Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:39 AM GMT

PDB ID	:	3FCU
Title	:	Structure of headpiece of integrin aIIBb3 in open conformation
Authors	:	Zhu, J.; Luo, B.-H.; Xiao, T.; Zhang, C.; Nishida, N.; Springer, T.A.
Deposited on	:	2008-11-22
Resolution	:	2.90 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:

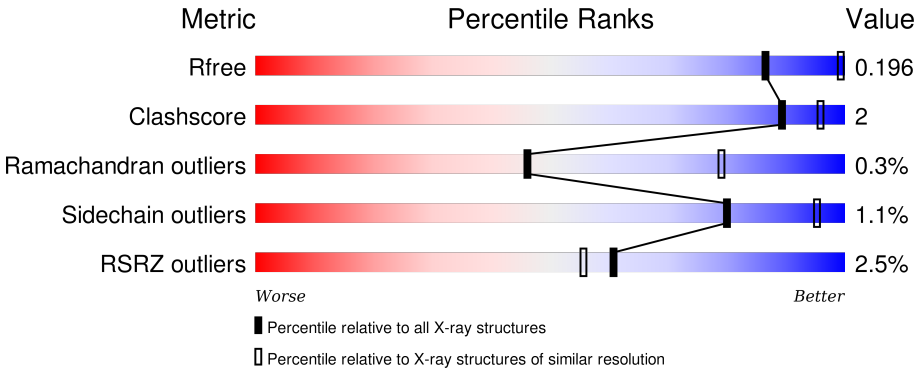
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	457	2% 91% 8%
1	C	457	94%
1	E	457	93% 6%
2	B	461	3% 92% 7%
2	D	461	2% 92% 6%

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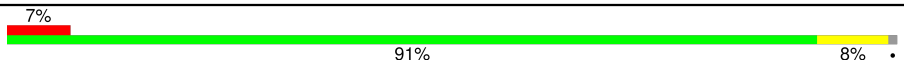
Mol	Chain	Length	Quality of chain
2	F	461	

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	CA	B	2003	-	-	-	X
3	CA	D	2003	-	-	-	X
6	MAN	B	3322	X	-	-	-
6	MAN	F	3322	X	-	-	-
7	CAC	B	462	-	-	-	X
8	MAN	D	3322	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21657 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 Integrin, alpha 2b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	1	0
			3511	2230	606	667	8			
1	C	451	Total	C	N	O	S	0	2	0
			3477	2207	602	660	8			
1	E	452	Total	C	N	O	S	0	2	0
			3485	2213	603	661	8			

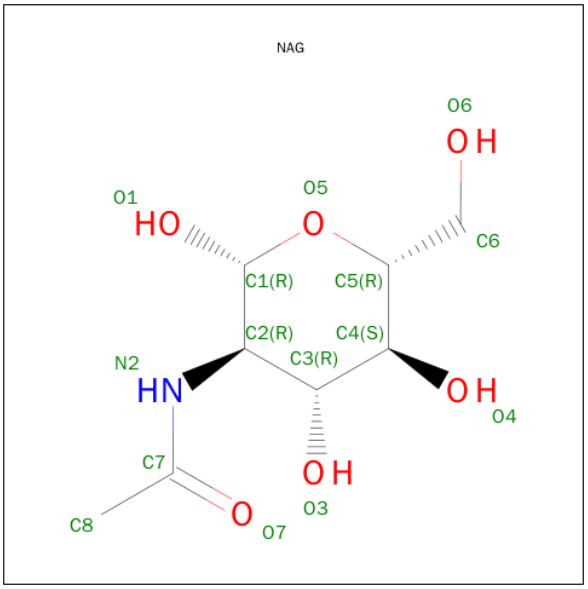
- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	455	Total	C	N	O	S	0	0	0
			3521	2196	601	692	32			
2	D	455	Total	C	N	O	S	0	0	0
			3521	2196	601	692	32			
2	F	455	Total	C	N	O	S	0	0	0
			3521	2196	601	692	32			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Ca	0	0
			2	2		
3	E	4	Total	Ca	0	0
			4	4		
3	B	2	Total	Ca	0	0
			2	2		
3	C	4	Total	Ca	0	0
			4	4		
3	A	4	Total	Ca	0	0
			4	4		
3	F	2	Total	Ca	0	0
			2	2		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0

