Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 05:15 PM EDT

PDB ID	:	2I9L
Title	:	Structure of Fab 7D11 from a neutralizing antibody against the poxvirus L1 protein
Authors	:	Su, H.P.; Golden, J.W.; Gittis, A.G.; Moss, B.; Hooper, J.W.; Garboczi, D.N.
Deposited on	:	2006-09-05
Resolution	:	3.10 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

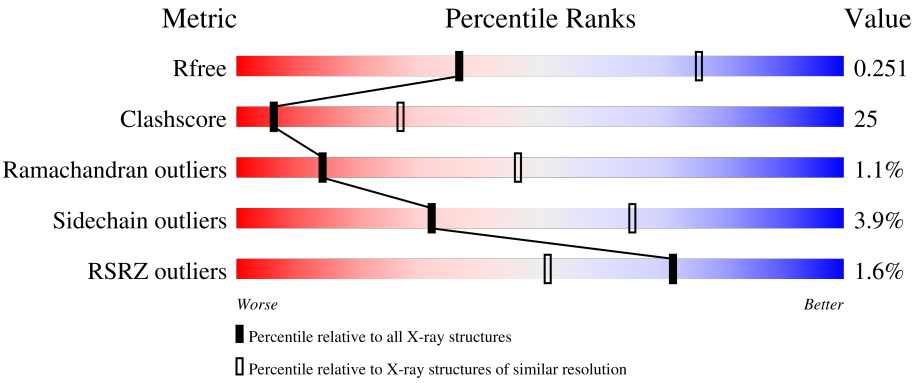
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	219	60% 37%
1	C	219	59% 38%
1	E	219	63% 35%
1	G	219	57% 41%
2	B	219	63% 34%

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Mol	Chain	Length	Quality of chain
2	D	219	63% 33% 5%
2	F	219	3% 63% 35%
2	H	219	59% 38%
3	I	184	56% 36% 6%
3	J	184	56% 36% 6%
3	K	184	3% 55% 37% 6%
3	L	184	56% 36% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	220	-	-	X	X
4	GOL	E	222	-	-	X	-
4	GOL	J	186	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18674 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 Antibody 7D11 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1696	1056	286	345	9			
1	C	219	Total	C	N	O	S	0	0	0
			1696	1056	286	345	9			
1	E	219	Total	C	N	O	S	0	0	0
			1696	1056	286	345	9			
1	G	219	Total	C	N	O	S	0	0	0
			1696	1056	286	345	9			

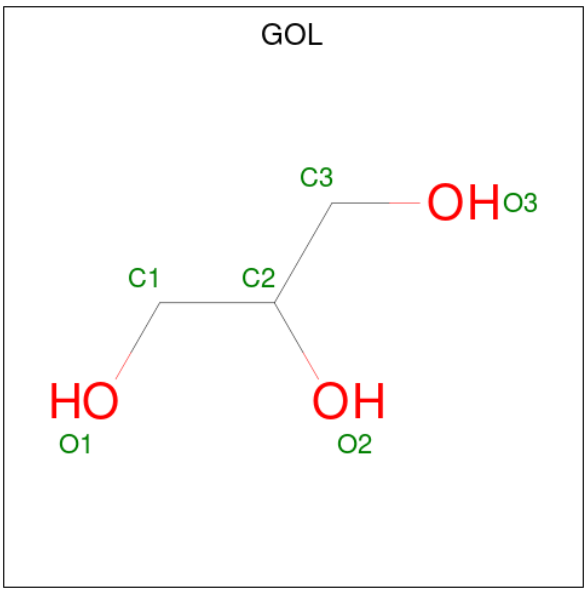
- Molecule 2 is a protein called Antibody 7D11 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	0
			1665	1056	272	329	8			
2	D	219	Total	C	N	O	S	0	0	0
			1665	1056	272	329	8			
2	F	219	Total	C	N	O	S	0	0	0
			1665	1056	272	329	8			
2	H	219	Total	C	N	O	S	0	0	0
			1665	1056	272	329	8			

- Molecule 3 is a protein called Virion membrane protein M25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	173	Total	C	N	O	S	0	0	0
			1292	795	220	268	9			
3	J	173	Total	C	N	O	S	0	0	0
			1292	795	220	268	9			
3	K	173	Total	C	N	O	S	0	0	0
			1292	795	220	268	9			
3	L	173	Total	C	N	O	S	0	0	0
			1292	795	220	268	9			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	J	1	Total C O 6 3 3	0	0
4	K	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0
5	C	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0

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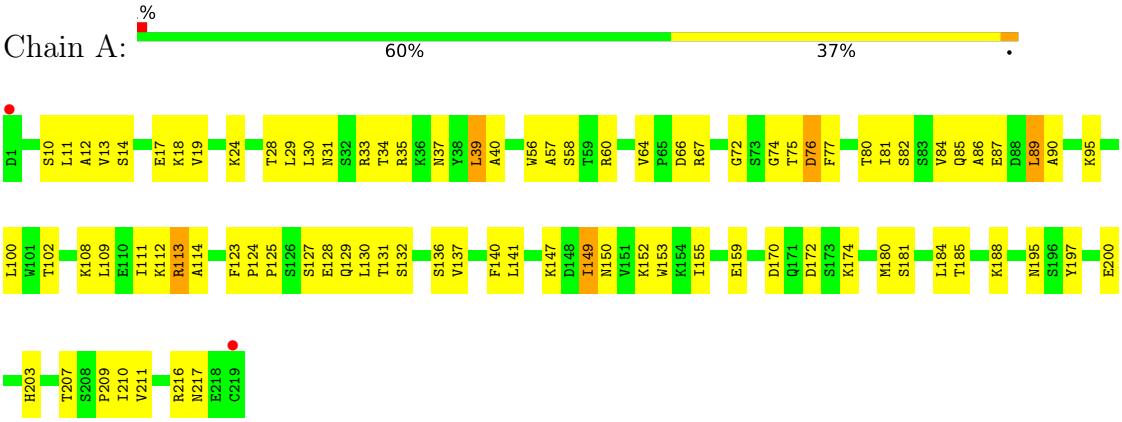
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total O 1 1	0	0
5	F	4	Total O 4 4	0	0
5	G	1	Total O 1 1	0	0
5	H	2	Total O 2 2	0	0
5	I	1	Total O 1 1	0	0
5	J	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

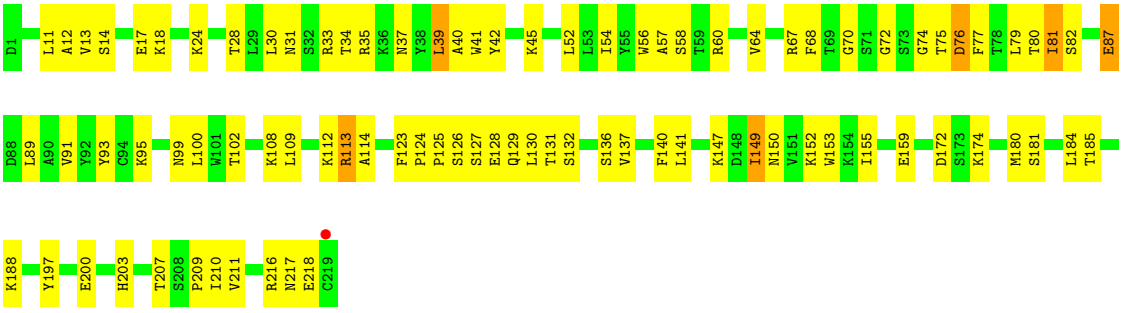
• Molecule 1: Antibody 7D11 light chain

Chain A:



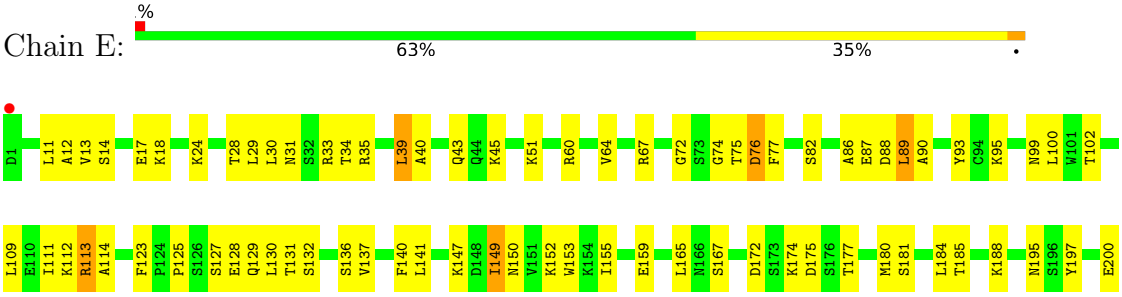
• Molecule 1: Antibody 7D11 light chain

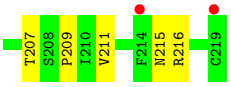
Chain C:



