WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:18 PM GMT

PDB ID   :   4OGA
Title   :   Insulin in complex with Site 1 of the human insulin receptor
Authors   :   Lawrence, M.C.; Menting, J.G.
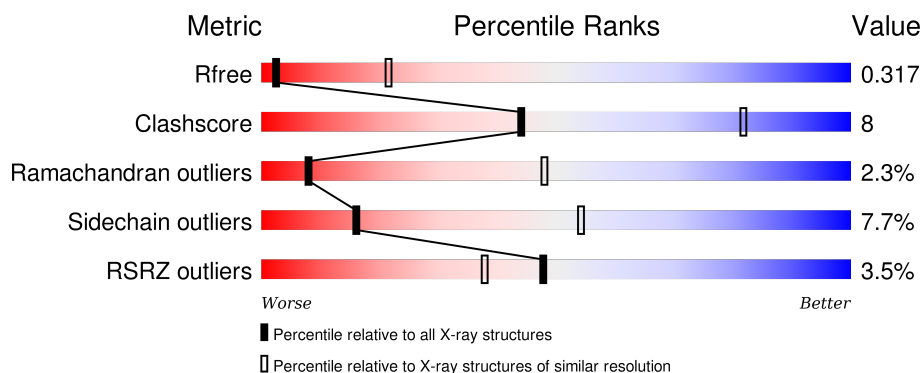Deposited on :   2014-01-15
Resolution :   3.50 Å(reported)

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 3.50 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	Percentile Ranks	Value
Rfree		0.317
Clashscore		8
Ramachandran outliers		2.3%
Sidechain outliers		7.7%
RSRZ outliers		3.5%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	21	5% / 38% / 48% / 14%
2	B	30	3% / 43% / 23% · / 30%
3	C	118	8% / 77% / 21% ·
4	D	114	5% / 72% / 25% ·
5	E	317	% / 79% / 11% · 9%

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Mol	Chain	Length	Quality of chain
6	F	16	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 4693 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 Insulin A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	S	0	0	0
			162	99	25	34	4			

- Molecule 2 is a protein called Insulin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	21	Total	C	N	O	S	0	0	0
			165	108	26	29	2			

- Molecule 3 is a protein called monoclonal antibody fab 83-7 fragment - heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	118	Total	C	N	O	S	0	0	0
			904	568	153	178	5			

- Molecule 4 is a protein called monoclonal antibody fab 83-7 fragment - light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	114	Total	C	N	O	S	0	0	0
			891	565	149	173	4			

- Molecule 5 is a protein called Insulin receptor domains L1-CR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	288	Total	C	N	O	S	0	0	0
			2301	1449	397	423	32			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	144	HIS	TYR	VARIANT	UNP P06213
E	311	SER	-	EXPRESSION TAG	UNP P06213

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Chain	Residue	Modelled	Actual	Comment	Reference
E	312	SER	-	EXPRESSION TAG	UNP P06213
E	313	SER	-	EXPRESSION TAG	UNP P06213
E	314	LEU	-	EXPRESSION TAG	UNP P06213
E	315	VAL	-	EXPRESSION TAG	UNP P06213
E	316	PRO	-	EXPRESSION TAG	UNP P06213
E	317	ARG	-	EXPRESSION TAG	UNP P06213

• Molecule 6 is a protein called Insulin receptor alpha-CT peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	F	15	129	86	21	22	0	0	0

• Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
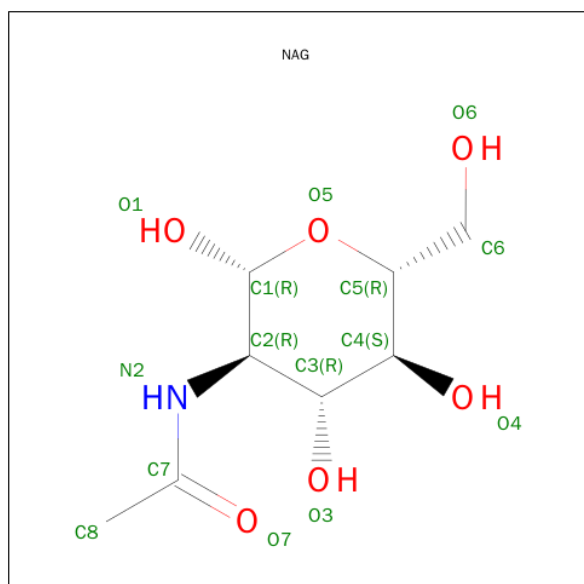
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	E	1	14	8	1	5	0	0
7	E	1	14	8	1	5	0	0
7	E	1	14	8	1	5	0	0

