Full wwPDB X-ray Structure Validation Report (i)

Mar 22, 2016 – 04:14 PM EDT

PDB ID	:	4ZXB
Title	:	Structure of the human insulin receptor ectodomain, IRDeltabeta construct, in complex with four Fab molecules
Authors	:	Croll, T.; Smith, B.J.; Margetts, M.B.; Whittaker, J.; Weiss, M.A.; Ward, C.W.; Lawrence, M.C.
Deposited on	:	2015-05-20
Resolution	:	3.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

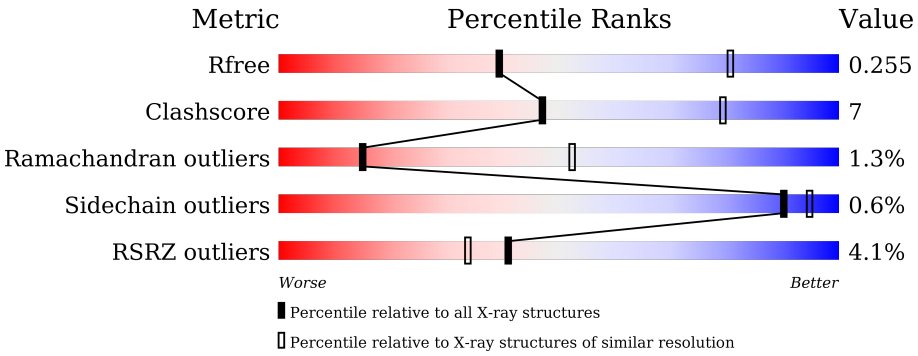
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 <=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	219	85% 12% ·
2	B	219	% 86% 12% ·
3	C	220	9% 67% 17% 15%
4	D	214	8% 77% 7% 15%
5	E	894	3% 71% 18% · 11%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12918 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 Fab 83-7 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1611	1018	266	319	8			

- Molecule 2 is a protein called Fab 83-7 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1706	1068	286	345	7			

- Molecule 3 is a protein called Fab 83-14 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	187	Total	C	N	O	S	0	0	0
			1427	917	234	271	5			

- Molecule 4 is a protein called Fab 83-14 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	182	Total	C	N	O	S	0	0	0
			1384	865	227	287	5			

- Molecule 5 is a protein called Insulin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	800	Total	C	N	O	S	0	0	0
			6473	4106	1117	1202	48			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	144	HIS	TYR	engineered mutation	UNP P06213
E	?	-	ARG	deletion	UNP P06213

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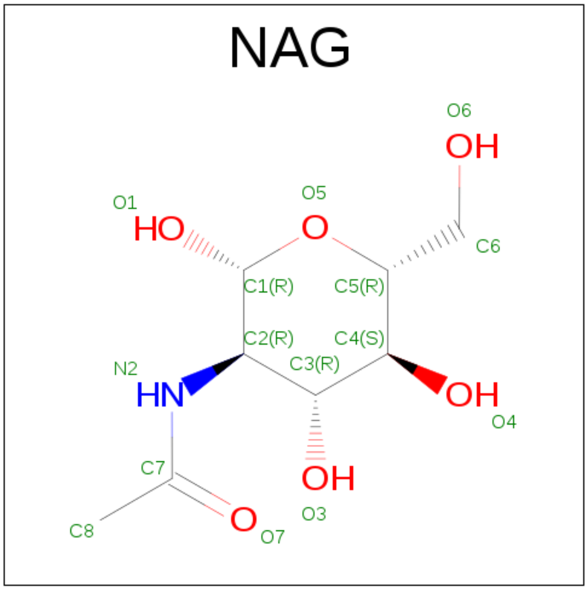
Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LYS	deletion	UNP P06213
E	?	-	ARG	deletion	UNP P06213
E	?	-	ARG	deletion	UNP P06213
E	?	-	VAL	deletion	UNP P06213
E	?	-	THR	deletion	UNP P06213
E	?	-	VAL	deletion	UNP P06213
E	?	-	ALA	deletion	UNP P06213
E	?	-	VAL	deletion	UNP P06213
E	?	-	PRO	deletion	UNP P06213
E	?	-	THR	deletion	UNP P06213
E	?	-	VAL	deletion	UNP P06213
E	?	-	ALA	deletion	UNP P06213
E	?	-	ALA	deletion	UNP P06213
E	?	-	PHE	deletion	UNP P06213
E	?	-	PRO	deletion	UNP P06213
E	?	-	ASN	deletion	UNP P06213
E	?	-	THR	deletion	UNP P06213
E	?	-	SER	deletion	UNP P06213
E	?	-	SER	deletion	UNP P06213
E	?	-	THR	deletion	UNP P06213
E	?	-	SER	deletion	UNP P06213
E	?	-	VAL	deletion	UNP P06213
E	750	ALA	PRO	engineered mutation	UNP P06213
E	751	GLY	THR	engineered mutation	UNP P06213
E	752	ASN	SER	engineered mutation	UNP P06213
E	753	ASN	PRO	engineered mutation	UNP P06213

