



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:28 PM GMT

PDB ID : 1FRT
Title : CRYSTAL STRUCTURE OF THE COMPLEX OF RAT NEONATAL FC
RECEPTOR WITH FC
Authors : Burmeister, W.P.; Bjorkman, P.J.
Deposited on : 1994-11-11
Resolution : 4.50 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

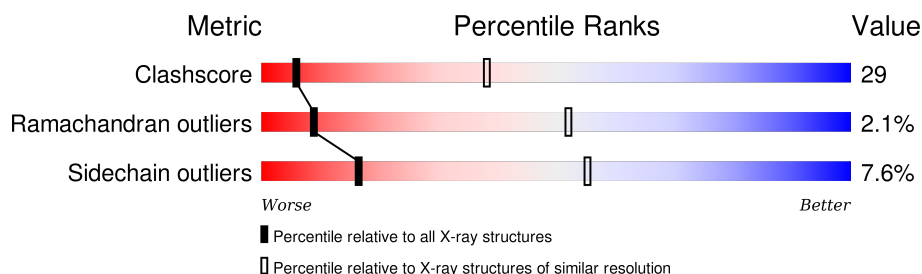
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)

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	A	269	
2	B	99	
3	C	205	

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
6	FUC	C	2	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4756 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 NEONATAL FC RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2138	1354	370	404	10			

- Molecule 2 is a protein called BETA 2-MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	528	137	152	4			

- Molecule 3 is a protein called IGG FC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	205	Total	C	N	O	S	0	0	0
			1649	1049	280	313	7			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	272	GLN	GLU	CONFLICT	GB 243866
C	283	GLN	GLU	CONFLICT	GB 243866
C	294	GLN	GLU	CONFLICT	GB 243866
C	312	ASN	ASP	CONFLICT	GB 243866
C	315	ASP	ASN	CONFLICT	GB 243866
C	356	GLU	ASP	CONFLICT	GB 243866
C	358	MET	LEU	CONFLICT	GB 243866

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 6 is a polymer of unknown type called SUGAR (9-MER).

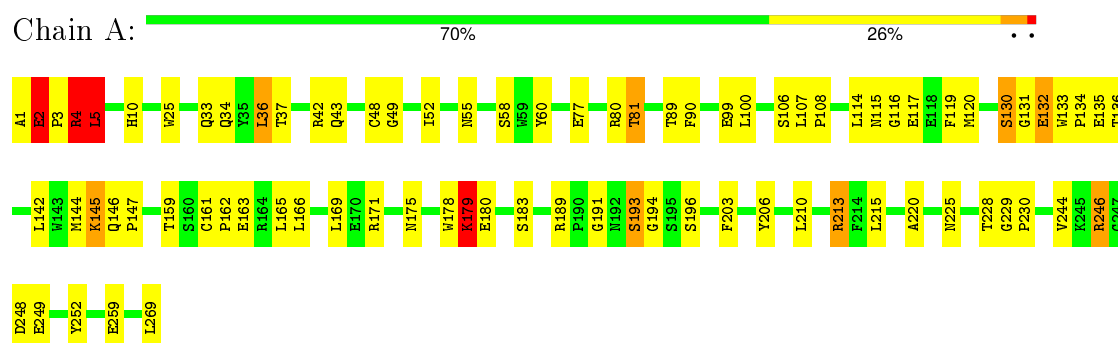
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	9	Total	C	N	O	0	0
			110	62	4	44		

3 Residue-property plots

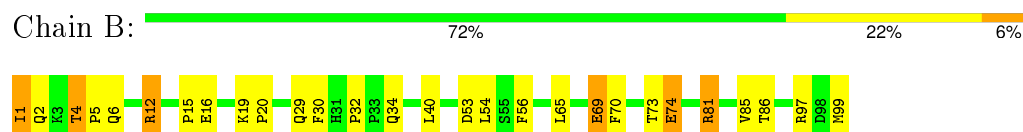
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

