Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:00 PM GMT

PDB ID	:	3SGJ
Title	:	Unique carbohydrate-carbohydrate interactions are required for high affinity binding between FcgIII and antibodies lacking core fucose
Authors	:	Ferrara, C.; Grau, S.; Jaeger, C.; Sondermann, P.; Bruenker, P.; Waldhauer, I.; Hennig, M.; Ruf, A.; Rufer, A.C.; Stihle, M.; Umana, P.; Benz, J.
Deposited on	:	2011-06-15
Resolution	:	2.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

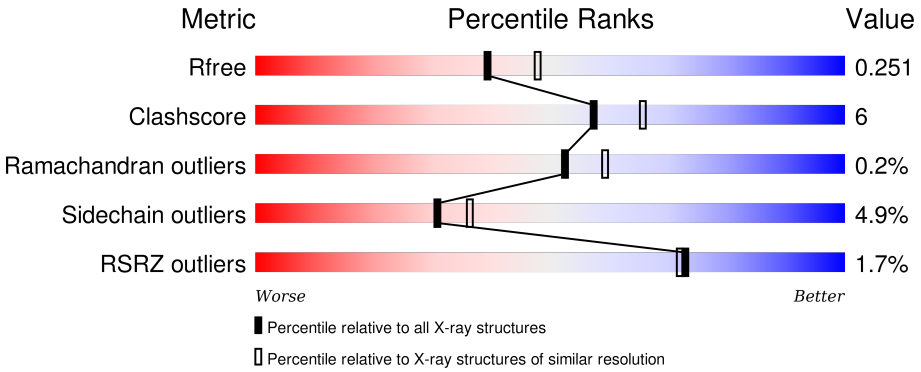
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 <=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	225	2% 82% 15%
1	B	225	2% 78% 16%
2	C	204	68% 15% 17%

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	FUC	A	508	X	-	-	-
4	MLI	A	509	-	-	-	X
5	MAN	B	501	X	-	-	-
6	MAN	C	304	X	-	-	-
6	MAN	C	305	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5443 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 human Fc fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1738	1107	291	332	8			
1	B	217	Total	C	N	O	S	0	0	0
			1726	1101	289	329	7			

- Molecule 2 is a protein called human Fcg3a receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	169	Total	C	N	O	S	0	0	0
			1365	870	233	258	4			

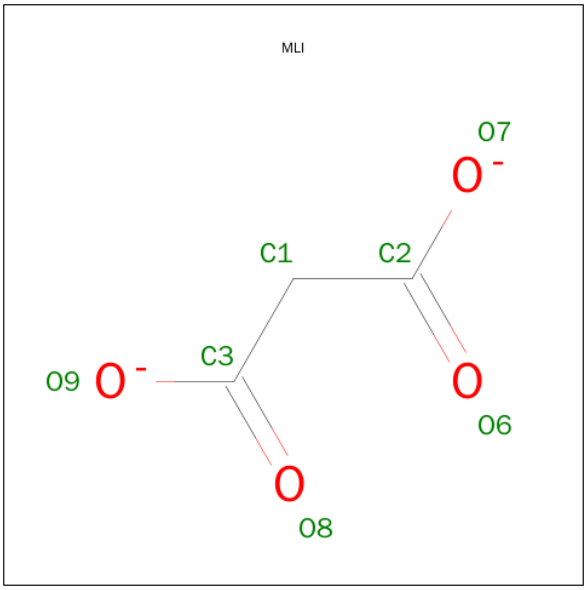
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	38	GLN	ASN	ENGINEERED MUTATION	UNP P08637
C	74	GLN	ASN	ENGINEERED MUTATION	UNP P08637
C	158	VAL	PHE	SEE REMARK 999	UNP P08637
C	169	GLN	ASN	ENGINEERED MUTATION	UNP P08637
C	191	GLY	-	EXPRESSION TAG	UNP P08637
C	192	LYS	-	EXPRESSION TAG	UNP P08637
C	193	LYS	-	EXPRESSION TAG	UNP P08637
C	194	LYS	-	EXPRESSION TAG	UNP P08637
C	195	LYS	-	EXPRESSION TAG	UNP P08637
C	196	LYS	-	EXPRESSION TAG	UNP P08637
C	197	LYS	-	EXPRESSION TAG	UNP P08637
C	198	GLY	-	EXPRESSION TAG	UNP P08637
C	199	HIS	-	EXPRESSION TAG	UNP P08637
C	200	HIS	-	EXPRESSION TAG	UNP P08637
C	201	HIS	-	EXPRESSION TAG	UNP P08637
C	202	HIS	-	EXPRESSION TAG	UNP P08637
C	203	HIS	-	EXPRESSION TAG	UNP P08637
C	204	HIS	-	EXPRESSION TAG	UNP P08637

