



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:50 PM GMT

PDB ID : 1MCO
Title : THREE-DIMENSIONAL STRUCTURE OF A HUMAN IMMUNOGLOBULIN WITH A HINGE DELETION
Authors : Guddat, L.W.; Edmundson, A.B.
Deposited on : 1993-02-25
Resolution : 3.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

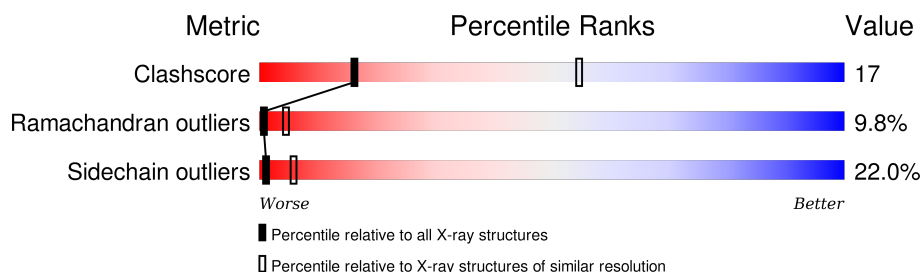
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	216	
2	H	428	

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
4	GUP	H	437	X	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5041 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 IGG1 MCG INTACT ANTIBODY (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1606	999	266	336	5			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	20	ILE	PHE	CONFLICT	PIR S14675
L	23	THR	SER	CONFLICT	PIR S14675
L	29	VAL	ILE	CONFLICT	PIR S14675
L	31	GLY	ASN	CONFLICT	PIR S14675
L	39	GLN	ARG	CONFLICT	PIR S14675
L	42	ALA	PRO	CONFLICT	PIR S14675
L	48	VAL	LEU	CONFLICT	PIR S14675
L	49	ILE	MET	CONFLICT	PIR S14675
L	54	ASN	THR	CONFLICT	PIR S14675
L	62	ASP	ASN	CONFLICT	PIR S14675
L	94	GLU	ALA	CONFLICT	PIR S14675
L	97	ASP	ASN	CONFLICT	PIR S14675
L	98	ASN	SER	CONFLICT	PIR S14675
L	99	PHE	LEU	CONFLICT	PIR S14675
L	100	VAL	ILE	CONFLICT	PIR S14675
L	103	THR	GLY	CONFLICT	PIR S14675
L	106	LYS	ARG	CONFLICT	PIR S14675
L	107	VAL	LEU	CONFLICT	PIR S14675
L	116	ASN	ALA	CONFLICT	PIR S14675
L	118	THR	SER	CONFLICT	PIR S14675
L	136	GLU	LEU	CONFLICT	PIR S14675
L	156	GLY	SER	CONFLICT	PIR S14675
L	167	LYS	THR	CONFLICT	PIR S14675

- Molecule 2 is a protein called IGG1 MCG INTACT ANTIBODY (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	428	Total	C	N	O	S	0	0	0
			3305	2108	551	635	11			

There are 67 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	GLN	DELETION	GB 243866
H	13	LYS	ARG	CONFLICT	GB 243866
H	16	GLU	GLN	CONFLICT	GB 243866
H	17	ALA	THR	CONFLICT	GB 243866
H	27	ASP	-	INSERTION	GB 243866
H	28	SER	PHE	CONFLICT	GB 243866
H	29	ILE	THR	CONFLICT	GB 243866
H	30	ASN	PHE	CONFLICT	GB 243866
H	32	ILE	-	INSERTION	GB 243866
H	33	LEU	ASP	CONFLICT	GB 243866
H	34	TYR	PHE	CONFLICT	GB 243866
H	36	TRP	MET	CONFLICT	GB 243866
H	37	SER	ASN	CONFLICT	GB 243866
H	39	ILE	VAL	CONFLICT	GB 243866
H	45	LYS	ARG	CONFLICT	GB 243866
H	52	TYR	PHE	CONFLICT	GB 243866
H	?	-	ARG	DELETION	GB 243866
H	?	-	ASP	DELETION	GB 243866
H	54	TYR	LYS	CONFLICT	GB 243866
H	55	TYR	ALA	CONFLICT	GB 243866
H	56	SER	LYS	CONFLICT	GB 243866
H	58	SER	TYR	CONFLICT	GB 243866
H	?	-	THR	DELETION	GB 243866
H	?	-	GLU	DELETION	GB 243866
H	61	GLY	-	INSERTION	GB 243866
H	65	LEU	VAL	CONFLICT	GB 243866
H	67	SER	GLY	CONFLICT	GB 243866
H	71	ILE	MET	CONFLICT	GB 243866
H	72	SER	LEU	CONFLICT	GB 243866
H	74	ASN	ASP	CONFLICT	GB 243866
H	81	TYR	SER	CONFLICT	GB 243866
H	82	SER	LEU	CONFLICT	GB 243866
H	83	LYS	ARG	CONFLICT	GB 243866
H	100	VAL	GLU	CONFLICT	GB 243866
H	101	PRO	GLY	CONFLICT	GB 243866
H	102	LEU	HIS	CONFLICT	GB 243866
H	103	VAL	THR	CONFLICT	GB 243866

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Chain	Residue	Modelled	Actual	Comment	Reference
H	104	VAL	ALA	CONFLICT	GB 243866
H	105	ASN	ALA	CONFLICT	GB 243866
H	?	-	PHE	DELETION	GB 243866
H	?	-	ASP	DELETION	GB 243866
H	?	-	TYR	DELETION	GB 243866
H	111	THR	SER	CONFLICT	GB 243866
H	152	GLN	GLU	CONFLICT	GB 243866
H	214	ARG	LYS	CONFLICT	GB 243866
H	?	-	GLU	DELETION	GB 243866
H	?	-	PRO	DELETION	GB 243866
H	?	-	LYS	DELETION	GB 243866
H	?	-	SER	DELETION	GB 243866
H	?	-	CYS	DELETION	GB 243866
H	?	-	ASP	DELETION	GB 243866
H	?	-	LYS	DELETION	GB 243866
H	?	-	THR	DELETION	GB 243866
H	?	-	HIS	DELETION	GB 243866
H	?	-	THR	DELETION	GB 243866
H	?	-	CYS	DELETION	GB 243866
H	?	-	PRO	DELETION	GB 243866
H	?	-	PRO	DELETION	GB 243866
H	?	-	CYS	DELETION	GB 243866
H	?	-	PRO	DELETION	GB 243866
H	257	GLN	GLU	CONFLICT	GB 243866
H	268	GLN	GLU	CONFLICT	GB 243866
H	279	GLN	GLU	CONFLICT	GB 243866
H	297	ASN	ASP	CONFLICT	GB 243866
H	300	ASP	ASN	CONFLICT	GB 243866
H	341	GLU	ASP	CONFLICT	GB 243866
H	343	MET	LEU	CONFLICT	GB 243866

- Molecule 3 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	8	Total	C	N	O	0	0
			105	59	4	42		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

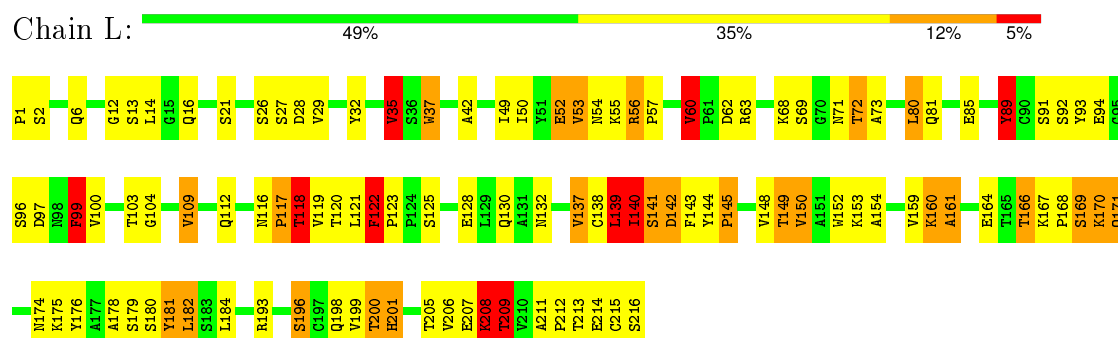
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	2	Total	C	N	O	0	0
			25	14	1	10		