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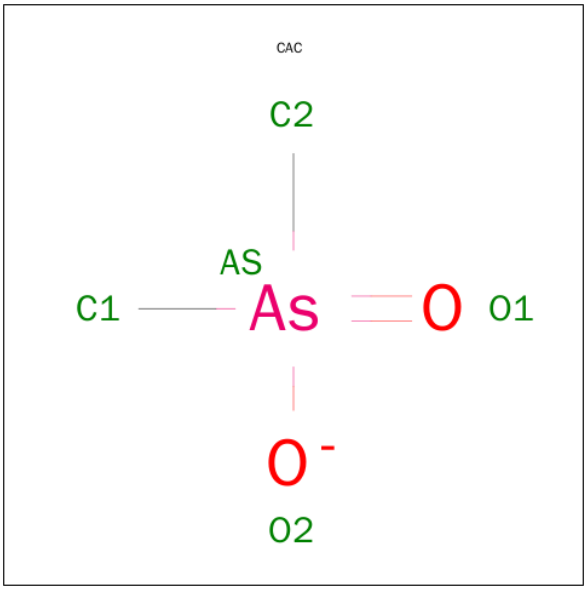
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	5	Total C N O 61 34 2 25	0	0
6	F	5	Total C N O 61 34 2 25	0	0

- Molecule 7 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total As C O 5 1 2 2	0	0
7	D	1	Total As C O 5 1 2 2	0	0
7	F	1	Total As C O 5 1 2 2	0	0

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

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

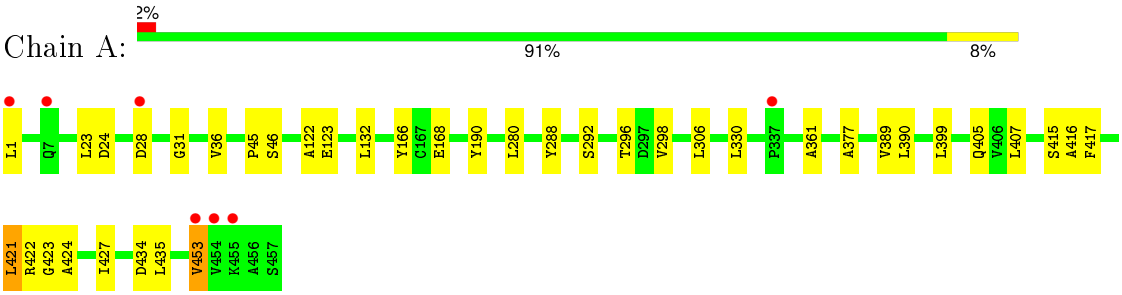
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	191	Total	O	0	0
			191	191		
9	C	56	Total	O	0	0
			56	56		
9	E	51	Total	O	0	0
			51	51		

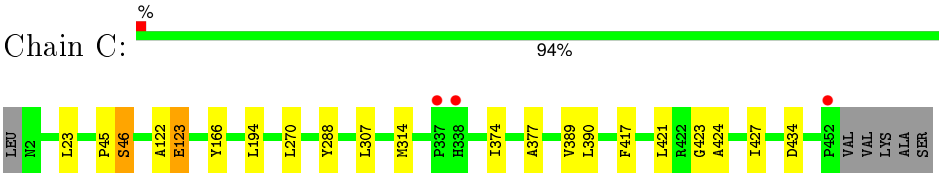
3 Residue-property plots (i)

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.

