Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:22 PM GMT

PDB ID	:	4LAJ
Title	:	Crystal structure of HIV-1 YU2 envelope gp120 glycoprotein in complex with CD4-mimetic miniprotein, M48U1, and llama single-domain, broadly neutralizing, co-receptor binding site antibody, JM4
Authors	:	Acharya, P.; Luongo, T.S.; Kwong, P.D.
Deposited on	:	2013-06-20
Resolution	:	2.14 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:

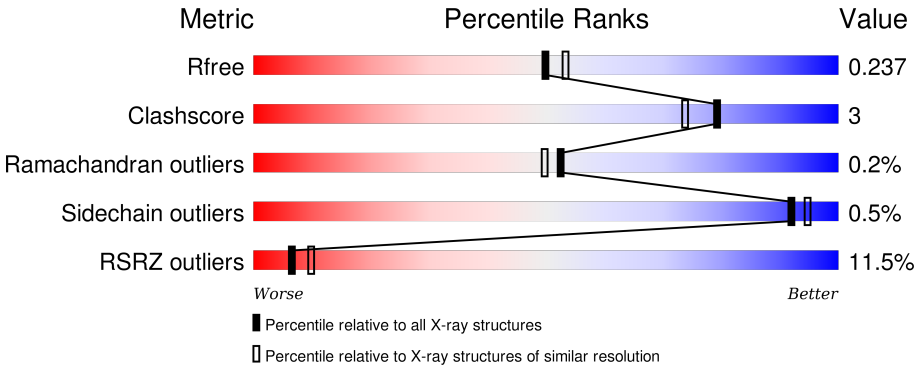
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.14 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	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (2.16-2.12)

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	376	12% 86% 5% 9%
1	B	376	9% 83% 7% 9%
1	F	376	9% 85% • 11%
1	J	376	9% 85% 5% 10%
2	C	28	7% 82% 18%

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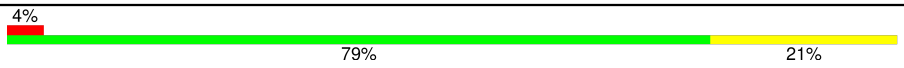
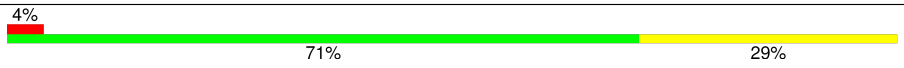
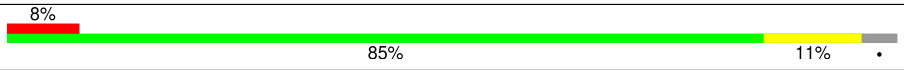
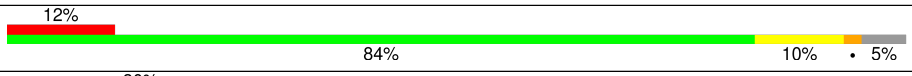
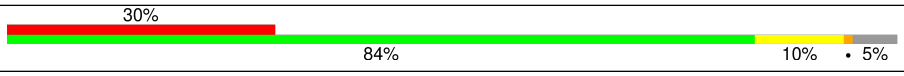
Mol	Chain	Length	Quality of chain
2	D	28	
2	G	28	
2	K	28	
3	H	129	
3	I	129	
3	L	129	
3	M	129	

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
4	NAG	A	502	-	-	-	X
4	NAG	A	506	-	-	-	X
4	NAG	A	509	-	-	-	X
4	NAG	B	502	-	-	-	X
4	NAG	B	503	-	-	-	X
4	NAG	F	506	-	-	-	X
4	NAG	J	502	-	-	-	X
4	NAG	J	505	-	-	-	X
4	NAG	J	507	-	-	-	X
5	EDO	A	510	-	-	-	X
5	EDO	A	511	-	-	-	X
5	EDO	A	512	-	-	-	X
5	EDO	B	509	-	-	-	X
5	EDO	B	510	-	-	-	X
5	EDO	J	510	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16384 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 HIV-1 YU2 gp120 envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	337	Total	C	N	O	S	0	6	0
			2660	1669	465	506	20			
1	F	334	Total	C	N	O	S	0	5	0
			2633	1654	461	498	20			
1	A	343	Total	C	N	O	S	0	4	0
			2702	1693	474	515	20			
1	B	341	Total	C	N	O	S	0	3	0
			2680	1681	470	509	20			

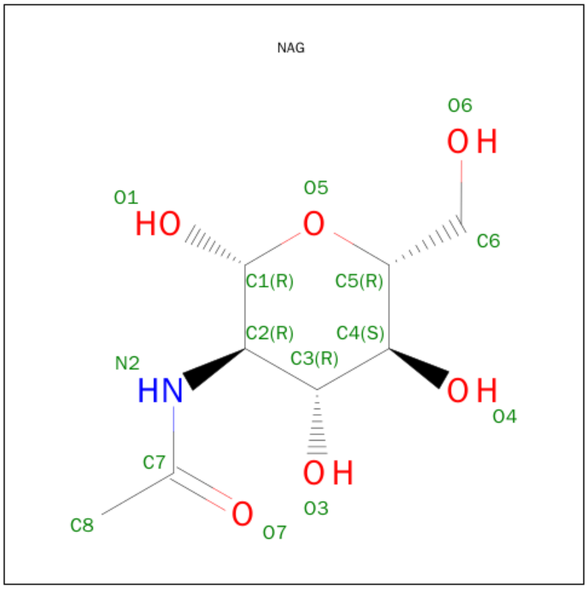
- Molecule 2 is a protein called CD4-mimetic miniprotein M48U1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	28	Total	C	N	O	S	0	1	1
			214	136	39	33	6			
2	D	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			
2	G	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			
2	C	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			

- Molecule 3 is a protein called Llama single domain antibody, JM4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	124	Total	C	N	O	S	0	0	0
			944	589	156	193	6			
3	M	123	Total	C	N	O	S	0	0	0
			939	586	155	192	6			
3	L	123	Total	C	N	O	S	0	0	0
			939	586	155	192	6			
3	I	125	Total	C	N	O	S	0	0	0
			949	592	157	194	6			

- 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	J	1	Total C N O 14 8 1 5	0	0
4	J	1	Total C N O 14 8 1 5	0	0
4	J	1	Total C N O 14 8 1 5	0	0
4	J	1	Total C N O 14 8 1 5	0	0
4	J	1	Total C N O 14 8 1 5	0	0
4	J	1	Total C N O 14 8 1 5	0	0
4	J	1	Total C N O 14 8 1 5	0	0
4	J	1	Total C N O 14 8 1 5	0	0
4	J	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0