• Molecule 8 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 9 is a polymer of unknown type called SUGAR (4-MER).

| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	E	4	Total	C	N	O	0	0
			49	28	2	19		

3 Residue-property plots ⓘ

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: Insulin A chain
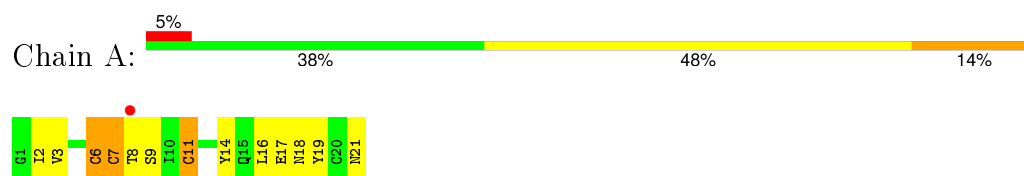
Chain A:

- Molecule 2: Insulin B chain
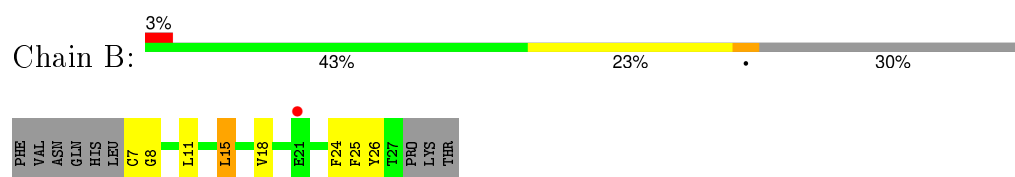
Chain B:

- Molecule 3: monoclonal antibody fab 83-7 fragment - heavy chain
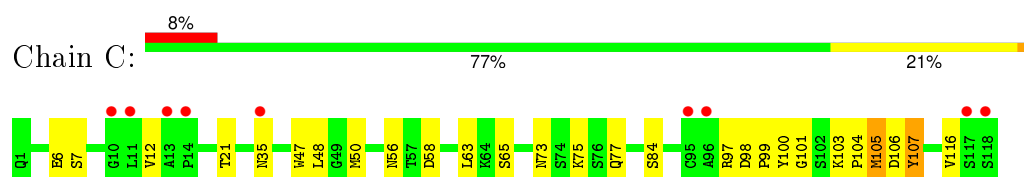
Chain C:

- Molecule 4: monoclonal antibody fab 83-7 fragment - light chain

Chain D:
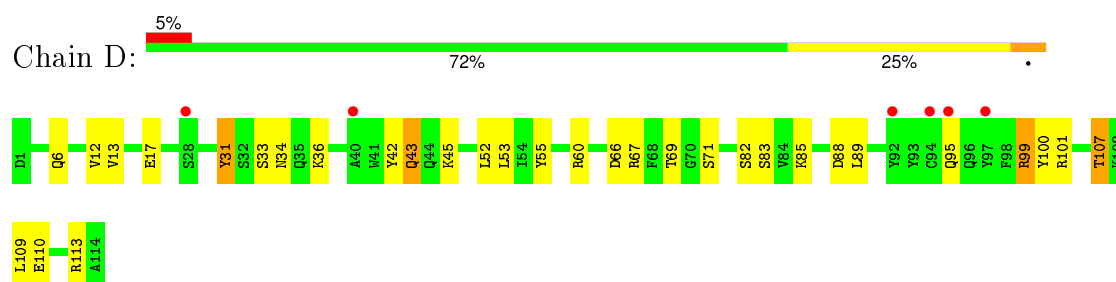
- Molecule 5: Insulin receptor domains L1-CR

Chain E:

T194 I195 E211 K224 C228 R229 N230 R236 C241 H247 F248 Q249 D250 Q260 K265 CYS LYS ASN SER ARG ARG GLN GLY CYS HIS Q276 Y277 V278 N282 E287 M294 L299 K310 SER SER SER LEU VAL PRO ARG
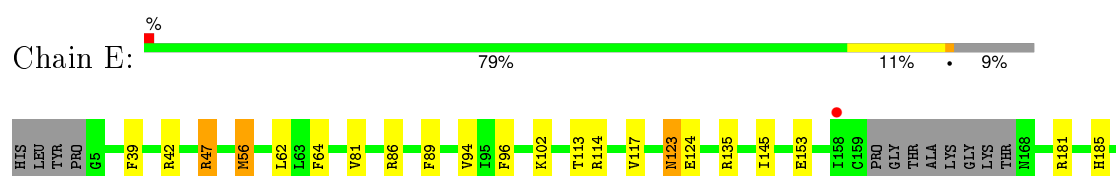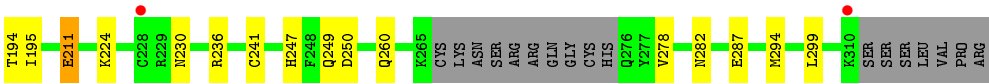
• Molecule 6: Insulin receptor alpha-CT peptide

Chain F:

50%   13%   31%   6%

THR F705 E706 D707 Y708 L709 V712 V713 R717 P718 S719

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, α, β, γ	169.04Å 169.04Å 169.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.78 – 3.50 19.65 – 3.50	Depositor EDS
% Data completeness (in resolution range)	93.3 (19.78-3.50) 93.6 (19.65-3.50)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	0.82 (at 3.52Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.264 , 0.284 0.281 , 0.317	Depositor DCC
R_{free} test set	940 reflections (4.93%)	DCC
Wilson B-factor (Å^2)	212.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 195.7	EDS
Estimated twinning fraction	0.056 for l,-k,h	Xtriage
L-test for twinning[2]	$<|L|> = 0.46$, $<L^2> = 0.29$	Xtriage
Outliers	0 of 19092 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4693	wwPDB-VP
Average B, all atoms (Å^2)	238.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BMA, NAG, 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	0.68	0/163	1.05	0/220
2	B	0.61	0/169	0.86	0/227
3	C	0.49	0/926	0.78	0/1258
4	D	0.52	0/910	0.73	1/1228 (0.1%)
5	E	0.51	0/2355	0.80	0/3192
6	F	0.66	0/134	0.91	0/183
All	All	0.52	0/4657	0.80	1/6308 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	82	SER	C-N-CA	5.24	134.80	121.70

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	162	0	149	7	0
2	B	165	0	152	10	0
3	C	904	0	879	28	0
4	D	891	0	882	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	2301	0	2201	20	0
6	F	129	0	119	3	0
7	E	42	0	39	0	0
8	E	50	0	43	0	0
9	E	49	0	43	0	0
All	All	4693	0	4507	74	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 8.

