Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:19 AM GMT

PDB ID	:	2GJ7
Title	:	Crystal Structure of a gE-gI/Fc complex
Authors	:	Sprague, E.R.; Wang, C.; Baker, D.; Bjorkman, P.J.
Deposited on	:	2006-03-30
Resolution	:	5.00 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:

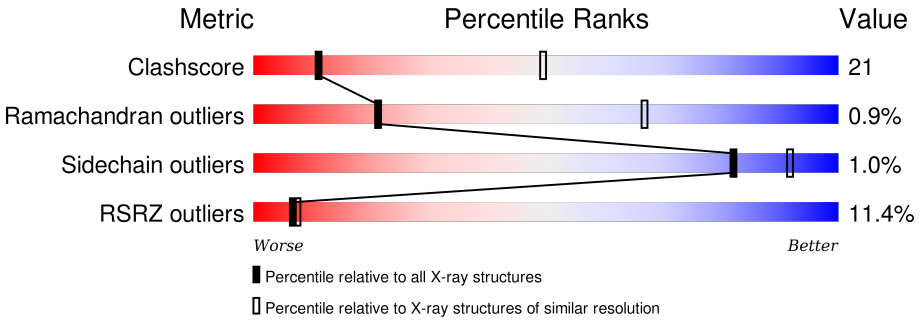
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1019 (6.22-3.66)
Ramachandran outliers	100387	1158 (6.22-3.60)
Sidechain outliers	100360	1136 (6.22-3.60)
RSRZ outliers	91569	1122 (6.22-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	227	15% 73% 18% 9%
1	B	227	14% 72% 19% • 9%
2	E	401	4% 34% 8% 57%
2	F	401	% 33% 8% 57%

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	A	2	-	-	-	X
3	FUC	A	8	X	-	-	-
3	NAG	B	2	-	-	-	X
3	NAG	B	5	-	-	-	X
3	FUC	B	8	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6148 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	207	Total	C	N	O	S	19	0	0
			1659	1056	279	317	7			
1	B	207	Total	C	N	O	S	11	0	0
			1659	1056	279	317	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	LEU	-	CLONING ARTIFACT	UNP P01857
A	222	GLU	-	CLONING ARTIFACT	UNP P01857
A	356	GLU	ASP	CONFLICT	UNP P01857
A	358	MET	LEU	CONFLICT	UNP P01857
B	221	LEU	-	CLONING ARTIFACT	UNP P01857
B	222	GLU	-	CLONING ARTIFACT	UNP P01857
B	356	GLU	ASP	CONFLICT	UNP P01857
B	358	MET	LEU	CONFLICT	UNP P01857

- Molecule 2 is a protein called Glycoprotein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	171	Total	C	N	O	S	0	0	0
			1319	829	229	250	11			
2	E	171	Total	C	N	O	S	0	0	0
			1319	829	229	250	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	420	ASP	-	CLONING ARTIFACT	UNP P04488
F	421	ILE	-	CLONING ARTIFACT	UNP P04488
E	420	ASP	-	CLONING ARTIFACT	UNP P04488
E	421	ILE	-	CLONING ARTIFACT	UNP P04488

- Molecule 3 is a polymer of unknown type called SUGAR (8-MER).

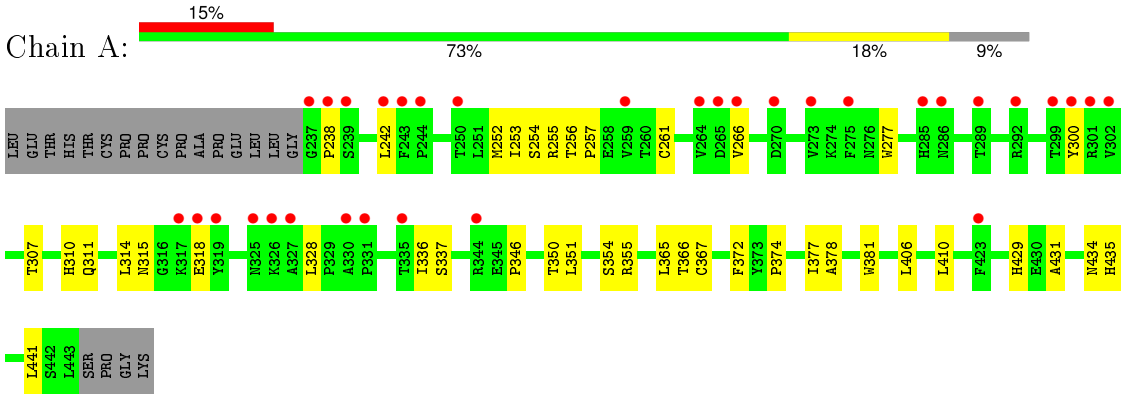
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	8	Total	C	N	O	0	0
			96	54	3	39		
3	B	8	Total	C	N	O	0	0
			96	54	3	39		

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.

