



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:01 PM GMT

PDB ID : 3SGK
Title : Unique carbohydrate/carbohydrate interactions are required for high affinity binding of FcγIII 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 : 2.40 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) : 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

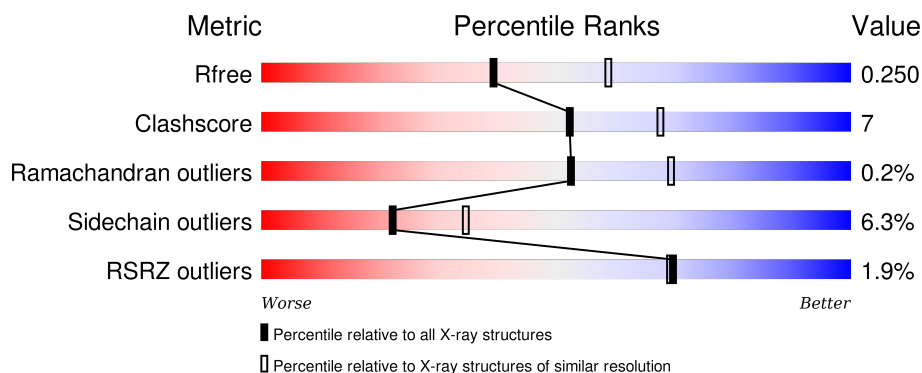
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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.

Mol	Chain	Length	Quality of chain
1	A	225	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 76%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 76% 15% • 7% </div> </div>
1	B	225	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 21%, green 72%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 72% 21% • 6% </div> </div>
2	C	204	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 63%, yellow 15%, orange 1%, grey 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 63% 15% • 19% </div> </div>

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	MLI	A	1	-	-	-	X
5	NAG	B	1445	X	-	-	-
5	MAN	B	1451	X	-	-	-
6	MAN	C	1471	X	-	-	-
6	MAN	C	1475	X	-	-	-
6	MAN	C	1476	X	-	-	-
6	MAN	C	1477	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5163 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 Fc fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1668	1061	281	320	6			
1	B	212	Total	C	N	O	S	0	0	0
			1694	1080	284	324	6			

- Molecule 2 is a protein called human Fcg3a receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	165	Total	C	N	O	S	0	0	0
			1331	850	229	248	4			

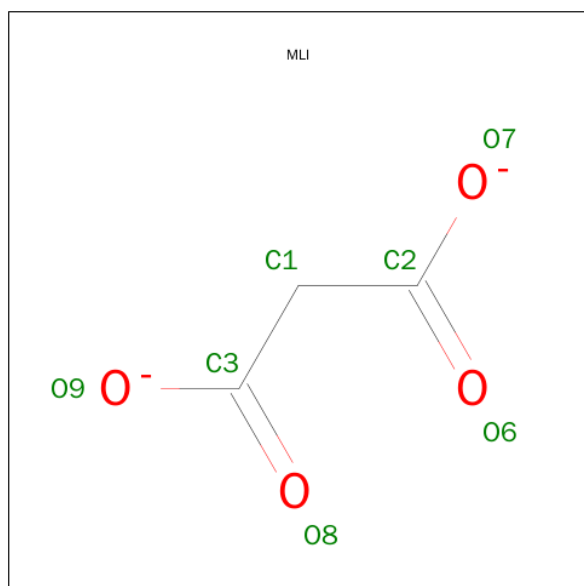
There are 18 discrepancies between the modelled and reference sequences:

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
			103	58	5	40		

- 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
			103	58	5	40		

- Molecule 6 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	8	Total	C	N	O	0	0
			94	52	2	40		