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0

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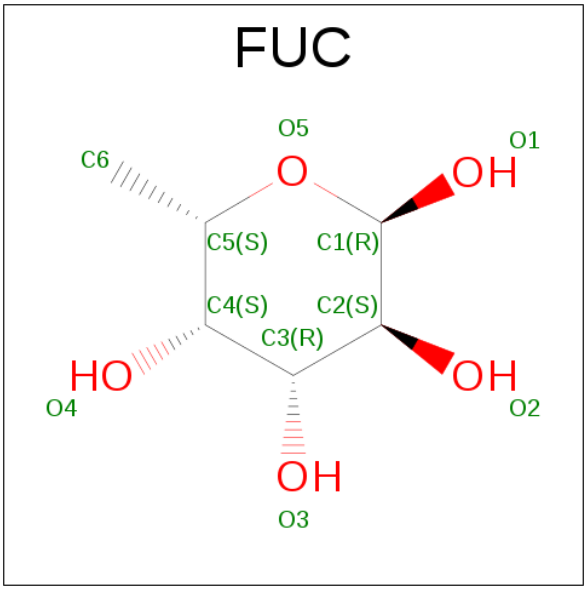
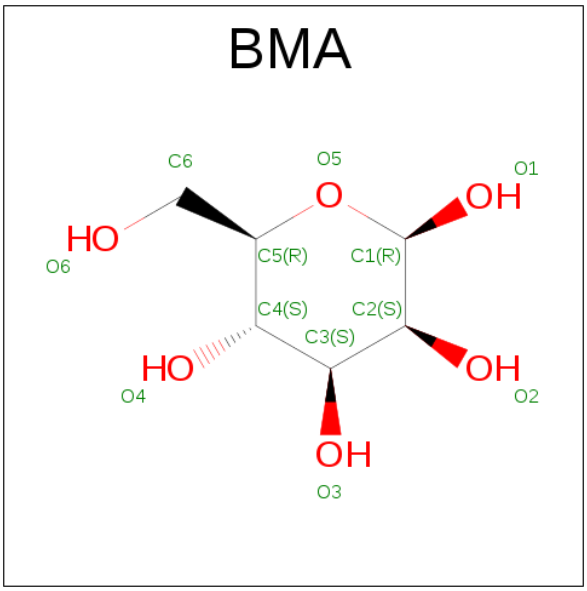
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0

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



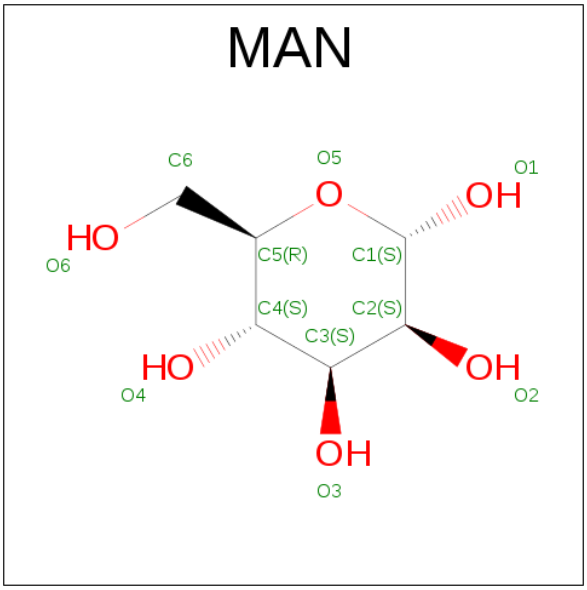
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total C O 10 6 4	0	0
7	E	1	Total C O 10 6 4	0	0
7	E	1	Total C O 10 6 4	0	0
7	E	1	Total C O 10 6 4	0	0
7	E	1	Total C O 10 6 4	0	0
7	E	1	Total C O 10 6 4	0	0

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total C O 11 6 5	0	0
8	E	1	Total C O 11 6 5	0	0

- Molecule 9 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



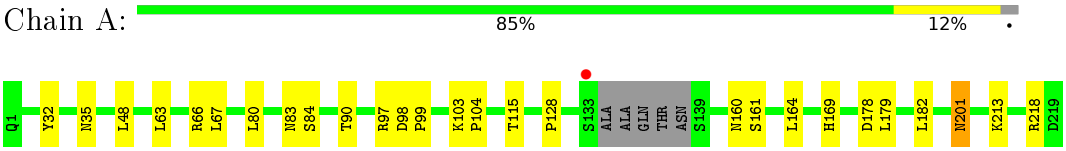
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	1	Total C O 11 6 5	0	0

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.

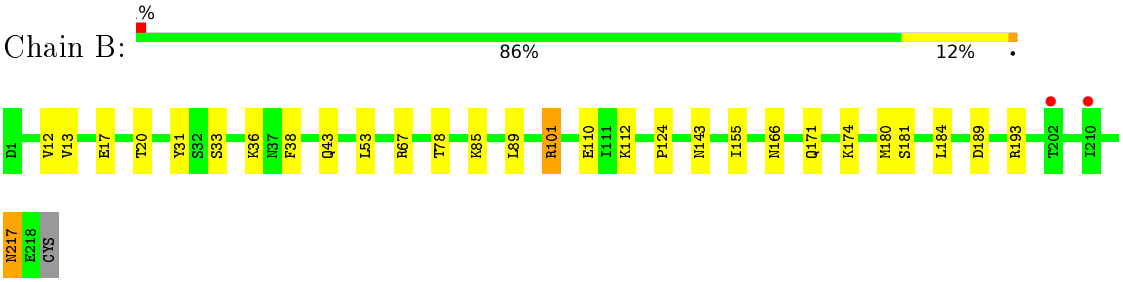
- Molecule 1: Fab 83-7 heavy chain

Chain A:



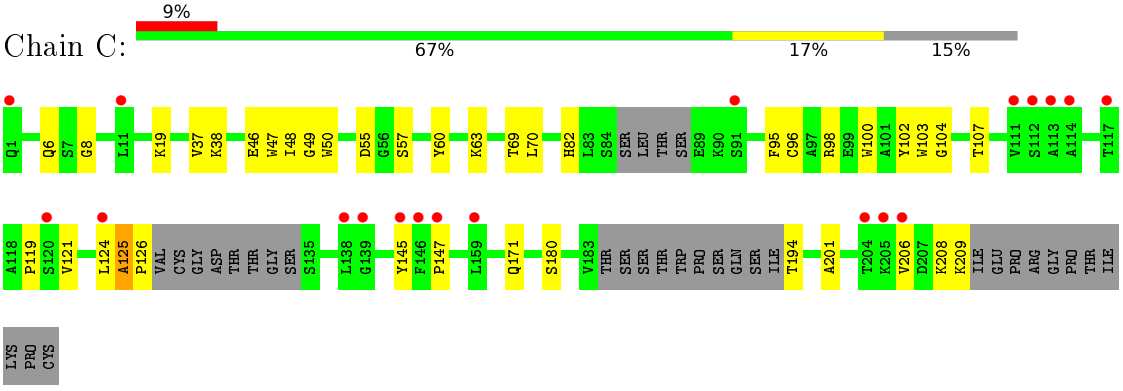
- Molecule 2: Fab 83-7 light chain

Chain B:



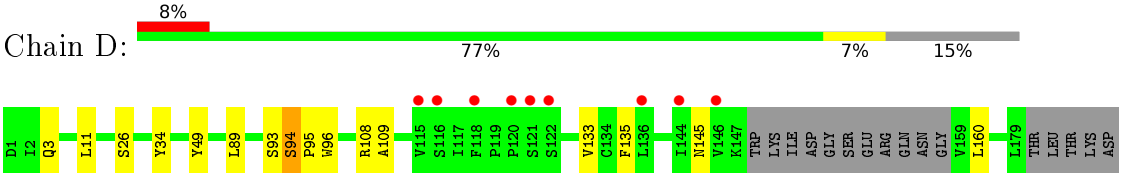
- Molecule 3: Fab 83-14 heavy chain

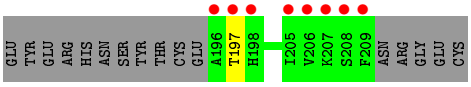
Chain C:



- Molecule 4: Fab 83-14 light chain

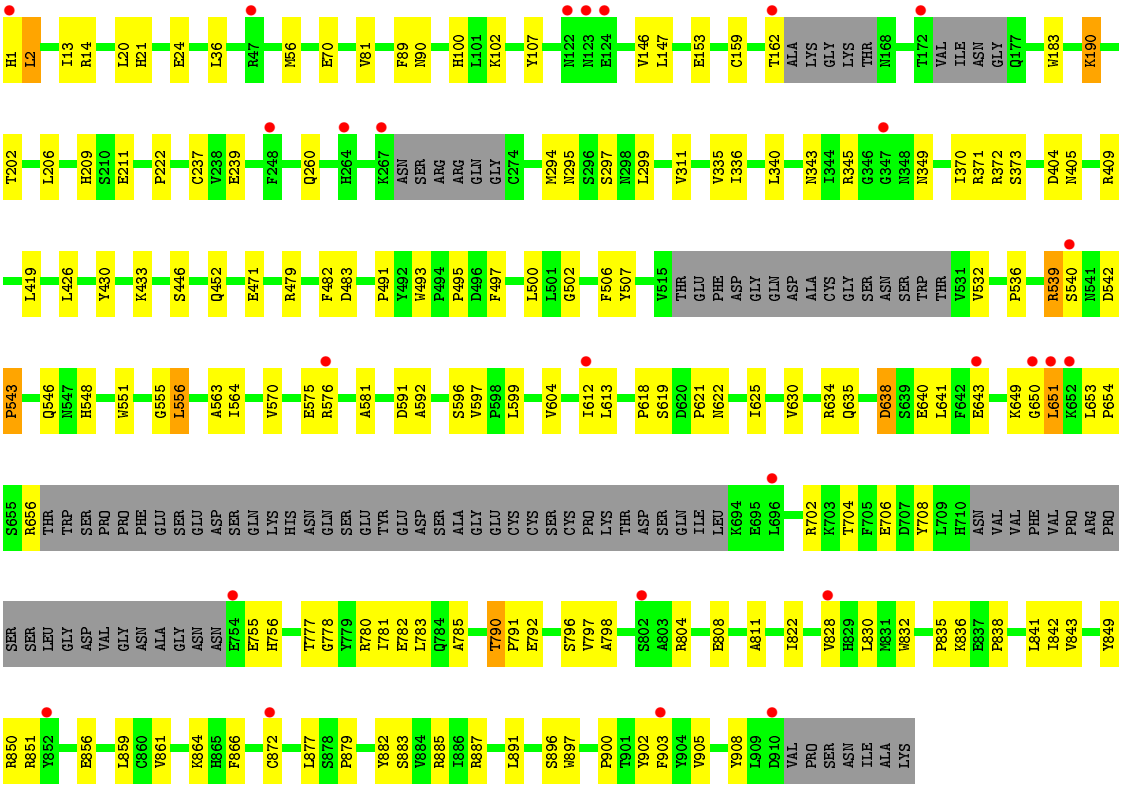
Chain D:





• Molecule 5: Insulin receptor

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	121.87Å 321.25Å 199.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.46 – 3.30 34.26 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (34.46-3.30) 98.0 (34.26-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.205 , 0.237 0.222 , 0.255	Depositor DCC
R_{free} test set	2911 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	106.7	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 89.9	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 57926 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12918	wwPDB-VP
Average B, all atoms (Å^2)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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, 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	0.54	0/1654	0.78	0/2261
2	B	0.48	0/1744	0.73	0/2363
3	C	0.47	0/1465	0.83	0/1995
4	D	0.54	0/1412	0.84	1/1914 (0.1%)
5	E	0.53	0/6631	0.84	3/8986 (0.0%)
All	All	0.52	0/12906	0.82	4/17519 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	555	GLY	C-N-CA	6.36	137.59	121.70
5	E	539	ARG	C-N-CA	5.45	135.31	121.70
4	D	93	SER	C-N-CA	5.33	135.04	121.70
5	E	295	ASN	N-CA-C	-5.08	97.28	111.00

