



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2017 – 12:13 AM EDT

PDB ID : 5D6D
Title : Crystal structure of GASDALIE IgG1 Fc in complex with FcgRIIIa
Authors : Ahmed, A.A.; Bjorkman, P.J.
Deposited on : unknown
Resolution : 3.13 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029824

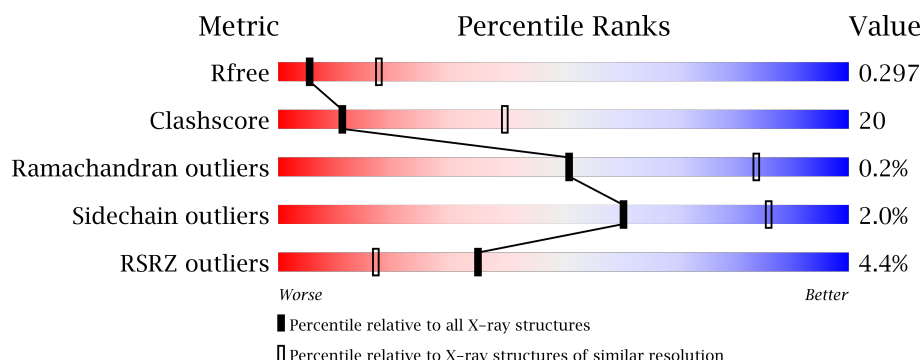
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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}	100719	1234 (3.18-3.10)
Clashscore	112137	1345 (3.18-3.10)
Ramachandran outliers	110173	1301 (3.18-3.10)
Sidechain outliers	110143	1301 (3.18-3.10)
RSRZ outliers	101464	1240 (3.18-3.10)

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	249	<div> <div>2%</div> <div>54%</div> <div>29%</div> <div>16%</div> </div>
1	B	249	<div> <div>%</div> <div>64%</div> <div>18%</div> <div>16%</div> </div>
2	C	240	<div> <div>8%</div> <div>49%</div> <div>15%</div> <div>35%</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
3	NAG	C	302	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4755 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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1630	1038	275	311	6			
1	B	208	Total	C	N	O	S	0	0	0
			1660	1057	278	319	6			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	MET	-	initiating methionine	UNP P01857
A	199	GLU	-	expression tag	UNP P01857
A	200	PHE	-	expression tag	UNP P01857
A	201	GLY	-	expression tag	UNP P01857
A	202	LEU	-	expression tag	UNP P01857
A	203	SER	-	expression tag	UNP P01857
A	204	TRP	-	expression tag	UNP P01857
A	205	LEU	-	expression tag	UNP P01857
A	206	PHE	-	expression tag	UNP P01857
A	207	LEU	-	expression tag	UNP P01857
A	208	VAL	-	expression tag	UNP P01857
A	209	ALA	-	expression tag	UNP P01857
A	210	ILE	-	expression tag	UNP P01857
A	211	LEU	-	expression tag	UNP P01857
A	212	LYS	-	expression tag	UNP P01857
A	213	GLY	-	expression tag	UNP P01857
A	214	VAL	-	expression tag	UNP P01857
A	215	GLN	-	expression tag	UNP P01857
A	216	CYS	-	expression tag	UNP P01857
A	217	GLU	-	expression tag	UNP P01857
A	218	VAL	-	expression tag	UNP P01857
A	219	GLN	-	expression tag	UNP P01857
A	220	LEU	-	expression tag	UNP P01857
A	221	LEU	-	expression tag	UNP P01857
A	222	GLU	-	expression tag	UNP P01857

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Chain	Residue	Modelled	Actual	Comment	Reference
A	223	THR	-	expression tag	UNP P01857
A	224	SER	-	expression tag	UNP P01857
A	236	ALA	GLY	engineered mutation	UNP P01857
A	239	ASP	SER	engineered mutation	UNP P01857
A	330	LEU	ALA	engineered mutation	UNP P01857
A	332	GLU	ILE	engineered mutation	UNP P01857
B	198	MET	-	initiating methionine	UNP P01857
B	199	GLU	-	expression tag	UNP P01857
B	200	PHE	-	expression tag	UNP P01857
B	201	GLY	-	expression tag	UNP P01857
B	202	LEU	-	expression tag	UNP P01857
B	203	SER	-	expression tag	UNP P01857
B	204	TRP	-	expression tag	UNP P01857
B	205	LEU	-	expression tag	UNP P01857
B	206	PHE	-	expression tag	UNP P01857
B	207	LEU	-	expression tag	UNP P01857
B	208	VAL	-	expression tag	UNP P01857
B	209	ALA	-	expression tag	UNP P01857
B	210	ILE	-	expression tag	UNP P01857
B	211	LEU	-	expression tag	UNP P01857
B	212	LYS	-	expression tag	UNP P01857
B	213	GLY	-	expression tag	UNP P01857
B	214	VAL	-	expression tag	UNP P01857
B	215	GLN	-	expression tag	UNP P01857
B	216	CYS	-	expression tag	UNP P01857
B	217	GLU	-	expression tag	UNP P01857
B	218	VAL	-	expression tag	UNP P01857
B	219	GLN	-	expression tag	UNP P01857
B	220	LEU	-	expression tag	UNP P01857
B	221	LEU	-	expression tag	UNP P01857
B	222	GLU	-	expression tag	UNP P01857
B	223	THR	-	expression tag	UNP P01857
B	224	SER	-	expression tag	UNP P01857
B	236	ALA	GLY	engineered mutation	UNP P01857
B	239	ASP	SER	engineered mutation	UNP P01857
B	330	LEU	ALA	engineered mutation	UNP P01857
B	332	GLU	ILE	engineered mutation	UNP P01857