3 Residue-property plots

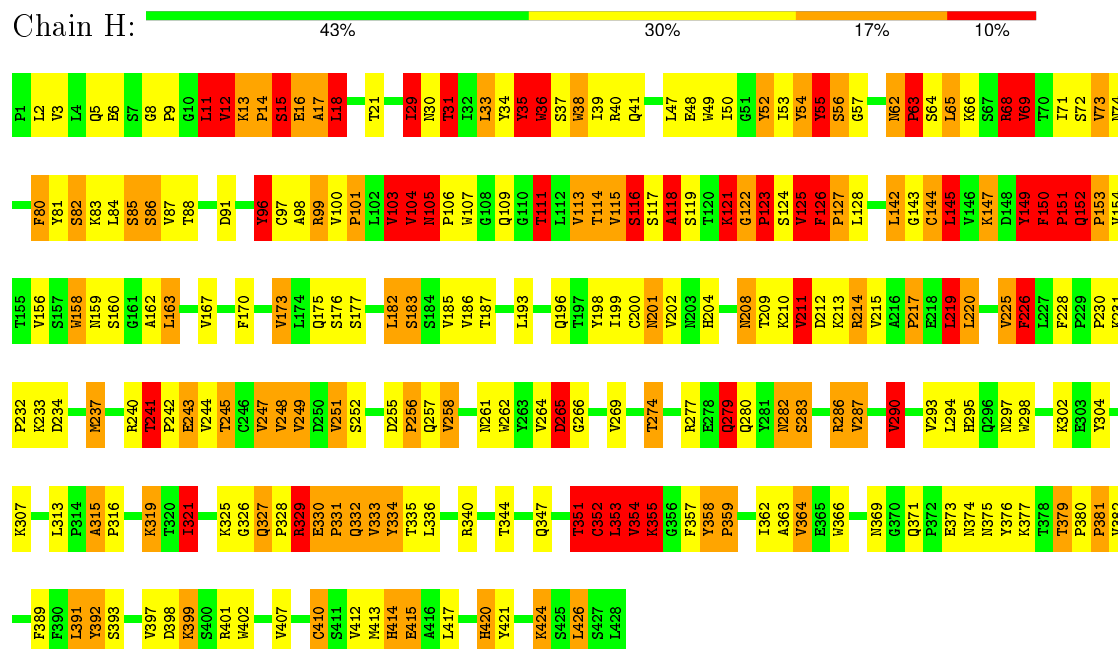
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: IGG1 MCG INTACT ANTIBODY (LIGHT CHAIN)



• Molecule 2: IGG1 MCG INTACT ANTIBODY (HEAVY CHAIN)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.40 Å 110.00 Å 186.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.232 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5041	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, GUP, NAG, SIA, GAL, FUL, MAN

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	L	0.95	2/1645 (0.1%)	2.06	73/2242 (3.3%)
2	H	1.09	17/3396 (0.5%)	2.47	227/4641 (4.9%)
All	All	1.05	19/5041 (0.4%)	2.35	300/6883 (4.4%)

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	L	0	2
2	H	0	10
4	H	1	0
All	All	1	12

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	85	SER	CA-CB	7.76	1.64	1.52
2	H	84	LEU	CA-CB	7.22	1.70	1.53
2	H	18	LEU	N-CA	6.62	1.59	1.46
2	H	243	GLU	CD-OE1	-6.51	1.18	1.25
2	H	84	LEU	CB-CG	6.04	1.70	1.52
2	H	243	GLU	CD-OE2	-5.89	1.19	1.25
2	H	17	ALA	CA-C	5.88	1.68	1.52
2	H	290	VAL	CB-CG1	-5.72	1.40	1.52
2	H	38	TRP	CD1-NE1	-5.54	1.28	1.38
2	H	18	LEU	CA-C	5.51	1.67	1.52
2	H	69	VAL	CA-CB	5.50	1.66	1.54
1	L	209	THR	CA-CB	5.41	1.67	1.53
2	H	36	TRP	CD1-NE1	-5.41	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	366	TRP	CD1-NE1	-5.27	1.28	1.38
2	H	262	TRP	CD1-NE1	-5.26	1.29	1.38
2	H	87	VAL	CA-CB	5.20	1.65	1.54
2	H	402	TRP	CD1-NE1	-5.10	1.29	1.38
2	H	107	TRP	CD1-NE1	-5.06	1.29	1.38
1	L	37	TRP	CD1-NE1	-5.05	1.29	1.38

