:A:239:VAL:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:TYR:HB3	2:B:215:ASN:HD21	1.84	0.43
2:D:84:SER:HB3	2:D:85:PRO:CD	2.48	0.43
2:F:223:PHE:CZ	2:F:254:THR:HG21	2.53	0.43
1:A:400:ARG:HG3	1:A:400:ARG:HH11	1.82	0.43
2:B:98:LYS:HA	2:B:98:LYS:HD2	1.80	0.43
2:B:120:LEU:HD22	2:B:155:ALA:CB	2.48	0.43
2:D:128:LEU:HD12	2:D:128:LEU:HA	1.85	0.43
1:E:103:VAL:HG23	1:E:104:ILE:N	2.33	0.43
1:E:112:HIS:NE2	1:E:126:PRO:HG3	2.34	0.43
2:B:86:GLN:H	2:B:86:GLN:CD	2.27	0.43
2:B:373:THR:CG2	2:B:379:VAL:HG22	2.44	0.43
2:B:25:TRP:CG	2:B:26:CYS:N	2.86	0.43
2:B:142:MET:HE3	2:B:344:ILE:HG22	2.00	0.43
2:D:82:GLN:HB3	2:D:107:VAL:HG12	2.01	0.43
2:D:84:SER:CB	2:D:85:PRO:CD	2.97	0.43
2:F:65:GLU:HG3	2:F:87:ARG:HB3	2.00	0.43
9:A:1429:HOH:O	2:B:216:ARG:HD3	2.18	0.43
2:D:70:SER:HB2	2:D:107:VAL:HG21	2.01	0.43
2:D:84:SER:HB2	2:D:103:GLN:N	2.23	0.43
1:A:298:VAL:HG11	1:A:399:LEU:HD11	2.00	0.43
2:B:104:VAL:HG21	2:B:355:VAL:CG1	2.45	0.43
2:B:136:THR:HA	2:B:204:ASN:HD21	1.84	0.43
2:B:341:LEU:HD13	2:B:341:LEU:HA	1.82	0.43
1:C:415:SER:HB2	1:C:442:ALA:HB2	2.01	0.43
2:D:390:LYS:HB2	2:D:390:LYS:HE3	1.86	0.43
1:E:91:GLN:HG3	1:E:111:GLN:HB2	2.01	0.43
1:E:327:ARG:NH1	1:E:346:LEU:HD23	2.34	0.43
2:F:60:GLU:HG3	2:F:61:ALA:H	1.83	0.42
2:F:91:ARG:HG2	2:F:430:THR:HB	2.00	0.42
2:F:102:ILE:CG2	2:F:397:PHE:HB2	2.49	0.42
3:I:1:NAG:O6	3:I:2:NAG:H82	2.18	0.42
1:C:243:GLU:N	1:C:304:HIS:HD2	2.16	0.42
2:F:257:ALA:O	2:F:258:LEU:HB2	2.19	0.42
1:A:356:PHE:CZ	1:A:376:VAL:HG11	2.53	0.42
1:C:94:GLY:C	1:C:96:SER:N	2.76	0.42
1:C:258:PRO:HA	1:C:289:PHE:O	2.19	0.42
1:C:363:LEU:HD21	1:C:435:LEU:HD13	2.02	0.42
2:F:34:GLY:O	2:F:36:PRO:HD3	2.19	0.42
2:F:71:ASP:O	2:F:107:VAL:CG2	2.67	0.42
1:A:3:LEU:HA	1:A:449:ARG:O	2.20	0.42
1:C:269:ILE:O	1:C:277:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:122:TYR:HB2	2:D:214:ARG:HG2	2.01	0.42
1:E:311:PRO:HA	1:E:356:PHE:O	2.18	0.42
1:A:28:ASP:O	1:A:30:HIS:N	2.53	0.42
1:A:417:PHE:CE1	1:A:437:VAL:HG11	2.54	0.42
2:B:110:TYR:HA	2:B:111:PRO:HD3	1.91	0.42
3:G:2:NAG:H3	3:G:3:MAN:O5	2.19	0.42
1:A:119:THR:O	1:A:119:THR:HG23	2.19	0.42
1:C:112:HIS:NE2	1:C:126:PRO:HG3	2.35	0.42
2:B:46:LYS:NZ	2:B:46:LYS:HB3	2.34	0.42
2:B:3:ASN:ND2	2:B:5:CYS:HB2	2.29	0.42
1:E:18:GLN:H	1:E:443:ASN:ND2	2.18	0.42
1:E:197:GLN:HG3	1:E:220:SER:HB3	2.02	0.42
1:C:407:LEU:HD13	1:C:448:TYR:CD2	2.54	0.42
2:F:281:TYR:CE1	2:F:283:ALA:HB3	2.54	0.42
2:F:287:MET:HE3	2:F:287:MET:HB2	1.98	0.42
2:B:82:GLN:NE2	2:B:107:VAL:H	2.17	0.42
1:C:231:PHE:N	1:C:231:PHE:CD1	2.87	0.42
2:D:65:GLU:HG2	2:D:87:ARG:HB3	2.01	0.42
1:A:333:GLN:O	1:A:335:ARG:NH2	2.54	0.41
1:A:433:PRO:O	1:A:450:ALA:HB2	2.20	0.41
2:B:141:GLN:HG2	2:B:341:LEU:HD12	2.02	0.41
2:B:249:THR:HA	2:B:309:ALA:O	2.19	0.41
2:B:400:GLU:CB	6:B:1006:NAG:H83	2.50	0.41
2:D:139:ALA:O	2:D:143:ARG:HB2	2.19	0.41
1:E:325:VAL:O	1:E:356:PHE:HB3	2.20	0.41
1:E:335:ARG:HG2	1:E:335:ARG:HH11	1.84	0.41
1:C:340:LEU:H	1:C:340:LEU:CD1	2.33	0.41
2:D:119:ASP:HB3	2:D:124:MET:HE2	2.02	0.41
1:E:297:ASP:O	1:E:372:ASN:HB2	2.20	0.41
1:A:377:ALA:HB2	1:A:421:LEU:HD11	2.02	0.41
1:A:430:ASN:O	1:A:432:TYR:HD1	2.03	0.41
2:B:390:LYS:HD2	2:B:390:LYS:N	2.35	0.41
1:C:314:MET:HE3	1:C:322:LEU:HD13	2.01	0.41
1:C:345:LEU:C	1:C:346:LEU:HD12	2.46	0.41
1:E:181:LEU:O	1:E:197:GLN:HA	2.21	0.41
1:E:409:SER:HB2	1:E:417:PHE:CD2	2.55	0.41
2:F:70:SER:OG	2:F:80:VAL:HG23	2.19	0.41
2:F:121:SER:O	2:F:124:MET:HB2	2.20	0.41
2:B:82:GLN:HE21	2:B:107:VAL:H	1.68	0.41
2:B:142:MET:HE2	2:B:142:MET:HA	2.02	0.41
2:F:354:LYS:HB2	2:F:354:LYS:HE3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PHE:CG	1:A:124:LYS:HE3	2.56	0.41
1:A:174:VAL:HG23	1:A:182:VAL:HB	2.02	0.41
2:D:44:LEU:O	2:D:49:CYS:HB2	2.21	0.41
1:E:174:VAL:CG2	1:E:239:VAL:HG23	2.49	0.41
2:F:161:VAL:HG12	2:F:162:SER:N	2.35	0.41
2:D:116:TYR:HB3	2:D:153:PHE:CB	2.50	0.41
1:E:198:ALA:HA	1:E:199:PRO:HD3	1.91	0.41
2:F:400:GLU:HB2	6:F:1020:NAG:C8	2.46	0.41
1:A:113:TRP:O	1:A:124:LYS:HA	2.20	0.41
2:B:103:GLN:HB3	2:B:396:SER:HB3	2.02	0.41
1:C:198:ALA:HA	1:C:199:PRO:HD3	1.93	0.41
1:C:335:ARG:O	1:C:336:GLY:C	2.61	0.41
2:D:117:LEU:HD12	2:D:117:LEU:HA	1.89	0.41
2:F:60:GLU:O	2:F:98:LYS:HE2	2.19	0.41
3:G:2:NAG:C3	3:G:3:MAN:O5	2.68	0.41
2:B:87:ARG:HA	2:B:426:ILE:O	2.20	0.41
2:B:93:ARG:HG3	2:B:96:ASP:HB2	2.02	0.41
2:B:97:SER:OG	2:B:402:LYS:HG3	2.19	0.41
2:B:245:LEU:HD23	2:B:305:ASN:HB2	2.02	0.41
1:C:432:TYR:HA	1:C:433:PRO:HD3	1.89	0.41
1:E:83:THR:HB	1:E:116:LEU:HB2	2.03	0.41
1:E:174:VAL:HG12	1:E:175:VAL:N	2.35	0.41
1:E:175:VAL:HA	1:E:180:GLU:O	2.21	0.41
1:E:395:GLN:CG	1:E:396:SER:N	2.84	0.41
2:F:84:SER:CB	2:F:85:PRO:HD3	2.49	0.41
2:F:112:VAL:O	2:F:149:LEU:HD12	2.21	0.41
2:F:219:PRO:HA	2:F:253:LYS:O	2.21	0.41
2:F:312:GLU:HA	2:F:315:VAL:HG23	2.03	0.41
2:F:410:LYS:HA	2:F:431:PHE:HB2	2.03	0.41
1:A:303:ARG:NH2	1:A:336:GLY:H	2.19	0.41
2:B:136:THR:HA	2:B:204:ASN:ND2	2.36	0.41
2:B:159:LYS:HA	2:B:160:PRO:HD3	1.87	0.41
2:D:60:GLU:HG3	2:D:61:ALA:H	1.85	0.41
2:B:269:ASN:ND2	2:B:290:PRO:HB3	2.35	0.40
1:C:410:PRO:HG2	1:C:411:PHE:CE2	2.56	0.40
2:D:119:ASP:HB2	2:D:249:THR:O	2.20	0.40
2:F:117:LEU:HD12	2:F:117:LEU:HA	1.89	0.40
4:H:2:NAG:O3	4:H:3:MAN:C5	2.69	0.40
1:A:244:PHE:HB2	1:A:252:GLU:HG3	2.02	0.40
2:B:377:ASN:N	2:B:377:ASN:HD22	2.19	0.40
2:B:399:ILE:HD13	2:B:416:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:436:ALA:O	2:B:437:CYS:HB2	2.21	0.40
2:D:120:LEU:HD12	2:D:120:LEU:HA	1.72	0.40
1:E:324:GLU:HG2	9:E:1442:HOH:O	2.21	0.40
1:A:114:ASN:ND2	1:A:115:VAL:N	2.68	0.40
1:A:314:MET:HE1	2:B:324:LEU:HB3	2.02	0.40
2:B:223:PHE:CD1	2:B:226:ILE:HD12	2.56	0.40
2:B:417:LYS:HB3	2:B:424:SER:CB	2.52	0.40
2:B:288:ASP:OD1	2:B:289:TYR:N	2.52	0.40
1:C:103:VAL:HG11	1:C:204:PHE:CE2	2.56	0.40
2:D:292:LEU:HA	2:D:295:MET:CE	2.51	0.40
1:E:77:ARG:HA	1:E:77:ARG:HD3	1.86	0.40
1:E:77:ARG:HG2	1:E:212:LEU:HD22	2.04	0.40
2:F:70:SER:CB	2:F:80:VAL:HG23	2.52	0.40
2:F:253:LYS:H	2:F:253:LYS:HG2	1.58	0.40
2:D:308:PHE:HB2	2:D:330:VAL:HG22	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	450/452 (100%)	404 (90%)	40 (9%)	6 (1%)	9	32
1	C	450/452 (100%)	409 (91%)	34 (8%)	7 (2%)	7	27
1	E	450/452 (100%)	414 (92%)	33 (7%)	3 (1%)	18	48
2	B	438/440 (100%)	390 (89%)	39 (9%)	9 (2%)	5	21
2	D	438/440 (100%)	387 (88%)	43 (10%)	8 (2%)	6	25
2	F	438/440 (100%)	386 (88%)	45 (10%)	7 (2%)	7	27
All	All	2664/2676 (100%)	2390 (90%)	234 (9%)	40 (2%)	8	28