- 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		

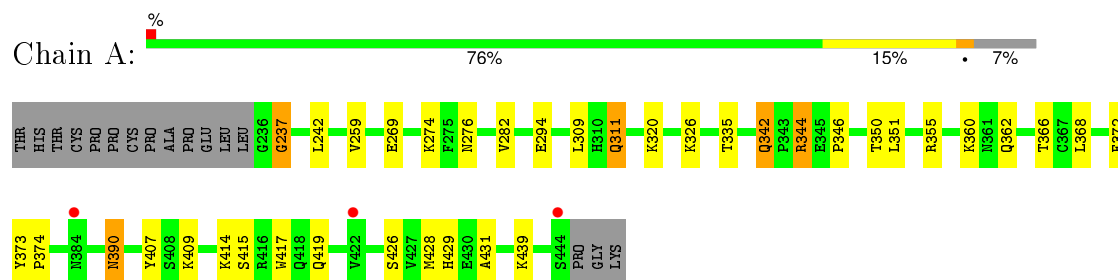
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	51	Total	O	0	0
			51	51		
8	B	30	Total	O	0	0
			30	30		
8	C	54	Total	O	0	0
			54	54		

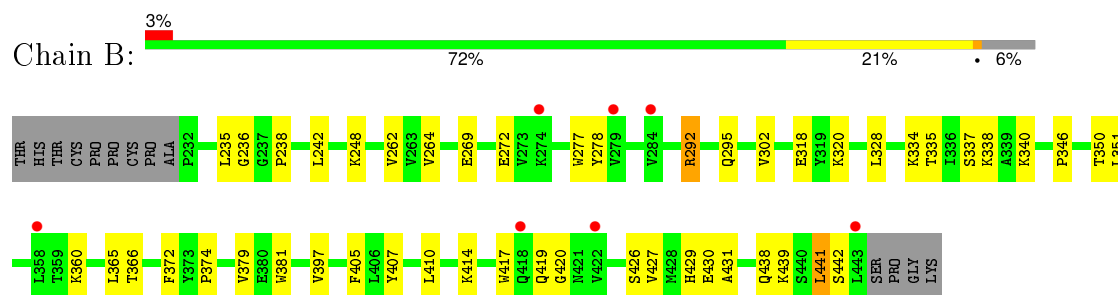
3 Residue-property plots [i](#)

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.

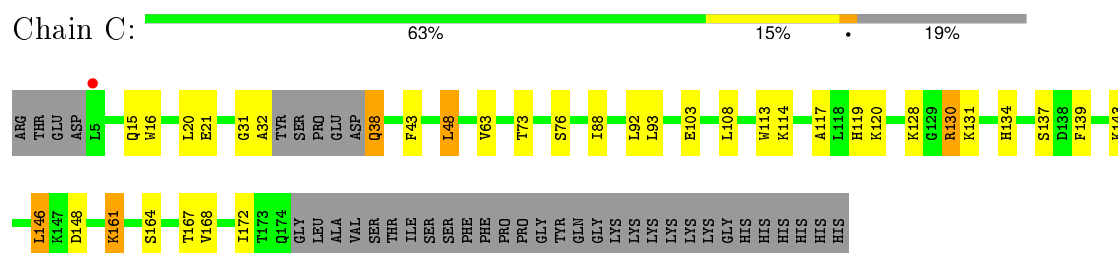
- Molecule 1: Fc fragment



- Molecule 1: Fc fragment



- Molecule 2: human Fcg3a receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.34Å 88.23Å 141.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 48.72 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.40) 100.0 (48.72-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0112	Depositor
R, R_{free}	0.205 , 0.250 0.208 , 0.250	Depositor DCC
R_{free} test set	1687 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 33659 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5163	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: BMA, NAG, MLI, 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	0.55	1/1714 (0.1%)	0.61	0/2335
1	B	0.54	3/1741 (0.2%)	0.60	0/2372
2	C	0.63	1/1366 (0.1%)	0.67	0/1854
All	All	0.57	5/4821 (0.1%)	0.62	0/6561

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
5	B	2	0
6	C	4	0
All	All	6	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	417	TRP	CD2-CE2	5.42	1.47	1.41
1	A	417	TRP	CD2-CE2	5.35	1.47	1.41
1	B	381	TRP	CD2-CE2	5.17	1.47	1.41
2	C	16	TRP	CD2-CE2	5.14	1.47	1.41
1	B	277	TRP	CD2-CE2	5.04	1.47	1.41

There are no bond angle outliers.