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

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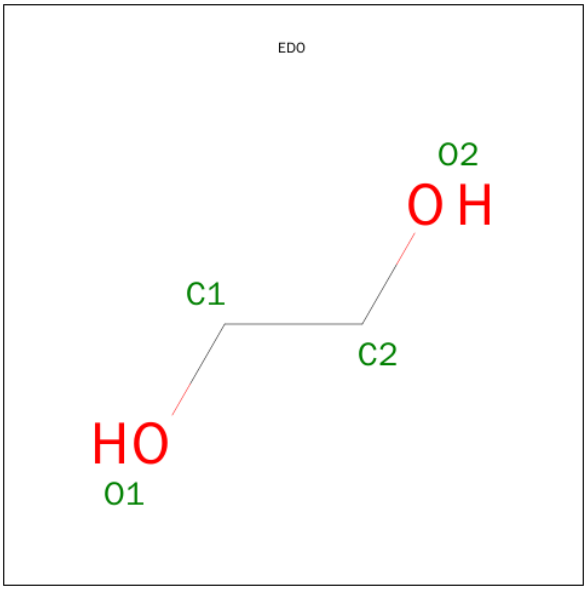
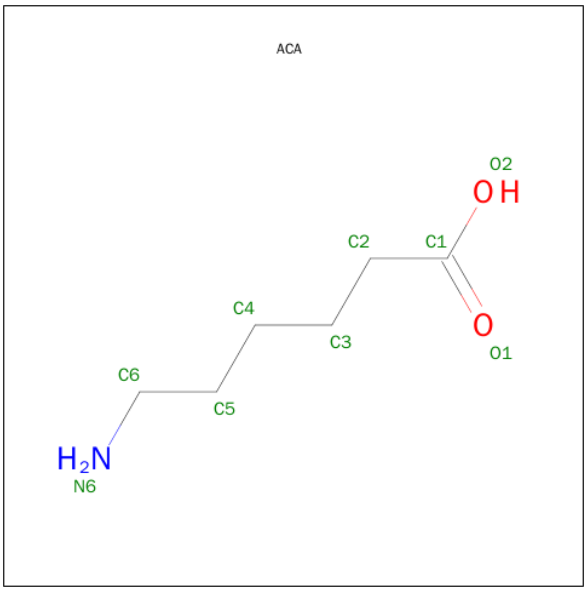
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is 6-AMINOHEXANOIC ACID (three-letter code: ACA) (formula: $C_6H_{13}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 9 6 1 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	73	Total O 73 73	0	0
7	F	111	Total O 111 111	0	0
7	A	114	Total O 114 114	0	0
7	B	139	Total O 139 139	0	0
7	K	4	Total O 4 4	0	0
7	D	10	Total O 10 10	0	0
7	G	3	Total O 3 3	0	0
7	C	10	Total O 10 10	0	0
7	H	37	Total O 37 37	0	0
7	M	9	Total O 9 9	0	0
7	L	25	Total O 25 25	0	0

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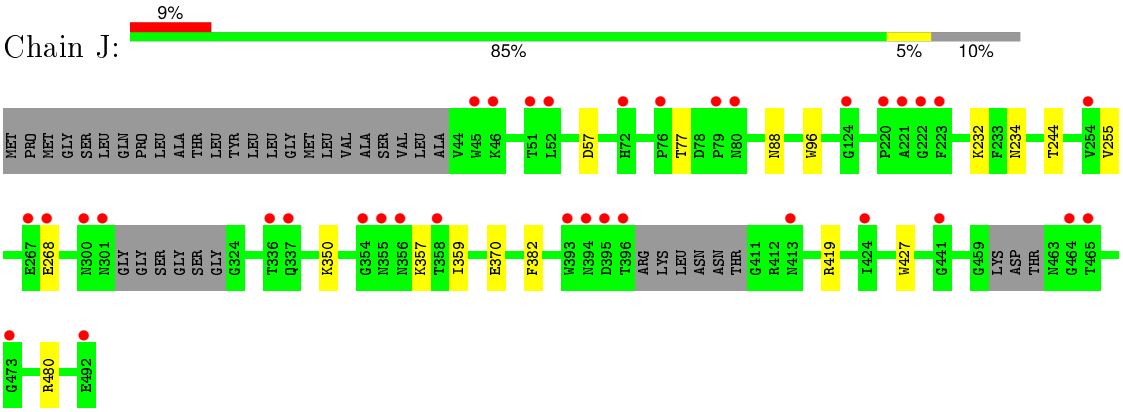
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	I	35	35	35	0	0

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.

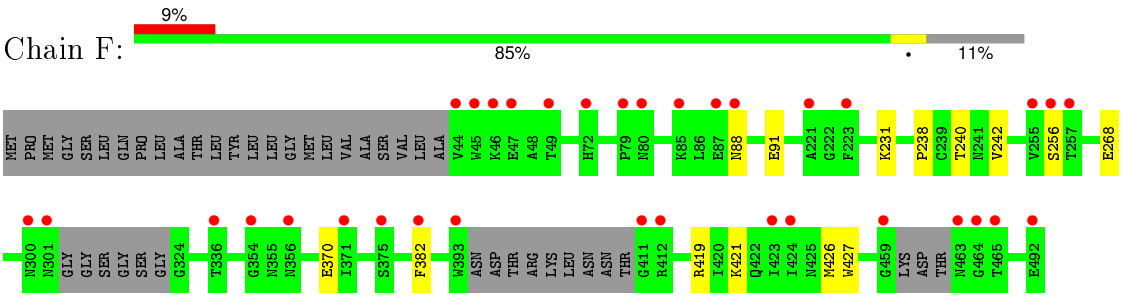
- Molecule 1: HIV-1 YU2 gp120 envelope glycoprotein

Chain J:



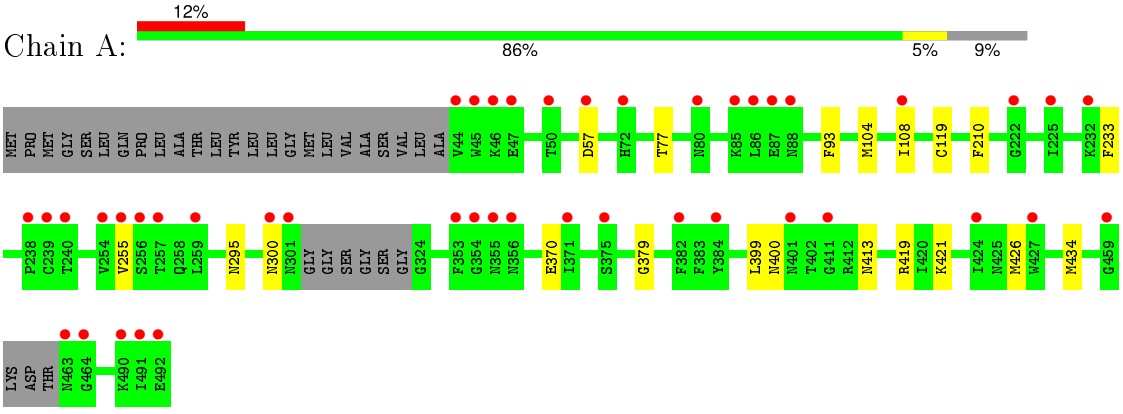
- Molecule 1: HIV-1 YU2 gp120 envelope glycoprotein

Chain F:



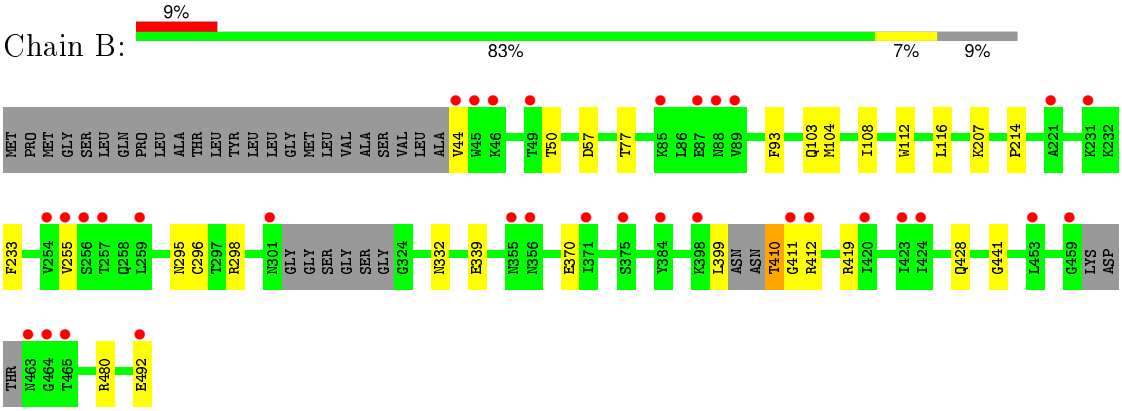
- Molecule 1: HIV-1 YU2 gp120 envelope glycoprotein

Chain A:



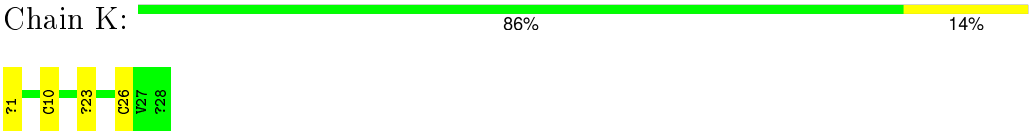
• Molecule 1: HIV-1 YU2 gp120 envelope glycoprotein

Chain B:



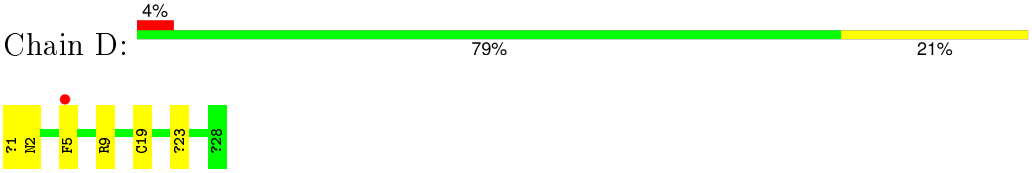
• Molecule 2: CD4-mimetic miniprotein M48U1

Chain K:



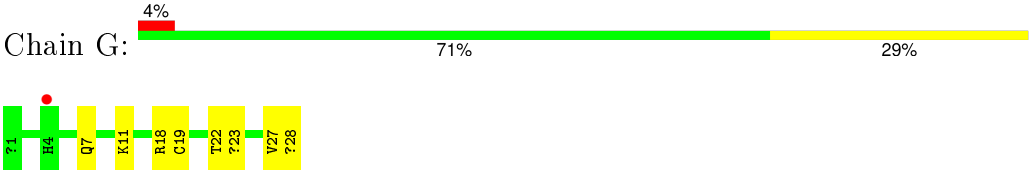
• Molecule 2: CD4-mimetic miniprotein M48U1

Chain D:



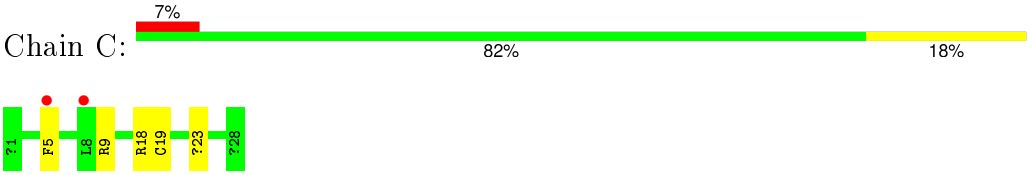
• Molecule 2: CD4-mimetic miniprotein M48U1

Chain G:



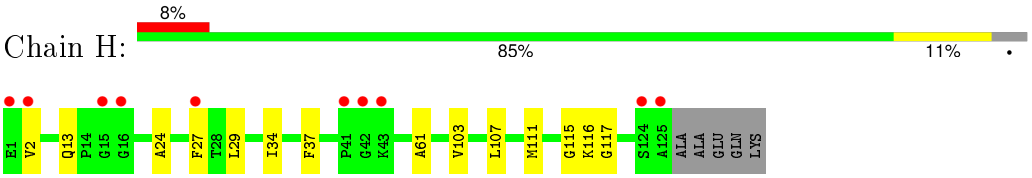
• Molecule 2: CD4-mimetic miniprotein M48U1

Chain C:



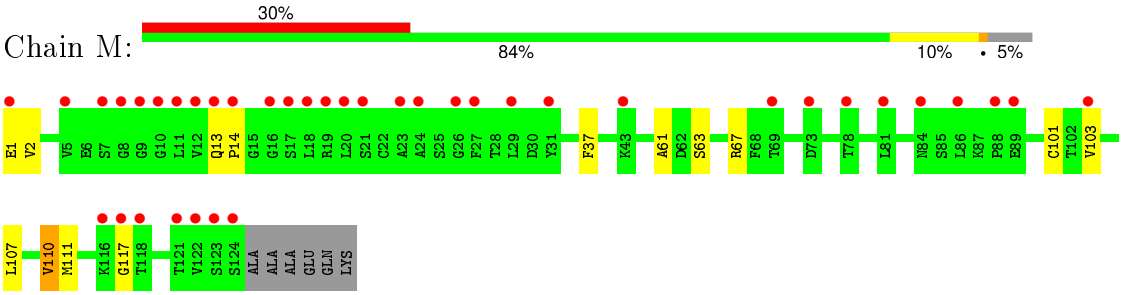
• Molecule 3: Llama single domain antibody, JM4

Chain H:



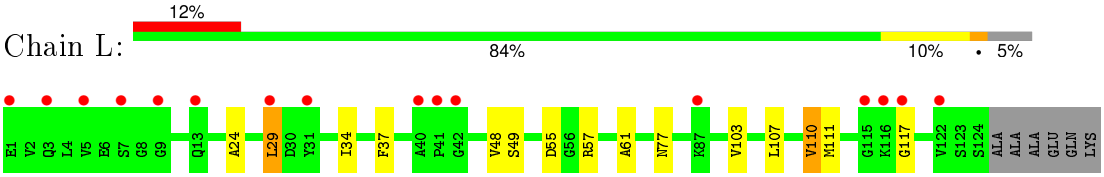
• Molecule 3: Llama single domain antibody, JM4

Chain M:



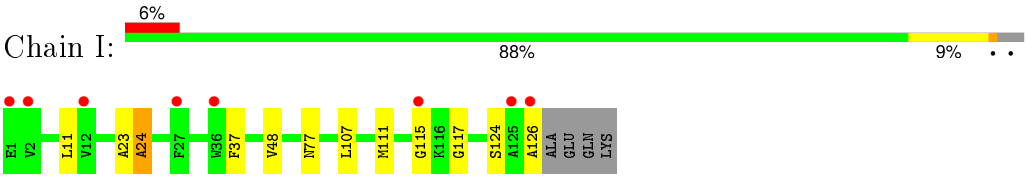
- Molecule 3: Llama single domain antibody, JM4

Chain L:



- Molecule 3: Llama single domain antibody, JM4

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.77Å 86.22Å 144.85Å 90.00° 102.88° 90.00°	Depositor
Resolution (Å)	38.80 – 2.14 38.80 – 2.13	Depositor EDS
% Data completeness (in resolution range)	76.7 (38.80-2.14) 71.7 (38.80-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.14Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.185 , 0.227 0.200 , 0.237	Depositor DCC
R_{free} test set	4976 reflections (5.66%)	DCC
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 99018 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16384	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.70% 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: ACA, DPR, EDO, MPT, NH2, U2X, NAG

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	0.28	0/2783	0.50	0/3775
1	B	0.28	0/2754	0.49	0/3734
1	F	0.27	0/2706	0.47	0/3670
1	J	0.28	0/2746	0.49	0/3724
2	C	0.53	1/176 (0.6%)	0.71	1/231 (0.4%)
2	D	0.55	1/176 (0.6%)	0.59	0/231
2	G	0.52	1/176 (0.6%)	0.46	0/231
2	K	0.35	0/184	0.58	0/242
3	H	0.30	0/962	0.56	0/1304
3	I	0.28	0/967	0.53	0/1311
3	L	0.30	0/957	0.56	0/1297
3	M	0.27	0/957	0.51	0/1297
All	All	0.29	3/15544 (0.0%)	0.51	1/21047 (0.0%)

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
2	D	0	1
2	K	0	2
3	H	0	1
3	I	0	1
3	L	0	1
3	M	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	19	CYS	C-N	6.18	1.48	1.34
2	G	19	CYS	C-N	5.92	1.47	1.34
2	C	19	CYS	C-N	5.88	1.47	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	19	CYS	C-N-CA	5.82	136.24	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	1	MPT	Mainchain
3	H	117	GLY	Peptide
3	I	117	GLY	Peptide
2	K	1	MPT	Peptide
3	L	117	GLY	Peptide
3	M	117	GLY	Peptide