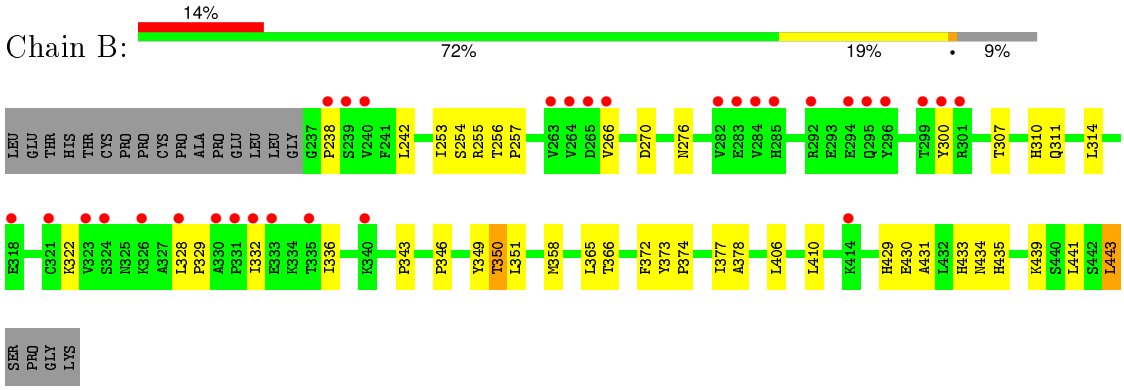
- Molecule 1: Ig gamma-1 chain C region

Chain A:



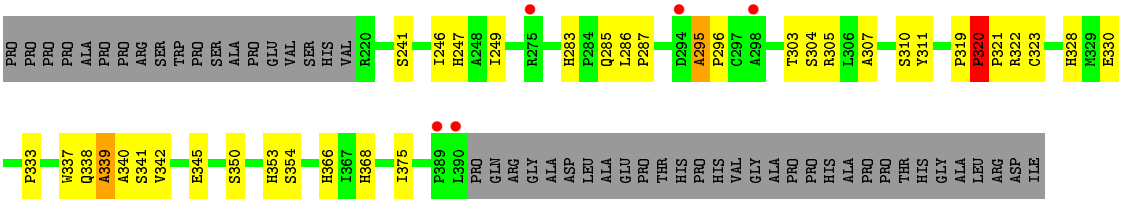
- Molecule 1: Ig gamma-1 chain C region

Chain B:

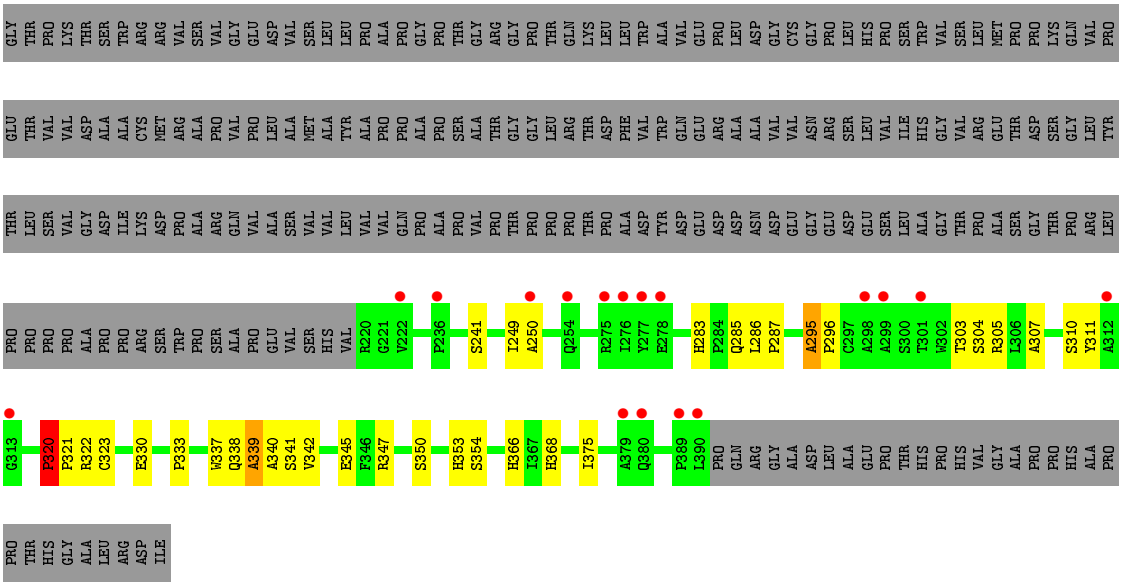


- Molecule 2: Glycoprotein E

Chain F:



- Molecule 2: Glycoprotein E



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	174.73Å 174.73Å 316.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.00 – 5.00 35.68 – 4.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (36.00-5.00) 99.5 (35.68-4.99)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.70 (at 5.08Å)	Xtriage
Refinement program	?	Depositor
R, R_{free}	(Not available) , (Not available) 0.515 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	210.3	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 62.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 21767 reflections	Xtriage
F_o,F_c correlation	0.63	EDS
Total number of atoms	6148	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: FUC, GAL, NAG, BMA, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.40	0/1705	0.61	0/2322
1	B	0.40	0/1705	0.61	0/2322
2	E	0.32	0/1359	0.64	0/1866
2	F	0.32	0/1359	0.64	0/1866
All	All	0.37	0/6128	0.62	0/8376

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
3	B	1	0
All	All	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	8	FUC	C1
3	B	8	FUC	C1

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	1659	0	1622	133	0
1	B	1659	0	1623	82	0
2	E	1319	0	1239	76	30
2	F	1319	0	1238	133	30
3	A	96	0	82	1	0
3	B	96	0	82	0	0
All	All	6148	0	5886	249	30

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 21.