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1451	MAN	C1
5	B	1445	NAG	C1

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Mol	Chain	Res	Type	Atom
6	C	1471	MAN	C1
6	C	1475	MAN	C1
6	C	1476	MAN	C1
6	C	1477	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	1668	0	1633	21	0
1	B	1694	0	1664	26	0
2	C	1331	0	1287	18	0
3	A	103	0	88	0	0
4	A	7	0	2	0	0
5	B	103	0	88	1	0
6	C	94	0	79	4	0
7	C	28	0	24	0	0
8	A	51	0	0	2	0
8	B	30	0	0	1	0
8	C	54	0	0	3	0
All	All	5163	0	4865	66	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 7.

All (66) 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)
6:C:1445:NAG:C8	8:C:243:HOH:O	2.05	1.03
1:B:350:THR:HB	1:B:441:LEU:HG	1.63	0.79
1:B:236:GLY:O	2:C:161:LYS:HE3	1.82	0.79
1:B:338:LYS:HE3	1:B:430:GLU:OE1	1.84	0.77
5:B:1452:NAG:H5	5:B:1454:NAG:H5	1.65	0.77
6:C:1445:NAG:H83	8:C:243:HOH:O	1.77	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.68	0.73
1:A:274:LYS:HE3	1:A:276:ASN:HD21	1.55	0.71
1:B:419:GLN:HG3	1:B:420:GLY:HA2	1.73	0.69
2:C:103:GLU:HA	2:C:143:LYS:HB2	1.74	0.69
6:C:1445:NAG:H81	8:C:243:HOH:O	1.82	0.68
1:B:238:PRO:HD2	1:B:328:LEU:HD21	1.76	0.68
1:A:326:LYS:HA	1:A:326:LYS:HE2	1.78	0.64
2:C:63:VAL:HG21	2:C:88:ILE:HD11	1.78	0.63
1:A:429:HIS:CD2	1:A:431:ALA:H	2.17	0.62
1:A:429:HIS:HD2	1:A:431:ALA:H	1.49	0.60
1:A:311:GLN:HE21	1:A:311:GLN:HA	1.66	0.60
1:B:379:VAL:HG22	1:B:427:VAL:HG22	1.83	0.60
1:A:428:MET:HE2	8:A:127:HOH:O	2.02	0.59
1:B:374:PRO:O	1:B:429:HIS:HE1	1.87	0.56
1:B:238:PRO:HD2	1:B:328:LEU:CD2	2.33	0.56
1:A:320:LYS:HG3	1:A:335:THR:HG22	1.88	0.55
1:B:338:LYS:HE2	1:B:374:PRO:HG3	1.89	0.54
1:B:360:LYS:O	1:B:414:LYS:HD3	2.07	0.54
1:A:415:SER:O	1:A:419:GLN:HG3	2.07	0.54
1:B:429:HIS:CD2	1:B:431:ALA:H	2.27	0.53
1:A:374:PRO:O	1:A:429:HIS:HE1	1.92	0.53
1:B:429:HIS:HD2	1:B:431:ALA:H	1.58	0.51
1:B:351:LEU:HB2	1:B:366:THR:HB	1.91	0.51
2:C:63:VAL:CG2	2:C:88:ILE:HD11	2.43	0.49
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.95	0.48
1:A:409:LYS:HB2	1:B:407:TYR:OH	2.13	0.48
1:B:278:TYR:HB2	1:B:320:LYS:HB3	1.96	0.48
1:B:426:SER:HB3	1:B:438:GLN:HG3	1.95	0.48
2:C:43:PHE:CE2	2:C:48:LEU:HD13	2.49	0.48
2:C:20:LEU:HD21	2:C:92:LEU:HB2	1.96	0.48
2:C:93:LEU:HD23	2:C:168:VAL:HG22	1.97	0.47
2:C:73:THR:H	2:C:76:SER:HB2	1.80	0.47
1:B:419:GLN:HG3	1:B:420:GLY:CA	2.43	0.47
1:B:269:GLU:HB2	8:B:40:HOH:O	2.13	0.47
2:C:119:HIS:HD2	2:C:120:LYS:HG3	1.79	0.46
1:A:342:GLN:HB2	8:A:65:HOH:O	2.15	0.46
2:C:130:ARG:NH2	2:C:148:ASP:OD1	2.49	0.45
1:A:360:LYS:O	1:A:414:LYS:HD3	2.16	0.45
6:C:1470:BMA:H62	6:C:1475:MAN:H2	1.54	0.44
1:A:344:ARG:HG2	1:A:373:TYR:HB3	1.99	0.44
1:A:350:THR:HG23	1:A:439:LYS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ARG:H	1:B:292:ARG:NE	2.15	0.44
1:B:318:GLU:HA	1:B:337:SER:HB3	2.00	0.43
1:A:368:LEU:HD13	1:A:407:TYR:CZ	2.53	0.43
1:B:334:LYS:HA	1:B:334:LYS:HD3	1.83	0.43
1:A:242:LEU:HD11	1:A:259:VAL:CG1	2.49	0.43
1:B:235:LEU:HD21	2:C:117:ALA:HB3	2.01	0.43
2:C:31:GLY:O	2:C:32:ALA:HB3	2.18	0.43
1:B:318:GLU:OE1	1:B:335:THR:HG21	2.19	0.42
1:A:351:LEU:HB2	1:A:366:THR:HB	2.01	0.42
2:C:21:GLU:OE2	2:C:63:VAL:HG23	2.19	0.42
1:B:346:PRO:HB3	1:B:372:PHE:HB3	2.02	0.42
1:A:237:GLY:HA2	2:C:134:HIS:CD2	2.54	0.41
2:C:146:LEU:HD12	2:C:172:ILE:HG22	2.00	0.41
1:B:397:VAL:HB	1:B:405:PHE:CE2	2.55	0.41
2:C:108:LEU:HD12	2:C:139:PHE:HD2	1.85	0.41
1:A:390:ASN:HD22	1:A:390:ASN:HA	1.73	0.41
2:C:113:TRP:CH2	2:C:114:LYS:HE2	2.57	0.40
2:C:38:GLN:HB3	2:C:38:GLN:HE21	1.70	0.40
1:A:414:LYS:HB3	1:A:414:LYS:HE2	1.94	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	207/225 (92%)	202 (98%)	4 (2%)	1 (0%)	34	48
1	B	210/225 (93%)	207 (99%)	3 (1%)	0	100	100
2	C	161/204 (79%)	157 (98%)	4 (2%)	0	100	100
All	All	578/654 (88%)	566 (98%)	11 (2%)	1 (0%)	52	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	GLY