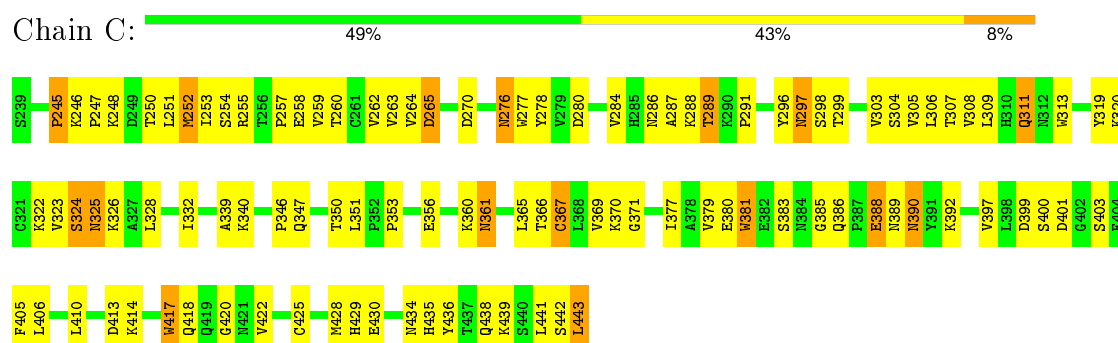
• Molecule 1: NEONATAL FC RECEPTOR



• Molecule 2: BETA 2-MICROGLOBULIN



• Molecule 3: IGG FC



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.00Å 145.00Å 216.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.50	Depositor
% Data completeness (in resolution range)	67.0 (20.00-4.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.423 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4756	wwPDB-VP
Average B, all atoms (Å ²)	199.0	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: FUC, GAL, NAG, BMA, 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	A	0.77	1/2200 (0.0%)	0.98	7/2991 (0.2%)
2	B	0.85	0/846	0.90	0/1149
3	C	1.40	5/1693 (0.3%)	1.26	1/2302 (0.0%)
All	All	1.05	6/4739 (0.1%)	1.08	8/6442 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
3	C	0	13
6	C	2	0
All	All	2	15

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	443	LEU	C-OXT	38.49	1.96	1.23
3	C	417	TRP	NE1-CE2	-8.12	1.26	1.37
3	C	277	TRP	NE1-CE2	-7.92	1.27	1.37
3	C	381	TRP	NE1-CE2	-7.75	1.27	1.37
3	C	313	TRP	NE1-CE2	-7.68	1.27	1.37
1	A	179	LYS	C-N	-5.03	1.22	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	LYS	O-C-N	-18.23	93.53	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	LEU	CA-CB-CG	8.04	133.80	115.30
1	A	4	ARG	N-CA-C	5.71	126.42	111.00
1	A	107	LEU	N-CA-C	-5.39	96.44	111.00
3	C	367	CYS	N-CA-CB	5.20	119.96	110.60
1	A	5	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	249	GLU	N-CA-C	5.06	124.67	111.00
1	A	166	LEU	CA-CB-CG	5.03	126.88	115.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	2	FUC	C5,C1

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	179	LYS	Mainchain
1	A	60	TYR	Sidechain
3	C	252	MET	Mainchain
3	C	276	ASN	Sidechain
3	C	325	ASN	Sidechain
3	C	361	ASN	Mainchain
3	C	380	GLU	Sidechain
3	C	386	GLN	Sidechain
3	C	388	GLU	Sidechain
3	C	390	ASN	Sidechain
3	C	399	ASP	Sidechain
3	C	401	ASP	Sidechain
3	C	413	ASP	Sidechain
3	C	418	GLN	Sidechain
3	C	438	GLN	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2138	0	2032	172	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	821	0	807	31	4
3	C	1649	0	1620	196	3
4	A	14	0	13	0	0
5	A	24	0	22	1	1
6	C	110	0	94	3	0
All	All	4756	0	4588	267	10

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 29.