All (249) 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:310:HIS:CD2	2:F:321:PRO:HB3	1.12	1.60
1:A:310:HIS:CG	2:F:321:PRO:CB	1.85	1.60
1:A:310:HIS:CG	2:F:321:PRO:HB3	1.07	1.56
1:A:314:LEU:HB2	2:F:322:ARG:NH1	1.36	1.38
1:A:252:MET:HE3	2:F:247:HIS:CE1	1.61	1.35
1:A:310:HIS:CD2	2:F:321:PRO:CB	2.01	1.34
1:A:254:SER:O	2:F:342:VAL:HG22	1.28	1.34
1:A:311:GLN:O	2:F:322:ARG:NH2	1.61	1.32
1:A:310:HIS:CB	2:F:321:PRO:CB	2.11	1.27
1:A:256:THR:CG2	2:F:340:ALA:HB3	1.59	1.26
1:A:256:THR:HG23	2:F:340:ALA:CB	1.21	1.25
1:B:434:ASN:ND2	2:E:249:ILE:HA	1.52	1.23
1:B:314:LEU:HB2	2:E:322:ARG:NH1	1.53	1.22
1:A:310:HIS:CB	2:F:321:PRO:HB2	1.67	1.22
1:A:311:GLN:O	2:F:322:ARG:CZ	1.91	1.18
1:B:433:HIS:NE2	2:E:250:ALA:O	1.76	1.17
1:A:435:HIS:NE2	2:F:319:PRO:HG3	1.57	1.17
1:B:434:ASN:HD21	2:E:250:ALA:N	1.39	1.16
1:B:253:ILE:HD13	2:E:321:PRO:CA	1.75	1.15
1:A:253:ILE:HB	2:F:320:PRO:HB2	1.23	1.15
1:B:307:THR:CG2	2:E:339:ALA:HB1	1.76	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ILE:CD1	2:E:321:PRO:HA	1.77	1.15
1:A:253:ILE:HB	2:F:320:PRO:CB	1.77	1.14
1:A:253:ILE:CD1	2:F:321:PRO:HA	1.78	1.13
1:B:434:ASN:ND2	2:E:250:ALA:H	1.46	1.13
1:A:307:THR:OG1	2:F:339:ALA:HB1	1.45	1.12
1:A:253:ILE:HD12	2:F:321:PRO:HA	1.29	1.12
1:A:311:GLN:HB2	2:F:322:ARG:CA	1.80	1.11
1:A:311:GLN:HA	2:F:322:ARG:HG2	1.27	1.09
1:A:310:HIS:HB2	2:F:321:PRO:C	1.74	1.07
1:A:310:HIS:HB3	2:F:321:PRO:HB2	1.07	1.07
1:B:307:THR:HG21	2:E:339:ALA:HB1	1.10	1.07
1:B:255:ARG:O	2:E:340:ALA:O	1.74	1.06
1:A:253:ILE:CD1	2:F:321:PRO:CA	2.33	1.05
1:A:314:LEU:CB	2:F:322:ARG:NH1	2.20	1.04
1:A:254:SER:HB3	2:F:246:ILE:HB	1.41	1.00
1:A:256:THR:HG23	2:F:340:ALA:HB3	1.20	1.00
1:A:253:ILE:CB	2:F:320:PRO:CB	2.40	1.00
1:B:434:ASN:HD22	2:E:249:ILE:HA	1.11	1.00
1:B:254:SER:HA	2:E:342:VAL:HG22	1.43	1.00
1:A:314:LEU:CB	2:F:322:ARG:HH11	1.74	0.99
1:A:311:GLN:HB2	2:F:322:ARG:HA	1.45	0.98
1:A:253:ILE:CB	2:F:320:PRO:HB3	1.95	0.97
1:A:257:PRO:HD2	2:F:340:ALA:HB1	1.45	0.97
1:A:311:GLN:CA	2:F:322:ARG:HG2	1.94	0.96
1:B:314:LEU:CB	2:E:322:ARG:NH1	2.28	0.96
1:A:256:THR:HG22	2:F:340:ALA:HB3	1.46	0.96
1:A:253:ILE:HD11	2:F:311:TYR:CE2	2.01	0.96
1:B:314:LEU:HB2	2:E:322:ARG:HH12	1.29	0.95
1:A:314:LEU:HB2	2:F:322:ARG:HH11	0.85	0.95
1:B:434:ASN:ND2	2:E:249:ILE:CA	2.29	0.94
1:A:253:ILE:CG1	2:F:311:TYR:CE2	2.50	0.94
1:A:310:HIS:HB3	2:F:321:PRO:CB	1.88	0.94
1:A:311:GLN:O	2:F:322:ARG:NH1	2.01	0.93
1:A:253:ILE:HD11	2:F:311:TYR:HE2	1.35	0.91
1:A:254:SER:O	2:F:342:VAL:CG2	2.16	0.91
1:A:311:GLN:HA	2:F:322:ARG:CG	2.01	0.90
1:A:253:ILE:HG21	2:F:320:PRO:HB3	1.54	0.90
1:B:314:LEU:HB2	2:E:322:ARG:HH11	1.37	0.89
1:B:256:THR:OG1	2:E:341:SER:CB	2.21	0.89
1:A:311:GLN:HA	2:F:322:ARG:CZ	2.03	0.88
1:A:252:MET:CE	2:F:247:HIS:CE1	2.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLN:HB2	2:F:322:ARG:CB	2.04	0.87
1:A:435:HIS:NE2	2:F:319:PRO:CG	2.37	0.87
1:A:238:PRO:HD2	1:A:328:LEU:HD13	1.56	0.87
1:A:252:MET:HE3	2:F:247:HIS:NE2	1.89	0.87
1:A:253:ILE:HG13	2:F:311:TYR:CE2	2.10	0.86
1:A:253:ILE:CG2	2:F:320:PRO:HB3	2.05	0.86
1:B:434:ASN:ND2	2:E:250:ALA:N	2.13	0.84
1:B:256:THR:HG21	2:E:339:ALA:HB3	1.57	0.84
1:B:307:THR:HG21	2:E:339:ALA:CB	2.04	0.83
1:A:253:ILE:CD1	2:F:311:TYR:CE2	2.62	0.83
1:A:253:ILE:CD1	2:F:311:TYR:HE2	1.90	0.83
1:B:256:THR:OG1	2:E:341:SER:HB2	1.78	0.82
1:B:242:LEU:HG	1:B:336:ILE:HG12	1.59	0.82
1:A:310:HIS:CD2	2:F:321:PRO:CG	2.64	0.81
1:A:242:LEU:HG	1:A:336:ILE:HG12	1.62	0.81
1:A:310:HIS:CG	2:F:321:PRO:CA	2.62	0.81
1:B:256:THR:HG21	2:E:339:ALA:CB	2.10	0.80
1:A:254:SER:CB	2:F:246:ILE:HB	2.11	0.80
1:A:311:GLN:HA	2:F:322:ARG:NH1	1.97	0.80
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.64	0.80