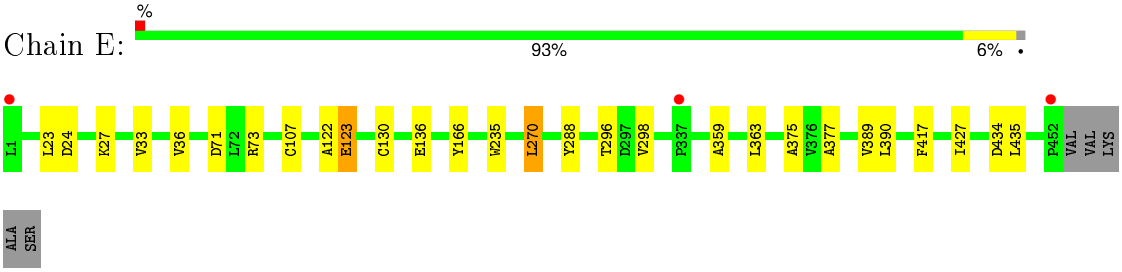
- Molecule 1: Integrin, alpha 2b



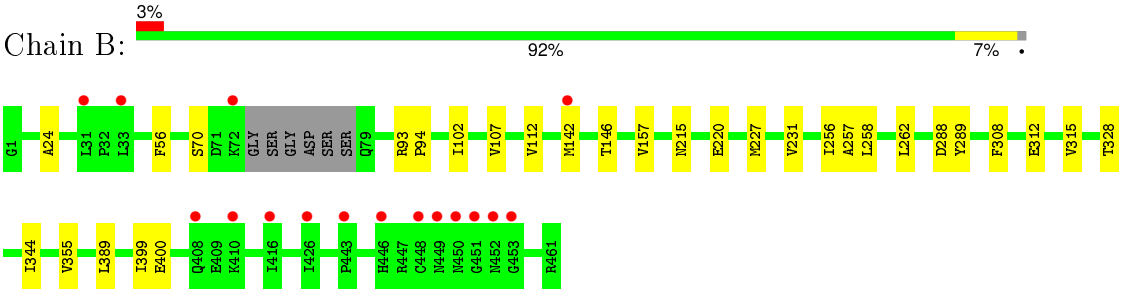
- Molecule 1: Integrin, alpha 2b



- Molecule 1: Integrin, alpha 2b

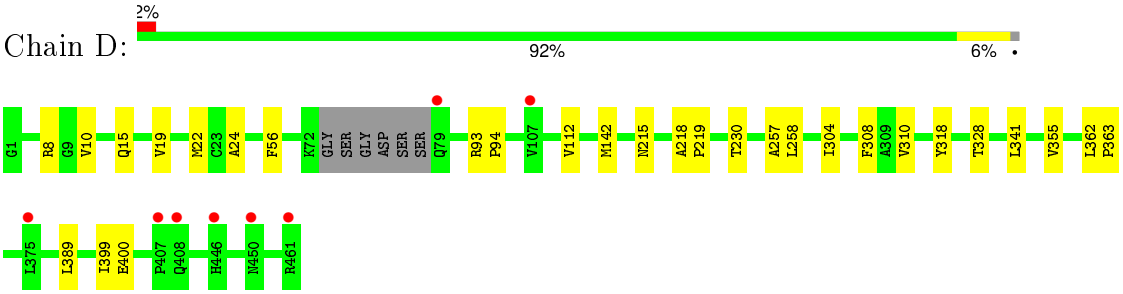


- Molecule 2: Integrin beta-3



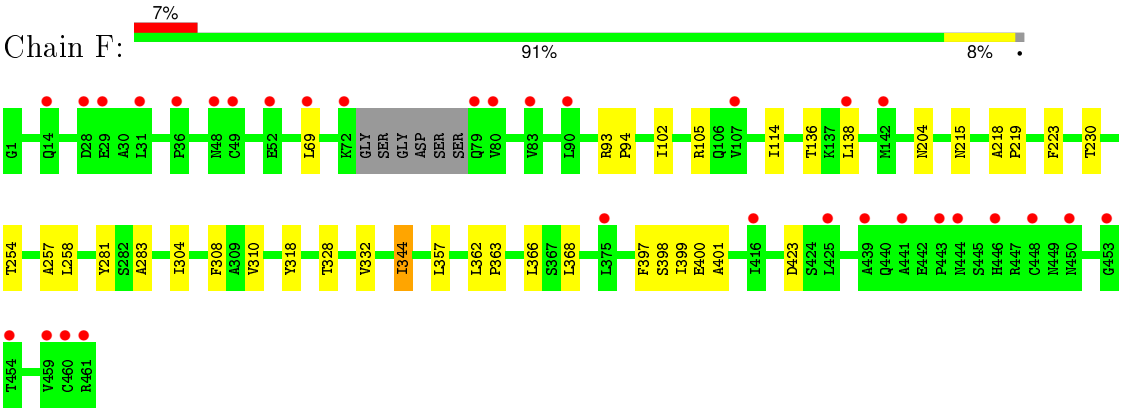
• Molecule 2: Integrin beta-3

Chain D:



• Molecule 2: Integrin beta-3

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α, β, γ	332.09Å 332.09Å 88.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.59 – 2.90 44.58 – 2.89	Depositor EDS
% Data completeness (in resolution range)	95.2 (44.59-2.90) 95.2 (44.58-2.89)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.174 , 0.197 0.175 , 0.196	Depositor DCC
R_{free} test set	3098 reflections (2.70%)	DCC
Wilson B-factor (Å^2)	63.7	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 118478 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21657	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: CAC, MG, CA, 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	0.33	0/3608	0.41	0/4916
1	C	0.32	0/3577	0.41	0/4873
1	E	0.33	0/3585	0.41	0/4884
2	B	0.30	0/3584	0.38	0/4858
2	D	0.30	0/3584	0.39	0/4858
2	F	0.30	0/3584	0.38	0/4858
All	All	0.31	0/21522	0.40	0/29247

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
6	B	1	0
6	F	1	0
8	D	1	0
All	All	3	0

There are no bond length outliers.

There are no bond angle outliers.