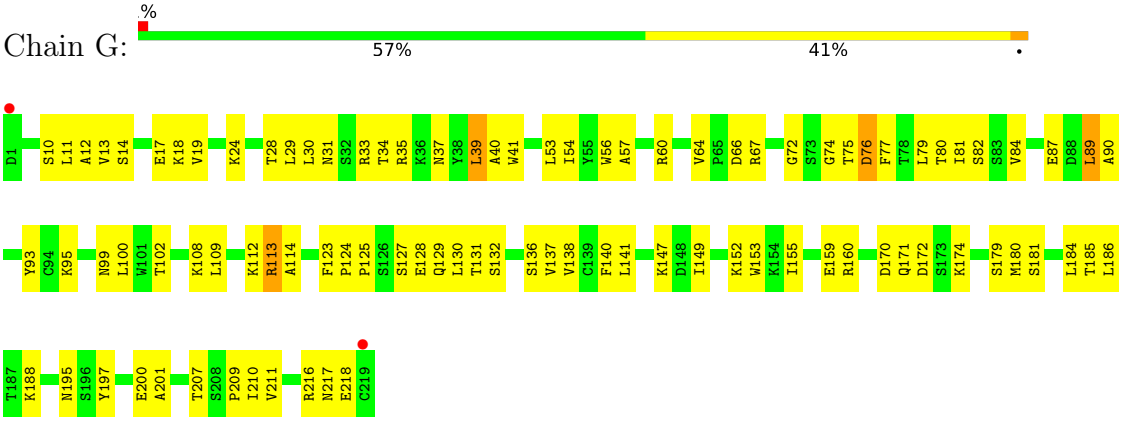
• Molecule 1: Antibody 7D11 light chain

Chain E:

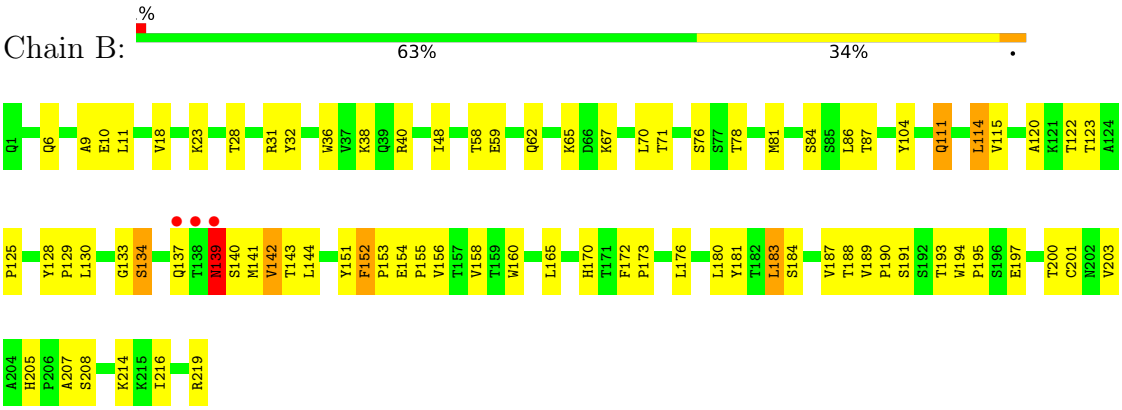




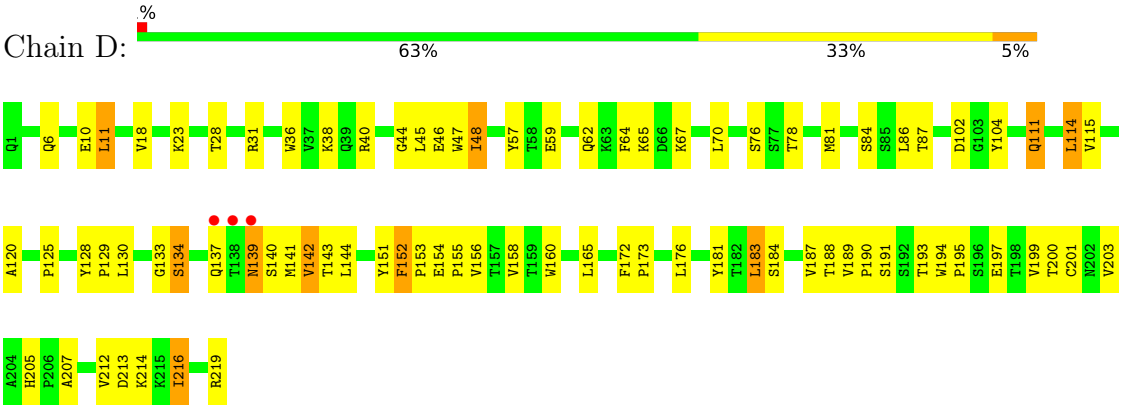
• Molecule 1: Antibody 7D11 light chain



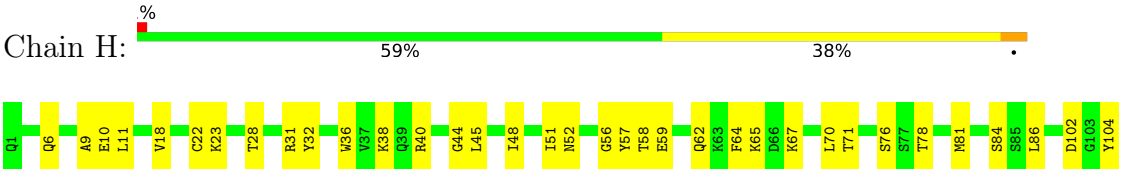
• Molecule 2: Antibody 7D11 heavy chain

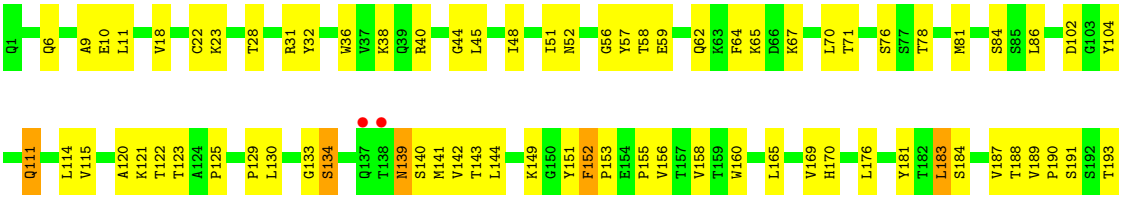


• Molecule 2: Antibody 7D11 heavy chain



• Molecule 2: Antibody 7D11 heavy chain



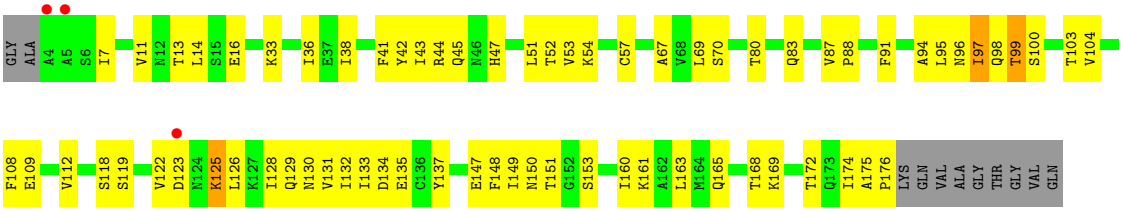


• Molecule 2: Antibody 7D11 heavy chain

Chain H:

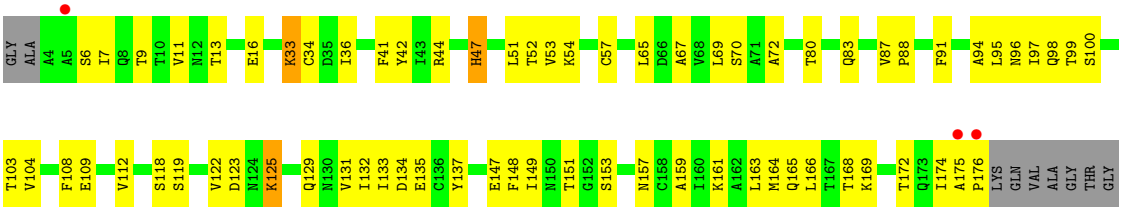
• Molecule 3: Virion membrane protein M25

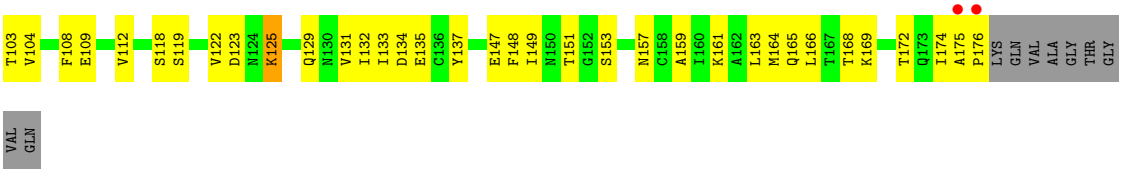
Chain I:



• Molecule 3: Virion membrane protein M25

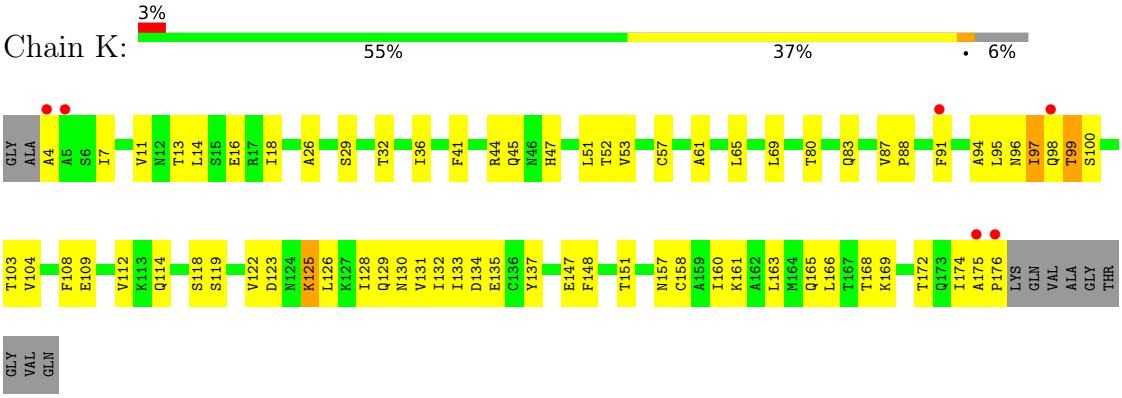
Chain J:





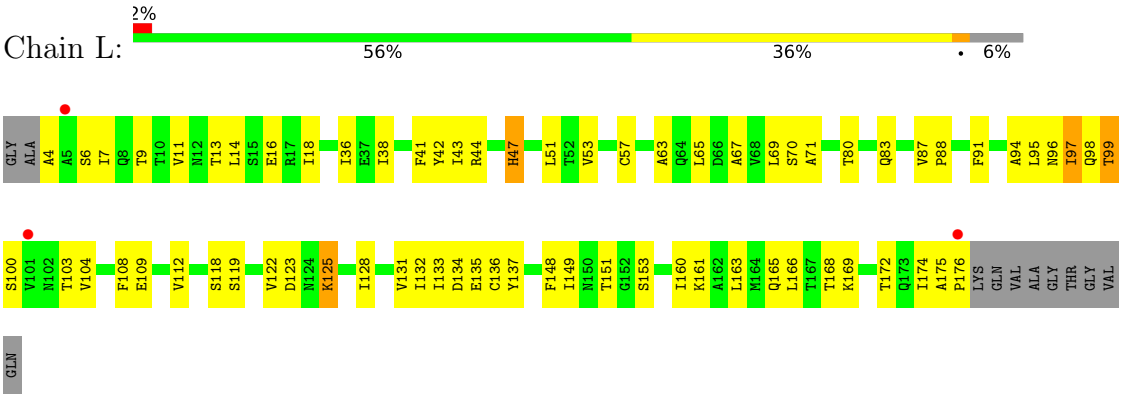
• Molecule 3: Virion membrane protein M25

Chain K:



• Molecule 3: Virion membrane protein M25

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	218.77Å 85.56Å 211.84Å 90.00° 119.60° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 46.05 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-3.10) 98.1 (46.05-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.259 0.233 , 0.251	Depositor DCC
R_{free} test set	3111 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	48.0	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	18674	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: GOL

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	0.42	0/1733	0.65	0/2348
1	C	0.42	0/1733	0.65	0/2348
1	E	0.43	0/1733	0.65	0/2348
1	G	0.44	0/1733	0.65	0/2348
2	B	0.52	1/1710 (0.1%)	0.71	0/2337
2	D	0.52	0/1710	0.72	0/2337
2	F	0.53	0/1710	0.70	0/2337
2	H	0.52	0/1710	0.71	0/2337
3	I	0.47	0/1306	0.69	0/1775
3	J	0.44	0/1306	0.69	0/1775
3	K	0.48	0/1306	0.68	0/1775
3	L	0.45	0/1306	0.69	0/1775
All	All	0.47	1/18996 (0.0%)	0.68	0/25840

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	H	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	139	ASN	CG-OD1	5.59	1.36	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	149	LYS	Mainchain

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	1696	0	1638	75	0
1	C	1696	0	1638	76	0
1	E	1696	0	1638	67	0
1	G	1696	0	1638	81	0
2	B	1665	0	1620	79	0
2	D	1665	0	1620	82	0
2	F	1665	0	1620	81	0
2	H	1665	0	1622	100	0
3	I	1292	0	1276	93	0
3	J	1292	0	1276	73	0
3	K	1292	0	1276	84	0
3	L	1292	0	1276	75	0
4	A	6	0	8	5	0
4	E	18	0	24	7	0
4	I	6	0	8	2	0
4	J	6	0	8	4	0
4	K	6	0	8	3	0
4	L	6	0	8	0	0
5	A	2	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	4	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
5	I	1	0	0	1	0
5	J	1	0	0	0	0
All	All	18674	0	18202	908	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 25.