1:B:254:SER:CA	2:E:342:VAL:HG22	2.11	0.78
1:B:253:ILE:HD13	2:E:321:PRO:HA	0.85	0.78
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.65	0.76
1:B:433:HIS:HE2	2:E:250:ALA:C	1.89	0.76
1:A:311:GLN:CA	2:F:322:ARG:CZ	2.63	0.76
1:A:253:ILE:CB	2:F:320:PRO:HB2	2.09	0.76
1:A:256:THR:CG2	2:F:340:ALA:CB	2.05	0.75
1:B:434:ASN:HD21	2:E:250:ALA:H	0.78	0.75
1:B:253:ILE:HG12	2:E:311:TYR:CE2	2.21	0.74
1:A:253:ILE:CG1	2:F:320:PRO:HB3	2.16	0.74
1:A:311:GLN:CB	2:F:322:ARG:HB3	2.18	0.74
2:E:338:GLN:HG3	2:E:341:SER:HB3	1.70	0.74
1:B:256:THR:OG1	2:E:341:SER:N	2.21	0.74
2:F:338:GLN:HG3	2:F:341:SER:HB3	1.70	0.73
1:A:311:GLN:CB	2:F:322:ARG:CB	2.67	0.73
1:A:311:GLN:C	2:F:322:ARG:CZ	2.57	0.72
1:A:435:HIS:CE1	2:F:319:PRO:CG	2.73	0.71
1:B:433:HIS:CE1	2:E:250:ALA:HB3	2.24	0.71
1:A:253:ILE:HG12	2:F:320:PRO:HB3	1.70	0.71
1:A:253:ILE:HD12	2:F:321:PRO:CA	2.08	0.71
1:B:256:THR:HG21	2:E:338:GLN:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:SER:C	2:F:342:VAL:HG22	2.11	0.70
1:A:310:HIS:CB	2:F:321:PRO:C	2.58	0.69
1:A:311:GLN:HB2	2:F:322:ARG:HB3	1.73	0.69
1:B:238:PRO:HD2	1:B:328:LEU:HD13	1.73	0.69
1:A:307:THR:OG1	2:F:339:ALA:CB	2.34	0.69
1:A:350:THR:HB	1:A:441:LEU:HD13	1.74	0.69
1:A:311:GLN:C	2:F:322:ARG:NH1	2.46	0.68
1:B:314:LEU:CB	2:E:322:ARG:HH12	2.02	0.68
1:A:311:GLN:CB	2:F:322:ARG:HA	2.22	0.67
1:A:307:THR:HG1	2:F:339:ALA:HB1	1.59	0.66
1:A:314:LEU:CA	2:F:322:ARG:NH1	2.58	0.66
1:A:311:GLN:N	2:F:322:ARG:HA	2.11	0.65
1:A:254:SER:HB2	2:F:342:VAL:HG21	1.78	0.65
1:B:434:ASN:HD22	2:E:249:ILE:CA	1.95	0.64
1:A:311:GLN:CA	2:F:322:ARG:NH1	2.61	0.63
1:A:310:HIS:CB	2:F:321:PRO:CA	2.75	0.63
1:B:310:HIS:HE1	2:E:340:ALA:O	1.82	0.63
1:B:311:GLN:HB2	2:E:322:ARG:HA	1.81	0.62
1:A:253:ILE:CG2	2:F:320:PRO:CB	2.74	0.62
1:B:257:PRO:HD2	2:E:340:ALA:CB	2.29	0.62
1:A:252:MET:CE	2:F:247:HIS:NE2	2.60	0.61
1:A:253:ILE:CG1	2:F:320:PRO:CB	2.77	0.61
1:B:314:LEU:CB	2:E:322:ARG:HH11	2.04	0.61
1:A:311:GLN:HB2	2:F:322:ARG:C	2.20	0.61
1:A:307:THR:HG23	2:F:340:ALA:HB2	1.81	0.61
1:B:256:THR:OG1	2:E:340:ALA:C	2.39	0.61
1:B:433:HIS:CE1	2:E:250:ALA:O	2.52	0.60
1:B:443:LEU:HD12	1:B:443:LEU:N	2.15	0.60
1:B:254:SER:HA	2:E:342:VAL:CG2	2.27	0.60
2:E:350:SER:H	2:E:353:HIS:HD2	1.50	0.59
1:A:311:GLN:CA	2:F:322:ARG:CG	2.73	0.59
1:B:257:PRO:HD2	2:E:340:ALA:HB3	1.83	0.59
1:B:350:THR:HB	1:B:441:LEU:HD13	1.85	0.59
1:A:311:GLN:H	2:F:322:ARG:HA	1.68	0.58
2:F:350:SER:H	2:F:353:HIS:HD2	1.50	0.58
2:F:241:SER:HB3	2:F:345:GLU:HG3	1.86	0.58
1:A:311:GLN:HB2	2:F:322:ARG:O	2.04	0.58
1:B:253:ILE:HG12	2:E:311:TYR:HE2	1.69	0.58
1:A:253:ILE:HD11	2:F:311:TYR:CD2	2.38	0.57
1:A:311:GLN:CB	2:F:322:ARG:CA	2.71	0.57
1:A:314:LEU:HD12	2:F:322:ARG:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:HIS:HB2	2:F:321:PRO:O	2.04	0.57
1:A:310:HIS:HB2	2:F:321:PRO:CA	2.34	0.57
1:A:311:GLN:N	2:F:322:ARG:HG2	2.20	0.56
2:E:241:SER:HB3	2:E:345:GLU:HG3	1.86	0.56
1:B:256:THR:HG23	2:E:340:ALA:HB3	1.87	0.56
1:A:255:ARG:O	2:F:340:ALA:O	2.20	0.56
1:B:434:ASN:ND2	2:E:249:ILE:C	2.58	0.56
1:A:314:LEU:HD12	2:F:322:ARG:CG	2.36	0.56
1:B:253:ILE:CG1	2:E:311:TYR:CE2	2.88	0.55
1:B:253:ILE:CG1	2:E:311:TYR:HE2	2.19	0.55
1:A:307:THR:CG2	2:F:340:ALA:HB2	2.36	0.55
2:E:283:HIS:CD2	2:E:286:LEU:HD12	2.42	0.55
2:E:320:PRO:HA	2:E:323:CYS:SG	2.47	0.55
1:A:314:LEU:N	2:F:322:ARG:HH12	2.03	0.55
2:F:320:PRO:HA	2:F:323:CYS:SG	2.47	0.54
2:F:283:HIS:CD2	2:F:286:LEU:HD12	2.42	0.54
1:B:256:THR:CG2	2:E:339:ALA:CB	2.84	0.54
1:B:351:LEU:HB2	1:B:366:THR:HB	1.90	0.54
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.89	0.53
1:A:311:GLN:HA	2:F:322:ARG:NE	2.22	0.53
1:A:435:HIS:CE1	2:F:319:PRO:HG2	2.43	0.52
1:B:429:HIS:O	1:B:435:HIS:HA	2.09	0.52