All (267) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:PRO:CB	3:C:252:MET:HE1	1.26	1.57
1:A:134:PRO:HB2	3:C:252:MET:CE	1.06	1.50
1:A:115:ASN:ND2	3:C:254:SER:HA	1.17	1.47
3:C:251:LEU:HD22	3:C:435:HIS:ND1	1.37	1.37
1:A:115:ASN:HD22	3:C:254:SER:CA	1.35	1.35
1:A:134:PRO:CB	3:C:252:MET:CE	1.81	1.35
1:A:117:GLU:H	3:C:253:ILE:CD1	1.36	1.35
1:A:114:LEU:HB3	3:C:253:ILE:CG2	1.55	1.34
1:A:117:GLU:O	3:C:253:ILE:HD12	1.24	1.29
1:A:135:GLU:OE1	3:C:252:MET:SD	1.92	1.27
1:A:135:GLU:OE2	3:C:252:MET:SD	1.92	1.27
1:A:135:GLU:CD	3:C:252:MET:SD	2.15	1.25
2:B:1:ILE:HD11	3:C:309:LEU:CA	1.67	1.24
1:A:114:LEU:CB	3:C:253:ILE:HG21	1.66	1.24
1:A:134:PRO:CG	3:C:252:MET:HE3	1.68	1.21
1:A:134:PRO:CG	3:C:436:TYR:HB2	1.70	1.21
1:A:178:TRP:CZ2	1:A:180:GLU:HB2	1.74	1.21
3:C:251:LEU:CD2	3:C:435:HIS:ND1	2.03	1.20
1:A:114:LEU:CB	3:C:253:ILE:CG2	2.19	1.19
1:A:117:GLU:H	3:C:253:ILE:HD11	1.03	1.17
1:A:134:PRO:CG	3:C:252:MET:CE	2.21	1.17
1:A:115:ASN:HB2	3:C:253:ILE:C	1.65	1.15
1:A:135:GLU:OE2	3:C:252:MET:CE	1.96	1.12
2:B:1:ILE:HD13	3:C:309:LEU:CD2	1.79	1.10
1:A:135:GLU:OE2	3:C:252:MET:HE2	1.51	1.09
1:A:135:GLU:OE2	3:C:252:MET:CG	1.99	1.08
2:B:1:ILE:CD1	3:C:309:LEU:HA	1.83	1.08
2:B:1:ILE:CD1	3:C:309:LEU:HD23	1.83	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLU:OE2	3:C:252:MET:HG2	1.55	1.07
1:A:117:GLU:N	3:C:253:ILE:CD1	2.17	1.06
1:A:117:GLU:N	3:C:253:ILE:HD11	1.69	1.06
1:A:134:PRO:HG2	3:C:252:MET:HE3	1.34	1.06
1:A:115:ASN:CB	3:C:253:ILE:O	2.04	1.05
3:C:251:LEU:HD13	3:C:435:HIS:HB3	1.34	1.05
1:A:115:ASN:CG	3:C:254:SER:HA	1.78	1.04
1:A:134:PRO:HG3	3:C:436:TYR:CB	1.87	1.04
1:A:178:TRP:CZ3	1:A:206:TYR:HB3	1.92	1.04
1:A:115:ASN:ND2	3:C:254:SER:CA	2.02	1.01
1:A:117:GLU:H	3:C:253:ILE:CG1	1.73	1.01
1:A:114:LEU:HB3	3:C:253:ILE:HG21	1.01	1.00
1:A:115:ASN:HB2	3:C:253:ILE:O	1.64	0.96
1:A:114:LEU:C	3:C:253:ILE:CG2	2.30	0.94
2:B:1:ILE:HD13	3:C:309:LEU:HD22	1.48	0.94
1:A:134:PRO:CD	3:C:252:MET:CE	2.45	0.93
1:A:114:LEU:CA	3:C:253:ILE:HG21	1.99	0.92
1:A:114:LEU:C	3:C:253:ILE:HG23	1.90	0.91
1:A:4:ARG:HG3	1:A:99:GLU:HG2	1.52	0.91
1:A:114:LEU:N	3:C:253:ILE:CD1	2.32	0.91
2:B:1:ILE:HD13	3:C:309:LEU:HD23	1.46	0.91
1:A:178:TRP:CH2	1:A:180:GLU:HB2	2.04	0.91
3:C:388:GLU:HG2	3:C:410:LEU:HD11	1.54	0.89
1:A:178:TRP:CE3	1:A:206:TYR:HB3	2.07	0.89
1:A:178:TRP:CZ3	1:A:206:TYR:CB	2.55	0.89
1:A:134:PRO:HG3	3:C:436:TYR:HB2	0.91	0.89
1:A:117:GLU:O	3:C:253:ILE:CD1	2.18	0.88
1:A:114:LEU:H	3:C:253:ILE:CD1	1.87	0.87
2:B:1:ILE:CD1	3:C:309:LEU:CD2	2.47	0.87
3:C:248:LYS:HG3	3:C:428:MET:HE1	1.56	0.87
1:A:134:PRO:CD	3:C:252:MET:HE2	2.04	0.86
2:B:1:ILE:HD11	3:C:309:LEU:HA	0.88	0.86
1:A:178:TRP:CZ2	1:A:180:GLU:CB	2.58	0.85
1:A:133:TRP:HA	3:C:434:ASN:O	1.77	0.85
1:A:114:LEU:HG	3:C:253:ILE:HG23	1.59	0.85
1:A:134:PRO:HD2	3:C:252:MET:HE2	1.59	0.84
1:A:134:PRO:CB	3:C:252:MET:HE2	2.06	0.84
1:A:114:LEU:N	3:C:253:ILE:HD13	1.66	0.84
1:A:115:ASN:C	3:C:253:ILE:HG12	1.97	0.83
1:A:115:ASN:HB3	3:C:253:ILE:O	1.77	0.83