All (300) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	290	VAL	CG1-CB-CG2	-23.59	73.15	110.90
2	H	290	VAL	CA-CB-CG1	-19.64	81.44	110.90
2	H	247	VAL	CG1-CB-CG2	-17.56	82.80	110.90
2	H	354	VAL	CG1-CB-CG2	-16.69	84.20	110.90
2	H	17	ALA	N-CA-CB	-15.06	89.02	110.10
2	H	17	ALA	O-C-N	-13.07	101.78	122.70
2	H	269	VAL	CG1-CB-CG2	-12.79	90.43	110.90
2	H	329	ARG	CA-C-N	-12.52	89.66	117.20
2	H	17	ALA	C-N-CA	12.46	152.86	121.70
2	H	145	LEU	CA-CB-CG	12.37	143.74	115.30
2	H	287	VAL	CG1-CB-CG2	-12.35	91.14	110.90
2	H	103	VAL	CG1-CB-CG2	-12.05	91.62	110.90
2	H	154	VAL	CG1-CB-CG2	-11.92	91.82	110.90
2	H	103	VAL	CA-CB-CG2	-11.77	93.25	110.90
2	H	382	VAL	CG1-CB-CG2	-11.64	92.28	110.90
2	H	68	ARG	NE-CZ-NH1	11.58	126.09	120.30
2	H	329	ARG	N-CA-C	11.16	141.12	111.00
2	H	84	LEU	N-CA-CB	-10.99	88.42	110.40
2	H	290	VAL	CA-CB-CG2	10.88	127.22	110.90
2	H	84	LEU	CB-CA-C	10.76	130.64	110.20
2	H	333	VAL	CG1-CB-CG2	-10.69	93.79	110.90
2	H	35	TYR	CB-CG-CD1	-10.40	114.76	121.00
2	H	353	LEU	CA-CB-CG	10.05	138.42	115.30
2	H	149	TYR	CB-CG-CD2	-9.85	115.09	121.00
2	H	186	VAL	CG1-CB-CG2	-9.78	95.26	110.90
2	H	103	VAL	CA-CB-CG1	9.51	125.17	110.90
2	H	415	GLU	N-CA-C	9.50	136.66	111.00
2	H	319	LYS	CA-CB-CG	-9.46	92.59	113.40
2	H	144	CYS	CA-CB-SG	-9.32	97.23	114.00
2	H	18	LEU	CA-CB-CG	9.30	136.69	115.30
2	H	247	VAL	CA-CB-CG1	9.28	124.82	110.90
2	H	11	LEU	CD1-CG-CD2	-9.25	82.74	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	364	VAL	CG1-CB-CG2	-9.25	96.11	110.90
2	H	264	VAL	CA-C-N	-9.20	96.97	117.20
2	H	244	VAL	CG1-CB-CG2	-9.11	96.32	110.90
1	L	117	PRO	N-CA-C	9.09	135.73	112.10
2	H	85	SER	CA-C-N	9.04	137.09	117.20
2	H	16	GLU	CA-C-N	9.04	137.09	117.20
2	H	87	VAL	CG1-CB-CG2	-8.91	96.64	110.90
2	H	258	VAL	CG1-CB-CG2	-8.90	96.67	110.90
2	H	151	PRO	CA-N-CD	-8.81	99.17	111.50
2	H	328	PRO	CA-C-N	-8.79	97.86	117.20
2	H	167	VAL	CG1-CB-CG2	-8.79	96.84	110.90
2	H	17	ALA	CB-CA-C	8.68	123.12	110.10
2	H	84	LEU	C-N-CA	8.66	143.36	121.70
2	H	226	PHE	CB-CG-CD2	-8.65	114.74	120.80
2	H	16	GLU	O-C-N	-8.57	108.99	122.70
2	H	103	VAL	CA-C-N	8.47	135.84	117.20
2	H	414	HIS	CA-C-N	-8.47	98.57	117.20
2	H	17	ALA	CA-C-N	8.46	135.80	117.20
2	H	113	VAL	CA-CB-CG2	-8.44	98.25	110.90
2	H	85	SER	C-N-CA	8.40	142.70	121.70
2	H	355	LYS	CG-CD-CE	-8.34	86.89	111.90
2	H	85	SER	O-C-N	-8.33	109.37	122.70
2	H	264	VAL	C-N-CA	8.28	142.39	121.70
2	H	81	TYR	CB-CG-CD2	-8.25	116.05	121.00
2	H	84	LEU	CA-C-N	8.24	135.32	117.20
2	H	36	TRP	CE2-CD2-CG	-8.24	100.71	107.30
2	H	214	ARG	NE-CZ-NH1	8.23	124.41	120.30
2	H	158	TRP	CE2-CD2-CG	-8.14	100.79	107.30
2	H	35	TYR	CB-CG-CD2	8.13	125.88	121.00
2	H	264	VAL	O-C-N	8.08	135.63	122.70
2	H	36	TRP	CG-CD2-CE3	7.97	141.07	133.90
1	L	118	THR	N-CA-C	7.96	132.49	111.00
1	L	89	TYR	CA-CB-CG	7.94	128.48	113.40
2	H	247	VAL	CA-CB-CG2	-7.93	99.01	110.90
2	H	329	ARG	CA-C-O	7.91	136.70	120.10
2	H	115	VAL	C-N-CA	7.89	141.42	121.70
2	H	126	PHE	CA-C-N	7.79	138.90	117.10
2	H	352	CYS	CA-CB-SG	7.75	127.96	114.00
2	H	88	THR	CA-CB-CG2	7.75	123.24	112.40
2	H	15	SER	N-CA-C	7.72	131.85	111.00
1	L	35	VAL	CA-CB-CG2	-7.68	99.37	110.90
2	H	220	LEU	CA-CB-CG	7.65	132.89	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	16	GLU	C-N-CA	7.62	140.76	121.70
2	H	262	TRP	CE2-CD2-CG	-7.61	101.21	107.30
2	H	115	VAL	CG1-CB-CG2	-7.60	98.74	110.90
2	H	244	VAL	CA-CB-CG2	-7.33	99.90	110.90
2	H	38	TRP	CE2-CD2-CG	-7.33	101.44	107.30
2	H	182	LEU	CA-CB-CG	7.26	131.99	115.30
2	H	121	LYS	CA-CB-CG	7.21	129.27	113.40
1	L	37	TRP	CE2-CD2-CG	-7.19	101.55	107.30
2	H	104	VAL	CG1-CB-CG2	-7.18	99.41	110.90
2	H	391	LEU	CD1-CG-CD2	-7.17	88.98	110.50
1	L	35	VAL	CA-CB-CG1	7.17	121.65	110.90
1	L	216	SER	N-CA-C	7.13	130.26	111.00
2	H	185	VAL	CA-CB-CG2	-7.10	100.24	110.90
1	L	53	VAL	CA-CB-CG2	-7.06	100.30	110.90
2	H	414	HIS	C-N-CA	7.01	139.21	121.70
2	H	329	ARG	NE-CZ-NH2	-6.99	116.81	120.30
2	H	321	ILE	CA-C-N	-6.98	101.84	117.20
1	L	53	VAL	CG1-CB-CG2	-6.93	99.82	110.90
2	H	86	SER	N-CA-C	6.92	129.69	111.00
2	H	158	TRP	CD1-CG-CD2	6.91	111.83	106.30
2	H	376	TYR	CA-CB-CG	6.89	126.50	113.40
2	H	282	ASN	N-CA-C	6.89	129.60	111.00
2	H	382	VAL	CA-CB-CG1	6.88	121.22	110.90
1	L	29	VAL	CG1-CB-CG2	-6.88	99.90	110.90
2	H	149	TYR	CB-CG-CD1	6.88	125.13	121.00
2	H	315	ALA	N-CA-CB	-6.87	100.48	110.10
2	H	126	PHE	CA-CB-CG	-6.87	97.42	113.90
1	L	139	LEU	CB-CA-C	-6.85	97.19	110.20
2	H	220	LEU	N-CA-C	6.84	129.47	111.00
2	H	355	LYS	CA-CB-CG	6.84	128.44	113.40
2	H	262	TRP	CG-CD2-CE3	6.81	140.03	133.90
2	H	103	VAL	O-C-N	-6.79	111.84	122.70
2	H	219	LEU	CA-CB-CG	6.79	130.91	115.30
2	H	185	VAL	CA-CB-CG1	6.77	121.06	110.90
2	H	65	LEU	CA-CB-CG	6.76	130.85	115.30
1	L	116	ASN	CA-C-N	6.76	136.02	117.10
1	L	117	PRO	C-N-CA	6.74	138.56	121.70
2	H	16	GLU	CA-CB-CG	6.74	128.22	113.40
1	L	37	TRP	CD1-CG-CD2	6.72	111.67	106.30
1	L	56	ARG	NE-CZ-NH1	6.64	123.62	120.30
2	H	290	VAL	N-CA-C	6.63	128.91	111.00
2	H	64	SER	N-CA-C	-6.62	93.13	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	52	TYR	CB-CG-CD2	-6.62	117.03	121.00
2	H	113	VAL	CA-CB-CG1	6.62	120.82	110.90
2	H	410	CYS	CA-CB-SG	6.61	125.91	114.00
1	L	100	VAL	CG1-CB-CG2	-6.61	100.32	110.90
2	H	366	TRP	CE2-CD2-CG	-6.60	102.02	107.30
2	H	391	LEU	CA-CB-CG	6.60	130.47	115.30
1	L	28	ASP	CA-CB-CG	6.58	127.87	113.40
2	H	38	TRP	CD1-CG-CD2	6.58	111.56	106.30
2	H	199	ILE	CG1-CB-CG2	-6.53	97.03	111.40
1	L	53	VAL	CA-CB-CG1	6.52	120.69	110.90
2	H	18	LEU	CA-C-O	6.51	133.78	120.10
2	H	173	VAL	CA-CB-CG2	-6.49	101.16	110.90
2	H	14	PRO	C-N-CA	6.49	137.93	121.70
2	H	69	VAL	CG1-CB-CG2	-6.49	100.52	110.90
2	H	417	LEU	CA-C-N	-6.48	102.95	117.20
2	H	265	ASP	N-CA-C	6.47	128.47	111.00
2	H	86	SER	CA-CB-OG	6.46	128.65	111.20
2	H	274	THR	CA-CB-CG2	6.46	121.45	112.40
1	L	140	ILE	CA-CB-CG2	-6.45	98.01	110.90
1	L	103	THR	CA-CB-CG2	6.45	121.42	112.40
1	L	141	SER	CA-C-N	-6.43	103.04	117.20
2	H	14	PRO	N-CA-C	6.43	128.82	112.10
2	H	16	GLU	N-CA-CB	-6.43	99.03	110.60
2	H	11	LEU	CA-CB-CG	6.42	130.08	115.30
2	H	33	LEU	CB-CA-C	-6.42	98.00	110.20
2	H	244	VAL	CA-CB-CG1	6.42	120.54	110.90
2	H	287	VAL	CA-CB-CG2	6.37	120.45	110.90
2	H	329	ARG	CA-CB-CG	6.35	127.36	113.40
1	L	112	GLN	N-CA-C	6.34	128.13	111.00
2	H	159	ASN	C-N-CA	6.33	137.51	121.70
2	H	262	TRP	CD1-CG-CD2	6.32	111.36	106.30
2	H	36	TRP	CD1-CG-CD2	6.30	111.34	106.30
2	H	240	ARG	NE-CZ-NH1	6.29	123.44	120.30
2	H	234	ASP	CB-CG-OD1	6.28	123.95	118.30
2	H	99	ARG	NE-CZ-NH1	6.27	123.43	120.30
2	H	426	LEU	CA-CB-CG	6.26	129.71	115.30
2	H	2	LEU	CA-CB-CG	6.26	129.70	115.30