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	3322	MAN	C1
8	D	3322	MAN	C1
6	F	3322	MAN	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	3511	0	3345	19	0
1	C	3477	0	3303	10	0
1	E	3485	0	3317	15	0
2	B	3521	0	3455	19	0
2	D	3521	0	3455	14	0
2	F	3521	0	3456	23	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
3	C	4	0	0	0	0
3	D	2	0	0	0	0
3	E	4	0	0	0	0
3	F	2	0	0	0	0
4	A	14	0	13	0	0
4	B	28	0	26	1	0
4	C	14	0	13	0	0
4	D	28	0	26	1	0
4	E	14	0	13	0	0
4	F	14	0	13	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	B	61	0	52	0	0
6	F	61	0	52	0	0
7	B	5	0	0	0	0
7	D	5	0	0	0	0
7	F	5	0	0	0	0
8	D	50	0	43	0	0
9	A	191	0	0	0	0
9	C	56	0	0	0	0
9	E	51	0	0	1	0
All	All	21657	0	20582	99	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 2.

All (99) 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)
2:B:112:VAL:HG11	2:B:142:MET:HE3	1.71	0.72
1:A:427:ILE:HG22	1:A:434:ASP:OD1	1.91	0.70
2:F:138:LEU:CD2	2:F:344:ILE:HD12	2.26	0.66
2:D:230:THR:HG23	2:D:304:ILE:HD12	1.79	0.63
2:D:8:ARG:HB2	2:D:10:VAL:HG13	1.80	0.62
2:F:138:LEU:HD23	2:F:344:ILE:HD12	1.84	0.59
1:C:427:ILE:HG22	1:C:434:ASP:OD1	2.03	0.59
1:E:427:ILE:HG22	1:E:434:ASP:OD1	2.03	0.59
2:F:400:GLU:HB2	4:F:3371:NAG:H83	1.86	0.58
2:F:223:PHE:CZ	2:F:254:THR:HG21	2.40	0.57
1:E:363:LEU:HD21	1:E:435:LEU:HD13	1.86	0.57
2:D:308:PHE:CE2	2:D:328:THR:HG21	2.40	0.57
1:A:377:ALA:HB2	1:A:421:LEU:HD22	1.86	0.57
2:D:400:GLU:HB2	4:D:3371:NAG:H83	1.86	0.57
2:F:281:TYR:CE1	2:F:283:ALA:HB3	2.41	0.55
1:A:330:LEU:HD22	1:A:399:LEU:HD12	1.89	0.54
2:B:400:GLU:HB2	4:B:3371:NAG:H83	1.90	0.53
2:B:142:MET:HE2	2:B:344:ILE:HG23	1.90	0.52
2:F:218:ALA:HB3	2:F:219:PRO:HD3	1.91	0.52
1:E:122:ALA:O	1:E:123:GLU:HB2	2.08	0.52
1:C:122:ALA:O	1:C:123:GLU:HB2	2.09	0.52
2:B:355:VAL:HG23	2:B:389:LEU:HD22	1.91	0.52
1:A:1:LEU:HD12	1:A:405:GLN:HG3	1.92	0.51
2:D:218:ALA:HB3	2:D:219:PRO:HD3	1.93	0.51
1:C:45:PRO:O	1:C:46:SER:CB	2.57	0.51
2:B:256:ILE:HD12	9:E:494:HOH:O	2.09	0.51
2:B:102:ILE:HG22	2:B:399:ILE:HD11	1.93	0.51
2:F:308:PHE:CE2	2:F:328:THR:HG21	2.45	0.51
1:C:377:ALA:HB2	1:C:421:LEU:HD11	1.93	0.50
2:F:230:THR:HG23	2:F:304:ILE:HD12	1.93	0.49
1:A:132:LEU:N	1:A:132:LEU:HD12	2.28	0.49
1:E:235:TRP:HZ2	1:E:270:LEU:HD11	1.77	0.49
2:D:112:VAL:HG21	2:D:142:MET:CE	2.42	0.49
1:E:296:THR:HG23	1:E:298:VAL:HG13	1.94	0.49
1:C:389:VAL:HG23	1:C:417:PHE:CE2	2.47	0.48
1:C:194:LEU:HD12	1:C:194:LEU:C	2.34	0.48
2:F:138:LEU:HD22	2:F:344:ILE:HD12	1.96	0.48
1:E:24:ASP:O	1:E:36:VAL:HG12	2.13	0.47
2:B:24:ALA:HB2	2:B:56:PHE:CD1	2.49	0.47
2:F:114:ILE:HD13	2:F:344:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ALA:O	1:A:123:GLU:HB2	2.14	0.47
2:D:257:ALA:O	2:D:258:LEU:HB2	2.15	0.47
2:F:399:ILE:HD12	2:F:399:ILE:N	2.30	0.47
2:B:312:GLU:O	2:B:315:VAL:HG12	2.15	0.46
2:B:257:ALA:O	2:B:258:LEU:HB2	2.15	0.46
2:F:332:VAL:O	2:F:332:VAL:HG13	2.14	0.46
1:E:71:ASP:OD1	1:E:73:ARG:HD3	2.16	0.46