All (908) 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:91:PHE:CE2	3:I:97:ILE:HB	1.16	1.60
3:I:91:PHE:HE2	3:I:97:ILE:CB	1.16	1.57
3:I:91:PHE:CE2	3:I:97:ILE:CB	1.83	1.50
3:I:91:PHE:CE2	3:I:97:ILE:CG2	2.06	1.38
3:I:91:PHE:HE2	3:I:97:ILE:CG2	1.38	1.33
1:C:100:LEU:HD21	2:D:59:GLU:OE2	1.28	1.31
3:K:91:PHE:CE2	3:K:104:VAL:HG13	1.80	1.16
2:F:140:SER:O	2:F:141:MET:HG2	1.43	1.15
3:I:38:ILE:HD11	3:I:150:ASN:HB2	1.16	1.14
3:K:14:LEU:HD21	3:K:163:LEU:HD21	1.30	1.13
3:I:43:ILE:HD12	3:I:133:ILE:HB	1.25	1.09
2:H:199:VAL:O	2:H:216:ILE:HD13	1.53	1.08
1:G:100:LEU:HD21	2:H:59:GLU:OE2	1.51	1.08
3:L:14:LEU:HD21	3:L:163:LEU:HD21	1.36	1.08
3:I:14:LEU:HD21	3:I:163:LEU:HD21	1.34	1.08
2:D:199:VAL:O	2:D:216:ILE:HD13	1.54	1.06
1:E:100:LEU:HD21	2:F:59:GLU:OE2	1.57	1.04
1:E:43:GLN:HE22	4:E:222:GOL:H31	1.18	1.04
1:A:100:LEU:HD21	2:B:59:GLU:OE2	1.57	1.03
3:L:91:PHE:CE2	3:L:104:VAL:HG13	1.93	1.02
3:J:91:PHE:CE2	3:J:104:VAL:HG13	1.97	0.99
3:I:91:PHE:CZ	3:I:97:ILE:HG21	1.97	0.99
2:F:140:SER:O	2:F:141:MET:CG	2.12	0.98
2:H:51:ILE:HD13	2:H:58:THR:HG23	1.45	0.97
3:K:87:VAL:CG1	3:K:91:PHE:CZ	2.47	0.97
2:H:51:ILE:HD13	2:H:58:THR:CG2	1.95	0.97
3:I:118:SER:HB3	5:I:187:HOH:O	1.61	0.97
3:K:91:PHE:CE2	3:K:104:VAL:CG1	2.48	0.96
3:I:38:ILE:HD11	3:I:150:ASN:CB	1.94	0.96
3:J:44:ARG:NE	3:L:44:ARG:HH21	1.64	0.96
3:I:91:PHE:CZ	3:I:97:ILE:HB	2.00	0.96
2:B:141:MET:HG2	2:B:142:VAL:H	1.28	0.96
3:I:91:PHE:CE2	3:I:97:ILE:HG22	2.01	0.96
3:K:87:VAL:HG12	3:K:91:PHE:CE2	2.01	0.95
2:B:141:MET:SD	2:B:188:THR:HG21	2.07	0.95
3:I:91:PHE:CZ	3:I:97:ILE:CG2	2.49	0.95
3:J:44:ARG:HE	3:L:44:ARG:HH21	1.15	0.94
3:K:87:VAL:HG12	3:K:91:PHE:CZ	2.01	0.94
2:D:23:LYS:HD3	2:D:78:THR:CG2	1.98	0.93
2:D:48:ILE:HD12	2:D:64:PHE:CE2	2.04	0.92
3:L:38:ILE:HD12	3:L:53:VAL:CG1	1.99	0.91
2:H:202:ASN:ND2	2:H:213:ASP:OD2	2.03	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:91:PHE:CZ	3:I:97:ILE:CB	2.53	0.90
3:I:91:PHE:CD2	3:I:97:ILE:HB	2.07	0.89
2:H:22:CYS:O	2:H:78:THR:HG23	1.72	0.89
2:B:141:MET:SD	2:B:188:THR:CG2	2.61	0.89
3:L:38:ILE:HD12	3:L:53:VAL:HG13	1.55	0.87
3:J:44:ARG:HE	3:L:44:ARG:NH2	1.73	0.86
1:C:100:LEU:CD2	2:D:59:GLU:OE2	2.20	0.86
3:K:91:PHE:CZ	3:K:104:VAL:HG13	2.11	0.86
3:J:94:ALA:HB2	3:J:169:LYS:HG3	1.59	0.85
1:A:149:ILE:HD12	1:A:203:HIS:HB2	1.59	0.85
1:E:51:LYS:NZ	4:E:222:GOL:O1	2.09	0.84
2:D:23:LYS:CD	2:D:78:THR:CG2	2.55	0.84
1:G:124:PRO:HD2	2:H:219:ARG:HH12	1.42	0.84
2:D:151:TYR:CE2	2:D:156:VAL:HG11	2.13	0.84
3:I:94:ALA:HB2	3:I:169:LYS:HG3	1.60	0.84
3:I:44:ARG:HG3	3:I:44:ARG:HH11	1.42	0.83
2:B:141:MET:HG2	2:B:142:VAL:N	1.92	0.83
3:K:94:ALA:HB2	3:K:169:LYS:HG3	1.58	0.83
3:L:94:ALA:HB2	3:L:169:LYS:HG3	1.60	0.83
3:K:91:PHE:CZ	3:K:104:VAL:CG1	2.62	0.83
1:C:149:ILE:HD12	1:C:203:HIS:HB2	1.59	0.83
2:D:23:LYS:CD	2:D:78:THR:HG22	2.08	0.83
2:D:11:LEU:HG	2:D:153:PRO:CG	2.09	0.83
3:K:44:ARG:HG3	3:K:44:ARG:HH11	1.43	0.83
3:J:129:GLN:OE1	4:J:186:GOL:H12	1.77	0.83
2:D:11:LEU:HG	2:D:153:PRO:HG3	1.58	0.82
2:H:51:ILE:HD12	2:H:57:TYR:O	1.80	0.82
3:J:133:ILE:HG22	3:J:134:ASP:H	1.44	0.82
2:F:37:VAL:HA	2:F:48:ILE:HD13	1.60	0.82
3:I:91:PHE:CD2	3:I:97:ILE:O	2.33	0.81
3:I:91:PHE:HD2	3:I:97:ILE:O	1.63	0.81
3:K:96:ASN:O	3:K:97:ILE:HG13	1.82	0.80
3:L:44:ARG:HG3	3:L:44:ARG:HH11	1.47	0.80
3:I:38:ILE:CD1	3:I:150:ASN:HB2	2.06	0.79
3:J:159:ALA:O	3:J:163:LEU:HD13	1.83	0.79
1:E:43:GLN:NE2	4:E:222:GOL:H31	1.97	0.79
3:L:91:PHE:CZ	3:L:104:VAL:HG13	2.18	0.79
3:K:133:ILE:HG22	3:K:134:ASP:H	1.47	0.78
1:E:149:ILE:HD13	1:E:150:ASN:N	1.99	0.78
3:J:108:PHE:HZ	3:J:163:LEU:HD12	1.47	0.78
3:I:133:ILE:HG22	3:I:134:ASP:H	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:69:LEU:HD21	3:J:112:VAL:HG21	1.65	0.78
3:J:96:ASN:O	3:J:97:ILE:HG13	1.85	0.77
2:F:38:LYS:N	2:F:48:ILE:HD11	2.00	0.77
1:G:53:LEU:HB3	1:G:54:ILE:HD12	1.66	0.76
3:J:44:ARG:HG3	3:J:44:ARG:HH11	1.48	0.76
2:F:151:TYR:CE2	2:F:156:VAL:HG11	2.21	0.76
3:J:54:LYS:HD3	3:J:149:ILE:HD12	1.66	0.76
2:F:76:SER:OG	2:F:78:THR:HG22	1.86	0.76
3:K:69:LEU:HD21	3:K:112:VAL:HG21	1.68	0.75
2:D:23:LYS:HA	2:D:78:THR:HG22	1.67	0.75
2:B:76:SER:OG	2:B:78:THR:HG22	1.86	0.75
2:D:23:LYS:HD2	2:D:78:THR:HG22	1.67	0.75
3:I:54:LYS:HD3	3:I:149:ILE:HD12	1.69	0.74
3:I:69:LEU:HD21	3:I:112:VAL:HG21	1.68	0.74
3:L:69:LEU:HD21	3:L:112:VAL:HG21	1.69	0.74
3:K:14:LEU:HD21	3:K:163:LEU:CD2	2.15	0.74
3:I:91:PHE:HZ	3:I:97:ILE:HG21	1.52	0.74
3:L:100:SER:O	3:L:104:VAL:HG23	1.88	0.74
1:A:124:PRO:HD2	2:B:219:ARG:HH12	1.50	0.74
2:H:143:THR:HG22	2:H:188:THR:OG1	1.86	0.74
2:F:143:THR:HG22	2:F:188:THR:OG1	1.87	0.74
2:H:165:LEU:HD21	2:H:187:VAL:HG21	1.70	0.74
3:L:133:ILE:HG22	3:L:134:ASP:H	1.51	0.74
2:B:141:MET:CG	2:B:142:VAL:H	2.01	0.73
2:B:125:PRO:HB3	2:B:151:TYR:HB3	1.70	0.73
2:H:67:LYS:HE2	2:H:84:SER:O	1.89	0.73
1:A:170:ASP:O	4:A:220:GOL:H11	1.87	0.73
2:D:67:LYS:HE2	2:D:84:SER:O	1.89	0.73
3:J:91:PHE:CZ	3:J:104:VAL:HG13	2.24	0.73
2:F:67:LYS:HE2	2:F:84:SER:O	1.90	0.72
2:D:143:THR:HG22	2:D:188:THR:OG1	1.89	0.72
2:F:10:GLU:HG2	2:F:18:VAL:HG21	1.71	0.72
2:B:129:PRO:HG3	2:B:214:LYS:HG2	1.72	0.72
2:F:129:PRO:HG3	2:F:214:LYS:HG2	1.71	0.72
3:K:29:SER:HG	3:K:32:THR:HG1	1.30	0.71