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	2702	0	2627	17	0
1	B	2680	0	2605	22	0
1	F	2633	0	2557	14	0
1	J	2660	0	2584	13	0
2	C	209	0	212	5	0
2	D	209	0	212	3	0
2	G	209	0	212	10	0
2	K	214	0	220	7	0
3	H	944	0	901	8	0
3	I	949	0	906	10	0
3	L	939	0	896	9	0
3	M	939	0	896	8	0
4	A	126	0	117	2	0
4	B	112	0	104	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	126	0	117	3	0
4	J	126	0	117	4	0
5	A	12	0	18	4	0
5	B	12	0	18	3	0
5	J	4	0	6	1	0
6	B	9	0	12	1	0
7	A	114	0	0	0	0
7	B	139	0	0	2	0
7	C	10	0	0	1	0
7	D	10	0	0	0	0
7	F	111	0	0	1	0
7	G	3	0	0	0	0
7	H	37	0	0	0	0
7	I	35	0	0	3	0
7	J	73	0	0	0	0
7	K	4	0	0	0	0
7	L	25	0	0	0	0
7	M	9	0	0	0	0
All	All	16384	0	15337	109	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 3.

All (109) 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:K:10:CYS:CB	2:K:26:CYS:SG	2.24	1.25
2:K:10:CYS:SG	2:K:26:CYS:SG	1.05	0.96
2:K:10:CYS:SG	2:K:26:CYS:CB	2.63	0.86
1:B:296:CYS:SG	7:B:717:HOH:O	2.33	0.85
1:J:370:GLU:HG2	2:K:23:U2X:H71	1.59	0.85
1:F:370:GLU:HG2	2:G:23:U2X:H71	1.62	0.82
1:B:480:ARG:NH2	7:B:651:HOH:O	2.19	0.76
1:B:370:GLU:HG2	2:C:23:U2X:H71	1.69	0.74
1:A:295:ASN:ND2	4:A:502:NAG:O7	2.21	0.73
1:F:382:PHE:HD1	2:G:23:U2X:H11	1.56	0.70
1:B:295:ASN:HD22	4:B:502:NAG:H81	1.57	0.69
4:F:509:NAG:O5	1:A:400:ASN:ND2	2.26	0.69
1:A:370:GLU:HG2	2:D:23:U2X:H71	1.77	0.67
3:I:24:ALA:O	7:I:232:HOH:O	2.13	0.66
1:J:350:LYS:NZ	1:J:357:LYS:O	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:115:GLY:O	7:I:225:HOH:O	2.14	0.64
1:B:57:ASP:OD1	1:B:77:THR:OG1	2.11	0.63
1:A:210:PHE:H	5:A:512:EDO:H11	1.66	0.60
4:J:503:NAG:H83	4:J:503:NAG:H3	1.83	0.59
2:G:7:GLN:O	2:G:11:LYS:HB2	2.03	0.59
1:F:231:LYS:HD3	1:F:268:GLU:HG3	1.86	0.58
2:D:5:PHE:CE2	2:D:9:ARG:HD2	2.38	0.58
3:L:55:ASP:OD2	3:L:57:ARG:NH2	2.37	0.57
2:G:18:ARG:CZ	2:G:27:VAL:HG21	2.35	0.57
2:C:18:ARG:NH2	7:C:609:HOH:O	2.38	0.56
1:F:240:THR:O	7:F:663:HOH:O	2.18	0.55
2:G:27:VAL:CG1	2:G:28:NH2:N	2.70	0.55
2:G:27:VAL:HG12	2:G:28:NH2:N	2.21	0.55
3:I:23:ALA:HA	3:I:24:ALA:HB2	1.89	0.54
2:K:10:CYS:CA	2:K:26:CYS:SG	2.94	0.53
1:J:234:ASN:HD22	4:J:502:NAG:H83	1.74	0.53
3:M:63:SER:O	3:M:67:ARG:NH2	2.40	0.53
1:B:428:GLN:OE1	5:B:509:EDO:O1	2.24	0.53
3:I:77:ASN:ND2	7:I:232:HOH:O	2.35	0.53
1:F:421:LYS:HD3	3:M:110:VAL:HG13	1.91	0.53
1:B:214:PRO:HG2	6:B:512:ACA:H52	1.92	0.52
3:I:23:ALA:CA	3:I:24:ALA:HB2	2.39	0.52
1:J:382:PHE:HD1	2:K:23:U2X:H11	1.74	0.52
1:A:104:MET:HE2	1:A:108:ILE:HD11	1.93	0.51
1:A:421:LYS:HD3	3:L:110:VAL:HG13	1.91	0.51
1:B:339:GLU:HB3	1:B:399:LEU:HD22	1.94	0.50
1:J:88:ASN:HD21	4:J:505:NAG:C2	2.24	0.50
3:H:61:ALA:N	3:H:103:VAL:HG21	2.27	0.50
1:A:419:ARG:HG2	3:L:107:LEU:HD13	1.94	0.50
1:B:255:VAL:HG12	2:C:23:U2X:H61	1.94	0.49
1:F:427:TRP:HA	2:G:22:THR:OG1	2.11	0.49
1:F:382:PHE:CD1	2:G:23:U2X:H11	2.42	0.49
1:A:379:GLY:CA	5:A:512:EDO:H12	2.43	0.49
3:M:61:ALA:N	3:M:103:VAL:HG21	2.28	0.49
1:J:419:ARG:HG2	3:H:107:LEU:HD13	1.94	0.48
3:M:37:PHE:HD1	3:M:111:MET:HE2	1.78	0.48
1:J:382:PHE:CD1	2:K:23:U2X:H11	2.49	0.48
1:A:379:GLY:HA2	5:A:512:EDO:H12	1.95	0.48
1:A:426:MET:HA	5:A:510:EDO:H22	1.95	0.48
3:I:37:PHE:HD2	3:I:111:MET:HE1	1.79	0.48
1:F:240:THR:OG1	4:F:509:NAG:H81	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ARG:HG2	3:I:107:LEU:HD13	1.95	0.48
1:B:116:LEU:HD22	5:B:510:EDO:O1	2.13	0.47
3:L:37:PHE:HD2	3:L:111:MET:HE1	1.79	0.47
3:L:37:PHE:HA	3:L:48:VAL:HG13	1.97	0.47
1:B:332:ASN:HD22	4:B:502:NAG:H2	1.80	0.47
4:F:509:NAG:H83	1:A:399:LEU:HD12	1.97	0.47
2:C:5:PHE:CE2	2:C:9:ARG:HD2	2.50	0.47
1:B:410:THR:CB	1:B:411:GLY:HA3	2.44	0.47
1:F:419:ARG:HG2	3:M:107:LEU:HD13	1.95	0.47
1:A:57:ASP:OD1	1:A:77:THR:OG1	2.22	0.46
3:L:48:VAL:HG22	3:L:49:SER:N	2.31	0.46
3:H:37:PHE:HD2	3:H:111:MET:HE1	1.79	0.46
3:I:23:ALA:HB1	3:I:24:ALA:HB2	1.97	0.46
4:J:503:NAG:C1	4:J:503:NAG:H82	2.46	0.46
3:H:29:LEU:HD22	3:H:34:ILE:HG13	1.98	0.46
1:J:350:LYS:HG3	1:J:359:ILE:CG1	2.46	0.46
3:I:11:LEU:HG	3:I:126:ALA:HB2	1.97	0.46
3:H:2:VAL:HG11	3:H:27:PHE:CZ	2.51	0.45
3:L:61:ALA:N	3:L:103:VAL:HG21	2.31	0.45
3:H:115:GLY:O	3:H:116:LYS:HG2	2.17	0.45
1:J:57:ASP:OD1	1:J:77:THR:OG1	2.26	0.45
1:J:96:TRP:CE3	1:J:480:ARG:HD3	2.51	0.45
1:A:255:VAL:HG12	2:D:23:U2X:H61	1.99	0.45
1:J:255:VAL:HG11	1:J:427:TRP:CD1	2.52	0.45
1:F:238:PRO:HB2	1:A:399:LEU:HD13	2.01	0.43
1:J:427:TRP:CD1	5:J:510:EDO:O2	2.72	0.43
3:M:101:CYS:HA	3:M:111:MET:HE3	2.00	0.43
3:H:24:ALA:HB3	3:H:29:LEU:HD21	2.00	0.43
3:L:29:LEU:HD22	3:L:34:ILE:HG13	2.00	0.43
1:F:231:LYS:HD3	1:F:268:GLU:CG	2.48	0.42
1:B:410:THR:HB	1:B:411:GLY:HA3	2.00	0.42
1:B:93:PHE:HB2	1:B:233:PHE:HZ	1.83	0.42
3:M:13:GLN:HG3	3:M:14:PRO:HD2	2.02	0.42
1:F:256:SER:HA	2:G:23:U2X:H52	2.02	0.42
3:L:24:ALA:O	3:L:77:ASN:ND2	2.53	0.42
1:J:232:LYS:HE3	1:J:268:GLU:HB2	2.02	0.41
1:F:91:GLU:HB3	1:F:242:VAL:HG21	2.03	0.41
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.86	0.41
4:A:502:NAG:H83	4:A:502:NAG:C1	2.50	0.41
1:A:119:CYS:N	1:A:434:MET:O	2.54	0.41
1:B:50:THR:O	1:B:103:GLN:NE2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:VAL:HA	1:B:492:GLU:H	1.86	0.41
1:A:300:ASN:ND2	1:A:300:ASN:O	2.47	0.41
3:I:23:ALA:CB	3:I:24:ALA:HB2	2.51	0.41
1:B:207:LYS:HD3	5:B:510:EDO:H22	2.03	0.41
3:H:37:PHE:CD2	3:H:111:MET:HE1	2.55	0.40
1:B:112:TRP:CE3	1:B:116:LEU:HD12	2.56	0.40
1:B:298:ARG:NH2	1:B:441:GLY:O	2.45	0.40
3:M:1:GLU:HG2	3:M:2:VAL:N	2.37	0.40
2:C:23:U2X:H71	2:C:23:U2X:HE11	1.85	0.40
1:F:426:MET:O	2:G:22:THR:OG1	2.27	0.40
1:B:411:GLY:HA3	1:B:412:ARG:HA	1.79	0.40
1:B:104:MET:CE	1:B:108:ILE:HD11	2.51	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	342/376 (91%)	326 (95%)	15 (4%)	1 (0%)	46 41
1	B	336/376 (89%)	323 (96%)	13 (4%)	0	100 100
1	F	330/376 (88%)	317 (96%)	12 (4%)	1 (0%)	46 41
1	J	336/376 (89%)	322 (96%)	14 (4%)	0	100 100
2	C	24/28 (86%)	24 (100%)	0	0	100 100
2	D	24/28 (86%)	24 (100%)	0	0	100 100
2	G	24/28 (86%)	24 (100%)	0	0	100 100
2	K	25/28 (89%)	23 (92%)	2 (8%)	0	100 100
3	H	122/129 (95%)	118 (97%)	4 (3%)	0	100 100
3	I	123/129 (95%)	118 (96%)	4 (3%)	1 (1%)	24 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	L	121/129 (94%)	116 (96%)	4 (3%)	1 (1%)	24 14
3	M	121/129 (94%)	117 (97%)	4 (3%)	0	100 100
All	All	1928/2132 (90%)	1852 (96%)	72 (4%)	4 (0%)	52 50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	88	ASN
1	A	413	ASN
3	I	24	ALA
3	L	29	LEU