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	1611	0	1582	26	0
2	B	1706	0	1648	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1427	0	1407	35	0
4	D	1384	0	1337	13	0
5	E	6473	0	6272	101	0
6	E	224	0	195	1	0
7	E	60	0	60	0	0
8	E	22	0	19	0	0
9	E	11	0	9	0	0
All	All	12918	0	12529	190	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (190) 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)
5:E:426:LEU:H	5:E:452:GLN:HE21	1.13	0.88
1:A:48:LEU:HD22	1:A:63:LEU:CD1	2.05	0.86
3:C:125:ALA:H	3:C:126:PRO:HD3	1.40	0.86
5:E:790:THR:HB	5:E:791:PRO:HD3	1.57	0.84
2:B:101:ARG:HH11	2:B:101:ARG:CG	1.93	0.81
5:E:755:GLU:HG2	5:E:756:HIS:N	1.99	0.77
2:B:12:VAL:HG12	2:B:110:GLU:HB2	1.65	0.76
3:C:6:GLN:HE21	3:C:104:GLY:HA3	1.50	0.75
5:E:755:GLU:HG2	5:E:756:HIS:H	1.51	0.75
1:A:35:ASN:ND2	1:A:98:ASP:HB2	2.01	0.74
1:A:48:LEU:HD22	1:A:63:LEU:HD12	1.69	0.73
3:C:46:GLU:OE1	3:C:63:LYS:HD3	1.89	0.72
5:E:599:LEU:HD11	5:E:619:SER:HB3	1.72	0.71
3:C:124:LEU:HD13	4:D:133:VAL:HG11	1.72	0.70
2:B:13:VAL:HG22	2:B:17:GLU:HB2	1.73	0.70
5:E:885:ARG:HE	5:E:897:TRP:HB3	1.55	0.69
3:C:60:TYR:HE1	3:C:70:LEU:HD13	1.58	0.69
5:E:70:GLU:O	5:E:102:LYS:HG2	1.93	0.68
5:E:471:GLU:HB2	5:E:581:ALA:HB2	1.75	0.68
1:A:35:ASN:HD21	1:A:98:ASP:HB2	1.58	0.67
2:B:101:ARG:HH11	2:B:101:ARG:HG3	1.58	0.67
3:C:98:ARG:NH2	5:E:546:GLN:HB3	2.11	0.66
3:C:102:TYR:HE1	5:E:546:GLN:HB2	1.62	0.64
5:E:651:LEU:H	5:E:651:LEU:HD23	1.62	0.64
5:E:785:ALA:H	5:E:796:SER:HB3	1.60	0.64
5:E:56:MET:HG3	5:E:81:VAL:HB	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:426:LEU:H	5:E:452:GLN:NE2	1.92	0.64
3:C:8:GLY:HA3	3:C:107:THR:HG23	1.79	0.64
1:A:48:LEU:CD2	1:A:63:LEU:HD12	2.29	0.63
5:E:808:GLU:HB2	5:E:811:ALA:HB2	1.80	0.63
1:A:99:PRO:HG2	1:A:103:LYS:HB2	1.81	0.63
1:A:161:SER:H	1:A:201:ASN:HD21	1.46	0.62
5:E:597:VAL:HG22	5:E:797:VAL:CG2	2.28	0.62
1:A:48:LEU:CD2	1:A:63:LEU:CD1	2.77	0.61
1:A:218:ARG:HH22	2:B:124:PRO:HB2	1.64	0.61
5:E:209:HIS:CD2	5:E:211:GLU:H	2.19	0.61
5:E:643:GLU:HA	5:E:864:LYS:HE3	1.82	0.61
5:E:89:PHE:O	5:E:90:ASN:HB3	2.02	0.60
5:E:879:PRO:HA	5:E:905:VAL:HG23	1.82	0.59
2:B:13:VAL:CG2	2:B:17:GLU:HB2	2.31	0.59
2:B:101:ARG:HH11	2:B:101:ARG:HG2	1.65	0.58
3:C:125:ALA:H	3:C:126:PRO:CD	2.11	0.58
5:E:822:ILE:HG12	5:E:828:VAL:HG22	1.86	0.57
1:A:218:ARG:HH12	2:B:124:PRO:HD2	1.69	0.57
5:E:704:THR:HG22	5:E:708:TYR:CE2	2.40	0.57
1:A:67:LEU:HD11	1:A:80:LEU:HD11	1.86	0.57
5:E:146:VAL:HG22	5:E:147:LEU:HG	1.87	0.56
2:B:31:TYR:HB2	2:B:38:PHE:CE1	2.41	0.56
5:E:294:MET:HG3	5:E:294:MET:O	2.05	0.56
5:E:634:ARG:HD2	5:E:777:THR:HG21	1.87	0.55
5:E:604:VAL:HB	5:E:612:ILE:HG13	1.88	0.55
5:E:885:ARG:NH1	5:E:900:PRO:HD3	2.21	0.55
1:A:160:ASN:HB2	1:A:164:LEU:HD13	1.88	0.55
5:E:190:LYS:HG3	6:E:1008:NAG:H81	1.88	0.55
5:E:345:ARG:NH2	5:E:372:ARG:HD2	2.23	0.55
3:C:180:SER:HB3	4:D:135:PHE:CE2	2.42	0.54
5:E:835:PRO:HD2	5:E:842:ILE:HD12	1.88	0.54
5:E:483:ASP:O	5:E:556:LEU:HB2	2.08	0.54
2:B:217:ASN:H	2:B:217:ASN:HD22	1.55	0.54
