Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:50 PM GMT

PDB ID	:	3V4P
Title	:	crystal structure of a4b7 headpiece complexed with Fab ACT-1
Authors	:	Yu, Y.; Zhu, J.; Springer, T.A.
Deposited on	:	2011-12-15
Resolution	:	3.15 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:

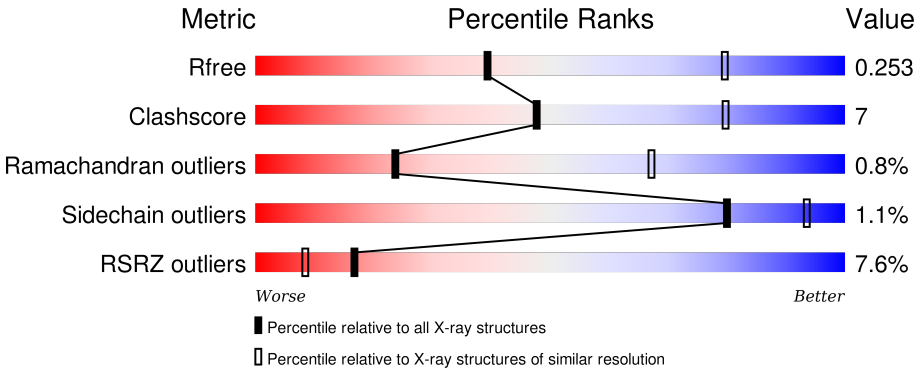
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.15 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	597	75% 22%
1	C	597	74% 22%
2	B	503	3% 61% 13% 25%
2	D	503	5% 62% 13% 25%
3	H	219	14% 83% 13%

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Mol	Chain	Length	Quality of chain
3	M	219	12% 86% 10%
4	L	217	28% 85% 14%
4	N	217	23% 87% 13%

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
5	CA	A	602	-	-	-	X
5	CA	A	603	-	-	-	X
8	15P	A	612	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21722 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-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	14	0	0
			4493	2834	773	864	22			
1	C	581	Total	C	N	O	S	19	0	0
			4496	2835	776	863	22			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	558	ALA	ARG	ENGINEERED MUTATION	UNP P13612
A	588	THR	-	EXPRESSION TAG	UNP P13612
A	589	GLY	-	EXPRESSION TAG	UNP P13612
A	590	GLY	-	EXPRESSION TAG	UNP P13612
A	591	LEU	-	EXPRESSION TAG	UNP P13612
A	592	GLU	-	EXPRESSION TAG	UNP P13612
A	593	ASN	-	EXPRESSION TAG	UNP P13612
A	594	LEU	-	EXPRESSION TAG	UNP P13612
A	595	TYR	-	EXPRESSION TAG	UNP P13612
A	596	PHE	-	EXPRESSION TAG	UNP P13612
A	597	GLN	-	EXPRESSION TAG	UNP P13612
C	558	ALA	ARG	ENGINEERED MUTATION	UNP P13612
C	588	THR	-	EXPRESSION TAG	UNP P13612
C	589	GLY	-	EXPRESSION TAG	UNP P13612
C	590	GLY	-	EXPRESSION TAG	UNP P13612
C	591	LEU	-	EXPRESSION TAG	UNP P13612
C	592	GLU	-	EXPRESSION TAG	UNP P13612
C	593	ASN	-	EXPRESSION TAG	UNP P13612
C	594	LEU	-	EXPRESSION TAG	UNP P13612
C	595	TYR	-	EXPRESSION TAG	UNP P13612
C	596	PHE	-	EXPRESSION TAG	UNP P13612
C	597	GLN	-	EXPRESSION TAG	UNP P13612

- Molecule 2 is a protein called Integrin beta-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	375	Total	C	N	O	S	6	2	0
			2922	1828	519	563	12			
2	D	375	Total	C	N	O	S	0	1	0
			2916	1824	518	562	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	494	SER	-	EXPRESSION TAG	UNP P26010
B	495	ARG	-	EXPRESSION TAG	UNP P26010
B	496	GLY	-	EXPRESSION TAG	UNP P26010
B	497	LEU	-	EXPRESSION TAG	UNP P26010
B	498	GLU	-	EXPRESSION TAG	UNP P26010
B	499	ASN	-	EXPRESSION TAG	UNP P26010
B	500	LEU	-	EXPRESSION TAG	UNP P26010
B	501	TYR	-	EXPRESSION TAG	UNP P26010
B	502	PHE	-	EXPRESSION TAG	UNP P26010
B	503	GLN	-	EXPRESSION TAG	UNP P26010
D	494	SER	-	EXPRESSION TAG	UNP P26010
D	495	ARG	-	EXPRESSION TAG	UNP P26010
D	496	GLY	-	EXPRESSION TAG	UNP P26010
D	497	LEU	-	EXPRESSION TAG	UNP P26010
D	498	GLU	-	EXPRESSION TAG	UNP P26010
D	499	ASN	-	EXPRESSION TAG	UNP P26010
D	500	LEU	-	EXPRESSION TAG	UNP P26010
D	501	TYR	-	EXPRESSION TAG	UNP P26010
D	502	PHE	-	EXPRESSION TAG	UNP P26010
D	503	GLN	-	EXPRESSION TAG	UNP P26010

- Molecule 3 is a protein called MONOCLONAL ANTIBODY Act-1 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	211	Total	C	N	O	S	0	0	0
			1607	1021	258	321	7			
3	M	211	Total	C	N	O	S	0	0	0
			1607	1021	258	321	7			

- Molecule 4 is a protein called MONOCLONAL ANTIBODY Act-1 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	217	Total	C	N	O	S	0	0	0
			1681	1054	282	339	6			

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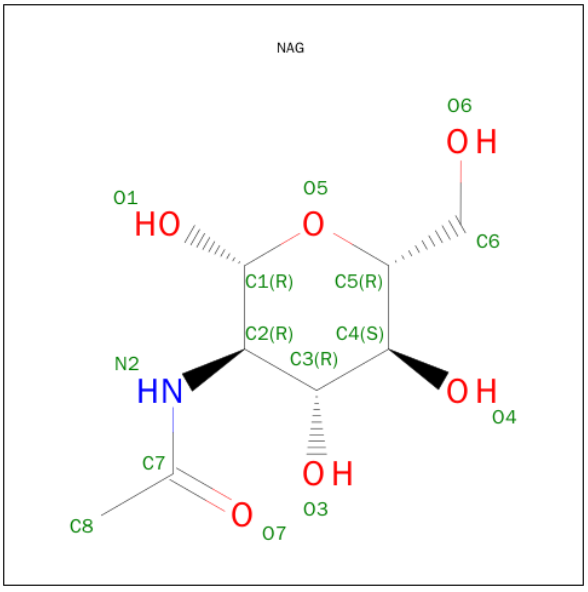
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	217	Total	C	N	O	S	0	0	0
			1681	1054	282	339	6			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Ca	0	0
			2	2		
5	A	3	Total	Ca	0	0
			3	3		
5	D	2	Total	Ca	0	0
			2	2		
5	C	3	Total	Ca	0	0
			3	3		

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



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

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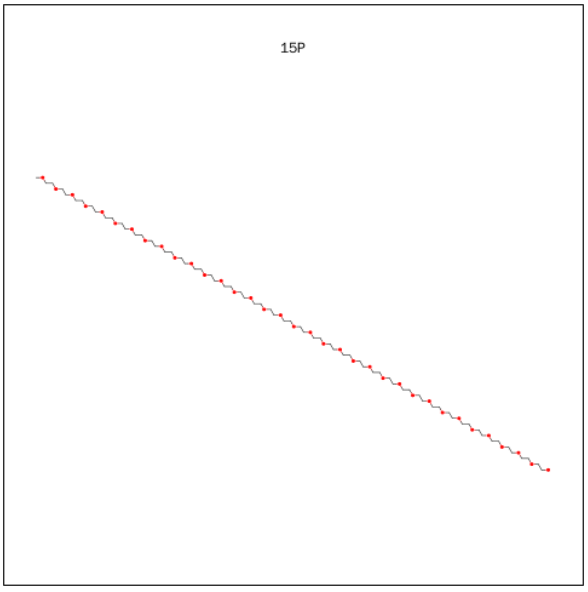
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 8 is POLYETHYLENE GLYCOL (N=34) (three-letter code: 15P) (formula: $C_{69}H_{140}O_{35}$).