- Molecule 2 is a protein called Low affinity immunoglobulin gamma Fc region receptor III-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	157	Total	C	N	O	S	0	0	0
			1217	775	211	227	4			

There are 51 discrepancies between the modelled and reference sequences:

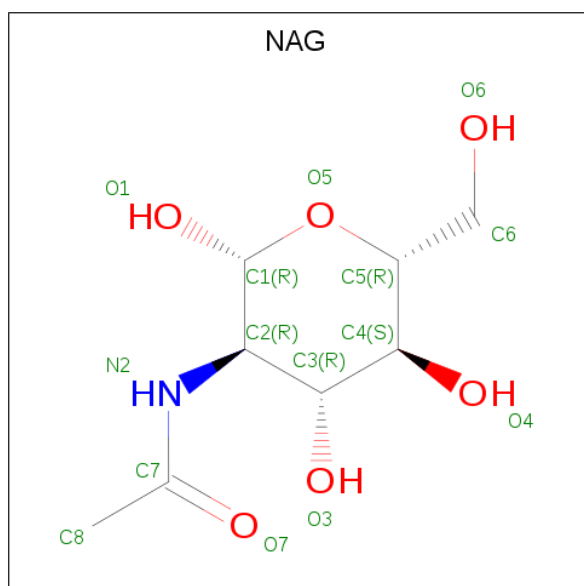
Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	MET	-	expression tag	UNP P08637
C	-16	TRP	-	expression tag	UNP P08637
C	-15	GLN	-	expression tag	UNP P08637
C	-14	LEU	-	expression tag	UNP P08637
C	-13	LEU	-	expression tag	UNP P08637
C	-12	LEU	-	expression tag	UNP P08637
C	-11	PRO	-	expression tag	UNP P08637
C	-10	THR	-	expression tag	UNP P08637
C	-9	ALA	-	expression tag	UNP P08637
C	-8	LEU	-	expression tag	UNP P08637
C	-7	LEU	-	expression tag	UNP P08637
C	-6	LEU	-	expression tag	UNP P08637
C	-5	LEU	-	expression tag	UNP P08637
C	38	GLN	ASN	engineered mutation	UNP P08637
C	74	GLN	ASN	engineered mutation	UNP P08637
C	169	GLN	ASN	engineered mutation	UNP P08637
C	188	SER	-	expression tag	UNP P08637
C	189	ARG	-	expression tag	UNP P08637
C	190	GLY	-	expression tag	UNP P08637
C	191	GLY	-	expression tag	UNP P08637
C	192	GLY	-	expression tag	UNP P08637
C	193	GLY	-	expression tag	UNP P08637
C	194	SER	-	expression tag	UNP P08637
C	195	GLY	-	expression tag	UNP P08637
C	196	GLY	-	expression tag	UNP P08637
C	197	GLY	-	expression tag	UNP P08637
C	198	GLY	-	expression tag	UNP P08637
C	199	HIS	-	expression tag	UNP P08637
C	200	VAL	-	expression tag	UNP P08637
C	201	LEU	-	expression tag	UNP P08637
C	202	ASN	-	expression tag	UNP P08637
C	203	ASP	-	expression tag	UNP P08637
C	204	ILE	-	expression tag	UNP P08637
C	205	PHE	-	expression tag	UNP P08637
C	206	GLU	-	expression tag	UNP P08637
C	207	ALA	-	expression tag	UNP P08637
C	208	GLN	-	expression tag	UNP P08637
C	209	LYS	-	expression tag	UNP P08637
C	210	ILE	-	expression tag	UNP P08637
C	211	GLU	-	expression tag	UNP P08637
C	212	TRP	-	expression tag	UNP P08637
C	213	HIS	-	expression tag	UNP P08637

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Chain	Residue	Modelled	Actual	Comment	Reference
C	214	GLU	-	expression tag	UNP P08637
C	215	THR	-	expression tag	UNP P08637
C	216	GLY	-	expression tag	UNP P08637
C	217	HIS	-	expression tag	UNP P08637
C	218	HIS	-	expression tag	UNP P08637
C	219	HIS	-	expression tag	UNP P08637
C	220	HIS	-	expression tag	UNP P08637
C	221	HIS	-	expression tag	UNP P08637
C	222	HIS	-	expression tag	UNP P08637

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



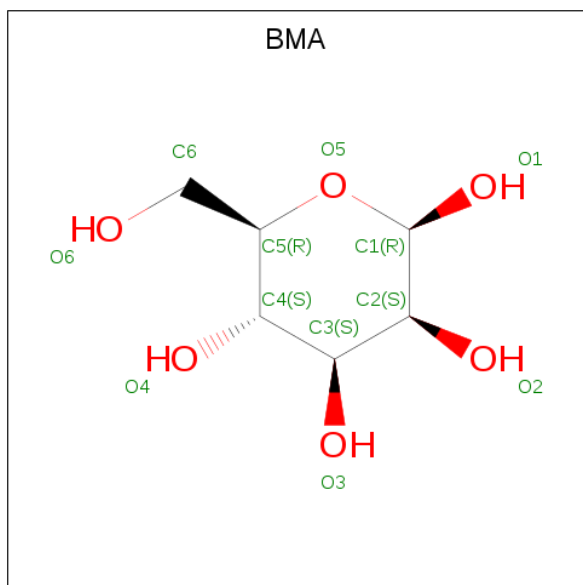
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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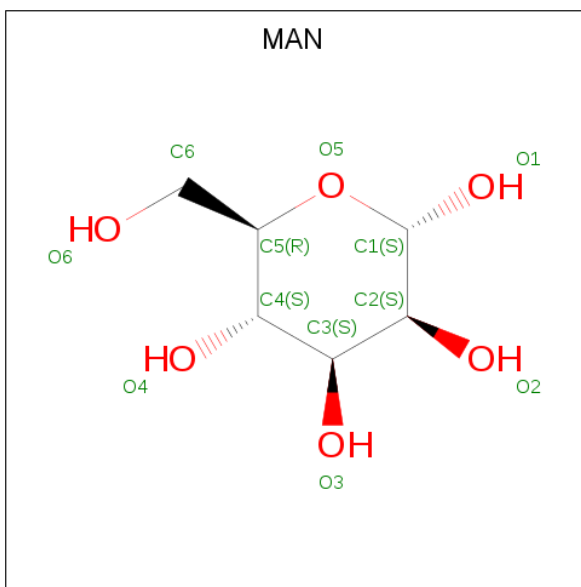
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