2	H	248	VAL	CA-C-N	-6.26	103.43	117.20
2	H	353	LEU	CA-C-N	-6.25	103.45	117.20
2	H	147	LYS	CG-CD-CE	-6.22	93.24	111.90
1	L	109	VAL	CA-CB-CG2	6.21	120.21	110.90
2	H	269	VAL	C-N-CA	6.17	137.13	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	122	PHE	CA-CB-CG	6.13	128.61	113.90
1	L	201	HIS	CA-CB-CG	-6.11	103.21	113.60
1	L	152	TRP	CE2-CD2-CG	-6.11	102.42	107.30
1	L	116	ASN	CA-CB-CG	6.09	126.80	113.40
1	L	117	PRO	CA-N-CD	-6.07	103.00	111.50
2	H	358	TYR	CB-CG-CD1	-6.07	117.36	121.00
2	H	68	ARG	CG-CD-NE	6.06	124.53	111.80
1	L	206	VAL	CG1-CB-CG2	-6.06	101.20	110.90
2	H	330	GLU	CA-CB-CG	6.03	126.67	113.40
1	L	141	SER	O-C-N	6.03	132.34	122.70
1	L	60	VAL	CA-CB-CG1	-6.02	101.87	110.90
2	H	329	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	H	366	TRP	CG-CD2-CE3	6.02	139.32	133.90
2	H	3	VAL	CG1-CB-CG2	-6.01	101.28	110.90
2	H	240	ARG	NE-CZ-NH2	-6.01	117.30	120.30
2	H	38	TRP	CG-CD2-CE3	5.99	139.29	133.90
2	H	62	ASN	CA-C-N	5.99	133.88	117.10
2	H	211	VAL	CA-CB-CG1	-5.98	101.93	110.90
1	L	118	THR	CA-C-N	-5.98	104.05	117.20
1	L	182	LEU	CA-CB-CG	5.97	129.03	115.30
1	L	168	PRO	N-CA-C	5.96	127.59	112.10
2	H	107	TRP	CE2-CD2-CG	-5.96	102.53	107.30
2	H	125	VAL	CG1-CB-CG2	5.96	120.43	110.90
2	H	293	VAL	CG1-CB-CG2	-5.95	101.37	110.90
2	H	421	TYR	CA-CB-CG	5.92	124.65	113.40
2	H	29	ILE	C-N-CA	5.91	136.48	121.70
2	H	344	THR	CA-CB-CG2	5.91	120.67	112.40
2	H	40	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	H	13	LYS	CA-CB-CG	5.86	126.30	113.40
1	L	60	VAL	CA-CB-CG2	5.86	119.69	110.90
1	L	89	TYR	CB-CG-CD2	-5.86	117.49	121.00
1	L	214	GLU	CA-C-N	5.85	130.07	117.20
2	H	402	TRP	CE2-CD2-CG	-5.84	102.63	107.30
1	L	35	VAL	CG1-CB-CG2	-5.83	101.57	110.90
2	H	83	LYS	CA-CB-CG	-5.83	100.57	113.40
2	H	80	PHE	CB-CG-CD2	-5.83	116.72	120.80
2	H	313	LEU	CB-CG-CD2	-5.81	101.12	111.00
2	H	173	VAL	CA-CB-CG1	5.80	119.60	110.90
1	L	122	PHE	CB-CG-CD1	5.79	124.85	120.80
2	H	414	HIS	O-C-N	5.78	131.95	122.70
2	H	364	VAL	CA-CB-CG1	5.78	119.57	110.90
2	H	113	VAL	CG1-CB-CG2	-5.78	101.66	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	326	GLY	CA-C-N	-5.77	104.51	117.20
2	H	96	TYR	CA-CB-CG	5.73	124.29	113.40
2	H	152	GLN	CA-CB-CG	-5.73	100.80	113.40
2	H	158	TRP	CG-CD2-CE3	5.71	139.04	133.90
1	L	193	ARG	NE-CZ-NH1	5.71	123.15	120.30
2	H	359	PRO	N-CA-C	5.71	126.94	112.10
1	L	148	VAL	CG1-CB-CG2	-5.69	101.79	110.90
1	L	207	GLU	N-CA-C	-5.68	95.66	111.00
2	H	31	THR	CA-CB-CG2	5.68	120.36	112.40
2	H	12	VAL	CA-C-N	5.68	129.70	117.20
2	H	251	VAL	C-N-CA	5.68	135.89	121.70
2	H	351	THR	CA-CB-CG2	-5.66	104.48	112.40
2	H	426	LEU	CB-CG-CD2	5.66	120.62	111.00
1	L	159	VAL	CA-CB-CG1	-5.65	102.43	110.90
2	H	251	VAL	CG1-CB-CG2	-5.64	101.87	110.90
1	L	138	CYS	CA-C-N	5.64	129.61	117.20
2	H	426	LEU	CD1-CG-CD2	-5.63	93.61	110.50
2	H	282	ASN	C-N-CA	5.63	135.76	121.70
2	H	420	HIS	CA-C-N	-5.62	104.83	117.20
2	H	40	ARG	CA-CB-CG	5.61	125.75	113.40
2	H	204	HIS	CA-CB-CG	5.60	123.12	113.60
1	L	93	TYR	CA-CB-CG	5.60	124.04	113.40
2	H	382	VAL	CA-CB-CG2	-5.58	102.52	110.90
2	H	279	GLN	CA-CB-CG	5.58	125.67	113.40
1	L	150	VAL	CA-CB-CG2	5.56	119.24	110.90
2	H	399	LYS	CA-CB-CG	5.56	125.63	113.40
2	H	379	THR	OG1-CB-CG2	-5.54	97.27	110.00
2	H	118	ALA	CB-CA-C	-5.53	101.80	110.10
2	H	34	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	L	72	THR	CA-CB-CG2	5.53	120.14	112.40
2	H	12	VAL	CA-CB-CG1	-5.52	102.61	110.90
2	H	366	TRP	CD1-CG-CD2	5.52	110.72	106.30
2	H	63	PRO	N-CA-C	5.51	126.44	112.10
1	L	170	LYS	CA-C-N	-5.48	105.14	117.20
2	H	104	VAL	N-CA-C	-5.48	96.21	111.00
2	H	381	PRO	N-CA-C	5.47	126.33	112.10
2	H	126	PHE	O-C-N	-5.47	110.70	121.10
1	L	56	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	L	167	LYS	N-CA-C	5.46	125.74	111.00
2	H	96	TYR	CA-C-N	-5.45	105.20	117.20
1	L	152	TRP	CD1-CG-CD2	5.44	110.65	106.30
2	H	241	THR	N-CA-CB	-5.43	99.98	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	160	LYS	CA-CB-CG	5.43	125.35	113.40
1	L	52	GLU	N-CA-C	5.42	125.65	111.00
2	H	49	TRP	CE2-CD2-CG	-5.41	102.97	107.30
2	H	225	VAL	CG1-CB-CG2	-5.40	102.25	110.90
1	L	150	VAL	CA-CB-CG1	-5.40	102.80	110.90
1	L	14	LEU	CA-CB-CG	5.38	127.68	115.30
2	H	81	TYR	CB-CG-CD1	5.37	124.22	121.00
2	H	401	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	L	72	THR	CA-CB-OG1	-5.34	97.78	109.00
2	H	116	SER	N-CA-C	5.34	125.42	111.00
2	H	14	PRO	O-C-N	5.32	131.22	122.70
2	H	328	PRO	O-C-N	5.32	131.21	122.70
2	H	264	VAL	N-CA-C	-5.31	96.66	111.00
2	H	121	LYS	CB-CA-C	-5.31	99.79	110.40
2	H	118	ALA	N-CA-CB	5.30	117.53	110.10
1	L	145	PRO	N-CA-C	5.30	125.88	112.10
2	H	65	LEU	N-CA-CB	-5.29	99.81	110.40
2	H	336	LEU	CA-CB-CG	5.29	127.48	115.30
2	H	331	PRO	CA-C-N	-5.29	105.56	117.20
2	H	298	TRP	CE2-CD2-CG	-5.27	103.09	107.30
2	H	154	VAL	CA-CB-CG1	5.27	118.80	110.90
1	L	63	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	H	34	TYR	CA-CB-CG	5.26	123.39	113.40
1	L	169	SER	CA-C-N	-5.25	105.64	117.20
2	H	214	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	H	182	LEU	CB-CG-CD2	-5.23	102.11	111.00
2	H	111	THR	CA-C-N	-5.21	105.73	117.20
2	H	334	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	L	161	ALA	CB-CA-C	-5.20	102.30	110.10
1	L	208	LYS	C-N-CA	5.18	134.66	121.70
2	H	116	SER	C-N-CA	5.18	134.64	121.70
1	L	89	TYR	CB-CG-CD1	5.17	124.10	121.00
2	H	186	VAL	CA-CB-CG1	5.17	118.66	110.90
2	H	415	GLU	CA-C-N	5.16	128.56	117.20
2	H	402	TRP	CA-CB-CG	5.15	123.49	113.70
2	H	105	ASN	CA-C-N	5.13	131.47	117.10
1	L	208	LYS	N-CA-C	5.12	124.83	111.00
1	L	154	ALA	C-N-CA	5.12	134.50	121.70
1	L	159	VAL	CA-CB-CG2	5.12	118.58	110.90
2	H	186	VAL	CA-CB-CG2	-5.11	103.23	110.90
2	H	68	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
1	L	128	GLU	CA-CB-CG	5.09	124.61	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	149	TYR	CA-CB-CG	5.09	123.08	113.40
2	H	241	THR	CA-CB-CG2	-5.09	105.27	112.40
2	H	153	PRO	N-CA-C	5.09	125.32	112.10
1	L	209	THR	CA-CB-CG2	5.07	119.50	112.40
2	H	274	THR	CA-CB-OG1	-5.07	98.36	109.00
2	H	36	TRP	CB-CG-CD1	-5.06	120.42	127.00
1	L	181	TYR	CA-CB-CG	5.05	123.00	113.40
2	H	234	ASP	CA-CB-CG	5.05	124.50	113.40
2	H	214	ARG	N-CA-C	5.04	124.61	111.00
1	L	150	VAL	CG1-CB-CG2	-5.04	102.84	110.90
1	L	152	TRP	CG-CD2-CE3	5.03	138.43	133.90
1	L	208	LYS	CA-CB-CG	5.03	124.46	113.40
1	L	99	PHE	CB-CG-CD1	5.02	124.32	120.80
1	L	141	SER	CA-CB-OG	5.02	124.75	111.20
2	H	111	THR	CA-CB-CG2	5.00	119.40	112.40
2	H	84	LEU	O-C-N	-5.00	114.70	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	437	GUP	C1