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	307/328 (94%)	307 (100%)	0	100 100
1	B	303/328 (92%)	302 (100%)	1 (0%)	94 97
1	F	297/328 (90%)	297 (100%)	0	100 100
1	J	302/328 (92%)	301 (100%)	1 (0%)	94 97
2	C	20/20 (100%)	20 (100%)	0	100 100
2	D	20/20 (100%)	19 (95%)	1 (5%)	30 25
2	G	20/20 (100%)	20 (100%)	0	100 100
2	K	21/20 (105%)	21 (100%)	0	100 100
3	H	103/106 (97%)	102 (99%)	1 (1%)	82 85
3	I	103/106 (97%)	101 (98%)	2 (2%)	65 68
3	L	103/106 (97%)	102 (99%)	1 (1%)	82 85
3	M	103/106 (97%)	102 (99%)	1 (1%)	82 85
All	All	1702/1816 (94%)	1694 (100%)	8 (0%)	92 95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	244	THR
1	B	410	THR
2	D	2	ASN
3	H	13	GLN
3	M	110	VAL
3	L	110	VAL
3	I	48	VAL
3	I	124	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	2	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DPR	C	21	2	6,7,8	0.61	0	7,8,10	1.23	1 (14%)
2	U2X	C	23	2	19,20,21	2.37	5 (26%)	22,25,27	1.76	6 (27%)
2	DPR	D	21	2	6,7,8	0.61	0	7,8,10	1.22	1 (14%)
2	U2X	D	23	2	19,20,21	2.34	4 (21%)	22,25,27	1.77	6 (27%)
2	DPR	G	21	2	6,7,8	0.61	0	7,8,10	1.22	1 (14%)
2	U2X	G	23	2	19,20,21	2.41	4 (21%)	22,25,27	1.82	5 (22%)
2	DPR	K	21	2	6,7,8	0.60	0	7,8,10	1.23	1 (14%)
2	U2X	K	23	2	19,20,21	2.43	4 (21%)	22,25,27	1.73	6 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DPR	C	21	2	-	0/0/9/11	0/1/1/1
2	U2X	C	23	2	-	0/9/19/21	0/2/2/2
2	DPR	D	21	2	-	0/0/9/11	0/1/1/1
2	U2X	D	23	2	-	0/9/19/21	0/2/2/2
2	DPR	G	21	2	-	0/0/9/11	0/1/1/1
2	U2X	G	23	2	-	0/9/19/21	0/2/2/2
2	DPR	K	21	2	-	0/0/9/11	0/1/1/1
2	U2X	K	23	2	-	0/9/19/21	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	23	U2X	CB-CA	-2.11	1.49	1.53
2	C	23	U2X	C4-C3	2.42	1.59	1.52
2	D	23	U2X	C4-C3	2.44	1.59	1.52
2	G	23	U2X	C4-C3	2.45	1.59	1.52
2	K	23	U2X	C4-C3	2.49	1.59	1.52
2	D	23	U2X	CE1-CZ	2.76	1.44	1.38
2	C	23	U2X	CE1-CZ	2.78	1.44	1.38
2	G	23	U2X	CE1-CZ	2.82	1.44	1.38
2	K	23	U2X	CE1-CZ	2.88	1.44	1.38
2	C	23	U2X	CE1-CD1	4.42	1.46	1.38
2	D	23	U2X	CE1-CD1	4.42	1.46	1.38
2	G	23	U2X	CE1-CD1	4.62	1.47	1.38
2	K	23	U2X	CE1-CD1	4.65	1.47	1.38
2	D	23	U2X	CE2-CD2	7.34	1.52	1.38
2	C	23	U2X	CE2-CD2	7.46	1.52	1.38
2	G	23	U2X	CE2-CD2	7.57	1.52	1.38
2	K	23	U2X	CE2-CD2	7.70	1.52	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	23	U2X	C1-C2-C3	-2.94	107.47	112.22
2	D	23	U2X	C1-C2-C3	-2.90	107.55	112.22
2	K	23	U2X	C1-C2-C3	-2.67	107.92	112.22
2	C	23	U2X	C1-C2-C3	-2.28	108.55	112.22
2	D	23	U2X	C5-C4-C3	-2.19	108.68	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	21	DPR	O-C-CA	-2.14	119.79	125.44
2	K	23	U2X	O-C-CA	-2.14	119.92	125.49
2	K	21	DPR	O-C-CA	-2.12	119.84	125.44
2	C	21	DPR	O-C-CA	-2.11	119.87	125.44
2	D	21	DPR	O-C-CA	-2.10	119.88	125.44
2	C	23	U2X	C5-C4-C3	-2.08	108.87	112.22
2	D	23	U2X	CG-CB-CA	2.07	118.88	114.21
2	K	23	U2X	CG-CB-CA	2.09	118.92	114.21
2	C	23	U2X	CG-CB-CA	2.40	119.62	114.21
2	G	23	U2X	CG-CB-CA	2.70	120.30	114.21
2	K	23	U2X	C4-C3-C7	2.94	117.66	111.47
2	G	23	U2X	C4-C3-C7	3.09	117.99	111.47
2	C	23	U2X	C4-C3-C7	3.19	118.21	111.47
2	D	23	U2X	C4-C3-C7	3.21	118.24	111.47
2	D	23	U2X	OH-C7-C3	3.37	115.75	107.97
2	C	23	U2X	C2-C3-C7	3.51	118.87	111.47
2	K	23	U2X	C2-C3-C7	3.59	119.04	111.47
2	G	23	U2X	C2-C3-C7	3.75	119.37	111.47
2	D	23	U2X	C2-C3-C7	3.76	119.39	111.47
2	C	23	U2X	OH-C7-C3	3.93	117.04	107.97
2	K	23	U2X	OH-C7-C3	3.96	117.09	107.97
2	G	23	U2X	OH-C7-C3	4.07	117.35	107.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	23	U2X	3	0
2	D	23	U2X	2	0
2	G	23	U2X	4	0
2	K	23	U2X	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

