Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:15 PM GMT

PDB ID	:	4HLZ
Title	:	Crystal Structure of Fab C179 in Complex with a H2N2 influenza virus hemagglutinin
Authors	:	Dreyfus, C.; Wilson, I.A.
Deposited on	:	2012-10-17
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

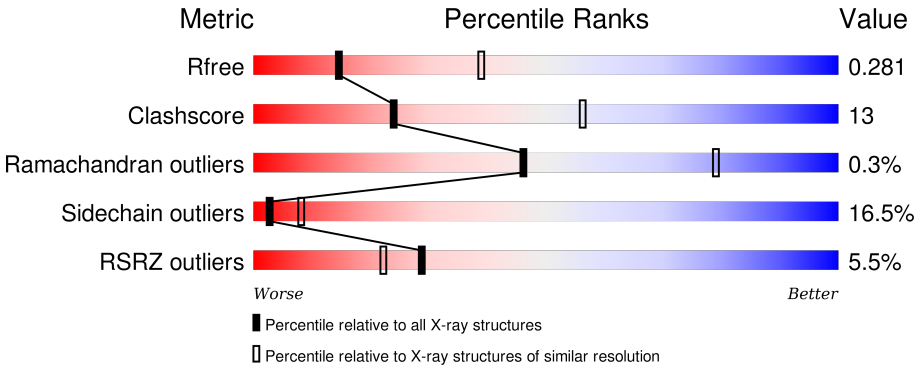
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	5% 65% 29% 5% •
1	C	327	3% 69% 28% • •
1	E	327	5% 66% 28% 5% •
2	B	174	% 72% 24% • •
2	D	174	2% 70% 25% • •

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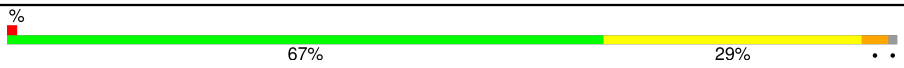
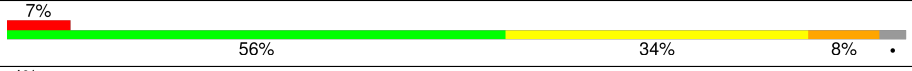
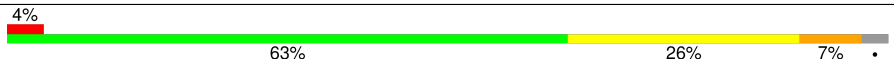
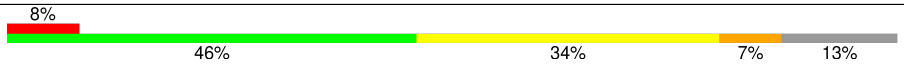
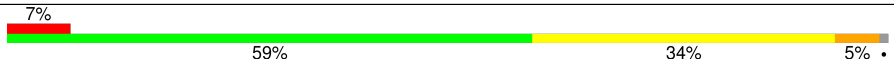
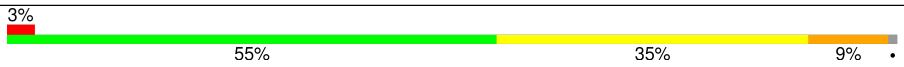
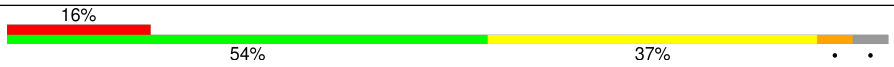
Mol	Chain	Length	Quality of chain
2	F	174	
3	G	229	
3	I	229	
3	K	229	
4	H	214	
4	J	214	
4	L	214	

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
6	NAG	A	403	-	-	-	X
7	SO4	F	201	-	-	X	-
7	SO4	H	301	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 21839 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	4	0
			2546	1600	441	490	15			
1	C	324	Total	C	N	O	S	0	4	0
			2546	1600	441	490	15			
1	E	324	Total	C	N	O	S	0	5	0
			2551	1605	441	490	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	EXPRESSION TAG	UNP C7S226
C	9	PRO	-	EXPRESSION TAG	UNP C7S226
E	9	PRO	-	EXPRESSION TAG	UNP C7S226

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	168	Total	C	N	O	S	0	1	0
			1370	854	235	272	9			
2	D	170	Total	C	N	O	S	0	1	0
			1384	862	237	276	9			
2	F	172	Total	C	N	O	S	0	1	0
			1404	876	240	279	9			

- Molecule 3 is a protein called Fab C179 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	223	Total	C	N	O	S	0	1	0
			1696	1071	283	334	8			
3	I	221	Total	C	N	O	S	0	0	0
			1675	1059	278	330	8			

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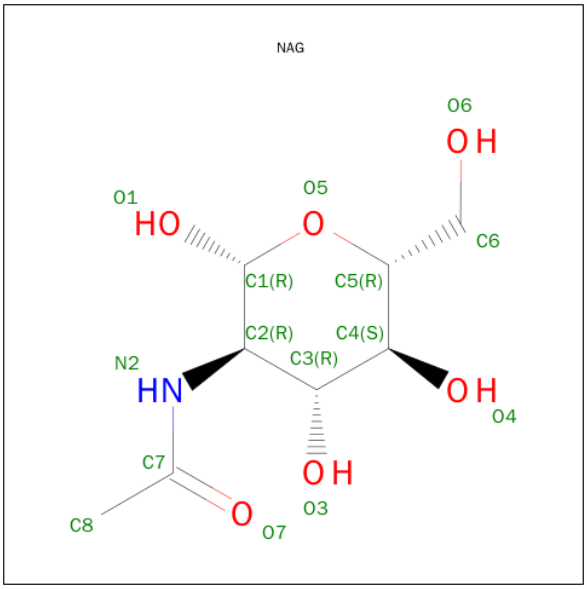
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	200	Total	C	N	O	S	0	0	0
			1532	970	253	302	7			

- Molecule 4 is a protein called Fab C179 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	211	Total	C	N	O	S	0	0	0
			1627	1021	270	330	6			
4	J	212	Total	C	N	O	S	0	0	0
			1635	1025	272	332	6			
4	L	205	Total	C	N	O	S	0	0	0
			1580	994	261	319	6			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

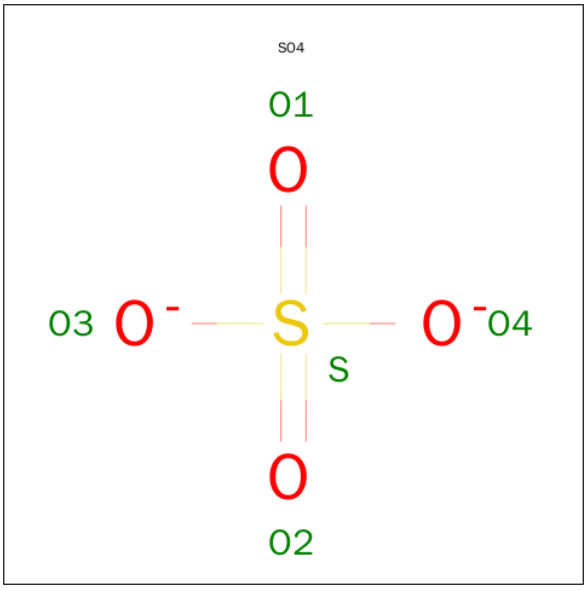


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	F	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	J	1	Total	O	S	0	0
			5	4	1		
7	L	1	Total	O	S	0	0
			5	4	1		

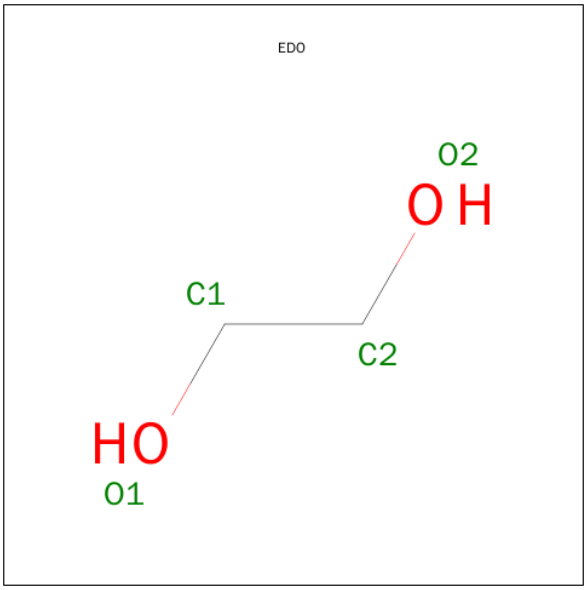
- Molecule 8 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 9 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	2	Total	C	N	O	0	0
			28	16	2	10		
9	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

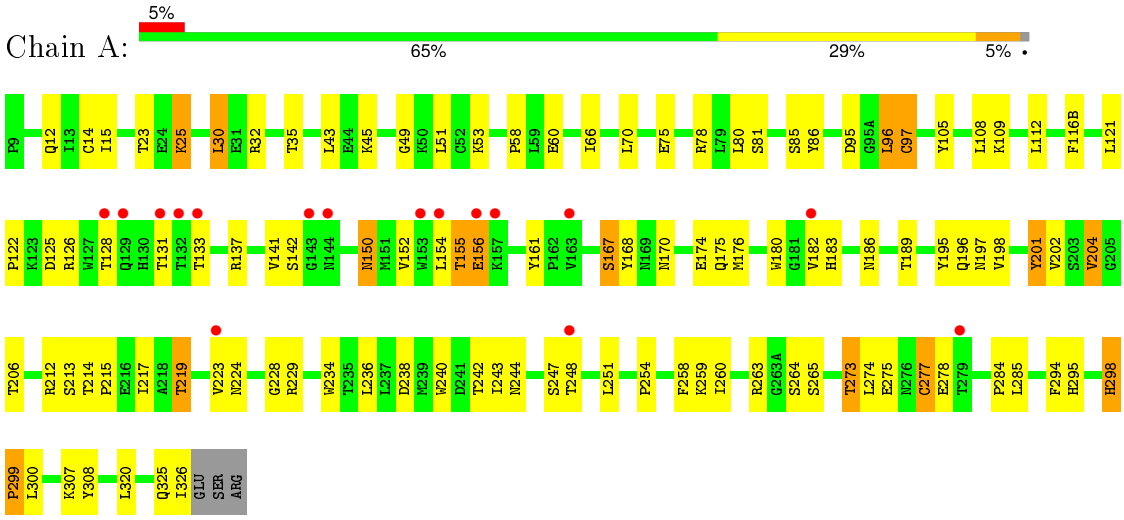


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	J	1	Total	C	O	0	0
			4	2	2		

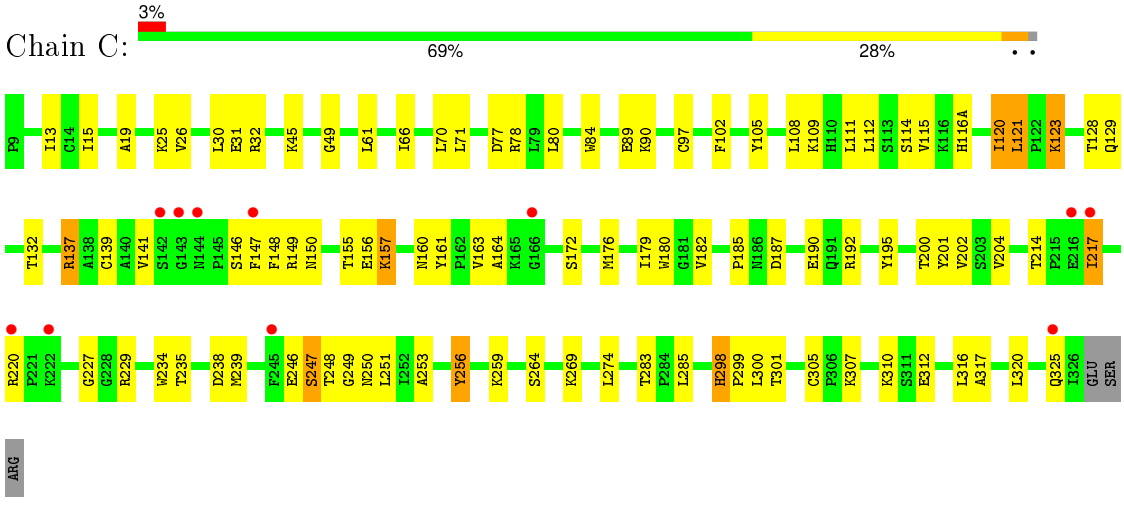
3 Residue-property plots (i)

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.

