Full wwPDB X-ray Structure Validation Report (i)

Jan 19, 2017 – 12:00 PM EST

PDB ID	:	3ZTJ
Title	:	Structure of influenza A neutralizing antibody selected from cultures of single human plasma cells in complex with human H3 Influenza haemagglutinin.
Authors	:	Voss, J.E.; Vachieri, S.G.; Gamblin, S.J.; Collins, P.J.; Haire, L.F.; Skehel, J.J.
Deposited on	:	2011-07-08
Resolution	:	3.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

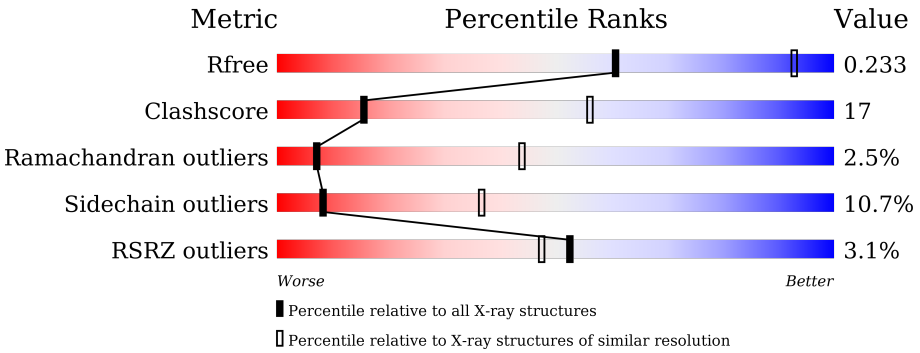
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 3.41 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	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)

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	329	58% 34% 5%
1	C	329	53% 37% 5%
1	E	329	64% 29%
2	B	175	65% 29%
2	D	175	59% 33% 6%
2	F	175	66% 25% 6%

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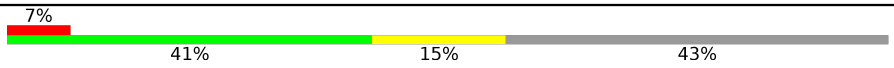
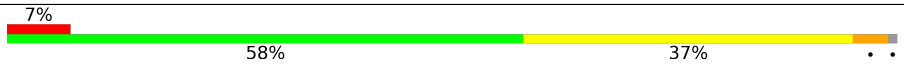
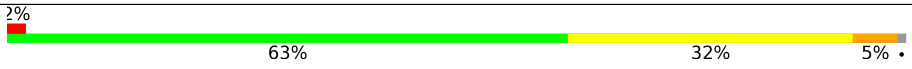
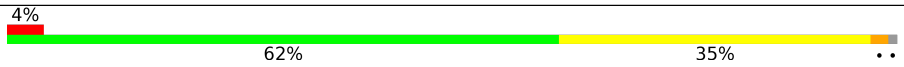
Mol	Chain	Length	Quality of chain
3	G	226	
3	I	226	
3	K	226	
4	H	218	
4	J	218	
4	L	218	

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	NAG	A	430	X	-	-	-
6	NAG	C	430	X	-	-	-
6	NAG	F	410	X	-	-	-
7	NAG	D	410	-	-	X	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20384 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 HEMAGGLUTININ HA1 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2451	1535	430	473	13			
1	C	316	Total	C	N	O	S	0	0	0
			2425	1521	422	469	13			
1	E	318	Total	C	N	O	S	0	0	0
			2451	1535	430	473	13			

- Molecule 2 is a protein called HEMAGGLUTININ HA2 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1392	863	244	279	6			
2	D	172	Total	C	N	O	S	0	0	0
			1382	856	243	277	6			
2	F	172	Total	C	N	O	S	0	0	0
			1379	854	244	275	6			

- Molecule 3 is a protein called FI6V3 ANTIBODY HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	129	Total	C	N	O	S	0	0	0
			1004	642	167	191	4			
3	I	226	Total	C	N	O	S	0	0	0
			1712	1089	285	332	6			
3	K	224	Total	C	N	O	S	0	0	0
			1697	1082	281	328	6			

- Molecule 4 is a protein called FI6V3 ANTIBODY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	107	Total	C	N	O	S	0	0	0
			771	485	129	154	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	216	Total	C	N	O	S	0	0	0
			1647	1035	278	329	5			
4	L	216	Total	C	N	O	S	0	0	0
			1623	1018	273	327	5			

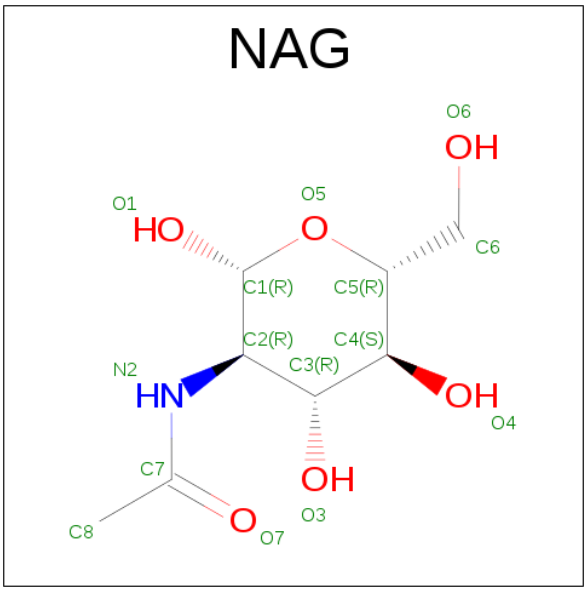
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			39	22	2	15		
5	A	3	Total	C	N	O	0	0
			39	22	2	15		
5	C	3	Total	C	N	O	0	0
			39	22	2	15		
5	E	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	B	2	Total	C	N	O	0	0
			28	16	2	10		
6	C	2	Total	C	N	O	0	0
			28	16	2	10		
6	C	2	Total	C	N	O	0	0
			28	16	2	10		
6	C	2	Total	C	N	O	0	0
			28	16	2	10		
6	E	2	Total	C	N	O	0	0
			28	16	2	10		
6	E	2	Total	C	N	O	0	0
			28	16	2	10		
6	E	2	Total	C	N	O	0	0
			28	16	2	10		
6	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



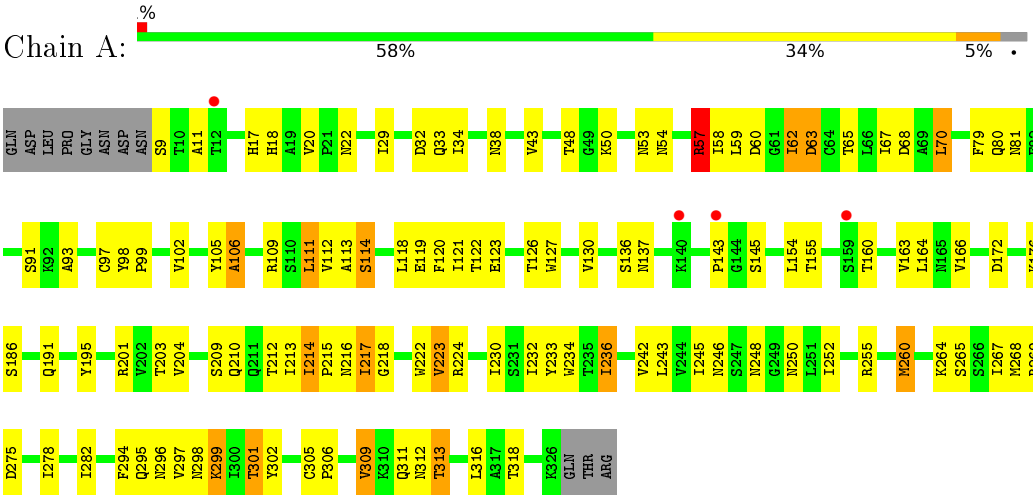
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	D	1	14	8	1	5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

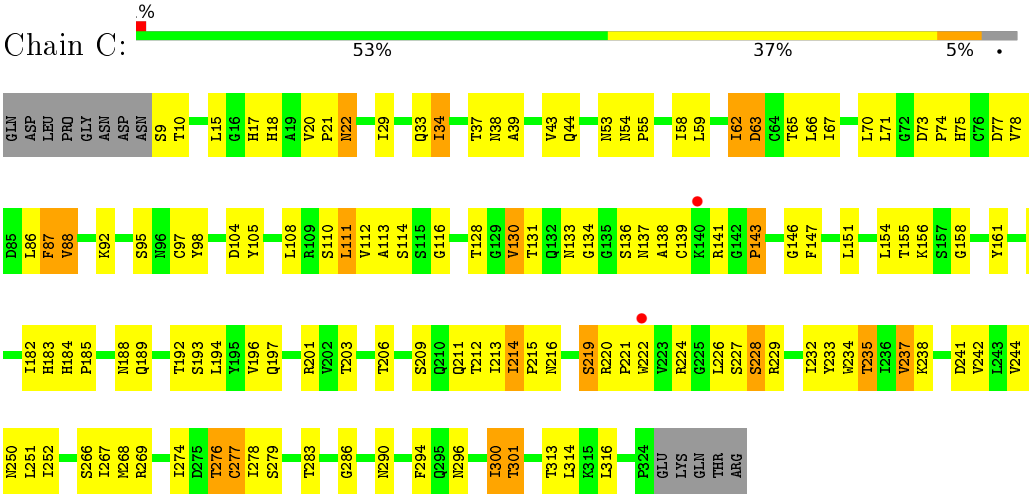
- Molecule 1: HEMAGGLUTININ HA1 CHAIN

Chain A:



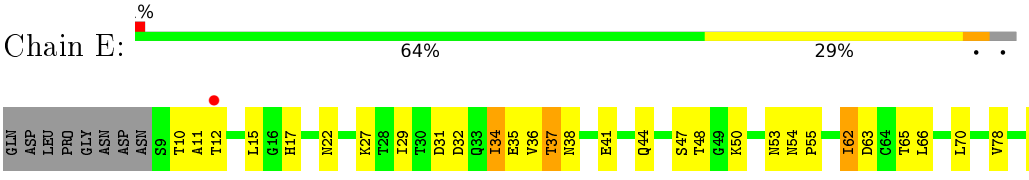
- Molecule 1: HEMAGGLUTININ HA1 CHAIN

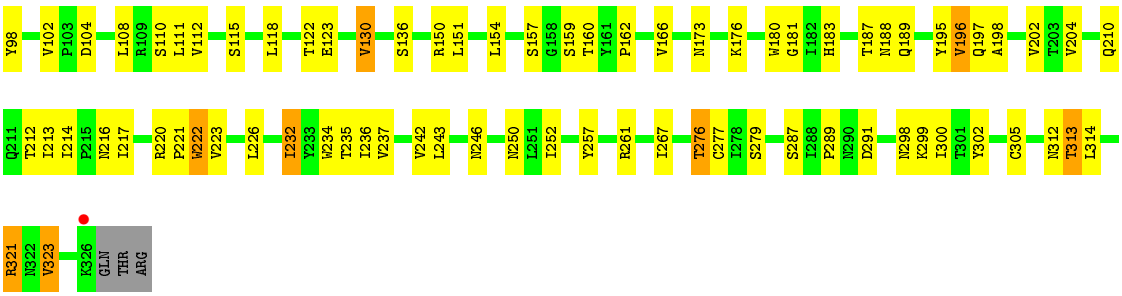
Chain C:



- Molecule 1: HEMAGGLUTININ HA1 CHAIN

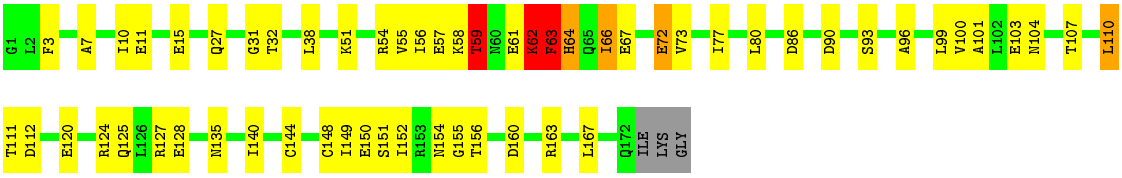
Chain E:





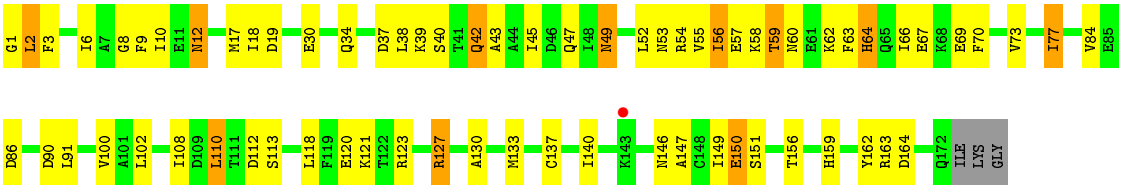
• Molecule 2: HEMAGGLUTININ HA2 CHAIN

Chain B:



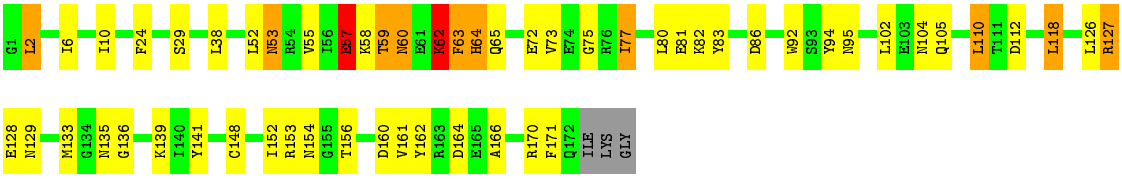
• Molecule 2: HEMAGGLUTININ HA2 CHAIN

Chain D:



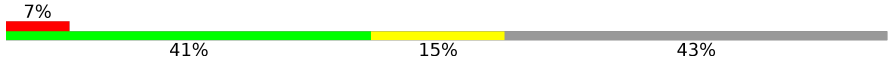
• Molecule 2: HEMAGGLUTININ HA2 CHAIN

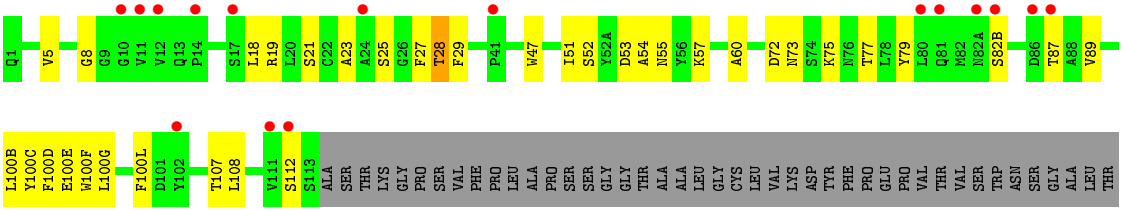
Chain F:



• Molecule 3: FI6V3 ANTIBODY HEAVY CHAIN

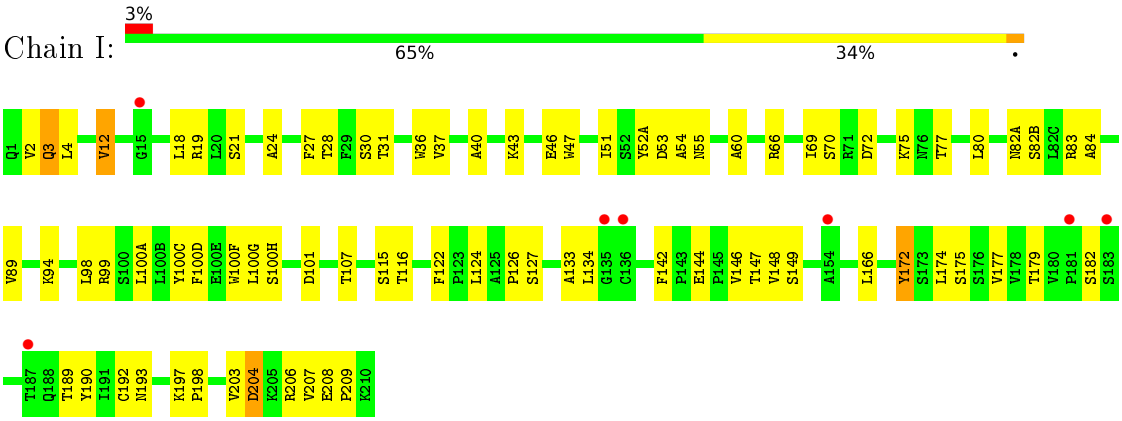
Chain G:





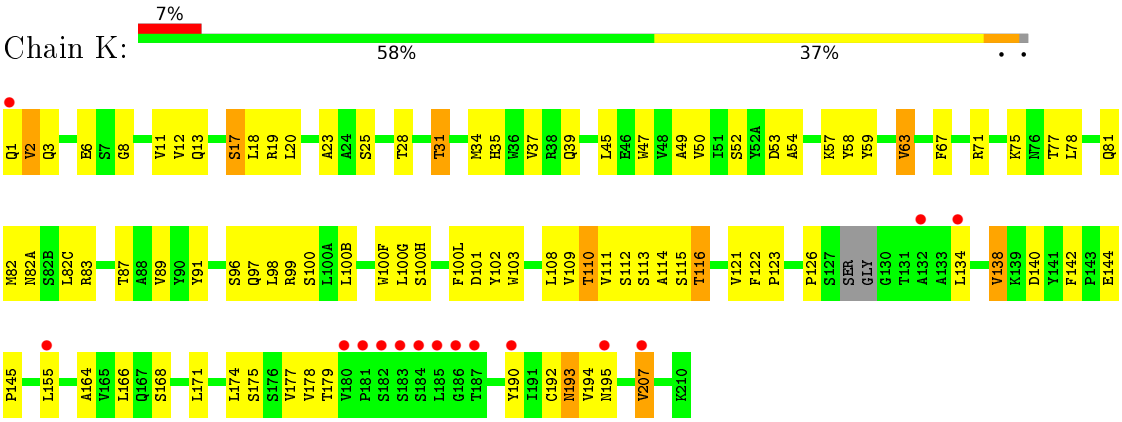
- Molecule 3: FI6V3 ANTIBODY HEAVY CHAIN

Chain I:



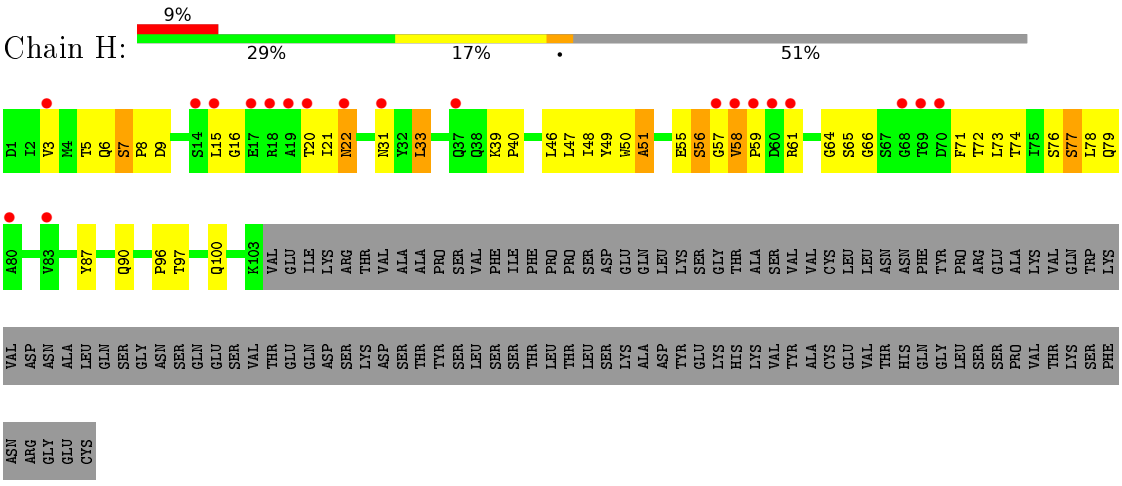
- Molecule 3: FI6V3 ANTIBODY HEAVY CHAIN

Chain K:



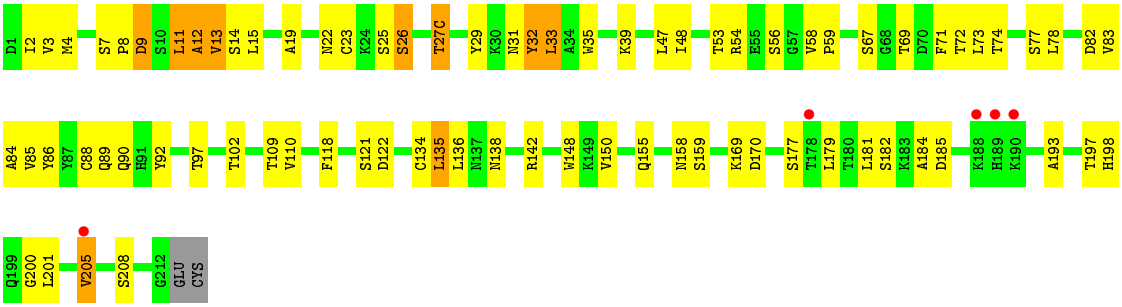
- Molecule 4: FI6V3 ANTIBODY LIGHT CHAIN

Chain H:



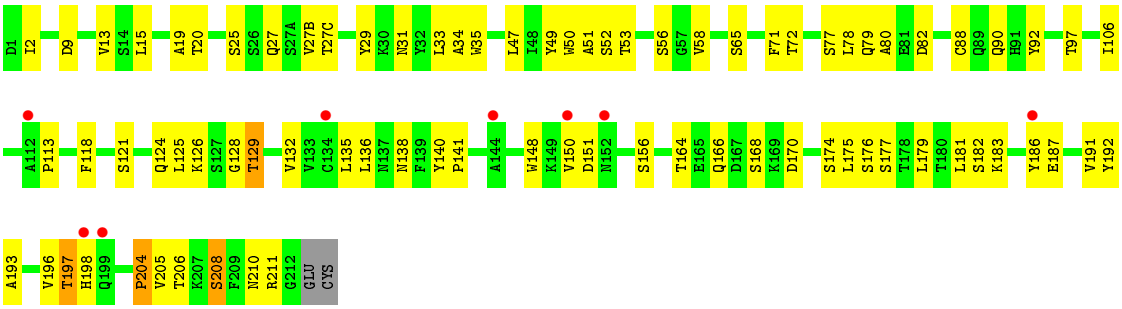
- Molecule 4: FI6V3 ANTIBODY LIGHT CHAIN

Chain J:



- Molecule 4: FI6V3 ANTIBODY LIGHT CHAIN

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	171.49Å 193.43Å 213.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	143.42 – 3.41 30.16 – 3.41	Depositor EDS
% Data completeness (in resolution range)	95.6 (143.42-3.41) 95.4 (30.16-3.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 3.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.234 , 0.284 0.236 , 0.233	Depositor DCC
R_{free} test set	4622 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	116.8	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 94.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	20384	wwPDB-VP
Average B, all atoms (Å^2)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: BMA, 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	0.73	0/2507	0.82	1/3417 (0.0%)
1	C	0.78	1/2481 (0.0%)	0.83	0/3384
1	E	0.78	1/2507 (0.0%)	0.86	1/3417 (0.0%)
2	B	0.87	4/1416 (0.3%)	0.82	1/1905 (0.1%)
2	D	0.92	3/1406 (0.2%)	0.87	2/1893 (0.1%)
2	F	0.86	2/1402 (0.1%)	0.85	1/1887 (0.1%)
3	G	0.52	0/1030	0.63	0/1401
3	I	0.67	0/1757	0.73	0/2399
3	K	0.73	0/1741	0.77	0/2376
4	H	0.54	0/792	0.63	0/1088
4	J	0.70	0/1686	0.77	0/2299
4	L	0.61	0/1662	0.71	0/2272
All	All	0.75	11/20387 (0.1%)	0.79	6/27738 (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	B	0	1
2	F	0	3
5	A	1	0
6	C	1	0
6	F	1	0
All	All	3	4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	150	GLU	CB-CG	7.17	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	59	THR	CA-CB	7.02	1.71	1.53
2	D	150	GLU	CG-CD	6.83	1.62	1.51
1	C	277	CYS	CB-SG	6.16	1.92	1.82
2	B	61	GLU	CG-CD	5.71	1.60	1.51
2	D	67	GLU	CG-CD	5.65	1.60	1.51
2	B	61	GLU	CD-OE2	5.53	1.31	1.25
2	F	60	ASN	CB-CG	5.35	1.63	1.51
2	B	59	THR	CA-CB	5.33	1.67	1.53
1	E	35	GLU	CG-CD	5.25	1.59	1.51
2	B	61	GLU	CB-CG	5.17	1.61	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	63	PHE	N-CA-C	-9.09	86.45	111.00
1	A	57	ARG	NE-CZ-NH1	8.39	124.49	120.30
2	D	54	ARG	NE-CZ-NH1	7.04	123.82	120.30
2	D	54	ARG	NE-CZ-NH2	-6.23	117.19	120.30
2	B	63	PHE	N-CA-CB	5.36	120.25	110.60
1	E	232	ILE	CB-CA-C	-5.00	101.59	111.60

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	430	NAG	C1
6	C	430	NAG	C1
6	F	410	NAG	C1

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	62	LYS	Peptide
2	F	57	GLU	Peptide
2	F	62	LYS	Peptide
2	F	75	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	2451	0	2395	90	0
1	C	2425	0	2364	99	0
1	E	2451	0	2395	68	0
2	B	1392	0	1298	60	0
2	D	1382	0	1276	77	0
2	F	1379	0	1285	46	0
3	G	1004	0	937	17	0
3	I	1712	0	1638	68	0
3	K	1697	0	1628	75	0
4	H	771	0	666	30	0
4	J	1647	0	1562	55	0
4	L	1623	0	1497	57	0
5	A	78	0	68	2	0
5	C	39	0	34	0	0
5	E	39	0	34	0	0
6	A	56	0	50	2	0
6	B	28	0	25	1	0
6	C	84	0	75	3	0
6	E	84	0	75	1	0
6	F	28	0	25	2	0
7	D	14	0	13	7	0
All	All	20384	0	19340	682	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 17.