3:C:284:VAL:HB	3:C:287:ALA:HB2	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:248:LYS:CG	3:C:428:MET:HE1	2.11	0.81
1:A:115:ASN:HB2	3:C:254:SER:N	1.94	0.81
1:A:134:PRO:HD2	3:C:252:MET:CE	2.10	0.81
1:A:132:GLU:N	3:C:434:ASN:OD1	2.14	0.80
1:A:115:ASN:CB	3:C:254:SER:HA	2.10	0.80
1:A:179:LYS:NZ	1:A:259:GLU:OE1	2.15	0.80
1:A:133:TRP:C	3:C:434:ASN:HB3	2.03	0.79
1:A:117:GLU:N	3:C:253:ILE:HG13	1.98	0.79
2:B:40:LEU:HD21	2:B:81:ARG:HH21	1.46	0.78
1:A:117:GLU:HG3	3:C:253:ILE:HG13	1.66	0.78
1:A:117:GLU:N	3:C:253:ILE:CG1	2.43	0.78
1:A:37:THR:HB	2:B:53:ASP:OD2	1.84	0.78
3:C:251:LEU:CD1	3:C:435:HIS:HB3	2.14	0.77
1:A:115:ASN:HD22	3:C:254:SER:C	1.86	0.77
1:A:114:LEU:CB	3:C:253:ILE:HG23	2.15	0.76
3:C:251:LEU:HD13	3:C:435:HIS:CB	2.15	0.76
1:A:114:LEU:CG	3:C:253:ILE:HG23	2.16	0.76
3:C:251:LEU:HD21	3:C:435:HIS:ND1	2.00	0.75
1:A:114:LEU:CA	3:C:253:ILE:CG2	2.63	0.75
1:A:178:TRP:HH2	1:A:180:GLU:OE1	1.69	0.75
1:A:178:TRP:CH2	1:A:180:GLU:CB	2.71	0.74
1:A:134:PRO:CB	3:C:436:TYR:HB2	2.18	0.74
1:A:10:HIS:HB3	2:B:56:PHE:CE2	2.22	0.73
1:A:134:PRO:CD	3:C:252:MET:HE3	2.15	0.72
3:C:420:GLY:HA2	3:C:443:LEU:HB3	1.69	0.72
1:A:133:TRP:CA	3:C:434:ASN:O	2.38	0.72
1:A:132:GLU:O	3:C:434:ASN:C	2.28	0.71
1:A:114:LEU:H	3:C:253:ILE:HD12	1.55	0.71
3:C:379:VAL:HG21	3:C:406:LEU:HD11	1.72	0.71
1:A:134:PRO:HB2	3:C:252:MET:HE2	1.55	0.71
1:A:134:PRO:HB3	3:C:436:TYR:CG	2.25	0.71
1:A:114:LEU:CG	3:C:253:ILE:CG2	2.68	0.70
2:B:2:GLN:OE1	3:C:288:LYS:NZ	2.24	0.70
3:C:287:ALA:HB3	3:C:306:LEU:HD11	1.73	0.69
1:A:161:CYS:HB3	1:A:162:PRO:HD3	1.74	0.69
1:A:117:GLU:C	3:C:253:ILE:HD12	2.10	0.69
1:A:135:GLU:CD	3:C:252:MET:CG	2.58	0.69
3:C:328:LEU:HD21	3:C:332:ILE:HG13	1.75	0.69
3:C:377:ILE:HG13	3:C:429:HIS:HB2	1.75	0.69
1:A:90:PHE:CE2	3:C:254:SER:HB3	2.27	0.69
3:C:351:LEU:HB2	3:C:366:THR:HB	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLU:HG2	1:A:80:ARG:HH12	1.58	0.68
1:A:133:TRP:N	3:C:434:ASN:HB3	2.08	0.68
1:A:178:TRP:HZ3	1:A:206:TYR:CB	2.01	0.68
1:A:178:TRP:CE2	1:A:180:GLU:HB2	2.29	0.68
1:A:134:PRO:HB3	3:C:436:TYR:CD1	2.29	0.67
1:A:178:TRP:CH2	1:A:180:GLU:OE1	2.47	0.67
1:A:114:LEU:HB3	3:C:253:ILE:HG22	1.68	0.67
1:A:179:LYS:HD2	1:A:259:GLU:HB2	1.75	0.67
3:C:250:THR:HG22	3:C:257:PRO:HB3	1.75	0.67
1:A:117:GLU:CB	3:C:253:ILE:HG13	2.26	0.66
1:A:178:TRP:HZ3	1:A:206:TYR:HB2	1.58	0.66
1:A:114:LEU:C	3:C:253:ILE:HG21	2.15	0.66
1:A:117:GLU:CG	3:C:253:ILE:HG13	2.27	0.65
2:B:4:THR:HG23	2:B:86:THR:HB	1.78	0.64
1:A:179:LYS:HD2	1:A:259:GLU:CB	2.27	0.64
3:C:381:TRP:CE3	3:C:410:LEU:HD22	2.33	0.64
1:A:115:ASN:HB2	3:C:254:SER:CA	2.28	0.63
3:C:417:TRP:HH2	3:C:441:LEU:HD22	1.64	0.62
3:C:276:ASN:HB2	3:C:322:LYS:HB3	1.81	0.61
3:C:259:VAL:HG23	3:C:308:VAL:HG21	1.82	0.61
1:A:133:TRP:CA	3:C:434:ASN:HB3	2.30	0.61
3:C:251:LEU:CD2	3:C:435:HIS:CE1	2.82	0.60
1:A:115:ASN:HD22	3:C:254:SER:HA	0.72	0.60
2:B:1:ILE:CG1	3:C:309:LEU:HD23	2.30	0.60
1:A:4:ARG:HB2	1:A:100:LEU:O	2.01	0.60
1:A:115:ASN:CB	3:C:254:SER:CA	2.79	0.59
1:A:213:ARG:HH11	1:A:213:ARG:HG2	1.66	0.59
3:C:371:GLY:HA2	3:C:403:SER:HB3	1.84	0.59
1:A:77:GLU:HG2	1:A:80:ARG:NH1	2.18	0.59