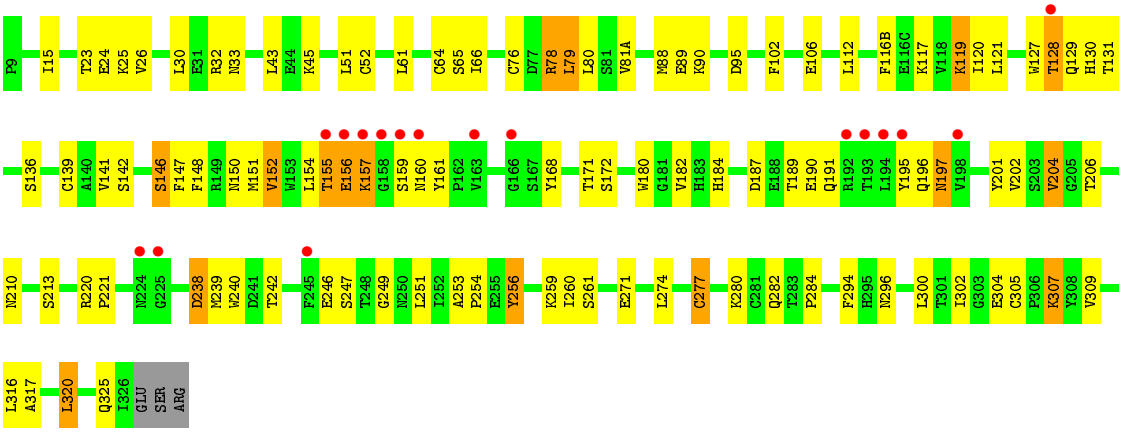
- Molecule 1: Hemagglutinin HA1



- Molecule 1: Hemagglutinin HA1

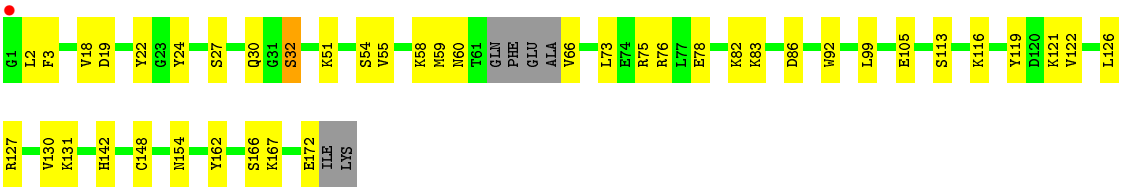


- Molecule 1: Hemagglutinin HA1



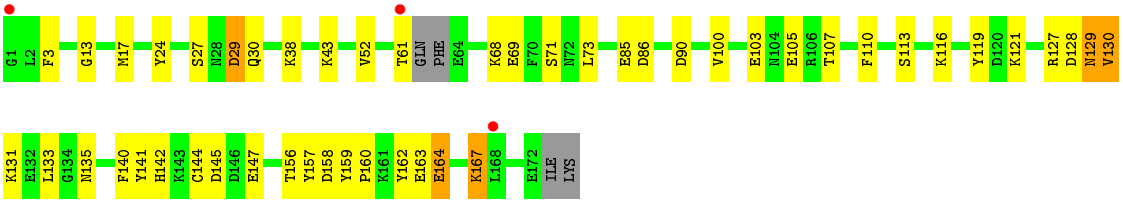
- Molecule 2: Hemagglutinin HA2

Chain B:



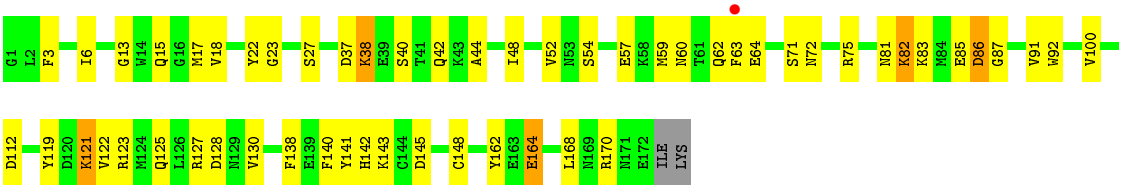
- Molecule 2: Hemagglutinin HA2

Chain D:



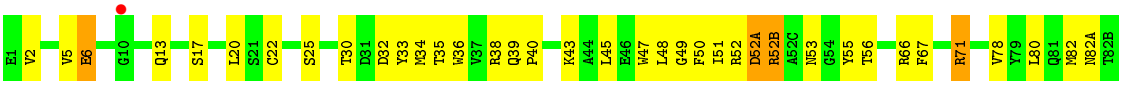
- Molecule 2: Hemagglutinin HA2

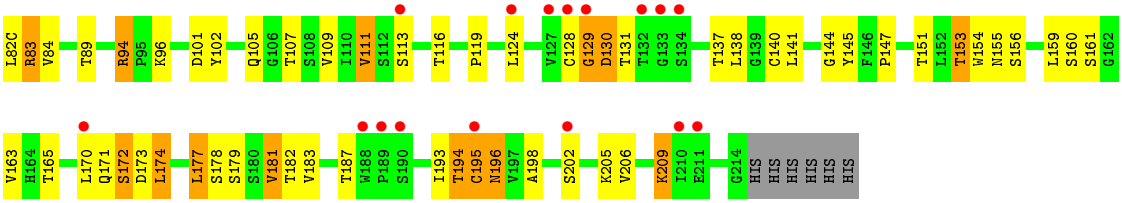
Chain F:



- Molecule 3: Fab C179 heavy chain

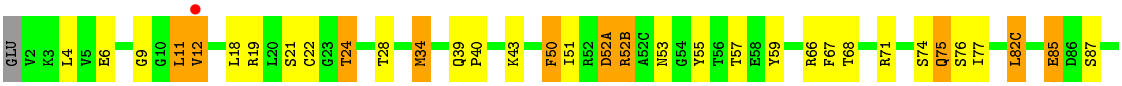
Chain G:

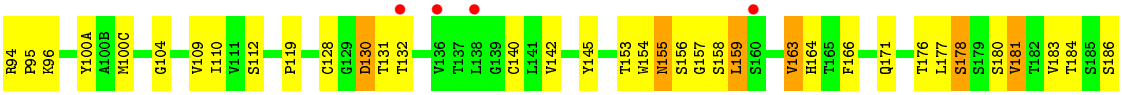


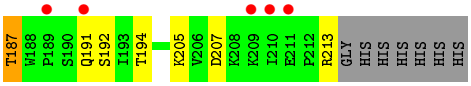


• Molecule 3: Fab C179 heavy chain

Chain I:

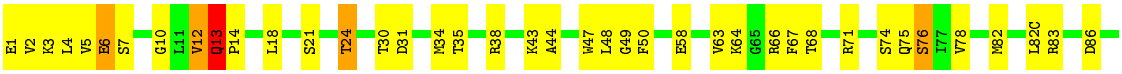


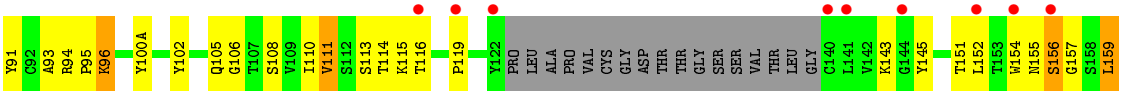


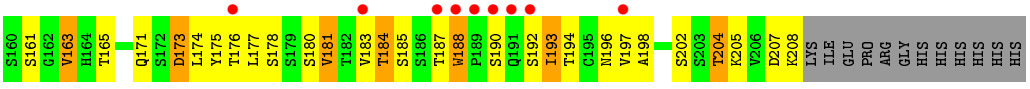


• Molecule 3: Fab C179 heavy chain

Chain K:

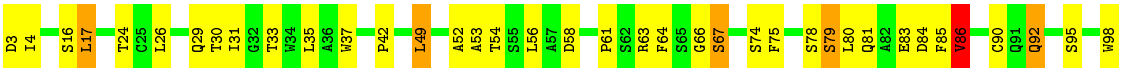


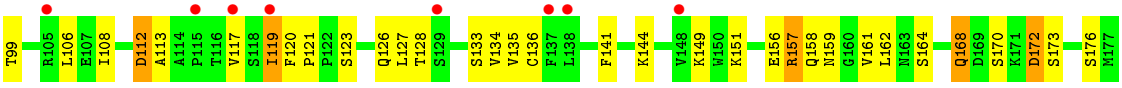


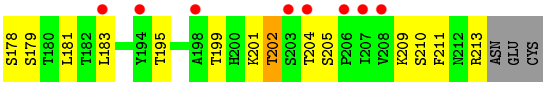


• Molecule 4: Fab C179 light chain

Chain H:

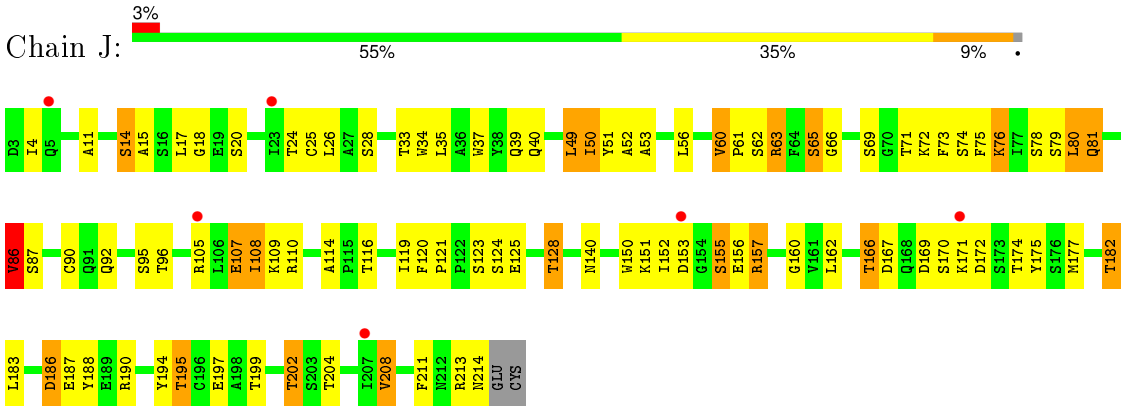






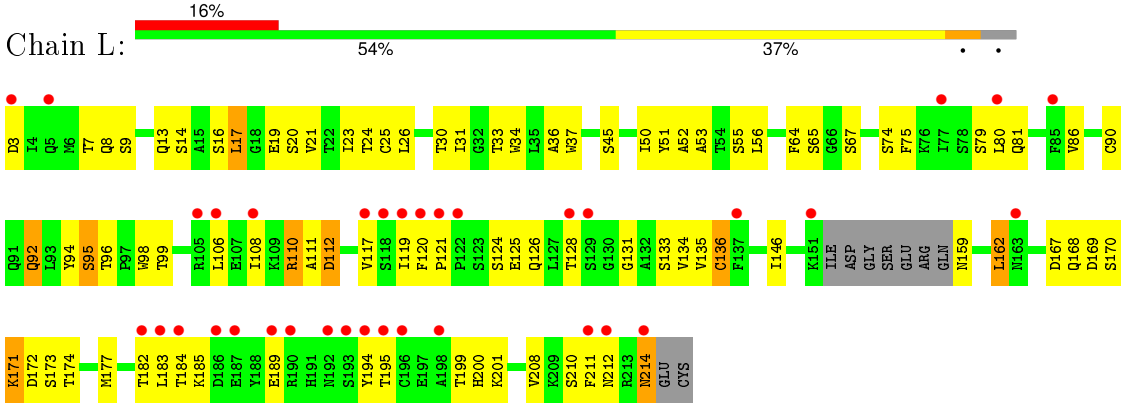
• Molecule 4: Fab C179 light chain

Chain J:



- Molecule 4: Fab C179 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	136.58Å 150.78Å 217.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.55 – 2.90 39.55 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.55-2.90) 98.6 (39.55-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.228 , 0.284 0.231 , 0.281	Depositor DCC
R_{free} test set	5001 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	86.1	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 72.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 98674 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21839	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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: SO4, BMA, NAG, EDO, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.47	1/2612 (0.0%)	0.66	1/3545 (0.0%)
1	C	0.46	0/2612	0.64	1/3545 (0.0%)
1	E	0.48	0/2620	0.66	0/3556
2	B	0.57	0/1399	0.69	0/1876
2	D	0.56	0/1413	0.68	0/1895
2	F	0.54	0/1435	0.67	0/1926
3	G	0.47	0/1742	0.67	1/2378 (0.0%)
3	I	0.46	0/1718	0.71	2/2347 (0.1%)
3	K	0.47	0/1571	0.66	1/2143 (0.0%)
4	H	0.44	0/1666	0.61	0/2264
4	J	0.40	0/1674	0.62	0/2275
4	L	0.42	0/1618	0.63	1/2199 (0.0%)
All	All	0.48	1/22080 (0.0%)	0.66	7/29949 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	299	PRO	N-CD	5.35	1.55	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	9	GLY	N-CA-C	-9.83	88.53	113.10
1	C	298	HIS	C-N-CD	6.03	141.07	128.40
3	K	13	GLN	C-N-CD	5.64	140.25	128.40
1	A	298	HIS	C-N-CD	5.56	140.07	128.40
4	L	3	ASP	CB-CG-OD2	5.25	123.02	118.30
3	G	52(A)	ASP	CB-CG-OD2	5.22	122.99	118.30
3	I	52(A)	ASP	CB-CG-OD2	5.21	122.99	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2546	0	2499	63	0
1	C	2546	0	2500	58	0
1	E	2551	0	2510	68	0
2	B	1370	0	1282	21	0
2	D	1384	0	1294	32	0
2	F	1404	0	1311	45	0
3	G	1696	0	1661	53	0
3	I	1675	0	1636	57	0
3	K	1532	0	1486	64	0
4	H	1627	0	1561	41	0
4	J	1635	0	1567	60	0
4	L	1580	0	1516	47	0
5	A	28	0	26	0	0
5	B	14	0	13	0	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
6	A	39	0	34	0	0
6	E	39	0	34	0	0
7	B	5	0	0	0	0
7	D	5	0	0	1	0
7	E	5	0	0	0	0
7	F	5	0	0	3	0
7	H	5	0	0	0	0
7	J	5	0	0	1	0
7	L	5	0	0	1	0
8	C	50	0	43	0	0
9	C	28	0	25	0	0
9	E	28	0	25	0	0
10	J	4	0	6	1	0
All	All	21839	0	21055	560	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 13.