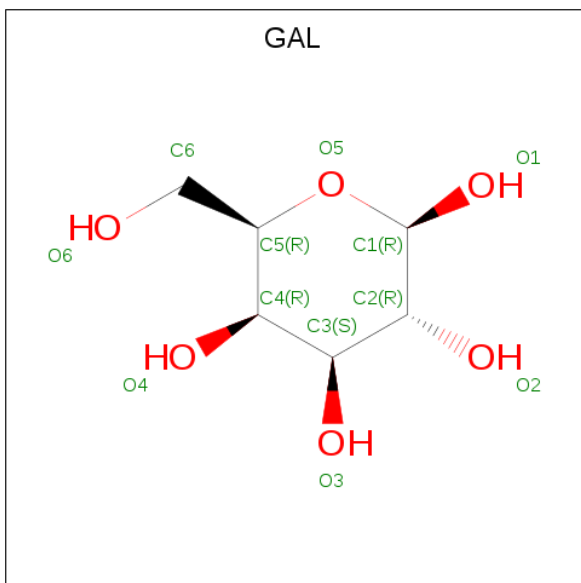
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



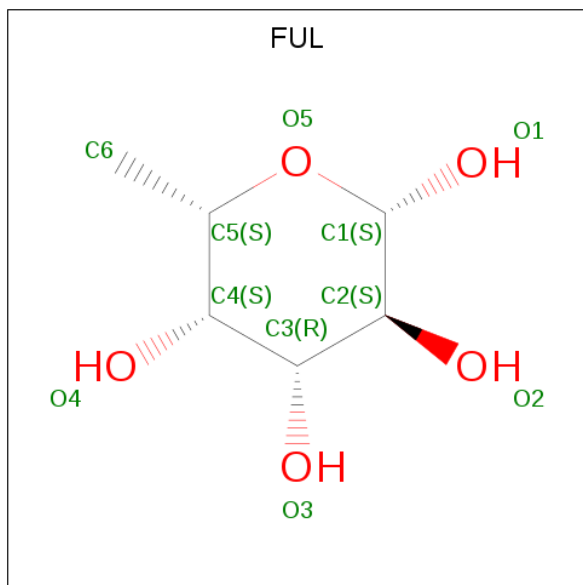
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



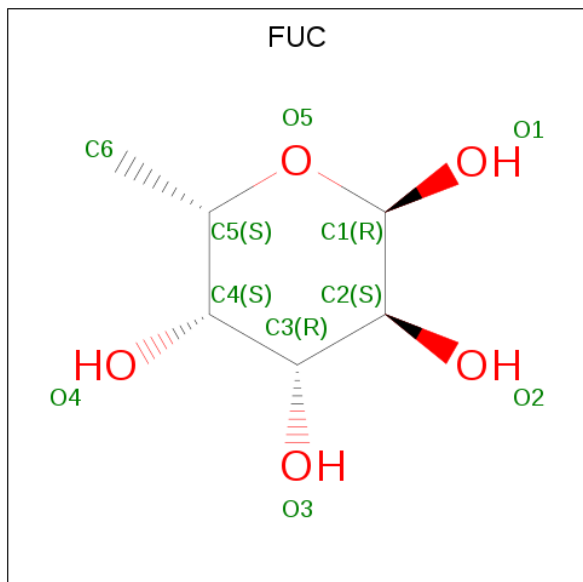
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is BETA-L-FUCOSE (three-letter code: FUL) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).