3:C:365:LEU:HB2	3:C:410:LEU:HB3	1.85	0.59
2:B:1:ILE:HD11	3:C:309:LEU:CB	2.33	0.58
1:A:203:PHE:HD2	2:B:12:ARG:O	1.86	0.58
1:A:134:PRO:CB	3:C:436:TYR:CB	2.83	0.57
3:C:246:LYS:HE2	3:C:248:LYS:HB3	1.87	0.57
1:A:133:TRP:C	3:C:434:ASN:O	2.43	0.56
3:C:383:SER:HB2	3:C:388:GLU:OE1	2.04	0.56
1:A:5:LEU:O	1:A:165:LEU:HD11	2.04	0.56
1:A:133:TRP:O	3:C:434:ASN:HB3	2.05	0.56
1:A:134:PRO:CA	3:C:252:MET:CE	2.77	0.56
2:B:15:PRO:O	2:B:16:GLU:HG3	2.05	0.56
5:A:403:NAG:O5	5:A:405:FUC:C1	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:THR:CB	2:B:53:ASP:OD2	2.54	0.55
1:A:159:THR:O	1:A:163:GLU:HG3	2.06	0.55
3:C:248:LYS:CB	3:C:428:MET:HE1	2.36	0.55
3:C:245:PRO:HB2	3:C:250:THR:HG23	1.89	0.55
3:C:245:PRO:HA	6:C:7:GAL:H61	1.88	0.55
1:A:244:VAL:HG11	1:A:252:TYR:CE2	2.42	0.54
1:A:81:THR:HG21	1:A:142:LEU:HD22	1.89	0.54
3:C:353:PRO:HD3	3:C:365:LEU:HD23	1.89	0.54
1:A:55:ASN:O	1:A:171:ARG:HD3	2.08	0.54
2:B:1:ILE:CD1	3:C:309:LEU:CA	2.62	0.53
1:A:34:GLN:HG2	1:A:48:CYS:SG	2.48	0.53
3:C:247:PRO:O	3:C:251:LEU:HG	2.09	0.53
1:A:115:ASN:O	2:B:1:ILE:N	2.42	0.53
1:A:115:ASN:O	3:C:253:ILE:O	2.26	0.53
3:C:291:PRO:HA	3:C:303:VAL:O	2.09	0.53
3:C:263:VAL:HG21	3:C:323:VAL:HG11	1.90	0.53
3:C:397:VAL:HG23	3:C:405:PHE:CE1	2.43	0.53
2:B:32:PRO:HB2	2:B:34:GLN:OE1	2.08	0.52
3:C:346:PRO:HD3	3:C:429:HIS:HD2	1.74	0.52
1:A:120:MET:HG3	1:A:130:SER:O	2.10	0.52
3:C:324:SER:O	3:C:328:LEU:HD23	2.10	0.52
2:B:1:ILE:HD11	3:C:309:LEU:HD23	1.82	0.52
1:A:132:GLU:C	3:C:434:ASN:CA	2.79	0.52
3:C:422:VAL:HG22	3:C:442:SER:HB3	1.92	0.51
1:A:131:GLY:O	1:A:132:GLU:HG3	2.10	0.51
3:C:258:GLU:HB2	6:C:7:GAL:H62	1.92	0.50
3:C:258:GLU:HB3	3:C:305:VAL:CG1	2.41	0.50
1:A:115:ASN:O	3:C:253:ILE:HG12	2.12	0.50
1:A:179:LYS:HA	1:A:206:TYR:O	2.09	0.50
1:A:178:TRP:CZ2	1:A:180:GLU:CG	2.94	0.50
1:A:134:PRO:HA	3:C:436:TYR:HB3	1.92	0.49
3:C:365:LEU:HD12	3:C:410:LEU:HD23	1.94	0.49
1:A:145:LYS:HG3	1:A:145:LYS:O	2.11	0.49
1:A:114:LEU:CD2	3:C:254:SER:OG	2.60	0.49
1:A:133:TRP:N	3:C:434:ASN:CB	2.75	0.49
3:C:251:LEU:HD21	3:C:435:HIS:CE1	2.45	0.48
1:A:178:TRP:CE3	1:A:206:TYR:CB	2.87	0.48
1:A:213:ARG:NH1	1:A:213:ARG:HG2	2.29	0.48
1:A:114:LEU:HD21	3:C:254:SER:OG	2.13	0.48
1:A:144:MET:O	1:A:146:GLN:N	2.47	0.48
1:A:132:GLU:N	1:A:133:TRP:CE3	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:THR:HG23	2:B:86:THR:CB	2.42	0.48
3:C:289:THR:HG23	3:C:304:SER:OG	2.14	0.48
1:A:178:TRP:HE3	1:A:206:TYR:CD2	2.32	0.48
1:A:115:ASN:ND2	3:C:254:SER:CB	2.72	0.47
1:A:33:GLN:NE2	1:A:206:TYR:OH	2.46	0.47
1:A:4:ARG:HB2	1:A:100:LEU:HB2	1.96	0.47
3:C:371:GLY:HA2	3:C:403:SER:CB	2.44	0.47
3:C:297:ASN:HB3	3:C:299:THR:HG22	1.96	0.47
3:C:328:LEU:HD21	3:C:332:ILE:CG1	2.44	0.47
3:C:245:PRO:HD3	3:C:259:VAL:HG22	1.97	0.47
1:A:134:PRO:HD3	3:C:434:ASN:O	2.14	0.47
1:A:117:GLU:CA	3:C:253:ILE:CD1	2.92	0.47
2:B:1:ILE:HG12	3:C:309:LEU:HD23	1.96	0.47
3:C:360:LYS:O	3:C:414:LYS:HD2	2.14	0.47
1:A:25:TRP:CZ2	2:B:54:LEU:HD23	2.50	0.46
3:C:365:LEU:HD22	3:C:441:LEU:HD13	1.97	0.46
1:A:116:GLY:N	3:C:253:ILE:HD11	2.31	0.46