- Molecule 3 is a polymer of unknown type called Low affinity immunoglobulin gamma Fc region receptor III-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	8	Total	C	N	O	0	0
			99	56	4	39		

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



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

- Molecule 5 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	8	Total	C	N	O	0	0
			99	56	4	39		

- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

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

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is water.

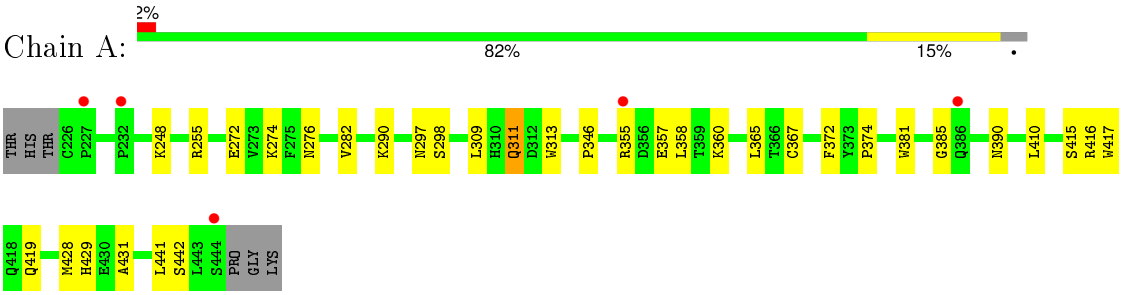
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	122	Total	O	0	0
			122	122		
8	B	111	Total	O	0	0
			111	111		
8	C	87	Total	O	0	0
			87	87		

3 Residue-property plots (i)

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.

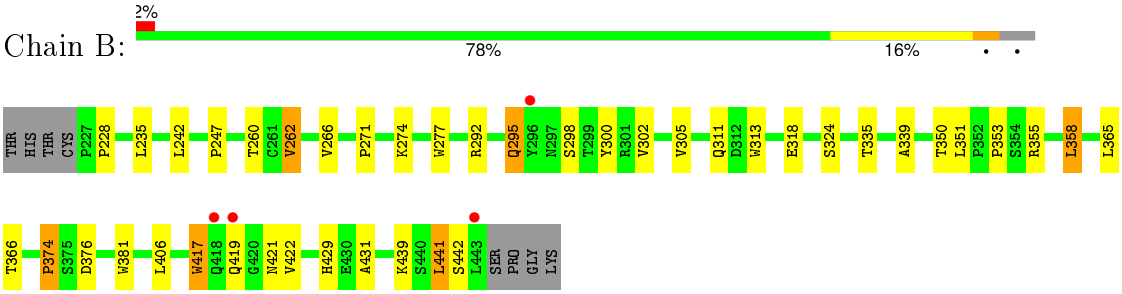
- Molecule 1: human Fc fragment

Chain A:



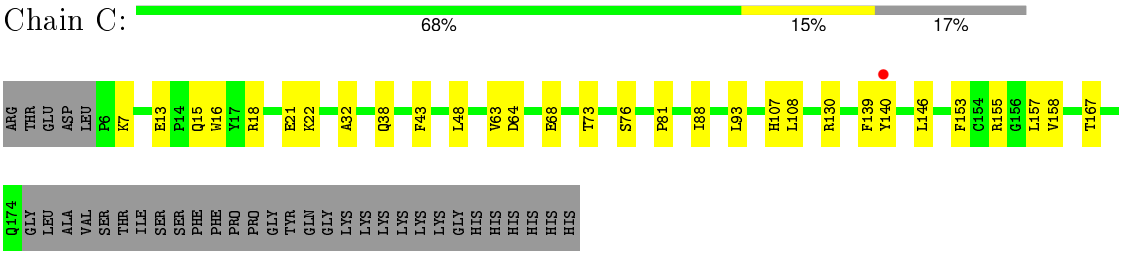
- Molecule 1: human Fc fragment

Chain B:



- Molecule 2: human Fcg3a receptor

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.65Å 88.48Å 140.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	140.29 – 2.20 49.77 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (140.29-2.20) 100.0 (49.77-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.6.0112	Depositor
R, R_{free}	0.195 , 0.252 0.195 , 0.251	Depositor DCC
R_{free} test set	2157 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 37.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 45936 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5443	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MAN, BMA, NAG, MLI, FUC

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	0.60	2/1788 (0.1%)	0.68	0/2440
1	B	0.60	4/1776 (0.2%)	0.66	0/2423
2	C	0.68	1/1403 (0.1%)	0.71	0/1906
All	All	0.62	7/4967 (0.1%)	0.68	0/6769

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
3	A	1	0
5	B	1	0
6	C	2	0
All	All	4	0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	16	TRP	CD2-CE2	6.09	1.48	1.41
1	B	381	TRP	CD2-CE2	5.76	1.48	1.41
1	B	277	TRP	CD2-CE2	5.50	1.48	1.41
1	B	313	TRP	CD2-CE2	5.25	1.47	1.41
1	A	417	TRP	CD2-CE2	5.22	1.47	1.41
1	A	313	TRP	CD2-CE2	5.09	1.47	1.41
1	B	417	TRP	CD2-CE2	5.08	1.47	1.41

There are no bond angle outliers.

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	508	FUC	C1
5	B	501	MAN	C1
6	C	304	MAN	C1
6	C	305	MAN	C1

There are no planarity outliers.

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	1738	0	1703	16	0
1	B	1726	0	1694	20	0
2	C	1365	0	1309	19	0
3	A	99	0	85	2	0
4	A	7	0	2	1	0
5	B	99	0	85	1	0
6	C	61	0	52	3	0
7	C	28	0	25	1	0
8	A	122	0	0	2	0
8	B	111	0	0	0	0
8	C	87	0	0	3	0
All	All	5443	0	4955	60	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 6.