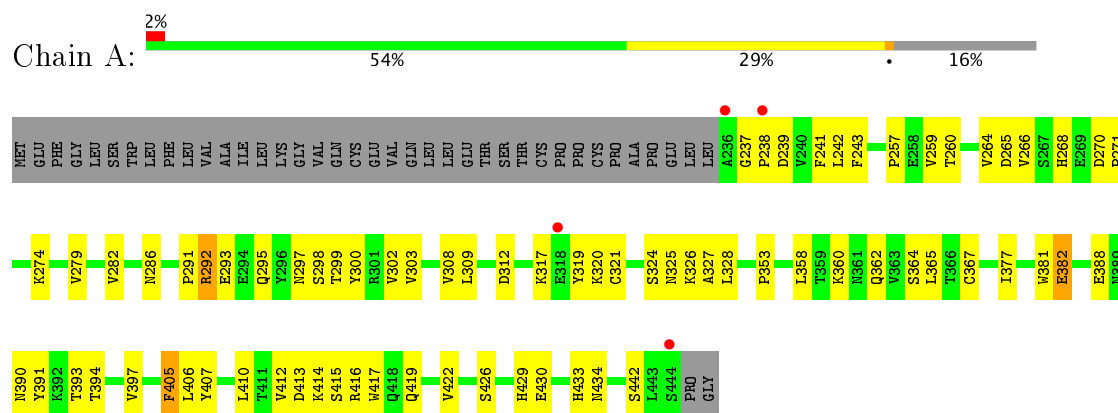


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			10	6	4		

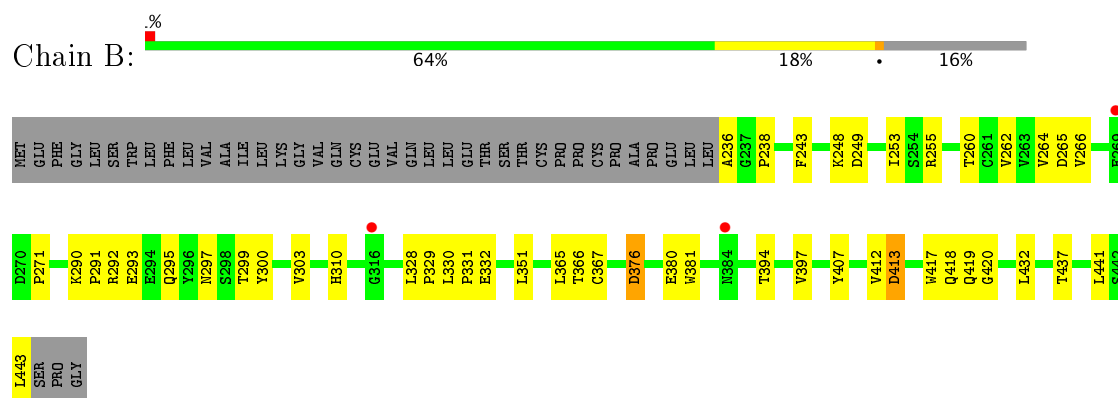
3 Residue-property plots [i](#)

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

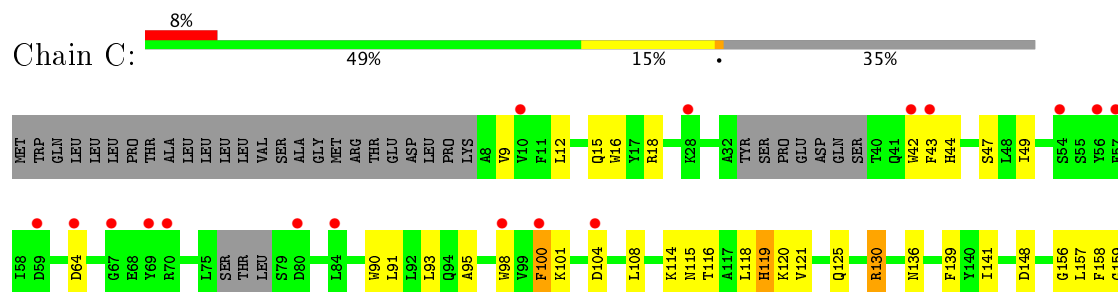
- Molecule 1: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region



- Molecule 2: Low affinity immunoglobulin gamma Fc region receptor III-A



V163	I170	T171	I172	T173	Q174	GLY	LEU	ALA	VAL	SER	THR	ILE	SER	SER	PHE	PHE	PRO	PRO	SER	ARG	GLY	GLY	GLY	GLY	GLY	GLY	GLY	HIS	VAL	LEU	ASN	ASP	ILE	PHE	GLU	ALA	GLN	LYS	ILE	GLU	THR	HIS	GLU	GLY	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.38 Å 94.50 Å 108.67 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.31 – 3.13 71.31 – 3.13	Depositor EDS
% Data completeness (in resolution range)	99.3 (71.31-3.13) 99.6 (71.31-3.13)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 3.13 Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.271 , 0.296 0.269 , 0.297	Depositor DCC
R_{free} test set	1396 reflections (9.99%)	DCC
Wilson B-factor (Å ²)	81.1	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4755	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, GAL, FUC, 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	A	0.90	0/1675	0.71	1/2290 (0.0%)
1	B	0.43	0/1706	0.60	0/2327
2	C	0.46	0/1249	0.57	0/1701
All	All	0.65	0/4630	0.63	1/6318 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ASP	C-N-CD	5.40	139.74	128.40

There are no chirality outliers.

There are no planarity outliers.

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	1630	0	1564	83	0
1	B	1660	0	1609	60	0
2	C	1217	0	1112	54	0
3	A	56	0	48	2	0
3	B	56	0	48	4	0
3	C	28	0	26	5	0
4	A	11	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	11	0	8	0	0
5	A	22	0	18	0	0
5	B	22	0	18	0	0
6	A	11	0	10	0	0
6	B	11	0	10	0	0
7	A	10	0	10	1	0
8	B	10	0	10	1	0
All	All	4755	0	4499	183	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 20.