1:A:253:ILE:HG21	2:F:320:PRO:CB	2.33	0.52
1:A:253:ILE:HG12	2:F:320:PRO:CB	2.40	0.52
1:A:374:PRO:O	1:A:429:HIS:HE1	1.93	0.52
2:F:333:PRO:O	2:F:353:HIS:HE1	1.93	0.51
1:A:365:LEU:HD12	1:A:410:LEU:HD23	1.92	0.51
1:A:314:LEU:HB2	2:F:322:ARG:CZ	2.28	0.51
1:A:307:THR:HG23	2:F:340:ALA:CB	2.41	0.51
2:E:333:PRO:O	2:E:353:HIS:HE1	1.93	0.50
2:F:338:GLN:HB3	2:F:345:GLU:OE2	2.11	0.50
2:E:338:GLN:HB3	2:E:345:GLU:OE2	2.11	0.50
1:B:253:ILE:CD1	2:E:311:TYR:HE2	2.24	0.50
1:B:429:HIS:CD2	1:B:431:ALA:H	2.29	0.50
1:B:253:ILE:HD11	2:E:311:TYR:HE2	1.77	0.50
1:A:351:LEU:HB2	1:A:366:THR:HB	1.93	0.50
1:B:433:HIS:HE2	2:E:250:ALA:CA	2.25	0.49
2:E:304:SER:HB3	2:E:330:GLU:OE2	2.12	0.49
2:F:304:SER:HB3	2:F:330:GLU:OE2	2.12	0.49
3:A:1:NAG:O6	3:A:8:FUC:H63	2.12	0.49
1:B:256:THR:CG2	2:E:339:ALA:HB3	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:THR:OG1	2:E:341:SER:HB3	2.11	0.49
1:A:257:PRO:CD	2:F:340:ALA:HB1	2.32	0.48
1:A:253:ILE:HG13	2:F:311:TYR:CZ	2.48	0.48
2:E:366:HIS:O	2:E:368:HIS:HD2	1.97	0.48
2:F:366:HIS:O	2:F:368:HIS:HD2	1.97	0.48
1:B:256:THR:CG2	2:E:338:GLN:O	2.60	0.48
1:A:377:ILE:HG12	1:A:378:ALA:H	1.78	0.47
1:A:434:ASN:CB	2:F:249:ILE:HA	2.43	0.47
1:A:256:THR:CA	2:F:340:ALA:CB	2.92	0.47
1:B:307:THR:HG23	2:E:339:ALA:HB1	1.87	0.47
1:A:406:LEU:HD12	1:A:406:LEU:C	2.35	0.47
1:A:310:HIS:HB2	2:F:322:ARG:N	2.28	0.47
1:B:256:THR:CB	2:E:338:GLN:O	2.62	0.47
2:F:333:PRO:O	2:F:353:HIS:CE1	2.68	0.47
2:E:333:PRO:O	2:E:353:HIS:CE1	2.68	0.47
2:E:338:GLN:HG3	2:E:341:SER:CB	2.42	0.47
1:B:374:PRO:O	1:B:429:HIS:HE1	1.98	0.47
1:B:310:HIS:CG	2:E:321:PRO:HB3	2.50	0.46
1:A:311:GLN:HA	2:F:322:ARG:CD	2.46	0.46
1:A:318:GLU:HA	1:A:337:SER:HB3	1.98	0.46
1:B:434:ASN:HD21	2:E:249:ILE:C	2.07	0.46
2:F:338:GLN:HG3	2:F:341:SER:CB	2.42	0.46
1:A:314:LEU:N	2:F:322:ARG:NH1	2.64	0.45
1:B:430:GLU:HA	1:B:435:HIS:CD2	2.51	0.45
1:A:429:HIS:CD2	1:A:431:ALA:H	2.35	0.45
1:A:377:ILE:HG12	1:A:378:ALA:N	2.31	0.45
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.51	0.45
1:B:256:THR:OG1	2:E:341:SER:CA	2.65	0.44
1:A:354:SER:HB2	1:B:349:TYR:HB3	1.99	0.44
1:A:429:HIS:O	1:A:435:HIS:HA	2.18	0.44
1:A:253:ILE:HG12	2:F:311:TYR:CE2	2.47	0.44
2:E:320:PRO:HB2	2:E:321:PRO:HD3	2.00	0.44
1:B:257:PRO:HD2	2:E:340:ALA:HB1	1.99	0.44
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.98	0.44
1:B:377:ILE:HG12	1:B:378:ALA:N	2.33	0.44
1:A:256:THR:HA	2:F:340:ALA:CB	2.47	0.43
2:E:295:ALA:HB3	2:E:296:PRO:CD	2.48	0.43
2:F:295:ALA:HB3	2:F:296:PRO:CD	2.49	0.43
1:B:377:ILE:HG12	1:B:378:ALA:H	1.82	0.43
1:B:406:LEU:HD12	1:B:406:LEU:C	2.39	0.43
2:F:307:ALA:HB1	2:F:337:TRP:CZ2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:CA	2:F:322:ARG:HH12	2.28	0.43
1:B:238:PRO:HD2	1:B:328:LEU:CD1	2.45	0.43
2:F:320:PRO:HB2	2:F:321:PRO:HD3	2.00	0.42
1:A:253:ILE:HA	2:F:321:PRO:HG3	2.02	0.42
2:F:319:PRO:HA	2:F:320:PRO:HD3	1.94	0.42
2:E:307:ALA:HB1	2:E:337:TRP:CZ2	2.54	0.42
1:B:254:SER:CB	2:E:342:VAL:CG2	2.97	0.42
2:E:295:ALA:HB3	2:E:296:PRO:HD3	2.01	0.42
1:B:266:VAL:HB	1:B:300:TYR:HB2	2.02	0.42
1:A:255:ARG:C	2:F:341:SER:HA	2.41	0.41
1:B:276:ASN:HB2	1:B:322:LYS:HB3	2.02	0.41
1:B:328:LEU:HD21	1:B:332:ILE:HD12	2.02	0.41
2:E:345:GLU:OE1	2:E:347:ARG:NH2	2.48	0.41
1:B:328:LEU:HA	1:B:329:PRO:HD2	1.87	0.41
2:F:354:SER:HA	2:F:375:ILE:O	2.20	0.41
2:F:295:ALA:HB3	2:F:296:PRO:HD3	2.01	0.41
1:A:256:THR:HB	2:F:341:SER:HB2	1.68	0.41
1:B:443:LEU:H	1:B:443:LEU:HD12	1.86	0.41
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.56	0.41
1:B:429:HIS:HD2	1:B:431:ALA:H	1.69	0.40
2:E:354:SER:HA	2:E:375:ILE:O	2.20	0.40
1:A:315:ASN:N	2:F:322:ARG:NH1	2.70	0.40
1:B:343:PRO:HA	1:B:373:TYR:O	2.21	0.40

