



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:29 PM GMT

PDB ID : 1FUJ
Title : PR3 (MYELOBLASTIN)
Authors : Fujinaga, M.; Chernaia, M.M.; Halenbeck, R.; Koths, K.; James, M.N.G.
Deposited on : 1996-01-25
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ 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

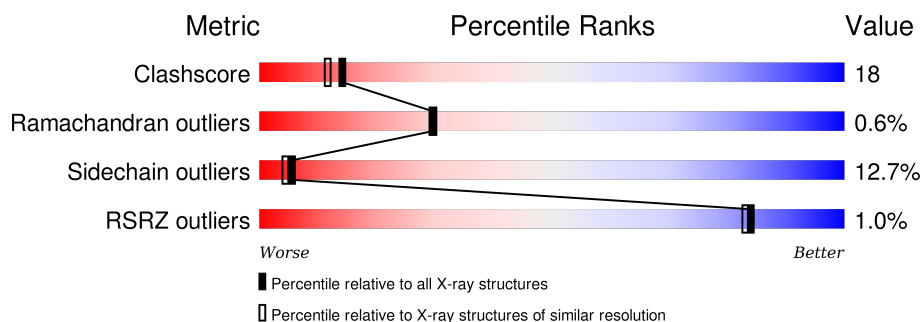
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	221	<div> <div></div> <div>65%30% . .</div> </div>
1	B	221	<div> <div></div> <div>56%38%5%</div> </div>
1	C	221	<div> <div></div> <div>61%33%5%</div> </div>
1	D	221	<div> <div></div> <div>60%34%5%</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
2	FUC	C	245	-	-	-	X
2	FUC	D	245	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7174 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 PR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1708	1083	311	303	11			
1	B	221	Total	C	N	O	S	0	0	0
			1708	1083	311	303	11			
1	C	221	Total	C	N	O	S	0	0	0
			1708	1083	311	303	11			
1	D	221	Total	C	N	O	S	0	0	0
			1708	1083	311	303	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ILE	VAL	CONFLICT	UNP P24158
B	103	ILE	VAL	CONFLICT	UNP P24158
C	103	ILE	VAL	CONFLICT	UNP P24158
D	103	ILE	VAL	CONFLICT	UNP P24158

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

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

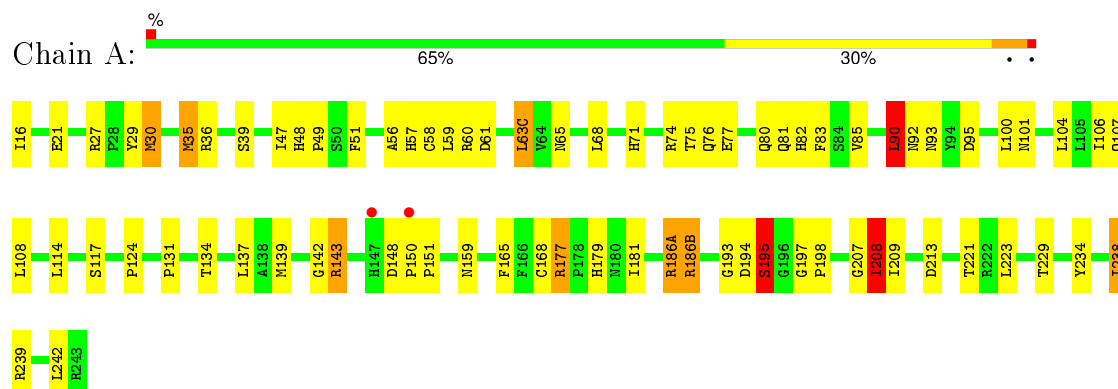
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total 74	O 74	0	0
3	B	48	Total 48	O 48	0	0
3	C	67	Total 67	O 67	0	0
3	D	57	Total 57	O 57	0	0

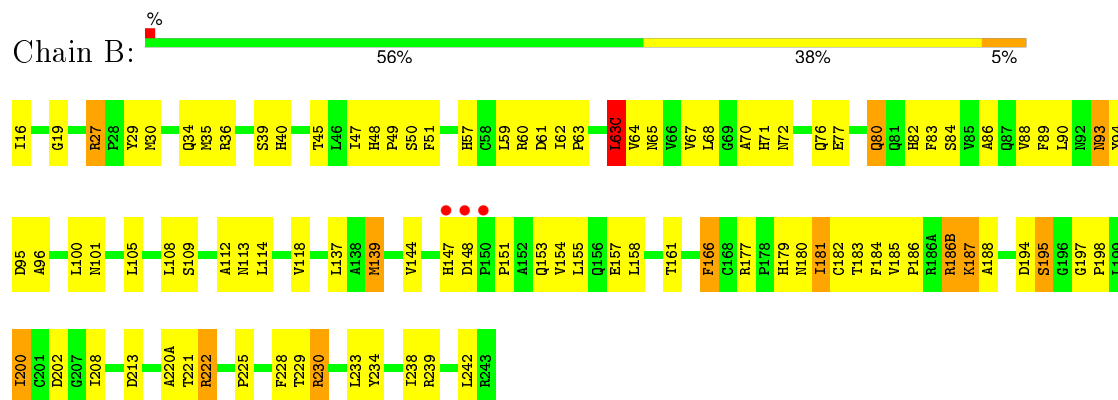
3 Residue-property plots [i](#)

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.