All (183) 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:B:501:NAG:O6	8:B:509:FUC:C1	1.82	1.28
1:B:330:LEU:HD12	1:B:331:PRO:HD2	1.38	1.03
1:A:237:GLY:O	1:A:328:LEU:HD23	1.63	0.97
2:C:157:LEU:HD11	3:C:301:NAG:C8	1.94	0.96
1:B:419:GLN:N	1:B:420:GLY:HA2	1.79	0.94
2:C:157:LEU:HD11	3:C:301:NAG:H83	1.46	0.94
2:C:64:ASP:O	3:C:302:NAG:H3	1.70	0.92
1:B:238:PRO:HB2	1:B:264:VAL:O	1.71	0.90
1:A:237:GLY:O	1:A:328:LEU:CD2	2.23	0.87
1:A:388:GLU:OE1	1:A:416:ARG:NH2	2.09	0.86
1:B:236:ALA:HB3	2:C:158:PHE:CD2	2.09	0.86
2:C:156:GLY:C	2:C:157:LEU:HD12	1.97	0.84
1:B:238:PRO:HB3	1:B:265:ASP:O	1.77	0.84
2:C:18:ARG:NH1	2:C:93:LEU:O	2.12	0.82
1:B:236:ALA:CB	2:C:158:PHE:CE2	2.63	0.82
1:A:265:ASP:HA	1:A:299:THR:HG21	1.61	0.82
1:B:328:LEU:HD12	1:B:328:LEU:O	1.80	0.81
1:B:328:LEU:HD13	1:B:330:LEU:O	1.80	0.81
1:A:274:LYS:HE2	1:A:324:SER:CB	2.12	0.80
1:B:262:VAL:HG23	1:B:303:VAL:HG22	1.63	0.78
1:A:382:GLU:OE2	1:A:426:SER:OG	2.02	0.78
1:A:388:GLU:OE1	1:A:416:ARG:NH1	2.18	0.76
1:B:330:LEU:HD12	1:B:331:PRO:CD	2.14	0.76
2:C:43:PHE:HA	2:C:47:SER:O	1.85	0.76
1:A:274:LYS:HE2	1:A:324:SER:HB2	1.65	0.75
1:B:236:ALA:HB3	2:C:158:PHE:HD2	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ALA:CB	2:C:158:PHE:HE2	1.97	0.74
1:B:330:LEU:CD1	1:B:331:PRO:HD2	2.17	0.73
1:B:418:GLN:HA	1:B:443:LEU:HD11	1.69	0.73
1:A:381:TRP:CE3	1:A:410:LEU:HD22	2.24	0.72
1:B:271:PRO:HB3	1:B:300:TYR:HE2	1.54	0.72
1:A:360:LYS:O	1:A:414:LYS:HE2	1.91	0.71
1:B:292:ARG:HD3	1:B:300:TYR:CG	2.25	0.70
2:C:100:PHE:O	2:C:172:ILE:HA	1.91	0.70
1:B:297:ASN:OD1	1:B:299:THR:HG23	1.93	0.69
2:C:157:LEU:HD11	3:C:301:NAG:H81	1.73	0.69
2:C:130:ARG:NH2	2:C:141:ILE:HD13	2.08	0.68
1:A:388:GLU:OE1	1:A:416:ARG:CZ	2.42	0.68
1:B:243:PHE:HB2	1:B:260:THR:OG1	1.95	0.67
2:C:157:LEU:N	2:C:157:LEU:HD12	2.10	0.66
1:A:242:LEU:HD12	1:A:260:THR:O	1.95	0.66
1:A:257:PRO:HG2	1:A:308:VAL:HG23	1.77	0.66
1:A:413:ASP:O	1:A:416:ARG:N	2.29	0.66
1:A:279:VAL:CG1	1:A:317:LYS:HD3	2.27	0.64
1:B:236:ALA:HB3	2:C:158:PHE:CE2	2.31	0.64
1:A:325:ASN:OD1	1:A:327:ALA:N	2.26	0.64
1:B:290:LYS:HB3	1:B:291:PRO:HD2	1.79	0.63
1:A:397:VAL:HG21	1:B:394:THR:HG22	1.81	0.62
1:B:271:PRO:HB3	1:B:300:TYR:CE2	2.32	0.62
1:A:239:ASP:CG	2:C:120:LYS:HZ1	2.02	0.62
2:C:118:LEU:C	2:C:119:HIS:ND1	2.53	0.62
7:A:508:FUL:O3	7:A:508:FUL:H63	2.00	0.62
2:C:42:TRP:HB2	2:C:49:ILE:CB	2.30	0.62
2:C:119:HIS:O	2:C:157:LEU:HD13	2.00	0.61
1:A:325:ASN:OD1	1:A:326:LYS:N	2.33	0.61
1:A:394:THR:HG22	1:B:397:VAL:HG21	1.81	0.61
1:A:299:THR:HG22	1:A:300:TYR:O	2.01	0.61
1:A:238:PRO:N	1:A:328:LEU:HD21	2.16	0.61
1:B:419:GLN:N	1:B:420:GLY:CA	2.59	0.61
1:A:237:GLY:C	1:A:328:LEU:HD21	2.21	0.60
2:C:116:THR:CB	2:C:158:PHE:CE1	2.84	0.60
1:A:266:VAL:H	1:A:299:THR:CG2	2.15	0.60
1:B:328:LEU:HD13	1:B:330:LEU:C	2.21	0.60