All (30) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:305:ARG:NH2	2:E:285:GLN:CB[3_444]	0.59	1.61
2:F:285:GLN:CB	2:E:305:ARG:NH2[3_444]	0.81	1.39
2:F:305:ARG:NH1	2:E:285:GLN:O[3_444]	1.28	0.92
2:F:303:THR:CB	2:E:303:THR:CB[3_444]	1.37	0.83
2:F:305:ARG:NH1	2:E:285:GLN:C[3_444]	1.40	0.80
2:F:285:GLN:O	2:E:305:ARG:NH1[3_444]	1.45	0.75
2:F:305:ARG:CZ	2:E:285:GLN:CB[3_444]	1.55	0.65
2:F:285:GLN:OE1	2:E:305:ARG:NE[3_444]	1.55	0.65
2:F:305:ARG:NE	2:E:285:GLN:OE1[3_444]	1.60	0.60
2:F:305:ARG:NH1	2:E:285:GLN:CA[3_444]	1.68	0.52
2:F:305:ARG:CZ	2:E:285:GLN:CA[3_444]	1.72	0.48
2:F:285:GLN:C	2:E:305:ARG:NH1[3_444]	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:285:GLN:CG	2:E:305:ARG:NH2[3_444]	1.77	0.43
2:F:285:GLN:CB	2:E:305:ARG:CZ[3_444]	1.79	0.41
2:F:305:ARG:NH2	2:E:285:GLN:CG[3_444]	1.83	0.37
2:F:305:ARG:NH2	2:E:285:GLN:CA[3_444]	1.84	0.36
2:F:305:ARG:NE	2:E:285:GLN:CD[3_444]	1.86	0.34
2:F:303:THR:CB	2:E:303:THR:CG2[3_444]	1.86	0.34
2:F:285:GLN:CD	2:E:305:ARG:NE[3_444]	1.87	0.33
2:F:303:THR:CG2	2:E:303:THR:CB[3_444]	1.89	0.31
2:F:285:GLN:CA	2:E:305:ARG:NH1[3_444]	1.94	0.26
2:F:310:SER:OG	2:E:287:PRO:CD[3_444]	1.98	0.22
2:F:285:GLN:CA	2:E:305:ARG:NH2[3_444]	2.01	0.19
2:F:310:SER:OG	2:E:287:PRO:CG[3_444]	2.03	0.17
2:F:285:GLN:CA	2:E:305:ARG:CZ[3_444]	2.04	0.16
2:F:328:HIS:CD2	2:E:287:PRO:CB[3_444]	2.06	0.14
2:F:287:PRO:CG	2:E:310:SER:OG[3_444]	2.12	0.08
2:F:305:ARG:CD	2:E:285:GLN:OE1[3_444]	2.12	0.08
2:F:328:HIS:NE2	2:E:287:PRO:CB[3_444]	2.14	0.06
2:F:305:ARG:CZ	2:E:285:GLN:O[3_444]	2.17	0.03