All (560) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:154:TRP:CZ3	3:I:163:VAL:HG21	1.64	1.32
3:I:154:TRP:HZ3	3:I:163:VAL:CG2	1.49	1.26
4:H:121:PRO:HG3	4:H:211:PHE:CE1	1.71	1.24
3:I:154:TRP:CZ3	3:I:163:VAL:CG2	2.20	1.23
4:H:121:PRO:HG3	4:H:211:PHE:CZ	1.88	1.09
3:K:184:THR:HG22	3:K:185:SER:H	1.22	1.04
1:C:298:HIS:HE1	1:C:300:LEU:HD12	1.21	0.99
1:C:298:HIS:CE1	1:C:300:LEU:HD12	1.98	0.99
3:G:34:MET:HG2	3:G:78:VAL:HG21	1.45	0.95
3:I:159:LEU:H	3:I:159:LEU:HD12	1.36	0.91
3:I:154:TRP:HZ3	3:I:163:VAL:HG21	0.74	0.91
3:K:12:VAL:HG21	3:K:18:LEU:HD13	1.51	0.90
3:K:6:GLU:H	3:K:105:GLN:HE22	1.20	0.89
3:K:154:TRP:HB2	3:K:159:LEU:HD11	1.54	0.89
3:K:35:THR:HG22	3:K:50:PHE:HB3	1.54	0.89
4:H:121:PRO:CG	4:H:211:PHE:CE1	2.56	0.89
3:I:130:ASP:O	3:I:131:THR:HG23	1.75	0.86
3:G:163:VAL:HG22	3:G:181:VAL:HG23	1.56	0.85
4:L:110:ARG:HG2	4:L:173:SER:HB2	1.59	0.84
4:H:54:THR:HG22	4:H:66:GLY:O	1.77	0.83
3:K:96:LYS:HB2	3:K:102:TYR:CE2	2.13	0.83
2:F:38:LYS:HZ1	4:L:33:THR:HG23	1.45	0.82
3:I:163:VAL:HG23	3:I:181:VAL:HG13	1.62	0.81
3:G:144:GLY:HA2	3:G:174:LEU:HD13	1.62	0.81
3:G:155:ASN:O	3:G:156:SER:OG	1.98	0.81
1:E:52:CYS:SG	1:E:277:CYS:CB	2.69	0.80
3:I:130:ASP:O	3:I:131:THR:CG2	2.29	0.80
1:C:316:LEU:HD23	2:D:100:VAL:HG13	1.64	0.80
1:E:52:CYS:SG	1:E:277:CYS:HB2	2.22	0.79
4:L:50:ILE:HG21	4:L:53:ALA:O	1.82	0.78
3:K:94:ARG:HH21	3:K:96:LYS:HA	1.46	0.78
4:L:195:THR:HG23	4:L:210:SER:HB2	1.65	0.77
3:I:154:TRP:CZ3	3:I:163:VAL:HG22	2.18	0.76
3:G:165:THR:HG23	3:G:179:SER:HB2	1.69	0.75
3:G:82(C):LEU:HB3	3:G:111:VAL:HG21	1.67	0.75
2:F:6:ILE:HD12	2:F:112:ASP:HA	1.68	0.75
4:H:195:THR:HG23	4:H:210:SER:HB2	1.70	0.74
3:G:83:ARG:O	3:G:111:VAL:HG11	1.87	0.74
3:G:52(A):ASP:OD1	3:G:53:ASN:HB2	1.88	0.74
3:I:159:LEU:N	3:I:159:LEU:HD12	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:184:THR:HG22	3:K:185:SER:N	2.03	0.72
3:I:191:GLN:NE2	3:I:192:SER:O	2.21	0.72
1:C:141:VAL:HG12	1:C:146:SER:HB2	1.72	0.72
4:J:92:GLN:HE21	4:J:95:SER:H	1.36	0.71
2:D:30:GLN:OE1	2:D:30:GLN:N	2.21	0.71
2:D:131:LYS:HD2	2:F:127[B]:ARG:HH22	1.54	0.71
3:K:1:GLU:HG2	3:K:2:VAL:N	2.06	0.71
3:I:213:ARG:HH12	4:J:124:SER:H	1.37	0.71
3:K:171:GLN:HB2	4:L:162:LEU:HD21	1.72	0.71
1:A:70:LEU:O	1:A:150:ASN:ND2	2.24	0.71
4:H:54:THR:HG22	4:H:67:SER:HA	1.74	0.70
4:J:14:SER:HB2	4:J:109:LYS:HG3	1.72	0.70
2:D:130:VAL:HG12	2:D:140:PHE:HA	1.73	0.70
4:H:172:ASP:N	4:H:172:ASP:OD1	2.24	0.70
1:A:97:CYS:O	1:A:224:ASN:ND2	2.25	0.70
1:C:150:ASN:HA	1:C:256:TYR:HE2	1.56	0.70
2:B:75:ARG:NH1	2:B:78:GLU:OE1	2.25	0.70
1:C:70:LEU:O	1:C:150:ASN:ND2	2.22	0.69
1:A:116(B):PHE:HE1	1:A:260:ILE:HG22	1.57	0.69
1:C:301:THR:OG1	1:C:305:CYS:SG	2.51	0.69
3:I:154:TRP:CH2	3:I:163:VAL:HG22	2.28	0.69
2:F:38:LYS:HZ1	4:L:33:THR:CG2	2.04	0.69
3:K:34:MET:HG2	3:K:78:VAL:HG21	1.75	0.68
3:K:152:LEU:HG	3:K:197:VAL:HG22	1.73	0.68
3:K:12:VAL:O	3:K:13:GLN:HG2	1.94	0.67
4:H:54:THR:CG2	4:H:67:SER:HA	2.25	0.67
4:L:119:ILE:HD12	4:L:211:PHE:HB3	1.76	0.67
1:A:294:PHE:CZ	2:B:59:MET:HG2	2.30	0.67
4:H:35:LEU:HD11	4:H:90:CYS:HB2	1.77	0.67
3:I:12:VAL:HG21	3:I:18:LEU:HD22	1.77	0.66
1:C:120:ILE:HD11	1:C:176:MET:SD	2.36	0.66
3:K:4:LEU:CD2	3:K:24:THR:HB	2.25	0.66
1:E:172:SER:HB2	1:E:259:LYS:HD2	1.77	0.66
4:J:188:TYR:O	4:J:213:ARG:NH2	2.28	0.66
3:K:161:SER:OG	4:L:171:LYS:NZ	2.29	0.66
4:L:194:TYR:HB2	4:L:211:PHE:HE2	1.61	0.66
4:L:112:ASP:OD1	4:L:112:ASP:N	2.29	0.65
3:I:40:PRO:HG2	3:I:43:LYS:HB2	1.79	0.65
4:L:110:ARG:NH1	4:L:111:ALA:O	2.30	0.65
3:K:38:ARG:HG2	3:K:48:LEU:HD21	1.79	0.65
3:K:163:VAL:HG13	3:K:181:VAL:HG23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307[A]:LYS:HE2	2:B:92:TRP:CG	2.33	0.64
1:E:191:GLN:NE2	1:E:197:ASN:O	2.31	0.64
2:D:164:GLU:HA	2:D:167:LYS:HG2	1.80	0.64
1:A:206:THR:HG22	1:A:243:ILE:HG13	1.78	0.64
1:C:180:TRP:CE2	1:C:204:VAL:HG21	2.34	0.63
4:L:92:GLN:HG2	4:L:94:TYR:H	1.63	0.63
3:K:13:GLN:O	3:K:111:VAL:HG23	1.99	0.63
1:A:299:PRO:HG2	1:A:300:LEU:HG	1.81	0.63
3:K:91:TYR:CE1	3:K:106:GLY:HA3	2.34	0.63
1:A:25:LYS:NZ	1:A:35:THR:OG1	2.30	0.62
4:H:157:ARG:NH1	4:H:159:ASN:O	2.31	0.62
3:K:12:VAL:HG12	3:K:12:VAL:O	1.98	0.62
1:C:150:ASN:HA	1:C:256:TYR:CE2	2.34	0.62
3:I:213:ARG:NH1	4:J:124:SER:H	1.97	0.62
4:J:187:GLU:HB3	4:J:190:ARG:HH21	1.64	0.62
4:L:125:GLU:HA	4:L:128:THR:HG22	1.82	0.62
4:J:183:LEU:HB3	4:J:187:GLU:HG3	1.82	0.62
4:H:80:LEU:HD13	4:H:85:PHE:CZ	2.35	0.61
2:F:38:LYS:NZ	7:F:201:SO4:O2	2.34	0.61
2:F:141:TYR:CE2	2:F:170:ARG:HD3	2.35	0.61
1:E:325:GLN:HG2	2:F:13:GLY:O	2.01	0.61
3:G:153:THR:HG23	3:G:196:ASN:HB2	1.83	0.61
3:I:119:PRO:HB3	3:I:145:TYR:HB3	1.81	0.61
4:L:185:LYS:O	4:L:189:GLU:N	2.33	0.60
4:L:92:GLN:HE21	4:L:95:SER:H	1.49	0.60
3:G:35:THR:HG22	3:G:50:PHE:HB3	1.83	0.60
2:F:38:LYS:NZ	4:L:33:THR:HG23	2.16	0.60
1:A:58:PRO:HD2	1:A:274:LEU:HD22	1.84	0.60
1:A:105:TYR:CE2	1:A:109:LYS:HE3	2.37	0.60
1:A:150:ASN:OD1	1:A:150:ASN:N	2.34	0.60
1:E:316:LEU:HD13	2:F:52:VAL:HG12	1.84	0.60
4:J:152:ILE:HG22	4:J:153:ASP:HB2	1.83	0.60
1:C:30:LEU:HB2	2:D:105:GLU:OE2	2.01	0.60
3:I:153:THR:HG22	3:I:154:TRP:H	1.66	0.59
1:C:155:THR:HG22	1:C:156:GLU:N	2.17	0.59
1:A:180:TRP:CE2	1:A:204:VAL:HG21	2.38	0.59
1:E:238:ASP:OD2	1:E:238:ASP:N	2.36	0.59
4:L:92:GLN:NE2	4:L:95:SER:O	2.35	0.59
1:C:77:ASP:HA	1:C:80:LEU:HG	1.84	0.59
3:K:91:TYR:CD1	3:K:106:GLY:CA	2.86	0.59
2:F:57:GLU:O	2:F:60:ASN:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLN:HG3	1:A:196:GLN:O	2.02	0.58
4:J:37:TRP:CZ3	4:J:90:CYS:HB3	2.37	0.58
1:C:155:THR:HG22	1:C:156:GLU:H	1.67	0.58
4:L:126:GLN:OE1	4:L:133:SER:N	2.22	0.58
1:C:61:LEU:HD12	1:C:89:GLU:HG3	1.84	0.58
1:E:294:PHE:HE1	1:E:307[A]:LYS:HZ3	1.50	0.58
3:I:12:VAL:HG11	3:I:82(C):LEU:HG	1.85	0.58
2:F:38:LYS:HG3	3:K:100(A):TYR:CZ	2.39	0.58
3:I:75:GLN:HB3	3:I:77:ILE:HG13	1.85	0.58
3:K:10:GLY:O	3:K:12:VAL:HG23	2.04	0.57
3:I:155:ASN:N	3:I:194:THR:O	2.37	0.57
4:H:141:PHE:HE2	4:H:176:SER:HA	1.69	0.57
1:C:180:TRP:HZ3	1:C:235:THR:HG22	1.68	0.57
2:F:82:LYS:HD3	2:F:86:ASP:OD2	2.04	0.57
3:K:76:SER:O	3:K:76:SER:OG	2.18	0.57
2:F:38:LYS:NZ	7:F:201:SO4:O4	2.38	0.57
3:G:128:CYS:C	3:G:130:ASP:H	2.08	0.57
3:G:172:SER:O	3:G:172:SER:OG	2.18	0.57
1:A:277:CYS:SG	1:A:278:GLU:N	2.78	0.57
1:E:159:SER:HA	1:E:196:GLN:NE2	2.19	0.56
4:H:31:ILE:HG21	4:H:92:GLN:HG3	1.86	0.56
1:C:108:LEU:HB2	1:C:234:TRP:CE2	2.39	0.56
2:B:126:LEU:HD13	2:B:130:VAL:HG11	1.86	0.56
3:K:183:VAL:HG22	3:K:184:THR:H	1.71	0.56
2:F:130:VAL:HG12	2:F:140:PHE:HA	1.88	0.56
2:D:129:ASN:ND2	2:D:159:TYR:HE1	2.04	0.56
4:J:92:GLN:NE2	4:J:95:SER:H	2.03	0.56
4:H:113:ALA:O	4:H:202:THR:HG21	2.04	0.56
4:J:52:ALA:O	4:J:53:ALA:HB3	2.06	0.56
3:K:12:VAL:CG1	3:K:12:VAL:O	2.54	0.56
1:C:71:LEU:O	1:C:148:PHE:HB3	2.06	0.56
4:J:20:SER:HB3	4:J:76:LYS:HZ1	1.70	0.55
4:J:37:TRP:HB2	4:J:50:ILE:HG23	1.89	0.55
2:D:30:GLN:HE22	2:D:145:ASP:HA	1.70	0.55
3:K:184:THR:CG2	3:K:185:SER:H	2.05	0.55
2:F:164:GLU:CD	2:F:164:GLU:H	2.10	0.55
2:B:54:SER:HB3	1:E:32:ARG:NH2	2.21	0.55
4:H:119:ILE:HG12	4:H:209:LYS:HB3	1.88	0.55
3:G:84:VAL:HA	3:G:111:VAL:CG1	2.36	0.55
1:E:130:HIS:HB3	1:E:155:THR:O	2.07	0.55
4:J:125:GLU:N	4:J:125:GLU:OE1	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:91:TYR:CE1	3:K:106:GLY:CA	2.90	0.55
3:G:33:TYR:O	3:G:35:THR:HG23	2.07	0.55
4:H:42:PRO:HD3	4:H:86:VAL:HG12	1.88	0.55
1:A:122:PRO:HD2	1:A:126:ARG:HH21	1.72	0.54
1:A:66:ILE:HD12	1:A:112:LEU:HD12	1.89	0.54
1:C:105:TYR:CE2	1:C:109:LYS:HE3	2.42	0.54
1:E:156:GLU:HB2	1:E:160:ASN:O	2.07	0.54
1:E:316:LEU:HD23	2:F:100:VAL:HG13	1.88	0.54
2:D:131:LYS:HD3	2:D:141:TYR:OH	2.07	0.54
3:I:130:ASP:C	3:I:131:THR:HG23	2.27	0.54
3:K:91:TYR:CD1	3:K:106:GLY:HA2	2.42	0.54
2:F:62:GLN:HB2	2:F:92:TRP:CE2	2.42	0.54
1:E:239:MET:HE2	1:E:239:MET:HA	1.90	0.54
4:J:152:ILE:HD12	4:J:157:ARG:HB2	1.89	0.53
2:F:62:GLN:NE2	2:F:63:PHE:O	2.41	0.53
4:L:212:ASN:OD1	4:L:214:ASN:ND2	2.40	0.53
3:G:172:SER:O	3:G:174:LEU:HG	2.07	0.53
4:J:33:THR:O	4:J:52:ALA:O	2.27	0.53
3:I:159:LEU:O	3:I:159:LEU:HD13	2.08	0.53
4:H:83:GLU:OE1	4:H:83:GLU:N	2.30	0.53
4:J:15:ALA:O	4:J:109:LYS:N	2.36	0.53
1:A:202:VAL:HG11	1:A:251:LEU:HD13	1.91	0.53
2:F:37:ASP:OD2	2:F:40:SER:OG	2.20	0.53
4:H:4:ILE:O	4:H:99:THR:HG21	2.09	0.53
3:I:153:THR:HG21	3:I:157:GLY:HA2	1.91	0.53
1:C:251:LEU:HD21	1:C:253:ALA:HB2	1.90	0.53
1:E:156:GLU:HB3	1:E:161:TYR:HD1	1.73	0.53