All (682) 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:D:52:LEU:O	2:D:56:ILE:HD11	1.43	1.17
2:D:56:ILE:N	2:D:56:ILE:HD12	1.68	1.08
2:D:56:ILE:H	2:D:56:ILE:HD12	1.15	1.00
4:L:13:VAL:HG11	4:L:19:ALA:HB2	1.45	0.98
1:C:53:ASN:HD21	1:C:276:THR:HG23	1.25	0.98
2:D:53:ASN:HD22	3:I:98:LEU:HD23	1.29	0.98
3:K:63:VAL:HG11	3:K:67:PHE:CE2	1.99	0.97
2:F:77:ILE:HD12	2:F:77:ILE:H	1.28	0.94
2:D:53:ASN:ND2	3:I:98:LEU:HD23	1.81	0.94
4:J:3:VAL:HG22	4:J:26:SER:OG	1.70	0.91
3:K:2:VAL:HG11	3:K:102:TYR:CE2	2.07	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:LEU:C	2:B:110:LEU:HD12	1.92	0.90
1:C:151:LEU:HD22	1:C:252:ILE:HG22	1.54	0.90
1:C:53:ASN:HD21	1:C:276:THR:CG2	1.84	0.89
2:F:53:ASN:ND2	3:K:98:LEU:HD23	1.88	0.88
3:K:2:VAL:HG21	3:K:102:TYR:CD2	2.08	0.88
4:J:22:ASN:OD1	4:J:72:THR:HG22	1.74	0.88
1:A:120:PHE:O	1:A:121:ILE:HD13	1.73	0.88
1:A:215:PRO:HG3	1:A:250:ASN:ND2	1.89	0.87
2:B:56:ILE:HG22	2:B:56:ILE:O	1.74	0.87
1:E:180:TRP:CE2	1:E:204:VAL:HG21	2.09	0.87
1:A:215:PRO:HG3	1:A:250:ASN:HD22	1.41	0.86
3:I:75:LYS:O	3:I:77:THR:HG23	1.76	0.85
2:D:52:LEU:O	2:D:56:ILE:CD1	2.25	0.83
2:F:57:GLU:N	2:F:57:GLU:OE1	2.11	0.83
3:K:63:VAL:HG11	3:K:67:PHE:CD2	2.14	0.83
3:I:133:ALA:HB2	3:I:179:THR:HG22	1.58	0.82
1:C:53:ASN:ND2	1:C:276:THR:HG23	1.95	0.82
1:C:15:LEU:HD12	2:D:118:LEU:HD23	1.60	0.82
2:D:63:PHE:O	2:D:64:HIS:O	1.96	0.82
3:I:69:ILE:HG23	3:I:69:ILE:O	1.80	0.79
2:D:38:LEU:HD23	3:I:100(F):TRP:CE2	2.17	0.79
4:L:2:ILE:HD11	4:L:90:GLN:HG2	1.63	0.79
3:I:116:THR:HG23	3:I:142:PHE:O	1.82	0.79
1:A:70:LEU:HD21	1:A:179:ILE:HG13	1.64	0.77
1:C:38:ASN:OD1	1:C:39:ALA:N	2.18	0.76
1:C:54:ASN:HB3	1:C:278:ILE:HD13	1.65	0.76
1:A:216:ASN:HB3	1:C:212:THR:HG21	1.68	0.76
4:L:47:LEU:HA	4:L:58:VAL:HG21	1.68	0.76
1:A:57:ARG:HG2	1:A:57:ARG:HH11	1.51	0.76
2:D:37:ASP:OD2	2:D:118:LEU:HD11	1.85	0.76
3:G:8:GLY:O	3:G:18:LEU:HD21	1.84	0.76
3:K:2:VAL:HG11	3:K:102:TYR:HE2	1.50	0.76
1:A:38:ASN:HB3	1:A:318:THR:HG23	1.68	0.75
1:C:67:ILE:HD12	1:C:108:LEU:HD23	1.68	0.75
3:K:63:VAL:CG1	3:K:67:PHE:CE2	2.70	0.74
1:C:67:ILE:CD1	1:C:108:LEU:HD23	2.17	0.74
1:C:139:CYS:HB3	1:C:146:GLY:O	1.86	0.74
2:D:38:LEU:HD23	3:I:100(F):TRP:CD2	2.22	0.74
1:C:86:LEU:HD12	1:C:266:SER:O	1.86	0.74
1:A:130:VAL:HG21	1:A:164:LEU:HD11	1.70	0.73
4:L:193:ALA:HB2	4:L:208:SER:OG	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:35:TRP:CZ3	4:L:88:CYS:HB3	2.23	0.73
4:L:148:TRP:CE3	4:L:179:LEU:HD22	2.23	0.73
3:I:18:LEU:HD12	3:I:19:ARG:H	1.53	0.72
4:J:4:MET:CE	4:J:23:CYS:SG	2.77	0.72
4:H:50:TRP:O	4:H:51:ALA:HB3	1.89	0.71
4:J:35:TRP:CZ3	4:J:88:CYS:HB3	2.25	0.71
1:E:196:VAL:HG12	1:E:197:GLN:NE2	2.06	0.71
4:H:33:LEU:HD13	4:H:71:PHE:CD2	2.26	0.71
4:L:47:LEU:HD23	4:L:58:VAL:HG22	1.72	0.71
1:E:53:ASN:ND2	1:E:276:THR:HG22	2.05	0.71
2:D:55:VAL:CG1	2:D:55:VAL:O	2.38	0.70
2:D:150:GLU:HG2	7:D:410:NAG:H5	1.73	0.70
3:K:155:LEU:HD21	3:K:178:VAL:HG21	1.74	0.70
1:C:15:LEU:CD1	2:D:118:LEU:HD23	2.21	0.70
4:J:47:LEU:O	4:J:48:ILE:HD13	1.92	0.70
4:J:22:ASN:OD1	4:J:72:THR:CG2	2.40	0.70
2:B:56:ILE:CG2	2:B:56:ILE:O	2.40	0.69
2:B:62:LYS:CB	2:B:63:PHE:HB2	2.23	0.69
3:I:69:ILE:CG2	3:I:69:ILE:O	2.40	0.69
3:K:63:VAL:CG1	3:K:67:PHE:CD2	2.75	0.69
4:L:150:VAL:HG13	4:L:192:TYR:CE1	2.26	0.69
1:A:204:VAL:HG22	1:A:245:ILE:HG12	1.74	0.69
1:A:53:ASN:HA	1:A:58:ILE:HD13	1.75	0.69
4:J:13:VAL:HG21	4:J:19:ALA:HB2	1.75	0.69
1:E:66:LEU:HD21	1:E:112:VAL:HG12	1.73	0.68
2:F:154:ASN:O	2:F:156:THR:HG23	1.92	0.68
1:A:102:VAL:HG13	1:A:232:ILE:HB	1.76	0.68
1:A:214:ILE:HG22	1:A:215:PRO:HD2	1.75	0.68
4:J:4:MET:HE1	4:J:23:CYS:SG	2.33	0.68
1:A:212:THR:HG21	1:E:216:ASN:HB3	1.74	0.67
2:F:77:ILE:H	2:F:77:ILE:CD1	2.03	0.67
1:E:183:HIS:ND1	1:E:195:TYR:OH	2.25	0.67
2:B:27:GLN:HA	2:B:32:THR:HG22	1.77	0.67
1:C:66:LEU:HD21	1:C:112:VAL:HG12	1.77	0.67
2:F:63:PHE:O	2:F:64:HIS:C	2.33	0.67
3:I:146:VAL:HG23	3:I:174:LEU:HD21	1.77	0.67
2:D:53:ASN:HA	2:D:56:ILE:HD11	1.76	0.67
4:H:90:GLN:HE21	4:H:97:THR:HG23	1.59	0.66
3:I:37:VAL:HG13	3:I:46:GLU:O	1.94	0.66
1:A:114:SER:HA	1:A:265:SER:O	1.95	0.66
1:A:268:MET:HE1	1:A:282:ILE:HG22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:13:GLN:HE21	3:K:113:SER:HA	1.59	0.66
3:I:28:THR:O	3:I:28:THR:HG22	1.97	0.65
6:E:440:NAG:H61	6:E:441:NAG:C7	2.26	0.65
1:E:65:THR:HG22	1:E:93:ALA:HB1	1.79	0.65
4:J:8:PRO:O	4:J:102:THR:HG23	1.96	0.65
1:E:298:ASN:ND2	1:E:300:ILE:HD12	2.12	0.65
1:E:17:HIS:HE1	1:E:323:VAL:HG23	1.61	0.65
1:E:220:ARG:HB3	1:E:221:PRO:CD	2.27	0.65
1:C:111:LEU:HD12	1:C:112:VAL:N	2.12	0.65
4:J:4:MET:HE3	4:J:23:CYS:SG	2.37	0.64
1:A:203:THR:HG23	1:A:212:THR:OG1	1.97	0.64
2:F:141:TYR:CD2	2:F:170:ARG:HG2	2.32	0.64
4:H:6:GLN:O	4:H:8:PRO:O	2.15	0.64
3:I:40:ALA:HB3	3:I:43:LYS:HB2	1.79	0.64
3:I:177:VAL:HG21	4:J:135:LEU:HD11	1.78	0.64
4:L:25:SER:OG	4:L:27:GLN:O	2.14	0.64
1:A:86:LEU:HD11	1:A:268:MET:HB2	1.79	0.64
4:L:31:ASN:HB3	4:L:51:ALA:HB2	1.80	0.64
3:K:17:SER:OG	3:K:82(A):ASN:HA	1.98	0.64
1:C:17:HIS:NE2	2:D:6:ILE:HG23	2.13	0.63
1:A:191:GLN:HB2	1:A:217:ILE:HD11	1.79	0.63
2:D:63:PHE:O	2:D:64:HIS:C	2.36	0.63
1:A:217:ILE:O	1:A:217:ILE:HG22	1.99	0.63
2:D:30:GLU:OE1	2:D:146:ASN:N	2.30	0.62
3:K:123:PRO:HB2	3:K:207:VAL:HG13	1.81	0.62
1:A:236:ILE:HD11	1:A:260:MET:SD	2.40	0.62
4:H:20:THR:HG22	4:H:74:THR:HG22	1.82	0.62
4:J:181:LEU:HD22	4:J:185:ASP:HB2	1.81	0.62
2:D:58:LYS:CD	2:D:58:LYS:O	2.47	0.62
2:F:161:VAL:HG12	2:F:162:TYR:CD1	2.35	0.62
4:H:50:TRP:O	4:H:51:ALA:CB	2.48	0.62
1:A:268:MET:HE1	1:A:282:ILE:CG2	2.30	0.61
4:L:121:SER:O	4:L:125:LEU:HD23	2.00	0.61
3:I:53:ASP:O	3:I:54:ALA:HB3	2.00	0.61
4:J:11:LEU:O	4:J:12:ALA:HB2	2.01	0.61
2:D:150:GLU:HG2	7:D:410:NAG:C5	2.31	0.61
4:L:136:LEU:HD21	4:L:196:VAL:HG11	1.82	0.61
2:B:62:LYS:CA	2:B:63:PHE:HB2	2.29	0.61
1:C:283:THR:OG1	1:C:286:GLY:O	2.16	0.61
1:A:186:SER:HA	1:A:218:GLY:O	2.01	0.61
1:C:220:ARG:HB3	1:C:221:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:LEU:N	1:E:15:LEU:HD22	2.16	0.60
1:A:57:ARG:CG	1:A:57:ARG:HH11	2.13	0.60
4:L:125:LEU:HD12	4:L:183:LYS:HG3	1.82	0.60
4:L:72:THR:O	4:L:72:THR:HG22	1.99	0.60
3:K:122:PHE:CE2	4:L:124:GLN:HG3	2.35	0.60
2:D:53:ASN:HA	2:D:56:ILE:CD1	2.32	0.60
3:K:35:HIS:CD2	3:K:100(L):PHE:CE2	2.90	0.60
1:C:70:LEU:HD13	1:C:112:VAL:HG21	1.84	0.60
1:C:88:VAL:O	1:C:88:VAL:HG12	2.00	0.60
1:A:70:LEU:HB2	1:A:118:LEU:HD21	1.84	0.60
1:C:20:VAL:HB	1:C:21:PRO:HD2	1.83	0.60
1:A:59:LEU:HD23	1:A:87:PHE:CD2	2.36	0.60
3:G:75:LYS:O	3:G:77:THR:HG23	2.02	0.60
4:L:2:ILE:C	4:L:2:ILE:HD12	2.22	0.59
2:B:110:LEU:C	2:B:110:LEU:CD1	2.68	0.59
1:C:70:LEU:CD1	1:C:112:VAL:HG21	2.32	0.59
1:A:97:CYS:O	1:A:224:ARG:NH1	2.36	0.59
2:F:6:ILE:HD12	2:F:112:ASP:HA	1.84	0.59
2:B:86:ASP:HB3	2:D:62:LYS:HD2	1.84	0.59
1:C:251:LEU:HD12	1:C:252:ILE:N	2.17	0.59
6:C:430:NAG:HO3	6:C:431:NAG:H61	1.68	0.59
2:F:156:THR:HG21	6:F:410:NAG:H82	1.85	0.58
2:F:63:PHE:O	2:F:65:GLN:N	2.36	0.58
2:B:144:CYS:SG	2:B:149:ILE:HG23	2.43	0.58
2:B:58:LYS:O	2:B:58:LYS:CG	2.51	0.58
1:A:97:CYS:O	1:A:98:TYR:C	2.41	0.58
1:C:156:LYS:HB3	1:C:194:LEU:O	2.03	0.58
2:D:56:ILE:N	2:D:56:ILE:CD1	2.48	0.58
1:A:99:PRO:HG3	1:A:223:VAL:HG12	1.85	0.58
2:B:62:LYS:HA	2:B:63:PHE:HB2	1.84	0.58
4:L:148:TRP:CG	4:L:179:LEU:HD13	2.38	0.58
4:J:27(C):THR:OG1	4:J:31:ASN:OD1	2.20	0.58
6:C:430:NAG:O3	6:C:431:NAG:H61	2.04	0.58
4:J:32:TYR:HB2	4:J:92:TYR:HB2	1.84	0.58
4:L:175:LEU:HD23	4:L:176:SER:N	2.18	0.58
4:L:47:LEU:HD23	4:L:58:VAL:CG2	2.34	0.58
2:D:53:ASN:ND2	3:I:99:ARG:HE	2.02	0.58
1:A:210:GLN:NE2	1:E:220:ARG:HH21	2.01	0.58
3:I:100(D):PHE:N	3:I:100(G):LEU:HD12	2.19	0.58
2:F:110:LEU:HD12	2:F:110:LEU:C	2.24	0.57
4:L:136:LEU:HD21	4:L:196:VAL:CG1	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:440:NAG:H61	6:C:441:NAG:H2	1.86	0.57
2:D:3:PHE:HB2	2:D:112:ASP:OD2	2.03	0.57
1:A:164:LEU:O	1:A:246:ASN:HA	2.04	0.57
2:D:52:LEU:C	2:D:56:ILE:HD11	2.23	0.57
2:D:63:PHE:C	2:D:64:HIS:O	2.42	0.57
3:K:112:SER:HB3	3:K:114:ALA:HB3	1.86	0.57
3:K:49:ALA:HB2	3:K:59:TYR:HD1	1.69	0.57
1:A:34:ILE:O	1:A:34:ILE:CG2	2.52	0.57
1:E:108:LEU:HD13	1:E:234:TRP:CE3	2.39	0.57
4:J:200:GLY:O	4:J:201:LEU:HD23	2.03	0.57
3:K:12:VAL:HG11	3:K:18:LEU:HB2	1.87	0.57
1:A:34:ILE:O	1:A:34:ILE:HG23	2.04	0.57
2:D:53:ASN:ND2	3:I:98:LEU:CD2	2.62	0.56
1:E:53:ASN:HD21	1:E:276:THR:HG22	1.68	0.56
1:E:212:THR:C	1:E:213:ILE:HD13	2.25	0.56
3:K:13:GLN:HE21	3:K:113:SER:CA	2.18	0.56
3:K:177:VAL:HG11	4:L:135:LEU:HD22	1.86	0.56
2:B:77:ILE:HD11	2:D:77:ILE:HD11	1.88	0.56
4:H:90:GLN:NE2	4:H:97:THR:HG23	2.20	0.56
1:C:188:ASN:O	1:C:192:THR:HG23	2.05	0.56
4:J:193:ALA:HB2	4:J:208:SER:HB3	1.87	0.56
2:B:62:LYS:HG2	2:B:63:PHE:N	2.20	0.56
3:I:100(D):PHE:H	3:I:100(G):LEU:HD12	1.70	0.56
4:L:118:PHE:O	4:L:132:VAL:HG13	2.05	0.56
3:K:144:GLU:OE2	3:K:164:ALA:HB3	2.06	0.56
4:L:128:GLY:O	4:L:129:THR:HG23	2.05	0.56
3:G:51:ILE:HD13	3:G:57:LYS:HG2	1.86	0.56
3:K:164:ALA:HA	3:K:174:LEU:HB3	1.87	0.56
2:F:53:ASN:ND2	3:K:99:ARG:HE	2.04	0.56
2:B:63:PHE:O	2:B:64:HIS:C	2.45	0.55
1:A:86:LEU:HD21	1:A:268:MET:CE	2.36	0.55
1:C:211:GLN:HE22	1:C:235:THR:HG23	1.72	0.55
1:C:147:PHE:CZ	1:C:252:ILE:HD12	2.42	0.55
3:I:100(A):LEU:HD22	3:I:100(C):TYR:CZ	2.41	0.55
3:I:51:ILE:O	3:I:51:ILE:HG23	2.07	0.55
3:K:12:VAL:HG21	3:K:82(C):LEU:HD13	1.89	0.55
4:L:33:LEU:HD23	4:L:34:ALA:N	2.21	0.55
3:K:39:GLN:HB2	3:K:45:LEU:HD23	1.89	0.55
2:B:110:LEU:O	2:B:110:LEU:HD12	2.07	0.55
2:B:149:ILE:HG22	2:B:152:ILE:HD12	1.89	0.55
1:C:77:ASP:C	1:C:79:PHE:H	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:GLY:O	2:D:3:PHE:N	2.39	0.55
4:H:65:SER:OG	4:H:66:GLY:N	2.39	0.55
4:L:148:TRP:CD2	4:L:179:LEU:HD13	2.42	0.55
1:A:230:ILE:CD1	1:A:252:ILE:HG13	2.37	0.55
1:C:151:LEU:HD22	1:C:252:ILE:CG2	2.32	0.55
2:D:17:MET:HA	2:D:34:GLN:HE22	1.71	0.55
1:E:226:LEU:HD23	1:E:226:LEU:N	2.22	0.55
4:H:58:VAL:HG22	4:H:59:PRO:HD2	1.89	0.55
2:B:3:PHE:HB2	2:B:112:ASP:OD2	2.08	0.54
1:C:111:LEU:HD12	1:C:112:VAL:H	1.71	0.54
3:I:36:TRP:CG	3:I:80:LEU:HD22	2.42	0.54
3:K:144:GLU:OE2	3:K:164:ALA:CB	2.54	0.54
2:B:77:ILE:CD1	2:D:77:ILE:HD11	2.37	0.54
3:I:2:VAL:HG12	3:I:3:GLN:N	2.22	0.54
3:K:13:GLN:NE2	3:K:112:SER:O	2.40	0.54
2:B:125:GLN:HE22	2:B:155:GLY:HA2	1.73	0.54
3:I:146:VAL:HG23	3:I:174:LEU:CD2	2.36	0.54
1:E:48:THR:HG21	1:E:50:LYS:HB2	1.87	0.54
2:F:126:LEU:HD21	2:F:152:ILE:HD13	1.89	0.54
2:D:55:VAL:HG12	2:D:55:VAL:O	2.05	0.54
4:L:27(C):THR:OG1	4:L:31:ASN:OD1	2.20	0.54
2:B:38:LEU:HD12	2:B:38:LEU:N	2.22	0.54
1:E:11:ALA:O	1:E:12:THR:HG23	2.08	0.54
1:E:27:LYS:HG2	1:E:32:ASP:O	2.08	0.54
2:F:10:ILE:HD13	2:F:136:GLY:HA3	1.89	0.54
4:J:182:SER:OG	4:J:184:ALA:HB3	2.07	0.54
2:D:53:ASN:CA	2:D:56:ILE:HD11	2.37	0.54
4:L:193:ALA:HB1	4:L:206:THR:HG23	1.90	0.54
1:C:97:CYS:HA	1:C:139:CYS:HA	1.90	0.53
2:D:58:LYS:CD	2:D:58:LYS:C	2.76	0.53
1:C:232:ILE:HG22	1:C:233:TYR:N	2.21	0.53
1:E:37:THR:OG1	1:E:38:ASN:N	2.40	0.53
1:A:60:ASP:HB2	1:A:274:ILE:HD11	1.90	0.53
1:A:98:TYR:CD1	1:A:99:PRO:HD2	2.43	0.53
4:J:54:ARG:HD2	4:J:58:VAL:HG12	1.91	0.53
4:J:85:VAL:HG12	4:J:86:TYR:N	2.22	0.53
6:A:440:NAG:H61	6:A:441:NAG:O7	2.08	0.53
2:B:103:GLU:O	2:B:107:THR:OG1	2.19	0.53
4:H:48:ILE:HG22	4:H:49:TYR:N	2.24	0.53
2:B:149:ILE:HD12	2:B:150:GLU:N	2.23	0.53
2:B:163:ARG:HG2	2:B:167:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG11	1:A:154:LEU:HB3	1.90	0.53
1:C:245:ILE:HG21	1:C:251:LEU:HD21	1.90	0.53
3:K:19:ARG:HG3	3:K:81:GLN:HA	1.90	0.53
3:K:37:VAL:HG22	3:K:47:TRP:HA	1.90	0.53
3:K:109:VAL:HG13	3:K:109:VAL:O	2.08	0.53
1:E:180:TRP:CD2	1:E:204:VAL:HG21	2.43	0.53
4:J:48:ILE:CD1	4:J:54:ARG:HA	2.39	0.53
3:G:100(D):PHE:H	3:G:100(G):LEU:HD12	1.75	0.52
3:K:100(H):SER:HB3	4:L:92:TYR:O	2.09	0.52
1:E:214:ILE:HD12	1:E:214:ILE:O	2.10	0.52
2:F:53:ASN:ND2	3:K:98:LEU:CD2	2.69	0.52
3:I:100(H):SER:OG	4:J:92:TYR:O	2.19	0.52
4:L:132:VAL:HG12	4:L:148:TRP:CH2	2.45	0.52
2:B:128:GLU:OE2	2:F:170:ARG:NH2	2.42	0.52
1:C:97:CYS:O	1:C:98:TYR:C	2.48	0.52
2:D:86:ASP:HB3	2:F:62:LYS:CD	2.39	0.52
2:B:62:LYS:HD2	2:F:86:ASP:HB3	1.90	0.52
3:I:197:LYS:N	3:I:198:PRO:CD	2.72	0.52
4:J:135:LEU:HD23	4:J:136:LEU:N	2.24	0.52
1:A:120:PHE:C	1:A:121:ILE:HD13	2.29	0.52
4:J:201:LEU:HD13	4:J:205:VAL:HB	1.91	0.52
1:C:167:THR:CG2	1:C:168:MET:N	2.72	0.52
1:C:161:TYR:CE1	1:C:249:GLY:HA2	2.45	0.52
1:C:87:PHE:HB3	1:C:267:ILE:HD12	1.92	0.52
3:K:194:VAL:HG12	3:K:195:ASN:N	2.25	0.52
3:I:30:SER:O	3:I:52(A):TYR:HB2	2.10	0.52
3:I:36:TRP:NE1	3:I:80:LEU:HB2	2.24	0.52
4:L:31:ASN:CB	4:L:51:ALA:HB2	2.39	0.52
1:C:237:VAL:HG12	1:C:241:ASP:HB3	1.92	0.52
3:K:138:VAL:HG23	3:K:174:LEU:HG	1.91	0.52
1:A:109:ARG:NE	1:A:267:ILE:HD13	2.25	0.52
4:H:73:LEU:O	4:H:74:THR:CG2	2.58	0.51
1:C:170:ASN:C	1:C:170:ASN:OD1	2.49	0.51
2:F:38:LEU:HD23	3:K:100(F):TRP:CZ2	2.45	0.51
3:K:28:THR:O	3:K:31:THR:HG23	2.09	0.51
2:B:62:LYS:CG	2:B:63:PHE:N	2.73	0.51
1:C:182:ILE:HD12	1:C:213:ILE:HB	1.93	0.51
2:D:156:THR:HG21	7:D:410:NAG:H83	1.92	0.51
4:L:92:TYR:CD1	4:L:92:TYR:O	2.64	0.51
4:J:33:LEU:HD13	4:J:71:PHE:CD2	2.44	0.51
4:H:58:VAL:HG13	4:H:59:PRO:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:147:THR:OG1	3:I:197:LYS:NZ	2.43	0.51
1:C:62:ILE:HG22	1:C:63:ASP:H	1.76	0.51
1:E:36:VAL:HG12	1:E:321:ARG:HA	1.91	0.51
4:L:79:GLN:O	4:L:82:ASP:HB2	2.11	0.51
1:C:170:ASN:OD1	1:C:171:ASN:N	2.43	0.51
1:C:70:LEU:HD23	1:C:71:LEU:HD23	1.92	0.51
2:D:150:GLU:O	2:D:151:SER:C	2.49	0.51
3:K:12:VAL:CG2	3:K:111:VAL:HG22	2.41	0.51
3:K:2:VAL:HG21	3:K:102:TYR:CE2	2.43	0.51
3:K:97:GLN:HE22	4:L:50:TRP:HZ2	1.59	0.51
1:C:130:VAL:HG12	1:C:155:THR:O	2.11	0.51
1:C:169:PRO:HA	1:C:242:VAL:HG23	1.92	0.51
1:C:33:GLN:O	1:C:34:ILE:HB	2.08	0.51
1:C:97:CYS:O	1:C:98:TYR:O	2.28	0.51
4:H:6:GLN:HE22	4:H:87:TYR:HA	1.74	0.51
1:C:147:PHE:HZ	1:C:252:ILE:HD12	1.76	0.51
2:D:37:ASP:OD2	2:D:118:LEU:CD1	2.56	0.51
1:E:29:ILE:HD11	2:F:102:LEU:HD23	1.93	0.51
4:H:16:GLY:HA2	4:H:77:SER:HB2	1.93	0.51
1:C:155:THR:HG22	1:C:156:LYS:H	1.75	0.51
1:E:180:TRP:CZ2	1:E:204:VAL:HG21	2.44	0.51
1:E:47:SER:OG	1:E:48:THR:N	2.44	0.51
3:G:47:TRP:HE3	3:G:60:ALA:HB2	1.76	0.51
4:H:33:LEU:HD13	4:H:71:PHE:CE2	2.45	0.51
4:H:73:LEU:O	4:H:74:THR:HG22	2.11	0.51
3:I:133:ALA:CB	3:I:179:THR:HG22	2.37	0.51
2:D:110:LEU:HD23	2:D:110:LEU:C	2.32	0.50
1:A:54:ASN:HB3	1:A:278:ILE:HD13	1.92	0.50
5:A:430:NAG:H62	5:A:431:NAG:HN2	1.76	0.50
3:I:124:LEU:HB3	4:J:118:PHE:CD2	2.46	0.50
2:B:55:VAL:HG13	2:B:99:LEU:HD21	1.93	0.50
2:F:141:TYR:O	2:F:166:ALA:HA	2.12	0.50
1:A:102:VAL:HG13	1:A:232:ILE:CB	2.41	0.50
2:D:49:ASN:CB	3:I:100(A):LEU:HD12	2.41	0.50
4:L:33:LEU:HD13	4:L:71:PHE:CD1	2.47	0.50
1:C:154:LEU:HD23	1:C:154:LEU:N	2.27	0.50
4:L:182:SER:O	4:L:183:LYS:C	2.50	0.50
2:B:58:LYS:O	2:B:59:THR:HG23	2.11	0.50
2:B:62:LYS:HG3	2:B:63:PHE:CB	2.42	0.50
1:E:181:GLY:O	1:E:252:ILE:N	2.36	0.50
4:H:39:LYS:O	4:H:40:PRO:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:91:LEU:HD23	2:F:92:TRP:CZ2	2.47	0.49
1:C:108:LEU:HD13	1:C:234:TRP:CE3	2.47	0.49
1:E:213:ILE:N	1:E:213:ILE:HD13	2.26	0.49
1:A:57:ARG:NH1	1:A:57:ARG:HG2	2.20	0.49
2:D:150:GLU:HG2	7:D:410:NAG:C1	2.42	0.49
1:E:34:ILE:O	1:E:34:ILE:HG23	2.12	0.49
4:L:47:LEU:HD22	4:L:58:VAL:HG13	1.93	0.49
1:A:298:ASN:OD1	1:A:299:LYS:N	2.45	0.49
2:B:100:VAL:HG23	2:B:101:ALA:N	2.28	0.49