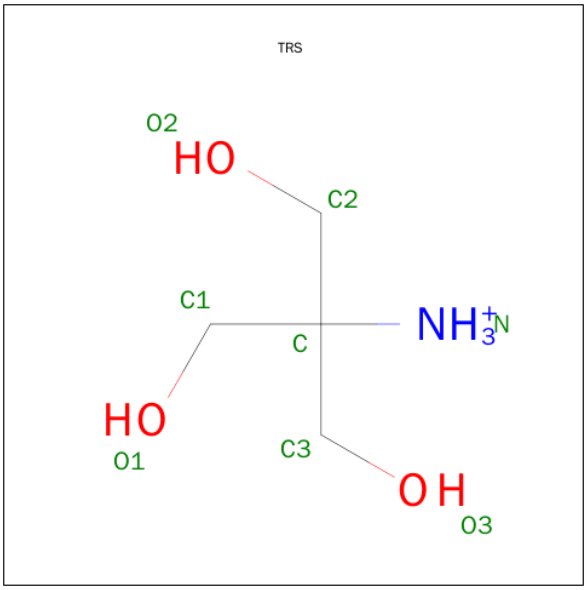


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 52 34 18	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Mg 1 1	0	0
9	D	1	Total Mg 1 1	0	0

- Molecule 10 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total C N O 8 4 1 3	0	0

- Molecule 11 is water.

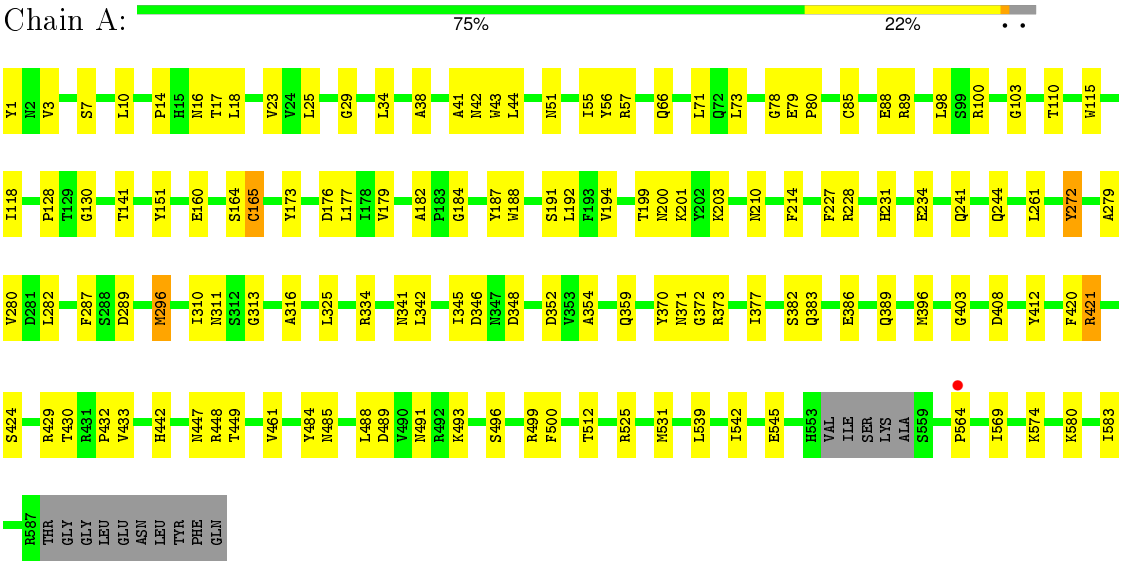
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	4	Total O 4 4	0	0
11	B	7	Total O 7 7	0	0
11	C	3	Total O 3 3	0	0
11	D	7	Total O 7 7	0	0

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.

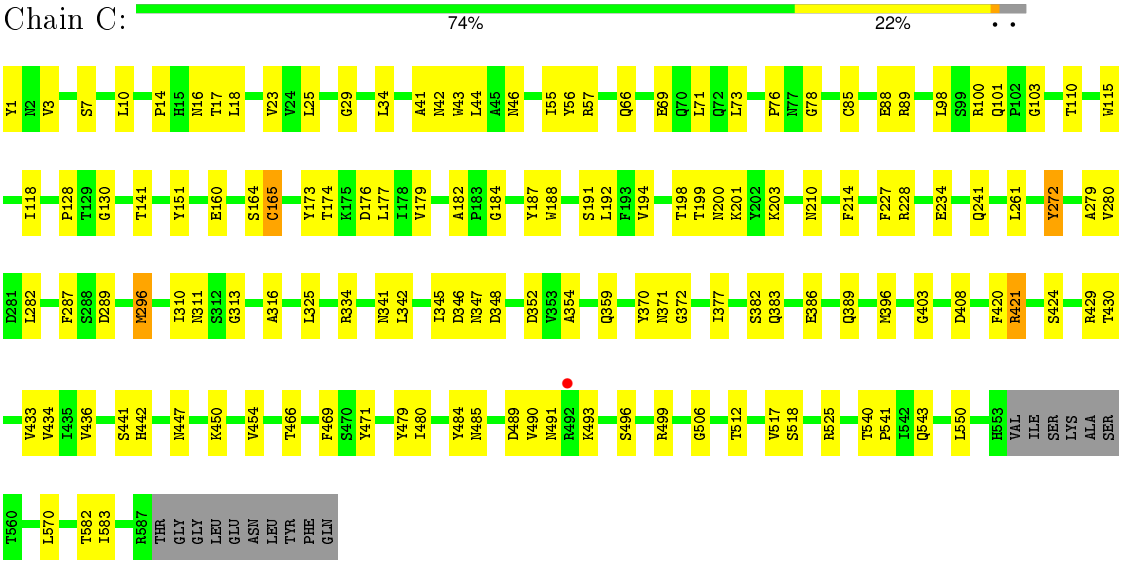
- Molecule 1: Integrin alpha-4

Chain A:



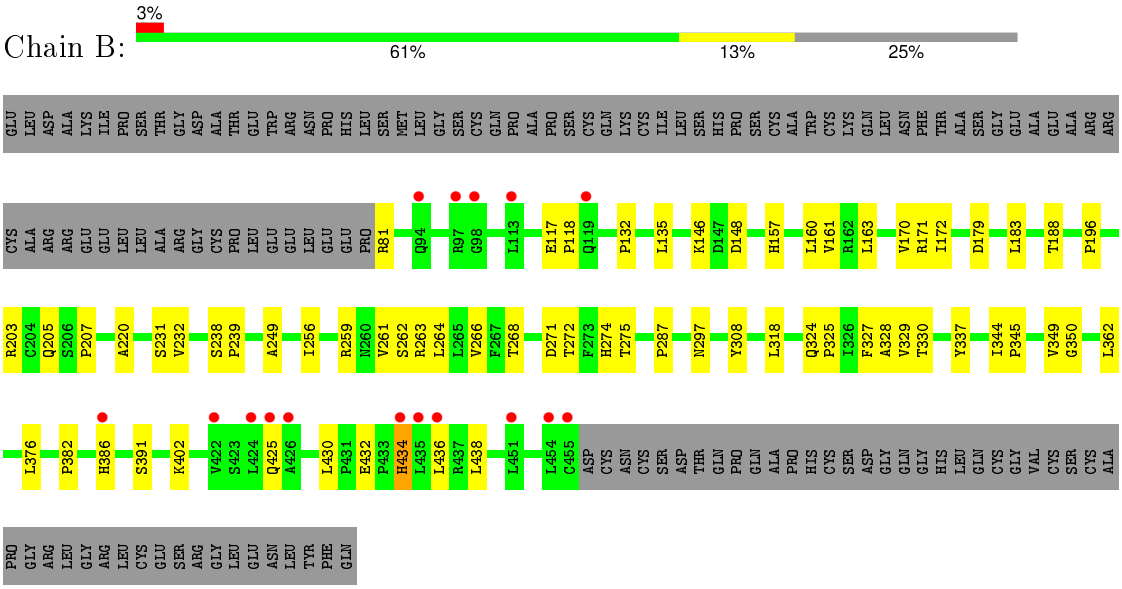
- Molecule 1: Integrin alpha-4

Chain C:



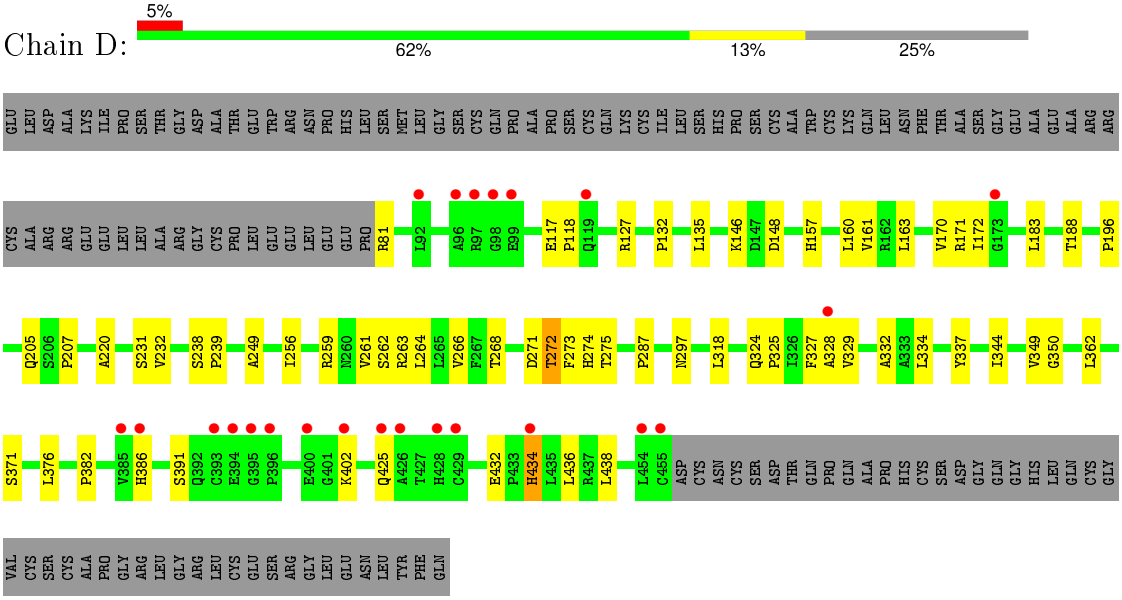
- Molecule 2: Integrin beta-7

Chain B:



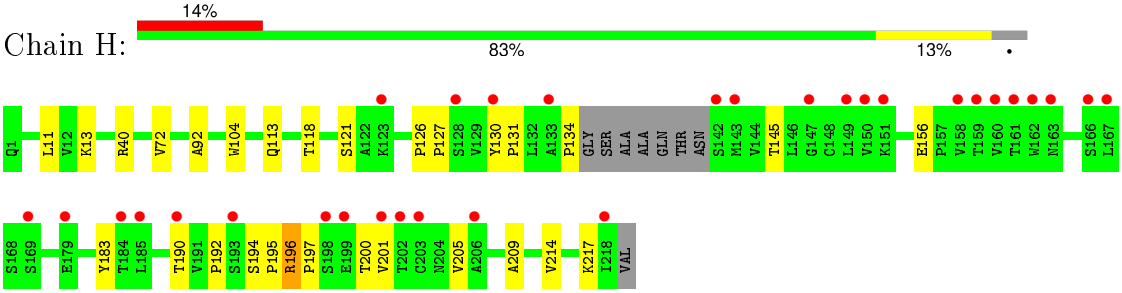
- Molecule 2: Integrin beta-7

Chain D:



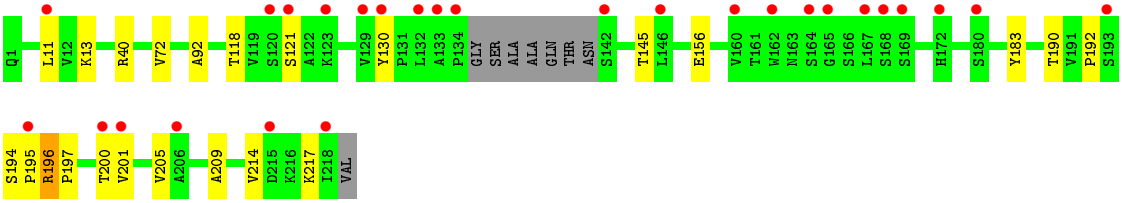
- Molecule 3: MONOCLONAL ANTIBODY Act-1 HEAVY CHAIN

Chain H:

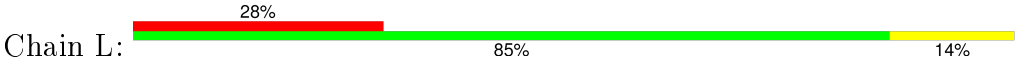


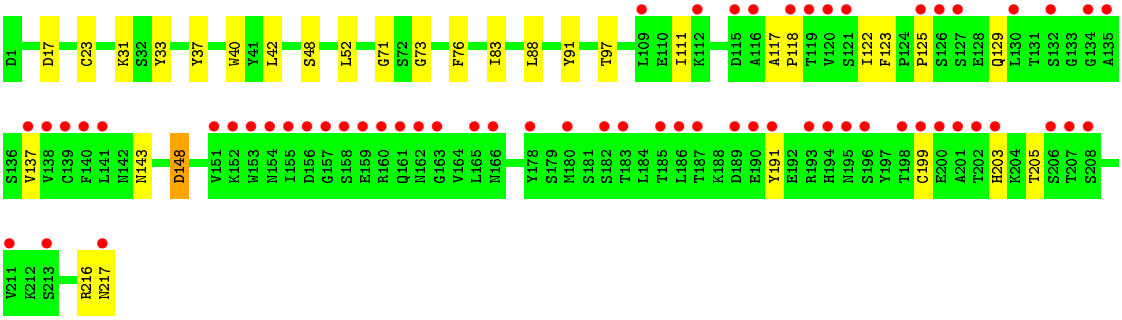
- Molecule 3: MONOCLONAL ANTIBODY Act-1 HEAVY CHAIN

Chain M:

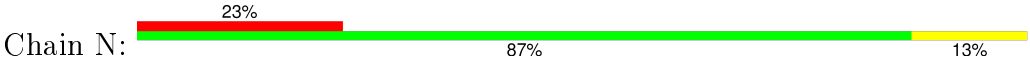


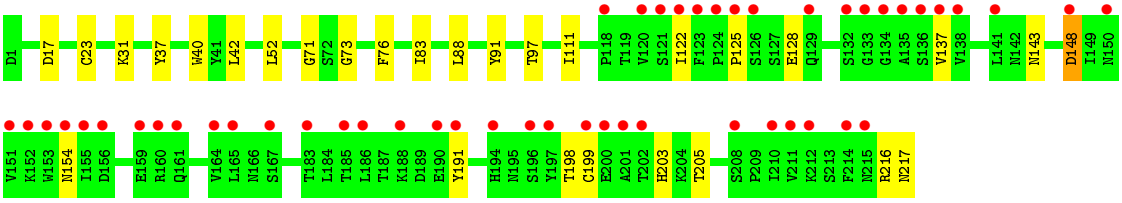
• Molecule 4: MONOCLONAL ANTIBODY Act-1 LIGHT CHAIN





• Molecule 4: MONOCLONAL ANTIBODY Act-1 LIGHT CHAIN





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	137.78Å 122.74Å 158.14Å 90.00° 115.38° 90.00°	Depositor
Resolution (Å)	46.13 – 3.15 46.13 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.13-3.15) 99.4 (46.13-3.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.220 , 0.251 0.224 , 0.253	Depositor DCC
R_{free} test set	1067 reflections (1.32%)	DCC
Wilson B-factor (Å^2)	54.1	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 84.5	EDS
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 82061 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	21722	wwPDB-VP
Average B, all atoms (Å^2)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: 15P, MG, BMA, NAG, CA, TRS, 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	0.25	0/4593	0.45	1/6221 (0.0%)
1	C	0.25	0/4596	0.45	1/6224 (0.0%)
2	B	0.23	0/2984	0.41	0/4053
2	D	0.23	0/2978	0.41	0/4044
3	H	0.22	0/1652	0.40	0/2259
3	M	0.22	0/1652	0.40	0/2259
4	L	0.22	0/1722	0.38	0/2340
4	N	0.22	0/1722	0.38	0/2340
All	All	0.23	0/21899	0.42	2/29740 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	348	ASP	CB-CG-OD1	5.16	122.94	118.30
1	C	348	ASP	CB-CG-OD1	5.11	122.90	118.30