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	126	PHE	Sidechain
2	H	15	SER	Mainchain
2	H	150	PHE	Peptide
2	H	152	GLN	Peptide
2	H	17	ALA	Mainchain
2	H	334	TYR	Sidechain
2	H	358	TYR	Peptide
2	H	380	PRO	Peptide
2	H	54	TYR	Sidechain
2	H	96	TYR	Sidechain
1	L	144	TYR	Sidechain,Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1606	0	1536	48	0
2	H	3305	0	3277	136	0
3	H	105	0	87	12	0
4	H	25	0	20	12	0
All	All	5041	0	4920	166	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 17.

All (166) 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)
3:H:432:BMA:HO3	4:H:437:GUP:C1	1.61	1.03
1:L:139:LEU:HG	2:H:147:LYS:HE3	1.60	0.84
2:H:226:PHE:CD2	3:H:432:BMA:H3	2.15	0.82
1:L:179:SER:HA	2:H:147:LYS:HE2	1.63	0.81
2:H:125:VAL:HG21	2:H:211:VAL:HG11	1.63	0.79
2:H:126:PHE:HB3	2:H:145:LEU:HD23	1.63	0.78
2:H:226:PHE:HZ	4:H:438:NAG:H2	1.49	0.77
1:L:125:SER:HB3	2:H:211:VAL:HG13	1.67	0.76
1:L:139:LEU:HD13	2:H:145:LEU:HG	1.66	0.75
2:H:248:VAL:HB	2:H:287:VAL:HG23	1.69	0.72
2:H:50:ILE:HB	2:H:65:LEU:HD23	1.72	0.71
2:H:226:PHE:HD2	3:H:432:BMA:H3	1.53	0.71
2:H:243:GLU:HG3	3:H:435:GAL:H62	1.72	0.71
1:L:145:PRO:HD2	1:L:201:HIS:NE2	2.07	0.70
2:H:333:VAL:HG12	2:H:424:LYS:HB2	1.74	0.69
1:L:179:SER:HA	2:H:147:LYS:CE	2.22	0.68
2:H:158:TRP:HZ3	2:H:198:TYR:HB3	1.58	0.68
2:H:100:VAL:HG13	2:H:103:VAL:O	1.93	0.67
2:H:226:PHE:CZ	4:H:438:NAG:H4	2.30	0.67
1:L:119:VAL:HA	1:L:139:LEU:O	1.94	0.67
2:H:200:CYS:O	2:H:212:ASP:HA	1.95	0.67
3:H:432:BMA:C3	4:H:437:GUP:C1	2.72	0.67
2:H:11:LEU:HD12	2:H:114:THR:HB	1.77	0.66
1:L:179:SER:HA	2:H:147:LYS:NZ	2.11	0.66
2:H:333:VAL:HG22	2:H:354:VAL:HG12	1.79	0.65
2:H:122:GLY:O	2:H:149:TYR:HA	1.95	0.65
1:L:137:VAL:HB	2:H:126:PHE:HE2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:277:ARG:O	2:H:287:VAL:HA	1.97	0.65
2:H:226:PHE:CZ	4:H:438:NAG:H2	2.32	0.64
2:H:127:PRO:HA	2:H:144:CYS:HA	1.79	0.64
2:H:170:PHE:HB2	2:H:183:SER:HB2	1.78	0.64
1:L:6:GLN:NE2	1:L:104:GLY:H	1.95	0.64
2:H:245:THR:HG23	2:H:290:VAL:HG13	1.81	0.63
2:H:31:THR:HB	2:H:73:VAL:HG11	1.80	0.62
2:H:329:ARG:HB2	2:H:357:PHE:HA	1.82	0.62
2:H:201:ASN:HA	2:H:211:VAL:O	1.99	0.62
2:H:11:LEU:HD22	2:H:118:ALA:HB2	1.82	0.62
2:H:29:ILE:HG23	2:H:30:ASN:H	1.64	0.62
1:L:1:PRO:HB3	2:H:63:PRO:HG3	1.81	0.61
2:H:99:ARG:HH21	2:H:106:PRO:HG2	1.65	0.61
2:H:226:PHE:CE2	4:H:437:GUP:C1	2.85	0.59
1:L:179:SER:HA	2:H:147:LYS:HZ3	1.68	0.58
2:H:357:PHE:O	2:H:389:PHE:HB2	2.04	0.58
1:L:137:VAL:HB	2:H:126:PHE:CE2	2.37	0.58
2:H:128:LEU:HG	2:H:145:LEU:HD22	1.86	0.57
2:H:354:VAL:HG21	2:H:364:VAL:HG21	1.86	0.57
1:L:179:SER:HB2	2:H:175:GLN:HE22	1.69	0.57
2:H:230:PRO:HB3	2:H:243:GLU:H	1.69	0.57
2:H:286:ARG:NH2	3:H:433:MAN:O3	2.38	0.57
2:H:261:ASN:HB2	2:H:307:LYS:HB3	1.85	0.56
1:L:139:LEU:HA	2:H:147:LYS:HZ2	1.70	0.56
1:L:139:LEU:HA	2:H:147:LYS:NZ	2.20	0.56
1:L:179:SER:CB	2:H:175:GLN:HE22	2.19	0.56
2:H:6:GLU:HB3	2:H:111:THR:HB	1.87	0.56
2:H:319:LYS:NZ	4:H:437:GUP:H3	2.21	0.56
2:H:335:THR:HA	2:H:352:CYS:HA	1.88	0.55
1:L:169:SER:HA	1:L:176:TYR:HD2	1.72	0.55
2:H:335:THR:HB	2:H:426:LEU:HD12	1.88	0.55
2:H:39:ILE:HG21	2:H:96:TYR:CD2	2.41	0.55
1:L:119:VAL:HG11	1:L:199:VAL:HG11	1.87	0.55
2:H:65:LEU:HD12	2:H:68:ARG:NH1	2.22	0.55
2:H:160:SER:H	2:H:201:ASN:ND2	2.04	0.55
2:H:249:VAL:HB	3:H:431:NAG:O3	2.07	0.55
3:H:435:GAL:H61	3:H:436:SIA:O1B	2.07	0.54
2:H:335:THR:HG23	2:H:424:LYS:HB3	1.90	0.54
2:H:123:PRO:HB3	2:H:149:TYR:HB3	1.90	0.53
1:L:137:VAL:HG11	2:H:124:SER:HB3	1.91	0.53
2:H:198:TYR:HD2	2:H:215:VAL:HG11	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:97:ASP:HB3	2:H:54:TYR:HB2	1.90	0.53
2:H:226:PHE:HZ	4:H:438:NAG:H4	1.72	0.53
2:H:226:PHE:CE2	3:H:432:BMA:H3	2.44	0.53
2:H:202:VAL:HB	2:H:211:VAL:HG23	1.90	0.53
2:H:304:TYR:HB2	2:H:321:ILE:HG22	1.89	0.53
1:L:149:THR:HB	1:L:200:THR:HG23	1.90	0.52
2:H:38:TRP:HB2	2:H:50:ILE:HG12	1.90	0.52
2:H:35:TYR:HB3	2:H:53:ILE:O	2.09	0.51
2:H:6:GLU:HG2	2:H:21:THR:O	2.10	0.51
2:H:362:ILE:HG12	2:H:391:LEU:HD21	1.92	0.51