2:D:15:GLN:O	2:D:19:VAL:HG23	2.15	0.46
1:E:390:LEU:HD12	1:E:390:LEU:N	2.31	0.46
1:C:390:LEU:HD12	1:C:390:LEU:N	2.31	0.46
2:F:93:ARG:HB2	2:F:94:PRO:HD2	1.98	0.45
1:E:363:LEU:CD2	1:E:435:LEU:HD13	2.46	0.45
1:A:280:LEU:HD11	1:A:306:LEU:HD23	1.99	0.45
2:B:112:VAL:HG11	2:B:142:MET:CE	2.45	0.45
2:B:308:PHE:CE2	2:B:328:THR:HG21	2.52	0.45
2:F:357:LEU:HD11	2:F:397:PHE:CD2	2.51	0.45
1:A:280:LEU:CD1	1:A:306:LEU:HD23	2.46	0.45
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.99	0.45
2:F:362:LEU:HD12	2:F:363:PRO:HD2	1.97	0.45
2:F:368:LEU:HD23	2:F:401:ALA:HA	1.98	0.44
1:E:363:LEU:HD11	1:E:375:ALA:HB2	1.99	0.44
2:D:355:VAL:HG23	2:D:389:LEU:HD22	2.00	0.44
2:D:93:ARG:HB2	2:D:94:PRO:HD2	1.99	0.44
2:B:70:SER:HB2	2:B:107:VAL:HG11	1.99	0.44
1:E:27:LYS:HG3	1:E:33:VAL:HG22	1.99	0.44
2:F:102:ILE:CG2	2:F:397:PHE:HB2	2.48	0.43
2:B:142:MET:HE2	2:B:344:ILE:CG2	2.48	0.43
1:A:390:LEU:HD12	1:A:390:LEU:N	2.33	0.43
2:B:142:MET:CE	2:B:344:ILE:HG23	2.48	0.43
1:A:24:ASP:O	1:A:36:VAL:HG12	2.18	0.43
2:F:69:LEU:HD13	2:F:105:ARG:HB2	2.00	0.43
2:D:310:VAL:HG11	2:D:318:TYR:CD2	2.53	0.43
1:C:307:LEU:HD11	1:C:374:ILE:HG21	2.01	0.43
1:E:107:CYS:HA	1:E:130:CYS:HA	2.00	0.43
2:F:310:VAL:HG11	2:F:318:TYR:CD2	2.53	0.42
2:B:157:VAL:O	2:B:220:GLU:HB3	2.19	0.42
1:A:415:SER:O	1:A:416:ALA:HB3	2.20	0.42
1:C:314:MET:HB2	1:C:314:MET:HE3	1.94	0.42
2:F:102:ILE:HG22	2:F:399:ILE:HD11	2.01	0.42
2:D:24:ALA:HB2	2:D:56:PHE:CD1	2.55	0.42
2:B:227:MET:O	2:B:231:VAL:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:389:VAL:HG23	1:E:417:PHE:CE2	2.55	0.41
1:A:389:VAL:HG23	1:A:417:PHE:CE2	2.55	0.41
1:A:296:THR:HG23	1:A:298:VAL:HG13	2.03	0.41
2:D:399:ILE:HD12	2:D:399:ILE:N	2.34	0.41
1:A:422:ARG:O	1:A:435:LEU:HD12	2.20	0.41
2:D:362:LEU:HD12	2:D:363:PRO:HD2	2.01	0.41
1:A:423:GLY:O	1:A:424:ALA:HB3	2.21	0.41
1:E:359:ALA:HB3	1:E:377:ALA:HB3	2.02	0.41
1:E:122:ALA:O	1:E:123:GLU:CB	2.69	0.41
2:F:363:PRO:HG2	2:F:366:LEU:HD12	2.03	0.41
1:C:423:GLY:O	1:C:424:ALA:HB3	2.21	0.41
1:A:361:ALA:HB2	1:A:421:LEU:HB3	2.01	0.40
1:A:377:ALA:HB2	1:A:421:LEU:CD2	2.50	0.40
1:A:168:GLU:OE1	2:B:262:LEU:O	2.39	0.40
2:B:288:ASP:OD1	2:B:289:TYR:N	2.54	0.40
2:F:257:ALA:O	2:F:258:LEU:HB2	2.21	0.40
2:F:136:THR:HG22	2:F:204:ASN:OD1	2.21	0.40
1:A:405:GLN:NE2	1:A:407:LEU:HD21	2.36	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	456/457 (100%)	435 (95%)	16 (4%)	5 (1%)	17 51
1	C	451/457 (99%)	436 (97%)	13 (3%)	2 (0%)	39 74
1	E	452/457 (99%)	440 (97%)	11 (2%)	1 (0%)	52 84
2	B	451/461 (98%)	437 (97%)	14 (3%)	0	100 100
2	D	451/461 (98%)	435 (96%)	16 (4%)	0	100 100
2	F	451/461 (98%)	434 (96%)	17 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2712/2754 (98%)	2617 (96%)	87 (3%)	8 (0%)	46 79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	SER
1	A	28	ASP
1	C	46	SER
1	A	31	GLY
1	E	123	GLU
1	C	123	GLU
1	A	45	PRO
1	A	453	VAL