43 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	$\#\|Z\| > 2$
4	NAG	A	501	1	14,14,15	0.13	0	15,19,21	0.52	0
4	NAG	A	502	-	14,14,15	0.30	0	15,19,21	0.51	0
4	NAG	A	503	1	14,14,15	0.21	0	15,19,21	0.50	0
4	NAG	A	504	1	14,14,15	0.24	0	15,19,21	0.55	0
4	NAG	A	505	1	14,14,15	0.17	0	15,19,21	0.41	0
4	NAG	A	506	1	14,14,15	0.39	0	15,19,21	0.41	0
4	NAG	A	507	1	14,14,15	0.28	0	15,19,21	0.34	0
4	NAG	A	508	1	14,14,15	0.46	0	15,19,21	0.95	1 (6%)
4	NAG	A	509	1	14,14,15	0.26	0	15,19,21	0.25	0
5	EDO	A	510	-	3,3,3	0.44	0	2,2,2	0.37	0
5	EDO	A	511	-	3,3,3	0.34	0	2,2,2	0.62	0
5	EDO	A	512	-	3,3,3	0.41	0	2,2,2	0.30	0
4	NAG	B	501	1	14,14,15	0.16	0	15,19,21	0.63	0
4	NAG	B	502	-	14,14,15	0.34	0	15,19,21	0.59	0
4	NAG	B	503	1	14,14,15	0.36	0	15,19,21	0.48	0
4	NAG	B	504	1	14,14,15	0.18	0	15,19,21	0.52	0
4	NAG	B	505	1	14,14,15	0.30	0	15,19,21	0.35	0
4	NAG	B	506	1	14,14,15	0.54	0	15,19,21	0.27	0
4	NAG	B	507	1	14,14,15	0.46	0	15,19,21	0.34	0
4	NAG	B	508	1	14,14,15	0.39	0	15,19,21	0.66	0
5	EDO	B	509	-	3,3,3	0.47	0	2,2,2	0.42	0
5	EDO	B	510	-	3,3,3	0.47	0	2,2,2	0.42	0
5	EDO	B	511	-	3,3,3	0.47	0	2,2,2	0.42	0
6	ACA	B	512	-	5,8,8	0.25	0	5,8,8	0.43	0
4	NAG	F	501	1	14,14,15	0.24	0	15,19,21	0.52	0
4	NAG	F	502	1	14,14,15	0.29	0	15,19,21	0.57	0
4	NAG	F	503	1	14,14,15	0.33	0	15,19,21	0.36	0
4	NAG	F	504	1	14,14,15	0.27	0	15,19,21	0.63	1 (6%)
4	NAG	F	505	1	14,14,15	0.33	0	15,19,21	0.37	0
4	NAG	F	506	1	14,14,15	0.46	0	15,19,21	0.79	1 (6%)
4	NAG	F	507	1	14,14,15	0.18	0	15,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	F	508	1	14,14,15	0.15	0	15,19,21	0.36	0
4	NAG	F	509	-	14,14,15	0.94	1 (7%)	15,19,21	0.62	0
4	NAG	J	501	1	14,14,15	0.37	0	15,19,21	0.36	0
4	NAG	J	502	1	14,14,15	0.12	0	15,19,21	0.58	0
4	NAG	J	503	1	14,14,15	0.23	0	15,19,21	1.01	2 (13%)
4	NAG	J	504	1	14,14,15	0.17	0	15,19,21	0.48	0
4	NAG	J	505	-	14,14,15	0.24	0	15,19,21	0.20	0
4	NAG	J	506	1	14,14,15	0.23	0	15,19,21	0.32	0
4	NAG	J	507	1	14,14,15	0.30	0	15,19,21	0.29	0
4	NAG	J	508	1	14,14,15	0.29	0	15,19,21	0.31	0
4	NAG	J	509	1	14,14,15	0.23	0	15,19,21	0.38	0
5	EDO	J	510	-	3,3,3	0.47	0	2,2,2	0.42	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
4	NAG	A	501	1	-	0/6/23/26	0/1/1/1
4	NAG	A	502	-	-	0/6/23/26	0/1/1/1
4	NAG	A	503	1	-	0/6/23/26	0/1/1/1
4	NAG	A	504	1	-	0/6/23/26	0/1/1/1
4	NAG	A	505	1	-	0/6/23/26	0/1/1/1
4	NAG	A	506	1	-	0/6/23/26	0/1/1/1
4	NAG	A	507	1	-	0/6/23/26	0/1/1/1
4	NAG	A	508	1	-	0/6/23/26	0/1/1/1
4	NAG	A	509	1	-	0/6/23/26	0/1/1/1
5	EDO	A	510	-	-	0/1/1/1	0/0/0/0
5	EDO	A	511	-	-	0/1/1/1	0/0/0/0
5	EDO	A	512	-	-	0/1/1/1	0/0/0/0
4	NAG	B	501	1	-	0/6/23/26	0/1/1/1
4	NAG	B	502	-	-	0/6/23/26	0/1/1/1
4	NAG	B	503	1	-	0/6/23/26	0/1/1/1
4	NAG	B	504	1	-	0/6/23/26	0/1/1/1
4	NAG	B	505	1	-	0/6/23/26	0/1/1/1
4	NAG	B	506	1	-	0/6/23/26	0/1/1/1
4	NAG	B	507	1	-	0/6/23/26	0/1/1/1
4	NAG	B	508	1	-	0/6/23/26	0/1/1/1
5	EDO	B	509	-	-	0/1/1/1	0/0/0/0
5	EDO	B	510	-	-	0/1/1/1	0/0/0/0
5	EDO	B	511	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ACA	B	512	-	-	0/4/6/6	0/0/0/0
4	NAG	F	501	1	-	0/6/23/26	0/1/1/1
4	NAG	F	502	1	-	0/6/23/26	0/1/1/1
4	NAG	F	503	1	-	0/6/23/26	0/1/1/1
4	NAG	F	504	1	-	0/6/23/26	0/1/1/1
4	NAG	F	505	1	-	0/6/23/26	0/1/1/1
4	NAG	F	506	1	-	0/6/23/26	0/1/1/1
4	NAG	F	507	1	-	0/6/23/26	0/1/1/1
4	NAG	F	508	1	-	0/6/23/26	0/1/1/1
4	NAG	F	509	-	-	0/6/23/26	0/1/1/1
4	NAG	J	501	1	-	0/6/23/26	0/1/1/1
4	NAG	J	502	1	-	0/6/23/26	0/1/1/1
4	NAG	J	503	1	-	0/6/23/26	0/1/1/1
4	NAG	J	504	1	-	0/6/23/26	0/1/1/1
4	NAG	J	505	-	-	0/6/23/26	0/1/1/1
4	NAG	J	506	1	-	0/6/23/26	0/1/1/1
4	NAG	J	507	1	-	0/6/23/26	0/1/1/1
4	NAG	J	508	1	-	0/6/23/26	0/1/1/1
4	NAG	J	509	1	-	0/6/23/26	0/1/1/1
5	EDO	J	510	-	-	0/1/1/1	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	509	NAG	O5-C1	-2.90	1.38	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	503	NAG	C1-O5-C5	2.01	114.80	112.25
4	F	504	NAG	C1-O5-C5	2.03	114.82	112.25
4	F	506	NAG	C1-O5-C5	2.93	115.96	112.25
4	A	508	NAG	C1-O5-C5	3.02	116.08	112.25
4	J	503	NAG	C2-N2-C7	3.03	126.94	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	NAG	2	0
5	A	510	EDO	1	0
5	A	512	EDO	3	0
4	B	502	NAG	2	0
5	B	509	EDO	1	0
5	B	510	EDO	2	0
6	B	512	ACA	1	0
4	F	509	NAG	3	0
4	J	502	NAG	1	0
4	J	503	NAG	2	0
4	J	505	NAG	1	0
5	J	510	EDO	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	343/376 (91%)	0.78	44 (12%) 5 7	33, 50, 99, 160	0
1	B	341/376 (90%)	0.61	33 (9%) 10 14	29, 45, 88, 140	0
1	F	334/376 (88%)	0.64	34 (10%) 9 13	36, 53, 97, 135	0
1	J	337/376 (89%)	0.75	35 (10%) 8 12	36, 60, 102, 133	0
2	C	24/28 (85%)	0.47	2 (8%) 14 19	21, 49, 70, 72	0
2	D	24/28 (85%)	0.34	1 (4%) 40 49	21, 51, 70, 76	0
2	G	24/28 (85%)	0.50	1 (4%) 40 49	21, 66, 81, 88	0
2	K	24/28 (85%)	0.39	0 100 100	21, 60, 79, 86	0
3	H	124/129 (96%)	0.46	10 (8%) 15 20	35, 53, 83, 131	0
3	I	125/129 (96%)	0.58	8 (6%) 23 30	34, 54, 83, 117	0
3	L	123/129 (95%)	0.73	16 (13%) 5 7	38, 63, 87, 113	0
3	M	123/129 (95%)	1.65	39 (31%) 1 1	47, 92, 134, 156	0
All	All	1946/2132 (91%)	0.72	223 (11%) 6 10	21, 55, 103, 160	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	44	VAL	16.1
3	M	123	SER	8.6
1	B	45	TRP	8.1
1	A	44	VAL	7.6
1	A	45	TRP	7.6
3	M	124	SER	7.5
1	F	44	VAL	7.3
1	A	492	GLU	7.3
1	A	301	ASN	6.9
3	M	18	LEU	6.7
1	F	492	GLU	6.3