1:B:365:LEU:HD22	1:B:441:LEU:HD23	1.82	0.60
1:A:268:HIS:O	1:A:271:PRO:HG3	2.02	0.59
1:A:364:SER:C	1:A:365:LEU:HD23	2.22	0.59
1:B:328:LEU:HD22	1:B:332:GLU:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ASP:HB2	1:A:264:VAL:HG23	1.85	0.59
1:A:415:SER:O	1:A:419:GLN:HG3	2.03	0.59
2:C:118:LEU:HD12	2:C:157:LEU:O	2.02	0.58
1:B:249:ASP:OD1	1:B:255:ARG:NE	2.32	0.57
1:A:381:TRP:CD2	1:A:410:LEU:HD22	2.38	0.57
1:A:266:VAL:N	1:A:299:THR:HG23	2.19	0.57
1:A:241:PHE:HZ	3:A:502:NAG:HO6	1.51	0.57
1:A:279:VAL:O	1:A:282:VAL:HG22	2.05	0.57
1:B:412:VAL:HG23	1:B:413:ASP:O	2.06	0.56
2:C:100:PHE:CD1	2:C:100:PHE:N	2.73	0.56
1:A:309:LEU:HD12	1:A:309:LEU:N	2.21	0.56
1:A:239:ASP:OD2	2:C:120:LYS:NZ	2.39	0.55
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.41	0.55
2:C:120:LYS:HB2	2:C:157:LEU:HD13	1.89	0.55
2:C:100:PHE:HB3	2:C:104:ASP:OD2	2.07	0.55
1:A:265:ASP:HA	1:A:299:THR:CG2	2.37	0.54
1:B:248:LYS:CE	1:B:380:GLU:OE2	2.56	0.54
2:C:114:LYS:O	2:C:115:ASN:C	2.46	0.54
1:A:238:PRO:CD	1:A:328:LEU:HD21	2.38	0.54
1:A:241:PHE:HE1	1:A:264:VAL:HG21	1.73	0.54
2:C:15:GLN:HG2	2:C:16:TRP:N	2.23	0.53
1:B:417:TRP:CH2	1:B:441:LEU:HG	2.43	0.53
1:B:238:PRO:CB	1:B:264:VAL:O	2.52	0.53
1:A:241:PHE:HZ	3:A:502:NAG:O6	1.90	0.52
2:C:158:PHE:O	2:C:159:GLY:C	2.45	0.52
1:A:266:VAL:H	1:A:299:THR:HG23	1.73	0.51
1:A:381:TRP:CE3	1:A:410:LEU:CD2	2.91	0.51
1:B:297:ASN:OD1	1:B:299:THR:CG2	2.58	0.51
2:C:157:LEU:N	2:C:157:LEU:CD1	2.73	0.51
1:A:362:GLN:HB3	1:A:412:VAL:O	2.11	0.51
1:A:358:LEU:O	1:A:414:LYS:NZ	2.43	0.51
1:A:268:HIS:O	1:A:271:PRO:HD3	2.11	0.51
2:C:119:HIS:N	2:C:119:HIS:ND1	2.59	0.51
1:A:391:TYR:HB3	1:A:410:LEU:HD13	1.93	0.51
2:C:95:ALA:HB3	2:C:98:TRP:CZ3	2.46	0.51
1:B:376:ASP:N	1:B:376:ASP:OD1	2.41	0.50
2:C:101:LYS:O	2:C:104:ASP:HB2	2.12	0.50
1:A:239:ASP:CG	2:C:120:LYS:NZ	2.64	0.50
2:C:100:PHE:HE1	2:C:170:ILE:HG23	1.76	0.50
1:B:295:GLN:HG2	3:B:501:NAG:H62	1.94	0.50
1:A:358:LEU:O	1:A:414:LYS:CE	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:98:TRP:HA	2:C:98:TRP:CE3	2.46	0.50
1:A:237:GLY:O	1:A:328:LEU:HD21	2.08	0.49
2:C:15:GLN:O	2:C:16:TRP:C	2.48	0.49
1:B:417:TRP:CE3	1:B:417:TRP:HA	2.48	0.49
1:A:242:LEU:HD12	1:A:243:PHE:H	1.77	0.48
1:B:238:PRO:HB3	1:B:265:ASP:C	2.32	0.48
1:A:265:ASP:CA	1:A:299:THR:HG21	2.39	0.48
1:A:237:GLY:C	1:A:328:LEU:CD2	2.80	0.48
1:A:353:PRO:HD2	1:A:417:TRP:CZ2	2.48	0.48
1:B:432:LEU:HD22	1:B:437:THR:OG1	2.13	0.48
2:C:42:TRP:CB	2:C:49:ILE:CB	2.92	0.48
1:A:291:PRO:O	1:A:292:ARG:C	2.49	0.48
1:B:248:LYS:HE2	1:B:380:GLU:OE2	2.14	0.48
1:A:238:PRO:CG	1:A:266:VAL:HG22	2.44	0.48
1:B:266:VAL:HB	1:B:300:TYR:HB2	1.96	0.47
1:B:295:GLN:HG2	3:B:501:NAG:C6	2.45	0.47
1:A:308:VAL:HG12	1:A:319:TYR:CE1	2.48	0.47
1:A:282:VAL:HG23	1:A:282:VAL:O	2.15	0.47