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	205/227 (90%)	203 (99%)	2 (1%)	0	100	100
1	B	205/227 (90%)	199 (97%)	5 (2%)	1 (0%)	34	77
2	E	169/401 (42%)	160 (95%)	6 (4%)	3 (2%)	11	54
2	F	169/401 (42%)	160 (95%)	6 (4%)	3 (2%)	11	54
All	All	748/1256 (60%)	722 (96%)	19 (2%)	7 (1%)	21	67

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	295	ALA
2	F	320	PRO
2	F	339	ALA
2	E	295	ALA
2	E	320	PRO
2	E	339	ALA
1	B	358	MET

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	193/210 (92%)	192 (100%)	1 (0%)	92 96
1	B	193/210 (92%)	189 (98%)	4 (2%)	61 85
2	E	144/332 (43%)	143 (99%)	1 (1%)	88 94
2	F	144/332 (43%)	143 (99%)	1 (1%)	88 94
All	All	674/1084 (62%)	667 (99%)	7 (1%)	82 92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	355	ARG
2	F	320	PRO
1	B	270	ASP
1	B	350	THR
1	B	439	LYS
1	B	443	LEU
2	E	320	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	429	HIS
1	A	438	GLN
2	F	283	HIS

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Mol	Chain	Res	Type
2	F	338	GLN
2	F	353	HIS
2	F	368	HIS
1	B	310	HIS
1	B	361	ASN
1	B	429	HIS
1	B	434	ASN
2	E	283	HIS
2	E	338	GLN
2	E	353	HIS
2	E	368	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

16 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	1	1,3	14,14,15	0.47	0	15,19,21	0.81	0
3	NAG	A	2	3	14,14,15	0.45	0	15,19,21	0.76	1 (6%)
3	BMA	A	3	3	11,11,12	0.64	0	14,15,17	0.63	0
3	MAN	A	4	3	11,11,12	0.49	0	14,15,17	0.62	0
3	NAG	A	5	3	14,14,15	0.49	0	15,19,21	0.71	1 (6%)
3	MAN	A	6	3	11,11,12	0.59	0	14,15,17	0.83	0
3	GAL	A	7	3	11,11,12	0.75	0	14,15,17	0.82	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FUC	A	8	3	10,10,11	0.73	0	14,14,16	1.28	3 (21%)
3	NAG	B	1	1,3	14,14,15	0.66	0	15,19,21	0.89	0
3	NAG	B	2	3	14,14,15	0.57	0	15,19,21	0.79	1 (6%)
3	BMA	B	3	3	11,11,12	0.83	1 (9%)	14,15,17	0.54	0
3	MAN	B	4	3	11,11,12	0.55	0	14,15,17	0.92	1 (7%)
3	NAG	B	5	3	14,14,15	0.49	0	15,19,21	0.83	1 (6%)
3	MAN	B	6	3	11,11,12	0.54	0	14,15,17	0.60	0
3	GAL	B	7	3	11,11,12	0.54	0	14,15,17	0.53	0
3	FUC	B	8	3	10,10,11	0.76	0	14,14,16	1.24	2 (14%)

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	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	0/6/23/26	0/1/1/1
3	BMA	A	3	3	-	0/2/19/22	0/1/1/1
3	MAN	A	4	3	-	0/2/19/22	0/1/1/1
3	NAG	A	5	3	-	0/6/23/26	0/1/1/1
3	MAN	A	6	3	-	0/2/19/22	0/1/1/1
3	GAL	A	7	3	-	0/2/19/22	0/1/1/1
3	FUC	A	8	3	1/1/4/5	0/0/17/20	0/1/1/1
3	NAG	B	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
3	MAN	B	4	3	-	0/2/19/22	0/1/1/1
3	NAG	B	5	3	-	0/6/23/26	0/1/1/1
3	MAN	B	6	3	-	0/2/19/22	0/1/1/1
3	GAL	B	7	3	-	0/2/19/22	0/1/1/1
3	FUC	B	8	3	1/1/4/5	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3	BMA	C2-C3	2.12	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2	NAG	C2-N2-C7	-2.43	119.91	123.04
3	B	5	NAG	C2-N2-C7	-2.16	120.27	123.04
3	A	2	NAG	C2-N2-C7	-2.15	120.28	123.04
3	A	5	NAG	C2-N2-C7	-2.00	120.47	123.04
3	A	8	FUC	C1-O5-C5	2.01	115.48	112.38
3	A	8	FUC	C3-C4-C5	2.33	113.65	109.72
3	A	7	GAL	C1-C2-C3	2.53	112.53	109.54
3	A	8	FUC	C1-C2-C3	2.63	112.65	109.54
3	B	4	MAN	C1-O5-C5	2.73	115.71	112.25
3	B	8	FUC	C1-C2-C3	2.78	112.83	109.54
3	B	8	FUC	C1-O5-C5	3.03	117.06	112.38