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	SER
2	B	85	PRO
1	C	101	SER
1	C	102	ASP
1	C	123	GLU
2	D	12	SER
2	D	49	CYS
2	D	84	SER
1	E	123	GLU
2	F	85	PRO
2	F	361	ASP
2	B	240	ASN
1	C	336	GLY
1	C	339	ALA
2	D	7	THR
2	D	72	LYS
1	E	101	SER
2	F	11	SER
1	A	31	GLY
2	B	11	SER
2	B	436	ALA
2	D	64	LEU
1	E	319	ASP
2	F	70	SER
1	A	319	ASP
1	C	319	ASP
2	D	361	ASP
2	B	34	GLY
2	B	51	PRO
2	B	73	GLY
2	B	233	ASP
2	B	374	CYS
1	C	334	PRO
2	F	199	GLN
1	A	60	ALA
1	A	222	SER
2	D	50	ALA
2	F	374	CYS
2	F	75	GLY
1	A	337	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	360/360 (100%)	323 (90%)	37 (10%)	7	23
1	C	360/360 (100%)	328 (91%)	32 (9%)	9	28
1	E	360/360 (100%)	327 (91%)	33 (9%)	8	27
2	B	392/392 (100%)	360 (92%)	32 (8%)	10	32
2	D	392/392 (100%)	357 (91%)	35 (9%)	9	28
2	F	392/392 (100%)	370 (94%)	22 (6%)	19	50
All	All	2256/2256 (100%)	2065 (92%)	191 (8%)	10	31

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	23	LEU
1	A	28	ASP
1	A	36	VAL
1	A	43	LEU
1	A	64	GLN
1	A	72	LEU
1	A	84	LEU
1	A	96	SER
1	A	103	VAL
1	A	119	THR
1	A	132	LEU
1	A	136	GLU
1	A	140	ARG
1	A	147	ARG
1	A	159	ASP
1	A	166	TYR
1	A	180	GLU
1	A	183	LEU
1	A	195	LEU
1	A	197	GLN
1	A	219	GLN