All (60) 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:248:LYS:HG3	1:A:428:MET:HE1	1.24	1.09
2:C:63:VAL:HG21	2:C:88:ILE:HD11	1.45	0.95
1:A:248:LYS:HG3	1:A:428:MET:CE	2.00	0.91
1:B:350:THR:HB	1:B:441:LEU:HG	1.53	0.90
2:C:68:GLU:HG3	2:C:81:PRO:HB3	1.66	0.78
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.66	0.77
1:B:429:HIS:CD2	1:B:431:ALA:H	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:68:GLU:HG3	2:C:81:PRO:CB	2.24	0.67
3:A:508:FUC:O3	6:C:302:NAG:H62	1.94	0.66
2:C:63:VAL:CG2	2:C:88:ILE:HD11	2.25	0.65
1:B:318:GLU:OE1	1:B:335:THR:HG21	1.97	0.64
1:A:311:GLN:HE21	1:A:311:GLN:HA	1.62	0.64
1:B:429:HIS:HD2	1:B:431:ALA:H	1.43	0.63
1:A:297:ASN:O	1:A:298:SER:HB3	1.98	0.63
2:C:38:GLN:NE2	2:C:73:THR:OG1	2.32	0.62
2:C:21:GLU:OE2	2:C:63:VAL:HG23	2.02	0.60
1:B:228:PRO:HG2	1:B:298:SER:HB2	1.83	0.60
1:A:274:LYS:HE3	1:A:276:ASN:HD21	1.67	0.59
1:A:357:GLU:O	1:A:360:LYS:HB2	2.04	0.58
2:C:155:ARG:HD3	8:C:447:HOH:O	2.04	0.57
1:A:374:PRO:O	1:A:429:HIS:HE1	1.87	0.57
1:A:416:ARG:HD3	8:A:676:HOH:O	2.04	0.56
1:A:429:HIS:HD2	1:A:431:ALA:H	1.53	0.56
2:C:43:PHE:CE2	2:C:48:LEU:HD13	2.40	0.56
1:B:271:PRO:HB2	1:B:292:ARG:NH1	2.21	0.55
3:A:502:NAG:HN2	3:A:508:FUC:H5	1.71	0.55
2:C:107:HIS:HD2	2:C:140:TYR:CZ	2.26	0.54
1:A:429:HIS:CD2	1:A:431:ALA:H	2.27	0.53
2:C:32:ALA:H	2:C:38:GLN:HE22	1.58	0.51
1:A:355:ARG:HA	1:A:358:LEU:HD23	1.92	0.51
1:B:351:LEU:HB2	1:B:366:THR:HB	1.92	0.51
2:C:108:LEU:HD12	2:C:139:PHE:HD2	1.76	0.51
6:C:301:NAG:H61	8:C:486:HOH:O	2.11	0.50
1:B:295:GLN:HG2	5:B:502:NAG:H62	1.93	0.50
2:C:64:ASP:OD1	7:C:307:NAG:O6	2.30	0.50
1:B:406:LEU:HD12	1:B:406:LEU:C	2.32	0.50
1:B:422:VAL:HG22	1:B:442:SER:OG	2.13	0.48
1:B:274:LYS:HB3	1:B:324:SER:HB2	1.95	0.47
1:B:417:TRP:HH2	1:B:441:LEU:HD22	1.78	0.47
1:B:353:PRO:HD3	1:B:365:LEU:HD23	1.97	0.47
1:B:419:GLN:HE21	1:B:421:ASN:HB2	1.80	0.46
2:C:18:ARG:NH1	2:C:93:LEU:O	2.47	0.46
1:A:365:LEU:HB3	1:A:441:LEU:HD23	1.97	0.46
1:B:266:VAL:HB	1:B:300:TYR:HB2	1.98	0.46
2:C:13:GLU:HG2	8:C:430:HOH:O	2.15	0.46
1:B:417:TRP:CH2	1:B:441:LEU:HD22	2.50	0.45
2:C:63:VAL:HG21	2:C:88:ILE:CD1	2.32	0.45
2:C:73:THR:H	2:C:76:SER:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLU:HG2	8:A:711:HOH:O	2.16	0.44
1:B:260:THR:HG22	1:B:262:VAL:HG12	1.99	0.44
1:B:339:ALA:HB3	1:B:374:PRO:HB3	1.99	0.43
6:C:303:BMA:H62	6:C:305:MAN:H2	1.50	0.42
2:C:93:LEU:HD22	2:C:153:PHE:HA	2.01	0.42
1:B:355:ARG:HA	1:B:358:LEU:HD23	2.02	0.42
1:B:247:PRO:HG3	1:B:376:ASP:OD1	2.20	0.42
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.55	0.42
4:A:509:MLI:O8	4:A:509:MLI:O6	2.34	0.41
1:A:365:LEU:HD12	1:A:410:LEU:HD23	2.02	0.41
2:C:38:GLN:HB3	2:C:73:THR:HB	2.02	0.41
2:C:21:GLU:O	2:C:22:LYS:HB2	2.21	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	A	217/225 (96%)	214 (99%)	2 (1%)	1 (0%)	34 35
1	B	215/225 (96%)	211 (98%)	4 (2%)	0	100 100
2	C	167/204 (82%)	162 (97%)	5 (3%)	0	100 100
All	All	599/654 (92%)	587 (98%)	11 (2%)	1 (0%)	52 59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	385	GLY

5.3.2 Protein sidechains (i)

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	203/208 (98%)	194 (96%)	9 (4%)	35	42
1	B	201/208 (97%)	190 (94%)	11 (6%)	27	30
2	C	152/183 (83%)	145 (95%)	7 (5%)	33	40
All	All	556/599 (93%)	529 (95%)	27 (5%)	31	36

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	ARG
1	A	282	VAL
1	A	290	LYS
1	A	309	LEU
1	A	311	GLN
1	A	390	ASN
1	A	415	SER
1	A	419	GLN
1	A	442	SER
1	B	235	LEU
1	B	242	LEU
1	B	262	VAL
1	B	295	GLN
1	B	302	VAL
1	B	305	VAL
1	B	311	GLN
1	B	358	LEU
1	B	374	PRO
1	B	439	LYS
1	B	441	LEU
2	C	7	LYS
2	C	15	GLN
2	C	130	ARG
2	C	146	LEU
2	C	157	LEU
2	C	158	VAL