2:B:31:TYR:CE2	2:B:33:SER:HB2	2.43	0.53
2:B:31:TYR:HB2	2:B:38:PHE:HE1	1.73	0.53
5:E:654:PRO:HG2	5:E:656:ARG:HH21	1.73	0.53
5:E:542:ASP:N	5:E:543:PRO:HD3	2.24	0.53
1:A:161:SER:H	1:A:201:ASN:ND2	2.06	0.53
5:E:345:ARG:HH21	5:E:372:ARG:HD2	1.73	0.52
1:A:90:THR:HG23	1:A:115:THR:HA	1.92	0.52
5:E:502:GLY:HA2	5:E:536:PRO:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:VAL:HB	3:C:206:VAL:HG11	1.91	0.52
3:C:60:TYR:CE1	3:C:70:LEU:HD13	2.43	0.52
2:B:43:GLN:HB2	2:B:53:LEU:HD11	1.92	0.51
3:C:124:LEU:HD13	4:D:133:VAL:CG1	2.39	0.51
5:E:336:ILE:HD12	5:E:340:LEU:HD11	1.91	0.51
5:E:613:LEU:HD22	5:E:781:ILE:HG21	1.91	0.51
3:C:47:TRP:HZ2	3:C:50:TRP:HD1	1.57	0.51
3:C:206:VAL:CG1	3:C:208:LYS:HD3	2.41	0.51
3:C:19:LYS:HB3	3:C:82:HIS:CD2	2.46	0.51
5:E:702:ARG:O	5:E:706:GLU:HG3	2.10	0.51
5:E:597:VAL:HG22	5:E:797:VAL:HG22	1.93	0.51
1:A:169:HIS:CE1	2:B:143:ASN:HD21	2.30	0.50
2:B:155:ILE:HD11	2:B:184:LEU:HD21	1.94	0.50
5:E:482:PHE:HA	5:E:591:ASP:HB2	1.93	0.50
5:E:597:VAL:HG22	5:E:797:VAL:HG23	1.92	0.50
2:B:180:MET:HG2	2:B:181:SER:N	2.26	0.50
5:E:373:SER:H	5:E:405:ASN:HD22	1.58	0.50
5:E:532:VAL:HG11	5:E:551:TRP:CE2	2.47	0.50
5:E:630:VAL:HG22	5:E:783:LEU:HD13	1.94	0.50
5:E:635:GLN:HE21	5:E:780:ARG:HB2	1.76	0.49
3:C:194:THR:OG1	3:C:209:LYS:HG2	2.12	0.49
5:E:546:GLN:HG3	5:E:548:HIS:HD2	1.77	0.49
4:D:145:ASN:HB3	4:D:197:THR:HB	1.93	0.49
5:E:373:SER:H	5:E:405:ASN:ND2	2.10	0.49
2:B:20:THR:HG23	2:B:78:THR:CG2	2.42	0.49
5:E:546:GLN:C	5:E:548:HIS:H	2.16	0.49
5:E:209:HIS:CD2	5:E:222:PRO:HB3	2.48	0.49
5:E:1:HIS:CD2	5:E:2:LEU:H	2.30	0.49
5:E:506:PHE:O	5:E:564:ILE:HA	2.13	0.48
3:C:124:LEU:CD1	4:D:133:VAL:HG11	2.39	0.48
5:E:877:LEU:N	5:E:877:LEU:HD12	2.29	0.48
3:C:38:LYS:HB2	3:C:48:ILE:HD11	1.96	0.47
5:E:592:ALA:HB1	5:E:622:ASN:O	2.14	0.47
5:E:851:ARG:HB2	5:E:882:TYR:CE2	2.49	0.47
5:E:830:LEU:HB2	5:E:872:CYS:HB3	1.96	0.47
1:A:67:LEU:HD11	1:A:80:LEU:CD1	2.44	0.47
5:E:404:ASP:HA	5:E:430:TYR:O	2.14	0.47
2:B:101:ARG:NH1	2:B:101:ARG:HG3	2.28	0.47
1:A:66:ARG:HB2	1:A:83:ASN:HB2	1.96	0.47
5:E:493:TRP:CE3	5:E:497:PHE:HB2	2.50	0.47
5:E:2:LEU:HD11	5:E:237:CYS:SG	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:108:ARG:HG2	4:D:109:ALA:N	2.31	0.46
5:E:859:LEU:HD23	5:E:872:CYS:SG	2.55	0.46
1:A:32:TYR:HE2	1:A:99:PRO:HB3	1.79	0.46
3:C:171:GLN:HB2	4:D:160:LEU:HD11	1.98	0.46
3:C:47:TRP:HD1	3:C:100:TRP:HH2	1.64	0.46
5:E:828:VAL:HG21	5:E:903:PHE:CE1	2.51	0.46
4:D:3:GLN:H	4:D:26:SER:CB	2.29	0.45
5:E:13:ILE:HD13	5:E:20:LEU:HA	1.97	0.45
2:B:67:ARG:NH1	2:B:85:LYS:HD2	2.31	0.45
2:B:36:LYS:HE3	5:E:239:GLU:OE2	2.17	0.45
5:E:260:GLN:HA	5:E:299:LEU:HD11	1.98	0.45
5:E:782:GLU:HG3	5:E:798:ALA:HB1	1.96	0.45
1:A:103:LYS:HB3	1:A:104:PRO:HD2	1.98	0.45
5:E:426:LEU:N	5:E:452:GLN:HE21	1.97	0.45
5:E:849:TYR:HA	5:E:883:SER:O	2.17	0.45
5:E:159:CYS:O	5:E:162:THR:HG23	2.16	0.45
4:D:89:LEU:HD11	4:D:96:TRP:HB3	1.97	0.44
5:E:202:THR:HG22	5:E:206:LEU:HB2	1.98	0.44
5:E:507:TYR:HA	5:E:563:ALA:O	2.17	0.44
5:E:621:PRO:HB3	5:E:625:ILE:HD11	1.98	0.44