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Mol	Chain	Res	Type	RSRZ
1	B	46	LYS	6.2
3	M	12	VAL	6.0
3	M	10	GLY	5.9
1	A	87	GLU	5.8
1	A	491[A]	ILE	5.7
3	M	88	PRO	5.6
1	J	221	ALA	5.5
3	M	1	GLU	5.5
1	J	355	ASN	5.4
1	B	87	GLU	5.2
3	M	121	THR	5.1
1	J	356	ASN	5.0
3	M	11	LEU	4.9
3	I	125	ALA	4.9
1	A	463	ASN	4.9
1	J	46	LYS	4.9
3	M	13	GLN	4.8
3	H	27	PHE	4.7
3	M	122	VAL	4.7
1	A	88	ASN	4.7
1	B	492	GLU	4.6
3	M	17	SER	4.5
1	F	301	ASN	4.5
1	F	464	GLY	4.3
1	A	401	ASN	4.3
1	J	45	TRP	4.3
3	M	27	PHE	4.3
1	J	492	GLU	4.3
3	M	69	THR	4.3
3	M	9	GLY	4.2
3	M	20	LEU	4.2
1	J	358[A]	THR	4.2
1	F	87	GLU	4.1
3	M	7	SER	4.0
1	B	88	ASN	4.0
1	J	354	GLY	4.0
1	J	222	GLY	3.9
1	A	356	ASN	3.9
1	F	371	ILE	3.9
3	M	86	LEU	3.8
1	F	412	ARG	3.8
1	J	80	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	J	79	PRO	3.8
3	L	41	PRO	3.8
3	H	43	LYS	3.8
1	B	411	GLY	3.7
1	F	88	ASN	3.7
1	F	356	ASN	3.6
1	J	301	ASN	3.6
3	M	8	GLY	3.6
1	A	464	GLY	3.6
1	A	255	VAL	3.5
1	J	76	PRO	3.5
1	F	463	ASN	3.5
1	F	46	LYS	3.5
1	F	72	HIS	3.5
3	M	89	GLU	3.5
3	M	16	GLY	3.5
3	I	27	PHE	3.5
1	J	395	ASP	3.4
1	J	465	THR	3.4
1	B	459	GLY	3.4
1	F	45	TRP	3.3
3	H	42	GLY	3.3
1	J	124	GLY	3.3
3	I	1	GLU	3.2
3	L	116	LYS	3.2
1	F	459	GLY	3.2
1	J	394	ASN	3.2
3	M	24	ALA	3.2
3	L	42	GLY	3.1
1	A	411	GLY	3.1
3	M	19	ARG	3.1
1	A	459	GLY	3.0
1	F	80	ASN	3.0
1	A	371	ILE	3.0
3	L	40	ALA	3.0
3	L	5	VAL	3.0
3	H	2	VAL	3.0
3	L	87	LYS	3.0
1	J	268	GLU	3.0
1	B	398	LYS	3.0
1	A	257	THR	3.0
1	B	412	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
3	M	117	GLY	2.9
3	M	14	PRO	2.9
1	J	336	THR	2.9
1	J	396	THR	2.9
1	B	259	LEU	2.9
1	J	223	PHE	2.9
1	A	46	LYS	2.9
3	I	115	GLY	2.9
1	F	85	LYS	2.9
3	H	15	GLY	2.8
1	J	300	ASN	2.8
1	J	220	PRO	2.8
3	M	84	ASN	2.8
1	A	424	ILE	2.8
1	B	465	THR	2.7
1	B	424	ILE	2.7
3	M	26	GLY	2.7
3	H	41	PRO	2.7
3	M	5	VAL	2.7
3	M	116	LYS	2.7
3	I	126	ALA	2.7
1	F	424	ILE	2.6
1	A	375	SER	2.6
1	J	72	HIS	2.6
3	L	1	GLU	2.6
1	J	52	LEU	2.6
1	B	85	LYS	2.6
1	A	256	SER	2.6
2	D	5	PHE	2.6
3	L	29	LEU	2.6
3	L	9	GLY	2.6
1	J	254	VAL	2.6
1	B	463	ASN	2.6
3	M	23	ALA	2.6
1	B	356	ASN	2.6
1	B	255	VAL	2.6
3	L	13	GLN	2.6
1	A	232	LYS	2.5
1	J	51	THR	2.5
1	F	300	ASN	2.5
1	B	453	LEU	2.5
1	J	267	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	382	PHE	2.5
1	A	86	LEU	2.5
1	F	255	VAL	2.5
1	B	371	ILE	2.5
1	J	464	GLY	2.5
3	L	117	GLY	2.5
1	A	353	PHE	2.5
2	C	8	LEU	2.5
1	A	239	CYS	2.5
1	A	354	GLY	2.5
1	F	465	THR	2.5
3	M	43	LYS	2.5
1	A	240	THR	2.5
1	F	375	SER	2.5
1	J	393	TRP	2.5
1	A	259	LEU	2.4
3	M	78	THR	2.4
1	F	354	GLY	2.4
1	A	47	GLU	2.4
1	A	85	LYS	2.4
1	F	393	TRP	2.4
1	J	473	GLY	2.4
1	B	221	ALA	2.4
1	A	80	ASN	2.4
1	B	301	ASN	2.4
3	L	7	SER	2.3
1	B	89	VAL	2.3
1	F	411	GLY	2.3
1	A	300	ASN	2.3
1	F	49	THR	2.3
3	M	81	LEU	2.3
3	L	122	VAL	2.3
1	F	47	GLU	2.3
1	A	72	HIS	2.3
1	A	490[A]	LYS	2.3
1	A	254	VAL	2.3
1	B	384	TYR	2.2
1	A	50	THR	2.2
3	M	29	LEU	2.2
3	M	31	TYR	2.2
3	M	118	THR	2.2
1	A	238	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	384	TYR	2.2
1	J	441	GLY	2.2
1	B	231	LYS	2.2
1	B	464	GLY	2.2
1	A	225	ILE	2.2
3	H	1	GLU	2.2
3	L	31	TYR	2.2
1	B	375	SER	2.2
1	F	423	ILE	2.2
1	F	223	PHE	2.2
1	B	423	ILE	2.2
1	J	337	GLN	2.1
1	B	256	SER	2.1
3	H	16	GLY	2.1
2	C	5	PHE	2.1
1	A	222	GLY	2.1
1	F	257	THR	2.1
1	B	49	THR	2.1
3	L	3	GLN	2.1
1	J	424	ILE	2.1
1	B	257	THR	2.1
1	A	382	PHE	2.1
3	I	36	TRP	2.1
1	B	254	VAL	2.1
1	F	336	THR	2.1
3	M	73	ASP	2.1
1	A	355	ASN	2.1
1	B	355	ASN	2.1
1	A	427	TRP	2.1
1	A	57	ASP	2.1
1	A	108	ILE	2.1
1	J	413	ASN	2.1
3	L	115	GLY	2.1
3	I	12	VAL	2.1
1	F	221	ALA	2.0
3	M	103	VAL	2.0
1	B	420	ILE	2.0
1	F	256	SER	2.0
3	H	124	SER	2.0
3	M	21	SER	2.0
3	H	125	ALA	2.0
2	G	4	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
3	I	2	VAL	2.0
1	F	79	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	U2X	K	23	19/20	0.94	0.22	-	35,46,57,59	0
2	DPR	C	21	7/8	0.92	0.14	-	19,19,24,25	0
2	DPR	D	21	7/8	0.92	0.11	-	19,19,24,25	0
2	U2X	D	23	19/20	0.96	0.23	-	32,39,47,47	0
2	DPR	G	21	7/8	0.93	0.14	-	19,19,24,25	0
2	U2X	C	23	19/20	0.95	0.20	-	25,38,46,50	0
2	DPR	K	21	7/8	0.93	0.14	-	19,19,24,25	0
2	U2X	G	23	19/20	0.96	0.18	-	35,41,50,58	0