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	4493	0	4351	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4496	0	4361	91	0
2	B	2922	0	2848	41	0
2	D	2916	0	2842	39	0
3	H	1607	0	1552	18	0
3	M	1607	0	1552	12	0
4	L	1681	0	1616	20	0
4	N	1681	0	1616	16	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
5	C	3	0	0	0	0
5	D	2	0	0	0	0
6	A	56	0	52	0	0
6	B	14	0	13	0	0
6	C	56	0	52	1	0
7	A	50	0	43	1	0
7	C	50	0	43	1	0
8	A	52	0	69	17	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	C	8	0	12	0	0
11	A	4	0	0	4	0
11	B	7	0	0	1	0
11	C	3	0	0	4	0
11	D	7	0	0	0	0
All	All	21722	0	21022	315	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 (315) 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:M:196:ARG:HD2	3:M:197:PRO:HA	1.59	0.83
3:H:196:ARG:HD2	3:H:197:PRO:HA	1.59	0.82
1:A:372:GLY:O	11:A:702:HOH:O	1.99	0.79
1:A:372:GLY:HA2	1:A:377:ILE:HG22	1.65	0.77
1:C:372:GLY:HA2	1:C:377:ILE:HG22	1.65	0.76
2:B:160:LEU:HD22	2:B:220:ALA:HB2	1.67	0.76
2:D:160:LEU:HD22	2:D:220:ALA:HB2	1.67	0.75
1:C:442:HIS:HE1	1:C:583:ILE:HB	1.53	0.74
1:A:442:HIS:HE1	1:A:583:ILE:HB	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:GLY:HA3	2:B:362:LEU:HD11	1.72	0.72
2:D:327:PHE:HB2	2:D:349:VAL:HG22	1.71	0.72
2:D:350:GLY:HA3	2:D:362:LEU:HD11	1.72	0.72
1:A:311:ASN:O	11:A:701:HOH:O	2.07	0.71
1:C:241:GLN:HE22	2:D:275:THR:HB	1.55	0.71
2:B:327:PHE:HB2	2:B:349:VAL:HG22	1.71	0.71
1:A:71:LEU:HB3	1:A:141:THR:HG21	1.73	0.71
1:C:71:LEU:HB3	1:C:141:THR:HG21	1.73	0.70
8:A:612:15P:H101	1:C:42:ASN:HD22	1.56	0.70
1:A:442:HIS:CE1	1:A:583:ILE:HB	2.26	0.69
1:A:16:ASN:HD22	8:A:612:15P:H252	1.57	0.68
2:D:146:LYS:HA	2:D:232:VAL:HG11	1.73	0.68
1:A:88:GLU:HB2	1:A:118:ILE:HG13	1.76	0.68
2:B:146:LYS:HA	2:B:232:VAL:HG11	1.74	0.68
1:C:88:GLU:HB2	1:C:118:ILE:HG13	1.76	0.67
1:C:372:GLY:O	11:C:702:HOH:O	2.13	0.67
1:C:430:THR:N	11:C:703:HOH:O	2.27	0.67
8:A:612:15P:H132	1:C:44:LEU:HD21	1.77	0.66
4:L:88:LEU:HD11	4:L:111:ILE:HD11	1.78	0.66
4:N:88:LEU:HD11	4:N:111:ILE:HD11	1.78	0.66
8:A:612:15P:H111	1:C:42:ASN:H	1.61	0.65
2:B:118:PRO:HB3	2:B:425:GLN:HB3	1.78	0.65
1:A:1:TYR:HA	1:A:383:GLN:HB2	1.79	0.64
1:C:1:TYR:HA	1:C:383:GLN:HB2	1.79	0.64
2:D:118:PRO:HB3	2:D:425:GLN:HB3	1.78	0.64
1:A:199:THR:O	1:A:201:LYS:N	2.31	0.63
2:D:382:PRO:HD3	2:D:436:LEU:HD21	1.80	0.63
1:C:199:THR:O	1:C:201:LYS:N	2.32	0.62
2:D:163:LEU:HB3	2:D:170:VAL:HG11	1.81	0.62
2:B:382:PRO:HD3	2:B:436:LEU:HD21	1.80	0.62
4:L:17:ASP:H	4:L:83:ILE:HG22	1.65	0.62
3:M:13:LYS:HG2	3:M:121:SER:HA	1.83	0.61
4:N:17:ASP:H	4:N:83:ILE:HG22	1.65	0.60
2:B:163:LEU:HB3	2:B:170:VAL:HG11	1.81	0.60
3:H:40:ARG:HG2	3:H:92:ALA:HB2	1.83	0.60
3:M:40:ARG:HG2	3:M:92:ALA:HB2	1.82	0.59
1:C:128:PRO:HD2	1:C:164:SER:HB3	1.85	0.59
1:A:128:PRO:HD2	1:A:164:SER:HB3	1.85	0.59
1:C:543:GLN:HG2	1:C:582:THR:HB	1.86	0.58
1:A:56:TYR:HE2	8:A:612:15P:H191	1.68	0.57
3:H:130:TYR:CG	4:L:129:GLN:HG2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ASN:O	11:C:701:HOH:O	2.18	0.57
1:A:17:THR:HB	1:A:41:ALA:HB2	1.86	0.57
4:L:216:ARG:HG2	4:L:217:ASN:H	1.71	0.56
1:A:545:GLU:HG2	1:A:580:LYS:HG2	1.86	0.56
3:M:200:THR:HG23	3:M:217:LYS:HD3	1.87	0.56
4:N:148:ASP:N	4:N:148:ASP:OD1	2.39	0.56
1:C:17:THR:HB	1:C:41:ALA:HB2	1.87	0.56
1:C:14:PRO:HB2	1:C:17:THR:HG21	1.88	0.56
3:H:200:THR:HG23	3:H:217:LYS:HD3	1.87	0.55
1:A:287:PHE:HB3	1:A:311:ASN:ND2	2.20	0.55
1:A:14:PRO:HB2	1:A:17:THR:HG21	1.89	0.55
2:B:132:PRO:HB2	2:B:261:VAL:HG11	1.87	0.55
1:A:100:ARG:NH2	1:A:103:GLY:O	2.40	0.55
4:L:148:ASP:OD1	4:L:148:ASP:N	2.39	0.55
1:C:493:LYS:HB2	1:C:496:SER:HB2	1.89	0.55
1:C:228:ARG:HD3	1:C:261:LEU:HD11	1.87	0.55
1:C:287:PHE:HB3	1:C:311:ASN:ND2	2.22	0.54
2:B:376:LEU:HD11	2:B:438:LEU:HB3	1.90	0.54
1:C:371:ASN:HB3	11:C:702:HOH:O	2.07	0.54
1:C:100:ARG:NH2	1:C:103:GLY:O	2.40	0.54
1:A:342:LEU:HB3	1:A:352:ASP:O	2.08	0.54
4:L:122:ILE:HD12	4:L:199:CYS:HB2	1.90	0.54
1:A:56:TYR:CE2	8:A:612:15P:H191	2.42	0.54
1:C:447:ASN:HB3	1:C:450:LYS:HG2	1.89	0.54
1:C:359:GLN:HE21	2:D:287:PRO:HG3	1.71	0.54
1:A:346:ASP:HB2	1:A:433:VAL:HG11	1.90	0.54
1:A:228:ARG:HD3	1:A:261:LEU:HD11	1.88	0.54
1:C:442:HIS:CE1	1:C:583:ILE:HB	2.39	0.54
2:D:264:LEU:HD23	2:D:324:GLN:HB2	1.90	0.54
2:B:135:LEU:HD11	2:B:266:VAL:HG23	1.89	0.54
2:D:376:LEU:HD11	2:D:438:LEU:HB3	1.90	0.54
2:D:135:LEU:HD11	2:D:266:VAL:HG23	1.89	0.53
1:A:228:ARG:HH11	1:A:261:LEU:HD11	1.74	0.53
2:B:264:LEU:HD23	2:B:324:GLN:HB2	1.90	0.53
4:N:122:ILE:HD12	4:N:199:CYS:HB2	1.90	0.53
2:B:205:GLN:HE21	2:B:231:SER:H	1.57	0.53
2:D:135:LEU:HB3	2:D:172:ILE:HG22	1.91	0.53
1:C:469:PHE:HB2	1:C:517:VAL:HG21	1.90	0.53
3:H:130:TYR:CD1	4:L:129:GLN:HG2	2.44	0.53
3:H:205:VAL:HB	3:H:214:VAL:HG13	1.91	0.53
3:M:205:VAL:HB	3:M:214:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:LEU:HB3	1:C:352:ASP:O	2.08	0.52
1:A:461:VAL:HG13	1:A:531:MET:HB3	1.91	0.52
1:A:491:ASN:HD21	1:A:542:ILE:HA	1.75	0.52
2:B:183:LEU:HG	2:B:188:THR:HG23	1.92	0.52
1:C:228:ARG:HH11	1:C:261:LEU:HD11	1.74	0.52
1:A:493:LYS:HB2	1:A:496:SER:HB2	1.92	0.52