2:B:31:TYR:CB	2:B:38:PHE:HE1	2.30	0.44
2:B:101:ARG:NH1	2:B:101:ARG:CG	2.63	0.44
2:B:189:ASP:O	2:B:193:ARG:HG3	2.16	0.44
3:C:47:TRP:HZ2	3:C:50:TRP:CD1	2.35	0.44
3:C:37:VAL:CG2	3:C:95:PHE:HB2	2.47	0.44
5:E:107:TYR:HA	5:E:183:TRP:CD1	2.52	0.44
3:C:50:TRP:CZ2	5:E:479:ARG:HD2	2.52	0.44
5:E:755:GLU:CG	5:E:756:HIS:N	2.77	0.44
5:E:861:VAL:HG12	5:E:866:PHE:HB2	1.99	0.44
5:E:640:GLU:H	5:E:640:GLU:CD	2.21	0.44
1:A:48:LEU:HD22	1:A:63:LEU:HD13	1.95	0.44
4:D:94:SER:HB2	4:D:95:PRO:HD3	2.00	0.44
3:C:147:PRO:HD2	3:C:201:ALA:CB	2.48	0.43
5:E:343:ASN:HD22	5:E:371:ARG:HH21	1.64	0.43
5:E:641:LEU:HB3	5:E:841:LEU:HD21	1.99	0.43
2:B:217:ASN:ND2	2:B:217:ASN:H	2.16	0.43
4:D:11:LEU:HD23	4:D:11:LEU:C	2.38	0.43
2:B:89:LEU:HD21	2:B:171:GLN:HB3	2.00	0.43
3:C:50:TRP:CE2	5:E:479:ARG:HD2	2.52	0.43
5:E:832:TRP:CH2	5:E:872:CYS:HB2	2.54	0.43
5:E:832:TRP:HH2	5:E:872:CYS:HB2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:34:TYR:HD1	4:D:49:TYR:HA	1.83	0.43
5:E:419:LEU:O	5:E:446:SER:HA	2.18	0.43
5:E:850:ARG:NH2	5:E:856:GLU:HB2	2.33	0.42
5:E:885:ARG:HH12	5:E:900:PRO:HD3	1.81	0.42
3:C:180:SER:HB3	4:D:135:PHE:CD2	2.54	0.42
5:E:755:GLU:CG	5:E:756:HIS:H	2.27	0.42
1:A:178:ASP:O	1:A:179:LEU:HD23	2.19	0.42
2:B:13:VAL:HA	2:B:112:LYS:HE2	2.01	0.42
5:E:653:LEU:HD21	5:E:891:LEU:HD23	2.01	0.42
1:A:35:ASN:HD21	1:A:98:ASP:CB	2.29	0.42
2:B:166:ASN:HB3	2:B:180:MET:HE3	2.00	0.42
5:E:21:HIS:O	5:E:24:GLU:HB2	2.19	0.42
5:E:778:GLY:HA2	5:E:804:ARG:HA	2.01	0.42
2:B:174:LYS:HA	2:B:174:LYS:HD3	1.43	0.42
5:E:654:PRO:HB2	5:E:656:ARG:HE	1.84	0.42
1:A:32:TYR:CD2	1:A:97:ARG:HD2	2.55	0.42
3:C:100:TRP:HE3	3:C:103:TRP:CZ2	2.38	0.42
3:C:125:ALA:N	3:C:126:PRO:CD	2.81	0.41
3:C:47:TRP:CZ2	3:C:49:GLY:HA2	2.55	0.41
5:E:596:SER:HB3	5:E:618:PRO:HB2	2.01	0.41
5:E:89:PHE:O	5:E:90:ASN:CB	2.67	0.41
3:C:47:TRP:HD1	3:C:100:TRP:CH2	2.38	0.41
1:A:128:PRO:HG3	1:A:213:LYS:HD2	2.03	0.41
3:C:119:PRO:HB3	3:C:145:TYR:HB3	2.02	0.41
5:E:14:ARG:HA	5:E:36:LEU:O	2.21	0.41
3:C:6:GLN:HE22	3:C:96:CYS:H	1.69	0.41
3:C:37:VAL:HG22	3:C:95:PHE:HB2	2.01	0.41
5:E:370:ILE:HD12	5:E:370:ILE:N	2.35	0.41
1:A:32:TYR:CE2	1:A:99:PRO:HB3	2.55	0.41
5:E:887:ARG:HB2	5:E:897:TRP:CD2	2.56	0.41
5:E:556:LEU:CD1	5:E:556:LEU:H	2.34	0.40
5:E:651:LEU:H	5:E:651:LEU:CD2	2.30	0.40
2:B:20:THR:HG23	2:B:78:THR:HG23	2.02	0.40
5:E:409:ARG:HG2	5:E:433:LYS:HB3	2.03	0.40
5:E:575:GLU:HB3	5:E:576:ARG:H	1.76	0.40
5:E:653:LEU:HD22	5:E:843:VAL:HG21	2.03	0.40
1:A:182:LEU:C	1:A:182:LEU:HD12	2.41	0.40
5:E:500:LEU:HA	5:E:570:VAL:HG12	2.02	0.40
5:E:882:TYR:O	5:E:902:TYR:HA	2.21	0.40
3:C:55:ASP:CG	3:C:57:SER:HB2	2.41	0.40
5:E:311:VAL:HG22	5:E:335:VAL:HB	2.04	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	210/219 (96%)	198 (94%)	11 (5%)	1 (0%)	34 71
2	B	216/219 (99%)	212 (98%)	4 (2%)	0	100 100
3	C	179/220 (81%)	169 (94%)	9 (5%)	1 (1%)	30 68
4	D	176/214 (82%)	171 (97%)	4 (2%)	1 (1%)	30 68
5	E	786/894 (88%)	715 (91%)	53 (7%)	18 (2%)	8 39
All	All	1567/1766 (89%)	1465 (94%)	81 (5%)	21 (1%)	15 52