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	194/208 (93%)	183 (94%)	11 (6%)	25	40
1	B	197/208 (95%)	185 (94%)	12 (6%)	23	36
2	C	148/183 (81%)	137 (93%)	11 (7%)	17	26
All	All	539/599 (90%)	505 (94%)	34 (6%)	22	35

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	GLU
1	A	282	VAL
1	A	294	GLU
1	A	309	LEU
1	A	311	GLN
1	A	342	GLN
1	A	344	ARG
1	A	355	ARG
1	A	362	GLN
1	A	390	ASN
1	A	426	SER
1	B	242	LEU
1	B	248	LYS
1	B	262	VAL
1	B	264	VAL
1	B	272	GLU
1	B	292	ARG
1	B	295	GLN
1	B	302	VAL
1	B	340	LYS
1	B	439	LYS
1	B	441	LEU

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Mol	Chain	Res	Type
1	B	442	SER
2	C	15	GLN
2	C	38	GLN
2	C	48	LEU
2	C	128	LYS
2	C	130	ARG
2	C	131	LYS
2	C	137	SER
2	C	146	LEU
2	C	161	LYS
2	C	164	SER
2	C	167	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	HIS
1	A	276	ASN
1	A	311	GLN
1	A	315	ASN
1	A	347	GLN
1	A	362	GLN
1	A	390	ASN
1	A	421	ASN
1	A	429	HIS
1	A	438	GLN
1	B	295	GLN
1	B	390	ASN
1	B	419	GLN
1	B	429	HIS
1	B	435	HIS
2	C	38	GLN
2	C	74	GLN
2	C	119	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 ⓘ