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
4	NAG	B	502	14/15	0.61	0.32	10.90	47,79,94,94	0
4	NAG	A	502	14/15	0.79	0.29	10.10	57,75,97,100	0
5	EDO	B	510	4/4	0.68	0.36	8.65	80,81,81,84	0
5	EDO	J	510	4/4	0.68	0.44	7.83	78,79,79,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	EDO	A	510	4/4	0.84	0.35	5.43	62,63,64,66	0
4	NAG	B	503	14/15	0.86	0.16	4.84	73,84,89,91	0
4	NAG	J	505	14/15	0.71	0.29	4.38	98,109,122,128	0
4	NAG	J	502	14/15	0.82	0.19	3.60	91,95,98,103	0
5	EDO	B	509	4/4	0.78	0.29	3.24	58,59,61,61	0
5	EDO	A	512	4/4	0.88	0.21	2.98	55,55,57,59	0
4	NAG	A	509	14/15	0.88	0.22	2.86	50,62,82,84	0
4	NAG	A	506	14/15	0.88	0.22	2.83	52,62,72,76	0
4	NAG	F	506	14/15	0.79	0.33	2.80	84,89,93,94	0
4	NAG	J	507	14/15	0.90	0.29	2.42	81,85,96,98	0
5	EDO	A	511	4/4	0.92	0.16	2.07	49,50,50,52	0
4	NAG	A	508	14/15	0.72	0.24	1.90	72,81,90,92	0
4	NAG	A	503	14/15	0.88	0.21	1.75	82,85,94,94	0
4	NAG	F	509	14/15	0.86	0.20	1.73	56,67,90,95	0
4	NAG	B	506	14/15	0.90	0.16	1.67	49,60,68,69	0
4	NAG	J	509	14/15	0.80	0.33	1.49	84,93,103,104	0
4	NAG	F	505	14/15	0.88	0.25	1.10	67,71,80,83	0
4	NAG	F	508	14/15	0.81	0.21	0.76	57,74,84,87	0
6	ACA	B	512	9/9	0.84	0.31	0.71	52,59,69,70	0
4	NAG	J	506	14/15	0.93	0.26	0.52	90,94,104,106	0
4	NAG	F	507	14/15	0.90	0.15	0.19	52,58,65,68	0
4	NAG	A	505	14/15	0.91	0.19	0.15	62,67,76,79	0
5	EDO	B	511	4/4	0.90	0.16	0.13	53,59,63,70	0
4	NAG	B	508	14/15	0.88	0.16	-0.23	50,72,78,83	0
4	NAG	B	505	14/15	0.91	0.12	-0.29	47,52,70,70	0
4	NAG	J	501	14/15	0.82	0.27	-0.36	90,98,103,104	0
4	NAG	F	504	14/15	0.97	0.15	-0.37	34,43,55,58	0
4	NAG	F	502	14/15	0.95	0.12	-0.38	52,62,71,74	0
4	NAG	A	507	14/15	0.91	0.14	-0.79	36,45,52,52	0
4	NAG	J	504	14/15	0.96	0.13	-1.07	52,55,64,64	0
4	NAG	B	504	14/15	0.95	0.13	-1.13	29,40,44,45	0
4	NAG	J	508	14/15	0.94	0.09	-1.17	45,50,59,61	0
4	NAG	A	504	14/15	0.97	0.12	-1.45	30,40,46,47	0
4	NAG	B	507	14/15	0.96	0.11	-1.65	34,44,48,50	0
4	NAG	F	501	14/15	0.95	0.18	-	62,70,79,87	0
4	NAG	A	501	14/15	0.85	0.27	-	66,75,80,86	0
4	NAG	F	503	14/15	0.61	0.45	-	115,130,142,143	0
4	NAG	B	501	14/15	0.88	0.20	-	61,69,76,80	0
4	NAG	J	503	14/15	0.81	0.37	-	97,104,107,107	0

6.5 Other polymers (i)

There are no such residues in this entry.