1:A:131:GLY:HA3	1:A:136:THR:HG21	1.96	0.46
1:A:4:ARG:HB2	1:A:100:LEU:CA	2.46	0.45
1:A:132:GLU:C	3:C:434:ASN:HA	2.37	0.45
1:A:132:GLU:O	3:C:434:ASN:CA	2.65	0.45
3:C:326:LYS:C	3:C:328:LEU:H	2.20	0.45
1:A:1:ALA:HB1	1:A:169:LEU:HB3	1.98	0.45
3:C:260:THR:HG22	3:C:262:VAL:HG23	1.98	0.45
1:A:134:PRO:N	3:C:252:MET:HE2	2.32	0.45
1:A:106:SER:HB2	1:A:162:PRO:CG	2.47	0.45
3:C:297:ASN:HB3	3:C:298:SER:H	1.45	0.45
2:B:73:THR:O	2:B:97:ARG:NH2	2.50	0.45
3:C:278:TYR:HB2	3:C:320:LYS:HB3	1.99	0.44
1:A:52:ILE:O	1:A:52:ILE:HG22	2.18	0.44
1:A:134:PRO:CA	3:C:252:MET:HE2	2.44	0.44
3:C:258:GLU:HG2	3:C:307:THR:HG22	1.98	0.44
1:A:134:PRO:CA	3:C:436:TYR:CB	2.95	0.44
1:A:115:ASN:CA	3:C:253:ILE:HG12	2.47	0.44
3:C:369:VAL:HG11	3:C:377:ILE:HD11	1.99	0.44
3:C:276:ASN:CB	3:C:322:LYS:HB3	2.48	0.44
1:A:134:PRO:HA	3:C:436:TYR:CB	2.48	0.44
1:A:134:PRO:N	3:C:434:ASN:O	2.51	0.43
1:A:33:GLN:CG	1:A:206:TYR:OH	2.66	0.43
3:C:245:PRO:HB2	3:C:250:THR:CG2	2.47	0.43
3:C:296:TYR:HD2	6:C:1:NAG:H62	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:SER:HB2	1:A:162:PRO:HG3	1.99	0.43
3:C:308:VAL:HG13	3:C:319:TYR:OH	2.17	0.43
3:C:389:ASN:HD22	3:C:389:ASN:HA	1.52	0.43
1:A:133:TRP:CD1	3:C:251:LEU:O	2.72	0.43
3:C:347:GLN:HB2	3:C:370:LYS:HG2	2.00	0.43
1:A:215:LEU:O	1:A:252:TYR:HA	2.19	0.43
3:C:264:VAL:O	3:C:265:ASP:HB2	2.18	0.43
3:C:286:ASN:HA	3:C:286:ASN:HD22	1.58	0.43
3:C:259:VAL:HG23	3:C:308:VAL:CG2	2.48	0.42
3:C:390:ASN:HD22	3:C:390:ASN:HA	1.58	0.42
1:A:228:THR:HG22	1:A:229:GLY:N	2.35	0.42
1:A:134:PRO:HD2	3:C:252:MET:HE3	1.88	0.42
1:A:134:PRO:CD	3:C:434:ASN:O	2.68	0.42
1:A:134:PRO:CB	3:C:436:TYR:CG	2.98	0.42
2:B:5:PRO:HB3	2:B:30:PHE:HB3	2.01	0.42
1:A:2:GLU:O	1:A:169:LEU:HD22	2.19	0.41
3:C:257:PRO:HG2	3:C:308:VAL:O	2.20	0.41
1:A:194:GLY:O	1:A:246:ARG:HB2	2.20	0.41
1:A:34:GLN:NE2	2:B:53:ASP:OD2	2.54	0.41
1:A:117:GLU:HB2	3:C:253:ILE:HG13	2.02	0.41
2:B:19:LYS:HA	2:B:20:PRO:HD3	1.89	0.41
2:B:40:LEU:HD11	2:B:81:ARG:HB2	2.02	0.41
1:A:215:LEU:HD23	1:A:220:ALA:HA	2.02	0.41
1:A:144:MET:C	1:A:146:GLN:H	2.24	0.41
3:C:430:GLU:HA	3:C:435:HIS:CD2	2.56	0.41
3:C:276:ASN:HB3	3:C:278:TYR:CE2	2.56	0.41
1:A:230:PRO:HG2	2:B:65:LEU:HD13	2.03	0.40
1:A:115:ASN:C	3:C:253:ILE:CG1	2.81	0.40
1:A:1:ALA:O	1:A:3:PRO:CD	2.69	0.40
3:C:361:ASN:HA	3:C:414:LYS:HD2	2.03	0.40
3:C:311:GLN:HG3	3:C:311:GLN:H	1.19	0.40
3:C:252:MET:O	3:C:255:ARG:HB2	2.22	0.40
1:A:117:GLU:CA	3:C:253:ILE:HG13	2.51	0.40
3:C:328:LEU:HD21	3:C:332:ILE:CD1	2.51	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:356:GLU:OE1	3:C:439:LYS:NZ[8_565]	1.04	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:GLU:OE1	2:B:74:GLU:OE1[6_755]	1.54	0.66
2:B:74:GLU:CG	2:B:74:GLU:OE1[6_755]	1.63	0.57
2:B:74:GLU:CD	2:B:74:GLU:OE1[6_755]	1.74	0.46
3:C:356:GLU:CD	3:C:439:LYS:NZ[8_565]	1.97	0.23
1:A:193:SER:CA	5:A:403:NAG:O7[6_755]	2.07	0.13
1:A:42:ARG:NH2	2:B:69:GLU:O[7_655]	2.11	0.09
1:A:193:SER:CB	1:A:225:ASN:ND2[6_755]	2.12	0.08
3:C:392:LYS:CE	3:C:400:SER:OG[8_565]	2.13	0.07
1:A:189:ARG:NH2	1:A:191:GLY:O[6_755]	2.16	0.04