1:C:86:LEU:HD11	1:C:268:MET:HB3	1.93	0.49
1:A:210:GLN:HE21	1:E:220:ARG:HH21	1.60	0.49
1:E:44:GLN:OE1	1:E:289:PRO:HG2	2.13	0.49
4:J:135:LEU:C	4:J:135:LEU:CD2	2.81	0.49
1:A:204:VAL:HG13	1:A:243:LEU:HD11	1.93	0.49
3:G:47:TRP:CE3	3:G:60:ALA:HB2	2.46	0.49
4:J:3:VAL:CG2	4:J:26:SER:OG	2.53	0.49
3:K:12:VAL:CG1	3:K:18:LEU:HB2	2.42	0.49
1:A:111:LEU:HD12	1:A:111:LEU:O	2.13	0.49
1:C:249:GLY:O	1:C:250:ASN:HB2	2.13	0.49
2:D:56:ILE:HD13	2:D:57:GLU:OE2	2.12	0.49
1:E:102:VAL:HG22	1:E:232:ILE:HB	1.94	0.49
1:E:15:LEU:HD13	2:F:24:PHE:CD2	2.48	0.49
3:G:53:ASP:O	3:G:54:ALA:HB3	2.12	0.49
2:F:53:ASN:HD21	3:K:98:LEU:HD23	1.76	0.49
4:L:132:VAL:HG12	4:L:148:TRP:HH2	1.77	0.49
1:A:230:ILE:HD12	1:A:252:ILE:HG13	1.95	0.49
1:C:141:ARG:O	1:C:143:PRO:HD2	2.13	0.49
1:C:22:ASN:N	1:C:22:ASN:OD1	2.44	0.49
2:D:133:MET:HB2	2:D:137:CYS:O	2.13	0.49
3:G:72:ASP:OD1	3:G:73:ASN:N	2.46	0.49
2:D:49:ASN:HB2	3:I:100(A):LEU:HD12	1.93	0.48
3:G:89:VAL:HG23	3:G:107:THR:O	2.11	0.48
1:C:138:ALA:HB2	1:C:226:LEU:HD12	1.94	0.48
1:C:43:VAL:HA	1:C:294:PHE:O	2.12	0.48
1:E:176:LYS:HD3	1:E:257:TYR:CD2	2.48	0.48
1:A:105:TYR:O	1:A:106:ALA:C	2.51	0.48
1:C:29:ILE:HD11	2:D:102:LEU:HD23	1.94	0.48
3:I:100(A):LEU:HD22	3:I:100(C):TYR:CE2	2.48	0.48
4:J:9:ASP:O	4:J:102:THR:HA	2.14	0.48
1:A:213:ILE:HG21	1:A:233:TYR:CE2	2.48	0.48
2:D:156:THR:CG2	7:D:410:NAG:H83	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:4:LEU:CD2	3:I:24:ALA:HB2	2.43	0.48
3:I:53:ASP:HB3	3:I:55:ASN:CG	2.34	0.48
4:L:33:LEU:HD23	4:L:34:ALA:H	1.77	0.48
1:A:62:ILE:HG22	1:A:63:ASP:H	1.77	0.48
2:D:42:GLN:HE22	3:I:100(H):SER:HB2	1.78	0.48
3:K:49:ALA:HB2	3:K:59:TYR:CD1	2.48	0.48
4:L:49:TYR:CZ	4:L:53:THR:HG21	2.48	0.48
1:A:59:LEU:HD23	1:A:87:PHE:CE2	2.48	0.48
1:C:220:ARG:HB3	1:C:221:PRO:CD	2.43	0.48
1:C:37:THR:O	1:C:38:ASN:HB2	2.14	0.48
4:H:21:ILE:HG22	4:H:22:ASN:N	2.28	0.48
3:K:134:LEU:HD11	3:K:190:TYR:CD2	2.49	0.48
3:K:8:GLY:HA3	3:K:20:LEU:HD23	1.96	0.48
1:A:163:VAL:HG22	1:A:248:ASN:HB3	1.96	0.48
1:C:155:THR:HG22	1:C:156:LYS:N	2.28	0.48
2:D:45:ILE:HD12	3:I:100(G):LEU:HD21	1.96	0.48
3:K:35:HIS:CD2	3:K:100(L):PHE:HE2	2.32	0.48
3:K:115:SER:O	3:K:116:THR:C	2.51	0.48
3:I:126:PRO:HG3	3:I:134:LEU:HD23	1.95	0.47
3:K:140:ASP:HB3	3:K:171:LEU:HD12	1.95	0.47
1:A:11:ALA:HB3	2:B:140:ILE:HD13	1.94	0.47
1:E:279:SER:OG	1:E:287:SER:HB2	2.14	0.47
1:E:305:CYS:O	2:F:59:THR:O	2.31	0.47
2:F:24:PHE:CD1	2:F:153:ARG:HD2	2.49	0.47
6:A:440:NAG:H61	6:A:441:NAG:C7	2.44	0.47
2:D:62:LYS:NZ	2:D:62:LYS:HB3	2.29	0.47
3:G:18:LEU:HD12	3:G:19:ARG:H	1.79	0.47
1:C:213:ILE:HG22	1:C:214:ILE:N	2.29	0.47
4:J:11:LEU:O	4:J:12:ALA:CB	2.63	0.47
4:J:148:TRP:HB3	4:J:179:LEU:HD22	1.95	0.47
4:J:25:SER:OG	4:J:69:THR:HA	2.14	0.47
2:B:128:GLU:OE1	2:B:128:GLU:HA	2.14	0.47
2:B:156:THR:HG21	6:B:410:NAG:HN2	1.78	0.47
1:C:66:LEU:HD13	1:C:87:PHE:CE2	2.49	0.47
1:E:298:ASN:CG	1:E:300:ILE:HD12	2.35	0.47
4:J:48:ILE:HD11	4:J:54:ARG:HG2	1.96	0.47
2:D:55:VAL:HG13	2:D:55:VAL:O	2.13	0.47
1:E:54:ASN:CG	1:E:55:PRO:HA	2.35	0.47
1:A:86:LEU:HD21	1:A:268:MET:HE3	1.95	0.47
1:C:77:ASP:C	1:C:79:PHE:N	2.67	0.47
4:J:150:VAL:CG2	4:J:155:GLN:HE21	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:4:LEU:HD23	3:I:24:ALA:HA	1.97	0.47
2:D:162:TYR:O	2:D:164:ASP:N	2.48	0.47
1:E:15:LEU:CD2	1:E:15:LEU:N	2.77	0.47
2:D:150:GLU:HG2	7:D:410:NAG:O5	2.15	0.47
2:D:38:LEU:H	2:D:38:LEU:HD12	1.80	0.47
2:D:56:ILE:C	2:D:57:GLU:OE2	2.53	0.47
1:A:268:MET:CE	1:A:282:ILE:CG2	2.92	0.46
3:I:12:VAL:HG12	3:I:12:VAL:O	2.15	0.46
4:J:73:LEU:HD12	4:J:74:THR:H	1.80	0.46
3:K:12:VAL:HG21	3:K:82(C):LEU:CD1	2.44	0.46
2:F:55:VAL:O	2:F:55:VAL:CG1	2.62	0.46
1:A:136:SER:C	1:A:145:SER:HB2	2.36	0.46
1:C:97:CYS:O	1:C:224:ARG:NH1	2.46	0.46
3:I:2:VAL:HG13	3:I:27:PHE:CD1	2.50	0.46
3:K:112:SER:HB3	3:K:114:ALA:CB	2.45	0.46
4:L:210:ASN:HD22	4:L:210:ASN:N	2.12	0.46
3:I:190:TYR:O	3:I:207:VAL:HG23	2.16	0.46
4:J:134:CYS:HB2	4:J:148:TRP:CH2	2.50	0.46
1:A:109:ARG:CZ	1:A:267:ILE:HD13	2.45	0.46
1:A:122:THR:HG23	1:A:255:ARG:HB3	1.97	0.46
1:A:274:ILE:HG22	1:A:275:ASP:N	2.31	0.46
1:C:133:ASN:HD22	1:C:133:ASN:N	2.13	0.46
3:G:47:TRP:CD1	4:H:96:PRO:HG2	2.51	0.46
4:J:158:ASN:ND2	4:J:179:LEU:HD11	2.30	0.46
4:L:27(B):VAL:HG21	4:L:33:LEU:HD12	1.97	0.46
1:E:154:LEU:N	1:E:154:LEU:HD23	2.30	0.46
1:E:220:ARG:HB3	1:E:221:PRO:HD2	1.97	0.46
3:K:35:HIS:CG	3:K:100(L):PHE:HE2	2.34	0.46
3:K:108:LEU:HD12	3:K:109:VAL:N	2.31	0.46
1:A:268:MET:CE	1:A:282:ILE:HG22	2.44	0.46
1:A:309:VAL:HG23	1:A:311:GLN:N	2.29	0.46
2:B:80:LEU:HD11	2:D:84:VAL:HG21	1.98	0.46
2:F:128:GLU:O	2:F:170:ARG:NH1	2.48	0.46
4:H:90:GLN:HE21	4:H:97:THR:CG2	2.28	0.46
3:I:133:ALA:HB2	3:I:179:THR:HA	1.96	0.46
1:C:88:VAL:CG1	1:C:88:VAL:O	2.64	0.46
1:E:313:THR:O	1:E:314:LEU:HD23	2.16	0.46
1:A:178:TYR:O	1:A:234:TRP:HA	2.16	0.46
2:D:130:ALA:HB2	2:D:140:ILE:HA	1.98	0.46
3:K:100(F):TRP:CZ3	3:K:100(G):LEU:HD23	2.51	0.46
3:K:53:ASP:O	3:K:54:ALA:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:136:LEU:CD2	4:L:196:VAL:HG11	2.44	0.46
1:A:177:LEU:HD12	1:A:178:TYR:N	2.31	0.45
1:C:214:ILE:N	1:C:214:ILE:HD12	2.31	0.45
1:E:188:ASN:OD1	1:E:217:ILE:HD13	2.17	0.45
1:E:180:TRP:CZ3	1:E:202:VAL:HG11	2.51	0.45
3:K:103:TRP:CD1	3:K:103:TRP:N	2.82	0.45
3:K:6:GLU:OE2	3:K:91:TYR:HA	2.16	0.45
1:C:300:ILE:C	1:C:301:THR:HG22	2.36	0.45
1:E:150:ARG:O	1:E:151:LEU:HD23	2.17	0.45
1:E:115:SER:HA	1:E:261:ARG:O	2.15	0.45
4:L:187:GLU:O	4:L:211:ARG:NH2	2.50	0.45
3:G:100(L):PHE:O	4:H:46:LEU:HD13	2.17	0.45
3:I:66:ARG:HB3	3:I:82(A):ASN:O	2.17	0.45
2:B:110:LEU:HD12	2:B:111:THR:N	2.29	0.45
1:A:63:ASP:HA	1:A:93:ALA:HA	1.96	0.45
1:A:70:LEU:HA	1:A:118:LEU:HD22	1.99	0.45
2:F:129:ASN:HA	2:F:166:ALA:HB1	1.99	0.45
3:I:83:ARG:O	3:I:84:ALA:C	2.55	0.45
2:D:1:GLY:O	2:D:2:LEU:C	2.55	0.45
2:F:156:THR:CG2	6:F:410:NAG:H82	2.47	0.45
4:L:175:LEU:HD23	4:L:176:SER:H	1.80	0.45
1:A:17:HIS:HD2	2:B:10:ILE:HG21	1.81	0.45
2:D:60:ASN:ND2	2:D:62:LYS:NZ	2.65	0.45
2:B:3:PHE:CE1	2:F:2:LEU:HD23	2.52	0.45
2:B:148:CYS:O	2:B:151:SER:OG	2.20	0.45
1:C:112:VAL:O	1:C:113:ALA:C	2.56	0.45
2:B:55:VAL:HG12	2:B:55:VAL:O	2.16	0.45
2:B:62:LYS:HA	2:B:63:PHE:CB	2.47	0.45
3:K:112:SER:HB2	3:K:142:PHE:CZ	2.51	0.45
2:B:120:GLU:O	2:B:124:ARG:HD2	2.17	0.44
1:C:228:SER:O	1:C:229:ARG:HG2	2.17	0.44
3:K:87:THR:HG23	3:K:110:THR:HA	1.99	0.44
1:A:137:ASN:ND2	1:A:145:SER:HB3	2.32	0.44
4:H:47:LEU:O	4:H:55:GLU:CB	2.65	0.44
3:I:134:LEU:HD13	3:I:207:VAL:HG11	1.98	0.44
3:I:28:THR:HG22	3:I:31:THR:OG1	2.17	0.44
4:L:31:ASN:O	4:L:33:LEU:N	2.48	0.44
5:A:431:NAG:H3	5:A:431:NAG:O7	2.18	0.44
2:D:127:ARG:HD3	2:D:159:HIS:CE1	2.53	0.44
1:E:97:CYS:O	1:E:98:TYR:C	2.54	0.44
1:A:312:ASN:OD1	1:A:313:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ILE:HG22	1:C:59:LEU:N	2.33	0.44
4:L:35:TRP:CH2	4:L:88:CYS:HB3	2.52	0.44
1:A:32:ASP:O	1:A:33:GLN:HG2	2.16	0.44
2:D:40:SER:O	2:D:43:ALA:HB3	2.17	0.44
1:C:219:SER:H	1:E:246:ASN:ND2	2.16	0.44
1:E:298:ASN:HD21	1:E:300:ILE:HD12	1.81	0.44
3:G:27:PHE:O	3:G:29:PHE:N	2.51	0.44
2:B:51:LYS:O	2:B:55:VAL:HG23	2.18	0.44
1:C:245:ILE:HG21	1:C:251:LEU:CD2	2.48	0.44
2:D:30:GLU:OE1	2:D:146:ASN:HB2	2.18	0.44
1:E:195:TYR:O	1:E:197:GLN:N	2.40	0.44
3:I:133:ALA:HB2	3:I:179:THR:CG2	2.40	0.44
1:C:104:ASP:O	1:C:105:TYR:C	2.54	0.44
1:C:44:GLN:O	1:C:296:ASN:N	2.51	0.44
2:D:53:ASN:HD22	3:I:98:LEU:CD2	2.13	0.44
1:E:222:TRP:O	1:E:223:VAL:HG23	2.18	0.44
1:E:237:VAL:HG21	1:E:243:LEU:HB2	1.99	0.44
3:I:94:LYS:NZ	3:I:101:ASP:OD2	2.41	0.44
4:J:48:ILE:HD13	4:J:54:ARG:HA	2.00	0.44
4:L:140:TYR:CD1	4:L:141:PRO:HA	2.52	0.44
1:A:120:PHE:CD1	1:A:121:ILE:N	2.86	0.44
1:C:167:THR:HG22	1:C:168:MET:N	2.32	0.44
2:F:92:TRP:HA	2:F:95:ASN:HB2	2.00	0.44
3:K:98:LEU:O	3:K:99:ARG:C	2.56	0.44
2:B:125:GLN:NE2	2:B:155:GLY:HA2	2.33	0.43
3:I:133:ALA:CB	3:I:179:THR:HA	2.48	0.43
3:K:17:SER:OG	3:K:82:MET:O	2.28	0.43
4:L:186:TYR:CE1	4:L:192:TYR:CE2	3.06	0.43
1:A:102:VAL:HG13	1:A:232:ILE:CG2	2.47	0.43
1:E:62:ILE:HG22	1:E:63:ASP:H	1.82	0.43
4:H:33:LEU:HD13	4:H:71:PHE:HD2	1.80	0.43
3:I:75:LYS:O	3:I:77:THR:CG2	2.57	0.43
4:J:2:ILE:HD13	4:J:2:ILE:HG21	1.74	0.43
3:K:75:LYS:O	3:K:77:THR:HG23	2.18	0.43
1:A:213:ILE:HG13	1:A:233:TYR:CE2	2.53	0.43
2:B:62:LYS:HB2	2:B:63:PHE:HB2	1.99	0.43
3:I:47:TRP:CE3	3:I:60:ALA:HB2	2.52	0.43
1:A:296:ASN:O	1:A:296:ASN:ND2	2.52	0.43
3:K:177:VAL:HG21	4:L:135:LEU:CD2	2.48	0.43
1:A:127:TRP:CH2	1:A:166:VAL:HG21	2.53	0.43
2:D:38:LEU:O	2:D:39:LYS:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HG22	1:A:63:ASP:N	2.32	0.43
2:B:86:ASP:HB3	2:D:62:LYS:CD	2.48	0.43
2:F:104:ASN:O	2:F:105:GLN:C	2.55	0.43
4:H:48:ILE:HD13	4:H:64:GLY:HA3	1.99	0.43
3:I:144:GLU:HG3	3:I:172:TYR:CE2	2.54	0.43
1:A:295:GLN:NE2	1:A:298:ASN:O	2.32	0.43
2:B:72:GLU:HG3	1:C:238:LYS:NZ	2.33	0.43
2:D:120:GLU:O	2:D:121:LYS:C	2.57	0.43
2:B:140:ILE:H	2:B:140:ILE:HD12	1.83	0.43
2:B:167:LEU:HD21	2:F:171:PHE:CD1	2.53	0.43
4:L:113:PRO:HD3	4:L:198:HIS:CD2	2.54	0.43
1:E:70:LEU:HD12	1:E:118:LEU:HD22	2.00	0.43
1:E:312:ASN:OD1	1:E:313:THR:HG22	2.19	0.43
4:H:5:THR:HG21	4:H:7:SER:OG	2.19	0.43
3:I:51:ILE:HD12	3:I:69:ILE:HG23	2.00	0.43
1:A:112:VAL:O	1:A:113:ALA:C	2.58	0.43
2:B:93:SER:O	2:B:96:ALA:N	2.52	0.43
2:D:47:GLN:HB3	2:D:110:LEU:HD11	2.00	0.43
2:D:12:ASN:HD22	2:D:12:ASN:C	2.22	0.43
2:B:86:ASP:CB	2:D:62:LYS:HD2	2.49	0.43
1:C:219:SER:H	1:E:246:ASN:HD22	1.66	0.43
3:G:52:SER:HB3	3:G:100(B):LEU:HD12	2.00	0.43
3:I:107:THR:O	3:I:107:THR:HG23	2.18	0.43
3:K:57:LYS:O	3:K:58:TYR:CD1	2.72	0.43
1:C:73:ASP:OD1	1:C:75:HIS:ND1	2.51	0.42
1:C:87:PHE:C	1:C:87:PHE:CD1	2.92	0.42
1:E:118:LEU:HA	1:E:118:LEU:HD23	1.83	0.42
1:E:62:ILE:HG22	1:E:63:ASP:N	2.34	0.42
3:I:148:VAL:HG12	3:I:149:SER:N	2.33	0.42
3:K:166:LEU:O	3:K:166:LEU:HD23	2.19	0.42
4:L:148:TRP:CZ2	4:L:179:LEU:HB2	2.54	0.42
1:C:183:HIS:O	1:C:185:PRO:HD3	2.19	0.42
1:C:84:TRP:CE2	1:C:116:GLY:HA2	2.54	0.42
4:J:89:GLN:HG2	4:J:90:GLN:N	2.33	0.42
4:L:33:LEU:HD13	4:L:71:PHE:CG	2.54	0.42
1:C:161:TYR:HB3	1:C:197:GLN:HE22	1.84	0.42
1:C:314:LEU:HB3	2:D:100:VAL:HG21	2.01	0.42
2:F:80:LEU:O	2:F:81:GLU:C	2.57	0.42
4:J:148:TRP:CB	4:J:179:LEU:HD22	2.50	0.42
4:J:54:ARG:HD2	4:J:58:VAL:CG1	2.48	0.42
4:L:197:THR:CG2	4:L:204:PRO:HG3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:ILE:HG22	2:B:10:ILE:O	2.19	0.42
1:C:54:ASN:HD22	1:C:55:PRO:HA	1.84	0.42
2:D:86:ASP:HB3	2:F:62:LYS:HD2	2.00	0.42
3:I:189:THR:CG2	3:I:206:ARG:HD2	2.50	0.42
2:B:149:ILE:HD12	2:B:149:ILE:C	2.40	0.42
3:K:193:ASN:N	3:K:193:ASN:OD1	2.52	0.42
3:K:190:TYR:O	3:K:207:VAL:HG23	2.19	0.42
2:B:31:GLY:O	2:B:32:THR:CG2	2.67	0.42
2:B:7:ALA:HA	4:J:29:TYR:OH	2.20	0.42
4:H:15:LEU:HD23	4:H:78:LEU:O	2.20	0.42
4:H:55:GLU:O	4:H:57:GLY:N	2.52	0.42
4:J:136:LEU:N	4:J:136:LEU:HD12	2.34	0.42
4:J:198:HIS:CD2	4:J:200:GLY:H	2.38	0.42
3:K:52:SER:HB3	3:K:100(B):LEU:HD12	2.00	0.42
1:C:245:ILE:CG2	1:C:251:LEU:CD2	2.97	0.42
1:E:122:THR:HG22	1:E:123:GLU:O	2.19	0.42
1:E:196:VAL:CG1	1:E:197:GLN:NE2	2.78	0.42
1:E:48:THR:CG2	1:E:50:LYS:HB2	2.50	0.42
4:J:47:LEU:HD12	4:J:47:LEU:HA	1.91	0.42
1:A:269:ARG:NH1	2:B:67:GLU:OE1	2.52	0.42
1:C:136:SER:OG	1:C:137:ASN:N	2.53	0.42
1:E:86:LEU:HD13	1:E:302:TYR:CG	2.55	0.42
4:J:78:LEU:HD11	4:J:82:ASP:HB2	2.01	0.42
1:C:216:ASN:HB3	1:E:212:THR:HG21	2.02	0.42
2:D:77:ILE:HD12	2:D:77:ILE:HG23	1.75	0.42
3:G:100(C):TYR:O	3:G:100(D):PHE:CD1	2.73	0.42
3:K:174:LEU:HD12	3:K:175:SER:N	2.34	0.42
1:A:43:VAL:HA	1:A:294:PHE:O	2.19	0.42
1:A:264:LYS:NZ	1:A:302:TYR:OH	2.46	0.42
1:C:184:HIS:HE1	1:C:216:ASN:HD22	1.68	0.42
3:K:112:SER:C	3:K:114:ALA:N	2.74	0.42
2:F:52:LEU:O	2:F:53:ASN:C	2.57	0.41
3:I:203:VAL:HG12	3:I:204:ASP:N	2.36	0.41
4:J:135:LEU:HD23	4:J:135:LEU:C	2.40	0.41
1:C:290:ASN:HB2	2:D:59:THR:HG21	2.02	0.41
2:B:66:ILE:HD13	2:F:83:TYR:CD1	2.55	0.41
4:H:55:GLU:O	4:H:56:SER:C	2.58	0.41
4:J:150:VAL:HB	4:J:155:GLN:HE21	1.85	0.41
1:A:316:LEU:HD12	2:B:104:ASN:OD1	2.21	0.41
1:A:97:CYS:O	1:A:98:TYR:O	2.37	0.41
2:F:94:TYR:C	2:F:94:TYR:CD1	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:98:LEU:O	3:I:99:ARG:C	2.58	0.41
4:L:151:ASP:OD1	4:L:191:VAL:N	2.51	0.41
2:F:133:MET:CE	2:F:135:ASN:HD21	2.32	0.41
3:I:53:ASP:HB3	3:I:55:ASN:OD1	2.20	0.41
3:I:72:ASP:OD2	3:I:75:LYS:HD3	2.21	0.41
4:J:148:TRP:CG	4:J:179:LEU:HD22	2.56	0.41
2:F:38:LEU:HD22	3:K:100(F):TRP:CD2	2.55	0.41
1:A:252:ILE:HG22	1:A:252:ILE:O	2.20	0.41
1:A:65:THR:OG1	1:A:68:ASP:OD2	2.36	0.41
1:C:203:THR:OG1	1:C:212:THR:HG23	2.20	0.41
1:C:104:ASP:HB3	1:C:234:TRP:HH2	1.86	0.41
2:D:69:GLU:C	2:D:70:PHE:CD1	2.94	0.41
1:E:15:LEU:HD12	2:F:118:LEU:HD21	2.02	0.41
1:E:130:VAL:HG13	1:E:162:PRO:HD2	2.03	0.41
1:E:267:ILE:HG21	1:E:267:ILE:HD13	1.75	0.41
2:F:77:ILE:N	2:F:77:ILE:CD1	2.80	0.41
1:A:301:THR:HB	1:A:305:CYS:SG	2.61	0.41
2:B:154:ASN:O	2:B:156:THR:HG23	2.21	0.41
4:J:39:LYS:HG2	4:J:84:ALA:HB2	2.03	0.41
3:K:50:VAL:HG13	3:K:50:VAL:O	2.20	0.41
1:C:214:ILE:HG22	1:C:215:PRO:HD2	2.03	0.41
1:C:10:THR:HB	2:D:140:ILE:O	2.20	0.41
4:J:2:ILE:HG23	4:J:26:SER:HB2	2.03	0.41
3:K:49:ALA:CB	3:K:59:TYR:CD1	3.03	0.41
4:L:106:ILE:HB	4:L:166:GLN:HE22	1.85	0.41
3:K:112:SER:CB	3:K:114:ALA:HB3	2.49	0.41
3:K:23:ALA:HA	3:K:77:THR:HG22	2.03	0.41
1:A:81:ASN:HA	1:A:119:GLU:HA	2.02	0.41
1:C:141:ARG:O	1:C:143:PRO:CD	2.69	0.41
3:G:5:VAL:O	3:G:23:ALA:N	2.49	0.41
1:C:33:GLN:HA	1:C:33:GLN:NE2	2.36	0.40
1:E:15:LEU:CD1	2:F:24:PHE:CD2	3.04	0.40
2:F:126:LEU:O	2:F:127:ARG:C	2.60	0.40
4:H:61:ARG:HB2	4:H:76:SER:CB	2.51	0.40
3:I:2:VAL:HG12	3:I:3:GLN:H	1.84	0.40
3:I:122:PHE:HB3	4:J:121:SER:OG	2.21	0.40
4:J:58:VAL:HG13	4:J:59:PRO:HD2	2.02	0.40
1:A:123:GLU:OE2	1:A:176:LYS:NZ	2.55	0.40
1:C:133:ASN:O	1:C:134:GLY:C	2.58	0.40
2:D:150:GLU:CG	7:D:410:NAG:C1	2.99	0.40
1:E:65:THR:HG22	1:E:93:ALA:CB	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:31:ASN:HB2	4:H:51:ALA:HB2	2.02	0.40
3:I:28:THR:O	3:I:28:THR:CG2	2.68	0.40
3:I:53:ASP:O	3:I:54:ALA:CB	2.65	0.40
1:A:130:VAL:HG13	1:A:155:THR:O	2.21	0.40
2:B:135:ASN:N	2:B:135:ASN:OD1	2.54	0.40
1:C:77:ASP:O	1:C:79:PHE:N	2.54	0.40
3:K:13:GLN:HE21	3:K:113:SER:C	2.24	0.40
3:K:3:GLN:HB3	3:K:25:SER:HB2	2.04	0.40
1:A:79:PHE:O	1:A:80:GLN:C	2.59	0.40
4:J:11:LEU:CD2	4:J:19:ALA:HB1	2.52	0.40
3:K:34:MET:HB3	3:K:78:LEU:HD22	2.03	0.40
4:L:148:TRP:CZ3	4:L:179:LEU:HD22	2.54	0.40
1:A:111:LEU:HD12	1:A:111:LEU:C	2.42	0.40
2:B:38:LEU:HB3	3:G:100(F):TRP:CZ3	2.56	0.40
4:L:50:TRP:O	4:L:51:ALA:HB3	2.21	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	316/329 (96%)	276 (87%)	32 (10%)	8 (2%)	7 44
1	C	314/329 (95%)	269 (86%)	36 (12%)	9 (3%)	6 41
1	E	316/329 (96%)	278 (88%)	33 (10%)	5 (2%)	12 53
2	B	170/175 (97%)	143 (84%)	23 (14%)	4 (2%)	7 45
2	D	170/175 (97%)	140 (82%)	23 (14%)	7 (4%)	3 32
2	F	170/175 (97%)	146 (86%)	20 (12%)	4 (2%)	7 45
3	G	127/226 (56%)	109 (86%)	14 (11%)	4 (3%)	5 40
3	I	224/226 (99%)	189 (84%)	33 (15%)	2 (1%)	21 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	K	220/226 (97%)	195 (89%)	22 (10%)	3 (1%)	14 56
4	H	105/218 (48%)	81 (77%)	21 (20%)	3 (3%)	6 41
4	J	214/218 (98%)	189 (88%)	19 (9%)	6 (3%)	6 42
4	L	214/218 (98%)	177 (83%)	28 (13%)	9 (4%)	3 31
All	All	2560/2844 (90%)	2192 (86%)	304 (12%)	64 (2%)	7 44