1:C:310:LYS:NZ	2:D:90:ASP:OD1	2.36	0.52
1:C:187:ASP:OD1	1:C:190:GLU:N	2.38	0.52
3:I:51:ILE:HD13	3:I:71:ARG:HD2	1.90	0.52
1:E:152:VAL:HG23	1:E:253:ALA:HB3	1.91	0.52
4:H:37:TRP:CE2	4:H:75:PHE:HB2	2.44	0.52
4:J:35:LEU:HD13	4:J:73:PHE:CG	2.44	0.52
3:K:43:LYS:HG3	3:K:44:ALA:H	1.74	0.52
4:L:37:TRP:CE2	4:L:75:PHE:HB2	2.43	0.52
1:E:119:LYS:HB3	1:E:256:TYR:CD1	2.44	0.52
4:J:152:ILE:O	4:J:155:SER:N	2.42	0.52
3:I:4:LEU:HD22	3:I:24:THR:HG22	1.91	0.52
1:C:32:ARG:NH2	2:F:54:SER:OG	2.41	0.52
3:G:40:PRO:HG2	3:G:43:LYS:HB3	1.92	0.52
3:K:173:ASP:N	3:K:173:ASP:OD2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:TYR:CE2	1:E:249:GLY:HA2	2.45	0.52
2:B:54:SER:HB3	1:E:32:ARG:HH22	1.74	0.52
1:E:150:ASN:HA	1:E:256:TYR:HE2	1.75	0.52
4:J:186:ASP:OD1	4:J:186:ASP:N	2.34	0.52
4:J:49:LEU:HD12	4:J:60:VAL:HG11	1.89	0.52
1:E:280:LYS:NZ	1:E:304:GLU:H	2.08	0.52
1:E:61:LEU:HD11	1:E:66:ILE:HD13	1.92	0.52
3:I:52(A):ASP:OD1	3:I:53:ASN:HB2	2.10	0.52
2:F:38:LYS:NZ	7:F:201:SO4:S	2.83	0.52
2:D:38:LYS:NZ	7:D:201:SO4:O2	2.43	0.52
4:L:92:GLN:NE2	4:L:95:SER:H	2.08	0.51
4:J:20:SER:HB3	4:J:76:LYS:NZ	2.26	0.51
4:H:126:GLN:OE1	4:H:133:SER:N	2.42	0.51
3:K:187:THR:OG1	3:K:188:TRP:N	2.43	0.51
1:C:229:ARG:NH2	1:E:206:THR:O	2.43	0.51
3:I:34:MET:HG2	3:I:94:ARG:HG3	1.91	0.51
3:K:155:ASN:ND2	3:K:193:ILE:HG12	2.26	0.51
4:J:197:GLU:HG3	4:J:208:VAL:HB	1.92	0.51
1:A:298:HIS:CG	1:A:299:PRO:HD2	2.46	0.51
1:E:129:GLN:CD	1:E:129:GLN:H	2.14	0.51
1:C:298:HIS:HE1	1:C:300:LEU:CD1	2.09	0.51
4:J:51:TYR:O	4:J:52:ALA:HB3	2.11	0.51
1:E:151:MET:HE1	1:E:254:PRO:HA	1.92	0.51
3:K:35:THR:HG22	3:K:50:PHE:CB	2.35	0.51
1:A:228:GLY:O	1:A:229:ARG:NH1	2.43	0.51
3:I:140:CYS:HB2	3:I:154:TRP:HE1	1.75	0.51
4:J:108:ILE:HD11	4:J:110:ARG:HD3	1.91	0.51
1:A:167:SER:HB2	1:A:244:ASN:HD21	1.74	0.51
1:E:117:LYS:NZ	1:E:150:ASN:OD1	2.29	0.50
1:A:244:ASN:OD1	1:E:221:PRO:HG3	2.10	0.50
4:J:61:PRO:HB2	4:J:63:ARG:HD2	1.93	0.50
3:I:164:HIS:NE2	4:J:140:ASN:OD1	2.34	0.50
1:E:128:THR:O	1:E:157:LYS:NZ	2.39	0.50
1:A:174:GLU:HB2	1:A:259:LYS:HE3	1.93	0.50
3:K:115:LYS:HD2	3:K:116:THR:H	1.77	0.50
2:B:3:PHE:CE2	2:B:113:SER:HB2	2.47	0.50
1:E:195:TYR:O	1:E:196:GLN:HB2	2.11	0.50
1:E:51:LEU:O	1:E:274:LEU:HD12	2.11	0.50
2:B:55:VAL:HG13	2:B:99:LEU:HD23	1.94	0.50
3:I:213:ARG:HH12	4:J:123:SER:HA	1.77	0.49
2:F:125:GLN:O	2:F:127[B]:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:PRO:HD3	1:E:300:LEU:O	2.12	0.49
3:K:31:ASP:HB3	3:K:71:ARG:NH2	2.26	0.49
2:D:38:LYS:HG2	3:I:100(A):TYR:CE2	2.46	0.49
1:E:45:LYS:HG2	1:E:296:ASN:HD21	1.77	0.49
4:J:169:ASP:OD1	4:J:172:ASP:HB3	2.13	0.49
3:G:30:THR:HG23	3:G:32:ASP:H	1.77	0.49
1:C:155:THR:HG22	1:C:156:GLU:HG2	1.94	0.49
3:G:161:SER:N	3:G:163:VAL:HG23	2.28	0.49
1:E:294:PHE:CE1	1:E:307[A]:LYS:HD3	2.47	0.49
3:K:35:THR:HG21	4:L:98:TRP:HZ3	1.78	0.49
3:I:12:VAL:CG2	3:I:18:LEU:HD22	2.42	0.49
3:I:155:ASN:HD22	3:I:155:ASN:C	2.16	0.49
1:E:64:CYS:HA	1:E:95:ASP:O	2.12	0.49
1:E:201:TYR:OH	1:E:246:GLU:OE2	2.31	0.49
1:C:13:ILE:HD11	2:D:24:TYR:HB3	1.94	0.49
2:B:83:LYS:NZ	2:D:85:GLU:OE2	2.46	0.48
3:K:1:GLU:HG2	3:K:2:VAL:HG23	1.95	0.48
3:G:52(A):ASP:OD1	3:G:53:ASN:N	2.43	0.48
4:J:114:ALA:HA	4:J:202:THR:HG21	1.95	0.48
1:E:139:CYS:HB2	1:E:146:SER:O	2.14	0.48
1:E:187:ASP:OD1	1:E:190:GLU:N	2.40	0.48
1:C:220:ARG:NH1	1:C:227:GLY:O	2.45	0.48
1:C:185:PRO:HD2	1:C:217:ILE:HG12	1.95	0.48
1:A:15:ILE:HD11	2:B:122:VAL:HG21	1.95	0.48
1:A:183:HIS:ND1	1:A:195:TYR:OH	2.29	0.48
3:I:213:ARG:HH12	4:J:124:SER:N	2.10	0.48
4:L:172:ASP:OD2	4:L:174:THR:OG1	2.29	0.48
3:G:155:ASN:HD22	3:G:159:LEU:HD12	1.79	0.47
1:A:284:PRO:HG2	1:A:298:HIS:CE1	2.49	0.47
3:K:155:ASN:CG	3:K:193:ILE:HG12	2.34	0.47
3:G:177:LEU:HG	3:G:178:SER:H	1.77	0.47
4:L:17:LEU:H	4:L:17:LEU:HD22	1.79	0.47
3:K:1:GLU:HG2	3:K:2:VAL:H	1.76	0.47
4:L:200:HIS:CD2	4:L:201:LYS:H	2.32	0.47
4:J:40:GLN:O	4:J:86:VAL:HG13	2.15	0.47
3:K:155:ASN:H	3:K:196:ASN:ND2	2.12	0.47
4:J:18:GLY:H	4:J:80:LEU:CB	2.27	0.47
4:J:124:SER:O	4:J:128:THR:OG1	2.32	0.47
4:J:50:ILE:HD13	4:J:66:GLY:HA3	1.97	0.47
1:A:202:VAL:HG22	1:A:247:SER:OG	2.14	0.47
3:K:83:ARG:O	3:K:111:VAL:HG11	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:32:ASP:OD1	3:G:52:ARG:NH2	2.34	0.47
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.50	0.47
4:J:151:LYS:O	4:J:195:THR:OG1	2.21	0.47
3:I:166:PHE:O	3:I:177:LEU:CD1	2.63	0.47
1:A:96:LEU:HD12	1:A:96:LEU:H	1.80	0.47
3:G:119:PRO:HB3	3:G:145:TYR:HB3	1.97	0.47
4:L:31:ILE:HG21	4:L:92:GLN:HG3	1.96	0.47
4:J:150:TRP:O	4:J:157:ARG:N	2.46	0.47
1:E:282:GLN:HB3	1:E:302[B]:ILE:HG23	1.97	0.47
1:C:161:TYR:CZ	1:C:249:GLY:HA2	2.50	0.47
3:G:124:LEU:HD11	3:G:141:LEU:HB2	1.96	0.47
3:G:83:ARG:C	3:G:111:VAL:HG11	2.35	0.46
2:F:127[A]:ARG:HB3	2:F:128:ASP:H	1.49	0.46
2:D:103:GLU:OE1	2:D:103:GLU:HA	2.13	0.46
1:A:170:ASN:HB3	1:A:240:TRP:N	2.31	0.46
3:G:194:THR:HA	3:G:209:LYS:HA	1.97	0.46
4:H:17:LEU:HD12	4:H:108:ILE:HD11	1.97	0.46
2:F:121:LYS:HG3	2:F:122:VAL:N	2.30	0.46
1:E:61:LEU:HD12	1:E:89:GLU:HB2	1.97	0.46
3:K:196:ASN:HB3	3:K:205:LYS:NZ	2.30	0.46
3:G:94:ARG:O	3:G:101:ASP:N	2.48	0.46
2:B:82:LYS:NZ	2:B:86:ASP:OD2	2.46	0.46
1:A:53:LYS:HG3	1:A:277:CYS:O	2.16	0.46
1:E:43:LEU:O	1:E:45:LYS:HE2	2.14	0.46
3:K:74:SER:OG	3:K:75:GLN:N	2.47	0.46
4:L:168:GLN:NE2	4:L:173:SER:O	2.48	0.46
1:A:15:ILE:HG13	2:B:119:TYR:HA	1.97	0.46
4:H:108:ILE:HG22	4:H:168:GLN:OE1	2.15	0.46
1:A:49:GLY:HA2	1:A:285:LEU:O	2.15	0.46
2:F:3:PHE:N	2:F:112:ASP:OD2	2.49	0.46
1:A:196:GLN:O	1:A:197:ASN:OD1	2.34	0.46
4:J:107:GLU:HG3	4:J:175:TYR:OH	2.16	0.46
2:B:162:TYR:O	2:B:166:SER:OG	2.29	0.46
3:G:2:VAL:HG21	3:G:102:TYR:CE2	2.50	0.46
1:C:26:VAL:HG21	1:C:317:ALA:HB2	1.97	0.46
3:G:116:THR:HG23	3:G:147:PRO:HD2	1.97	0.46
2:F:42:GLN:HG2	4:L:51:TYR:CE1	2.51	0.46
4:L:52:ALA:O	4:L:53:ALA:HB3	2.16	0.46
1:A:25:LYS:CE	1:A:35:THR:OG1	2.64	0.46
4:H:162:LEU:O	4:H:179:SER:HA	2.16	0.46
1:A:58:PRO:HB3	1:A:86:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LEU:HA	1:C:30:LEU:HD12	1.73	0.46
3:I:94:ARG:HG2	3:I:95:PRO:HD2	1.96	0.46
1:C:123:LYS:NZ	1:C:132:THR:O	2.49	0.46
3:G:39:GLN:HB2	3:G:45:LEU:HD23	1.98	0.46
1:A:201:TYR:HE2	1:A:248:THR:HG23	1.81	0.46
3:K:94:ARG:HA	3:K:95:PRO:HD3	1.81	0.46
4:J:34:TRP:NE1	7:J:301:SO4:O1	2.48	0.46
1:E:180:TRP:CE2	1:E:204:VAL:HG21	2.51	0.46
3:K:82:MET:HB3	3:K:82(C):LEU:HD21	1.98	0.46
1:C:66:ILE:HB	1:C:105:TYR:OH	2.17	0.45
3:G:171:GLN:HB2	4:H:162:LEU:HD11	1.98	0.45
2:F:87:GLY:O	2:F:91:VAL:HG23	2.17	0.45
4:L:51:TYR:O	4:L:52:ALA:HB3	2.16	0.45
4:J:92:GLN:NE2	4:J:95:SER:O	2.43	0.45
3:G:171:GLN:HG3	4:H:162:LEU:HD11	1.99	0.45
1:C:129:GLN:O	1:C:157:LYS:HB3	2.16	0.45
1:A:43:LEU:HD23	1:A:45:LYS:HE3	1.98	0.45
1:A:298:HIS:CD2	1:A:299:PRO:HD2	2.51	0.45
1:E:280:LYS:HG3	1:E:304:GLU:HG2	1.98	0.45
4:L:34:TRP:CD1	4:L:34:TRP:N	2.85	0.45
3:G:17:SER:HA	3:G:82(C):LEU:HD23	1.98	0.45
2:B:142:HIS:CD2	2:B:162:TYR:HB3	2.52	0.45
4:H:61:PRO:HB2	4:H:64:PHE:CD2	2.52	0.45
4:H:63:ARG:HH21	4:H:84:ASP:CG	2.20	0.45
2:F:123:ARG:HB2	2:F:138:PHE:CZ	2.52	0.45
1:C:111:LEU:O	1:C:115:VAL:HG23	2.16	0.45
2:D:107:THR:O	2:D:110:PHE:HB3	2.16	0.45
1:C:201:TYR:OH	1:C:246:GLU:OE2	2.32	0.45
1:C:102:PHE:HZ	1:C:179:ILE:HD13	1.81	0.45
1:E:184:HIS:HB3	1:E:220:ARG:NH2	2.32	0.45
1:A:307[A]:LYS:HE2	2:B:92:TRP:CD2	2.51	0.45
2:F:62:GLN:HB2	2:F:92:TRP:CZ2	2.52	0.45
3:K:66:ARG:HH22	3:K:86:ASP:CG	2.20	0.45
1:A:14:CYS:O	2:B:24:TYR:HA	2.16	0.45
2:F:71:SER:O	2:F:75:ARG:NH1	2.49	0.45
1:E:260:ILE:O	1:E:260:ILE:HG13	2.16	0.45
3:I:52(B):ARG:HB2	3:I:55:TYR:OH	2.17	0.45
4:L:8:GLN:HE21	4:L:23:ILE:HG21	1.80	0.45
1:A:58:PRO:HB3	1:A:86:TYR:CZ	2.52	0.45
1:E:247:SER:OG	1:E:249:GLY:O	2.35	0.45
1:A:170:ASN:HB3	1:A:240:TRP:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:SER:HB2	1:C:259:LYS:HD2	1.99	0.45
1:E:150:ASN:HA	1:E:256:TYR:CE2	2.52	0.44
3:I:66:ARG:C	3:I:67:PHE:HD1	2.21	0.44
4:L:13:GLN:HG3	4:L:14:SER:N	2.33	0.44
4:J:187:GLU:HA	4:J:190:ARG:HE	1.82	0.44
3:I:85:GLU:H	3:I:85:GLU:HG3	1.55	0.44
1:E:247:SER:HB2	1:E:251:LEU:HD12	1.99	0.44
1:A:168:TYR:O	1:A:242:THR:HA	2.18	0.44
3:K:47:TRP:CH2	3:K:49:GLY:HA2	2.53	0.44
3:K:202:SER:OG	3:K:204:THR:OG1	2.28	0.44
3:K:93:ALA:HA	3:K:102:TYR:O	2.18	0.44
4:J:37:TRP:HD1	4:J:50:ILE:HG12	1.81	0.44
4:H:120:PHE:HB2	4:H:135:VAL:HB	1.99	0.44
3:K:6:GLU:HA	3:K:21:SER:O	2.18	0.44
4:L:50:ILE:HG23	4:L:55:SER:O	2.18	0.44