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Mol	Chain	Res	Type
1	A	226	SER
1	A	227	ASN
1	A	252	GLU
1	A	264	LEU
1	A	270	LEU
1	A	277	LEU
1	A	288	TYR
1	A	312	LEU
1	A	317	ARG
1	A	337	PRO
1	A	348	THR
1	A	355	ARG
1	A	373	ASP
1	A	399	LEU
1	A	452	PRO
2	B	3	ASN
2	B	27	SER
2	B	49	CYS
2	B	55	GLU
2	B	67	ARG
2	B	79	GLN
2	B	120	LEU
2	B	136	THR
2	B	138	LEU
2	B	140	THR
2	B	142	MET
2	B	145	LEU
2	B	187	MET
2	B	193	VAL
2	B	202	ARG
2	B	214	ARG
2	B	239	ARG
2	B	240	ASN
2	B	246	LEU
2	B	294	LEU
2	B	314	VAL
2	B	332	VAL
2	B	341	LEU
2	B	342	GLN
2	B	362	LEU
2	B	364	GLU
2	B	376	ASN

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Mol	Chain	Res	Type
2	B	406	CYS
2	B	407	PRO
2	B	409	GLU
2	B	425	LEU
2	B	437	CYS
1	C	2	ASN
1	C	6	VAL
1	C	64	GLN
1	C	72	LEU
1	C	103	VAL
1	C	132	LEU
1	C	147	ARG
1	C	158	ASN
1	C	162	TRP
1	C	165	ARG
1	C	166	TYR
1	C	183	LEU
1	C	195	LEU
1	C	197	GLN
1	C	212	LEU
1	C	243	GLU
1	C	251	THR
1	C	252	GLU
1	C	264	LEU
1	C	270	LEU
1	C	277	LEU
1	C	280	LEU
1	C	288	TYR
1	C	312	LEU
1	C	317	ARG
1	C	329	TYR
1	C	334	PRO
1	C	337	PRO
1	C	348	THR
1	C	355	ARG
1	C	400	ARG
1	C	408	ASP
2	D	46	LYS
2	D	48	ASN
2	D	80	VAL
2	D	84	SER
2	D	92	LEU

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Mol	Chain	Res	Type
2	D	105	ARG
2	D	117	LEU
2	D	120	LEU
2	D	138	LEU
2	D	145	LEU
2	D	161	VAL
2	D	174	GLU
2	D	193	VAL
2	D	202	ARG
2	D	206	GLU
2	D	214	ARG
2	D	239	ARG
2	D	246	LEU
2	D	249	THR
2	D	294	LEU
2	D	303	ASN
2	D	314	VAL
2	D	322	SER
2	D	339	ASN
2	D	341	LEU
2	D	342	GLN
2	D	352	ARG
2	D	361	ASP
2	D	362	LEU
2	D	365	GLU
2	D	376	ASN
2	D	403	VAL
2	D	407	PRO
2	D	409	GLU
2	D	433	CYS
1	E	1	LEU
1	E	2	ASN
1	E	8	LEU
1	E	23	LEU
1	E	41	ARG
1	E	72	LEU
1	E	76	THR
1	E	103	VAL
1	E	132	LEU
1	E	135	PRO
1	E	147	ARG
1	E	165	ARG

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Mol	Chain	Res	Type
1	E	166	TYR
1	E	183	LEU
1	E	195	LEU
1	E	197	GLN
1	E	212	LEU
1	E	252	GLU
1	E	264	LEU
1	E	270	LEU
1	E	277	LEU
1	E	280	LEU
1	E	288	TYR
1	E	307	LEU
1	E	312	LEU
1	E	317	ARG
1	E	334	PRO
1	E	337	PRO
1	E	338	HIS
1	E	348	THR
1	E	366	LEU
1	E	373	ASP
1	E	395	GLN
2	F	10	VAL
2	F	40	LEU
2	F	49	CYS
2	F	77	SER
2	F	85	PRO
2	F	86	GLN
2	F	120	LEU
2	F	179	ASP
2	F	202	ARG
2	F	206	GLU
2	F	214	ARG
2	F	239	ARG
2	F	246	LEU
2	F	253	LYS
2	F	294	LEU
2	F	319	GLN
2	F	323	GLU
2	F	354	LYS
2	F	361	ASP
2	F	407	PRO
2	F	433	CYS

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Mol	Chain	Res	Type
2	F	437	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	18	GLN
1	A	114	ASN
1	A	158	ASN
1	A	197	GLN
1	A	219	GLN
1	A	227	ASN
1	A	291	HIS
1	A	351	GLN
1	A	372	ASN
1	A	443	ASN
2	B	3	ASN
2	B	14	GLN
2	B	15	GLN
2	B	82	GLN
2	B	141	GLN
2	B	204	ASN
2	B	279	ASN
2	B	319	GLN
2	B	376	ASN
2	B	377	ASN
2	B	408	GLN
2	B	438	GLN
2	B	440	GLN
1	C	2	ASN
1	C	47	GLN
1	C	114	ASN
1	C	158	ASN
1	C	227	ASN
1	C	304	HIS
1	C	338	HIS
1	C	372	ASN
1	C	388	GLN
1	C	395	GLN
1	C	443	ASN
1	C	444	GLN
2	D	15	GLN

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Mol	Chain	Res	Type
2	D	82	GLN
2	D	106	GLN
2	D	132	GLN
2	D	199	GLN
2	D	204	ASN
2	D	280	HIS
2	D	319	GLN
2	D	339	ASN
2	D	376	ASN
2	D	377	ASN
2	D	408	GLN
2	D	440	GLN
1	E	2	ASN
1	E	18	GLN
1	E	30	HIS
1	E	177	GLN
1	E	197	GLN
1	E	219	GLN
1	E	227	ASN
1	E	304	HIS
2	F	15	GLN
2	F	48	ASN
2	F	86	GLN
2	F	204	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](#)

13 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	G	1	3,2	14,14,15	0.39	0	17,19,21	0.73	1 (5%)
3	NAG	G	2	3	14,14,15	0.50	0	17,19,21	0.83	1 (5%)
3	MAN	G	3	3	11,11,12	0.69	0	15,15,17	1.30	1 (6%)
3	BMA	G	4	3	11,11,12	0.45	0	15,15,17	0.39	0
4	NAG	H	1	4,2	14,14,15	0.43	0	17,19,21	0.79	1 (5%)
4	NAG	H	2	4	14,14,15	0.63	0	17,19,21	0.86	0
4	MAN	H	3	4	11,11,12	0.72	0	15,15,17	1.05	2 (13%)
4	BMA	H	4	4	11,11,12	0.47	0	15,15,17	0.52	0
4	MAN	H	5	4	11,11,12	0.55	0	15,15,17	0.53	0
3	NAG	I	1	3,2	14,14,15	0.42	0	17,19,21	0.75	0
3	NAG	I	2	3	14,14,15	0.71	0	17,19,21	0.85	1 (5%)
3	MAN	I	3	3	11,11,12	0.62	0	15,15,17	0.88	1 (6%)
3	BMA	I	4	3	11,11,12	0.49	0	15,15,17	0.57	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
3	NAG	G	1	3,2	-	3/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	MAN	G	3	3	-	1/2/19/22	0/1/1/1
3	BMA	G	4	3	-	2/2/19/22	0/1/1/1
4	NAG	H	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	MAN	H	3	4	-	2/2/19/22	0/1/1/1
4	BMA	H	4	4	-	0/2/19/22	0/1/1/1
4	MAN	H	5	4	-	2/2/19/22	0/1/1/1
3	NAG	I	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	MAN	I	3	3	-	1/2/19/22	0/1/1/1
3	BMA	I	4	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	MAN	C3-C4-C5	3.52	116.61	110.23
4	H	3	MAN	C1-C2-C3	2.52	113.32	109.64
3	I	2	NAG	C4-C3-C2	2.47	114.64	111.02
3	I	3	MAN	C1-C2-C3	2.44	113.20	109.64
3	G	2	NAG	C2-N2-C7	-2.32	119.79	122.90
3	G	1	NAG	C2-N2-C7	-2.22	119.92	122.90
4	H	1	NAG	C2-N2-C7	-2.14	120.03	122.90
4	H	3	MAN	C3-C4-C5	2.05	113.95	110.23

There are no chirality outliers.