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ALA
2	D	64	HIS
2	D	127	ARG
2	D	163	ARG
2	F	58	LYS
2	F	64	HIS
3	G	28	THR
4	H	51	ALA
4	H	56	SER
4	J	12	ALA
4	J	56	SER
1	A	217	ILE
2	B	59	THR
2	B	64	HIS
1	C	158	GLY
1	E	210	GLN
1	E	277	CYS
2	F	60	ASN
4	J	15	LEU
4	J	83	VAL
4	L	138	ASN
4	L	204	PRO
1	A	62	ILE
1	A	172	ASP
1	A	201	ARG
1	A	297	VAL
2	B	127	ARG
1	C	62	ILE
1	C	143	PRO
1	C	196	VAL
1	C	279	SER
2	D	2	LEU

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Mol	Chain	Res	Type
2	D	147	ALA
3	G	82(B)	SER
3	G	100(E)	GLU
3	I	209	PRO
4	L	15	LEU
4	L	29	TYR
4	L	78	LEU
1	C	201	ARG
2	D	49	ASN
1	E	62	ILE
3	G	87	THR
3	K	126	PRO
4	L	174	SER
1	A	143	PRO
1	E	198	ALA
2	F	127	ARG
4	H	9	ASP
3	I	127	SER
4	J	110	VAL
4	J	138	ASN
3	K	101	ASP
4	L	52	SER
4	L	80	ALA
1	A	306	PRO
2	B	11	GLU
1	C	34	ILE
1	C	277	CYS
4	L	126	LYS
1	C	244	VAL
2	D	8	GLY
1	E	196	VAL
3	K	145	PRO