3:I:100:SER:O	3:I:104:VAL:HG23	1.90	0.71
3:K:100:SER:O	3:K:104:VAL:HG23	1.89	0.71
1:A:86:ALA:HA	1:A:111:ILE:HD13	1.71	0.71
3:I:43:ILE:CD1	3:I:133:ILE:HB	2.14	0.71
2:B:143:THR:HG22	2:B:188:THR:OG1	1.90	0.71
3:I:38:ILE:HD13	3:I:53:VAL:HG11	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:40:ARG:HG2	2:H:40:ARG:HH11	1.56	0.71
3:I:96:ASN:O	3:I:97:ILE:HG12	1.91	0.70
2:B:153:PRO:HD2	2:B:207:ALA:HB1	1.73	0.70
2:H:153:PRO:HD2	2:H:207:ALA:HB1	1.73	0.70
2:H:151:TYR:CE2	2:H:156:VAL:HG11	2.27	0.70
2:D:129:PRO:HG3	2:D:214:LYS:HG2	1.73	0.70
1:E:86:ALA:HA	1:E:111:ILE:HD13	1.74	0.70
2:F:37:VAL:CA	2:F:48:ILE:HD13	2.22	0.70
3:J:100:SER:O	3:J:104:VAL:HG23	1.90	0.70
2:F:40:ARG:HG2	2:F:40:ARG:HH11	1.57	0.70
1:A:14:SER:HB2	1:A:17:GLU:OE2	1.91	0.69
1:A:149:ILE:HG13	1:A:150:ASN:H	1.57	0.69
2:H:129:PRO:HG3	2:H:214:LYS:HG2	1.72	0.69
3:K:87:VAL:HG11	3:K:91:PHE:CZ	2.28	0.69
1:G:124:PRO:CD	2:H:219:ARG:HH12	2.05	0.69
2:H:125:PRO:HB3	2:H:151:TYR:HB3	1.73	0.69
2:B:67:LYS:HE2	2:B:84:SER:O	1.92	0.69
3:I:14:LEU:HD21	3:I:163:LEU:CD2	2.19	0.69
3:K:91:PHE:HE2	3:K:104:VAL:CG1	2.04	0.69
1:C:149:ILE:HG13	1:C:150:ASN:H	1.58	0.69
3:K:14:LEU:CD2	3:K:163:LEU:HD21	2.17	0.69
1:C:127:SER:O	1:C:131:THR:HG23	1.93	0.68
2:F:153:PRO:HD2	2:F:207:ALA:HB1	1.75	0.68
2:H:51:ILE:HD12	2:H:52:ASN:H	1.58	0.68
1:C:14:SER:HB2	1:C:17:GLU:OE2	1.93	0.68
1:E:127:SER:O	1:E:131:THR:HG23	1.93	0.68
3:I:14:LEU:CD2	3:I:163:LEU:HD21	2.20	0.68
3:L:14:LEU:HD21	3:L:163:LEU:CD2	2.20	0.68
3:L:38:ILE:HD12	3:L:53:VAL:HG11	1.73	0.68
3:L:14:LEU:CD2	3:L:163:LEU:HD21	2.21	0.68
1:A:127:SER:O	1:A:131:THR:HG23	1.94	0.68
2:B:10:GLU:HG2	2:B:18:VAL:HG21	1.75	0.68
2:F:140:SER:C	2:F:141:MET:HG2	2.13	0.68
2:F:165:LEU:HD21	2:F:187:VAL:HG21	1.75	0.68
1:E:14:SER:HB2	1:E:17:GLU:OE2	1.93	0.68
3:L:18:ILE:HD13	3:L:71:ALA:HB3	1.75	0.68
2:D:23:LYS:HD3	2:D:78:THR:HG21	1.76	0.67
2:D:10:GLU:HG2	2:D:18:VAL:HG21	1.75	0.67
2:D:40:ARG:HH11	2:D:40:ARG:HG2	1.60	0.67
3:K:129:GLN:OE1	4:K:186:GOL:H12	1.94	0.67
2:F:58:THR:H	3:K:125:LYS:HD2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:PRO:HD2	2:D:219:ARG:HH12	1.59	0.67
3:I:174:ILE:HG13	3:I:175:ALA:N	2.10	0.67
3:J:157:ASN:HB2	4:J:186:GOL:H11	1.77	0.67
1:A:172:ASP:HB2	4:A:220:GOL:H2	1.77	0.66
1:G:127:SER:O	1:G:131:THR:HG23	1.96	0.66
2:H:10:GLU:HG2	2:H:18:VAL:HG21	1.78	0.66
3:K:174:ILE:HG13	3:K:175:ALA:N	2.11	0.66
3:I:133:ILE:HG22	3:I:134:ASP:N	2.11	0.66
3:K:161:LYS:O	3:K:165:GLN:HG3	1.96	0.66
1:G:14:SER:HB2	1:G:17:GLU:OE2	1.96	0.65
3:J:133:ILE:HG22	3:J:134:ASP:N	2.11	0.65
2:F:48:ILE:HD12	2:F:48:ILE:N	2.11	0.65
2:B:40:ARG:HG2	2:B:40:ARG:HH11	1.61	0.65
2:F:37:VAL:HA	2:F:48:ILE:CD1	2.26	0.65
2:F:125:PRO:HB3	2:F:151:TYR:HB3	1.77	0.65
2:H:158:VAL:HG22	2:H:203:VAL:HG22	1.78	0.65
1:C:68:PHE:CD2	1:C:81:ILE:HD12	2.31	0.65
2:H:51:ILE:HD11	2:H:56:GLY:HA2	1.79	0.65
3:J:108:PHE:HZ	3:J:163:LEU:CD1	2.08	0.65
1:A:180:MET:HG2	1:A:181:SER:N	2.12	0.65
3:L:96:ASN:O	3:L:97:ILE:HG12	1.96	0.65
1:E:100:LEU:HD21	2:F:59:GLU:CD	2.17	0.64
1:E:28:THR:HA	1:E:75:THR:HG22	1.79	0.64
1:G:28:THR:HA	1:G:75:THR:HG22	1.80	0.64
3:J:57:CYS:HA	3:J:151:THR:O	1.98	0.64
1:A:149:ILE:HG13	1:A:150:ASN:N	2.12	0.64
1:G:180:MET:HG2	1:G:181:SER:N	2.13	0.64
2:D:125:PRO:HB3	2:D:151:TYR:HB3	1.78	0.64
2:H:48:ILE:HD13	2:H:64:PHE:CE2	2.32	0.64
3:L:128:ILE:HD12	3:L:128:ILE:H	1.62	0.63
1:C:180:MET:HG2	1:C:181:SER:N	2.12	0.63
2:B:151:TYR:CE2	2:B:156:VAL:HG11	2.33	0.63
2:D:151:TYR:CE2	2:D:156:VAL:CG1	2.80	0.63
3:I:57:CYS:HA	3:I:151:THR:O	1.99	0.63
3:J:54:LYS:HD3	3:J:149:ILE:CD1	2.28	0.63
2:H:216:ILE:N	2:H:216:ILE:HD12	2.14	0.63
3:I:38:ILE:HD12	3:I:38:ILE:H	1.63	0.63
2:D:46:GLU:O	2:D:48:ILE:HD13	1.99	0.63
1:C:149:ILE:HG13	1:C:150:ASN:N	2.14	0.63
3:I:38:ILE:HD13	3:I:53:VAL:CG1	2.28	0.63
2:D:23:LYS:HD2	2:D:78:THR:CG2	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:10:GLU:HG2	2:F:18:VAL:CG2	2.28	0.63
2:H:151:TYR:CE2	2:H:156:VAL:CG1	2.82	0.63
3:L:57:CYS:HA	3:L:151:THR:O	1.98	0.63
3:J:100:SER:OG	3:J:103:THR:HG23	1.99	0.62
1:A:149:ILE:CD1	1:A:203:HIS:HB2	2.29	0.62
2:D:216:ILE:N	2:D:216:ILE:HD12	2.14	0.62
3:L:100:SER:OG	3:L:103:THR:HG23	1.99	0.62
1:E:180:MET:HG2	1:E:181:SER:N	2.12	0.62
2:H:165:LEU:HD21	2:H:187:VAL:CG2	2.29	0.62
1:C:28:THR:HA	1:C:75:THR:HG22	1.81	0.62
3:K:96:ASN:C	3:K:97:ILE:HG13	2.20	0.62
3:K:133:ILE:HG22	3:K:134:ASP:N	2.15	0.62
2:B:28:THR:HB	2:B:31:ARG:CG	2.30	0.62
2:H:28:THR:HB	2:H:31:ARG:CG	2.29	0.62
2:D:11:LEU:HB2	2:D:153:PRO:HG2	1.82	0.62
2:B:10:GLU:HG2	2:B:18:VAL:CG2	2.30	0.62
2:H:129:PRO:HG3	2:H:214:LYS:CG	2.30	0.62
3:I:91:PHE:HE2	3:I:97:ILE:HG22	1.38	0.62
2:D:129:PRO:HG3	2:D:214:LYS:CG	2.30	0.61
3:J:42:TYR:CD1	3:J:132:ILE:HD12	2.35	0.61
2:B:129:PRO:HG3	2:B:214:LYS:CG	2.30	0.61
3:I:42:TYR:O	3:I:43:ILE:HD13	1.99	0.61
3:I:134:ASP:OD1	3:K:44:ARG:NH1	2.33	0.61
2:B:158:VAL:HG22	2:B:203:VAL:HG22	1.81	0.61
1:C:45:LYS:HE2	1:C:87:GLU:O	2.00	0.61
2:D:10:GLU:HG2	2:D:18:VAL:CG2	2.30	0.61
2:H:141:MET:HE1	2:H:188:THR:HG21	1.82	0.61
3:K:128:ILE:HD12	3:K:128:ILE:H	1.64	0.61
1:A:28:THR:HA	1:A:75:THR:HG22	1.81	0.61
3:I:54:LYS:HB3	3:I:149:ILE:HD13	1.83	0.61