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	365/364 (100%)	358 (98%)	7 (2%)	65 89
1	C	361/364 (99%)	357 (99%)	4 (1%)	80 95
1	E	362/364 (100%)	357 (99%)	5 (1%)	74 93
2	B	405/409 (99%)	403 (100%)	2 (0%)	92 98
2	D	405/409 (99%)	402 (99%)	3 (1%)	88 97
2	F	405/409 (99%)	401 (99%)	4 (1%)	82 95
All	All	2303/2319 (99%)	2278 (99%)	25 (1%)	80 95

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR
1	A	190	TYR
1	A	288	TYR

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Mol	Chain	Res	Type
1	A	292	SER
1	A	421	LEU
1	A	453	VAL
2	B	146	THR
2	B	215	ASN
1	C	23	LEU
1	C	166	TYR
1	C	270	LEU
1	C	288	TYR
2	D	22	MET
2	D	215	ASN
2	D	341	LEU
1	E	23	LEU
1	E	136	GLU
1	E	166	TYR
1	E	270	LEU
1	E	288	TYR
2	F	215	ASN
2	F	344	ILE
2	F	398	SER
2	F	423	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	451	GLN
1	C	2	ASN
2	D	428	GLN
1	E	197	GLN
1	E	395	GLN
2	F	316	ASN
2	F	342	GLN
2	F	428	GLN
2	F	449	ASN

5.3.3 RNA

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)

14 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	$\#\|Z\|>2$
6	NAG	B	3320	2,6	14,14,15	0.51	0	15,19,21	0.97	1 (6%)
6	NAG	B	3321	6	14,14,15	0.52	0	15,19,21	0.51	0
6	MAN	B	3322	6	11,11,12	0.57	0	14,15,17	0.75	0
6	MAN	B	3323	6	11,11,12	0.56	0	14,15,17	0.72	0
6	MAN	B	3324	6	11,11,12	0.53	0	14,15,17	0.74	0
8	NAG	D	3320	8,2	14,14,15	0.54	0	15,19,21	0.90	1 (6%)
8	NAG	D	3321	8	14,14,15	0.42	0	15,19,21	0.82	0
8	MAN	D	3322	8	11,11,12	0.56	0	14,15,17	0.49	0
8	MAN	D	3323	8	11,11,12	0.56	0	14,15,17	0.63	0
6	NAG	F	3320	2,6	14,14,15	0.55	0	15,19,21	0.82	1 (6%)
6	NAG	F	3321	6	14,14,15	0.49	0	15,19,21	0.56	0
6	MAN	F	3322	6	11,11,12	0.54	0	14,15,17	0.58	0
6	MAN	F	3323	6	11,11,12	0.51	0	14,15,17	0.69	0
6	MAN	F	3324	6	11,11,12	0.53	0	14,15,17	0.77	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	B	3320	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	3321	6	-	0/6/23/26	0/1/1/1
6	MAN	B	3322	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	B	3323	6	-	0/2/19/22	0/1/1/1
6	MAN	B	3324	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	D	3320	8,2	-	0/6/23/26	0/1/1/1
8	NAG	D	3321	8	-	0/6/23/26	0/1/1/1
8	MAN	D	3322	8	1/1/4/5	0/2/19/22	0/1/1/1
8	MAN	D	3323	8	-	0/2/19/22	0/1/1/1
6	NAG	F	3320	2,6	-	0/6/23/26	0/1/1/1
6	NAG	F	3321	6	-	0/6/23/26	0/1/1/1
6	MAN	F	3322	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	F	3323	6	-	0/2/19/22	0/1/1/1
6	MAN	F	3324	6	-	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})
6	F	3320	NAG	C1-O5-C5	2.19	115.03	112.25
8	D	3320	NAG	C1-O5-C5	2.66	115.62	112.25
6	B	3320	NAG	C1-O5-C5	3.09	116.17	112.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	3322	MAN	C1
6	F	3322	MAN	C1
8	D	3322	MAN	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

Of 35 ligands modelled in this entry, 24 are monoatomic - leaving 11 for Mogul analysis.