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	279/290 (96%)	249 (89%)	30 (11%)	8 36
1	C	276/290 (95%)	238 (86%)	38 (14%)	4 24
1	E	279/290 (96%)	249 (89%)	30 (11%)	8 36
2	B	145/149 (97%)	134 (92%)	11 (8%)	16 55
2	D	142/149 (95%)	125 (88%)	17 (12%)	6 30
2	F	142/149 (95%)	127 (89%)	15 (11%)	8 37
3	G	102/191 (53%)	95 (93%)	7 (7%)	19 60
3	I	185/191 (97%)	170 (92%)	15 (8%)	15 51
3	K	184/191 (96%)	164 (89%)	20 (11%)	8 36
4	H	74/193 (38%)	65 (88%)	9 (12%)	6 29
4	J	181/193 (94%)	158 (87%)	23 (13%)	5 27
4	L	173/193 (90%)	157 (91%)	16 (9%)	11 44
All	All	2162/2469 (88%)	1931 (89%)	231 (11%)	8 37

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	18	HIS
1	A	20	VAL
1	A	22	ASN
1	A	29	ILE
1	A	48	THR
1	A	50	LYS
1	A	57	ARG
1	A	63	ASP
1	A	67	ILE
1	A	70	LEU
1	A	83	THR
1	A	91	SER
1	A	111	LEU
1	A	114	SER
1	A	126	THR
1	A	160	THR
1	A	195	TYR
1	A	209	SER
1	A	214	ILE
1	A	222	TRP
1	A	223	VAL

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Mol	Chain	Res	Type
1	A	236	ILE
1	A	242	VAL
1	A	260	MET
1	A	271	ASP
1	A	299	LYS
1	A	301	THR
1	A	309	VAL
1	A	313	THR
2	B	15	GLU
2	B	54	ARG
2	B	57	GLU
2	B	62	LYS
2	B	63	PHE
2	B	66	ILE
2	B	72	GLU
2	B	73	VAL
2	B	90	ASP
2	B	110	LEU
2	B	160	ASP
1	C	9	SER
1	C	18	HIS
1	C	22	ASN
1	C	63	ASP
1	C	65	THR
1	C	74	PRO
1	C	78	VAL
1	C	82	GLU
1	C	83	THR
1	C	87	PHE
1	C	88	VAL
1	C	92	LYS
1	C	95	SER
1	C	110	SER
1	C	111	LEU
1	C	114	SER
1	C	128	THR
1	C	130	VAL
1	C	131	THR
1	C	189	GLN
1	C	193	SER
1	C	206	THR
1	C	209	SER