26 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	1445	1,3	14,14,15	0.57	0	15,19,21	1.17	1 (6%)
3	NAG	A	1447	3	14,14,15	0.69	0	15,19,21	1.56	1 (6%)
3	BMA	A	1448	3	11,11,12	0.21	0	14,15,17	1.05	1 (7%)
3	MAN	A	1450	3	11,11,12	0.71	0	14,15,17	1.12	0
3	MAN	A	1451	3	11,11,12	0.58	0	14,15,17	0.96	0
3	NAG	A	1452	3	14,14,15	0.55	0	15,19,21	1.01	1 (6%)
3	NAG	A	1453	3	14,14,15	0.56	0	15,19,21	1.01	1 (6%)
3	NAG	A	1454	3	14,14,15	0.55	0	15,19,21	1.12	2 (13%)
5	NAG	B	1445	1,5	14,14,15	0.55	0	15,19,21	1.58	2 (13%)
5	NAG	B	1447	5	14,14,15	0.59	0	15,19,21	1.56	3 (20%)
5	BMA	B	1448	5	11,11,12	0.65	0	14,15,17	2.79	7 (50%)
5	MAN	B	1450	5	11,11,12	0.70	0	14,15,17	0.98	0
5	MAN	B	1451	5	11,11,12	0.82	0	14,15,17	1.58	3 (21%)
5	NAG	B	1452	5	14,14,15	0.51	0	15,19,21	0.83	0
5	NAG	B	1453	5	14,14,15	0.53	0	15,19,21	1.89	3 (20%)
5	NAG	B	1454	5	14,14,15	0.52	0	15,19,21	1.34	1 (6%)
6	NAG	C	1445	2,6	14,14,15	0.82	0	15,19,21	3.09	7 (46%)
6	NAG	C	1447	6	14,14,15	0.74	1 (7%)	15,19,21	0.71	0
7	NAG	C	1460	2,7	14,14,15	0.50	0	15,19,21	1.32	2 (13%)
7	NAG	C	1461	2,7	14,14,15	0.50	0	15,19,21	1.59	3 (20%)
6	BMA	C	1470	6	11,11,12	0.66	0	14,15,17	2.89	6 (42%)
6	MAN	C	1471	6	11,11,12	0.82	0	14,15,17	3.39	5 (35%)
6	MAN	C	1472	6	11,11,12	0.59	0	14,15,17	1.13	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	C	1475	6	11,11,12	0.78	0	14,15,17	1.09	1 (7%)
6	MAN	C	1476	6	11,11,12	0.63	0	14,15,17	1.32	2 (14%)
6	MAN	C	1477	6	11,11,12	0.82	0	14,15,17	0.91	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1445	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1447	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1448	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1450	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1451	3	-	0/2/19/22	0/1/1/1
3	NAG	A	1452	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1453	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1454	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1445	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	B	1447	5	-	0/6/23/26	0/1/1/1
5	BMA	B	1448	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1450	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1451	5	1/1/4/5	0/2/19/22	0/1/1/1
5	NAG	B	1452	5	-	0/6/23/26	0/1/1/1
5	NAG	B	1453	5	-	0/6/23/26	0/1/1/1
5	NAG	B	1454	5	-	0/6/23/26	0/1/1/1
6	NAG	C	1445	2,6	-	0/6/23/26	0/1/1/1
6	NAG	C	1447	6	-	0/6/23/26	0/1/1/1
7	NAG	C	1460	2,7	-	0/6/23/26	0/1/1/1
7	NAG	C	1461	2,7	-	0/6/23/26	0/1/1/1
6	BMA	C	1470	6	-	0/2/19/22	0/1/1/1
6	MAN	C	1471	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	C	1472	6	-	0/2/19/22	0/1/1/1
6	MAN	C	1475	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	C	1476	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	C	1477	6	1/1/4/5	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1447	NAG	O5-C1	-2.13	1.40	1.43