1:B:293:GLU:HG2	1:B:293:GLU:O	2.15	0.47
1:B:295:GLN:CG	3:B:501:NAG:H62	2.45	0.47
1:A:295:GLN:HB2	1:A:299:THR:O	2.14	0.47
1:B:253:ILE:O	1:B:310:HIS:NE2	2.45	0.47
2:C:9:VAL:HG23	2:C:9:VAL:O	2.15	0.47
1:A:413:ASP:O	1:A:414:LYS:C	2.54	0.46
1:A:393:THR:HG23	1:A:406:LEU:HD13	1.97	0.46
1:A:266:VAL:N	1:A:299:THR:CG2	2.79	0.46
2:C:120:LYS:HB2	2:C:157:LEU:CD1	2.45	0.46
2:C:125:GLN:NE2	2:C:148:ASP:O	2.49	0.46
1:B:243:PHE:HB2	1:B:260:THR:HG1	1.81	0.45
1:A:413:ASP:O	1:A:416:ARG:HB2	2.17	0.45
1:B:290:LYS:CB	1:B:291:PRO:HD2	2.44	0.45
1:A:292:ARG:HG2	1:A:292:ARG:H	1.62	0.45
2:C:98:TRP:HE3	2:C:98:TRP:HA	1.81	0.45
1:B:297:ASN:OD1	1:B:299:THR:OG1	2.27	0.44
1:B:236:ALA:HB2	2:C:158:PHE:HE2	1.79	0.44
1:B:236:ALA:HB2	2:C:158:PHE:CE2	2.49	0.44
2:C:12:LEU:HB2	2:C:15:GLN:HA	2.00	0.44
1:A:422:VAL:HA	1:A:442:SER:HB2	1.99	0.44
1:A:394:THR:HG22	1:B:397:VAL:CG2	2.47	0.44
1:A:407:TYR:CD2	1:B:407:TYR:HB3	2.52	0.44
1:B:417:TRP:HH2	1:B:441:LEU:HG	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:64:ASP:O	3:C:302:NAG:C3	2.55	0.44
1:A:390:ASN:O	1:A:410:LEU:HD12	2.18	0.43
1:B:292:ARG:HD3	1:B:300:TYR:HB3	2.00	0.43
1:A:259:VAL:HG23	1:A:308:VAL:CG1	2.48	0.43
1:A:405:PHE:C	1:A:405:PHE:CD1	2.91	0.43
1:B:328:LEU:HD12	1:B:328:LEU:C	2.39	0.43
1:A:365:LEU:HD23	1:A:365:LEU:N	2.33	0.43
1:A:279:VAL:HG12	1:A:317:LYS:HD3	2.00	0.42
2:C:12:LEU:HD12	2:C:15:GLN:O	2.19	0.42
1:A:302:VAL:HG12	1:A:303:VAL:N	2.34	0.42
1:A:239:ASP:OD1	2:C:120:LYS:NZ	2.44	0.42
1:A:242:LEU:HD12	1:A:243:PHE:N	2.34	0.42
2:C:91:LEU:HD11	2:C:163:VAL:HG23	2.01	0.42
1:A:241:PHE:HE1	1:A:264:VAL:CG2	2.33	0.42
2:C:108:LEU:HB2	2:C:139:PHE:HB3	2.01	0.42
1:A:238:PRO:HG3	1:A:266:VAL:HG22	2.01	0.42
2:C:44:HIS:O	2:C:47:SER:HB3	2.20	0.41
1:B:329:PRO:HD2	2:C:90:TRP:CZ2	2.55	0.41
1:B:330:LEU:O	1:B:331:PRO:C	2.59	0.41
1:A:239:ASP:HB2	1:A:264:VAL:CG2	2.49	0.41
2:C:90:TRP:HZ3	2:C:158:PHE:CD2	2.39	0.41
1:A:413:ASP:O	1:A:415:SER:N	2.54	0.41
1:B:417:TRP:HA	1:B:417:TRP:HE3	1.85	0.41
1:A:309:LEU:HB2	1:A:312:ASP:HB2	2.03	0.41
1:A:377:ILE:HG13	1:A:429:HIS:HB2	2.02	0.41
1:A:433:HIS:ND1	1:A:434:ASN:CG	2.74	0.41
1:B:351:LEU:HB2	1:B:366:THR:HB	2.03	0.41
2:C:130:ARG:NH2	2:C:141:ILE:CD1	2.80	0.41
1:A:297:ASN:O	1:A:298:SER:CB	2.68	0.40
2:C:121:VAL:HG21	2:C:136:ASN:HA	2.02	0.40
1:A:320:LYS:HG2	1:A:321:CYS:N	2.36	0.40
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.57	0.40
1:A:433:HIS:O	1:A:434:ASN:HB2	2.21	0.40
1:B:292:ARG:HD3	1:B:300:TYR:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	207/249 (83%)	202 (98%)	4 (2%)	1 (0%)	32	71
1	B	206/249 (83%)	195 (95%)	11 (5%)	0	100	100
2	C	151/240 (63%)	140 (93%)	11 (7%)	0	100	100
All	All	564/738 (76%)	537 (95%)	26 (5%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	ASN