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Mol	Chain	Res	Type
1	C	214	ILE
1	C	219	SER
1	C	222	TRP
1	C	227	SER
1	C	228	SER
1	C	235	THR
1	C	237	VAL
1	C	247	SER
1	C	269	ARG
1	C	274	ILE
1	C	276	THR
1	C	300	ILE
1	C	301	THR
1	C	313	THR
1	C	316	LEU
2	D	9	PHE
2	D	10	ILE
2	D	12	ASN
2	D	18	ILE
2	D	19	ASP
2	D	42	GLN
2	D	56	ILE
2	D	59	THR
2	D	66	ILE
2	D	73	VAL
2	D	77	ILE
2	D	90	ASP
2	D	108	ILE
2	D	110	LEU
2	D	113	SER
2	D	123	ARG
2	D	149	ILE
1	E	10	THR
1	E	22	ASN
1	E	31	ASP
1	E	34	ILE
1	E	37	THR
1	E	41	GLU
1	E	78	VAL
1	E	104	ASP
1	E	110	SER
1	E	111	LEU

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Mol	Chain	Res	Type
1	E	130	VAL
1	E	136	SER
1	E	157	SER
1	E	159	SER
1	E	160	THR
1	E	166	VAL
1	E	173	ASN
1	E	187	THR
1	E	189	GLN
1	E	222	TRP
1	E	235	THR
1	E	236	ILE
1	E	242	VAL
1	E	250	ASN
1	E	276	THR
1	E	291	ASP
1	E	299	LYS
1	E	313	THR
1	E	321	ARG
1	E	323	VAL
2	F	2	LEU
2	F	29	SER
2	F	53	ASN
2	F	57	GLU
2	F	62	LYS
2	F	72	GLU
2	F	73	VAL
2	F	77	ILE
2	F	82	LYS
2	F	110	LEU
2	F	118	LEU
2	F	139	LYS
2	F	148	CYS
2	F	160	ASP
2	F	164	ASP
3	G	21	SER
3	G	25	SER
3	G	28	THR
3	G	55	ASN
3	G	79	TYR
3	G	108	LEU
3	G	112	SER

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Mol	Chain	Res	Type
4	H	3	VAL
4	H	7	SER
4	H	22	ASN
4	H	33	LEU
4	H	58	VAL
4	H	72	THR
4	H	77	SER
4	H	79	GLN
4	H	100	GLN
3	I	3	GLN
3	I	12	VAL
3	I	21	SER
3	I	70	SER
3	I	82(B)	SER
3	I	89	VAL
3	I	115	SER
3	I	166	LEU
3	I	172	TYR
3	I	175	SER
3	I	182	SER
3	I	192	CYS
3	I	193	ASN
3	I	204	ASP
3	I	208	GLU
4	J	7	SER
4	J	9	ASP
4	J	11	LEU
4	J	13	VAL
4	J	14	SER
4	J	26	SER
4	J	27(C)	THR
4	J	32	TYR
4	J	33	LEU
4	J	53	THR
4	J	67	SER
4	J	77	SER
4	J	97	THR
4	J	109	THR
4	J	122	ASP
4	J	135	LEU
4	J	142	ARG
4	J	159	SER

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Mol	Chain	Res	Type
4	J	169	LYS
4	J	170	ASP
4	J	177	SER
4	J	197	THR
4	J	205	VAL
3	K	1	GLN
3	K	2	VAL
3	K	11	VAL
3	K	17	SER
3	K	31	THR
3	K	63	VAL
3	K	71	ARG
3	K	83	ARG
3	K	89	VAL
3	K	96	SER
3	K	100	SER
3	K	110	THR
3	K	116	THR
3	K	121	VAL
3	K	138	VAL
3	K	168	SER
3	K	179	THR
3	K	192	CYS
3	K	193	ASN
3	K	207	VAL
4	L	9	ASP
4	L	20	THR
4	L	56	SER
4	L	65	SER
4	L	77	SER
4	L	97	THR
4	L	129	THR
4	L	156	SER
4	L	164	THR
4	L	168	SER
4	L	170	ASP
4	L	177	SER
4	L	181	LEU
4	L	197	THR
4	L	205	VAL
4	L	208	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	18	HIS
1	A	54	ASN
1	A	171	ASN
1	A	188	ASN
1	A	210	GLN
2	B	27	GLN
2	B	53	ASN
2	B	78	GLN
2	B	125	GLN
2	B	168	ASN
1	C	33	GLN
1	C	53	ASN
1	C	54	ASN
1	C	133	ASN
1	C	197	GLN
1	C	211	GLN
1	C	216	ASN
2	D	12	ASN
2	D	34	GLN
2	D	53	ASN
2	D	60	ASN
1	E	17	HIS
1	E	33	GLN
1	E	96	ASN
1	E	189	GLN
1	E	197	GLN
1	E	216	ASN
1	E	296	ASN
2	F	49	ASN
2	F	53	ASN
2	F	146	ASN
3	G	1	GLN
3	G	3	GLN
4	H	6	GLN
4	H	31	ASN
4	H	42	GLN
3	I	1	GLN
3	I	167	GLN
3	I	188	GLN
4	J	124	GLN
4	J	155	GLN

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Mol	Chain	Res	Type
4	J	189	HIS
4	J	198	HIS
3	K	13	GLN
3	K	81	GLN
3	K	100(I)	GLN
4	L	37	GLN
4	L	42	GLN
4	L	124	GLN
4	L	138	ASN
4	L	155	GLN
4	L	198	HIS
4	L	210	ASN

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

32 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	$\#\|Z\| > 2$
5	NAG	A	430	1,5	14,14,15	0.75	0	15,19,21	1.60	6 (40%)
5	NAG	A	431	5	14,14,15	1.03	1 (7%)	15,19,21	2.14	4 (26%)
5	BMA	A	432	5	11,11,12	1.30	2 (18%)	15,15,17	1.76	5 (33%)
6	NAG	A	440	1,6	14,14,15	1.00	1 (7%)	15,19,21	2.08	7 (46%)
6	NAG	A	441	6	14,14,15	1.23	2 (14%)	15,19,21	1.96	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	A	450	1,5	14,14,15	0.73	1 (7%)	15,19,21	0.90	1 (6%)
5	NAG	A	451	5	14,14,15	0.78	0	15,19,21	1.11	3 (20%)
5	BMA	A	452	5	11,11,12	0.91	0	15,15,17	1.84	4 (26%)
6	NAG	A	460	1,6	14,14,15	0.59	0	15,19,21	1.18	1 (6%)
6	NAG	A	461	6	14,14,15	1.26	2 (14%)	15,19,21	1.69	5 (33%)
6	NAG	B	410	2,6	14,14,15	1.21	1 (7%)	15,19,21	1.22	3 (20%)
6	NAG	B	411	6	14,14,15	1.30	2 (14%)	15,19,21	1.81	6 (40%)
6	NAG	C	430	1,6	14,14,15	1.47	2 (14%)	15,19,21	1.62	2 (13%)
6	NAG	C	431	6	14,14,15	1.30	2 (14%)	15,19,21	2.98	6 (40%)
6	NAG	C	440	1,6	14,14,15	1.00	1 (7%)	15,19,21	2.99	7 (46%)
6	NAG	C	441	6	14,14,15	1.33	1 (7%)	15,19,21	1.27	1 (6%)
5	NAG	C	450	1,5	14,14,15	0.60	0	15,19,21	1.49	3 (20%)
5	NAG	C	451	5	14,14,15	0.63	0	15,19,21	1.99	3 (20%)
5	BMA	C	452	5	11,11,12	0.72	0	15,15,17	1.24	2 (13%)
6	NAG	C	460	1,6	14,14,15	0.78	0	15,19,21	1.51	3 (20%)
6	NAG	C	461	6	14,14,15	1.15	1 (7%)	15,19,21	1.91	4 (26%)
6	NAG	E	430	1,6	14,14,15	1.14	2 (14%)	15,19,21	2.19	4 (26%)
6	NAG	E	431	6	14,14,15	1.26	2 (14%)	15,19,21	1.93	2 (13%)
6	NAG	E	440	1,6	14,14,15	0.86	0	15,19,21	1.93	6 (40%)
6	NAG	E	441	6	14,14,15	1.11	3 (21%)	15,19,21	1.79	3 (20%)
5	NAG	E	450	1,5	14,14,15	0.68	0	15,19,21	1.01	1 (6%)
5	NAG	E	451	5	14,14,15	0.96	1 (7%)	15,19,21	1.13	2 (13%)
5	BMA	E	452	5	11,11,12	1.01	0	15,15,17	2.13	7 (46%)
6	NAG	E	460	1,6	14,14,15	0.98	0	15,19,21	1.91	3 (20%)
6	NAG	E	461	6	14,14,15	1.17	1 (7%)	15,19,21	1.61	2 (13%)
6	NAG	F	410	2,6	14,14,15	1.27	1 (7%)	15,19,21	1.77	4 (26%)
6	NAG	F	411	6	14,14,15	0.93	0	15,19,21	2.00	3 (20%)

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
5	NAG	A	430	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	A	431	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	A	432	5	-	0/2/19/22	0/1/1/1
6	NAG	A	440	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	441	6	-	0/6/23/26	0/1/1/1
5	NAG	A	450	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	451	5	-	0/6/23/26	0/1/1/1
5	BMA	A	452	5	-	0/2/19/22	0/1/1/1
6	NAG	A	460	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	461	6	-	0/6/23/26	0/1/1/1
6	NAG	B	410	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	411	6	-	0/6/23/26	0/1/1/1
6	NAG	C	430	1,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	C	431	6	-	0/6/23/26	0/1/1/1
6	NAG	C	440	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	441	6	-	0/6/23/26	0/1/1/1
5	NAG	C	450	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	451	5	-	0/6/23/26	0/1/1/1
5	BMA	C	452	5	-	0/2/19/22	0/1/1/1
6	NAG	C	460	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	461	6	-	0/6/23/26	0/1/1/1
6	NAG	E	430	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	431	6	-	0/6/23/26	0/1/1/1
6	NAG	E	440	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	441	6	-	0/6/23/26	0/1/1/1
5	NAG	E	450	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	451	5	-	0/6/23/26	0/1/1/1
5	BMA	E	452	5	-	0/2/19/22	0/1/1/1
6	NAG	E	460	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	461	6	-	0/6/23/26	0/1/1/1
6	NAG	F	410	2,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	F	411	6	-	0/6/23/26	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	451	NAG	O5-C1	-2.09	1.40	1.43
6	E	441	NAG	C4-C3	2.06	1.57	1.52
5	A	450	NAG	C1-C2	2.07	1.55	1.52
6	A	461	NAG	C4-C3	2.10	1.57	1.52
5	A	431	NAG	C1-C2	2.11	1.55	1.52
6	E	441	NAG	C3-C2	2.12	1.57	1.52
6	E	430	NAG	C1-C2	2.15	1.55	1.52
6	A	440	NAG	C4-C5	2.18	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	430	NAG	C3-C2	2.19	1.57	1.52
6	E	441	NAG	C1-C2	2.20	1.55	1.52
6	A	441	NAG	C1-C2	2.22	1.55	1.52
6	C	461	NAG	C1-C2	2.26	1.55	1.52
5	A	432	BMA	C1-C2	2.29	1.57	1.52
6	B	411	NAG	C4-C5	2.33	1.58	1.53
6	C	431	NAG	C2-N2	2.35	1.50	1.46
6	C	440	NAG	C4-C3	2.35	1.58	1.52
6	E	430	NAG	C4-C3	2.39	1.58	1.52
6	B	410	NAG	C1-C2	2.46	1.56	1.52
6	A	461	NAG	C1-C2	2.47	1.56	1.52
6	E	431	NAG	C4-C3	2.50	1.59	1.52
6	E	431	NAG	C1-C2	2.51	1.56	1.52
5	A	432	BMA	C2-C3	2.56	1.56	1.52
6	E	461	NAG	C1-C2	2.66	1.56	1.52
6	A	441	NAG	C3-C2	2.70	1.58	1.52
6	B	411	NAG	C1-C2	2.97	1.56	1.52
6	C	431	NAG	C1-C2	3.07	1.56	1.52
6	F	410	NAG	C1-C2	3.37	1.57	1.52
6	C	441	NAG	C1-C2	3.73	1.57	1.52
6	C	430	NAG	C1-C2	4.30	1.58	1.52