2:H:362:ILE:HD11	2:H:364:VAL:HG23	1.93	0.50
3:H:435:GAL:H2	3:H:436:SIA:O1B	2.11	0.50
2:H:38:TRP:CZ2	2:H:82:SER:HB2	2.47	0.50
2:H:62:ASN:O	2:H:66:LYS:N	2.45	0.50
1:L:68:LYS:HA	1:L:73:ALA:HA	1.93	0.50
1:L:80:LEU:HD23	1:L:109:VAL:HG12	1.92	0.50
2:H:226:PHE:HE2	4:H:437:GUP:C1	2.25	0.50
2:H:121:LYS:H	2:H:150:PHE:HB3	1.77	0.49
2:H:226:PHE:CE1	4:H:438:NAG:H4	2.46	0.49
2:H:331:PRO:HD3	2:H:414:HIS:HD2	1.77	0.49
2:H:290:VAL:HG12	3:H:436:SIA:O1A	2.13	0.49
1:L:49:ILE:HG22	1:L:60:VAL:HG11	1.95	0.48
2:H:226:PHE:HB3	2:H:228:PHE:CE2	2.48	0.48
2:H:101:PRO:HD3	2:H:106:PRO:HD3	1.94	0.48
1:L:92:SER:O	1:L:99:PHE:HB2	2.13	0.48
2:H:98:ALA:HB1	2:H:104:VAL:HG13	1.96	0.48
1:L:6:GLN:HE22	1:L:89:TYR:HB3	1.79	0.47
2:H:55:TYR:O	2:H:56:SER:HB2	2.14	0.47
2:H:18:LEU:HD21	2:H:113:VAL:HG22	1.96	0.47
2:H:119:SER:HB3	2:H:121:LYS:HE2	1.97	0.47
2:H:243:GLU:HG3	3:H:435:GAL:C6	2.44	0.47
1:L:137:VAL:HA	1:L:181:TYR:HA	1.96	0.47
2:H:392:TYR:HD1	2:H:392:TYR:HA	1.59	0.47
2:H:241:THR:HA	2:H:242:PRO:HD2	1.91	0.46
2:H:381:PRO:HD3	2:H:391:LEU:HD23	1.97	0.46
2:H:279:GLN:HE22	2:H:286:ARG:HB3	1.80	0.46
1:L:120:THR:HB	2:H:126:PHE:HD1	1.80	0.46
1:L:122:PHE:CD2	2:H:127:PRO:HD3	2.51	0.46
2:H:31:THR:HG23	2:H:55:TYR:O	2.16	0.46
1:L:169:SER:O	2:H:173:VAL:HG22	2.16	0.46
2:H:145:LEU:HB2	2:H:182:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:364:VAL:HG22	2:H:412:VAL:HG13	1.98	0.46
2:H:156:VAL:HG13	2:H:202:VAL:HG22	1.98	0.46
1:L:35:VAL:HG23	1:L:92:SER:OG	2.16	0.46
2:H:297:ASN:O	2:H:302:LYS:HB2	2.16	0.46
2:H:12:VAL:N	2:H:116:SER:H	2.14	0.45
2:H:233:LYS:O	2:H:237:MET:HB2	2.16	0.45
1:L:153:LYS:HD3	1:L:196:SER:HB2	1.97	0.45
1:L:12:GLY:HA2	1:L:16:GLN:OE1	2.16	0.45
2:H:125:VAL:HG11	2:H:211:VAL:HG21	1.99	0.45
1:L:85:GLU:OE2	1:L:109:VAL:HG22	2.16	0.45
1:L:50:ILE:HD13	1:L:56:ARG:HB2	1.99	0.45
1:L:140:ILE:HB	1:L:178:ALA:HB3	1.99	0.45
2:H:256:PRO:O	2:H:258:VAL:HG23	2.17	0.45
1:L:171:GLN:HB2	1:L:175:LYS:O	2.17	0.44
2:H:363:ALA:HB3	2:H:413:MET:HB2	1.99	0.44
2:H:331:PRO:CD	2:H:414:HIS:HD2	2.29	0.44
2:H:41:GLN:HB2	2:H:47:LEU:HD23	1.99	0.44
2:H:99:ARG:HE	2:H:106:PRO:HG2	1.82	0.44
2:H:315:ALA:HA	2:H:316:PRO:HD2	1.73	0.44
2:H:225:VAL:HG22	2:H:248:VAL:HG22	2.00	0.43
2:H:351:THR:HG22	2:H:352:CYS:H	1.81	0.43
1:L:122:PHE:HD2	2:H:127:PRO:HD3	1.82	0.43
1:L:37:TRP:HB2	1:L:50:ILE:HB	2.00	0.43
2:H:142:LEU:HD21	2:H:193:LEU:HD11	1.99	0.43
1:L:1:PRO:HD3	2:H:63:PRO:HD2	2.00	0.43
2:H:198:TYR:CD2	2:H:215:VAL:HG11	2.53	0.43
2:H:332:GLN:HB2	2:H:355:LYS:HG3	2.00	0.43
2:H:36:TRP:HZ2	2:H:97:CYS:SG	2.42	0.43
1:L:211:ALA:HA	1:L:212:PRO:HD3	1.84	0.43
1:L:166:THR:HB	2:H:177:SER:CB	2.49	0.43
2:H:319:LYS:HZ2	4:H:437:GUP:H3	1.83	0.42
1:L:27:SER:O	1:L:94:GLU:HA	2.19	0.42
1:L:137:VAL:HG12	1:L:180:SER:O	2.19	0.42
2:H:330:GLU:HA	2:H:331:PRO:HD2	1.92	0.42
2:H:347:GLN:HA	2:H:398:ASP:HA	2.01	0.42
1:L:164:GLU:O	1:L:180:SER:HA	2.20	0.42
2:H:245:THR:HG23	2:H:290:VAL:CG1	2.48	0.42
2:H:12:VAL:O	2:H:115:VAL:HA	2.19	0.42
1:L:139:LEU:HD22	1:L:141:SER:HB3	2.02	0.42
2:H:125:VAL:CG1	2:H:211:VAL:HG21	2.50	0.42
2:H:352:CYS:HB3	2:H:393:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:TRP:HD1	2:H:37:SER:H	1.66	0.42
2:H:126:PHE:CE2	2:H:147:LYS:HD2	2.55	0.42
2:H:36:TRP:CZ2	2:H:97:CYS:SG	3.13	0.42
2:H:65:LEU:HG	2:H:69:VAL:HB	2.02	0.41
2:H:335:THR:HG22	2:H:352:CYS:HB2	2.02	0.41
2:H:333:VAL:HA	2:H:353:LEU:O	2.20	0.41
2:H:212:ASP:O	2:H:213:LYS:HD2	2.20	0.41
1:L:200:THR:HA	1:L:205:THR:HA	2.02	0.41
2:H:128:LEU:O	2:H:143:GLY:N	2.52	0.41
2:H:327:GLN:HE22	2:H:329:ARG:NH1	2.19	0.41
2:H:126:PHE:HB3	2:H:145:LEU:CD2	2.44	0.40
2:H:162:ALA:O	2:H:163:LEU:HB2	2.20	0.40
2:H:66:LYS:C	2:H:68:ARG:H	2.24	0.40
2:H:255:ASP:N	2:H:256:PRO:HD3	2.35	0.40
2:H:226:PHE:HZ	4:H:438:NAG:C2	2.24	0.40
2:H:8:GLY:H	2:H:9:PRO:HD3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	L	214/216 (99%)	164 (77%)	32 (15%)	18 (8%)	1	6
2	H	426/428 (100%)	304 (71%)	77 (18%)	45 (11%)	0	3
All	All	640/644 (99%)	468 (73%)	109 (17%)	63 (10%)	1	4