All (27) torsion outliers are listed below:

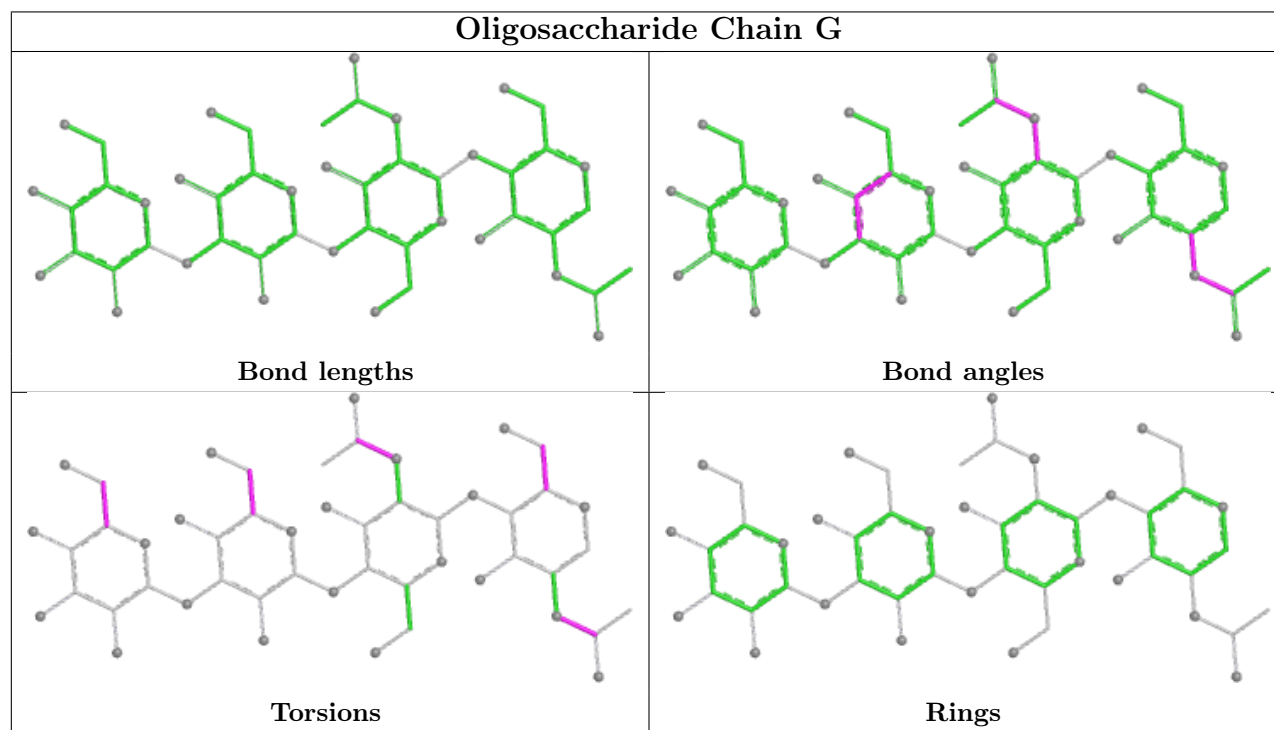
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	I	2	NAG	C1-C2-N2-C7
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
4	H	5	MAN	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	H	5	MAN	C4-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2
3	I	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C8-C7-N2-C2
4	H	1	NAG	C4-C5-C6-O6
3	G	4	BMA	C4-C5-C6-O6
3	G	2	NAG	O7-C7-N2-C2
3	I	4	BMA	O5-C5-C6-O6
3	G	4	BMA	O5-C5-C6-O6
4	H	3	MAN	O5-C5-C6-O6
4	H	3	MAN	C4-C5-C6-O6
3	I	1	NAG	O7-C7-N2-C2
3	G	3	MAN	O5-C5-C6-O6
3	I	3	MAN	O5-C5-C6-O6
3	I	4	BMA	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C3-C2-N2-C7