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	125	ALA
4	D	94	SER
5	E	153	GLU
5	E	539	ARG
5	E	540	SER
5	E	543	PRO
5	E	556	LEU
5	E	649	LYS
5	E	790	THR
5	E	896	SER
5	E	100	HIS
5	E	638	ASP
5	E	2	LEU
5	E	297	SER
5	E	650	GLY
5	E	792	GLU
1	A	84	SER
5	E	495	PRO

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Mol	Chain	Res	Type
5	E	836	LYS
5	E	908	TYR
5	E	838	PRO

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	187/190 (98%)	186 (100%)	1 (0%)	92 95
2	B	196/197 (100%)	194 (99%)	2 (1%)	82 91
3	C	157/187 (84%)	156 (99%)	1 (1%)	90 95
4	D	161/190 (85%)	161 (100%)	0	100 100
5	E	729/809 (90%)	724 (99%)	5 (1%)	88 94
All	All	1430/1573 (91%)	1421 (99%)	9 (1%)	90 95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
2	B	101	ARG
2	B	217	ASN
3	C	69	THR
5	E	190	LYS
5	E	349	ASN
5	E	491	PRO
5	E	638	ASP
5	E	651	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	83	ASN

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Mol	Chain	Res	Type
1	A	110	GLN
1	A	201	ASN
2	B	95	GLN
2	B	143	ASN
2	B	217	ASN
3	C	5	GLN
3	C	6	GLN
4	D	161	ASN
5	E	1	HIS
5	E	34	GLN
5	E	209	HIS
5	E	260	GLN
5	E	343	ASN
5	E	405	ASN
5	E	407	ASN
5	E	452	GLN
5	E	513	GLN
5	E	546	GLN
5	E	548	HIS
5	E	610	GLN
5	E	635	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

25 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	$\#\|Z\| > 2$
6	NAG	E	1001	5	14,14,15	0.36	0	15,19,21	0.61	0
6	NAG	E	1002	5,7,6	14,14,15	0.31	0	15,19,21	0.47	0
6	NAG	E	1003	6	14,14,15	0.30	0	15,19,21	0.46	0
7	FUC	E	1004	6	10,10,11	0.42	0	13,14,16	0.61	0
6	NAG	E	1005	5,6	14,14,15	0.40	0	15,19,21	1.31	2 (13%)
6	NAG	E	1006	8,6	14,14,15	0.33	0	15,19,21	0.80	1 (6%)
8	BMA	E	1007	6	11,11,12	0.41	0	15,15,17	0.74	0
6	NAG	E	1008	5	14,14,15	0.28	0	15,19,21	0.61	0
6	NAG	E	1009	5,7,6	14,14,15	0.32	0	15,19,21	0.84	1 (6%)
6	NAG	E	1010	6	14,14,15	0.42	0	15,19,21	0.56	0
7	FUC	E	1011	6	10,10,11	0.49	0	13,14,16	0.72	0
6	NAG	E	1012	5,7,6	14,14,15	0.29	0	15,19,21	0.80	1 (6%)
6	NAG	E	1013	8,6	14,14,15	0.36	0	15,19,21	0.62	0
8	BMA	E	1014	9,6	11,11,12	0.31	0	15,15,17	0.42	0
9	MAN	E	1015	8,6	11,11,12	0.47	0	15,15,17	0.93	1 (6%)
6	NAG	E	1016	9	14,14,15	0.33	0	15,19,21	0.78	1 (6%)
7	FUC	E	1017	6	10,10,11	0.52	0	13,14,16	0.71	0
6	NAG	E	1018	5,7	14,14,15	0.41	0	15,19,21	0.71	1 (6%)
7	FUC	E	1019	6	10,10,11	0.42	0	13,14,16	0.53	0
6	NAG	E	1020	5	14,14,15	0.35	0	15,19,21	0.78	1 (6%)
6	NAG	E	1021	5,7,6	14,14,15	0.35	0	15,19,21	0.45	0
6	NAG	E	1022	6	14,14,15	0.35	0	15,19,21	0.81	1 (6%)
7	FUC	E	1023	6	10,10,11	0.42	0	13,14,16	0.49	0
6	NAG	E	1024	5,7	14,14,15	0.42	0	15,19,21	0.81	0
7	FUC	E	1025	6	10,10,11	0.48	0	13,14,16	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
6	NAG	E	1001	5	-	0/6/23/26	0/1/1/1
6	NAG	E	1002	5,7,6	-	0/6/23/26	0/1/1/1
6	NAG	E	1003	6	-	0/6/23/26	0/1/1/1
7	FUC	E	1004	6	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	E	1005	5,6	-	0/6/23/26	0/1/1/1
6	NAG	E	1006	8,6	-	0/6/23/26	0/1/1/1
8	BMA	E	1007	6	-	0/2/19/22	0/1/1/1
6	NAG	E	1008	5	-	0/6/23/26	0/1/1/1
6	NAG	E	1009	5,7,6	-	0/6/23/26	0/1/1/1
6	NAG	E	1010	6	-	0/6/23/26	0/1/1/1
7	FUC	E	1011	6	-	0/0/17/20	0/1/1/1
6	NAG	E	1012	5,7,6	-	0/6/23/26	0/1/1/1
6	NAG	E	1013	8,6	-	0/6/23/26	0/1/1/1
8	BMA	E	1014	9,6	-	0/2/19/22	0/1/1/1
9	MAN	E	1015	8,6	-	0/2/19/22	0/1/1/1
6	NAG	E	1016	9	-	0/6/23/26	0/1/1/1
7	FUC	E	1017	6	-	0/0/17/20	0/1/1/1
6	NAG	E	1018	5,7	-	0/6/23/26	0/1/1/1
7	FUC	E	1019	6	-	0/0/17/20	0/1/1/1
6	NAG	E	1020	5	-	0/6/23/26	0/1/1/1
6	NAG	E	1021	5,7,6	-	0/6/23/26	0/1/1/1
6	NAG	E	1022	6	-	0/6/23/26	0/1/1/1
7	FUC	E	1023	6	-	0/0/17/20	0/1/1/1
6	NAG	E	1024	5,7	-	0/6/23/26	0/1/1/1
7	FUC	E	1025	6	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	1005	NAG	O4-C4-C5	2.06	114.66	109.23
6	E	1016	NAG	C1-O5-C5	2.30	115.52	112.14
6	E	1018	NAG	C1-O5-C5	2.35	115.59	112.14
6	E	1006	NAG	C1-O5-C5	2.42	115.69	112.14
6	E	1022	NAG	C1-O5-C5	2.57	115.91	112.14
6	E	1009	NAG	C1-O5-C5	2.57	115.91	112.14
6	E	1020	NAG	C1-O5-C5	2.68	116.08	112.14
9	E	1015	MAN	C1-O5-C5	2.74	116.17	112.14
6	E	1012	NAG	C1-O5-C5	2.79	116.24	112.14
6	E	1005	NAG	C1-O5-C5	4.28	118.44	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1008	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	214/219 (97%)	-0.08	1 (0%) 91 90	78, 111, 146, 168	0
2	B	218/219 (99%)	0.02	2 (0%) 85 82	84, 121, 155, 175	0
3	C	187/220 (85%)	0.54	19 (10%) 9 7	87, 155, 199, 214	0
4	D	182/214 (85%)	0.54	17 (9%) 11 9	78, 123, 204, 217	0
5	E	800/894 (89%)	0.21	26 (3%) 50 43	72, 135, 186, 228	0
All	All	1601/1766 (90%)	0.22	65 (4%) 41 34	72, 129, 190, 228	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	208	SER	7.4
5	E	267	LYS	5.2
4	D	196	ALA	5.1
4	D	115	VAL	4.4
3	C	139	GLY	4.1
4	D	206	VAL	4.1
5	E	754	GLU	3.7
3	C	112	SER	3.7
2	B	210	ILE	3.6
4	D	197	THR	3.6
5	E	162	THR	3.5
3	C	146	PHE	3.4
3	C	159	LEU	3.2
3	C	138	LEU	3.1
4	D	146	VAL	3.0
5	E	123	ASN	3.0
4	D	144	ILE	3.0
3	C	147	PRO	2.9
5	E	1	HIS	2.9
5	E	910	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	11	LEU	2.9
5	E	612	ILE	2.9
4	D	121	SER	2.8
4	D	120	PRO	2.8
4	D	116	SER	2.8
5	E	903	PHE	2.7
3	C	205	LYS	2.7
4	D	209	PHE	2.7
5	E	802	SER	2.7
5	E	122	ASN	2.7
4	D	122	SER	2.7
1	A	133	SER	2.6
5	E	643	GLU	2.6
5	E	248	PHE	2.6
4	D	207	LYS	2.6
5	E	264	HIS	2.6
5	E	540	SER	2.6
5	E	872	CYS	2.5
5	E	124	GLU	2.5
3	C	120	SER	2.5
3	C	1	GLN	2.5
5	E	651	LEU	2.5
5	E	696	LEU	2.4
4	D	205	ILE	2.4
3	C	111	VAL	2.4
3	C	114	ALA	2.4
5	E	652	LYS	2.4
3	C	206	VAL	2.4
5	E	576	ARG	2.4
3	C	204	THR	2.4
5	E	347	GLY	2.3
3	C	117	THR	2.2
3	C	91	SER	2.2
5	E	650	GLY	2.2
4	D	118	PHE	2.2
3	C	124	LEU	2.1
5	E	47	ARG	2.1
3	C	145	TYR	2.1
2	B	202	THR	2.1
3	C	113	ALA	2.1
5	E	852	TYR	2.1
4	D	136	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	172	THR	2.1
5	E	828	VAL	2.0
4	D	198	HIS	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)