3:I:39:GLN:HA	3:I:40:PRO:HD2	1.89	0.44
2:F:62:GLN:OE1	2:F:92:TRP:CD1	2.70	0.44
1:E:26:VAL:HG21	1:E:317:ALA:HB2	2.00	0.44
4:L:119:ILE:HG22	4:L:136:CYS:SG	2.58	0.44
2:D:133:LEU:HB2	2:D:135:ASN:OD1	2.17	0.44
4:L:120:PHE:HA	4:L:121:PRO:HD2	1.87	0.44
3:G:198:ALA:HB2	3:G:205:LYS:HD3	2.00	0.44
1:E:171:THR:HA	1:E:240:TRP:HZ3	1.82	0.44
1:E:121:LEU:HD12	1:E:254:PRO:HG2	1.99	0.44
3:G:47:TRP:CH2	3:G:49:GLY:HA2	2.53	0.44
1:C:137:ARG:H	1:C:137:ARG:NE	2.15	0.44
1:E:112:LEU:HD23	1:E:112:LEU:HA	1.69	0.44
1:A:131:THR:HB	1:A:155:THR:HG23	1.99	0.44
4:J:63:ARG:H	4:J:63:ARG:HG3	1.34	0.44
3:I:52(B):ARG:HA	3:I:55:TYR:CE2	2.53	0.44
2:B:76:ARG:NH1	2:D:69:GLU:O	2.48	0.44
4:J:78:SER:OG	4:J:79:SER:N	2.49	0.44
3:G:6:GLU:OE1	3:G:105:GLN:N	2.51	0.44
3:I:6:GLU:OE1	3:I:104:GLY:HA3	2.18	0.44
4:H:78:SER:OG	4:H:79:SER:N	2.50	0.44
3:K:5:VAL:HA	3:K:105:GLN:OE1	2.18	0.43
4:L:50:ILE:CG2	4:L:53:ALA:O	2.60	0.43
1:E:307[A]:LYS:HE2	1:E:309:VAL:HG13	2.00	0.43
1:C:238:ASP:OD1	1:C:239:MET:N	2.50	0.43
2:D:17:MET:HB2	2:D:17:MET:HE3	1.75	0.43
1:A:168:TYR:CE2	1:A:170:ASN:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:GLN:HG2	2:D:13:GLY:O	2.18	0.43
3:K:156:SER:HB3	3:K:157:GLY:H	1.57	0.43
3:G:154:TRP:CZ3	3:G:195:CYS:HB2	2.53	0.43
1:A:274:LEU:HD12	1:A:275:GLU:H	1.84	0.43
3:G:36:TRP:CE2	3:G:80:LEU:HB2	2.53	0.43
3:I:57:THR:HG1	3:I:59:TYR:HE2	1.65	0.43
3:K:50:PHE:C	3:K:50:PHE:CD1	2.91	0.43
2:F:38:LYS:HZ2	2:F:38:LYS:HB2	1.84	0.43
1:A:116(B):PHE:CE1	1:A:260:ILE:HG22	2.45	0.43
1:E:184:HIS:HB3	1:E:220:ARG:HH22	1.84	0.43
1:A:186:ASN:OD1	1:A:219:THR:HA	2.19	0.43
1:E:294:PHE:HE1	1:E:307[A]:LYS:NZ	2.16	0.43
1:E:161:TYR:CD1	1:E:195:TYR:HA	2.54	0.43
4:J:172:ASP:OD2	4:J:174:THR:OG1	2.37	0.43
4:J:166:THR:OG1	4:J:167:ASP:N	2.49	0.43
3:K:1:GLU:OE1	3:K:102:TYR:OH	2.22	0.43
1:C:164:ALA:O	1:C:246:GLU:HA	2.19	0.43
3:K:63:VAL:HB	3:K:67:PHE:CG	2.53	0.43
4:L:108:ILE:HG23	4:L:173:SER:HB3	2.01	0.43
4:J:188:TYR:HA	4:J:194:TYR:OH	2.19	0.43
3:K:151:THR:HB	3:K:198:ALA:HB3	2.01	0.43
1:C:112:LEU:HD23	1:C:112:LEU:HA	1.59	0.43
3:I:11:LEU:O	3:I:110:ILE:O	2.37	0.43
1:A:25:LYS:HZ1	1:A:35:THR:HG1	1.62	0.43
1:E:147:PHE:CG	1:E:148:PHE:N	2.86	0.43
2:F:142:HIS:CD2	2:F:162:TYR:HB3	2.53	0.43
4:L:34:TRP:NE1	7:L:301:SO4:O3	2.36	0.43
1:C:298:HIS:ND1	1:C:299:PRO:HD2	2.34	0.43
1:E:316:LEU:CD1	2:F:52:VAL:HG12	2.48	0.43
1:C:195:TYR:CZ	1:C:250:ASN:HA	2.54	0.43
1:C:49:GLY:HA2	1:C:285:LEU:O	2.19	0.43
4:J:37:TRP:CH2	4:J:90:CYS:HB3	2.53	0.42
3:I:166:PHE:HD2	4:J:166:THR:HG22	1.83	0.42
4:H:151:LYS:HB2	4:H:195:THR:HB	2.01	0.42
2:F:17:MET:HE1	2:F:23:GLY:HA3	2.01	0.42
1:C:202:VAL:HA	1:C:247:SER:HB2	2.01	0.42
3:G:67:PHE:N	3:G:67:PHE:CD1	2.87	0.42
3:G:52(B)[B]:ARG:HG3	3:G:55:TYR:CE2	2.54	0.42
3:I:205:LYS:NZ	3:I:207:ASP:OD1	2.43	0.42
3:K:13:GLN:HG3	3:K:14:PRO:O	2.19	0.42
2:F:38:LYS:NZ	2:F:38:LYS:HB2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:84:VAL:HA	3:G:111:VAL:HG12	2.00	0.42
1:A:180:TRP:NE1	1:A:204:VAL:HG21	2.33	0.42
2:D:160:PRO:HA	2:D:163:GLU:HB2	2.01	0.42
1:A:108:LEU:HD13	1:A:234:TRP:CD2	2.54	0.42
3:I:130:ASP:O	3:I:131:THR:HG22	2.14	0.42
4:J:110:ARG:HA	4:J:110:ARG:HD2	1.81	0.42
4:H:56:LEU:HD21	4:H:64:PHE:O	2.19	0.42
1:A:156:GLU:HB2	1:A:161:TYR:HB2	2.01	0.42
4:J:26:LEU:HD13	4:J:72:LYS:HG2	2.01	0.42
3:G:173:ASP:OD1	3:G:173:ASP:N	2.52	0.42
2:D:156:THR:OG1	2:D:157:TYR:N	2.51	0.42
1:A:214:THR:HA	1:A:215:PRO:HD3	1.81	0.42
4:J:120:PHE:HA	4:J:121:PRO:HD3	1.82	0.42
3:K:119:PRO:HB3	3:K:145:TYR:HB3	2.01	0.42
2:B:2:LEU:HD23	2:D:3:PHE:HZ	1.84	0.42
3:G:129:GLY:O	3:G:130:ASP:HB2	2.19	0.42
4:J:65:SER:OG	4:J:76:LYS:HG2	2.19	0.42
1:A:176:MET:HA	1:A:258:PHE:O	2.20	0.42
2:D:121:LYS:HB2	2:D:121:LYS:HE3	1.72	0.42
1:C:120:ILE:HG22	1:C:121:LEU:N	2.33	0.42
1:A:167:SER:HB2	1:A:244:ASN:ND2	2.33	0.42
4:L:56:LEU:HD11	4:L:64:PHE:O	2.19	0.42
4:H:33:THR:HG23	4:H:33:THR:O	2.19	0.42
1:E:247:SER:CB	1:E:251:LEU:HD12	2.50	0.42
2:F:140:PHE:HB3	2:F:142:HIS:O	2.19	0.42
4:H:49:LEU:HA	4:H:49:LEU:HD12	1.57	0.42
4:L:19:GLU:O	4:L:80:LEU:HD23	2.18	0.42
3:I:166:PHE:O	3:I:177:LEU:HD11	2.20	0.42
3:G:67:PHE:CE1	3:G:82:MET:HB3	2.55	0.42
1:E:127:TRP:CZ3	1:E:154:LEU:HD21	2.55	0.42
2:B:27:SER:HB3	2:B:32:SER:HB2	2.01	0.42
2:D:43:LYS:HE3	2:D:43:LYS:HB3	1.90	0.42
2:F:164:GLU:CD	2:F:164:GLU:N	2.72	0.42
4:J:17:LEU:HA	4:J:80:LEU:HB3	2.01	0.42
1:E:90:LYS:HB3	1:E:271:GLU:OE1	2.20	0.42
2:D:142:HIS:CD2	2:D:162:TYR:HB3	2.54	0.42
1:A:273:THR:OG1	1:A:274:LEU:N	2.52	0.41
4:J:18:GLY:H	4:J:80:LEU:HB3	1.85	0.41
1:C:15:ILE:HG13	2:D:119:TYR:HA	2.02	0.41
1:A:284:PRO:HD3	1:A:300:LEU:O	2.20	0.41
4:H:158:GLN:HG2	4:H:159:ASN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ASP:OD2	1:C:149:ARG:NH2	2.53	0.41
1:A:175:GLN:HG2	1:A:236:LEU:HG	2.02	0.41
3:I:159:LEU:CD1	3:I:159:LEU:N	2.73	0.41
1:A:105:TYR:CZ	1:A:109:LYS:HE3	2.55	0.41
3:K:143:LYS:HG3	3:K:176:THR:HG23	2.03	0.41
1:C:155:THR:CG2	1:C:156:GLU:N	2.83	0.41
3:I:155:ASN:O	3:I:155:ASN:ND2	2.43	0.41
1:C:90:LYS:O	1:C:269:LYS:NZ	2.43	0.41
4:H:52:ALA:O	4:H:53:ALA:HB3	2.20	0.41
2:D:29:ASP:OD2	2:D:29:ASP:N	2.36	0.41
4:L:36:ALA:O	4:L:90:CYS:HA	2.21	0.41
4:L:120:PHE:HB2	4:L:135:VAL:HB	2.03	0.41
3:G:38:ARG:HD3	3:G:48:LEU:HD21	2.01	0.41
3:I:50:PHE:C	3:I:50:PHE:CD1	2.94	0.41
1:E:320:LEU:HD23	1:E:320:LEU:H	1.85	0.41
2:F:6:ILE:HD12	2:F:112:ASP:CA	2.45	0.41
4:L:194:TYR:HB2	4:L:211:PHE:CE2	2.48	0.41
3:G:50:PHE:C	3:G:50:PHE:CD1	2.94	0.41
4:H:141:PHE:CE2	4:H:176:SER:HA	2.54	0.41
2:D:129:ASN:OD1	2:D:157:TYR:OH	2.38	0.41
2:F:81:ASN:O	2:F:85:GLU:HG3	2.21	0.41
3:I:184:THR:O	3:I:187:THR:OG1	2.37	0.41
3:K:13:GLN:C	3:K:111:VAL:HG23	2.41	0.41
1:E:325:GLN:OE1	2:F:15:GLN:HB2	2.21	0.41
3:K:155:ASN:OD1	3:K:193:ILE:HG12	2.21	0.41
3:G:51:ILE:HD13	3:G:71:ARG:HG2	2.03	0.41
1:C:84:TRP:CZ3	1:C:116(A):HIS:HA	2.56	0.41
3:K:4:LEU:HD23	3:K:24:THR:HB	2.00	0.41
1:A:51:LEU:O	1:A:274:LEU:HD12	2.21	0.41
1:C:155:THR:CG2	1:C:156:GLU:H	2.32	0.41
4:J:35:LEU:HB3	4:J:53:ALA:HB2	2.03	0.41
4:J:80:LEU:HD12	4:J:81:GLN:H	1.85	0.41
3:I:177:LEU:HG	3:I:178:SER:N	2.36	0.41
3:G:171:GLN:HB2	4:H:162:LEU:HD21	2.03	0.41
1:C:123:LYS:O	1:C:132:THR:HG21	2.21	0.41
3:I:52(B):ARG:HB2	3:I:55:TYR:CZ	2.56	0.41
1:C:19:ALA:HB2	2:D:13:GLY:HA3	2.02	0.41
2:F:44:ALA:O	2:F:48:ILE:HG12	2.21	0.41
1:E:78:ARG:HG3	1:E:79:LEU:HD13	2.03	0.41
1:A:30:LEU:HD12	1:A:30:LEU:HA	1.73	0.41
1:A:75:GLU:HG3	1:A:95:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:ILE:HG13	2:F:119:TYR:HA	2.02	0.41
4:J:121:PRO:HG3	4:J:211:PHE:CE2	2.56	0.41
4:J:11:ALA:H	10:J:302:EDO:H21	1.85	0.41
4:L:106:LEU:HD12	4:L:106:LEU:HA	1.88	0.41
2:F:83:LYS:HZ3	2:F:83:LYS:HG3	1.77	0.41
3:G:52:ARG:NH2	3:G:53:ASN:OD1	2.54	0.40
2:D:38:LYS:HG2	3:I:100(A):TYR:CZ	2.56	0.40
2:B:51:LYS:O	2:B:55:VAL:HG23	2.21	0.40
4:H:112:ASP:N	4:H:112:ASP:OD1	2.38	0.40
4:H:121:PRO:CG	4:H:211:PHE:CZ	2.80	0.40
3:I:18:LEU:HD12	3:I:18:LEU:HA	1.82	0.40
3:G:35:THR:HG21	4:H:98:TRP:HZ3	1.86	0.40
4:H:161:VAL:HG22	4:H:181:LEU:HD12	2.03	0.40
1:E:168:TYR:O	1:E:242:THR:HA	2.22	0.40
4:J:160:GLY:O	4:J:182:THR:OG1	2.36	0.40
3:G:66:ARG:HB3	3:G:82(A):ASN:O	2.21	0.40
3:K:1:GLU:CG	3:K:2:VAL:N	2.73	0.40
4:L:126:GLN:HG2	4:L:131:GLY:O	2.21	0.40
2:B:76:ARG:HB3	2:D:68:LYS:HD3	2.03	0.40
1:A:295:HIS:O	1:A:308:TYR:HA	2.21	0.40
1:A:121:LEU:HD12	1:A:254:PRO:HG2	2.03	0.40
1:E:106:GLU:H	1:E:106:GLU:CD	2.21	0.40
1:C:200:THR:HA	1:C:248:THR:OG1	2.21	0.40
4:L:37:TRP:CZ3	4:L:90:CYS:HB3	2.57	0.40
2:F:168:LEU:HD23	2:F:168:LEU:HA	1.92	0.40
3:G:128:CYS:O	3:G:130:ASP:N	2.54	0.40
1:E:129:GLN:HB2	1:E:130:HIS:ND1	2.36	0.40
3:G:96:LYS:HB2	3:G:96:LYS:HE3	1.92	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	325/327 (99%)	316 (97%)	9 (3%)	0	100	100
1	C	325/327 (99%)	315 (97%)	10 (3%)	0	100	100
1	E	326/327 (100%)	309 (95%)	17 (5%)	0	100	100
2	B	165/174 (95%)	157 (95%)	8 (5%)	0	100	100
2	D	167/174 (96%)	153 (92%)	14 (8%)	0	100	100
2	F	171/174 (98%)	162 (95%)	9 (5%)	0	100	100
3	G	222/229 (97%)	204 (92%)	16 (7%)	2 (1%)	21	57
3	I	219/229 (96%)	207 (94%)	11 (5%)	1 (0%)	34	71
3	K	196/229 (86%)	177 (90%)	16 (8%)	3 (2%)	13	42
4	H	209/214 (98%)	200 (96%)	8 (4%)	1 (0%)	34	71
4	J	210/214 (98%)	195 (93%)	14 (7%)	1 (0%)	34	71
4	L	201/214 (94%)	190 (94%)	10 (5%)	1 (0%)	34	71
All	All	2736/2832 (97%)	2585 (94%)	142 (5%)	9 (0%)	46	79