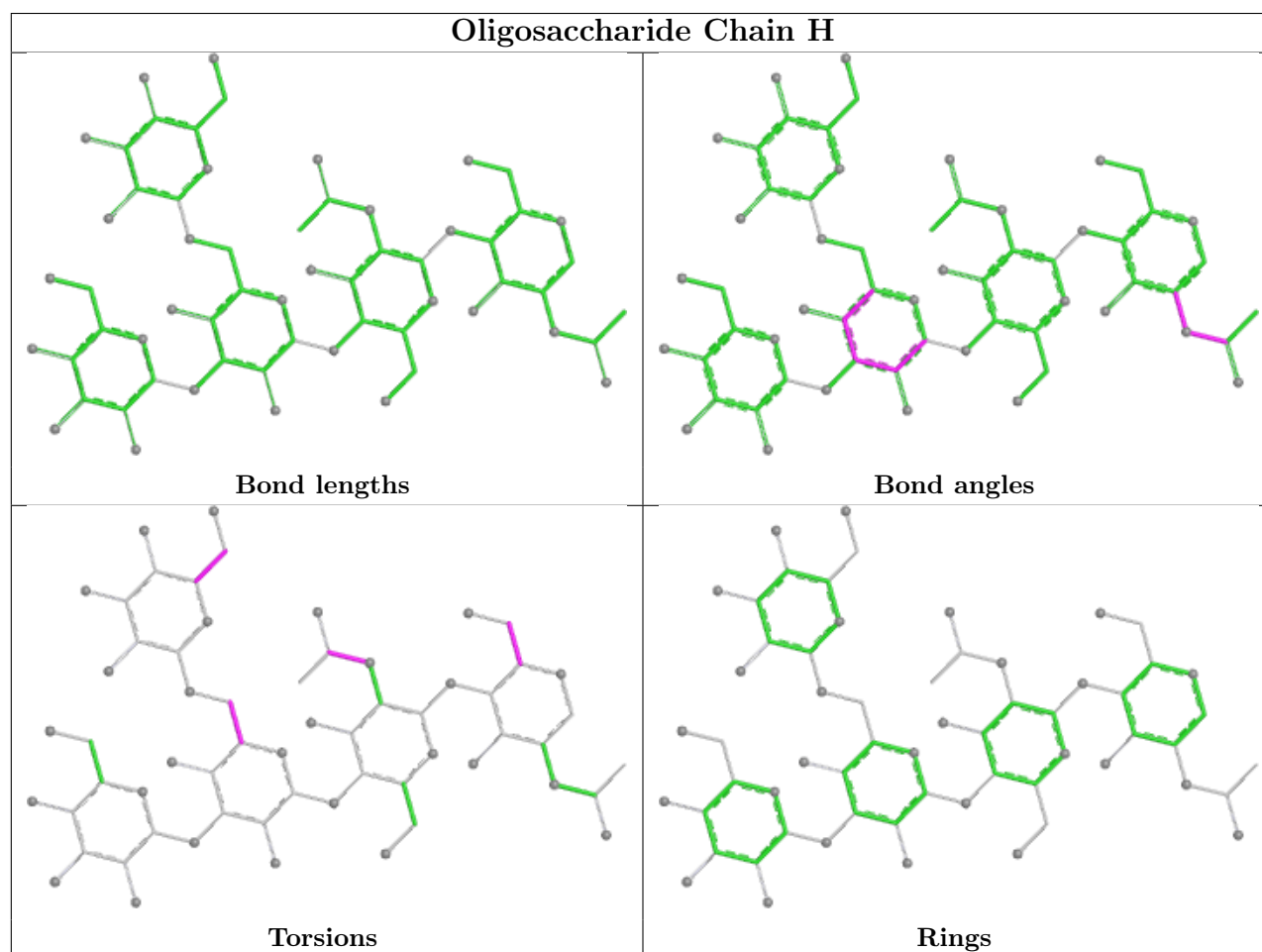
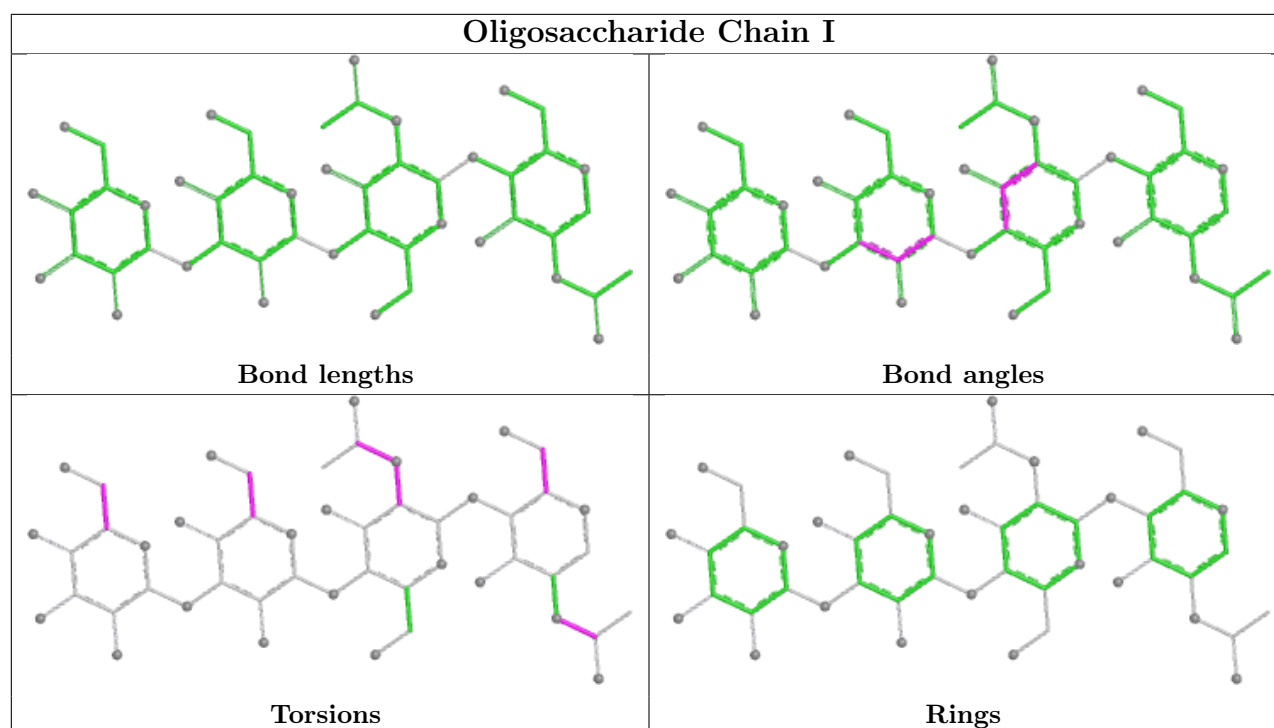
There are no ring outliers.

12 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	2	0
3	G	2	NAG	5	0
3	I	4	BMA	1	0
3	G	1	NAG	1	0
4	H	2	NAG	4	0
3	G	4	BMA	1	0
3	I	3	MAN	3	0
4	H	4	BMA	1	0
3	I	1	NAG	6	0
3	G	3	MAN	5	0
4	H	3	MAN	3	0
3	I	2	NAG	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry

Of 31 ligands modelled in this entry, 21 are monoatomic - leaving 10 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	$\# Z > 2$
6	NAG	B	1006	2	14,14,15	0.53	0	17,19,21	0.69	1 (5%)
7	CAC	D	1302	8	2,4,4	1.89	1 (50%)	4,6,6	5.17	2 (50%)
6	NAG	D	1007	2	14,14,15	0.56	0	17,19,21	0.59	0
6	NAG	E	1014	1	14,14,15	0.72	0	17,19,21	0.61	0
7	CAC	F	1303	8	2,4,4	1.74	1 (50%)	4,6,6	5.39	2 (50%)
6	NAG	F	1015	2	14,14,15	0.61	0	17,19,21	0.64	0
7	CAC	B	1301	8	2,4,4	1.90	1 (50%)	4,6,6	5.42	2 (50%)
6	NAG	B	1001	2	14,14,15	0.49	0	17,19,21	0.77	0
6	NAG	F	1020	2	14,14,15	0.44	0	17,19,21	0.80	1 (5%)
6	NAG	D	1013	2	14,14,15	0.50	0	17,19,21	0.90	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
6	NAG	B	1006	2	-	4/6/23/26	0/1/1/1
6	NAG	D	1007	2	-	2/6/23/26	0/1/1/1
6	NAG	E	1014	1	-	4/6/23/26	0/1/1/1
6	NAG	F	1015	2	-	4/6/23/26	0/1/1/1
6	NAG	B	1001	2	-	4/6/23/26	0/1/1/1
6	NAG	F	1020	2	-	2/6/23/26	0/1/1/1
6	NAG	D	1013	2	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1302	CAC	AS-C1	2.52	1.96	1.90
7	B	1301	CAC	AS-C1	2.45	1.96	1.90
7	F	1303	CAC	AS-C1	2.27	1.95	1.90