2:D:70:LEU:CD1	2:D:81:MET:HG2	2.31	0.61
3:I:54:LYS:HD3	3:I:149:ILE:CD1	2.30	0.61
1:A:19:VAL:HG23	1:A:81:ILE:HD13	1.83	0.61
3:K:45:GLN:OE1	3:K:137:TYR:OH	2.16	0.61
3:L:42:TYR:CD1	3:L:132:ILE:HD12	2.35	0.61
3:I:161:LYS:O	3:I:165:GLN:HG3	2.00	0.61
2:B:123:THR:HG21	2:B:180:LEU:HD21	1.81	0.61
2:H:31:ARG:HH12	3:L:63:ALA:CB	2.14	0.61
3:L:161:LYS:O	3:L:165:GLN:HG3	2.00	0.61
2:F:114:LEU:HD13	2:F:155:PRO:HG3	1.82	0.60
2:H:153:PRO:HD2	2:H:207:ALA:CB	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:100:SER:OG	3:I:103:THR:HG23	2.01	0.60
3:I:128:ILE:H	3:I:128:ILE:HD12	1.66	0.60
2:D:38:LYS:HB3	2:D:48:ILE:HD11	1.82	0.60
1:A:12:ALA:HB1	1:A:112:LYS:HG3	1.83	0.60
2:H:122:THR:O	2:H:123:THR:CG2	2.50	0.60
1:A:34:THR:O	1:A:35:ARG:HB2	2.01	0.60
3:J:54:LYS:HB3	3:J:149:ILE:HD13	1.83	0.60
2:B:70:LEU:CD1	2:B:81:MET:HG2	2.32	0.60
1:C:129:GLN:O	1:C:132:SER:HB3	2.01	0.60
2:F:129:PRO:HG3	2:F:214:LYS:CG	2.31	0.60
3:K:87:VAL:CG1	3:K:91:PHE:CE2	2.80	0.60
1:G:19:VAL:HG23	1:G:81:ILE:HD13	1.83	0.60
3:K:91:PHE:CZ	3:K:104:VAL:HG11	2.37	0.60
2:H:23:LYS:HD3	2:H:78:THR:OG1	2.01	0.60
1:A:18:LYS:HE3	1:A:82:SER:HA	1.85	0.59
2:D:70:LEU:HD12	2:D:81:MET:HG2	1.83	0.59
1:C:34:THR:O	1:C:35:ARG:HB2	2.01	0.59
2:D:28:THR:HB	2:D:31:ARG:CG	2.33	0.59
1:G:129:GLN:O	1:G:132:SER:HB3	2.02	0.59
2:H:122:THR:O	2:H:123:THR:HG23	2.03	0.59
3:L:91:PHE:CZ	3:L:104:VAL:CG1	2.83	0.59
3:J:161:LYS:O	3:J:165:GLN:HG3	2.01	0.59
3:L:133:ILE:HG22	3:L:134:ASP:N	2.17	0.59
1:C:42:TYR:CE1	1:C:52:LEU:HD13	2.38	0.59
1:E:34:THR:O	1:E:35:ARG:HB2	2.02	0.59
1:G:113:ARG:HG2	1:G:114:ALA:H	1.68	0.59
2:D:114:LEU:HD13	2:D:155:PRO:HG3	1.84	0.59
1:G:53:LEU:CB	1:G:54:ILE:HD12	2.32	0.59
2:H:10:GLU:HG2	2:H:18:VAL:CG2	2.33	0.59
1:C:81:ILE:HD13	1:C:81:ILE:N	2.17	0.59
2:D:158:VAL:HG22	2:D:203:VAL:HG22	1.85	0.59
3:L:131:VAL:O	3:L:132:ILE:HD13	2.03	0.58
2:B:70:LEU:HD12	2:B:81:MET:HG2	1.85	0.58
2:B:114:LEU:HD13	2:B:155:PRO:HG3	1.84	0.58
4:A:220:GOL:O2	2:B:170:HIS:CE1	2.56	0.58
3:K:57:CYS:HA	3:K:151:THR:O	2.02	0.58
1:A:129:GLN:O	1:A:132:SER:HB3	2.02	0.58
1:C:149:ILE:CD1	1:C:203:HIS:HB2	2.31	0.58
1:E:123:PHE:CD2	2:F:130:LEU:HB3	2.39	0.58
2:B:123:THR:HG21	2:B:180:LEU:CD2	2.33	0.58
2:B:153:PRO:HD2	2:B:207:ALA:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:LYS:HE3	1:C:82:SER:HA	1.85	0.58
1:G:34:THR:O	1:G:35:ARG:HB2	2.03	0.58
3:I:126:LEU:HD23	3:K:96:ASN:HB3	1.85	0.58
1:E:18:LYS:HE3	1:E:82:SER:HA	1.86	0.58
1:C:80:THR:C	1:C:81:ILE:HD13	2.25	0.57
2:F:46:GLU:O	2:F:48:ILE:HD12	2.03	0.57
2:H:70:LEU:CD1	2:H:81:MET:HG2	2.34	0.57
2:H:28:THR:CG2	2:H:31:ARG:HG2	2.34	0.57
3:J:131:VAL:O	3:J:132:ILE:HD13	2.04	0.57
1:E:129:GLN:O	1:E:132:SER:HB3	2.04	0.57
3:J:157:ASN:CB	4:J:186:GOL:H11	2.34	0.57
1:C:123:PHE:CD2	2:D:130:LEU:HB3	2.39	0.57
2:D:11:LEU:HG	2:D:153:PRO:HG2	1.84	0.57
3:I:130:ASN:HB3	3:I:132:ILE:HD11	1.86	0.57
2:F:153:PRO:HD2	2:F:207:ALA:CB	2.34	0.57
1:A:210:ILE:H	1:A:210:ILE:HD12	1.70	0.57
2:D:28:THR:CG2	2:D:31:ARG:HG2	2.35	0.57
1:G:18:LYS:HE3	1:G:82:SER:HA	1.87	0.57
2:H:51:ILE:HD13	2:H:58:THR:HG22	1.82	0.57
3:K:100:SER:OG	3:K:103:THR:HG23	2.04	0.57
1:E:113:ARG:HG2	1:E:114:ALA:N	2.19	0.57
2:F:28:THR:CG2	2:F:31:ARG:HG2	2.34	0.57
1:A:113:ARG:HG2	1:A:114:ALA:H	1.70	0.57
2:F:70:LEU:CD1	2:F:81:MET:HG2	2.34	0.57
3:L:42:TYR:CE1	3:L:132:ILE:HD12	2.40	0.57
1:G:141:LEU:HD23	1:G:149:ILE:HD13	1.86	0.57
2:H:70:LEU:HD12	2:H:81:MET:HG2	1.86	0.57
3:I:119:SER:HB3	3:K:114:GLN:OE1	2.05	0.57
3:J:44:ARG:HH21	3:L:44:ARG:HH22	1.53	0.57
1:E:113:ARG:HG2	1:E:114:ALA:H	1.70	0.56
2:F:158:VAL:HG22	2:F:203:VAL:HG22	1.86	0.56
1:C:210:ILE:H	1:C:210:ILE:HD12	1.70	0.56
1:G:113:ARG:HG2	1:G:114:ALA:N	2.20	0.56
3:K:4:ALA:O	3:K:7:ILE:HD13	2.05	0.56
2:B:58:THR:H	3:I:125:LYS:HD2	1.71	0.56
2:F:38:LYS:H	2:F:48:ILE:HD11	1.66	0.56
3:I:42:TYR:C	3:I:43:ILE:HD13	2.26	0.56
3:J:96:ASN:C	3:J:97:ILE:HG13	2.25	0.56
3:J:137:TYR:CE2	3:J:172:THR:HG22	2.41	0.56
1:E:136:SER:OG	2:F:149:LYS:HE3	2.06	0.56
3:J:13:THR:O	3:J:16:GLU:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:130:ASN:HB3	3:K:132:ILE:HD11	1.88	0.56
1:E:12:ALA:HB1	1:E:112:LYS:HG3	1.88	0.56
2:H:114:LEU:HD23	2:H:115:VAL:N	2.21	0.56
2:H:194:TRP:CG	2:H:195:PRO:HA	2.41	0.56
3:L:4:ALA:O	3:L:7:ILE:HD13	2.05	0.56
2:D:183:LEU:C	2:D:183:LEU:HD23	2.26	0.56
2:F:151:TYR:CE2	2:F:156:VAL:CG1	2.88	0.56
1:G:124:PRO:CG	2:H:219:ARG:HH12	2.18	0.56
1:G:210:ILE:HD12	1:G:210:ILE:H	1.70	0.56
2:B:194:TRP:CG	2:B:195:PRO:HA	2.41	0.56
1:C:200:GLU:HG3	1:C:211:VAL:CG1	2.36	0.56
2:F:120:ALA:HB3	2:F:152:PHE:CE2	2.41	0.56
2:F:55:THR:CG2	3:K:61:ALA:HB2	2.35	0.56
3:J:44:ARG:HG3	3:J:44:ARG:NH1	2.21	0.56
3:J:133:ILE:HD11	3:J:164:MET:SD	2.45	0.56
1:G:124:PRO:O	2:H:219:ARG:NH2	2.38	0.55
1:G:12:ALA:HB1	1:G:112:LYS:HG3	1.87	0.55
2:H:140:SER:HA	2:H:191:SER:OG	2.06	0.55
2:D:199:VAL:O	2:D:216:ILE:CD1	2.42	0.55
3:J:44:ARG:NE	3:L:44:ARG:NH2	2.39	0.55
2:F:165:LEU:HD21	2:F:187:VAL:CG2	2.34	0.55
1:A:113:ARG:HG2	1:A:114:ALA:N	2.21	0.55
3:J:91:PHE:CZ	3:J:104:VAL:CG1	2.89	0.55
1:A:12:ALA:HB3	1:A:112:LYS:HE3	1.88	0.55
3:K:13:THR:O	3:K:16:GLU:HG3	2.06	0.55
1:C:60:ARG:HG2	1:C:60:ARG:HH21	1.72	0.55