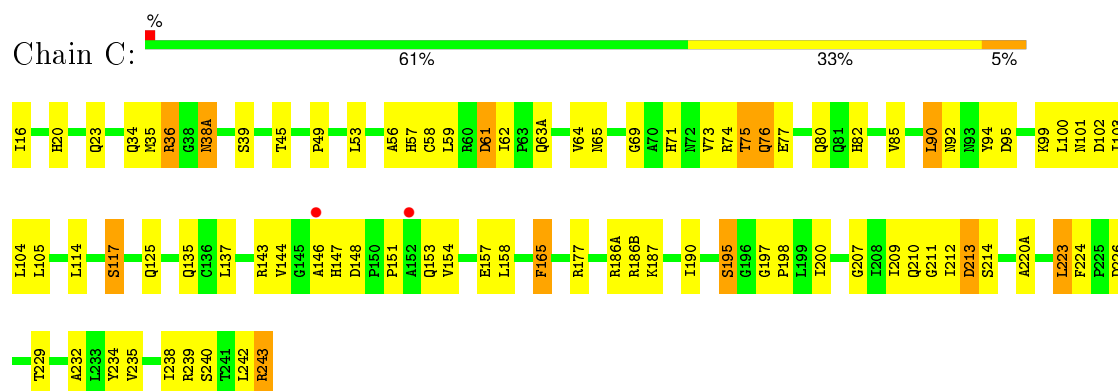
• Molecule 1: PR3



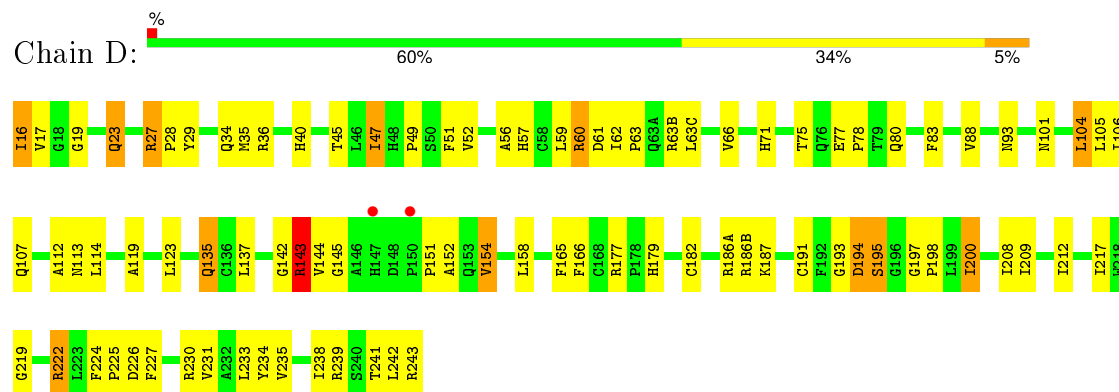
• Molecule 1: PR3



• Molecule 1: PR3



- Molecule 1: PR3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.60Å 54.07Å 113.51Å 90.00° 90.69° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 68.74 – 1.98	Depositor EDS
% Data completeness (in resolution range)	93.4 (10.00-2.20) 89.6 (68.74-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.98Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , (Not available) 0.177 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.716	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 124.6	EDS
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 65602 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7174	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: NAG, FUC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.97	2/1754 (0.1%)	1.09	6/2393 (0.3%)
1	B	0.92	0/1754	1.08	3/2393 (0.1%)
1	C	0.90	0/1754	1.01	1/2393 (0.0%)
1	D	0.91	0/1754	1.03	6/2393 (0.3%)
All	All	0.92	2/7016 (0.0%)	1.05	16/9572 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	SER	CA-CB	5.68	1.61	1.52
1	A	195	SER	CB-OG	5.40	1.49	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	LEU	CA-CB-CG	7.78	133.19	115.30
1	A	63(C)	LEU	CA-CB-CG	-6.91	99.41	115.30
1	A	208	ILE	CG1-CB-CG2	-6.29	97.56	111.40
1	A	108	LEU	CB-CG-CD2	-5.91	100.96	111.00
1	D	200	ILE	CG1-CB-CG2	-5.83	98.56	111.40
1	A	181	ILE	N-CA-C	-5.41	96.39	111.00
1	B	200	ILE	CG1-CB-CG2	-5.34	99.65	111.40
1	B	63(C)	LEU	CA-CB-CG	5.33	127.57	115.30
1	D	143	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	D	137	LEU	CB-CG-CD2	-5.27	102.04	111.00
1	C	226	ASP	N-CA-C	-5.13	97.16	111.00
1	D	194	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	226	ASP	N-CA-C	-5.09	97.25	111.00
1	D	145	GLY	N-CA-C	-5.09	100.38	113.10
1	A	238	ILE	CG1-CB-CG2	-5.07	100.24	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	181	ILE	CG1-CB-CG2	-5.06	100.27	111.40

There are no chirality outliers.

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	1708	0	1672	54	0
1	B	1708	0	1672	69	0
1	C	1708	0	1672	59	0
1	D	1708	0	1672	70	0
2	A	24	0	22	1	0
2	B	24	0	22	2	0
2	C	24	0	22	1	0
2	D	24	0	22	1	0
3	A	74	0	0	3	0
3	B	48	0	0	3	0
3	C	67	0	0	2	0
3	D	57	0	0	2	0
All	All	7174	0	6776	249	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 18.