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1301	CAC	O1-AS-C2	8.85	122.50	111.50
7	F	1303	CAC	O1-AS-C2	8.85	122.50	111.50
7	D	1302	CAC	O1-AS-C2	8.75	122.38	111.50
7	B	1301	CAC	O1-AS-C1	-5.88	104.19	111.50
7	F	1303	CAC	O1-AS-C1	-5.87	104.20	111.50
7	D	1302	CAC	O1-AS-C1	-5.21	105.02	111.50
6	D	1013	NAG	C2-N2-C7	-2.76	119.20	122.90
6	F	1020	NAG	C2-N2-C7	-2.25	119.89	122.90
6	B	1006	NAG	C2-N2-C7	-2.06	120.15	122.90

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1001	NAG	C8-C7-N2-C2
6	B	1001	NAG	O7-C7-N2-C2
6	D	1007	NAG	C8-C7-N2-C2
6	D	1007	NAG	O7-C7-N2-C2
6	D	1013	NAG	C8-C7-N2-C2
6	D	1013	NAG	O7-C7-N2-C2
6	E	1014	NAG	C8-C7-N2-C2
6	E	1014	NAG	O7-C7-N2-C2
6	F	1015	NAG	C8-C7-N2-C2
6	F	1015	NAG	O7-C7-N2-C2
6	F	1020	NAG	C8-C7-N2-C2
6	F	1020	NAG	O7-C7-N2-C2
6	B	1006	NAG	O5-C5-C6-O6
6	B	1001	NAG	O5-C5-C6-O6
6	B	1006	NAG	C4-C5-C6-O6
6	B	1001	NAG	C4-C5-C6-O6
6	B	1006	NAG	C8-C7-N2-C2
6	E	1014	NAG	C4-C5-C6-O6
6	D	1013	NAG	O5-C5-C6-O6
6	B	1006	NAG	O7-C7-N2-C2
6	F	1015	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	D	1013	NAG	C4-C5-C6-O6
6	E	1014	NAG	O5-C5-C6-O6
6	F	1015	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1006	NAG	2	0
7	D	1302	CAC	1	0
7	F	1303	CAC	1	0
6	F	1015	NAG	1	0
7	B	1301	CAC	1	0
6	F	1020	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	3
2	D	2
1	C	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	122:ALA	C	123:GLU	N	1.64
1	D	7:THR	C	8:ARG	N	1.19
1	D	84:SER	C	85:PRO	N	1.17
1	C	100:TRP	C	101:SER	N	1.09
1	C	101:SER	C	102:ASP	N	1.07
1	E	100:TRP	C	101:SER	N	1.06
1	A	122:ALA	C	123:GLU	N	1.04
1	E	123:GLU	C	124:LYS	N	0.96

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	452/452 (100%)	0.35	24 (5%)	32	25	19, 51, 89, 113	2 (0%)
1	C	452/452 (100%)	0.03	12 (2%)	56	47	24, 47, 85, 108	2 (0%)
1	E	452/452 (100%)	0.09	11 (2%)	59	50	26, 45, 78, 107	2 (0%)
2	B	440/440 (100%)	0.98	55 (12%)	8	7	31, 75, 118, 120	8 (1%)
2	D	440/440 (100%)	0.88	51 (11%)	9	8	27, 65, 108, 120	8 (1%)
2	F	440/440 (100%)	1.36	89 (20%)	3	2	36, 94, 120, 120	8 (1%)
All	All	2676/2676 (100%)	0.61	242 (9%)	15	13	19, 58, 117, 120	30 (1%)

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	74	SER	26.7
2	B	73	GLY	26.3
1	A	337	PRO	23.6
2	F	74	SER	20.1
2	F	73	GLY	18.9
2	D	78	SER	18.6
2	B	72	LYS	18.0
2	D	72	LYS	17.5
2	F	77	SER	17.2
2	B	78	SER	16.8
2	D	77	SER	16.4
2	D	76	ASP	15.9
2	B	75	GLY	15.6
2	B	77	SER	15.4
2	B	74	SER	15.3
2	F	72	LYS	15.2
2	F	75	GLY	14.6
2	F	78	SER	14.6
1	C	337	PRO	14.3