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	$\#\|Z\|>2$
4	NAG	A	3015	1	14,14,15	0.58	0	15,19,21	0.60	0
4	NAG	B	3099	2	14,14,15	0.55	0	15,19,21	0.54	0
4	NAG	B	3371	2	14,14,15	0.47	0	15,19,21	0.51	0
7	CAC	B	462	-	0,4,4	0.00	-	0,6,6	0.00	-
4	NAG	C	3015	1	14,14,15	0.45	0	15,19,21	0.65	0
4	NAG	D	3099	2	14,14,15	0.63	0	15,19,21	0.65	0
4	NAG	D	3371	2	14,14,15	0.44	0	15,19,21	0.54	0
7	CAC	D	462	-	0,4,4	0.00	-	0,6,6	0.00	-
4	NAG	E	3015	1	14,14,15	0.61	0	15,19,21	0.61	0
4	NAG	F	3371	2	14,14,15	0.50	0	15,19,21	0.61	0
7	CAC	F	462	-	0,4,4	0.00	-	0,6,6	0.00	-

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
4	NAG	A	3015	1	-	0/6/23/26	0/1/1/1
4	NAG	B	3099	2	-	0/6/23/26	0/1/1/1
4	NAG	B	3371	2	-	0/6/23/26	0/1/1/1
7	CAC	B	462	-	-	0/0/0/0	0/0/0/0
4	NAG	C	3015	1	-	0/6/23/26	0/1/1/1
4	NAG	D	3099	2	-	0/6/23/26	0/1/1/1
4	NAG	D	3371	2	-	0/6/23/26	0/1/1/1
7	CAC	D	462	-	-	0/0/0/0	0/0/0/0
4	NAG	E	3015	1	-	0/6/23/26	0/1/1/1
4	NAG	F	3371	2	-	0/6/23/26	0/1/1/1
7	CAC	F	462	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3371	NAG	1	0
4	D	3371	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	3371	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	457/457 (100%)	0.17	7 (1%)	76	74	37, 53, 90, 144	0
1	C	451/457 (98%)	0.15	3 (0%)	89	88	37, 52, 85, 133	0
1	E	452/457 (98%)	0.15	3 (0%)	89	88	39, 52, 85, 133	0
2	B	455/461 (98%)	0.30	16 (3%)	48	40	45, 80, 125, 139	1 (0%)
2	D	455/461 (98%)	0.31	8 (1%)	71	68	45, 80, 125, 139	1 (0%)
2	F	455/461 (98%)	0.46	32 (7%)	19	13	45, 80, 124, 139	1 (0%)
All	All	2725/2754 (98%)	0.26	69 (2%)	61	55	37, 60, 122, 144	3 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	LEU	4.9
1	C	337	PRO	4.7
1	E	452	PRO	4.6
2	F	31	LEU	4.6
2	F	454	THR	4.3
2	B	446	HIS	4.3
2	F	461	ARG	4.2
2	F	446	HIS	4.1
2	F	448	CYS	4.1
2	F	72	LYS	4.1
2	B	453	GLY	4.0
2	F	444	ASN	3.9
2	F	443	PRO	3.9
2	F	453	GLY	3.9
2	F	460	CYS	3.9
2	B	452	ASN	3.8
2	D	79	GLN	3.7
1	C	452	PRO	3.6
2	F	450	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	72	LYS	3.5
2	F	107	VAL	3.4
1	A	455	LYS	3.4
2	D	408	GLN	3.4
1	A	453	VAL	3.2
1	C	338	HIS	3.2
2	B	450	ASN	3.2
2	D	375	LEU	3.2
2	D	446	HIS	3.1
2	B	410	LYS	3.1
2	B	451	GLY	3.1
2	F	375	LEU	2.9
2	D	107	VAL	2.9
2	D	407	PRO	2.8
2	D	450	ASN	2.7
2	F	36	PRO	2.7
2	B	443	PRO	2.7
2	F	425	LEU	2.7
2	F	90	LEU	2.6
2	F	79	GLN	2.6
1	A	1	LEU	2.6
2	F	29	GLU	2.6
2	B	416	ILE	2.6
2	F	80	VAL	2.5
2	F	441	ALA	2.5
2	B	33	LEU	2.4
2	B	142	MET	2.4
2	F	142	MET	2.4
2	B	408	GLN	2.4
2	F	14	GLN	2.4
2	B	449	ASN	2.4
1	E	337	PRO	2.3
1	A	454	VAL	2.3
1	A	337	PRO	2.3
2	B	426	ILE	2.3
2	F	52	GLU	2.2
2	B	31	LEU	2.2
2	F	439	ALA	2.2
2	F	48	ASN	2.2
2	F	28	ASP	2.2
2	F	83	VAL	2.2
2	F	459	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	28	ASP	2.1