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	8	FUC	C1
3	B	8	FUC	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	NAG	1	0
3	A	8	FUC	1	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	207/227 (91%)	1.09	33 (15%) 3 4	9, 24, 36, 50	5 (2%)
1	B	207/227 (91%)	0.90	31 (14%) 3 5	10, 25, 45, 56	4 (1%)
2	E	171/401 (42%)	0.76	17 (9%) 9 9	11, 18, 28, 36	0
2	F	171/401 (42%)	0.43	5 (2%) 55 45	0, 0, 0, 0	0
All	All	756/1256 (60%)	0.81	86 (11%) 7 7	0, 19, 37, 56	9 (1%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	ASP	14.0
1	A	237	GLY	12.6
2	E	390	LEU	11.9
1	A	238	PRO	11.0
2	F	390	LEU	9.4
1	A	266	VAL	7.1
1	A	264	VAL	6.7
2	E	389	PRO	6.2
2	F	389	PRO	6.1
1	B	301	ARG	6.1
1	A	331	PRO	4.7
1	B	263	VAL	4.7
1	B	264	VAL	4.7
1	A	326	LYS	4.5
1	A	325	ASN	4.5
1	B	331	PRO	4.4
1	B	240	VAL	4.3
1	B	300	TYR	4.3
1	B	239	SER	4.3
1	B	333	GLU	4.3
1	B	296	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	332	ILE	4.0
1	A	330	ALA	4.0
1	A	301	ARG	3.9
1	A	318	GLU	3.8
1	A	239	SER	3.7
1	B	294	GLU	3.7
2	E	254	GLN	3.7
2	E	379	ALA	3.3
1	B	340	LYS	3.3
1	B	238	PRO	3.2
1	A	243	PHE	3.2
1	A	302	VAL	3.2
1	A	292	ARG	3.2
1	A	299	THR	3.1
1	A	259	VAL	3.1
1	B	282	VAL	3.1
1	B	285	HIS	3.1
2	E	236	PRO	3.1
1	A	300	TYR	3.1
2	E	277	TYR	3.0
1	A	242	LEU	3.0
1	B	266	VAL	2.9
1	B	330	ALA	2.9
2	E	275	ARG	2.9
1	A	423	PHE	2.9
1	A	250	THR	2.8
1	A	270	ASP	2.8
1	A	319	TYR	2.8
2	F	294	ASP	2.7
2	E	250	ALA	2.7
1	B	324	SER	2.7
2	E	298	ALA	2.7
2	E	299	ALA	2.6
2	E	313	GLY	2.6
2	E	312	ALA	2.6
1	A	286	ASN	2.5
1	B	292	ARG	2.5
1	A	335	THR	2.4
2	E	301	THR	2.4
1	B	283	GLU	2.4
1	A	327	ALA	2.3
1	B	335	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	275	ARG	2.3
2	F	298	ALA	2.3
1	A	273	VAL	2.3
1	A	344	ARG	2.3
1	A	244	PRO	2.3
2	E	278	GLU	2.2
2	E	380	GLN	2.2
1	B	323	VAL	2.2
1	A	275	PHE	2.2
1	B	299	THR	2.2
2	E	276	ILE	2.2
1	B	328	LEU	2.1
1	A	289	THR	2.1
1	A	317	LYS	2.1
1	B	265	ASP	2.1
1	B	284	VAL	2.1
1	B	326	LYS	2.1
2	E	222	VAL	2.1
1	A	285	HIS	2.1
1	B	318	GLU	2.0
1	B	414	LYS	2.0
1	B	295	GLN	2.0
1	B	321	CYS	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, 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
3	NAG	B	2	14/15	0.31	1.30	1.19	29,34,36,38	0
3	NAG	A	2	14/15	0.80	1.06	-0.06	23,27,30,31	0
3	NAG	B	5	14/15	0.53	0.47	-0.26	29,33,37,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	5	14/15	0.68	0.36	-0.71	33,36,39,42	0
3	GAL	B	7	11/12	0.83	0.28	-0.98	48,52,55,58	0
3	GAL	A	7	11/12	0.62	0.37	-1.14	47,53,56,61	0
3	MAN	A	6	11/12	0.21	0.75	-	39,44,46,47	0
3	BMA	A	3	11/12	0.43	0.61	-	30,33,36,40	0
3	MAN	B	6	11/12	0.58	0.77	-	40,42,43,44	0
3	BMA	B	3	11/12	0.45	0.47	-	25,28,33,34	0
3	FUC	A	8	10/11	-0.02	0.75	-	62,68,74,74	0
3	MAN	A	4	11/12	0.57	0.58	-	36,37,40,40	0
3	FUC	B	8	10/11	-0.19	0.83	-	57,60,63,64	0
3	NAG	B	1	14/15	0.30	0.84	-	40,42,45,54	0
3	NAG	A	1	14/15	0.59	0.85	-	31,33,43,54	0
3	MAN	B	4	11/12	0.26	0.58	-	27,29,32,36	0

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.