2:D:183:LEU:HG	2:D:188:THR:HG23	1.92	0.52
2:D:205:GLN:HE21	2:D:231:SER:H	1.57	0.52
1:A:57:ARG:HD3	1:A:71:LEU:HD21	1.92	0.52
1:A:408:ASP:OD2	1:A:429:ARG:HD2	2.10	0.52
2:D:238:SER:N	2:D:239:PRO:HD2	2.25	0.52
2:B:261:VAL:O	2:B:263:ARG:HG3	2.10	0.51
2:B:238:SER:N	2:B:239:PRO:HD2	2.24	0.51
2:B:135:LEU:HB3	2:B:172:ILE:HG22	1.92	0.51
1:A:184:GLY:HA2	1:A:188:TRP:CD1	2.45	0.51
1:C:57:ARG:HD3	1:C:71:LEU:HD21	1.92	0.51
1:C:184:GLY:HA2	1:C:188:TRP:CD1	2.46	0.51
4:N:216:ARG:HG2	4:N:217:ASN:H	1.75	0.51
8:A:612:15P:H14	1:C:16:ASN:HD21	1.75	0.51
2:D:261:VAL:O	2:D:263:ARG:HG3	2.10	0.51
1:C:491:ASN:C	1:C:493:LYS:H	2.14	0.51
1:C:18:LEU:HD22	1:C:420:PHE:HD2	1.76	0.51
1:C:408:ASP:OD2	1:C:429:ARG:HD2	2.11	0.51
1:C:485:ASN:HB3	1:C:512:THR:HG22	1.93	0.50
2:B:330:THR:HG21	11:B:2106:HOH:O	2.11	0.50
1:A:41:ALA:HA	8:A:612:15P:H231	1.92	0.50
1:C:272:TYR:HB2	1:C:296:MET:HB2	1.94	0.50
1:A:396:MET:HG3	1:A:421:ARG:HG3	1.92	0.50
2:D:127:ARG:NH2	2:D:371:SER:OG	2.44	0.50
1:A:241:GLN:HE22	2:B:275:THR:HB	1.77	0.50
2:B:261:VAL:HG12	2:B:262:SER:N	2.27	0.50
1:C:179:VAL:HG22	1:C:194:VAL:HG12	1.93	0.50
1:A:210:ASN:ND2	1:A:210:ASN:O	2.45	0.50
1:A:359:GLN:HE21	2:B:287:PRO:HG3	1.77	0.50
1:A:489:ASP:OD2	1:A:499:ARG:HD3	2.12	0.50
1:C:342:LEU:HD22	1:C:354:ALA:HB2	1.94	0.49
1:A:231:HIS:CD2	7:A:609:MAN:H62	2.47	0.49
1:C:346:ASP:HB2	1:C:433:VAL:HG11	1.94	0.49
1:A:429:ARG:HH12	1:A:564:PRO:HD2	1.78	0.49
1:A:179:VAL:HG22	1:A:194:VAL:HG12	1.93	0.49
1:A:18:LEU:HD22	1:A:420:PHE:HD2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:TYR:HB2	1:A:296:MET:HB2	1.94	0.49
1:C:10:LEU:HD11	1:C:424:SER:HB2	1.95	0.49
4:N:42:LEU:HB2	4:N:52:LEU:HD11	1.95	0.49
1:A:342:LEU:HD22	1:A:354:ALA:HB2	1.94	0.49
4:L:42:LEU:HB2	4:L:52:LEU:HD11	1.95	0.49
2:D:261:VAL:HG12	2:D:262:SER:N	2.28	0.48
1:C:396:MET:HG3	1:C:421:ARG:HG3	1.94	0.48
1:C:280:VAL:O	1:C:289:ASP:HB2	2.13	0.48
4:L:42:LEU:HD13	4:L:91:TYR:CZ	2.48	0.48
1:C:25:LEU:HD12	1:C:403:GLY:HA2	1.95	0.48
1:C:489:ASP:O	1:C:493:LYS:HE3	2.13	0.48
2:B:268:THR:HA	2:B:328:ALA:O	2.14	0.48
4:L:125:PRO:HD3	4:L:137:VAL:HG22	1.95	0.48
1:A:10:LEU:HD11	1:A:424:SER:HB2	1.96	0.48
1:C:489:ASP:OD2	1:C:499:ARG:HD3	2.13	0.48
2:D:272:THR:OG1	2:D:273:PHE:N	2.45	0.48
1:A:16:ASN:ND2	8:A:612:15P:H252	2.27	0.48
1:A:484:TYR:OH	1:A:525:ARG:HD3	2.13	0.48
2:B:179:ASP:OD1	2:B:308:TYR:OH	2.26	0.48
1:A:280:VAL:O	1:A:289:ASP:HB2	2.13	0.48
1:C:261:LEU:HD13	1:C:316:ALA:HB2	1.96	0.47
4:N:125:PRO:HD3	4:N:137:VAL:HG22	1.95	0.47
4:N:203:HIS:CE1	4:N:205:THR:HG1	2.33	0.47
3:H:156:GLU:HG2	3:H:183:TYR:CE2	2.48	0.47
1:C:334:ARG:HG3	1:C:359:GLN:OE1	2.15	0.47
4:N:71:GLY:HA3	4:N:76:PHE:HA	1.96	0.47
1:C:210:ASN:O	1:C:210:ASN:ND2	2.47	0.47
1:A:1:TYR:HD1	1:A:569:ILE:HD13	1.79	0.47
4:N:42:LEU:HD13	4:N:91:TYR:CZ	2.49	0.47
1:C:436:VAL:HA	1:C:471:TYR:HA	1.96	0.47
2:D:268:THR:HA	2:D:328:ALA:O	2.14	0.47
3:H:13:LYS:HG2	3:H:121:SER:HA	1.96	0.47
1:A:7:SER:HB3	1:A:429:ARG:HH11	1.79	0.47
1:C:194:VAL:HG23	1:C:203:LYS:HB2	1.97	0.47
3:M:156:GLU:HG2	3:M:183:TYR:CE2	2.49	0.47
2:B:196:PRO:HG3	2:B:207:PRO:HD3	1.97	0.47
3:M:145:THR:HG22	3:M:190:THR:HG23	1.97	0.47
1:A:42:ASN:H	8:A:612:15P:C23	2.28	0.47
1:A:23:VAL:HG13	1:A:34:LEU:HD11	1.97	0.47
2:B:132:PRO:HB2	2:B:261:VAL:CG1	2.46	0.47
1:A:334:ARG:HG3	1:A:359:GLN:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:125:PRO:HG2	4:L:191:TYR:CE1	2.50	0.47
2:D:386:HIS:HB2	2:D:425:GLN:HG3	1.96	0.46
1:A:194:VAL:HG23	1:A:203:LYS:HB2	1.97	0.46
2:D:196:PRO:HG3	2:D:207:PRO:HD3	1.95	0.46
2:D:324:GLN:HA	2:D:325:PRO:HD3	1.71	0.46
1:C:7:SER:HB3	1:C:429:ARG:HH11	1.80	0.46
4:N:125:PRO:HG2	4:N:191:TYR:CE1	2.50	0.46
1:A:261:LEU:HD13	1:A:316:ALA:HB2	1.97	0.46
1:C:434:VAL:HG23	1:C:570:LEU:HA	1.97	0.46
4:L:71:GLY:HA3	4:L:76:PHE:HA	1.96	0.46
1:A:227:PHE:HD1	1:A:234:GLU:HB2	1.80	0.46
2:B:329:VAL:HG11	2:B:337:TYR:CD2	2.51	0.46
2:D:325:PRO:HG2	2:D:344:ILE:HG21	1.98	0.46
1:A:165:CYS:HB2	1:A:182:ALA:HB1	1.98	0.46
2:B:203:ARG:HB3	3:H:104:TRP:CD1	2.51	0.46
1:A:25:LEU:HD12	1:A:403:GLY:HA2	1.96	0.46
1:A:371:ASN:HB3	11:A:702:HOH:O	2.16	0.46
1:C:434:VAL:HG23	1:C:570:LEU:HD23	1.98	0.46
1:C:227:PHE:HD1	1:C:234:GLU:HB2	1.80	0.46
1:A:289:ASP:OD1	1:A:310:ILE:HA	2.16	0.46
1:C:479:TYR:HA	1:C:518:SER:HA	1.97	0.46
1:A:429:ARG:HB3	11:A:704:HOH:O	2.15	0.46
1:C:165:CYS:HB2	1:C:182:ALA:HB1	1.98	0.46
1:C:23:VAL:HG13	1:C:34:LEU:HD11	1.97	0.46
1:C:289:ASP:OD1	1:C:310:ILE:HA	2.15	0.46
1:A:227:PHE:CD1	1:A:234:GLU:HB2	2.51	0.46
4:L:203:HIS:CE1	4:L:205:THR:HG1	2.33	0.45
2:B:386:HIS:HB2	2:B:425:GLN:HG3	1.96	0.45
2:B:325:PRO:HG2	2:B:344:ILE:HG21	1.98	0.45
3:H:145:THR:HG22	3:H:190:THR:HG23	1.97	0.45
1:C:85:CYS:HB2	1:C:151:TYR:CE1	2.51	0.45
2:B:432:GLU:HB2	2:B:434:HIS:NE2	2.31	0.45
1:C:73:LEU:HD23	1:C:141:THR:HB	1.98	0.45
1:A:44:LEU:HD22	8:A:612:15P:H131	1.97	0.45
1:C:89:ARG:NH2	6:C:604:NAG:O6	2.42	0.45
1:A:447:ASN:C	1:A:449:THR:H	2.20	0.45
2:D:329:VAL:HG11	2:D:337:TYR:CD2	2.51	0.45
1:A:73:LEU:HD23	1:A:141:THR:HB	1.99	0.45
8:A:612:15P:H161	1:C:69:GLU:HA	1.99	0.45