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:D:49:PRO:HG3	1:D:114:LEU:HD11	1.46	0.98
1:C:59:LEU:HD22	1:C:62:ILE:HD11	1.51	0.92
1:D:63:PRO:HD2	1:D:63(C):LEU:HD12	1.53	0.91
1:B:230:ARG:HG2	1:B:233:LEU:HD13	1.56	0.86
1:D:123:LEU:HD23	1:D:209:ILE:HD11	1.60	0.83
1:B:77:GLU:HB2	1:B:80:GLN:HG3	1.63	0.81
1:C:95:ASP:HB3	1:C:100:LEU:HB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ARG:HA	1:A:151:PRO:HA	1.63	0.79
1:A:90:LEU:HD22	1:A:104:LEU:HG	1.69	0.74
1:C:49:PRO:HG3	1:C:114:LEU:HD11	1.69	0.74
1:B:63:PRO:HB2	1:B:63(C):LEU:HD13	1.69	0.73
1:C:90:LEU:HG	1:C:104:LEU:HD12	1.70	0.72
1:D:77:GLU:HB2	1:D:80:GLN:NE2	2.05	0.71
1:D:105:LEU:HD23	1:D:241:THR:HG21	1.72	0.71
1:C:57:HIS:CE1	1:C:195:SER:HB3	2.26	0.70
1:B:166:PHE:HD2	1:C:165:PHE:HE1	1.39	0.70
1:D:101:ASN:H	1:D:179:HIS:HE1	1.40	0.70
1:A:30:MET:SD	1:A:139:MET:HE3	2.32	0.69
1:B:222:ARG:HG2	1:B:222:ARG:HH11	1.57	0.69
1:A:198:PRO:HB3	1:A:209:ILE:HD12	1.73	0.69
1:C:65:ASN:HD21	1:C:82:HIS:HB3	1.58	0.67
1:D:49:PRO:HG3	1:D:114:LEU:CD1	2.23	0.67
1:B:86:ALA:HB2	1:B:109:SER:HA	1.76	0.66
1:D:77:GLU:HB2	1:D:80:GLN:HE21	1.57	0.65
1:B:184:PHE:CE2	1:B:186:PRO:HA	2.31	0.65
1:D:123:LEU:CD2	1:D:209:ILE:HD11	2.26	0.65
1:C:190:ILE:HD12	1:C:213:ASP:HB3	1.78	0.65
1:C:59:LEU:CD2	1:C:62:ILE:HD11	2.27	0.64
1:C:187:LYS:HG2	1:C:220(A):ALA:HB1	1.79	0.63
1:D:51:PHE:CE2	1:D:107:GLN:HG3	2.34	0.62
1:A:101:ASN:H	1:A:179:HIS:HE1	1.46	0.62
1:B:62:ILE:HD13	1:B:64:VAL:HG22	1.82	0.62
1:D:105:LEU:HD23	1:D:241:THR:CG2	2.29	0.62
1:B:49:PRO:HG3	1:B:114:LEU:HD11	1.81	0.62
1:D:77:GLU:HB2	1:D:80:GLN:HG3	1.82	0.62
1:A:137:LEU:HD12	1:A:159:ASN:HA	1.82	0.62
1:A:101:ASN:H	1:A:179:HIS:CE1	2.18	0.61
1:C:74:ARG:HD2	1:C:153:GLN:NE2	2.16	0.60
1:D:23:GLN:HA	1:D:23:GLN:NE2	2.16	0.60
1:D:144:VAL:HG13	1:D:152:ALA:HB2	1.82	0.60
1:B:65:ASN:HD21	1:B:82:HIS:HB3	1.65	0.60
1:D:101:ASN:H	1:D:179:HIS:CE1	2.19	0.60
1:A:27:ARG:HB3	1:A:139:MET:HE1	1.84	0.59
1:C:53:LEU:HD23	1:C:209:ILE:HD13	1.84	0.59
1:B:230:ARG:CG	1:B:233:LEU:HD13	2.31	0.59
1:A:239:ARG:HD3	3:A:301:HOH:O	2.03	0.59
1:C:143:ARG:HA	1:C:151:PRO:HA	1.84	0.59
1:C:239:ARG:O	1:C:243:ARG:HD2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186(A):ARG:HG3	1:A:186(B):ARG:HD3	1.85	0.58
1:D:59:LEU:HD22	1:D:104:LEU:HD21	1.86	0.58
1:D:135:GLN:HA	1:D:135:GLN:HE21	1.67	0.58
1:A:48:HIS:HB3	1:A:51:PHE:HB2	1.84	0.58
1:D:52:VAL:HG21	1:D:66:VAL:HG11	1.84	0.58
1:D:238:ILE:O	1:D:242:LEU:HD13	2.04	0.58
1:D:144:VAL:CG1	1:D:152:ALA:HB2	2.34	0.58
1:A:16:ILE:N	1:A:194:ASP:OD2	2.37	0.58
1:C:62:ILE:HD13	1:C:64:VAL:CG2	2.34	0.57
1:C:95:ASP:CB	1:C:100:LEU:HB2	2.35	0.57
1:C:63(A):GLN:NE2	1:C:85:VAL:HG12	2.19	0.57
1:D:23:GLN:HA	1:D:23:GLN:HE21	1.69	0.57
1:A:186(A):ARG:CG	1:A:186(B):ARG:HD3	2.34	0.57
1:D:45:THR:OG1	1:D:198:PRO:HB3	2.04	0.57
1:C:75:THR:HG22	1:C:76:GLN:H	1.70	0.56
1:B:200:ILE:HD13	2:B:245:FUC:H62	1.87	0.56
1:C:77:GLU:HB2	1:C:80:GLN:HG3	1.88	0.56
1:C:59:LEU:HD22	1:C:62:ILE:CD1	2.31	0.56
1:D:19:GLY:HA2	1:D:158:LEU:HD13	1.86	0.56
1:D:47:ILE:HG12	1:D:123:LEU:HD21	1.87	0.56
1:B:63:PRO:HB2	1:B:63(C):LEU:CD1	2.36	0.56
1:A:51:PHE:CD2	1:A:242:LEU:HD22	2.42	0.55
1:B:16:ILE:N	1:B:194:ASP:OD2	2.40	0.55
1:D:71:HIS:CD2	1:D:154:VAL:HG22	2.41	0.55
1:A:234:TYR:O	1:A:238:ILE:HG13	2.05	0.55
1:D:28:PRO:HG2	1:D:119:ALA:HB3	1.89	0.55
1:B:93:ASN:N	1:B:93:ASN:OD1	2.40	0.55
1:C:187:LYS:HE3	1:C:220(A):ALA:O	2.06	0.54
1:B:197:GLY:HA3	3:B:247:HOH:O	2.08	0.54
1:D:57:HIS:NE2	1:D:195:SER:HB3	2.22	0.54
1:C:232:ALA:HA	1:C:235:VAL:HG23	1.90	0.54
1:A:124:PRO:HD3	1:A:209:ILE:O	2.07	0.54
1:B:27:ARG:HG2	1:B:139:MET:SD	2.48	0.54
1:C:207:GLY:H	2:C:245:FUC:HO4	1.56	0.54
1:D:77:GLU:CB	1:D:80:GLN:HG3	2.38	0.53
1:B:95:ASP:HB3	1:B:100:LEU:HB2	1.88	0.53
1:A:197:GLY:HA3	3:A:248:HOH:O	2.09	0.53