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	A	267/269 (99%)	248 (93%)	13 (5%)	6 (2%)	8	51
2	B	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
3	C	201/205 (98%)	178 (89%)	17 (8%)	6 (3%)	5	44
All	All	565/573 (99%)	517 (92%)	36 (6%)	12 (2%)	9	52

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
3	C	265	ASP
3	C	297	ASN
3	C	339	ALA
1	A	49	GLY
1	A	145	LYS
3	C	324	SER
1	A	193	SER
3	C	385	GLY
1	A	132	GLU

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Mol	Chain	Res	Type
3	C	340	LYS
1	A	147	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	227/227 (100%)	208 (92%)	19 (8%)	14	51
2	B	95/95 (100%)	84 (88%)	11 (12%)	7	35
3	C	192/192 (100%)	183 (95%)	9 (5%)	32	69
All	All	514/514 (100%)	475 (92%)	39 (8%)	16	55

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	4	ARG
1	A	5	LEU
1	A	36	LEU
1	A	43	GLN
1	A	58	SER
1	A	81	THR
1	A	89	THR
1	A	108	PRO
1	A	119	PHE
1	A	130	SER
1	A	175	ASN
1	A	183	SER
1	A	196	SER
1	A	210	LEU
1	A	213	ARG
1	A	246	ARG
1	A	248	ASP
1	A	269	LEU
2	B	1	ILE