1:C:227:PHE:CD1	1:C:234:GLU:HB2	2.51	0.45
1:A:85:CYS:HB2	1:A:151:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:PHE:CE2	1:C:313:GLY:HA2	2.51	0.45
1:A:115:TRP:HB3	1:A:130:GLY:HA2	1.97	0.45
1:A:287:PHE:CE2	1:A:313:GLY:HA2	2.52	0.45
1:C:198:THR:HG21	7:C:607:NAG:H82	1.98	0.45
1:C:115:TRP:HB3	1:C:130:GLY:HA2	1.97	0.45
2:D:432:GLU:HB2	2:D:434:HIS:NE2	2.31	0.44
1:C:282:LEU:HD13	1:C:377:ILE:HG23	2.00	0.44
1:C:176:ASP:HB3	1:C:177:LEU:HD12	2.00	0.44
2:D:391:SER:H	2:D:402:LYS:HE3	1.83	0.44
1:A:373:ARG:NH1	1:A:574:LYS:HA	2.32	0.44
1:A:346:ASP:O	1:A:433:VAL:HG21	2.17	0.44
1:C:441:SER:HB2	1:C:466:THR:HB	2.00	0.44
3:H:126:PRO:HA	3:H:127:PRO:HD3	1.85	0.44
3:H:134:PRO:HD3	4:L:123:PHE:CE1	2.52	0.44
1:A:282:LEU:HD13	1:A:377:ILE:HG23	2.00	0.44
1:C:279:ALA:O	1:C:341:ASN:ND2	2.49	0.44
1:A:493:LYS:HD2	1:A:496:SER:HB2	1.99	0.44
1:A:191:SER:O	1:A:192:LEU:HD23	2.18	0.44
1:A:485:ASN:HB3	1:A:512:THR:HG22	2.00	0.44
2:B:171:ARG:HD3	2:B:259:ARG:HD3	2.00	0.44
3:M:201:VAL:O	3:M:217:LYS:HG3	2.18	0.43
2:B:249:ALA:HA	2:B:256:ILE:HD11	1.99	0.43
1:C:480:ILE:HD12	1:C:480:ILE:HA	1.89	0.43
1:A:386:GLU:HG2	1:A:389:GLN:HG3	2.00	0.43
2:B:324:GLN:HA	2:B:325:PRO:HD3	1.71	0.43
1:C:386:GLU:HG2	1:C:389:GLN:HG3	2.00	0.43
3:H:201:VAL:O	3:H:217:LYS:HG3	2.18	0.43
1:A:279:ALA:O	1:A:341:ASN:ND2	2.51	0.43
8:A:612:15P:H152	1:C:56:TYR:HE2	1.84	0.43
2:B:81:ARG:HA	2:B:117:GLU:OE1	2.18	0.43
2:B:391:SER:H	2:B:402:LYS:HE3	1.83	0.43
1:C:442:HIS:HE1	1:C:583:ILE:CB	2.28	0.43
1:C:3:VAL:HA	1:C:430:THR:HA	2.01	0.43
4:N:31:LYS:HE2	4:N:97:THR:HA	1.99	0.43
1:C:98:LEU:HD23	1:C:110:THR:HB	2.00	0.42
1:A:160:GLU:HB3	1:A:187:TYR:CE2	2.54	0.42
1:C:191:SER:O	1:C:192:LEU:HD23	2.18	0.42
1:C:160:GLU:HB3	1:C:187:TYR:CE2	2.54	0.42
1:A:244:GLN:HE21	1:A:244:GLN:HB3	1.71	0.42
2:D:81:ARG:HA	2:D:117:GLU:OE1	2.18	0.42
1:A:98:LEU:HD23	1:A:110:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:130:TYR:HA	3:H:131:PRO:HD3	1.88	0.42
1:A:176:ASP:HB3	1:A:177:LEU:HD12	2.00	0.42
2:D:239:PRO:O	2:D:274:HIS:CD2	2.73	0.42
2:D:171:ARG:HD3	2:D:259:ARG:HD3	2.00	0.42
1:C:43:TRP:CH2	1:C:89:ARG:HD2	2.55	0.42
1:A:412:TYR:CZ	1:A:432:PRO:HA	2.54	0.42
2:D:132:PRO:HB2	2:D:261:VAL:CG1	2.49	0.42
2:D:259:ARG:O	2:D:261:VAL:N	2.53	0.42
3:M:11:LEU:HB3	3:M:118:THR:HB	2.01	0.42
2:D:249:ALA:HA	2:D:256:ILE:HD11	2.00	0.42
4:L:31:LYS:HE2	4:L:97:THR:HA	2.00	0.42
8:A:612:15P:H142	1:C:56:TYR:CE2	2.55	0.42
3:M:194:SER:HB2	3:M:195:PRO:HD3	2.01	0.42
3:M:130:TYR:HD1	4:N:128:GLU:HB2	1.84	0.42
3:H:11:LEU:HB3	3:H:118:THR:HB	2.01	0.42
2:B:259:ARG:O	2:B:261:VAL:N	2.52	0.42
4:N:31:LYS:HE3	4:N:37:TYR:CE2	2.54	0.42
3:M:192:PRO:O	3:M:195:PRO:HD2	2.20	0.42
2:B:318:LEU:HD13	2:B:325:PRO:HG3	2.01	0.41
1:A:43:TRP:CH2	1:A:89:ARG:HD2	2.55	0.41
4:L:117:ALA:HA	4:L:118:PRO:HD3	1.89	0.41
1:A:42:ASN:H	8:A:612:15P:H231	1.85	0.41
3:H:194:SER:HB2	3:H:195:PRO:HD3	2.01	0.41
2:D:318:LEU:HD13	2:D:325:PRO:HG3	2.02	0.41
1:A:10:LEU:O	1:A:66:GLN:HG3	2.20	0.41
4:L:31:LYS:HE3	4:L:37:TYR:CE2	2.55	0.41
1:C:241:GLN:NE2	2:D:275:THR:HB	2.27	0.41
1:C:10:LEU:O	1:C:66:GLN:HG3	2.21	0.41
1:C:325:LEU:HD22	1:C:370:TYR:CE2	2.55	0.41
1:C:46:ASN:ND2	1:C:76:PRO:O	2.50	0.41
1:A:51:ASN:HD21	8:A:612:15P:H261	1.86	0.41
1:A:1:TYR:HB3	1:A:382:SER:HB3	2.03	0.41
1:C:187:TYR:HB2	1:C:214:PHE:CD1	2.56	0.41
1:A:17:THR:HB	1:A:38:ALA:HB1	2.03	0.41
1:C:345:ILE:HG22	1:C:352:ASP:OD2	2.21	0.41
2:B:430:LEU:HD13	2:B:434:HIS:CD2	2.56	0.41
1:A:187:TYR:HB2	1:A:214:PHE:CD1	2.56	0.41
3:H:192:PRO:O	3:H:195:PRO:HD2	2.20	0.41
1:C:540:THR:HA	1:C:541:PRO:HD3	1.88	0.41
1:A:325:LEU:HD22	1:A:370:TYR:CE2	2.56	0.41
3:H:113:GLN:HA	4:L:48:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ILE:HG22	1:A:352:ASP:OD2	2.22	0.40
2:B:344:ILE:HA	2:B:345:PRO:HD3	1.94	0.40
2:B:239:PRO:O	2:B:274:HIS:CD2	2.74	0.40
1:C:484:TYR:OH	1:C:525:ARG:HD3	2.21	0.40
1:C:101:GLN:HG3	1:C:174:THR:O	2.21	0.40
1:A:3:VAL:HA	1:A:430:THR:HA	2.03	0.40
4:N:154:ASN:HB2	4:N:198:THR:HB	2.03	0.40
2:B:203:ARG:HD3	4:L:33:TYR:CZ	2.56	0.40
1:C:347:ASN:ND2	1:C:347:ASN:O	2.55	0.40
1:A:488:LEU:HD13	1:A:500:PHE:HB3	2.04	0.40
1:A:16:ASN:HD21	8:A:612:15P:H302	1.85	0.40
2:D:239:PRO:HB3	2:D:272:THR:HG23	2.03	0.40
1:A:79:GLU:HA	1:A:80:PRO:HD3	1.99	0.40
2:D:157:HIS:O	2:D:161:VAL:HG23	2.21	0.40
4:L:23:CYS:HB2	4:L:40:TRP:CH2	2.57	0.40
1:C:1:TYR:HB3	1:C:382:SER:HB3	2.03	0.40
4:N:23:CYS:HB2	4:N:40:TRP:CH2	2.57	0.40
2:B:157:HIS:O	2:B:161:VAL:HG23	2.21	0.40
2:D:332:ALA:C	2:D:334:LEU:H	2.25	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	578/597 (97%)	520 (90%)	53 (9%)	5 (1%)	21	65
1	C	577/597 (97%)	523 (91%)	48 (8%)	6 (1%)	19	63
2	B	375/503 (75%)	328 (88%)	44 (12%)	3 (1%)	24	67
2	D	374/503 (74%)	330 (88%)	42 (11%)	2 (0%)	34	76
3	H	207/219 (94%)	186 (90%)	20 (10%)	1 (0%)	34	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	207/219 (94%)	186 (90%)	20 (10%)	1 (0%)	34	76
4	L	215/217 (99%)	201 (94%)	12 (6%)	2 (1%)	21	65
4	N	215/217 (99%)	201 (94%)	12 (6%)	2 (1%)	21	65
All	All	2748/3072 (90%)	2475 (90%)	251 (9%)	22 (1%)	24	67