1:E:149:ILE:HD13	1:E:150:ASN:C	2.27	0.55
2:B:38:LYS:HB2	2:B:48:ILE:HD11	1.89	0.55
1:C:12:ALA:HB1	1:C:112:LYS:HG3	1.88	0.55
1:C:100:LEU:HD21	2:D:59:GLU:CD	2.21	0.55
3:I:137:TYR:CE2	3:I:172:THR:HG22	2.42	0.55
3:J:161:LYS:HD3	4:J:186:GOL:O3	2.07	0.55
3:I:131:VAL:C	3:I:132:ILE:HD12	2.27	0.55
3:J:42:TYR:CE1	3:J:132:ILE:HD12	2.42	0.55
2:B:141:MET:HG3	2:B:189:VAL:O	2.07	0.54
2:F:70:LEU:HD12	2:F:81:MET:HG2	1.88	0.54
1:C:113:ARG:HG2	1:C:114:ALA:H	1.72	0.54
1:E:12:ALA:HB3	1:E:112:LYS:HE3	1.89	0.54
3:K:52:THR:HG23	3:K:147:GLU:HG3	1.88	0.54
3:K:174:ILE:HG13	3:K:175:ALA:H	1.72	0.54
3:I:36:ILE:HD13	3:I:153:SER:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:44:ARG:CZ	3:L:44:ARG:HH21	2.21	0.54
1:C:217:ASN:O	1:C:218:GLU:HG2	2.07	0.54
1:G:81:ILE:N	1:G:81:ILE:HD12	2.21	0.54
3:J:36:ILE:HD13	3:J:153:SER:HA	1.89	0.54
3:J:174:ILE:HD12	3:J:175:ALA:N	2.21	0.54
2:B:140:SER:HA	2:B:191:SER:OG	2.07	0.54
1:G:200:GLU:HG3	1:G:211:VAL:CG1	2.37	0.54
2:H:114:LEU:HD13	2:H:155:PRO:HG3	1.88	0.54
1:A:81:ILE:HD12	1:A:81:ILE:N	2.22	0.54
2:H:28:THR:HB	2:H:31:ARG:HG3	1.89	0.54
1:A:123:PHE:CD2	2:B:130:LEU:HB3	2.43	0.54
2:F:160:TRP:CZ3	2:F:201:CYS:HB2	2.43	0.54
2:H:51:ILE:HD11	2:H:56:GLY:CA	2.38	0.54
3:I:96:ASN:C	3:I:97:ILE:HG12	2.27	0.54
3:I:128:ILE:HD12	3:I:128:ILE:N	2.23	0.54
2:D:18:VAL:HG12	2:D:86:LEU:HD11	1.90	0.54
2:F:183:LEU:C	2:F:183:LEU:HD23	2.28	0.54
3:I:13:THR:O	3:I:16:GLU:HG3	2.08	0.54
3:I:174:ILE:HG13	3:I:175:ALA:H	1.72	0.54
3:L:174:ILE:HD12	3:L:175:ALA:N	2.22	0.54
2:B:18:VAL:HG12	2:B:86:LEU:HD11	1.90	0.54
3:J:44:ARG:HH21	3:L:44:ARG:NH2	2.06	0.54
1:C:113:ARG:HG2	1:C:114:ALA:N	2.22	0.54
2:F:28:THR:HB	2:F:31:ARG:CG	2.37	0.54
3:I:44:ARG:NH1	3:K:134:ASP:HB2	2.23	0.54
3:J:137:TYR:CD2	3:J:172:THR:HG22	2.43	0.54
3:K:128:ILE:HD12	3:K:128:ILE:N	2.23	0.54
3:L:36:ILE:HD13	3:L:153:SER:HA	1.89	0.53
3:L:137:TYR:CE2	3:L:172:THR:HG22	2.43	0.53
1:A:67:ARG:HB2	1:A:82:SER:OG	2.07	0.53
2:F:18:VAL:HG12	2:F:86:LEU:HD11	1.90	0.53
2:B:28:THR:CG2	2:B:31:ARG:HG2	2.38	0.53
1:G:141:LEU:HD12	1:G:141:LEU:N	2.23	0.53
1:G:172:ASP:OD2	1:G:174:LYS:HB3	2.08	0.53
1:A:30:LEU:HD12	1:A:31:ASN:H	1.72	0.53
1:A:172:ASP:OD2	1:A:174:LYS:HB3	2.08	0.53
1:E:200:GLU:HG3	1:E:211:VAL:CG1	2.39	0.53
1:G:217:ASN:O	1:G:218:GLU:HG2	2.09	0.53
3:I:44:ARG:HG3	3:I:44:ARG:NH1	2.16	0.53
3:I:137:TYR:CD2	3:I:172:THR:HG22	2.44	0.53
3:K:96:ASN:O	3:K:97:ILE:CG1	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:128:ILE:HD12	3:L:128:ILE:N	2.23	0.53
1:E:45:LYS:NZ	4:E:222:GOL:H32	2.24	0.53
2:F:40:ARG:HG2	2:F:40:ARG:NH1	2.23	0.53
2:H:48:ILE:HD13	2:H:64:PHE:CD2	2.43	0.53
2:H:51:ILE:HD12	2:H:52:ASN:N	2.24	0.53
3:K:41:PHE:CE2	3:K:51:LEU:HB3	2.44	0.53
3:K:131:VAL:C	3:K:132:ILE:HD12	2.29	0.53
3:K:137:TYR:CE2	3:K:172:THR:HG22	2.44	0.53
3:K:157:ASN:HB2	4:K:186:GOL:H11	1.91	0.53
3:L:118:SER:O	3:L:122:VAL:HG22	2.09	0.53
1:A:200:GLU:HG3	1:A:211:VAL:CG1	2.38	0.53
1:G:136:SER:OG	1:G:185:THR:HG23	2.09	0.53
3:J:119:SER:O	3:J:123:ASP:HB2	2.08	0.53
3:K:91:PHE:CE2	3:K:104:VAL:HG11	2.41	0.53
3:L:13:THR:O	3:L:16:GLU:HG3	2.09	0.53
3:L:137:TYR:CD2	3:L:172:THR:HG22	2.44	0.53
1:A:172:ASP:CB	4:A:220:GOL:H2	2.38	0.53
2:H:160:TRP:CZ3	2:H:201:CYS:HB2	2.44	0.53
2:B:151:TYR:CE2	2:B:156:VAL:CG1	2.92	0.52
1:G:30:LEU:HD12	1:G:31:ASN:H	1.74	0.52
2:H:40:ARG:HG2	2:H:40:ARG:NH1	2.23	0.52
2:D:194:TRP:CG	2:D:195:PRO:HA	2.44	0.52
1:A:210:ILE:HD12	1:A:210:ILE:N	2.25	0.52
2:H:18:VAL:HG12	2:H:86:LEU:HD11	1.90	0.52
3:K:137:TYR:CD2	3:K:172:THR:HG22	2.45	0.52
2:B:28:THR:HB	2:B:31:ARG:HG3	1.92	0.52
2:F:194:TRP:CG	2:F:195:PRO:HA	2.44	0.52
2:H:151:TYR:CZ	2:H:156:VAL:HG11	2.44	0.52
3:L:18:ILE:CD1	3:L:71:ALA:HB3	2.39	0.52
1:E:141:LEU:N	1:E:141:LEU:HD12	2.25	0.52
1:G:210:ILE:HD12	1:G:210:ILE:N	2.25	0.52
1:C:39:LEU:HG	1:C:40:ALA:N	2.25	0.52
2:D:140:SER:HA	2:D:191:SER:OG	2.10	0.52
3:I:161:LYS:HD3	4:I:186:GOL:O1	2.10	0.51
2:D:160:TRP:CZ3	2:D:201:CYS:HB2	2.46	0.51
3:L:96:ASN:C	3:L:97:ILE:HG12	2.30	0.51
1:C:172:ASP:OD2	1:C:174:LYS:HB3	2.09	0.51
1:G:12:ALA:HB3	1:G:112:LYS:HE3	1.92	0.51
1:G:124:PRO:HD2	2:H:219:ARG:NH1	2.18	0.51
3:I:44:ARG:HH11	3:I:44:ARG:CG	2.17	0.51
3:K:91:PHE:HE2	3:K:104:VAL:CG2	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:36:TRP:CD2	2:F:81:MET:HG3	2.46	0.51
1:G:60:ARG:HG2	1:G:60:ARG:HH21	1.74	0.51
2:H:22:CYS:C	2:H:78:THR:HG23	2.29	0.51
2:H:216:ILE:N	2:H:216:ILE:CD1	2.73	0.51
2:D:40:ARG:HG2	2:D:40:ARG:NH1	2.26	0.51
1:E:30:LEU:HD12	1:E:31:ASN:H	1.75	0.51
2:F:38:LYS:N	2:F:48:ILE:CD1	2.72	0.51
1:G:67:ARG:HB2	1:G:82:SER:OG	2.10	0.51
3:I:38:ILE:HD11	3:I:150:ASN:CG	2.30	0.51
3:I:38:ILE:HD12	3:I:38:ILE:N	2.26	0.51
3:K:91:PHE:HD2	3:K:99:THR:HG21	1.76	0.51
2:B:183:LEU:HD23	2:B:183:LEU:C	2.31	0.51
1:E:172:ASP:OD2	1:E:174:LYS:HB3	2.11	0.51
2:H:122:THR:C	2:H:123:THR:HG23	2.31	0.51
3:I:96:ASN:O	3:I:97:ILE:CG1	2.58	0.51
3:J:52:THR:HG23	3:J:147:GLU:HG3	1.92	0.51
1:C:136:SER:OG	1:C:185:THR:HG23	2.11	0.51
1:C:210:ILE:HD12	1:C:210:ILE:N	2.25	0.51
1:A:60:ARG:HG2	1:A:60:ARG:HH21	1.76	0.51
2:D:28:THR:HB	2:D:31:ARG:HG3	1.92	0.51
2:D:216:ILE:N	2:D:216:ILE:CD1	2.74	0.51
1:G:141:LEU:HD23	1:G:149:ILE:CD1	2.41	0.51