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Mol	Chain	Res	Type
2	B	4	THR
2	B	6	GLN
2	B	12	ARG
2	B	29	GLN
2	B	69	GLU
2	B	70	PHE
2	B	74	GLU
2	B	81	ARG
2	B	85	VAL
2	B	99	MET
3	C	245	PRO
3	C	270	ASP
3	C	280	ASP
3	C	289	THR
3	C	311	GLN
3	C	325	ASN
3	C	350	THR
3	C	367	CYS
3	C	425	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	55	ASN
1	A	115	ASN
1	A	141	ASN
1	A	175	ASN
1	A	217	ASN
1	A	251	HIS
3	C	276	ASN
3	C	283	GLN
3	C	286	ASN
3	C	294	GLN
3	C	311	GLN
3	C	384	ASN
3	C	389	ASN
3	C	390	ASN
3	C	421	ASN
3	C	438	GLN

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 ⓘ

11 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$
5	NAG	A	403	1,5	14,14,15	0.99	1 (7%)	15,19,21	1.16	1 (6%)
5	FUC	A	405	5	10,10,11	1.02	1 (10%)	14,14,16	0.84	1 (7%)
6	NAG	C	1	3,6	14,14,15	0.74	0	15,19,21	1.46	1 (6%)
6	FUC	C	2	6	10,10,11	0.78	0	14,14,16	1.56	2 (14%)
6	NAG	C	3	6	14,14,15	1.07	1 (7%)	15,19,21	1.45	2 (13%)
6	BMA	C	4	6	11,11,12	0.65	0	14,15,17	1.47	1 (7%)
6	MAN	C	5	6	11,11,12	0.75	1 (9%)	14,15,17	1.88	2 (14%)
6	NAG	C	6	6	14,14,15	0.74	0	15,19,21	1.62	1 (6%)
6	GAL	C	7	6	11,11,12	0.66	0	14,15,17	1.84	3 (21%)
6	MAN	C	8	6	11,11,12	0.56	0	14,15,17	1.74	1 (7%)
6	NAG	C	9	6	14,14,15	0.72	0	15,19,21	1.67	1 (6%)

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
5	NAG	A	403	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FUC	A	405	5	-	0/0/17/20	0/1/1/1
6	NAG	C	1	3,6	-	0/6/23/26	0/1/1/1
6	FUC	C	2	6	2/2/4/5	0/0/17/20	0/1/1/1
6	NAG	C	3	6	-	0/6/23/26	0/1/1/1
6	BMA	C	4	6	-	0/2/19/22	0/1/1/1
6	MAN	C	5	6	-	0/2/19/22	0/1/1/1
6	NAG	C	6	6	-	0/6/23/26	0/1/1/1
6	GAL	C	7	6	-	0/2/19/22	0/1/1/1
6	MAN	C	8	6	-	0/2/19/22	0/1/1/1
6	NAG	C	9	6	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	5	MAN	C2-C3	2.04	1.55	1.52
5	A	403	NAG	C1-C2	2.06	1.55	1.52
6	C	3	NAG	C1-C2	2.24	1.55	1.52
5	A	405	FUC	C1-C2	2.58	1.58	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	7	GAL	O5-C1-C2	-2.66	106.54	110.86
5	A	405	FUC	C2-C3-C4	-2.45	106.87	111.04
5	A	403	NAG	C2-N2-C7	2.04	125.67	123.04
6	C	2	FUC	C1-C2-C3	2.05	111.96	109.54
6	C	7	GAL	O2-C2-C1	2.08	113.38	109.21
6	C	3	NAG	C2-N2-C7	2.16	125.81	123.04
6	C	5	MAN	C1-C2-C3	2.52	112.52	109.54
6	C	4	BMA	C1-O5-C5	4.44	117.89	112.25
6	C	3	NAG	C1-O5-C5	4.49	117.94	112.25
6	C	2	FUC	C1-O5-C5	4.82	119.82	112.38
6	C	1	NAG	C1-O5-C5	4.98	118.57	112.25
6	C	6	NAG	C1-O5-C5	5.19	118.84	112.25
6	C	7	GAL	C1-O5-C5	5.43	119.14	112.25
6	C	5	MAN	C1-O5-C5	5.84	119.66	112.25
6	C	8	MAN	C1-O5-C5	5.96	119.81	112.25
6	C	9	NAG	C1-O5-C5	6.14	120.04	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	2	FUC	C5
6	C	2	FUC	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	403	NAG	1	1
5	A	405	FUC	1	0
6	C	1	NAG	1	0
6	C	7	GAL	2	0

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
4	NAG	A	401	1	14,14,15	0.67	0	15,19,21	1.04	1 (6%)

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
4	NAG	A	401	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	401	NAG	C4-C3-C2	-2.93	106.68	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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.