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	12	VAL
4	L	86	VAL
3	G	130	ASP
4	J	86	VAL
4	H	86	VAL
3	K	184	THR
3	I	12	VAL
3	K	13	GLN
3	G	129	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	288/288 (100%)	245 (85%)	43 (15%)	4	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	288/288 (100%)	260 (90%)	28 (10%)	10 30
1	E	289/288 (100%)	249 (86%)	40 (14%)	4 13
2	B	147/151 (97%)	128 (87%)	19 (13%)	5 16
2	D	148/151 (98%)	129 (87%)	19 (13%)	5 16
2	F	150/151 (99%)	136 (91%)	14 (9%)	11 32
3	G	192/197 (98%)	153 (80%)	39 (20%)	1 4
3	I	190/197 (96%)	153 (80%)	37 (20%)	2 5
3	K	173/197 (88%)	139 (80%)	34 (20%)	1 5
4	H	184/187 (98%)	142 (77%)	42 (23%)	1 3
4	J	185/187 (99%)	140 (76%)	45 (24%)	1 2
4	L	179/187 (96%)	139 (78%)	40 (22%)	1 3
All	All	2413/2469 (98%)	2013 (83%)	400 (17%)	3 8

All (400) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	23	THR
1	A	25	LYS
1	A	30	LEU
1	A	32	ARG
1	A	60	GLU
1	A	78	ARG
1	A	80	LEU
1	A	81	SER
1	A	85	SER
1	A	96	LEU
1	A	97	CYS
1	A	125	ASP
1	A	128	THR
1	A	133	THR
1	A	137	ARG
1	A	141	VAL
1	A	142	SER
1	A	150	ASN
1	A	152	VAL
1	A	154	LEU
1	A	155	THR