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1471	MAN	C1-C2-C3	-9.98	97.73	109.54
5	B	1448	BMA	C3-C4-C5	-5.99	99.75	110.20
6	C	1471	MAN	C1-O5-C5	-5.87	104.80	112.25
6	C	1445	NAG	C3-C2-N2	-4.73	99.24	110.56
6	C	1470	BMA	O5-C5-C6	-4.46	97.70	107.35
6	C	1445	NAG	C3-C4-C5	-3.59	103.93	110.20
6	C	1445	NAG	C8-C7-N2	-3.50	109.41	116.11
5	B	1451	MAN	C1-C2-C3	-3.10	105.88	109.54
5	B	1451	MAN	O5-C1-C2	-2.90	106.16	110.86
5	B	1448	BMA	O4-C4-C5	-2.86	101.66	109.24
6	C	1475	MAN	C1-O5-C5	-2.81	108.68	112.25
6	C	1470	BMA	O3-C3-C4	-2.78	104.07	110.34
3	A	1448	BMA	O4-C4-C3	-2.32	105.12	110.34
6	C	1471	MAN	O5-C1-C2	-2.20	107.29	110.86
7	C	1460	NAG	C6-C5-C4	-2.20	107.60	113.02
5	B	1445	NAG	C3-C4-C5	-2.13	106.48	110.20
6	C	1470	BMA	C1-C2-C3	-2.09	107.07	109.54
3	A	1452	NAG	C4-C3-C2	-2.02	108.09	111.23
6	C	1476	MAN	C1-C2-C3	2.00	111.91	109.54
5	B	1448	BMA	O5-C5-C6	2.01	111.71	107.35
6	C	1470	BMA	C3-C4-C5	2.11	113.88	110.20
6	C	1471	MAN	O2-C2-C1	2.25	113.71	109.21
3	A	1454	NAG	C1-O5-C5	2.27	115.14	112.25
3	A	1454	NAG	O7-C7-N2	2.28	126.51	121.86
7	C	1461	NAG	O5-C5-C6	2.29	112.30	107.35
5	B	1447	NAG	O4-C4-C3	2.38	115.69	110.34
3	A	1445	NAG	C1-O5-C5	2.53	115.46	112.25
7	C	1461	NAG	C2-N2-C7	2.56	126.33	123.04
3	A	1453	NAG	C1-O5-C5	2.59	115.54	112.25
5	B	1447	NAG	C1-O5-C5	2.73	115.71	112.25
6	C	1445	NAG	O7-C7-N2	2.78	127.52	121.86
5	B	1448	BMA	C1-O5-C5	2.81	115.81	112.25
5	B	1451	MAN	C3-C4-C5	2.91	115.26	110.20
6	C	1472	MAN	C1-O5-C5	2.96	116.01	112.25
6	C	1471	MAN	C3-C4-C5	3.03	115.48	110.20
5	B	1453	NAG	C3-C2-N2	3.11	118.02	110.56
5	B	1448	BMA	O3-C3-C4	3.13	117.38	110.34
5	B	1447	NAG	C2-N2-C7	3.42	127.43	123.04
6	C	1445	NAG	C1-O5-C5	3.76	117.03	112.25
7	C	1461	NAG	C1-O5-C5	3.77	117.03	112.25
5	B	1448	BMA	O4-C4-C3	3.78	118.84	110.34
6	C	1445	NAG	C4-C3-C2	3.81	117.16	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1476	MAN	C1-O5-C5	3.88	117.17	112.25
7	C	1460	NAG	C1-O5-C5	3.93	117.23	112.25
5	B	1453	NAG	C1-O5-C5	3.95	117.26	112.25
5	B	1454	NAG	C1-O5-C5	4.00	117.32	112.25
5	B	1453	NAG	C2-N2-C7	4.06	128.25	123.04
5	B	1448	BMA	O3-C3-C2	4.90	118.85	110.00
5	B	1445	NAG	C1-O5-C5	5.02	118.62	112.25
3	A	1447	NAG	C1-O5-C5	5.06	118.67	112.25
6	C	1470	BMA	O3-C3-C2	5.63	120.16	110.00
6	C	1470	BMA	C1-O5-C5	6.14	120.05	112.25
6	C	1445	NAG	C2-N2-C7	7.34	132.47	123.04