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Mol	Chain	Res	Type	RSRZ
1	E	337	PRO	14.3
2	D	75	GLY	13.7
2	D	79	GLN	13.1
2	F	76	ASP	13.1
2	D	73	GLY	12.8
1	E	336	GLY	11.9
2	B	76	ASP	11.0
2	B	79	GLN	10.9
2	F	79	GLN	10.3
1	A	336	GLY	10.0
2	F	11	SER	9.2
1	C	336	GLY	8.9
2	B	11	SER	7.4
1	C	1	LEU	7.4
1	E	1	LEU	6.8
2	B	10	VAL	6.6
2	D	439	ALA	6.5
2	F	10	VAL	6.3
1	A	452	PRO	6.0
2	B	9	GLY	6.0
1	A	1	LEU	6.0
2	B	439	ALA	5.7
2	F	7	THR	5.3
2	F	30	ALA	5.2
2	D	10	VAL	5.1
2	B	33	LEU	4.9
2	B	84	SER	4.7
2	F	58	VAL	4.4
2	D	409	GLU	4.4
2	D	30	ALA	4.3
2	F	6	THR	4.3
2	F	8	ARG	4.3
2	F	80	VAL	4.2
2	F	33	LEU	4.2
1	E	123	GLU	4.1
2	D	33	LEU	4.1
1	A	29	SER	4.1
2	F	435	CYS	4.1
2	F	436	ALA	4.0
1	A	6	VAL	3.9
2	F	439	ALA	3.8
2	F	81	THR	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	440	GLN	3.6
2	D	437	CYS	3.6
2	F	410	LYS	3.6
2	F	407	PRO	3.6
2	F	83	VAL	3.5
1	E	338	HIS	3.5
2	D	31	LEU	3.4
2	B	8	ARG	3.4
1	A	30	HIS	3.4
2	F	437	CYS	3.3
2	D	410	LYS	3.3
2	F	431	PHE	3.3
2	F	440	GLN	3.3
2	F	108	GLU	3.3
1	A	338	HIS	3.3
2	B	81	THR	3.2
2	B	410	LYS	3.2
2	B	440	GLN	3.2
2	D	9	GLY	3.2
2	F	438	GLN	3.2
2	F	35	SER	3.1
2	F	9	GLY	3.1
2	D	61	ALA	3.1
2	D	80	VAL	3.1
2	F	409	GLU	3.1
2	B	435	CYS	3.1
2	B	32	PRO	3.1
2	F	422	LYS	3.1
1	E	339	ALA	3.0
1	A	303	ARG	3.0
2	F	107	VAL	3.0
2	F	64	LEU	3.0
1	C	338	HIS	3.0
2	B	31	LEU	3.0
2	F	84	SER	3.0
2	B	437	CYS	3.0
2	D	108	GLU	2.9
1	A	318	ALA	2.9
2	F	388	GLY	2.9
2	D	412	LYS	2.9
1	A	45	PRO	2.9
2	D	83	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	419	VAL	2.9
2	D	179	ASP	2.8
2	F	147	SER	2.8
1	E	321	LYS	2.8
2	B	54	ILE	2.8
2	F	12	SER	2.8
1	C	122	ALA	2.7
2	B	70	SER	2.7
2	B	91	ARG	2.7
2	F	26	CYS	2.7
2	F	56	PHE	2.7
2	B	3	ASN	2.7
2	B	2	PRO	2.7
2	D	32	PRO	2.7
2	D	11	SER	2.7
2	F	243	SER	2.7
1	C	123	GLU	2.7
2	B	85	PRO	2.7
2	F	424	SER	2.7
2	F	88	ILE	2.7
2	F	426	ILE	2.7
2	D	107	VAL	2.7
2	B	12	SER	2.7
2	D	84	SER	2.7
1	A	339	ALA	2.6
2	F	20	SER	2.6
2	D	8	ARG	2.6
1	A	296	THR	2.6
2	F	391	ILE	2.6
2	F	22	MET	2.6
2	F	179	ASP	2.6
1	C	450	ALA	2.6
1	A	27	LYS	2.6
2	F	40	LEU	2.6
1	A	7	GLN	2.6
2	F	428	GLN	2.6
2	B	420	GLY	2.6
2	F	420	GLY	2.6
2	D	64	LEU	2.6
2	B	80	VAL	2.6
2	F	70	SER	2.5
2	F	32	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	63	VAL	2.5
2	F	430	THR	2.5
1	E	318	ALA	2.5
2	B	412	LYS	2.5
2	B	27	SER	2.5
2	F	373	THR	2.5
2	D	241	ASP	2.5
2	F	241	ASP	2.5
2	B	64	LEU	2.5
2	F	92	LEU	2.5
2	B	433	CYS	2.5
2	F	85	PRO	2.4
1	C	101	SER	2.4
2	D	89	ALA	2.4
2	D	438	GLN	2.4
2	F	110	TYR	2.4
1	E	158	ASN	2.4
1	C	197	GLN	2.4
2	F	61	ALA	2.4
2	F	68	PRO	2.4
2	B	83	VAL	2.4
1	C	335	ARG	2.4
2	F	149	LEU	2.4
2	D	355	VAL	2.4
1	A	320	ARG	2.4
2	B	108	GLU	2.4
1	C	339	ALA	2.4
2	D	50	ALA	2.4
2	D	408	GLN	2.4
2	F	54	ILE	2.4
2	B	379	VAL	2.3
2	D	6	THR	2.3
1	A	5	PRO	2.3
2	F	36	PRO	2.3
2	F	37	ARG	2.3
2	B	431	PHE	2.3
1	A	28	ASP	2.3
2	B	50	ALA	2.3
2	D	13	CYS	2.3
2	F	69	LEU	2.3
2	D	63	VAL	2.3
2	F	42	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	142	MET	2.3
2	F	14	GLN	2.3
2	B	36	PRO	2.3
2	D	29	GLU	2.3
2	D	7	THR	2.3
2	D	178	TYR	2.3
2	D	403	VAL	2.3
2	B	22	MET	2.2
2	D	375	LEU	2.2
1	A	2	ASN	2.2
2	B	380	ILE	2.2
2	F	82	GLN	2.2
2	B	49	CYS	2.2
2	B	385	SER	2.2
2	F	335	MET	2.2
2	F	387	MET	2.2
2	D	106	GLN	2.2
1	E	452	PRO	2.2
2	F	63	VAL	2.2
2	D	81	THR	2.2
2	F	5	CYS	2.2
2	B	24	ALA	2.2
2	F	4	ILE	2.2
2	B	438	GLN	2.2
2	F	143	ARG	2.1
1	E	451	GLN	2.1
2	F	71	ASP	2.1
2	B	1	GLY	2.1
1	A	31	GLY	2.1
2	F	101	SER	2.1
2	F	307	ILE	2.1
2	F	374	CYS	2.1
2	F	34	GLY	2.1
1	C	58	TRP	2.1
2	D	413	SER	2.1
1	A	451	GLN	2.1
2	B	387	MET	2.1
1	A	364	GLY	2.1
1	A	400	ARG	2.1
2	B	47	ASP	2.1
2	D	430	THR	2.1
2	F	62	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	126	ASP	2.1
2	B	88	ILE	2.1
2	D	70	SER	2.0
2	B	51	PRO	2.0
2	F	31	LEU	2.0
2	D	91	ARG	2.0
1	A	316	SER	2.0
2	B	425	LEU	2.0
2	D	92	LEU	2.0
2	F	48	ASN	2.0
2	F	91	ARG	2.0
2	F	411	GLU	2.0
2	F	432	ASP	2.0

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](#)

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.

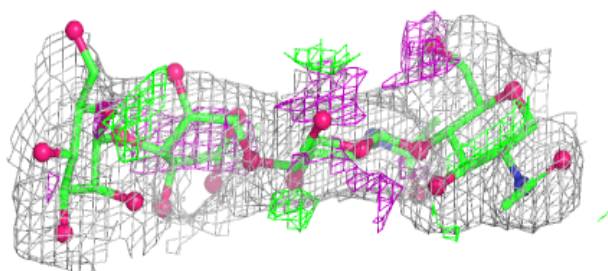
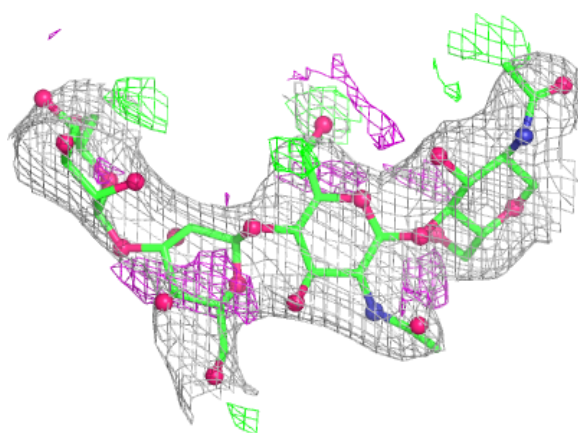
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	H	5	11/12	0.34	0.17	117,118,119,119	0
3	MAN	G	3	11/12	0.40	0.17	103,107,108,111	0
4	MAN	H	3	11/12	0.47	0.15	103,110,113,116	0
3	BMA	G	4	11/12	0.50	0.17	112,113,114,115	0
4	NAG	H	2	14/15	0.55	0.17	77,81,87,95	0
4	BMA	H	4	11/12	0.58	0.17	115,116,117,117	0
3	BMA	I	4	11/12	0.60	0.17	102,103,104,104	0
3	MAN	I	3	11/12	0.62	0.13	97,101,102,103	0
3	NAG	I	2	14/15	0.72	0.15	77,81,86,91	0
3	NAG	G	2	14/15	0.77	0.15	77,82,88,96	0
3	NAG	I	1	14/15	0.88	0.12	53,59,66,69	0
3	NAG	G	1	14/15	0.91	0.10	53,59,61,69	0
4	NAG	H	1	14/15	0.94	0.08	48,52,58,68	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