1:C:38(A):ASN:HB3	1:C:39:SER:HB3	1.90	0.53
1:A:229:THR:HG23	3:A:258:HOH:O	2.09	0.53
1:D:34:GLN:HG2	1:D:40:HIS:HA	1.89	0.53
1:C:73:VAL:HG22	1:C:153:GLN:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:HIS:CE1	1:A:195:SER:HB3	2.43	0.53
1:D:187:LYS:HA	1:D:222:ARG:HD2	1.90	0.53
1:A:168:CYS:SG	1:A:177:ARG:N	2.81	0.53
1:C:137:LEU:HD12	1:C:158:LEU:O	2.09	0.52
1:A:58:CYS:C	1:A:59:LEU:HD12	2.30	0.52
1:D:60:ARG:O	1:D:62:ILE:HD12	2.09	0.52
1:B:94:TYR:CE2	1:B:96:ALA:HB2	2.44	0.52
1:A:35:MET:HB2	1:A:39:SER:OG	2.09	0.52
1:C:36:ARG:HH11	1:C:36:ARG:HB3	1.73	0.52
1:C:210:GLN:NE2	3:C:306:HOH:O	2.40	0.52
1:A:47:ILE:HD12	1:A:242:LEU:HD11	1.92	0.52
1:D:16:ILE:HD13	1:D:194:ASP:OD2	2.09	0.52
1:D:19:GLY:CA	1:D:158:LEU:HD13	2.40	0.51
1:D:59:LEU:HD22	1:D:104:LEU:CD2	2.41	0.51
1:B:200:ILE:HD12	1:B:200:ILE:O	2.11	0.51
1:B:27:ARG:HD3	1:B:157:GLU:OE1	2.11	0.51
1:B:34:GLN:HG2	1:B:40:HIS:HA	1.93	0.51
1:D:234:TYR:O	1:D:238:ILE:HG13	2.11	0.51
1:A:85:VAL:HG13	1:A:106:ILE:HG23	1.91	0.51
1:A:186(A):ARG:HG3	1:A:186(B):ARG:N	2.25	0.51
1:B:183:THR:HG1	1:B:228:PHE:HE1	1.59	0.51
1:B:180:ASN:O	1:B:230:ARG:NH1	2.45	0.50
1:D:104:LEU:HD23	1:D:106:ILE:HG13	1.92	0.50
1:B:45:THR:OG1	1:B:198:PRO:HG3	2.11	0.50
1:A:49:PRO:HG3	1:A:114:LEU:HD11	1.93	0.50
1:C:71:HIS:O	1:C:154:VAL:HA	2.12	0.50
1:D:59:LEU:CD2	1:D:88:VAL:HG11	2.41	0.50
1:C:186(B):ARG:HH11	1:C:186(B):ARG:HG2	1.77	0.50
1:D:57:HIS:CE1	1:D:195:SER:HB3	2.47	0.49
1:C:103:ILE:HD13	1:C:234:TYR:CD2	2.47	0.49
1:C:213:ASP:OD1	1:C:213:ASP:N	2.44	0.49
1:D:16:ILE:N	1:D:194:ASP:OD2	2.45	0.49
1:A:65:ASN:HD21	1:A:82:HIS:HB3	1.77	0.49
1:C:105:LEU:HD11	1:C:238:ILE:HG23	1.93	0.49
1:A:131:PRO:O	1:A:134:THR:HG23	2.13	0.49
1:C:58:CYS:C	1:C:59:LEU:HD23	2.33	0.49
1:B:144:VAL:CG2	1:B:148:ASP:HB3	2.42	0.49
1:B:200:ILE:CD1	2:B:245:FUC:H62	2.43	0.49
1:A:36:ARG:HG2	1:A:65:ASN:HB2	1.94	0.49
1:B:182:CYS:HB3	1:B:225:PRO:HB2	1.94	0.49
1:C:197:GLY:HA3	3:C:264:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:TYR:HE1	1:A:139:MET:HE2	1.78	0.48
1:D:59:LEU:HD23	1:D:88:VAL:HG11	1.95	0.48
1:A:90:LEU:HD22	1:A:104:LEU:CG	2.40	0.48
1:B:36:ARG:NH1	1:B:84:SER:HB3	2.28	0.48
1:B:67:VAL:HG22	1:B:82:HIS:ND1	2.29	0.48
1:B:51:PHE:CD2	1:B:242:LEU:HD22	2.48	0.48
1:C:38(A):ASN:HB3	1:C:39:SER:CB	2.43	0.48
1:D:200:ILE:O	2:D:245:FUC:H4	2.13	0.48
1:B:48:HIS:HB3	1:B:51:PHE:HB2	1.95	0.48
1:B:70:ALA:HA	1:B:77:GLU:OE1	2.14	0.47
1:D:56:ALA:HA	1:D:104:LEU:HD13	1.97	0.47
1:B:89:PHE:HB2	1:B:105:LEU:HB2	1.96	0.47
1:B:71:HIS:O	1:B:154:VAL:HA	2.14	0.47
1:B:222:ARG:NH1	1:B:222:ARG:HG2	2.27	0.47
1:C:211:GLY:HA2	1:C:229:THR:O	2.14	0.47
1:A:68:LEU:HD12	1:A:83:PHE:CE1	2.49	0.47
1:D:19:GLY:HA2	1:D:158:LEU:CD1	2.44	0.47
1:B:230:ARG:O	1:B:233:LEU:HB2	2.15	0.47
1:B:83:PHE:CZ	1:B:112:ALA:HA	2.49	0.47
1:C:69:GLY:HA2	1:C:117:SER:O	2.14	0.47
1:A:21:GLU:OE2	1:A:71:HIS:NE2	2.40	0.47
1:B:59:LEU:HG	1:B:62:ILE:HD11	1.97	0.47
1:D:212:ILE:HD12	1:D:231:VAL:HG22	1.97	0.47
1:A:165:PHE:CZ	1:D:165:PHE:HB2	2.51	0.46
1:D:197:GLY:HA3	3:D:248:HOH:O	2.16	0.46
1:D:45:THR:HG22	1:D:47:ILE:CD1	2.46	0.46
1:A:27:ARG:O	1:A:30:MET:HB2	2.14	0.46
1:A:51:PHE:CE1	1:A:107:GLN:HB2	2.50	0.46
1:A:57:HIS:NE2	1:A:195:SER:HB3	2.31	0.46
1:B:68:LEU:O	1:B:80:GLN:HA	2.15	0.46
1:B:27:ARG:HG2	1:B:139:MET:CE	2.45	0.46
1:A:77:GLU:HB2	1:A:80:GLN:HG3	1.97	0.46
1:C:57:HIS:NE2	1:C:195:SER:HB3	2.30	0.46
1:A:186(B):ARG:H	1:A:186(B):ARG:HG2	1.45	0.46
1:B:187:LYS:HD2	1:B:220(A):ALA:O	2.15	0.46
1:C:45:THR:OG1	1:C:198:PRO:HB3	2.15	0.46
1:D:182:CYS:HB3	1:D:225:PRO:HB2	1.97	0.46
1:D:17:VAL:HG23	1:D:191:CYS:HB2	1.97	0.46
1:D:83:PHE:CZ	1:D:112:ALA:HA	2.51	0.46
1:C:59:LEU:N	1:C:59:LEU:HD23	2.31	0.45
1:B:184:PHE:HE2	1:B:186:PRO:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:LYS:CG	1:C:220(A):ALA:HB1	2.44	0.45