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	440	NAG	O3-C3-C2	-6.91	94.58	109.37
6	C	440	NAG	O5-C5-C4	-3.98	103.55	110.13
5	E	452	BMA	O5-C5-C4	-3.94	103.60	110.13
6	A	440	NAG	O3-C3-C2	-3.14	102.66	109.37
5	C	451	NAG	C2-N2-C7	-3.13	119.04	123.11
5	E	450	NAG	C4-C3-C2	-3.10	106.53	111.34
6	E	440	NAG	C4-C3-C2	-2.98	106.72	111.34
6	E	440	NAG	O5-C5-C4	-2.80	105.50	110.13
6	C	431	NAG	O7-C7-C8	-2.77	116.96	122.07
5	A	430	NAG	C1-O5-C5	-2.72	108.14	112.14
6	E	441	NAG	O5-C5-C4	-2.50	105.99	110.13
6	E	440	NAG	O7-C7-C8	-2.47	117.52	122.07
6	F	410	NAG	O5-C5-C4	-2.43	106.11	110.13
6	B	411	NAG	O7-C7-C8	-2.37	117.70	122.07
5	A	430	NAG	O5-C5-C4	-2.32	106.29	110.13
5	A	430	NAG	O3-C3-C2	-2.32	104.42	109.37
6	A	441	NAG	C1-O5-C5	-2.24	108.85	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	450	NAG	C4-C3-C2	-2.22	107.89	111.34
5	E	452	BMA	C3-C4-C5	-2.22	106.28	110.23
6	A	461	NAG	O3-C3-C2	-2.20	104.66	109.37
6	E	460	NAG	C8-C7-N2	-2.20	111.89	116.10
5	A	451	NAG	O7-C7-C8	-2.09	118.23	122.07
6	C	460	NAG	O3-C3-C2	-2.06	104.97	109.37
6	A	441	NAG	O7-C7-C8	-2.06	118.29	122.07
5	A	450	NAG	C2-N2-C7	-2.05	120.44	123.11
5	E	451	NAG	O3-C3-C2	-2.01	105.08	109.37
6	E	430	NAG	O3-C3-C4	2.01	114.89	110.36
5	A	451	NAG	O7-C7-N2	2.02	125.97	121.84
5	A	430	NAG	O4-C4-C5	2.04	114.61	109.23
6	A	440	NAG	O6-C6-C5	2.05	118.15	111.30
5	A	431	NAG	O5-C5-C6	2.05	111.73	107.34
5	E	452	BMA	O2-C2-C1	2.06	113.36	109.23
6	F	410	NAG	C2-N2-C7	2.07	125.80	123.11
6	E	440	NAG	C3-C4-C5	2.07	113.92	110.23
6	A	440	NAG	O3-C3-C4	2.09	115.07	110.36
6	A	460	NAG	C3-C4-C5	2.09	113.96	110.23
6	A	461	NAG	O4-C4-C3	2.10	115.09	110.36
6	E	460	NAG	O7-C7-N2	2.10	126.13	121.84
6	B	411	NAG	O4-C4-C5	2.12	114.81	109.23
5	A	452	BMA	O2-C2-C1	2.13	113.49	109.23
6	B	410	NAG	C2-N2-C7	2.13	125.88	123.11
5	A	432	BMA	C1-O5-C5	2.16	115.31	112.14
6	B	411	NAG	O5-C5-C4	2.17	113.72	110.13
6	B	410	NAG	C3-C4-C5	2.19	114.13	110.23
5	A	451	NAG	C4-C3-C2	2.23	114.80	111.34
5	A	430	NAG	C3-C4-C5	2.28	114.28	110.23
5	C	450	NAG	O4-C4-C3	2.29	115.53	110.36
5	A	430	NAG	C6-C5-C4	2.32	118.80	112.99
5	C	452	BMA	C1-O5-C5	2.33	115.57	112.14
5	A	432	BMA	O5-C5-C4	2.33	114.00	110.13
6	A	461	NAG	C1-O5-C5	2.34	115.58	112.14
6	E	440	NAG	O4-C4-C3	2.37	115.69	110.36
6	A	440	NAG	O5-C5-C6	2.38	112.43	107.34
5	A	431	NAG	C3-C4-C5	2.38	114.47	110.23
6	A	441	NAG	O5-C5-C6	2.39	112.46	107.34
6	C	440	NAG	O3-C3-C4	2.40	115.78	110.36
6	C	460	NAG	C4-C3-C2	2.41	115.08	111.34
6	B	411	NAG	C3-C4-C5	2.44	114.59	110.23
6	C	440	NAG	O4-C4-C3	2.48	115.94	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	451	NAG	C1-O5-C5	2.48	115.78	112.14
5	C	452	BMA	C3-C4-C5	2.52	114.71	110.23
6	F	411	NAG	C4-C3-C2	2.57	115.33	111.34
6	A	440	NAG	C6-C5-C4	2.60	119.50	112.99
5	E	452	BMA	C6-C5-C4	2.60	119.51	112.99
6	A	461	NAG	C2-N2-C7	2.60	126.49	123.11
6	C	431	NAG	C3-C4-C5	2.61	114.88	110.23
5	A	432	BMA	O2-C2-C1	2.61	114.47	109.23
6	C	431	NAG	O7-C7-N2	2.63	127.22	121.84
6	E	440	NAG	O6-C6-C5	2.66	120.20	111.30
6	B	411	NAG	C1-O5-C5	2.69	116.10	112.14
6	B	411	NAG	C2-N2-C7	2.71	126.63	123.11
5	A	452	BMA	C1-C2-C3	2.81	112.96	109.55
6	C	461	NAG	C3-C4-C5	2.82	115.26	110.23
5	E	452	BMA	C1-C2-C3	2.85	113.01	109.55
5	A	432	BMA	C1-C2-C3	2.91	113.07	109.55
6	E	441	NAG	C2-N2-C7	2.91	126.90	123.11
6	C	441	NAG	C3-C4-C5	2.92	115.44	110.23
6	B	410	NAG	C4-C3-C2	2.96	115.93	111.34
6	A	440	NAG	C1-O5-C5	2.99	116.54	112.14
5	E	452	BMA	O3-C3-C4	3.06	117.27	110.36
5	A	452	BMA	C2-C3-C4	3.11	116.47	111.05
6	C	461	NAG	C4-C3-C2	3.22	116.33	111.34
6	C	460	NAG	C3-C4-C5	3.23	116.00	110.23
6	F	410	NAG	O5-C5-C6	3.25	114.31	107.34
6	C	431	NAG	C4-C3-C2	3.27	116.41	111.34
6	C	430	NAG	C4-C3-C2	3.28	116.43	111.34
5	E	452	BMA	O5-C5-C6	3.29	114.38	107.34
6	E	431	NAG	C3-C4-C5	3.29	116.09	110.23
6	E	430	NAG	C4-C3-C2	3.35	116.54	111.34
5	A	432	BMA	C3-C4-C5	3.36	116.22	110.23
6	C	430	NAG	C2-N2-C7	3.39	127.51	123.11
6	F	410	NAG	C4-C3-C2	3.48	116.75	111.34
5	A	431	NAG	C4-C3-C2	3.48	116.75	111.34
6	C	461	NAG	C2-N2-C7	3.52	127.68	123.11
6	A	461	NAG	C4-C3-C2	3.59	116.92	111.34
6	E	461	NAG	C4-C3-C2	3.65	117.00	111.34
6	E	461	NAG	C2-N2-C7	3.70	127.92	123.11
6	F	411	NAG	C3-C4-C5	3.79	116.98	110.23
5	A	452	BMA	C3-C4-C5	3.88	117.14	110.23
6	C	440	NAG	C4-C3-C2	3.92	117.42	111.34
6	C	440	NAG	C3-C4-C5	4.01	117.37	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	440	NAG	O4-C4-C5	4.02	119.82	109.23
6	C	461	NAG	C1-O5-C5	4.03	118.06	112.14
5	C	450	NAG	C1-O5-C5	4.11	118.18	112.14
5	C	451	NAG	O5-C5-C4	4.15	117.00	110.13
6	E	441	NAG	C4-C3-C2	4.23	117.90	111.34
6	C	440	NAG	C1-O5-C5	4.29	118.45	112.14
6	E	430	NAG	C2-N2-C7	4.58	129.06	123.11
6	E	431	NAG	C4-C3-C2	4.77	118.74	111.34
5	C	451	NAG	C1-O5-C5	4.82	119.22	112.14
6	A	441	NAG	C4-C3-C2	5.00	119.09	111.34
6	F	411	NAG	C1-O5-C5	5.20	119.78	112.14
6	E	430	NAG	C3-C4-C5	5.30	119.67	110.23
6	C	431	NAG	C2-N2-C7	5.64	130.44	123.11
5	A	431	NAG	C2-N2-C7	5.94	130.83	123.11
6	E	460	NAG	C2-N2-C7	6.00	130.91	123.11
6	C	431	NAG	C1-O5-C5	7.96	123.84	112.14

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	430	NAG	C1
6	F	410	NAG	C1
5	A	430	NAG	C1

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	430	NAG	1	0
5	A	431	NAG	2	0
6	A	440	NAG	2	0
6	A	441	NAG	2	0
6	B	410	NAG	1	0
6	C	430	NAG	2	0
6	C	431	NAG	2	0
6	C	440	NAG	1	0
6	C	441	NAG	1	0
6	E	440	NAG	1	0
6	E	441	NAG	1	0
6	F	410	NAG	2	0

5.6 Ligand geometry (i)

1 ligand is 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	D	410	2	14,14,15	1.26	1 (7%)	15,19,21	1.50	3 (20%)

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	D	410	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	410	NAG	C4-C5	2.69	1.59	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	410	NAG	O7-C7-C8	-2.29	117.86	122.07
7	D	410	NAG	O5-C5-C4	2.01	113.46	110.13
7	D	410	NAG	C3-C4-C5	3.57	116.60	110.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	410	NAG	7	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	318/329 (96%)	-0.05	4 (1%) 79 73	110, 138, 165, 184	0
1	C	316/329 (96%)	-0.22	2 (0%) 90 86	104, 126, 153, 180	0
1	E	318/329 (96%)	-0.17	2 (0%) 90 86	106, 125, 149, 185	0
2	B	172/175 (98%)	-0.10	0 100 100	98, 143, 196, 219	0
2	D	172/175 (98%)	-0.27	1 (0%) 90 86	97, 135, 196, 233	0
2	F	172/175 (98%)	-0.16	0 100 100	102, 138, 195, 226	0
3	G	129/226 (57%)	0.62	16 (12%) 5 6	163, 221, 268, 289	0
3	I	226/226 (100%)	0.08	7 (3%) 52 47	114, 150, 223, 253	0
3	K	224/226 (99%)	0.10	15 (6%) 21 19	109, 141, 229, 251	0
4	H	107/218 (49%)	0.95	20 (18%) 2 2	189, 240, 266, 273	0
4	J	216/218 (99%)	-0.02	5 (2%) 64 58	113, 142, 196, 223	0
4	L	216/218 (99%)	0.19	8 (3%) 45 40	121, 183, 215, 234	0
All	All	2586/2844 (90%)	0.01	80 (3%) 52 47	97, 140, 233, 289	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	10	GLY	6.3
4	H	15	LEU	5.4
3	K	190	TYR	4.3
4	H	14	SER	4.0
4	H	69	THR	3.9
4	H	20	THR	3.8
3	K	187	THR	3.7
3	K	185	LEU	3.6
4	H	68	GLY	3.6
3	K	195	ASN	3.6
3	I	183	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	143	PRO	3.5
1	E	12	THR	3.5
3	K	181	PRO	3.4
4	H	58	VAL	3.3
3	G	11	VAL	3.2
4	L	199	GLN	3.2
3	G	112	SER	3.1
3	K	1	GLN	3.1
4	H	37	GLN	3.1
4	H	31	ASN	3.1
1	A	159	SER	3.1
3	G	86	ASP	3.0
3	G	80	LEU	3.0
3	I	15	GLY	3.0
3	I	136	CYS	3.0
4	H	59	PRO	3.0
4	J	189	HIS	2.9
3	G	82(A)	ASN	2.9
3	G	14	PRO	2.9
3	K	132	ALA	2.8
4	J	190	LYS	2.8
3	G	24	ALA	2.7
4	H	19	ALA	2.7
1	A	140	LYS	2.7
4	H	70	ASP	2.7
4	L	144	ALA	2.7
3	K	134	LEU	2.7
2	D	143	LYS	2.7
1	C	140	LYS	2.6
3	G	81	GLN	2.6
3	I	135	GLY	2.6
4	H	61	ARG	2.6
4	H	83	VAL	2.6
3	K	180	VAL	2.6
3	K	183	SER	2.6
3	K	186	GLY	2.5
3	G	17	SER	2.5
1	E	326	LYS	2.5
4	L	152	ASN	2.5
4	L	150	VAL	2.5
1	A	12	THR	2.4
3	I	181	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
3	K	182	SER	2.4
3	G	12	VAL	2.3
3	K	184	SER	2.3
3	G	41	PRO	2.3
4	H	60	ASP	2.3
4	H	57	GLY	2.3
4	J	188	LYS	2.3
3	G	111	VAL	2.2
4	L	186	TYR	2.2
3	I	187	THR	2.2
4	L	134	CYS	2.2
3	G	87	THR	2.2
4	L	198	HIS	2.1
4	H	80	ALA	2.1
4	H	18	ARG	2.1
4	H	3	VAL	2.1
3	G	82(B)	SER	2.1
1	C	222	TRP	2.1
3	I	154	ALA	2.1
4	J	178	THR	2.1
3	K	155	LEU	2.1
4	L	112	ALA	2.0
3	K	207	VAL	2.0
3	G	102	TYR	2.0
4	H	22	ASN	2.0
4	H	17	GLU	2.0
4	J	205	VAL	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	E	460	14/15	0.92	0.30	1.01	156,164,172,180	0
6	NAG	A	460	14/15	0.92	0.27	0.96	152,160,164,170	0
6	NAG	C	430	14/15	0.86	0.18	0.22	170,180,186,193	0
5	NAG	C	451	14/15	0.93	0.31	0.12	210,221,233,237	0
5	NAG	A	450	14/15	0.96	0.23	-0.05	192,203,213,213	0
6	NAG	E	440	14/15	0.91	0.19	-0.13	162,171,175,184	0
6	NAG	E	430	14/15	0.88	0.18	-0.31	175,187,190,191	0
6	NAG	C	440	14/15	0.83	0.18	-0.31	172,183,192,204	0
5	NAG	A	451	14/15	0.91	0.25	-0.48	209,217,228,228	0
5	NAG	A	430	14/15	0.87	0.17	-0.53	178,188,193,196	0
5	NAG	E	450	14/15	0.96	0.19	-0.57	155,164,168,171	0
5	NAG	C	450	14/15	0.95	0.12	-1.14	183,195,200,203	0
6	NAG	A	440	14/15	0.86	0.15	-1.30	180,186,194,202	0
6	NAG	C	441	14/15	0.84	0.33	-	207,214,219,222	0
6	NAG	E	441	14/15	0.88	0.20	-	191,197,204,209	0
5	BMA	E	452	11/12	0.82	0.19	-	201,205,212,213	0
6	NAG	B	411	14/15	0.76	0.54	-	267,273,284,291	0
5	BMA	A	432	11/12	0.88	0.30	-	214,220,223,226	0
5	BMA	A	452	11/12	0.60	0.20	-	230,232,237,240	0
6	NAG	E	431	14/15	0.89	0.23	-	190,200,204,205	0
6	NAG	C	461	14/15	0.93	0.33	-	167,171,175,178	0
6	NAG	C	460	14/15	0.95	0.24	-	143,149,159,160	0
6	NAG	C	431	14/15	0.70	0.34	-	200,206,210,215	0
6	NAG	F	411	14/15	0.81	0.49	-	258,264,271,277	0
6	NAG	A	441	14/15	0.91	0.17	-	212,217,225,226	0
5	NAG	E	451	14/15	0.92	0.23	-	177,183,195,196	0
6	NAG	A	461	14/15	0.82	0.34	-	181,188,190,191	0
6	NAG	E	461	14/15	0.88	0.40	-	190,196,203,203	0
6	NAG	F	410	14/15	0.85	0.30	-	223,239,248,250	0
5	BMA	C	452	11/12	0.61	0.21	-	243,248,254,258	0
5	NAG	A	431	14/15	0.88	0.23	-	197,203,217,217	0
6	NAG	B	410	14/15	0.71	0.29	-	232,248,258,261	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
7	NAG	D	410	14/15	0.61	0.37	2.11	201,215,222,225	0

6.5 Other polymers (i)

There are no such residues in this entry.