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, 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
6	NAG	E	1005	14/15	0.96	0.19	-0.80	138,152,170,180	0
6	NAG	E	1008	14/15	0.92	0.15	-1.22	134,150,160,163	0
6	NAG	E	1021	14/15	0.88	0.26	-	155,179,193,198	0
9	MAN	E	1015	11/12	0.85	0.34	-	185,197,203,208	0
8	BMA	E	1007	11/12	0.67	0.29	-	160,165,169,169	0
7	FUC	E	1017	10/11	0.95	0.15	-	161,170,173,174	0
6	NAG	E	1016	14/15	0.84	0.33	-	160,168,180,181	0
6	NAG	E	1018	14/15	0.85	0.16	-	181,187,195,196	0
6	NAG	E	1024	14/15	0.80	0.28	-	152,159,173,184	0
6	NAG	E	1013	14/15	0.85	0.33	-	153,185,196,200	0
6	NAG	E	1012	14/15	0.90	0.13	-	147,159,171,177	0
6	NAG	E	1022	14/15	0.85	0.34	-	173,193,201,203	0
6	NAG	E	1020	14/15	0.84	0.25	-	155,162,168,169	0
7	FUC	E	1019	10/11	0.85	0.33	-	178,184,186,189	0
6	NAG	E	1003	14/15	0.80	0.36	-	179,204,207,207	0
6	NAG	E	1009	14/15	0.94	0.14	-	135,148,159,159	0
7	FUC	E	1011	10/11	0.83	0.28	-	146,154,162,162	0
8	BMA	E	1014	11/12	0.82	0.33	-	186,198,199,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	NAG	E	1006	14/15	0.94	0.15	-	133,151,167,174	0
7	FUC	E	1004	10/11	0.90	0.33	-	177,185,193,194	0
6	NAG	E	1002	14/15	0.90	0.27	-	177,187,197,204	0
6	NAG	E	1010	14/15	0.88	0.23	-	146,173,183,183	0
7	FUC	E	1023	10/11	0.92	0.17	-	180,188,194,201	0
6	NAG	E	1001	14/15	0.84	0.19	-	152,163,168,169	0
7	FUC	E	1025	10/11	0.85	0.44	-	187,197,205,206	0

6.5 Other polymers

There are no such residues in this entry.