1:D:208:ILE:HD13	3:D:295:HOH:O	2.16	0.45
1:A:56:ALA:HA	1:A:104:LEU:HB2	1.99	0.45
1:C:212:ILE:HB	1:C:229:THR:HB	1.99	0.45
1:A:101:ASN:ND2	1:A:234:TYR:OH	2.44	0.45
1:B:202:ASP:O	1:B:208:ILE:HD12	2.17	0.45
1:A:35:MET:HB3	1:A:35:MET:HE3	1.59	0.45
1:C:186(B):ARG:NH1	1:C:186(B):ARG:HG2	2.32	0.45
1:C:61:ASP:N	1:C:61:ASP:OD1	2.50	0.45
1:B:83:PHE:CB	1:B:108:LEU:HD22	2.46	0.45
1:B:72:ASN:HA	1:B:153:GLN:O	2.17	0.45
1:B:101:ASN:HA	1:B:234:TYR:OH	2.17	0.45
1:C:74:ARG:HD2	1:C:153:GLN:HE21	1.82	0.45
1:A:95:ASP:HB3	1:A:100:LEU:HB2	1.99	0.44
1:A:198:PRO:CB	1:A:209:ILE:HD12	2.45	0.44
1:D:51:PHE:CZ	1:D:107:GLN:HG3	2.52	0.44
1:C:56:ALA:N	1:C:102:ASP:OD1	2.50	0.44
1:D:61:ASP:O	1:D:62:ILE:HG13	2.17	0.44
1:B:100:LEU:HD23	1:B:100:LEU:HA	1.76	0.44
1:B:83:PHE:HB2	1:B:108:LEU:HD22	2.00	0.44
1:B:57:HIS:NE2	1:B:195:SER:HB3	2.33	0.44
1:B:19:GLY:HA2	1:B:158:LEU:HD13	2.00	0.44
1:D:105:LEU:HD12	1:D:105:LEU:HA	1.68	0.44
1:B:77:GLU:HB2	1:B:80:GLN:CG	2.41	0.44
1:B:234:TYR:O	1:B:238:ILE:HG13	2.18	0.44
1:C:223:LEU:HD13	1:C:224:PHE:CZ	2.53	0.44
1:D:230:ARG:HD2	1:D:233:LEU:HD21	1.99	0.44
1:A:186(A):ARG:HB2	1:A:186(A):ARG:HE	1.57	0.43
1:B:185:VAL:HG11	1:B:188:ALA:HB3	1.99	0.43
1:B:137:LEU:HB3	1:B:200:ILE:HD11	2.00	0.43
1:C:95:ASP:O	1:C:99:LYS:N	2.52	0.43
1:A:238:ILE:HD13	1:A:238:ILE:HG21	1.67	0.43
1:C:20:HIS:O	1:C:157:GLU:N	2.40	0.43
1:D:142:GLY:HA2	1:D:193:GLY:HA3	2.00	0.43
1:D:235:VAL:O	1:D:239:ARG:HG3	2.18	0.43
1:B:63:PRO:CB	1:B:63(C):LEU:HD13	2.45	0.43
1:B:137:LEU:HD12	1:B:137:LEU:HA	1.85	0.43
1:D:77:GLU:HA	1:D:78:PRO:HD3	1.82	0.43
1:A:142:GLY:HA2	1:A:193:GLY:HA3	2.01	0.43
1:C:197:GLY:O	1:C:212:ILE:HA	2.19	0.43
1:D:143:ARG:HB3	1:D:191:CYS:SG	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:THR:HG22	1:A:76:GLN:N	2.34	0.43
1:C:198:PRO:HB2	1:C:200:ILE:HD13	2.00	0.42
1:B:113:ASN:HD22	1:B:113:ASN:HA	1.76	0.42
1:D:27:ARG:HB3	1:D:27:ARG:HE	1.70	0.42
1:D:62:ILE:HA	1:D:63:PRO:HD3	1.89	0.42
1:B:242:LEU:N	1:B:242:LEU:HD23	2.34	0.42
1:D:59:LEU:HA	1:D:59:LEU:HD12	1.76	0.42
1:A:208:ILE:HG23	1:A:208:ILE:HD13	1.55	0.42
1:A:100:LEU:HA	1:A:179:HIS:CE1	2.54	0.42
1:C:198:PRO:HB2	1:C:200:ILE:CD1	2.50	0.42
1:C:75:THR:HG22	1:C:76:GLN:N	2.34	0.42
1:D:182:CYS:HB3	1:D:225:PRO:CB	2.50	0.42
1:B:48:HIS:CG	1:B:49:PRO:HD2	2.55	0.41
1:C:223:LEU:HA	1:C:223:LEU:HD23	1.49	0.41
1:B:186(B):ARG:HB2	1:B:186(B):ARG:HE	1.68	0.41
1:D:45:THR:HG21	1:D:209:ILE:HG21	2.01	0.41
1:C:36:ARG:HA	1:C:65:ASN:HB2	2.02	0.41
1:D:60:ARG:HA	1:D:60:ARG:HD2	1.65	0.41
1:C:94:TYR:HA	1:C:101:ASN:HB2	2.03	0.41
1:D:217:ILE:HD11	1:D:227:PHE:CE1	2.56	0.41
1:B:179:HIS:HB2	3:B:273:HOH:O	2.19	0.41
1:D:83:PHE:HZ	1:D:112:ALA:HA	1.85	0.41
1:B:88:VAL:HA	1:B:105:LEU:O	2.20	0.41
1:D:217:ILE:O	1:D:219:GLY:N	2.45	0.41
1:A:68:LEU:O	1:A:80:GLN:HA	2.21	0.41
1:B:83:PHE:HZ	1:B:112:ALA:HA	1.85	0.41
1:C:16:ILE:O	1:C:144:VAL:HG12	2.20	0.41
1:A:142:GLY:N	1:A:194:ASP:OD1	2.51	0.41
1:B:114:LEU:HA	1:B:118:VAL:O	2.20	0.40
1:D:52:VAL:HG21	1:D:66:VAL:CG1	2.49	0.40
1:A:208:ILE:HD12	1:A:208:ILE:HG21	1.74	0.40
1:B:155:LEU:HD12	1:B:155:LEU:HA	1.84	0.40
1:A:207:GLY:N	2:A:245:FUC:O4	2.43	0.40
1:B:166:PHE:HD2	1:C:165:PHE:CE1	2.29	0.40
1:D:29:TYR:HA	1:D:119:ALA:O	2.22	0.40
1:B:27:ARG:HG3	1:B:29:TYR:OH	2.21	0.40
1:B:229:THR:HG23	3:B:291:HOH:O	2.22	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	219/221 (99%)	204 (93%)	14 (6%)	1 (0%)	34	35
1	B	219/221 (99%)	197 (90%)	20 (9%)	2 (1%)	21	19
1	C	219/221 (99%)	201 (92%)	17 (8%)	1 (0%)	34	35
1	D	219/221 (99%)	205 (94%)	13 (6%)	1 (0%)	34	35
All	All	876/884 (99%)	807 (92%)	64 (7%)	5 (1%)	30	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	PRO
1	C	146	ALA
1	D	151	PRO
1	A	150	PRO
1	B	39	SER