All (74) 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:C:99:PRO:HG2	3:C:103:LYS:HB2	1.45	0.94
2:B:24:PHE:HE2	5:E:39:PHE:HE2	1.13	0.90
4:D:60:ARG:HH11	4:D:66:ASP:HA	1.38	0.89
4:D:99:ARG:HA	4:D:99:ARG:HE	1.39	0.88
4:D:12:VAL:HG12	4:D:110:GLU:HB2	1.59	0.85
2:B:24:PHE:CE2	5:E:39:PHE:HE2	1.98	0.82
4:D:43:GLN:HB2	4:D:53:LEU:HD11	1.68	0.76
3:C:35:ASN:HD22	3:C:47:TRP:HE1	1.36	0.74
1:A:2:ILE:HG12	2:B:11:LEU:HD21	1.72	0.72
3:C:99:PRO:HD2	3:C:103:LYS:O	1.92	0.70
2:B:24:PHE:HE2	5:E:39:PHE:CE2	2.05	0.68
5:E:102:LYS:HD3	5:E:124:GLU:HB3	1.76	0.66
3:C:58:ASP:HB3	4:D:100:TYR:HD1	1.60	0.64
3:C:47:TRP:CE3	4:D:101:ARG:O	2.51	0.63
3:C:104:PRO:HG2	4:D:55:TYR:HB3	1.81	0.62
6:F:709:LEU:O	6:F:713:VAL:HB	2.00	0.61
3:C:47:TRP:CD2	4:D:101:ARG:O	2.53	0.61
4:D:60:ARG:NH1	4:D:66:ASP:HA	2.14	0.60
5:E:241:CYS:H	5:E:247:HIS:CE1	2.21	0.59
3:C:104:PRO:HA	4:D:101:ARG:HH12	1.68	0.59
3:C:101:GLY:H	5:E:236:ARG:NH2	2.04	0.56
1:A:16:LEU:HG	2:B:15:LEU:HD12	1.87	0.55
3:C:47:TRP:CE2	4:D:101:ARG:HB2	2.42	0.55
4:D:31:TYR:HE1	5:E:282:ASN:OD1	1.89	0.55
3:C:106:ASP:O	3:C:107:TYR:HB2	2.07	0.54
3:C:105:MET:HB2	4:D:42:TYR:OH	2.07	0.54
2:B:15:LEU:HD23	2:B:24:PHE:CE1	2.43	0.53
3:C:97:ARG:O	3:C:105:MET:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:CYS:C	1:A:9:SER:H	2.12	0.53
5:E:62:LEU:HD13	5:E:94:VAL:CG1	2.39	0.52
4:D:99:ARG:NE	4:D:99:ARG:HA	2.13	0.52
2:B:25:PHE:CD1	2:B:26:TYR:N	2.78	0.52
1:A:14:TYR:O	1:A:17:GLU:N	2.37	0.51
4:D:67:ARG:NH2	4:D:88:ASP:OD1	2.43	0.51
1:A:3:VAL:HG21	6:F:707:ASP:O	2.12	0.48
5:E:56:MET:HG3	5:E:81:VAL:HB	1.95	0.48
3:C:48:LEU:HD22	3:C:63:LEU:HD11	1.95	0.48
4:D:89:LEU:HD12	4:D:109:LEU:O	2.13	0.48
3:C:35:ASN:ND2	4:D:101:ARG:HD2	2.30	0.47
3:C:104:PRO:CG	4:D:55:TYR:HB3	2.44	0.47
4:D:34:ASN:ND2	4:D:36:LYS:HG3	2.30	0.46
2:B:15:LEU:HD23	2:B:24:PHE:HE1	1.80	0.46
3:C:106:ASP:O	3:C:107:TYR:CB	2.63	0.46
3:C:105:MET:CE	4:D:95:GLN:HE22	2.28	0.46
4:D:43:GLN:CB	4:D:53:LEU:HD11	2.43	0.45
4:D:31:TYR:HE1	5:E:282:ASN:CG	2.20	0.45
4:D:60:ARG:HE	4:D:60:ARG:HB2	1.58	0.45
5:E:64:PHE:HA	5:E:96:PHE:O	2.18	0.44
3:C:47:TRP:NE1	4:D:101:ARG:HB2	2.33	0.44
5:E:117:VAL:HG12	5:E:145:ILE:HD11	2.00	0.44
3:C:99:PRO:HG2	3:C:103:LYS:CB	2.33	0.44
5:E:47:ARG:NH1	5:E:47:ARG:HB3	2.33	0.44
4:D:6:GLN:NE2	4:D:107:THR:HG23	2.33	0.44
5:E:181:ARG:HA	5:E:181:ARG:HD3	1.82	0.44
3:C:21:THR:HG21	3:C:77:GLN:HE21	1.83	0.43
5:E:123:ASN:HD22	5:E:123:ASN:H	1.66	0.43
3:C:58:ASP:HB3	4:D:100:TYR:CD1	2.48	0.43
3:C:47:TRP:HZ2	3:C:50:MET:HG2	1.83	0.43
5:E:211:GLU:OE2	5:E:230:ASN:ND2	2.51	0.43
2:B:24:PHE:CE2	5:E:39:PHE:CE2	2.91	0.43
4:D:43:GLN:NE2	4:D:45:LYS:HG3	2.33	0.43
3:C:75:LYS:O	3:C:77:GLN:HG3	2.18	0.43
5:E:260:GLN:HA	5:E:299:LEU:HD11	2.01	0.42
3:C:12:VAL:O	3:C:116:VAL:HA	2.20	0.42
6:F:708:TYR:O	6:F:712:VAL:HG12	2.21	0.41
4:D:13:VAL:CG2	4:D:17:GLU:HB3	2.51	0.41
3:C:35:ASN:HD21	4:D:101:ARG:HD2	1.85	0.41
3:C:6:GLU:OE1	3:C:6:GLU:N	2.52	0.41
1:A:6:CYS:HB3	1:A:11:CYS:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLU:HA	2:B:18:VAL:HG11	2.01	0.41
5:E:278:VAL:CG1	5:E:294:MET:HG3	2.51	0.41
3:C:104:PRO:HD2	4:D:52:LEU:HD21	2.04	0.40
5:E:195:ILE:HG13	5:E:195:ILE:H	1.72	0.40
4:D:99:ARG:CA	4:D:99:ARG:HE	2.23	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	19/21 (90%)	11 (58%)	6 (32%)	2 (10%)	1	8
2	B	19/30 (63%)	16 (84%)	2 (10%)	1 (5%)	2	25
3	C	116/118 (98%)	108 (93%)	3 (3%)	5 (4%)	3	31
4	D	112/114 (98%)	104 (93%)	6 (5%)	2 (2%)	11	53
5	E	282/317 (89%)	261 (93%)	19 (7%)	2 (1%)	26	72
6	F	13/16 (81%)	11 (85%)	1 (8%)	1 (8%)	1	14
All	All	561/616 (91%)	511 (91%)	37 (7%)	13 (2%)	8	48