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	C	200	ASN
4	L	73	GLY
4	N	73	GLY
1	A	29	GLY
1	A	448	ARG
1	C	29	GLY
2	D	272	THR
1	A	539	LEU
2	B	434	HIS
2	D	434	HIS
3	H	209	ALA
4	L	143	ASN
3	M	209	ALA
4	N	143	ASN
2	B	272[A]	THR
2	B	272[B]	THR
1	C	454	VAL
1	C	490	VAL
1	C	506	GLY
1	A	78	GLY
1	C	78	GLY

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	486/500 (97%)	480 (99%)	6 (1%)	78 93
1	C	487/500 (97%)	480 (99%)	7 (1%)	74 91
2	B	325/431 (75%)	321 (99%)	4 (1%)	78 93
2	D	324/431 (75%)	320 (99%)	4 (1%)	78 93
3	H	183/188 (97%)	181 (99%)	2 (1%)	80 93
3	M	183/188 (97%)	181 (99%)	2 (1%)	80 93
4	L	194/194 (100%)	193 (100%)	1 (0%)	92 97
4	N	194/194 (100%)	193 (100%)	1 (0%)	92 97
All	All	2376/2626 (90%)	2349 (99%)	27 (1%)	80 93

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ILE
1	A	165	CYS
1	A	173	TYR
1	A	272	TYR
1	A	296	MET
1	A	421	ARG
2	B	148	ASP
2	B	271[A]	ASP
2	B	271[B]	ASP
2	B	297	ASN
1	C	55	ILE
1	C	165	CYS
1	C	173	TYR
1	C	272	TYR
1	C	296	MET
1	C	421	ARG
1	C	550	LEU
2	D	148	ASP
2	D	271[A]	ASP
2	D	271[B]	ASP
2	D	297	ASN
3	H	72	VAL
3	H	196	ARG
4	L	148	ASP
3	M	72	VAL
3	M	196	ARG
4	N	148	ASP

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	211	GLN
1	A	242	HIS
1	A	347	ASN
1	A	404	GLN
2	B	154	GLN
2	B	291	HIS
2	B	324	GLN
1	C	16	ASN
1	C	42	ASN
1	C	211	GLN
1	C	242	HIS
1	C	347	ASN
1	C	404	GLN
1	C	442	HIS
2	D	154	GLN
2	D	291	HIS
2	D	324	GLN
3	H	59	ASN
4	L	47	GLN
4	L	50	GLN
3	M	59	ASN
4	N	47	GLN
4	N	50	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	$\#\|Z\| > 2$
7	NAG	A	606	1,7	14,14,15	0.60	0	15,19,21	0.67	0
7	NAG	A	607	7	14,14,15	0.52	0	15,19,21	0.70	0
7	BMA	A	608	7	11,11,12	0.79	0	14,15,17	1.65	2 (14%)
7	MAN	A	609	7	11,11,12	0.43	0	14,15,17	1.61	1 (7%)
7	NAG	C	606	1,7	14,14,15	0.56	0	15,19,21	1.26	2 (13%)
7	NAG	C	607	7	14,14,15	0.60	0	15,19,21	0.82	0
7	BMA	C	608	7	11,11,12	0.57	0	14,15,17	0.98	1 (7%)
7	MAN	C	609	7	11,11,12	0.56	0	14,15,17	0.65	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
7	NAG	A	606	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	607	7	-	0/6/23/26	0/1/1/1
7	BMA	A	608	7	-	0/2/19/22	0/1/1/1
7	MAN	A	609	7	-	0/2/19/22	0/1/1/1
7	NAG	C	606	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	607	7	-	0/6/23/26	0/1/1/1
7	BMA	C	608	7	-	0/2/19/22	0/1/1/1
7	MAN	C	609	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	606	NAG	C3-C4-C5	2.59	114.72	110.20
7	C	606	NAG	C2-N2-C7	2.60	126.38	123.04
7	C	608	BMA	C1-C2-C3	2.72	112.76	109.54
7	A	608	BMA	C2-C3-C4	2.98	116.11	111.04
7	A	608	BMA	C1-C2-C3	5.02	115.48	109.54
7	A	609	MAN	C1-O5-C5	5.59	119.34	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	609	MAN	1	0
7	C	607	NAG	1	0

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 12 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	$\#\|Z\| > 2$
6	NAG	A	604	1	14,14,15	0.53	0	15,19,21	0.65	0
6	NAG	A	605	1	14,14,15	0.51	0	15,19,21	0.69	0
6	NAG	A	610	1	14,14,15	0.51	0	15,19,21	0.80	1 (6%)
6	NAG	A	611	1	14,14,15	0.52	0	15,19,21	0.57	0
8	15P	A	612	-	51,51,103	0.54	0	50,50,102	1.53	3 (6%)
6	NAG	B	2004	2	14,14,15	0.98	1 (7%)	15,19,21	1.57	1 (6%)
6	NAG	C	604	1	14,14,15	0.56	0	15,19,21	0.70	0
6	NAG	C	605	1	14,14,15	0.53	0	15,19,21	0.63	0
6	NAG	C	610	1	14,14,15	0.49	0	15,19,21	0.76	0
6	NAG	C	611	1	14,14,15	0.50	0	15,19,21	0.79	1 (6%)
10	TRS	C	612	-	7,7,7	2.25	1 (14%)	9,9,9	1.88	3 (33%)

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	A	604	1	-	0/6/23/26	0/1/1/1
6	NAG	A	605	1	-	0/6/23/26	0/1/1/1
6	NAG	A	610	1	-	0/6/23/26	0/1/1/1
6	NAG	A	611	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	15P	A	612	-	-	0/49/49/101	0/0/0/0
6	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
6	NAG	C	604	1	-	0/6/23/26	0/1/1/1
6	NAG	C	605	1	-	0/6/23/26	0/1/1/1
6	NAG	C	610	1	-	0/6/23/26	0/1/1/1
6	NAG	C	611	1	-	0/6/23/26	0/1/1/1
10	TRS	C	612	-	-	0/9/9/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	612	TRS	C-N	-4.77	1.43	1.50
6	B	2004	NAG	C1-C2	2.79	1.56	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	612	15P	C29-O14-C28	2.02	122.00	113.31
8	A	612	15P	O15-C30-C29	2.08	119.62	110.36
8	A	612	15P	O11-C23-C24	2.10	119.69	110.36
6	C	611	NAG	C1-O5-C5	2.10	114.91	112.25
6	A	610	NAG	C1-O5-C5	2.18	115.01	112.25
10	C	612	TRS	O2-C2-C	2.93	117.11	111.18
10	C	612	TRS	O3-C3-C	2.95	117.16	111.18
10	C	612	TRS	O1-C1-C	3.44	118.13	111.18
6	B	2004	NAG	C1-O5-C5	5.42	119.13	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	612	15P	17	0
6	C	604	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	582/597 (97%)	0.01	1 (0%)	95	94	38, 89, 161, 227	3 (0%)
1	C	581/597 (97%)	0.01	1 (0%)	95	94	47, 96, 166, 236	4 (0%)
2	B	375/503 (74%)	0.25	16 (4%)	39	23	51, 126, 203, 263	0
2	D	375/503 (74%)	0.32	23 (6%)	25	12	69, 131, 198, 240	0
3	H	211/219 (96%)	0.69	31 (14%)	3	2	83, 168, 230, 247	0
3	M	211/219 (96%)	0.82	27 (12%)	5	2	101, 176, 231, 246	0
4	L	217/217 (100%)	1.25	61 (28%)	1	0	93, 167, 249, 274	0
4	N	217/217 (100%)	1.10	50 (23%)	1	1	102, 168, 251, 276	0
All	All	2769/3072 (90%)	0.38	210 (7%)	17	8	38, 125, 224, 276	7 (0%)

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	455	CYS	14.7
4	N	186	LEU	10.8
2	B	455	CYS	10.1
4	N	185	THR	9.8
3	H	206	ALA	9.0
4	L	135	ALA	8.9
4	N	197	TYR	8.6
4	L	155	ILE	7.7
4	L	186	LEU	7.4
3	M	167	LEU	7.2
4	N	126	SER	7.0
4	N	134	GLY	6.8
4	N	135	ALA	6.7
3	M	134	PRO	6.7
4	L	189	ASP	6.7
4	L	154	ASN	6.7