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	26	SER
1	L	52	GLU

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Mol	Chain	Res	Type
1	L	96	SER
1	L	117	PRO
1	L	123	PRO
1	L	132	ASN
1	L	209	THR
1	L	213	THR
1	L	215	CYS
2	H	15	SER
2	H	29	ILE
2	H	56	SER
2	H	85	SER
2	H	86	SER
2	H	101	PRO
2	H	122	GLY
2	H	151	PRO
2	H	153	PRO
2	H	163	LEU
2	H	208	ASN
2	H	217	PRO
2	H	220	LEU
2	H	251	VAL
2	H	252	SER
2	H	257	GLN
2	H	282	ASN
2	H	283	SER
2	H	359	PRO
1	L	42	ALA
1	L	57	PRO
1	L	118	THR
1	L	142	ASP
1	L	161	ALA
2	H	33	LEU
2	H	116	SER
2	H	219	LEU
2	H	265	ASP
2	H	280	GLN
2	H	295	HIS
2	H	325	LYS
2	H	340	ARG
2	H	369	ASN
1	L	170	LYS
1	L	208	LYS

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Mol	Chain	Res	Type
2	H	104	VAL
2	H	118	ALA
2	H	123	PRO
2	H	152	GLN
1	L	53	VAL
1	L	130	GLN
2	H	55	TYR
2	H	63	PRO
2	H	103	VAL
2	H	117	SER
2	H	68	ARG
2	H	266	GLY
2	H	329	ARG
2	H	256	PRO
2	H	14	PRO
2	H	105	ASN
2	H	127	PRO
2	H	57	GLY
2	H	69	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	L	181/181 (100%)	143 (79%)	38 (21%)	1	7
2	H	383/383 (100%)	297 (78%)	86 (22%)	1	5
All	All	564/564 (100%)	440 (78%)	124 (22%)	1	6

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	SER
1	L	13	SER
1	L	21	SER
1	L	32	TYR

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Mol	Chain	Res	Type
1	L	35	VAL
1	L	54	ASN
1	L	55	LYS
1	L	60	VAL
1	L	62	ASP
1	L	69	SER
1	L	71	ASN
1	L	72	THR
1	L	80	LEU
1	L	81	GLN
1	L	89	TYR
1	L	91	SER
1	L	99	PHE
1	L	118	THR
1	L	121	LEU
1	L	122	PHE
1	L	137	VAL
1	L	139	LEU
1	L	140	ILE
1	L	142	ASP
1	L	143	PHE
1	L	149	THR
1	L	150	VAL
1	L	160	LYS
1	L	166	THR
1	L	171	GLN
1	L	174	ASN
1	L	182	LEU
1	L	184	LEU
1	L	196	SER
1	L	198	GLN
1	L	200	THR
1	L	208	LYS
1	L	209	THR
2	H	5	GLN
2	H	11	LEU
2	H	12	VAL
2	H	13	LYS
2	H	16	GLU
2	H	18	LEU
2	H	29	ILE
2	H	31	THR

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Mol	Chain	Res	Type
2	H	35	TYR
2	H	36	TRP
2	H	48	GLU
2	H	52	TYR
2	H	55	TYR
2	H	68	ARG
2	H	69	VAL
2	H	71	ILE
2	H	72	SER
2	H	73	VAL
2	H	74	ASN
2	H	80	PHE
2	H	82	SER
2	H	91	ASP
2	H	96	TYR
2	H	105	ASN
2	H	109	GLN
2	H	111	THR
2	H	114	THR
2	H	121	LYS
2	H	123	PRO
2	H	125	VAL
2	H	142	LEU
2	H	145	LEU
2	H	149	TYR
2	H	150	PHE
2	H	151	PRO
2	H	152	GLN
2	H	176	SER
2	H	183	SER
2	H	187	THR
2	H	196	GLN
2	H	201	ASN
2	H	208	ASN
2	H	209	THR
2	H	210	LYS
2	H	211	VAL
2	H	214	ARG
2	H	217	PRO
2	H	219	LEU
2	H	226	PHE
2	H	231	LYS

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Mol	Chain	Res	Type
2	H	232	PRO
2	H	237	MET
2	H	241	THR
2	H	245	THR
2	H	247	VAL
2	H	249	VAL
2	H	265	ASP
2	H	274	THR
2	H	279	GLN
2	H	283	SER
2	H	286	ARG
2	H	290	VAL
2	H	294	LEU
2	H	321	ILE
2	H	327	GLN
2	H	329	ARG
2	H	332	GLN
2	H	351	THR
2	H	352	CYS
2	H	353	LEU
2	H	354	VAL
2	H	355	LYS
2	H	371	GLN
2	H	373	GLU
2	H	374	ASN
2	H	375	ASN
2	H	377	LYS
2	H	379	THR
2	H	392	TYR
2	H	397	VAL
2	H	399	LYS
2	H	407	VAL
2	H	410	CYS
2	H	415	GLU
2	H	420	HIS
2	H	424	LYS

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

Mol	Chain	Res	Type
1	L	6	GLN
1	L	39	GLN

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Mol	Chain	Res	Type
1	L	98	ASN
1	L	171	GLN
1	L	198	GLN
2	H	79	GLN
2	H	109	GLN
2	H	175	GLN
2	H	196	GLN
2	H	201	ASN
2	H	208	ASN
2	H	257	GLN
2	H	279	GLN
2	H	280	GLN
2	H	327	GLN
2	H	332	GLN
2	H	371	GLN
2	H	375	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

10 carbohydrates 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	H	429	3,2	14,14,15	2.26	6 (42%)	15,19,21	4.43	9 (60%)
3	FUL	H	430	3	10,10,11	1.42	1 (10%)	14,14,16	1.07	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	H	431	3	14,14,15	1.48	2 (14%)	15,19,21	3.79	6 (40%)
3	BMA	H	432	3,4	11,11,12	2.18	4 (36%)	14,15,17	4.52	9 (64%)
3	MAN	H	433	3	11,11,12	1.92	3 (27%)	14,15,17	2.79	6 (42%)
3	NAG	H	434	3	14,14,15	1.59	3 (21%)	15,19,21	2.64	5 (33%)
3	GAL	H	435	3	11,11,12	3.51	8 (72%)	14,15,17	4.18	10 (71%)
3	SIA	H	436	3	16,20,21	2.74	5 (31%)	18,28,31	2.92	7 (38%)
4	GUP	H	437	3,4	11,11,12	3.93	4 (36%)	14,15,17	5.47	7 (50%)
4	NAG	H	438	4	14,14,15	2.27	5 (35%)	15,19,21	3.09	8 (53%)