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1451	MAN	C1
6	C	1471	MAN	C1
5	B	1445	NAG	C1
6	C	1477	MAN	C1
6	C	1476	MAN	C1
6	C	1475	MAN	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1452	NAG	1	0
5	B	1454	NAG	1	0
6	C	1445	NAG	3	0
6	C	1470	BMA	1	0
6	C	1475	MAN	1	0

5.6 Ligand geometry

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	1	-	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	1	-	-	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.

No monomer is involved in short contacts.

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](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	209/225 (92%)	-0.02	3 (1%) 78 77	35, 56, 101, 118	0
1	B	212/225 (94%)	0.23	7 (3%) 50 50	47, 74, 96, 108	0
2	C	165/204 (80%)	0.02	1 (0%) 90 90	39, 53, 82, 102	0
All	All	586/654 (89%)	0.08	11 (1%) 70 69	35, 61, 95, 118	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	284	VAL	3.9
1	B	422	VAL	3.5
1	A	444	SER	3.2
1	A	384	ASN	3.1
1	B	418	GLN	2.8
1	B	443	LEU	2.7
1	B	279	VAL	2.5
2	C	5	LEU	2.5
1	B	274	LYS	2.4
1	A	422	VAL	2.0
1	B	358	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	B	1453	14/15	0.88	0.17	1.11	63,71,78,80	0
5	NAG	B	1445	14/15	0.94	0.14	0.09	40,43,47,50	0
3	NAG	A	1453	14/15	0.95	0.14	-0.23	40,50,56,58	0
7	NAG	C	1460	14/15	0.94	0.12	-1.09	33,37,46,47	0
6	NAG	C	1445	14/15	0.96	0.09	-2.81	28,31,33,34	0
3	NAG	A	1445	14/15	0.97	0.10	-3.23	23,28,30,32	0
6	MAN	C	1472	11/12	0.83	0.29	-	50,54,56,56	0
6	MAN	C	1471	11/12	0.94	0.18	-	43,49,52,56	0
5	MAN	B	1450	11/12	0.97	0.09	-	56,58,64,65	0
3	NAG	A	1447	14/15	0.97	0.11	-	29,32,35,36	0
6	MAN	C	1477	11/12	0.80	0.18	-	82,87,90,90	0
3	MAN	A	1451	11/12	0.95	0.11	-	51,56,63,64	0
3	MAN	A	1450	11/12	0.97	0.11	-	39,41,45,45	0
5	NAG	B	1447	14/15	0.96	0.13	-	40,42,47,51	0
3	NAG	A	1454	14/15	0.95	0.18	-	50,54,64,67	0
6	BMA	C	1470	11/12	0.92	0.10	-	38,44,51,58	0
6	NAG	C	1447	14/15	0.97	0.11	-	30,32,35,37	0
5	NAG	B	1454	14/15	0.93	0.13	-	72,80,83,92	0
6	MAN	C	1476	11/12	0.84	0.22	-	72,80,82,83	0
5	BMA	B	1448	11/12	0.94	0.10	-	52,55,62,68	0
3	NAG	A	1452	14/15	0.92	0.13	-	60,67,71,72	0
5	MAN	B	1451	11/12	0.91	0.10	-	59,62,65,65	0
6	MAN	C	1475	11/12	0.88	0.15	-	62,70,83,85	0
3	BMA	A	1448	11/12	0.98	0.11	-	35,37,42,48	0
5	NAG	B	1452	14/15	0.94	0.10	-	65,70,75,77	0
7	NAG	C	1461	14/15	0.88	0.21	-	50,55,60,63	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MLI	A	1	7/7	0.82	0.32	7.05	59,60,67,76	0

6.5 Other polymers

There are no such residues in this entry.