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Mol	Chain	Res	Type
2	C	167	THR

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	276	ASN
1	A	311	GLN
1	A	315	ASN
1	A	390	ASN
1	A	429	HIS
1	B	276	ASN
1	B	295	GLN
1	B	347	GLN
1	B	390	ASN
1	B	418	GLN
1	B	419	GLN
1	B	429	HIS
1	B	433	HIS
2	C	15	GLN
2	C	38	GLN
2	C	107	HIS
2	C	134	HIS

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

23 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	A	501	1,3	14,14,15	0.52	0	15,19,21	1.06	1 (6%)
3	NAG	A	502	3	14,14,15	0.68	0	15,19,21	0.93	1 (6%)
3	BMA	A	503	3	11,11,12	0.32	0	14,15,17	1.15	0
3	MAN	A	504	3	11,11,12	0.60	0	14,15,17	0.98	0
3	NAG	A	505	3	14,14,15	0.52	0	15,19,21	1.04	1 (6%)
3	MAN	A	506	3	11,11,12	0.61	0	14,15,17	1.41	2 (14%)
3	NAG	A	507	3	14,14,15	0.46	0	15,19,21	1.00	0
3	FUC	A	508	3	10,10,11	0.79	0	14,14,16	1.86	4 (28%)
5	MAN	B	501	5	11,11,12	1.37	1 (9%)	14,15,17	1.96	4 (28%)
5	NAG	B	502	1,5	14,14,15	0.65	0	15,19,21	1.44	2 (13%)
5	NAG	B	503	5	14,14,15	0.62	0	15,19,21	1.43	2 (13%)
5	BMA	B	504	5	11,11,12	0.50	0	14,15,17	1.73	4 (28%)
5	MAN	B	505	5	11,11,12	0.60	0	14,15,17	1.19	2 (14%)
5	NAG	B	506	5	14,14,15	0.58	0	15,19,21	1.68	3 (20%)
5	NAG	B	507	5	14,14,15	0.53	0	15,19,21	2.13	4 (26%)
5	FUC	B	508	5	10,10,11	0.88	0	14,14,16	2.36	4 (28%)
6	NAG	C	301	2,6	14,14,15	1.82	1 (7%)	15,19,21	2.17	4 (26%)
6	NAG	C	302	6	14,14,15	0.72	1 (7%)	15,19,21	1.47	4 (26%)
6	BMA	C	303	6	11,11,12	0.46	0	14,15,17	1.16	2 (14%)
6	MAN	C	304	6	11,11,12	0.70	0	14,15,17	2.27	3 (21%)
6	MAN	C	305	6	11,11,12	0.68	0	14,15,17	1.49	2 (14%)
7	NAG	C	306	2,7	14,14,15	1.94	1 (7%)	15,19,21	2.22	4 (26%)
7	NAG	C	307	7	14,14,15	0.55	0	15,19,21	1.34	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
3	NAG	A	501	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	502	3	-	0/6/23/26	0/1/1/1
3	BMA	A	503	3	-	0/2/19/22	0/1/1/1
3	MAN	A	504	3	-	0/2/19/22	0/1/1/1
3	NAG	A	505	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	A	506	3	-	0/2/19/22	0/1/1/1
3	NAG	A	507	3	-	0/6/23/26	0/1/1/1
3	FUC	A	508	3	1/1/4/5	0/0/17/20	0/1/1/1
5	MAN	B	501	5	1/1/4/5	0/2/19/22	0/1/1/1
5	NAG	B	502	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	503	5	-	0/6/23/26	0/1/1/1
5	BMA	B	504	5	-	0/2/19/22	0/1/1/1
5	MAN	B	505	5	-	0/2/19/22	0/1/1/1
5	NAG	B	506	5	-	0/6/23/26	0/1/1/1
5	NAG	B	507	5	-	0/6/23/26	0/1/1/1
5	FUC	B	508	5	-	0/0/17/20	0/1/1/1
6	NAG	C	301	2,6	-	0/6/23/26	0/1/1/1
6	NAG	C	302	6	-	0/6/23/26	0/1/1/1
6	BMA	C	303	6	-	0/2/19/22	0/1/1/1
6	MAN	C	304	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	C	305	6	1/1/4/5	0/2/19/22	0/1/1/1
7	NAG	C	306	2,7	-	0/6/23/26	0/1/1/1
7	NAG	C	307	7	-	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)
7	C	306	NAG	O5-C1	-6.66	1.32	1.43
6	C	301	NAG	O5-C1	-6.49	1.32	1.43
5	B	501	MAN	O5-C1	-4.23	1.36	1.43
6	C	302	NAG	O5-C1	-2.19	1.40	1.43