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
2	B	8	GLY
3	C	100	TYR
3	C	105	MET
4	D	33	SER
4	D	83	SER
5	E	153	GLU

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Mol	Chain	Res	Type
1	A	19	TYR
3	C	84	SER
5	E	114	ARG
6	F	717	ARG
3	C	65	SER
3	C	107	TYR

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	20/20 (100%)	15 (75%)	5 (25%)	1	4
2	B	17/26 (65%)	15 (88%)	2 (12%)	6	31
3	C	101/101 (100%)	97 (96%)	4 (4%)	38	75
4	D	100/100 (100%)	92 (92%)	8 (8%)	15	52
5	E	268/293 (92%)	253 (94%)	15 (6%)	26	66
6	F	15/16 (94%)	9 (60%)	6 (40%)	0	1
All	All	521/556 (94%)	481 (92%)	40 (8%)	16	54

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	CYS
1	A	7	CYS
1	A	8	THR
1	A	11	CYS
1	A	21	ASN
2	B	7	CYS
2	B	15	LEU
3	C	7	SER
3	C	56	ASN
3	C	73	ASN
3	C	98	ASP
4	D	31	TYR

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Mol	Chain	Res	Type
4	D	43	GLN
4	D	69	THR
4	D	71	SER
4	D	85	LYS
4	D	99	ARG
4	D	107	THR
4	D	113	ARG
5	E	42	ARG
5	E	47	ARG
5	E	56	MET
5	E	86	ARG
5	E	89	PHE
5	E	113	THR
5	E	123	ASN
5	E	135	ARG
5	E	185	HIS
5	E	194	THR
5	E	211	GLU
5	E	224	LYS
5	E	249	GLN
5	E	250	ASP
5	E	287	GLU
6	F	705	PHE
6	F	707	ASP
6	F	709	LEU
6	F	712	VAL
6	F	713	VAL
6	F	717	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
3	C	3	GLN
3	C	35	ASN
3	C	86	GLN
4	D	43	GLN
4	D	95	GLN
5	E	32	HIS
5	E	123	ASN
5	E	152	ASN
5	E	247	HIS

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Mol	Chain	Res	Type
5	E	281	ASN

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)