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	H	429	3,2	-	0/6/23/26	0/1/1/1
3	FUL	H	430	3	-	0/0/17/20	0/1/1/1
3	NAG	H	431	3	-	0/6/23/26	0/1/1/1
3	BMA	H	432	3,4	-	0/2/19/22	0/1/1/1
3	MAN	H	433	3	-	0/2/19/22	0/1/1/1
3	NAG	H	434	3	-	0/6/23/26	0/1/1/1
3	GAL	H	435	3	-	0/2/19/22	0/1/1/1
3	SIA	H	436	3	-	0/14/34/38	0/1/1/1
4	GUP	H	437	3,4	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	H	438	4	-	0/6/23/26	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	438	NAG	C8-C7	-4.11	1.42	1.50
4	H	438	NAG	C2-N2	-3.90	1.39	1.46
3	H	433	MAN	O3-C3	-3.56	1.34	1.43
3	H	435	GAL	O4-C4	-3.08	1.35	1.43
4	H	438	NAG	C7-N2	-3.08	1.22	1.34
4	H	438	NAG	O7-C7	-3.01	1.16	1.23
4	H	437	GUP	C1-C2	-2.81	1.45	1.52
3	H	436	SIA	C8-C7	2.00	1.57	1.53
3	H	434	NAG	C8-C7	2.04	1.54	1.50
3	H	436	SIA	C9-C8	2.54	1.59	1.52
3	H	432	BMA	C4-C5	2.57	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	433	MAN	O2-C2	2.58	1.49	1.43
3	H	431	NAG	O5-C5	2.58	1.49	1.43
3	H	434	NAG	C1-C2	2.62	1.56	1.52
3	H	429	NAG	C6-C5	2.64	1.61	1.51
3	H	432	BMA	C6-C5	2.75	1.61	1.51
3	H	435	GAL	C6-C5	2.75	1.61	1.51
3	H	432	BMA	C2-C3	2.76	1.56	1.52
3	H	433	MAN	C4-C3	2.80	1.59	1.52
3	H	435	GAL	O5-C5	2.81	1.49	1.43
3	H	429	NAG	C8-C7	2.89	1.56	1.50
3	H	429	NAG	C2-N2	2.95	1.51	1.46
3	H	430	FUL	C2-C3	3.16	1.56	1.52
3	H	431	NAG	C3-C2	3.18	1.59	1.52
3	H	429	NAG	C4-C5	3.20	1.59	1.53
4	H	437	GUP	C2-C3	3.24	1.57	1.52
3	H	436	SIA	C3-C4	3.25	1.58	1.52
3	H	434	NAG	C4-C5	3.34	1.60	1.53
3	H	429	NAG	C4-C3	3.39	1.61	1.52
4	H	438	NAG	C4-C5	3.47	1.60	1.53
3	H	435	GAL	C2-C3	3.48	1.57	1.52
3	H	435	GAL	C1-C2	3.69	1.61	1.52
3	H	429	NAG	C1-C2	3.98	1.58	1.52
4	H	437	GUP	C4-C5	4.15	1.61	1.53
3	H	435	GAL	C4-C5	4.32	1.62	1.53
3	H	432	BMA	C4-C3	4.55	1.64	1.52
3	H	436	SIA	C6-C5	4.83	1.61	1.53
3	H	435	GAL	O3-C3	5.15	1.55	1.43
3	H	435	GAL	C4-C3	6.09	1.68	1.52
3	H	436	SIA	C3-C2	8.16	1.66	1.52
4	H	437	GUP	O5-C1	11.20	1.62	1.43

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	431	NAG	O3-C3-C4	-7.90	92.54	110.34
4	H	437	GUP	C1-C2-C3	-7.87	100.23	109.54
4	H	437	GUP	O5-C1-C2	-6.67	100.04	110.86
3	H	432	BMA	O3-C3-C2	-5.30	100.43	110.00
3	H	434	NAG	O4-C4-C3	-4.79	99.56	110.34
3	H	433	MAN	C2-C3-C4	-4.67	103.10	111.04
3	H	435	GAL	O2-C2-C3	-4.29	101.48	110.12
4	H	438	NAG	C8-C7-N2	-4.10	108.26	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	436	SIA	C6-C5-N5	-3.83	104.39	111.07
4	H	438	NAG	C3-C4-C5	-3.77	103.63	110.20
4	H	438	NAG	C4-C3-C2	-3.76	105.39	111.23
3	H	435	GAL	C2-C3-C4	-3.48	105.13	111.04
3	H	433	MAN	C3-C4-C5	-3.38	104.31	110.20
3	H	435	GAL	O4-C4-C5	-3.10	101.02	109.24
3	H	429	NAG	O4-C4-C5	-2.79	101.86	109.24
3	H	436	SIA	C3-C4-C5	-2.67	108.50	111.47
3	H	436	SIA	O8-C8-C9	-2.61	103.12	109.22
3	H	429	NAG	C4-C3-C2	-2.61	107.17	111.23
4	H	438	NAG	O7-C7-C8	-2.42	117.61	122.06
3	H	434	NAG	C4-C3-C2	-2.41	107.49	111.23
3	H	429	NAG	O4-C4-C3	-2.37	105.00	110.34
3	H	429	NAG	O7-C7-C8	-2.12	118.17	122.06
3	H	431	NAG	O7-C7-C8	-2.05	118.30	122.06
3	H	431	NAG	C2-N2-C7	2.00	125.61	123.04
3	H	433	MAN	O4-C4-C5	2.00	114.54	109.24
3	H	434	NAG	C6-C5-C4	2.13	118.28	113.02
3	H	436	SIA	C5-N5-C10	2.15	128.63	123.10
3	H	433	MAN	O5-C1-C2	2.19	114.42	110.86
3	H	435	GAL	O4-C4-C3	2.25	115.40	110.34
3	H	429	NAG	C3-C2-N2	2.26	115.97	110.56
3	H	432	BMA	O6-C6-C5	2.37	119.16	111.33
3	H	430	FUL	C1-O5-C5	2.43	116.13	112.38
3	H	431	NAG	C8-C7-N2	2.51	120.91	116.11
4	H	438	NAG	O4-C4-C5	2.55	115.99	109.24
3	H	432	BMA	O2-C2-C1	2.58	114.38	109.21
4	H	437	GUP	C3-C4-C5	2.61	114.75	110.20
3	H	436	SIA	O6-C6-C5	2.66	112.84	108.48
3	H	435	GAL	O5-C1-C2	2.78	115.37	110.86
3	H	433	MAN	O3-C3-C4	2.85	116.75	110.34
3	H	432	BMA	C6-C5-C4	2.95	120.29	113.02
3	H	436	SIA	C9-C8-C7	3.02	119.56	112.48
3	H	432	BMA	C1-C2-C3	3.11	113.22	109.54
3	H	431	NAG	C1-O5-C5	3.23	116.34	112.25
4	H	437	GUP	O2-C2-C3	3.35	116.86	110.12
4	H	437	GUP	O5-C5-C6	3.44	114.81	107.35
3	H	432	BMA	O4-C4-C3	3.66	118.58	110.34
3	H	435	GAL	O3-C3-C4	3.97	119.28	110.34
4	H	438	NAG	C1-O5-C5	4.18	117.55	112.25
4	H	438	NAG	C6-C5-C4	4.19	123.35	113.02
3	H	429	NAG	C1-O5-C5	4.19	117.57	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	434	NAG	C1-O5-C5	4.30	117.70	112.25
4	H	437	GUP	C6-C5-C4	4.54	124.22	113.02
3	H	429	NAG	C6-C5-C4	5.20	125.85	113.02
3	H	435	GAL	C6-C5-C4	5.51	126.61	113.02
4	H	438	NAG	O7-C7-N2	6.00	134.10	121.86
3	H	429	NAG	C3-C4-C5	6.35	121.28	110.20
3	H	435	GAL	C3-C4-C5	6.47	121.48	110.20
3	H	434	NAG	C2-N2-C7	6.66	131.60	123.04
3	H	432	BMA	C1-O5-C5	6.69	120.74	112.25
3	H	435	GAL	C1-O5-C5	6.98	121.11	112.25
3	H	433	MAN	C1-O5-C5	7.02	121.16	112.25
3	H	435	GAL	C1-C2-C3	7.22	118.08	109.54
3	H	432	BMA	O5-C1-C2	7.68	123.32	110.86
3	H	436	SIA	C7-C6-C5	9.52	128.74	114.32
3	H	432	BMA	O3-C3-C4	10.37	133.69	110.34
3	H	431	NAG	C4-C3-C2	10.71	127.89	111.23
3	H	429	NAG	C2-N2-C7	12.99	139.72	123.04
4	H	437	GUP	O6-C6-C5	16.03	164.30	111.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	437	GUP	C1

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	431	NAG	1	0
3	H	432	BMA	5	0
3	H	433	MAN	1	0
3	H	435	GAL	4	0
3	H	436	SIA	3	0
4	H	437	GUP	6	0
4	H	438	NAG	6	0

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.