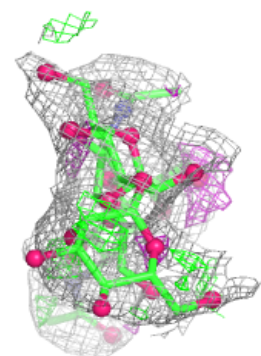
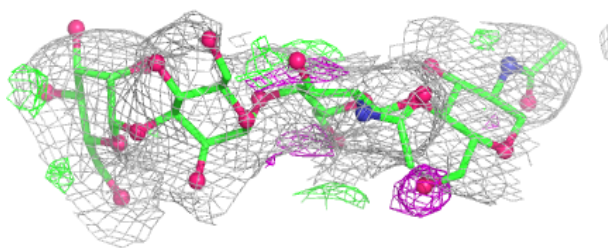
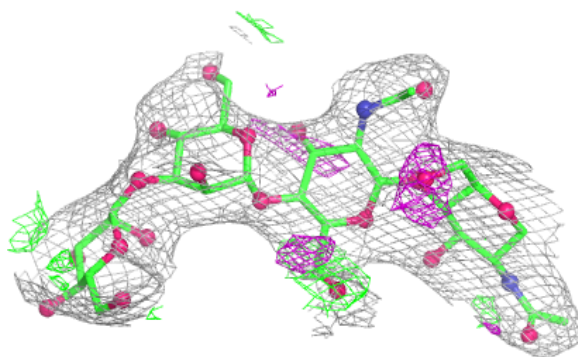
Electron density around Chain G:

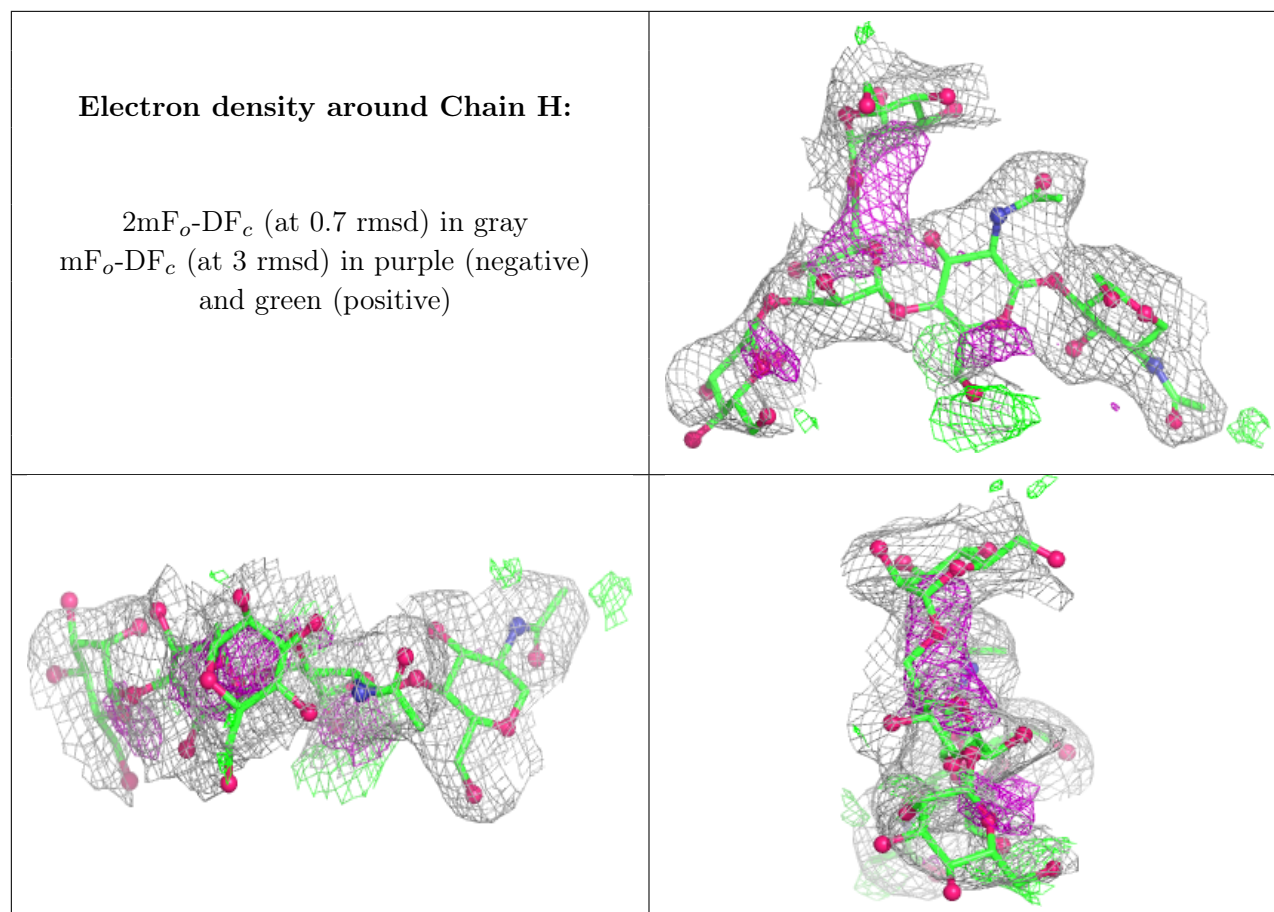
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain I:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





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
6	NAG	E	1014	14/15	0.33	0.19	87,92,95,95	0
6	NAG	D	1007	14/15	0.50	0.18	101,104,105,105	0
6	NAG	B	1001	14/15	0.54	0.14	109,111,113,114	0
6	NAG	F	1015	14/15	0.57	0.16	118,119,120,120	0
6	NAG	F	1020	14/15	0.70	0.16	109,112,113,114	0
6	NAG	D	1013	14/15	0.77	0.16	92,94,96,96	0
6	NAG	B	1006	14/15	0.77	0.13	102,103,103,103	0
5	CA	F	1416	1/1	0.92	0.09	63,63,63,63	0
5	CA	A	1406	1/1	0.92	0.09	73,73,73,73	0
5	CA	A	1405	1/1	0.93	0.08	75,75,75,75	0
5	CA	A	1407	1/1	0.93	0.09	68,68,68,68	0
5	CA	D	1409	1/1	0.94	0.05	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	E	1420	1/1	0.94	0.09	51,51,51,51	0
7	CAC	B	1301	5/5	0.94	0.17	100,101,102,102	0
7	CAC	F	1303	5/5	0.94	0.17	114,114,115,115	0
5	CA	C	1414	1/1	0.95	0.06	68,68,68,68	0
5	CA	E	1421	1/1	0.95	0.08	65,65,65,65	0
7	CAC	D	1302	5/5	0.95	0.15	96,96,98,98	0
5	CA	C	1411	1/1	0.95	0.08	58,58,58,58	0
5	CA	C	1412	1/1	0.96	0.06	46,46,46,46	0
5	CA	B	1402	1/1	0.96	0.04	48,48,48,48	0
5	CA	A	1404	1/1	0.97	0.07	61,61,61,61	0
5	CA	F	1417	1/1	0.97	0.04	42,42,42,42	0
5	CA	C	1413	1/1	0.97	0.08	70,70,70,70	0
8	MG	F	1415	1/1	0.98	0.04	32,32,32,32	0
5	CA	E	1419	1/1	0.99	0.04	35,35,35,35	0
5	CA	B	1403	1/1	0.99	0.03	28,28,28,28	0
5	CA	D	1410	1/1	0.99	0.02	24,24,24,24	0
8	MG	B	1401	1/1	0.99	0.03	24,24,24,24	0
8	MG	D	1408	1/1	0.99	0.04	18,18,18,18	0
5	CA	E	1418	1/1	0.99	0.04	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.