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	187/187 (100%)	166 (89%)	21 (11%)	7	6
1	B	187/187 (100%)	161 (86%)	26 (14%)	4	3
1	C	187/187 (100%)	162 (87%)	25 (13%)	5	4
1	D	187/187 (100%)	164 (88%)	23 (12%)	6	5
All	All	748/748 (100%)	653 (87%)	95 (13%)	5	4

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	MET
1	A	35	MET
1	A	60	ARG
1	A	61	ASP
1	A	63(C)	LEU
1	A	74	ARG
1	A	81	GLN
1	A	90	LEU
1	A	92	ASN
1	A	93	ASN
1	A	117	SER
1	A	143	ARG
1	A	148	ASP
1	A	177	ARG
1	A	186(A)	ARG
1	A	186(B)	ARG
1	A	195	SER
1	A	208	ILE
1	A	213	ASP
1	A	221	THR
1	A	223	LEU
1	B	27	ARG
1	B	30	MET
1	B	35	MET
1	B	47	ILE
1	B	50	SER
1	B	60	ARG
1	B	61	ASP
1	B	63(C)	LEU
1	B	76	GLN
1	B	80	GLN
1	B	90	LEU
1	B	93	ASN
1	B	139	MET
1	B	147	HIS
1	B	161	THR
1	B	166	PHE
1	B	177	ARG
1	B	181	ILE
1	B	186(B)	ARG
1	B	187	LYS
1	B	195	SER