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Mol	Chain	Res	Type	RSRZ
4	N	138	VAL	6.4
4	N	160	ARG	6.2
4	L	159	GLU	6.2
3	H	184	THR	5.9
3	M	168	SER	5.8
4	N	154	ASN	5.8
2	B	426	ALA	5.7
2	D	454	LEU	5.7
2	D	98	GLY	5.7
4	N	136	SER	5.5
3	H	150	VAL	5.4
4	N	161	GLN	5.4
4	L	198	THR	5.3
2	D	97	ARG	5.3
4	L	156	ASP	5.3
4	L	183	THR	5.3
2	D	426	ALA	5.3
3	M	146	LEU	5.3
4	L	185	THR	5.2
4	L	127	SER	5.0
4	N	118	PRO	5.0
3	M	120	SER	4.9
4	L	187	THR	4.9
2	D	428	HIS	4.9
4	L	201	ALA	4.7
4	L	200	GLU	4.7
2	D	395	GLY	4.6
4	N	125	PRO	4.6
3	H	218	ILE	4.5
2	D	96	ALA	4.5
4	L	141	LEU	4.5
3	M	215	ASP	4.4
4	N	210	ILE	4.4
3	H	142	SER	4.4
4	N	211	VAL	4.3
2	D	434	HIS	4.3
3	H	166	SER	4.3
3	M	133	ALA	4.3
4	N	133	GLY	4.2
1	C	492	ARG	4.2
4	L	116	ALA	4.2
3	M	218	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
3	H	163	ASN	4.2
4	N	153	TRP	4.2
2	D	425	GLN	4.1
4	L	125	PRO	4.1
4	N	121	SER	4.1
3	M	142	SER	4.1
2	D	394	GLU	4.1
4	N	183	THR	4.1
3	H	169	SER	4.1
2	B	435	LEU	4.0
4	N	202	THR	4.0
4	L	119	THR	4.0
4	L	152	LYS	4.0
4	N	137	VAL	3.9
4	L	138	VAL	3.9
2	D	119	GLN	3.9
4	N	199	CYS	3.9
4	L	211	VAL	3.8
4	N	155	ILE	3.7
3	H	158	VAL	3.7
3	M	169	SER	3.7
4	N	152	LYS	3.7
3	M	165	GLY	3.7
2	B	386	HIS	3.6
4	L	158	SER	3.6
3	H	167	LEU	3.5
4	L	199	CYS	3.5
3	H	201	VAL	3.5
4	L	213	SER	3.5
3	M	180	SER	3.5
4	L	166	ASN	3.5
4	L	163	GLY	3.5
4	N	200	GLU	3.5
3	H	161	THR	3.4
4	L	120	VAL	3.4
3	H	193	SER	3.4
3	H	159	THR	3.4
4	N	151	VAL	3.4
2	B	434	HIS	3.4
4	N	165	LEU	3.4
4	L	118	PRO	3.3
4	L	126	SER	3.3

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Mol	Chain	Res	Type	RSRZ
3	H	202	THR	3.3
4	L	137	VAL	3.3
3	H	185	LEU	3.3
4	N	120	VAL	3.3
2	B	454	LEU	3.3
3	H	149	LEU	3.3
3	M	200	THR	3.2
4	L	153	TRP	3.2
3	H	128	SER	3.2
4	L	191	TYR	3.1
4	N	132	SER	3.1
3	M	195	PRO	3.1
4	L	121	SER	3.1
4	L	217	ASN	3.0
4	N	156	ASP	3.0
4	L	140	PHE	3.0
3	M	123	LYS	3.0
4	N	196	SER	3.0
3	H	162	TRP	3.0
3	H	133	ALA	3.0
4	N	148	ASP	3.0
4	N	122	ILE	3.0
4	L	195	ASN	3.0
2	B	425	GLN	3.0
4	L	112	LYS	3.0
4	L	193	ARG	2.9
4	L	202	THR	2.9
3	H	123	LYS	2.9
4	L	139	CYS	2.9
4	L	206	SER	2.9
3	H	179	GLU	2.9
4	N	208	SER	2.9
4	N	141	LEU	2.9
4	N	159	GLU	2.9
4	L	196	SER	2.8
4	N	215	ASN	2.8
3	M	160	VAL	2.8
2	D	393	CYS	2.8
2	D	386	HIS	2.7
4	L	162	ASN	2.7
4	L	109	LEU	2.7
4	N	129	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
3	M	11	LEU	2.7
2	D	99	GLU	2.7
3	M	162	TRP	2.7
4	N	214	PHE	2.6
4	L	151	VAL	2.6
2	D	396	PRO	2.6
3	M	121	SER	2.6
4	N	124	PRO	2.6
4	L	161	GLN	2.6
2	D	173	GLY	2.6
4	N	201	ALA	2.6
3	M	201	VAL	2.5
3	H	160	VAL	2.5
2	B	94	GLN	2.5
3	M	164	SER	2.5
4	L	190	GLU	2.5
2	B	98	GLY	2.5
2	D	402	LYS	2.5
2	B	119	GLN	2.5
3	H	198	SER	2.5
2	B	424	LEU	2.5
1	A	564	PRO	2.4
4	N	191	TYR	2.4
4	L	194	HIS	2.4
4	N	150	ASN	2.4
4	L	178	TYR	2.4
2	D	429	CYS	2.4
4	L	207	THR	2.4
2	D	92	LEU	2.4
3	M	132	LEU	2.4
4	N	188	LYS	2.3
3	H	147	GLY	2.3
3	M	130	TYR	2.3
2	B	422	VAL	2.3
4	L	134	GLY	2.3
2	B	113	LEU	2.3
4	L	182	SER	2.3
4	N	167	SER	2.3
3	H	143	MET	2.3
2	D	328	ALA	2.3
4	N	190	GLU	2.3
4	L	180	MET	2.3

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Mol	Chain	Res	Type	RSRZ
4	N	164	VAL	2.3
3	M	206	ALA	2.2
4	N	212	LYS	2.2
4	N	123	PHE	2.2
2	B	97	ARG	2.2
2	D	385	VAL	2.2
3	M	129	VAL	2.2
3	H	151	LYS	2.2
3	M	172	HIS	2.2
4	N	194	HIS	2.2
4	L	160	ARG	2.1
4	L	203	HIS	2.1
4	L	165	LEU	2.1
4	L	208	SER	2.1
4	L	130	LEU	2.1
3	H	130	TYR	2.1
4	L	157	GLY	2.1
3	H	203	CYS	2.0
4	L	132	SER	2.0
4	L	115	ASP	2.0
3	H	199	GLU	2.0
3	M	193	SER	2.0
3	H	190	THR	2.0
2	D	400	GLU	2.0
2	B	436	LEU	2.0
2	B	451	LEU	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
7	NAG	C	606	14/15	0.92	0.22	-0.13	60,152,181,188	0
7	NAG	A	606	14/15	0.96	0.17	-0.92	45,111,145,158	0
7	NAG	C	607	14/15	0.89	0.19	-	130,154,204,205	0
7	NAG	A	607	14/15	0.94	0.15	-	58,121,166,179	0
7	BMA	A	608	11/12	0.81	0.20	-	112,197,215,224	0
7	BMA	C	608	11/12	0.83	0.15	-	182,203,226,244	0
7	MAN	A	609	11/12	0.76	0.20	-	115,192,228,245	0
7	MAN	C	609	11/12	0.65	0.42	-	180,237,249,252	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
5	CA	A	602	1/1	0.91	0.26	3.39	78,78,78,78	0
8	15P	A	612	52/104	0.95	0.29	2.39	3,88,137,176	0
5	CA	A	603	1/1	0.94	0.28	2.13	69,69,69,69	0
5	CA	C	603	1/1	0.98	0.28	1.77	68,68,68,68	0
6	NAG	C	611	14/15	0.88	0.24	1.77	135,147,173,176	0
5	CA	C	602	1/1	0.96	0.24	0.08	86,86,86,86	0
5	CA	A	601	1/1	0.88	0.23	-0.00	81,81,81,81	0
6	NAG	A	610	14/15	0.90	0.17	-0.26	133,157,188,195	0
6	NAG	C	610	14/15	0.85	0.24	-0.45	119,164,193,202	0
6	NAG	C	604	14/15	0.95	0.19	-0.61	52,87,127,156	0
9	MG	B	2001	1/1	0.80	0.19	-0.98	100,100,100,100	0
6	NAG	A	604	14/15	0.97	0.18	-1.00	47,75,103,114	0
5	CA	D	2002	1/1	0.87	0.12	-1.05	132,132,132,132	0
5	CA	C	601	1/1	0.88	0.20	-1.13	86,86,86,86	0
5	CA	B	2003	1/1	0.98	0.19	-1.14	87,87,87,87	0
9	MG	D	2001	1/1	0.96	0.10	-2.37	104,104,104,104	0
5	CA	B	2002	1/1	0.78	0.10	-2.50	125,125,125,125	0
5	CA	D	2003	1/1	0.91	0.12	-2.54	115,115,115,115	0
6	NAG	A	611	14/15	0.91	0.24	-	110,149,210,214	0
6	NAG	B	2004	14/15	0.84	0.22	-	143,177,230,235	0
6	NAG	A	605	14/15	0.90	0.20	-	67,160,177,193	0
10	TRS	C	612	8/8	0.78	0.22	-	114,148,166,167	0
6	NAG	C	605	14/15	0.88	0.21	-	69,157,189,199	0

6.5 Other polymers (i)

There are no such residues in this entry.