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	306	NAG	C1-O5-C5	-6.69	103.76	112.25
6	C	301	NAG	C1-O5-C5	-5.29	105.53	112.25
5	B	507	NAG	C4-C3-C2	-4.58	104.11	111.23
5	B	501	MAN	O5-C1-C2	-4.38	103.75	110.86
3	A	506	MAN	O2-C2-C3	-3.73	102.62	110.12
5	B	504	BMA	C3-C4-C5	-3.37	104.31	110.20
5	B	501	MAN	C1-C2-C3	-3.26	105.68	109.54
5	B	502	NAG	C3-C4-C5	-3.25	104.52	110.20
3	A	501	NAG	C3-C4-C5	-3.09	104.81	110.20
7	C	306	NAG	C2-N2-C7	-2.59	119.72	123.04
3	A	508	FUC	O3-C3-C2	-2.58	105.34	110.00
6	C	303	BMA	C1-C2-C3	-2.37	106.74	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	503	NAG	O7-C7-C8	-2.31	117.82	122.06
7	C	306	NAG	C4-C3-C2	-2.25	107.73	111.23
6	C	302	NAG	O3-C3-C4	-2.16	105.48	110.34
5	B	506	NAG	O7-C7-C8	-2.15	118.12	122.06
5	B	505	MAN	O2-C2-C3	-2.14	105.82	110.12
5	B	504	BMA	O6-C6-C5	-2.03	104.61	111.33
3	A	502	NAG	O4-C4-C5	-2.03	103.86	109.24
3	A	506	MAN	O2-C2-C1	2.04	113.30	109.21
6	C	302	NAG	C1-O5-C5	2.07	114.88	112.25
3	A	505	NAG	C1-O5-C5	2.19	115.03	112.25
7	C	306	NAG	O5-C5-C6	2.27	112.27	107.35
5	B	501	MAN	C3-C4-C5	2.45	114.46	110.20
6	C	303	BMA	C1-O5-C5	2.52	115.44	112.25
5	B	508	FUC	C3-C4-C5	2.53	113.98	109.72
5	B	502	NAG	C1-O5-C5	2.58	115.53	112.25
5	B	507	NAG	C1-O5-C5	2.60	115.55	112.25
5	B	505	MAN	O5-C5-C6	2.62	113.01	107.35
5	B	504	BMA	O3-C3-C4	2.64	116.28	110.34
6	C	305	MAN	C1-O5-C5	2.69	115.66	112.25
6	C	301	NAG	C3-C4-C5	2.70	114.90	110.20
3	A	508	FUC	O5-C5-C6	2.72	110.62	106.13
6	C	302	NAG	C4-C3-C2	2.78	115.55	111.23
6	C	301	NAG	C3-C2-N2	2.79	117.23	110.56
7	C	307	NAG	C1-O5-C5	2.86	115.88	112.25
6	C	302	NAG	C3-C4-C5	2.92	115.28	110.20
5	B	506	NAG	C1-O5-C5	3.10	116.19	112.25
5	B	501	MAN	C1-O5-C5	3.13	116.22	112.25
5	B	503	NAG	C1-O5-C5	3.16	116.26	112.25
6	C	301	NAG	C2-N2-C7	3.30	127.28	123.04
3	A	508	FUC	C3-C4-C5	3.58	115.75	109.72
5	B	504	BMA	O3-C3-C2	3.76	116.79	110.00
6	C	304	MAN	O5-C1-C2	3.78	116.99	110.86
5	B	508	FUC	O5-C5-C6	3.78	112.38	106.13
5	B	507	NAG	C2-N2-C7	3.89	128.03	123.04
3	A	508	FUC	C2-C3-C4	3.92	117.70	111.04
6	C	305	MAN	C3-C4-C5	3.97	117.11	110.20
5	B	507	NAG	C3-C2-N2	4.13	120.46	110.56
5	B	508	FUC	C2-C3-C4	4.38	118.49	111.04
5	B	506	NAG	C3-C4-C5	4.39	117.85	110.20
5	B	508	FUC	C1-C2-C3	4.67	115.07	109.54
6	C	304	MAN	C1-O5-C5	4.71	118.22	112.25
6	C	304	MAN	C1-C2-C3	5.55	116.11	109.54