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Mol	Chain	Res	Type
1	B	213	ASP
1	B	221	THR
1	B	222	ARG
1	B	230	ARG
1	B	239	ARG
1	C	23	GLN
1	C	34	GLN
1	C	35	MET
1	C	36	ARG
1	C	38(A)	ASN
1	C	61	ASP
1	C	75	THR
1	C	76	GLN
1	C	90	LEU
1	C	92	ASN
1	C	117	SER
1	C	125	GLN
1	C	135	GLN
1	C	147	HIS
1	C	148	ASP
1	C	165	PHE
1	C	177	ARG
1	C	186(A)	ARG
1	C	195	SER
1	C	213	ASP
1	C	214	SER
1	C	223	LEU
1	C	240	SER
1	C	242	LEU
1	C	243	ARG
1	D	16	ILE
1	D	23	GLN
1	D	27	ARG
1	D	35	MET
1	D	36	ARG
1	D	47	ILE
1	D	60	ARG
1	D	63(B)	ARG
1	D	75	THR
1	D	93	ASN
1	D	104	LEU
1	D	113	ASN

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Mol	Chain	Res	Type
1	D	135	GLN
1	D	143	ARG
1	D	154	VAL
1	D	166	PHE
1	D	177	ARG
1	D	186(A)	ARG
1	D	186(B)	ARG
1	D	195	SER
1	D	222	ARG
1	D	224	PHE
1	D	243	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	63(A)	GLN
1	A	65	ASN
1	A	92	ASN
1	A	93	ASN
1	A	101	ASN
1	A	153	GLN
1	A	179	HIS
1	A	210	GLN
1	B	34	GLN
1	B	65	ASN
1	B	76	GLN
1	B	80	GLN
1	B	113	ASN
1	B	210	GLN
1	C	38(A)	ASN
1	C	63(A)	GLN
1	C	65	ASN
1	C	210	GLN
1	D	23	GLN
1	D	48	HIS
1	D	63(A)	GLN
1	D	80	GLN
1	D	87	GLN
1	D	101	ASN
1	D	113	ASN
1	D	135	GLN

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Mol	Chain	Res	Type
1	D	179	HIS
1	D	210	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

8 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$
2	NAG	A	244	1,2	14,14,15	1.47	2 (14%)	15,19,21	1.82	5 (33%)
2	FUC	A	245	2	10,10,11	0.62	0	14,14,16	2.72	9 (64%)
2	NAG	B	244	1,2	14,14,15	1.32	3 (21%)	15,19,21	2.65	9 (60%)
2	FUC	B	245	2	10,10,11	0.77	0	14,14,16	3.02	6 (42%)
2	NAG	C	244	1,2	14,14,15	1.58	1 (7%)	15,19,21	1.45	3 (20%)
2	FUC	C	245	2	10,10,11	0.83	0	14,14,16	1.30	3 (21%)
2	NAG	D	244	1,2	14,14,15	1.66	3 (21%)	15,19,21	1.99	6 (40%)
2	FUC	D	245	2	10,10,11	0.69	0	14,14,16	2.52	7 (50%)

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
2	NAG	A	244	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	245	2	-	0/0/17/20	0/1/1/1
2	NAG	B	244	1,2	-	0/6/23/26	0/1/1/1
2	FUC	B	245	2	-	0/0/17/20	0/1/1/1
2	NAG	C	244	1,2	-	0/6/23/26	0/1/1/1
2	FUC	C	245	2	-	0/0/17/20	0/1/1/1
2	NAG	D	244	1,2	-	0/6/23/26	0/1/1/1
2	FUC	D	245	2	-	0/0/17/20	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	244	NAG	O5-C1	-2.51	1.39	1.43
2	A	244	NAG	O5-C1	-2.42	1.39	1.43
2	D	244	NAG	O5-C1	-2.32	1.39	1.43
2	B	244	NAG	C1-C2	2.06	1.55	1.52
2	D	244	NAG	O7-C7	2.07	1.28	1.23
2	B	244	NAG	C8-C7	2.72	1.56	1.50
2	A	244	NAG	C8-C7	4.00	1.58	1.50
2	C	244	NAG	C8-C7	4.14	1.58	1.50
2	D	244	NAG	C8-C7	4.68	1.60	1.50