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Mol	Chain	Res	Type
1	A	156	GLU
1	A	167	SER
1	A	182	VAL
1	A	189	THR
1	A	198	VAL
1	A	201	TYR
1	A	204	VAL
1	A	212	ARG
1	A	213	SER
1	A	217	ILE
1	A	219	THR
1	A	223	VAL
1	A	238	ASP
1	A	263	ARG
1	A	264	SER
1	A	265	SER
1	A	273	THR
1	A	277	CYS
1	A	320	LEU
1	A	325	GLN
1	A	326	ILE
2	B	18	VAL
2	B	19	ASP
2	B	22	TYR
2	B	30	GLN
2	B	32	SER
2	B	58	LYS
2	B	60	ASN
2	B	66	VAL
2	B	73	LEU
2	B	105	GLU
2	B	116	LYS
2	B	121	LYS
2	B	127[A]	ARG
2	B	127[B]	ARG
2	B	131	LYS
2	B	148	CYS
2	B	154	ASN
2	B	167	LYS
2	B	172	GLU
1	C	25	LYS
1	C	31	GLU

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Mol	Chain	Res	Type
1	C	45	LYS
1	C	78	ARG
1	C	97	CYS
1	C	114	SER
1	C	120	ILE
1	C	121	LEU
1	C	123	LYS
1	C	128	THR
1	C	137	ARG
1	C	139	CYS
1	C	147	PHE
1	C	157	LYS
1	C	160	ASN
1	C	163	VAL
1	C	182	VAL
1	C	192	ARG
1	C	214	THR
1	C	217	ILE
1	C	247	SER
1	C	256	TYR
1	C	264	SER
1	C	274	LEU
1	C	283	THR
1	C	307[A]	LYS
1	C	312	GLU
1	C	320	LEU
2	D	27	SER
2	D	29	ASP
2	D	52	VAL
2	D	61	THR
2	D	71	SER
2	D	73	LEU
2	D	86	ASP
2	D	113	SER
2	D	116	LYS
2	D	127[A]	ARG
2	D	127[B]	ARG
2	D	128	ASP
2	D	129	ASN
2	D	130	VAL
2	D	144	CYS
2	D	147	GLU

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Mol	Chain	Res	Type
2	D	158	ASP
2	D	164	GLU
2	D	167	LYS
1	E	23	THR
1	E	24	GLU
1	E	25	LYS
1	E	30	LEU
1	E	33	ASN
1	E	65	SER
1	E	76	CYS
1	E	78	ARG
1	E	79	LEU
1	E	80	LEU
1	E	81(A)	VAL
1	E	88	MET
1	E	102	PHE
1	E	116(B)	PHE
1	E	119	LYS
1	E	120	ILE
1	E	128	THR
1	E	131	THR
1	E	136	SER
1	E	141	VAL
1	E	142	SER
1	E	146	SER
1	E	152	VAL
1	E	155	THR
1	E	156	GLU
1	E	157	LYS
1	E	182	VAL
1	E	189	THR
1	E	197	ASN
1	E	202	VAL
1	E	204	VAL
1	E	210	ASN
1	E	213	SER
1	E	238	ASP
1	E	256	TYR
1	E	261	SER
1	E	277	CYS
1	E	305	CYS
1	E	307[A]	LYS

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Mol	Chain	Res	Type
1	E	320	LEU
2	F	18	VAL
2	F	22	TYR
2	F	27	SER
2	F	38	LYS
2	F	59	MET
2	F	64	GLU
2	F	72	ASN
2	F	82	LYS
2	F	86	ASP
2	F	121	LYS
2	F	143	LYS
2	F	145	ASP
2	F	148	CYS
2	F	164	GLU
3	G	5	VAL
3	G	6	GLU
3	G	13	GLN
3	G	20	LEU
3	G	22	CYS
3	G	25	SER
3	G	52(B)[A]	ARG
3	G	52(B)[B]	ARG
3	G	56	THR
3	G	71	ARG
3	G	83	ARG
3	G	89	THR
3	G	94	ARG
3	G	107	THR
3	G	109	VAL
3	G	111	VAL
3	G	113	SER
3	G	131	THR
3	G	137	THR
3	G	138	LEU
3	G	140	CYS
3	G	151	THR
3	G	153	THR
3	G	160	SER
3	G	170	LEU
3	G	172	SER
3	G	174	LEU

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Mol	Chain	Res	Type
3	G	177	LEU
3	G	181	VAL
3	G	182	THR
3	G	183	VAL
3	G	187	THR
3	G	193	ILE
3	G	194	THR
3	G	195	CYS
3	G	196	ASN
3	G	202	SER
3	G	206	VAL
3	G	209	LYS
4	H	3	ASP
4	H	16	SER
4	H	17	LEU
4	H	24	THR
4	H	26	LEU
4	H	29	GLN
4	H	30	THR
4	H	49	LEU
4	H	58	ASP
4	H	67	SER
4	H	74	SER
4	H	79	SER
4	H	81	GLN
4	H	86	VAL
4	H	92	GLN
4	H	95	SER
4	H	106	LEU
4	H	112	ASP
4	H	117	VAL
4	H	119	ILE
4	H	123	SER
4	H	127	LEU
4	H	128	THR
4	H	134	VAL
4	H	136	CYS
4	H	144	LYS
4	H	149	LYS
4	H	156	GLU
4	H	157	ARG
4	H	164	SER

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Mol	Chain	Res	Type
4	H	168	GLN
4	H	170	SER
4	H	172	ASP
4	H	173	SER
4	H	178	SER
4	H	183	LEU
4	H	199	THR
4	H	201	LYS
4	H	202	THR
4	H	204	THR
4	H	205	SER
4	H	213	ARG
3	I	11	LEU
3	I	19	ARG
3	I	21	SER
3	I	22	CYS
3	I	24	THR
3	I	28	THR
3	I	34	MET
3	I	50	PHE
3	I	52(B)	ARG
3	I	68	THR
3	I	74	SER
3	I	75	GLN
3	I	76	SER
3	I	82(C)	LEU
3	I	85	GLU
3	I	87	SER
3	I	96	LYS
3	I	100(C)	MET
3	I	109	VAL
3	I	112	SER
3	I	128	CYS
3	I	130	ASP
3	I	132	THR
3	I	142	VAL
3	I	155	ASN
3	I	156	SER
3	I	158	SER
3	I	159	LEU
3	I	163	VAL
3	I	171	GLN

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Mol	Chain	Res	Type
3	I	176	THR
3	I	178	SER
3	I	180	SER
3	I	181	VAL
3	I	183	VAL
3	I	186	SER
3	I	187	THR
4	J	4	ILE
4	J	14	SER
4	J	24	THR
4	J	25	CYS
4	J	28	SER
4	J	39	GLN
4	J	49	LEU
4	J	50	ILE
4	J	56	LEU
4	J	60	VAL
4	J	62	SER
4	J	63	ARG
4	J	65	SER
4	J	69	SER
4	J	71	THR
4	J	74	SER
4	J	75	PHE
4	J	76	LYS
4	J	80	LEU
4	J	81	GLN
4	J	86	VAL
4	J	87	SER
4	J	96	THR
4	J	105	ARG
4	J	107	GLU
4	J	108	ILE
4	J	116	THR
4	J	119	ILE
4	J	128	THR
4	J	155	SER
4	J	156	GLU
4	J	157	ARG
4	J	162	LEU
4	J	166	THR
4	J	170	SER

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Mol	Chain	Res	Type
4	J	171	LYS
4	J	177	MET
4	J	182	THR
4	J	186	ASP
4	J	195	THR
4	J	199	THR
4	J	202	THR
4	J	204	THR
4	J	208	VAL
4	J	214	ASN
3	K	3	LYS
3	K	6	GLU
3	K	7	SER
3	K	24	THR
3	K	30	THR
3	K	58	GLU
3	K	64	LYS
3	K	68	THR
3	K	76	SER
3	K	96	LYS
3	K	108	SER
3	K	110	ILE
3	K	111	VAL
3	K	113	SER
3	K	114	THR
3	K	156	SER
3	K	159	LEU
3	K	163	VAL
3	K	165	THR
3	K	173	ASP
3	K	174	LEU
3	K	175	TYR
3	K	177	LEU
3	K	178	SER
3	K	180	SER
3	K	181	VAL
3	K	188	TRP
3	K	190	SER
3	K	192	SER
3	K	193	ILE
3	K	194	THR
3	K	204	THR

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Mol	Chain	Res	Type
3	K	207	ASP
3	K	208	LYS
4	L	7	THR
4	L	9	SER
4	L	16	SER
4	L	17	LEU
4	L	20	SER
4	L	21	VAL
4	L	24	THR
4	L	25	CYS
4	L	26	LEU
4	L	30	THR
4	L	45	SER
4	L	65	SER
4	L	67	SER
4	L	74	SER
4	L	79	SER
4	L	81	GLN
4	L	92	GLN
4	L	95	SER
4	L	96	THR
4	L	99	THR
4	L	110	ARG
4	L	112	ASP
4	L	117	VAL
4	L	124	SER
4	L	134	VAL
4	L	136	CYS
4	L	146	ILE
4	L	159	ASN
4	L	162	LEU
4	L	167	ASP
4	L	169	ASP
4	L	170	SER
4	L	171	LYS
4	L	177	MET
4	L	182	THR
4	L	183	LEU
4	L	184	THR
4	L	199	THR
4	L	208	VAL
4	L	214	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	129	ASN
3	G	39	GLN
3	G	155	ASN
4	H	40	GLN
4	H	212	ASN
3	I	191	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

14 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	A	402	1,6	14,14,15	0.51	0	15,19,21	1.04	0
6	NAG	A	403	6	14,14,15	0.55	0	15,19,21	1.27	3 (20%)
6	BMA	A	404	6	11,11,12	0.65	0	14,15,17	0.64	0
8	NAG	C	401	1,8	14,14,15	0.49	0	15,19,21	1.24	1 (6%)
8	NAG	C	402	8	14,14,15	0.48	0	15,19,21	0.91	0
8	BMA	C	403	8	11,11,12	0.56	0	14,15,17	1.23	2 (14%)
8	MAN	C	404	8	11,11,12	0.53	0	14,15,17	0.65	0
9	NAG	C	405	1,9	14,14,15	0.43	0	15,19,21	0.79	0
9	NAG	C	406	9	14,14,15	0.42	0	15,19,21	0.74	0
6	NAG	E	403	1,6	14,14,15	0.46	0	15,19,21	1.58	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	E	404	6	14,14,15	0.48	0	15,19,21	1.27	2 (13%)
6	BMA	E	405	6	11,11,12	0.53	0	14,15,17	0.89	0
9	NAG	E	406	9,1	14,14,15	0.52	0	15,19,21	0.80	0
9	NAG	E	407	9	14,14,15	0.44	0	15,19,21	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	402	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	403	6	-	0/6/23/26	0/1/1/1
6	BMA	A	404	6	-	0/2/19/22	0/1/1/1
8	NAG	C	401	1,8	-	0/6/23/26	0/1/1/1
8	NAG	C	402	8	-	0/6/23/26	0/1/1/1
8	BMA	C	403	8	-	0/2/19/22	0/1/1/1
8	MAN	C	404	8	-	0/2/19/22	0/1/1/1
9	NAG	C	405	1,9	-	0/6/23/26	0/1/1/1
9	NAG	C	406	9	-	0/6/23/26	0/1/1/1
6	NAG	E	403	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	404	6	-	0/6/23/26	0/1/1/1
6	BMA	E	405	6	-	0/2/19/22	0/1/1/1
9	NAG	E	406	9,1	-	0/6/23/26	0/1/1/1
9	NAG	E	407	9	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	401	NAG	C2-N2-C7	-4.23	117.61	123.04
6	E	404	NAG	C4-C3-C2	-2.61	107.18	111.23
8	C	403	BMA	C1-O5-C5	-2.57	108.99	112.25
6	A	403	NAG	O7-C7-C8	-2.16	118.09	122.06
6	A	403	NAG	O7-C7-N2	2.07	126.09	121.86
8	C	403	BMA	O5-C5-C6	2.18	112.07	107.35
6	E	403	NAG	C2-N2-C7	2.22	125.89	123.04
6	E	404	NAG	C1-O5-C5	2.50	115.42	112.25
6	A	403	NAG	C2-N2-C7	3.13	127.06	123.04
6	E	403	NAG	C1-O5-C5	4.26	117.65	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