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	304	MAN	C1
5	B	501	MAN	C1
6	C	305	MAN	C1
3	A	508	FUC	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAG	1	0
3	A	508	FUC	2	0
5	B	502	NAG	1	0
6	C	301	NAG	1	0
6	C	302	NAG	1	0
6	C	303	BMA	1	0
6	C	305	MAN	1	0
7	C	307	NAG	1	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	MLI	A	509	-	0,6,6	0.00	-	0,7,7	0.00	-

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	MLI	A	509	-	-	0/0/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	509	MLI	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	219/225 (97%)	0.08	5 (2%)	64	63	24, 37, 66, 81	0
1	B	217/225 (96%)	-0.13	4 (1%)	71	70	27, 41, 64, 88	0
2	C	169/204 (82%)	-0.08	1 (0%)	90	90	24, 34, 56, 87	0
All	All	605/654 (92%)	-0.04	10 (1%)	73	72	24, 38, 64, 88	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	SER	4.4
1	B	296	TYR	3.7
1	A	232	PRO	2.6
1	B	418	GLN	2.5
2	C	140	TYR	2.2
1	B	443	LEU	2.2
1	B	419	GLN	2.2
1	A	386	GLN	2.1
1	A	355	ARG	2.1
1	A	227	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	B	507	14/15	0.92	0.14	0.41	44,48,54,56	0
7	NAG	C	306	14/15	0.94	0.12	-0.01	28,31,36,36	0
5	NAG	B	502	14/15	0.96	0.12	-0.67	30,33,38,41	0
3	NAG	A	505	14/15	0.94	0.10	-1.20	37,42,46,47	0
6	NAG	C	301	14/15	0.89	0.12	-1.33	37,43,51,53	0
5	NAG	B	503	14/15	0.96	0.09	-2.67	25,28,30,33	0
3	NAG	A	501	14/15	0.95	0.10	-3.67	28,31,44,53	0
6	MAN	C	304	11/12	0.44	0.33	-	88,97,99,102	0
3	MAN	A	506	11/12	0.88	0.13	-	50,58,66,69	0
5	MAN	B	501	11/12	0.90	0.14	-	56,59,61,69	0
3	MAN	A	504	11/12	0.94	0.10	-	37,38,39,41	0
3	BMA	A	503	11/12	0.97	0.11	-	31,34,37,41	0
6	MAN	C	305	11/12	0.73	0.28	-	97,100,103,104	0
6	NAG	C	302	14/15	0.86	0.15	-	52,58,69,71	0
3	FUC	A	508	10/11	0.81	0.24	-	64,73,77,86	0
5	FUC	B	508	10/11	0.85	0.22	-	54,60,63,65	0
3	NAG	A	507	14/15	0.76	0.20	-	78,83,88,92	0
5	BMA	B	504	11/12	0.95	0.09	-	35,40,43,51	0
6	BMA	C	303	11/12	0.70	0.23	-	77,85,92,93	0
5	MAN	B	505	11/12	0.97	0.07	-	37,41,43,44	0
3	NAG	A	502	14/15	0.98	0.10	-	29,30,31,31	0
7	NAG	C	307	14/15	0.94	0.11	-	36,38,40,40	0
5	NAG	B	506	14/15	0.83	0.18	-	65,78,87,89	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	MLI	A	509	7/7	0.90	0.21	3.33	40,43,46,48	0

6.5 Other polymers

There are no such residues in this entry.