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	245	FUC	C1-C2-C3	-4.64	104.05	109.54
2	B	244	NAG	C3-C4-C5	-4.58	102.21	110.20
2	B	244	NAG	O5-C5-C6	-4.50	97.61	107.35
2	D	244	NAG	C1-O5-C5	-4.04	107.12	112.25
2	B	245	FUC	C6-C5-C4	-3.08	107.02	113.08
2	C	244	NAG	O5-C5-C6	-2.95	100.95	107.35
2	B	244	NAG	O4-C4-C3	-2.91	103.79	110.34
2	B	244	NAG	C8-C7-N2	-2.72	110.91	116.11
2	D	244	NAG	O5-C5-C6	-2.58	101.75	107.35
2	A	244	NAG	O5-C5-C6	-2.56	101.80	107.35
2	B	244	NAG	C1-O5-C5	-2.34	109.28	112.25
2	A	245	FUC	C6-C5-C4	-2.23	108.69	113.08
2	A	244	NAG	C1-O5-C5	-2.22	109.44	112.25
2	D	245	FUC	C1-C2-C3	-2.18	106.96	109.54
2	A	245	FUC	C1-C2-C3	-2.07	107.09	109.54
2	D	244	NAG	O3-C3-C4	-2.01	105.81	110.34
2	C	245	FUC	C6-C5-C4	2.04	117.09	113.08
2	B	245	FUC	O2-C2-C1	2.08	113.37	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	245	FUC	C3-C4-C5	2.08	113.23	109.72
2	D	245	FUC	O2-C2-C1	2.20	113.62	109.21
2	C	245	FUC	O4-C4-C3	2.21	115.32	110.34
2	B	244	NAG	O3-C3-C2	2.21	113.50	109.11
2	C	244	NAG	O4-C4-C5	2.23	115.16	109.24
2	B	244	NAG	C6-C5-C4	2.28	118.65	113.02
2	A	245	FUC	O3-C3-C2	2.34	114.22	110.00
2	A	245	FUC	C2-C3-C4	2.39	115.10	111.04
2	D	244	NAG	C2-N2-C7	2.45	126.19	123.04
2	D	245	FUC	C2-C3-C4	2.47	115.24	111.04
2	D	245	FUC	O3-C3-C2	2.63	114.75	110.00
2	A	244	NAG	O4-C4-C5	2.70	116.40	109.24
2	C	245	FUC	C2-C3-C4	2.72	115.65	111.04
2	D	245	FUC	O5-C5-C6	2.79	110.74	106.13
2	A	244	NAG	C2-N2-C7	3.01	126.91	123.04
2	B	245	FUC	C3-C4-C5	3.11	114.95	109.72
2	D	244	NAG	O4-C4-C5	3.11	117.48	109.24
2	A	245	FUC	O2-C2-C1	3.11	115.44	109.21
2	D	244	NAG	C4-C3-C2	3.13	116.09	111.23
2	A	244	NAG	C4-C3-C2	3.35	116.44	111.23
2	D	245	FUC	O4-C4-C3	3.36	117.91	110.34
2	C	244	NAG	C2-N2-C7	3.38	127.38	123.04
2	B	244	NAG	O4-C4-C5	3.43	118.32	109.24
2	B	244	NAG	O7-C7-C8	3.64	128.75	122.06
2	A	245	FUC	O4-C4-C3	3.81	118.92	110.34
2	B	245	FUC	O5-C5-C6	4.35	113.33	106.13
2	A	245	FUC	O5-C5-C6	4.47	113.52	106.13
2	A	245	FUC	O5-C1-C2	5.54	119.84	110.86
2	D	245	FUC	O5-C1-C2	5.64	120.00	110.86
2	B	245	FUC	O5-C1-C2	7.17	122.48	110.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	245	FUC	1	0
2	B	245	FUC	2	0
2	C	245	FUC	1	0
2	D	245	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 [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	221/221 (100%)	-0.57	2 (0%) 85 85	9, 24, 68, 100	0
1	B	221/221 (100%)	-0.54	3 (1%) 78 77	12, 28, 68, 98	0
1	C	221/221 (100%)	-0.52	2 (0%) 85 85	9, 26, 72, 100	0
1	D	221/221 (100%)	-0.50	2 (0%) 85 85	8, 27, 67, 100	0
All	All	884/884 (100%)	-0.53	9 (1%) 84 83	8, 27, 69, 100	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	150	PRO	5.3
1	B	148	ASP	4.3
1	D	147	HIS	3.1
1	C	146	ALA	3.0
1	C	152	ALA	2.5
1	A	147	HIS	2.3
1	A	150	PRO	2.2
1	B	150	PRO	2.2
1	B	147	HIS	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](#)

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(\AA^2)	Q<0.9
2	FUC	C	245	10/11	0.74	0.24	8.82	42,100,100,100	0
2	FUC	D	245	10/11	0.86	0.20	6.03	26,65,100,100	0
2	FUC	A	245	10/11	0.94	0.13	0.67	27,46,100,100	0
2	FUC	B	245	10/11	0.93	0.12	0.18	26,45,83,100	0
2	NAG	B	244	14/15	0.88	0.12	-	33,62,100,100	0
2	NAG	D	244	14/15	0.83	0.18	-	26,92,100,100	0
2	NAG	A	244	14/15	0.87	0.14	-	25,70,100,100	0
2	NAG	C	244	14/15	0.71	0.20	-	47,100,100,100	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.