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	184/230 (80%)	179 (97%)	5 (3%)	50	81
1	B	191/230 (83%)	189 (99%)	2 (1%)	80	92
2	C	126/209 (60%)	123 (98%)	3 (2%)	54	83
All	All	501/669 (75%)	491 (98%)	10 (2%)	60	86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	292	ARG
1	A	293	GLU

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Mol	Chain	Res	Type
1	A	382	GLU
1	A	405	PHE
1	A	430	GLU
1	B	376	ASP
1	B	413	ASP
2	C	100	PHE
2	C	119	HIS
2	C	130	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	433	HIS
1	B	434	ASN
2	C	134	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

20 ligands 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	1,3,7	14,14,15	0.69	0	15,19,21	0.75	1 (6%)
3	NAG	A	502	3,4	14,14,15	0.60	0	15,19,21	0.72	0
4	BMA	A	503	3,5	11,11,12	0.56	0	13,15,17	1.16	1 (7%)
5	MAN	A	504	3,4	11,11,12	0.57	0	13,15,17	0.70	0
3	NAG	A	505	5,6	14,14,15	0.52	0	15,19,21	0.95	1 (6%)
5	MAN	A	506	3,4	11,11,12	0.44	0	13,15,17	0.68	0
6	GAL	A	507	3	11,11,12	0.54	0	13,15,17	0.63	1 (7%)
7	FUL	A	508	3	9,10,11	1.34	1 (11%)	13,14,16	1.47	3 (23%)
3	NAG	A	509	5	14,14,15	0.62	0	15,19,21	0.90	0
3	NAG	B	501	1,3	14,14,15	1.20	1 (7%)	15,19,21	2.92	2 (13%)
3	NAG	B	502	3,4	14,14,15	0.47	0	15,19,21	0.83	0
4	BMA	B	503	3,5	11,11,12	0.65	0	13,15,17	0.54	0
5	MAN	B	504	3,4	11,11,12	0.60	0	13,15,17	0.66	0
3	NAG	B	505	5,6	14,14,15	0.51	0	15,19,21	0.78	1 (6%)
5	MAN	B	506	3,4	11,11,12	0.50	0	13,15,17	0.55	0
6	GAL	B	507	3	11,11,12	0.63	0	13,15,17	0.35	0
3	NAG	B	508	5	14,14,15	0.29	0	15,19,21	0.57	0
8	FUC	B	509	-	9,10,11	0.95	0	13,14,16	2.16	4 (30%)
3	NAG	C	301	2	14,14,15	1.88	1 (7%)	15,19,21	1.95	3 (20%)
3	NAG	C	302	2	14,14,15	0.27	0	15,19,21	0.53	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	501	1,3,7	-	0/6/23/26	0/1/1/1
3	NAG	A	502	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	503	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	504	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	505	5,6	-	0/6/23/26	0/1/1/1
5	MAN	A	506	3,4	-	0/2/19/22	0/1/1/1
6	GAL	A	507	3	-	0/2/19/22	0/1/1/1
7	FUL	A	508	3	-	0/0/17/20	0/1/1/1
3	NAG	A	509	5	-	0/6/23/26	0/1/1/1
3	NAG	B	501	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	502	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	503	3,5	-	0/2/19/22	0/1/1/1
5	MAN	B	504	3,4	-	0/2/19/22	0/1/1/1
3	NAG	B	505	5,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	B	506	3,4	-	0/2/19/22	0/1/1/1
6	GAL	B	507	3	-	0/2/19/22	0/1/1/1
3	NAG	B	508	5	-	0/6/23/26	0/1/1/1
8	FUC	B	509	-	-	0/0/17/20	0/1/1/1
3	NAG	C	301	2	-	0/6/23/26	0/1/1/1
3	NAG	C	302	2	1/1/5/7	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	NAG	O5-C1	-6.74	1.32	1.43
3	B	501	NAG	O6-C6	-3.93	1.25	1.42
7	A	508	FUL	C2-C3	-2.20	1.49	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	NAG	C1-O5-C5	-4.78	105.57	112.17
7	A	508	FUL	C6-C5-C4	-2.56	108.52	113.07
3	B	501	NAG	C2-N2-C7	-2.44	119.38	122.94
7	A	508	FUL	O2-C2-C3	-2.38	105.50	110.17
3	B	505	NAG	C2-N2-C7	-2.26	119.64	122.94
7	A	508	FUL	O5-C1-C2	-2.25	107.27	110.79
3	A	501	NAG	C2-N2-C7	-2.13	119.83	122.94
3	A	505	NAG	C4-C3-C2	2.01	113.97	111.02
6	A	507	GAL	C1-C2-C3	2.10	112.32	109.65
8	B	509	FUC	C6-C5-C4	2.14	116.88	113.07
3	C	301	NAG	C3-C4-C5	2.65	114.89	110.22
8	B	509	FUC	C3-C4-C5	2.75	114.00	109.68
3	C	301	NAG	C2-N2-C7	2.97	127.28	122.94
4	A	503	BMA	C1-C2-C3	3.18	113.69	109.65
8	B	509	FUC	C1-C2-C3	4.28	115.08	109.65
8	B	509	FUC	C2-C3-C4	4.36	118.47	110.88
3	B	501	NAG	O6-C6-C5	10.82	147.75	111.34

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	302	NAG	C1

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAG	2	0
7	A	508	FUL	1	0
3	B	501	NAG	4	0
8	B	509	FUC	1	0
3	C	301	NAG	3	0
3	C	302	NAG	2	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, 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	209/249 (83%)	0.31	4 (1%) 67 48	12, 25, 48, 63	0
1	B	208/249 (83%)	0.47	3 (1%) 75 58	10, 28, 55, 84	0
2	C	157/240 (65%)	0.62	18 (11%) 5 2	15, 37, 89, 114	0
All	All	574/738 (77%)	0.45	25 (4%) 35 17	10, 29, 72, 114	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	PRO	4.2
1	B	384	ASN	4.1
2	C	54	SER	3.9
2	C	67	GLY	3.6
2	C	10	VAL	3.0
2	C	28	LYS	3.0
2	C	104	ASP	3.0
1	A	444	SER	2.9
2	C	59	ASP	2.8
1	A	236	ALA	2.7
2	C	172	ILE	2.7
2	C	42	TRP	2.6
2	C	69	TYR	2.5
2	C	57	PHE	2.4
2	C	98	TRP	2.3
2	C	80	ASP	2.3
2	C	64	ASP	2.3
2	C	84	LEU	2.3
2	C	56	TYR	2.3
2	C	43	PHE	2.2
1	A	318	GLU	2.1
2	C	70	ARG	2.1
2	C	100	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	316	GLY	2.1
1	B	269	GLU	2.1

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](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
6	GAL	B	507	11/12	0.82	0.35	1.50	26,46,58,63	0
6	GAL	A	507	11/12	0.88	0.39	0.80	27,39,50,53	0
3	NAG	C	302	14/15	0.75	0.33	0.14	61,73,88,91	0
3	NAG	C	301	14/15	0.80	0.30	-0.15	30,41,67,68	0
3	NAG	A	505	14/15	0.92	0.23	-0.71	23,36,43,48	0
3	NAG	A	501	14/15	0.89	0.22	-0.88	34,41,52,59	0
3	NAG	B	502	14/15	0.85	0.23	-1.14	29,51,63,63	0
3	NAG	A	509	14/15	0.71	0.37	-	54,80,90,98	0
5	MAN	A	506	11/12	0.86	0.26	-	48,62,70,71	0
7	FUL	A	508	10/11	0.87	0.21	-	53,68,83,94	0
4	BMA	A	503	11/12	0.85	0.25	-	34,41,48,56	0
3	NAG	B	501	14/15	0.88	0.17	-	43,58,73,80	0
5	MAN	B	504	11/12	0.92	0.15	-	35,45,49,50	0
5	MAN	A	504	11/12	0.93	0.20	-	30,36,41,44	0
3	NAG	B	508	14/15	0.71	0.40	-	76,96,108,127	0
3	NAG	B	505	14/15	0.89	0.22	-	31,38,57,59	0
5	MAN	B	506	11/12	0.90	0.20	-	58,67,75,79	0
8	FUC	B	509	10/11	0.76	0.34	-	75,85,91,92	0
4	BMA	B	503	11/12	0.93	0.18	-	36,47,52,54	0
3	NAG	A	502	14/15	0.93	0.24	-	33,40,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.