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
8	NAG	E	503	8,5	14,14,15	0.32	0	15,19,21	1.23	2 (13%)
8	NAG	E	504	8	14,14,15	0.42	0	15,19,21	0.45	0
8	BMA	E	505	8	11,11,12	0.21	0	14,15,17	0.76	0
8	MAN	E	506	8	11,11,12	0.31	0	14,15,17	0.61	0
9	NAG	E	508	9,5	14,14,15	0.33	0	15,19,21	0.70	0
9	FUC	E	509	9	10,10,11	0.43	0	14,14,16	0.89	1 (7%)
9	NAG	E	510	9	14,14,15	0.20	0	15,19,21	0.65	0
9	BMA	E	511	9	11,11,12	0.29	0	14,15,17	0.69	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
8	NAG	E	503	8,5	-	0/6/23/26	0/1/1/1
8	NAG	E	504	8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	E	505	8	-	0/2/19/22	0/1/1/1
8	MAN	E	506	8	-	0/2/19/22	0/1/1/1
9	NAG	E	508	9,5	-	0/6/23/26	0/1/1/1
9	FUC	E	509	9	-	0/0/17/20	0/1/1/1
9	NAG	E	510	9	-	0/6/23/26	0/1/1/1
9	BMA	E	511	9	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	503	NAG	O4-C4-C3	2.11	115.09	110.34
9	E	509	FUC	C1-O5-C5	2.84	116.77	112.38
8	E	503	NAG	C1-O5-C5	3.40	116.57	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

3 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	#$|Z| > 2$
7	NAG	E	501	5	14,14,15	0.35	0	15,19,21	0.90	1 (6%)
7	NAG	E	502	5	14,14,15	0.30	0	15,19,21	0.75	1 (6%)
7	NAG	E	507	5	14,14,15	0.35	0	15,19,21	0.91	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	E	501	5	-	0/6/23/26	0/1/1/1
7	NAG	E	502	5	-	0/6/23/26	0/1/1/1
7	NAG	E	507	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	502	NAG	C1-O5-C5	2.48	115.40	112.25
7	E	507	NAG	C2-N2-C7	2.64	126.44	123.04
7	E	501	NAG	C1-O5-C5	3.28	116.41	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	21/21 (100%)	-0.25	1 (4%)	34	27	221, 244, 251, 260	0
2	B	21/30 (70%)	-0.47	1 (4%)	34	27	214, 232, 258, 277	0
3	C	118/118 (100%)	0.25	9 (7%)	17	14	195, 266, 299, 304	0
4	D	114/114 (100%)	0.02	6 (5%)	30	23	198, 230, 265, 276	0
5	E	288/317 (90%)	-0.20	3 (1%)	84	76	183, 225, 279, 300	0
6	F	15/16 (93%)	-0.09	0	100	100	196, 219, 265, 277	0
All	All	577/616 (93%)	-0.07	20 (3%)	48	38	183, 235, 289, 304	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	117	SER	6.9
3	C	96	ALA	5.6
4	D	40	ALA	5.2
3	C	35	ASN	4.7
3	C	95	CYS	4.5
5	E	228	CYS	3.4
3	C	118	SER	3.3
4	D	95	GLN	3.3
3	C	11	LEU	3.0
3	C	14	PRO	2.8
3	C	13	ALA	2.7
4	D	97	TYR	2.6
5	E	310	LYS	2.6
2	B	21	GLU	2.3
3	C	10	GLY	2.3
1	A	8	THR	2.2
5	E	158	ILE	2.2
4	D	94	CYS	2.2
4	D	28	SER	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	92	TYR	2.2

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	NAG	E	503	14/15	0.84	0.21	-0.37	211,215,221,224	0
8	MAN	E	506	11/12	0.90	0.49	-	264,266,270,273	0
8	BMA	E	505	11/12	0.85	0.30	-	250,256,261,263	0
8	NAG	E	504	14/15	0.94	0.24	-	228,234,239,243	0
9	BMA	E	511	11/12	0.67	0.44	-	310,315,316,316	0
9	NAG	E	510	14/15	0.88	0.38	-	294,297,303,307	0
9	FUC	E	509	10/11	0.93	0.20	-	259,265,268,270	0
9	NAG	E	508	14/15	0.87	0.20	-	263,274,279,288	0

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
7	NAG	E	507	14/15	0.88	0.21	-0.89	244,256,262,265	0
7	NAG	E	502	14/15	0.81	0.22	-	282,293,297,297	0
7	NAG	E	501	14/15	0.83	0.32	-	294,297,299,300	0

6.5 Other polymers (i)

There are no such residues in this entry.