13 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	$\#\|Z\| > 2$
5	NAG	A	401	1	14,14,15	0.48	0	15,19,21	1.11	1 (6%)
5	NAG	A	405	1	14,14,15	0.57	0	15,19,21	1.06	1 (6%)
7	SO4	B	201	-	4,4,4	0.34	0	6,6,6	0.36	0
5	NAG	B	202	2	14,14,15	0.73	0	15,19,21	1.27	2 (13%)
7	SO4	D	201	-	4,4,4	0.24	0	6,6,6	0.22	0
5	NAG	E	401	1	14,14,15	0.38	0	15,19,21	1.37	2 (13%)
7	SO4	E	402	-	4,4,4	0.18	0	6,6,6	0.14	0
7	SO4	F	201	-	4,4,4	0.26	0	6,6,6	0.25	0
5	NAG	F	202	2	14,14,15	0.54	0	15,19,21	0.90	1 (6%)
7	SO4	H	301	-	4,4,4	0.17	0	6,6,6	0.13	0
7	SO4	J	301	-	4,4,4	0.10	0	6,6,6	0.13	0
10	EDO	J	302	-	3,3,3	0.60	0	2,2,2	0.24	0
7	SO4	L	301	-	4,4,4	0.24	0	6,6,6	0.29	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
5	NAG	A	401	1	-	0/6/23/26	0/1/1/1
5	NAG	A	405	1	-	0/6/23/26	0/1/1/1
7	SO4	B	201	-	-	0/0/0/0	0/0/0/0
5	NAG	B	202	2	-	0/6/23/26	0/1/1/1
7	SO4	D	201	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	401	1	-	0/6/23/26	0/1/1/1
7	SO4	E	402	-	-	0/0/0/0	0/0/0/0
7	SO4	F	201	-	-	0/0/0/0	0/0/0/0
5	NAG	F	202	2	-	0/6/23/26	0/1/1/1
7	SO4	H	301	-	-	0/0/0/0	0/0/0/0
7	SO4	J	301	-	-	0/0/0/0	0/0/0/0
10	EDO	J	302	-	-	0/1/1/1	0/0/0/0
7	SO4	L	301	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	401	NAG	C2-N2-C7	-2.79	119.45	123.04
5	F	202	NAG	C2-N2-C7	-2.62	119.67	123.04
5	B	202	NAG	C1-O5-C5	2.63	115.58	112.25
5	B	202	NAG	C2-N2-C7	2.86	126.72	123.04
5	A	405	NAG	C1-O5-C5	3.13	116.22	112.25
5	A	401	NAG	C1-O5-C5	3.77	117.04	112.25
5	E	401	NAG	C1-O5-C5	4.04	117.37	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	201	SO4	1	0
7	F	201	SO4	3	0
7	J	301	SO4	1	0
10	J	302	EDO	1	0
7	L	301	SO4	1	0

5.7 Other polymers (i)

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	324/327 (99%)	0.07	16 (4%) 33 27	44, 95, 147, 177	2 (0%)
1	C	324/327 (99%)	0.05	11 (3%) 49 41	49, 100, 147, 169	2 (0%)
1	E	324/327 (99%)	0.20	17 (5%) 31 24	49, 105, 153, 223	2 (0%)
2	B	168/174 (96%)	0.05	1 (0%) 90 89	45, 67, 108, 138	0
2	D	170/174 (97%)	0.12	3 (1%) 71 68	44, 79, 145, 169	0
2	F	172/174 (98%)	0.11	1 (0%) 90 89	44, 82, 126, 176	0
3	G	223/229 (97%)	0.30	17 (7%) 17 11	30, 100, 151, 246	0
3	I	221/229 (96%)	0.25	10 (4%) 37 31	45, 95, 166, 190	0
3	K	200/229 (87%)	0.48	18 (9%) 12 7	32, 89, 195, 245	0
4	H	211/214 (98%)	0.45	16 (7%) 17 11	42, 108, 155, 185	0
4	J	212/214 (99%)	0.15	6 (2%) 56 50	49, 122, 158, 213	0
4	L	205/214 (95%)	0.75	35 (17%) 2 1	46, 120, 185, 268	0
All	All	2754/2832 (97%)	0.24	151 (5%) 29 22	30, 97, 158, 268	6 (0%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	189	PRO	13.6
4	L	194	TYR	7.6
4	L	121	PRO	6.6
4	L	117	VAL	6.1
3	K	188	TRP	5.5
4	H	208	VAL	5.4
1	E	198	VAL	5.4
3	K	187	THR	5.4
4	L	119	ILE	5.3
3	K	152	LEU	5.2
3	K	192	SER	5.1

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Mol	Chain	Res	Type	RSRZ
3	G	133	GLY	4.8
4	L	120	PHE	4.7
3	K	156	SER	4.6
3	K	197	VAL	4.5
3	K	190	SER	4.4
4	H	207	ILE	4.4
4	L	129	SER	4.4
4	H	203	SER	4.4
1	E	157	LYS	4.3
2	B	1	GLY	4.2
4	H	137	PHE	4.1
4	L	182	THR	4.1
3	I	211	GLU	4.1
3	I	189	PRO	4.0
4	L	183	LEU	4.0
1	E	160	ASN	4.0
4	L	118	SER	4.0
3	K	122	TYR	4.0
1	A	163	VAL	3.8
1	E	155	THR	3.8
4	H	194	TYR	3.8
3	I	138	LEU	3.8
4	L	214	ASN	3.8
2	D	61	THR	3.8
4	L	137	PHE	3.7
4	L	198	ALA	3.6
3	I	191	GLN	3.6
4	H	206	PRO	3.5
3	K	191	GLN	3.5
2	D	168	LEU	3.4
1	A	143	GLY	3.4
4	L	85	PHE	3.4
4	L	195	THR	3.4
3	G	170	LEU	3.4
1	E	158	GLY	3.3
4	H	129	SER	3.3
4	L	151	LYS	3.2
1	A	132	THR	3.2
4	L	186	ASP	3.2
1	A	144	ASN	3.2
4	L	190	ARG	3.1
1	C	222	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
4	L	128	THR	3.1
4	L	122	PRO	3.1
1	E	194	LEU	3.1
3	I	136	VAL	3.1
4	H	138	LEU	3.1
1	A	154	LEU	3.1
1	E	195	TYR	3.1
4	H	148	VAL	3.1
4	L	196	CYS	3.1
4	L	3	ASP	3.1
4	H	183	LEU	3.1
1	E	128	THR	3.0
4	H	119	ILE	3.0
1	A	131	THR	3.0
3	K	154	TRP	3.0
1	C	245	PHE	3.0
4	L	192	ASN	3.0
1	E	156	GLU	2.9
1	C	143	GLY	2.9
3	G	127	VAL	2.9
4	L	187	GLU	2.9
3	G	210	ILE	2.9
1	A	128	THR	2.9
4	L	189	GLU	2.9
3	K	116	THR	2.9
3	G	188	TRP	2.8
1	A	279	THR	2.8
3	G	134	SER	2.8
3	K	141	LEU	2.7
3	G	10	GLY	2.7
4	L	184	THR	2.7
3	G	190	SER	2.7
1	E	245	PHE	2.7
3	K	183	VAL	2.7
3	G	113	SER	2.6
4	L	106	LEU	2.6
1	A	133	THR	2.6
1	A	157	LYS	2.6
3	G	132	THR	2.6
1	C	147	PHE	2.6
3	I	209	LYS	2.6
3	G	195	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
4	H	204	THR	2.6
3	I	160	SER	2.6
4	L	193	SER	2.6
3	K	140	CYS	2.5
1	A	182	VAL	2.5
1	E	225	GLY	2.5
1	E	159	SER	2.5
3	I	132	THR	2.5
4	L	80	LEU	2.5
4	H	117	VAL	2.5
4	J	5	GLN	2.5
4	L	108	ILE	2.5
3	G	124	LEU	2.4
4	L	163	ASN	2.4
4	L	5	GLN	2.4
1	C	216	GLU	2.4
3	K	144	GLY	2.4
1	E	224	ASN	2.4
1	C	166	GLY	2.4
4	H	115	PRO	2.4
3	K	119	PRO	2.3
4	H	105	ARG	2.3
4	J	105	ARG	2.3
3	G	211	GLU	2.3
1	E	193	THR	2.3
4	L	105	ARG	2.3
1	A	129	GLN	2.3
1	C	142	SER	2.3
4	H	198	ALA	2.3
1	E	166	GLY	2.3
4	J	23	ILE	2.3
1	A	248	THR	2.3
1	C	220	ARG	2.2
3	I	12	VAL	2.2
3	K	176	THR	2.2
4	J	207	ILE	2.2
1	C	217	ILE	2.2
3	I	210	ILE	2.2
1	A	153	TRP	2.2
3	G	202	SER	2.2
1	E	192	ARG	2.2
2	F	63	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
4	L	77	ILE	2.2
4	J	153	ASP	2.1
3	G	128	CYS	2.1
4	L	211	PHE	2.1
1	A	156	GLU	2.1
3	G	129	GLY	2.1
4	L	212	ASN	2.1
1	E	163	VAL	2.1
3	G	189	PRO	2.1
2	D	1	GLY	2.0
4	J	171	LYS	2.0
1	C	325	GLN	2.0
1	A	223	VAL	2.0
1	C	144	ASN	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	A	403	14/15	0.87	0.28	2.25	97,113,135,138	0
8	NAG	C	401	14/15	0.89	0.26	1.39	94,109,131,134	0
9	NAG	C	405	14/15	0.86	0.17	-	134,152,166,178	0
8	BMA	C	403	11/12	0.87	0.30	-	103,119,135,148	0
6	NAG	A	402	14/15	0.86	0.16	-	90,122,136,143	0
6	NAG	E	404	14/15	0.88	0.25	-	89,125,140,155	0
6	NAG	E	403	14/15	0.89	0.30	-	78,117,137,139	0
9	NAG	E	407	14/15	0.78	0.35	-	143,165,173,175	0
9	NAG	C	406	14/15	0.75	0.32	-	135,182,189,192	0
8	NAG	C	402	14/15	0.92	0.38	-	82,112,130,131	0
9	NAG	E	406	14/15	0.93	0.16	-	108,135,153,164	0
6	BMA	A	404	11/12	0.80	0.32	-	105,121,129,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	MAN	C	404	11/12	0.86	0.28	-	145,159,166,169	0
6	BMA	E	405	11/12	0.70	0.33	-	143,165,176,185	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	SO4	H	301	5/5	0.95	0.24	2.59	84,88,102,104	0
7	SO4	D	201	5/5	0.96	0.22	1.73	80,90,96,101	0
7	SO4	F	201	5/5	0.96	0.26	1.34	84,89,95,99	0
7	SO4	B	201	5/5	0.99	0.21	0.55	54,69,74,74	0
5	NAG	F	202	14/15	0.86	0.17	0.17	100,114,121,125	0
5	NAG	B	202	14/15	0.85	0.15	-0.44	103,114,125,125	0
7	SO4	J	301	5/5	0.92	0.17	-0.73	110,123,135,151	0
7	SO4	L	301	5/5	0.92	0.16	-1.65	89,106,111,123	0
5	NAG	A	401	14/15	0.86	0.19	-	129,142,146,150	0
7	SO4	E	402	5/5	0.88	0.16	-	107,124,128,130	0
10	EDO	J	302	4/4	0.89	0.08	-	72,74,76,81	0
5	NAG	A	405	14/15	0.88	0.32	-	113,129,153,159	0
5	NAG	E	401	14/15	0.89	0.20	-	92,106,121,124	0

6.5 Other polymers (i)

There are no such residues in this entry.