2	F	416	ILE	2.1
1	A	7	GLN	2.1
2	D	461	ARG	2.1
2	F	69	LEU	2.1
2	B	448	CYS	2.1
2	F	138	LEU	2.1
2	F	49	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
6	NAG	B	3320	14/15	0.94	0.16	-	55,62,65,72	0
6	MAN	F	3323	11/12	0.93	0.20	-	111,117,120,121	0
8	MAN	D	3323	11/12	0.91	0.29	-	106,113,114,115	0
6	MAN	B	3322	11/12	0.77	0.28	-	118,126,137,144	0
6	MAN	F	3322	11/12	0.86	0.25	-	118,123,135,142	0
8	MAN	D	3322	11/12	0.84	0.23	-	106,114,118,119	0
6	NAG	B	3321	14/15	0.93	0.18	-	80,86,96,108	0
6	MAN	F	3324	11/12	0.68	0.45	-	144,146,147,147	0
6	NAG	F	3321	14/15	0.94	0.16	-	89,98,102,110	0
6	MAN	B	3324	11/12	0.63	0.39	-	147,148,149,149	0
8	NAG	D	3321	14/15	0.94	0.18	-	89,94,99,103	0
8	NAG	D	3320	14/15	0.95	0.14	-	49,59,68,80	0
6	MAN	B	3323	11/12	0.84	0.24	-	119,125,127,127	0
6	NAG	F	3320	14/15	0.95	0.17	-	52,62,73,78	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, 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	CA	B	2003	1/1	1.00	0.23	3.78	37,37,37,37	0
3	CA	D	2003	1/1	0.99	0.24	3.01	40,40,40,40	0
7	CAC	B	462	5/5	0.96	0.25	2.57	103,106,109,109	0
7	CAC	F	462	5/5	0.94	0.23	1.68	122,122,124,126	0
3	CA	F	2003	1/1	0.99	0.23	1.25	42,42,42,42	0
7	CAC	D	462	5/5	0.95	0.21	0.97	91,96,99,101	0
4	NAG	F	3371	14/15	0.88	0.26	0.62	117,123,126,127	0
3	CA	E	2004	1/1	0.98	0.21	0.36	57,57,57,57	0
3	CA	C	2004	1/1	1.00	0.18	0.19	53,53,53,53	0
4	NAG	B	3371	14/15	0.87	0.19	0.13	112,118,120,120	0
3	CA	E	2005	1/1	0.95	0.18	0.12	42,42,42,42	0
5	MG	B	2001	1/1	0.97	0.18	-0.37	39,39,39,39	0
3	CA	C	2005	1/1	0.98	0.17	-0.41	43,43,43,43	0
4	NAG	D	3371	14/15	0.83	0.17	-0.51	92,111,115,115	0
5	MG	F	2001	1/1	0.96	0.15	-0.64	37,37,37,37	0
3	CA	E	2006	1/1	0.98	0.16	-0.71	62,62,62,62	0
3	CA	C	2006	1/1	0.95	0.14	-0.72	63,63,63,63	0
3	CA	A	2004	1/1	0.99	0.14	-0.73	56,56,56,56	0
3	CA	A	2006	1/1	0.94	0.14	-1.03	61,61,61,61	0
3	CA	A	2005	1/1	0.96	0.12	-1.31	66,66,66,66	0
3	CA	A	2007	1/1	0.96	0.06	-2.06	74,74,74,74	0
3	CA	C	2007	1/1	0.94	0.07	-2.20	78,78,78,78	0
5	MG	D	2001	1/1	0.93	0.15	-2.41	43,43,43,43	0
3	CA	E	2007	1/1	0.97	0.04	-3.12	65,65,65,65	0
4	NAG	C	3015	14/15	0.85	0.25	-	117,124,126,127	0
5	MG	A	458	1/1	0.97	0.05	-	61,61,61,61	0
4	NAG	A	3015	14/15	0.74	0.39	-	118,126,129,131	0
5	MG	C	458	1/1	0.96	0.02	-	72,72,72,72	0
4	NAG	B	3099	14/15	0.77	0.31	-	131,136,139,141	0
3	CA	D	2002	1/1	0.93	0.16	-	74,74,74,74	0
4	NAG	E	3015	14/15	0.77	0.32	-	104,106,108,108	14
4	NAG	D	3099	14/15	0.81	0.36	-	128,131,135,135	0
5	MG	E	458	1/1	0.96	0.06	-	68,68,68,68	0
3	CA	F	2002	1/1	0.98	0.11	-	66,66,66,66	0
3	CA	B	2002	1/1	0.90	0.15	-	72,72,72,72	0

6.5 Other polymers (i)

There are no such residues in this entry.