3:L:44:ARG:HH11	3:L:44:ARG:CG	2.23	0.51
1:C:12:ALA:HB3	1:C:112:LYS:HE3	1.92	0.50
2:H:165:LEU:CD2	2:H:187:VAL:HG21	2.39	0.50
3:J:108:PHE:CZ	3:J:163:LEU:CD1	2.92	0.50
2:D:47:TRP:C	2:D:48:ILE:HD13	2.32	0.50
2:H:143:THR:C	2:H:144:LEU:HD12	2.31	0.50
3:K:95:LEU:O	3:K:96:ASN:HB2	2.11	0.50
1:E:60:ARG:HG2	1:E:60:ARG:HH21	1.77	0.50
2:H:199:VAL:O	2:H:216:ILE:CD1	2.42	0.50
3:I:118:SER:O	3:I:122:VAL:HG22	2.11	0.50
3:I:119:SER:O	3:I:123:ASP:HB2	2.12	0.50
1:A:152:LYS:NZ	1:A:152:LYS:HB2	2.27	0.50
2:F:114:LEU:HD23	2:F:115:VAL:N	2.26	0.50
3:L:47:HIS:HB2	3:L:137:TYR:CD1	2.46	0.50
1:A:141:LEU:N	1:A:141:LEU:HD12	2.26	0.50
1:A:56:TRP:O	1:A:57:ALA:HB3	2.11	0.50
3:K:44:ARG:HH11	3:K:44:ARG:CG	2.18	0.50
1:C:30:LEU:HD12	1:C:31:ASN:H	1.75	0.50
3:K:47:HIS:HB2	3:K:137:TYR:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LEU:N	1:C:141:LEU:HD12	2.26	0.50
1:E:39:LEU:HG	1:E:40:ALA:N	2.25	0.50
1:E:152:LYS:HB2	1:E:152:LYS:NZ	2.27	0.50
3:I:45:GLN:OE1	3:I:137:TYR:OH	2.20	0.50
2:B:114:LEU:HD23	2:B:115:VAL:N	2.26	0.49
1:C:56:TRP:O	1:C:57:ALA:HB3	2.11	0.49
2:H:23:LYS:CD	2:H:78:THR:OG1	2.59	0.49
1:G:147:LYS:O	1:G:147:LYS:HG2	2.12	0.49
3:I:41:PHE:CE2	3:I:51:LEU:HB3	2.47	0.49
3:J:118:SER:O	3:J:122:VAL:HG22	2.13	0.49
3:K:69:LEU:HD13	3:K:109:GLU:HG2	1.93	0.49
3:K:119:SER:O	3:K:123:ASP:HB2	2.12	0.49
2:D:120:ALA:HB3	2:D:152:PHE:CE2	2.47	0.49
2:H:183:LEU:C	2:H:183:LEU:HD23	2.32	0.49
3:I:174:ILE:O	3:I:176:PRO:HD3	2.12	0.49
4:A:220:GOL:HO2	2:B:170:HIS:CE1	2.30	0.49
2:B:160:TRP:CZ3	2:B:201:CYS:HB2	2.47	0.49
2:D:205:HIS:NE2	2:D:207:ALA:HB3	2.27	0.49
2:F:140:SER:HA	2:F:191:SER:OG	2.13	0.49
2:F:205:HIS:NE2	2:F:207:ALA:HB3	2.28	0.49
2:H:51:ILE:HD11	2:H:56:GLY:C	2.33	0.49
1:A:39:LEU:HG	1:A:40:ALA:N	2.26	0.49
1:E:60:ARG:HG3	1:E:64:VAL:HB	1.95	0.49
2:H:36:TRP:CD2	2:H:81:MET:HG3	2.48	0.49
2:D:48:ILE:HD13	2:D:48:ILE:N	2.28	0.49
3:K:118:SER:O	3:K:122:VAL:HG22	2.12	0.49
1:A:60:ARG:HG3	1:A:64:VAL:HB	1.95	0.49
2:H:48:ILE:HD13	2:H:64:PHE:CZ	2.48	0.49
3:J:47:HIS:HB2	3:J:137:TYR:CD1	2.47	0.49
2:F:46:GLU:O	2:F:48:ILE:CD1	2.61	0.49
3:I:91:PHE:CE2	3:I:97:ILE:O	2.66	0.49
3:K:36:ILE:HD12	3:K:126:LEU:O	2.13	0.49
2:B:40:ARG:HG2	2:B:40:ARG:NH1	2.26	0.48
3:I:47:HIS:HB2	3:I:137:TYR:CD1	2.47	0.48
1:E:67:ARG:HB2	1:E:82:SER:OG	2.14	0.48
1:E:147:LYS:O	1:E:147:LYS:HG2	2.12	0.48
2:F:165:LEU:CD2	2:F:187:VAL:HG21	2.43	0.48
1:G:60:ARG:HG3	1:G:64:VAL:HB	1.95	0.48
2:H:31:ARG:NH1	3:L:63:ALA:CB	2.76	0.48
3:I:7:ILE:O	3:I:11:VAL:HG13	2.13	0.48
1:A:147:LYS:O	1:A:147:LYS:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:SER:O	2:D:78:THR:HG23	2.14	0.48
3:L:174:ILE:O	3:L:176:PRO:HD3	2.14	0.48
1:G:152:LYS:HB2	1:G:152:LYS:NZ	2.28	0.48
1:A:155:ILE:HD12	1:A:197:TYR:CD1	2.49	0.48
2:B:205:HIS:NE2	2:B:207:ALA:HB3	2.27	0.48
3:J:95:LEU:O	3:J:96:ASN:HB2	2.13	0.48
1:C:37:ASN:CB	1:C:57:ALA:HB2	2.43	0.48
1:E:45:LYS:CE	4:E:222:GOL:H32	2.44	0.48
2:F:141:MET:HA	2:F:190:PRO:HA	1.96	0.48
1:G:155:ILE:HD12	1:G:197:TYR:CD1	2.48	0.48
2:H:120:ALA:HB3	2:H:152:PHE:CE2	2.47	0.48
3:I:43:ILE:HD12	3:I:133:ILE:CB	2.18	0.48
3:L:41:PHE:CE2	3:L:51:LEU:HB3	2.48	0.48
1:C:54:ILE:HD13	1:C:70:GLY:HA3	1.96	0.48
2:B:139:ASN:OD1	2:B:139:ASN:N	2.46	0.48
2:B:143:THR:C	2:B:144:LEU:HD12	2.34	0.48
1:C:152:LYS:HB2	1:C:152:LYS:NZ	2.29	0.47
2:F:139:ASN:OD1	2:F:139:ASN:N	2.47	0.47
1:G:216:ARG:NH2	1:G:216:ARG:HB3	2.29	0.47
3:J:41:PHE:CE2	3:J:51:LEU:HB3	2.49	0.47
3:K:91:PHE:CD2	3:K:99:THR:HG21	2.49	0.47
1:C:60:ARG:HG3	1:C:64:VAL:HB	1.96	0.47
1:E:136:SER:OG	1:E:185:THR:HG23	2.14	0.47
2:H:202:ASN:CG	2:H:213:ASP:OD2	2.51	0.47
2:B:165:LEU:HD21	2:B:187:VAL:HG21	1.95	0.47
2:D:114:LEU:HD23	2:D:115:VAL:N	2.29	0.47
2:F:48:ILE:N	2:F:48:ILE:CD1	2.77	0.47
1:G:39:LEU:HG	1:G:40:ALA:N	2.29	0.47
2:H:141:MET:HA	2:H:190:PRO:HA	1.96	0.47
1:A:100:LEU:HD21	2:B:59:GLU:CD	2.32	0.47
1:C:147:LYS:HG2	1:C:147:LYS:O	2.13	0.47
3:K:108:PHE:O	3:K:112:VAL:HG23	2.14	0.47
3:L:44:ARG:HG3	3:L:44:ARG:NH1	2.20	0.47
3:L:96:ASN:O	3:L:97:ILE:CG1	2.61	0.47
3:L:149:ILE:HD12	3:L:149:ILE:N	2.29	0.47
1:A:37:ASN:CB	1:A:57:ALA:HB2	2.45	0.47
2:B:141:MET:HA	2:B:190:PRO:HA	1.96	0.47
2:D:36:TRP:CD2	2:D:81:MET:HG3	2.50	0.47
1:E:155:ILE:HD12	1:E:197:TYR:CD1	2.49	0.47
3:I:98:GLN:O	3:I:99:THR:HB	2.15	0.47
2:B:28:THR:HB	2:B:31:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:139:ASN:N	2:H:139:ASN:OD1	2.47	0.47
1:A:136:SER:OG	1:A:185:THR:HG23	2.14	0.47
2:B:36:TRP:CD2	2:B:81:MET:HG3	2.49	0.47
1:C:128:GLU:O	1:C:132:SER:HB2	2.14	0.47
1:C:155:ILE:HD12	1:C:197:TYR:CD1	2.50	0.47
1:C:200:GLU:HG3	1:C:211:VAL:HG12	1.96	0.47
2:D:143:THR:C	2:D:144:LEU:HD12	2.34	0.47
2:D:165:LEU:HD21	2:D:187:VAL:HG21	1.97	0.47
1:G:19:VAL:CG2	1:G:81:ILE:HD13	2.45	0.47
3:L:95:LEU:O	3:L:96:ASN:HB2	2.14	0.47
2:B:104:TYR:CE1	3:I:33:LYS:HD3	2.50	0.47
1:E:13:VAL:CG2	1:E:17:GLU:HB2	2.45	0.47
2:H:176:LEU:HD13	2:H:181:TYR:CZ	2.49	0.47
3:L:119:SER:O	3:L:123:ASP:HB2	2.15	0.47
2:D:6:GLN:HB2	2:D:111:GLN:OE1	2.15	0.47
2:D:183:LEU:HD23	2:D:184:SER:N	2.30	0.47
2:F:28:THR:HB	2:F:31:ARG:HG3	1.97	0.47
2:H:141:MET:CE	2:H:188:THR:HG21	2.44	0.47
3:I:44:ARG:NH1	3:I:44:ARG:CG	2.76	0.47
3:L:38:ILE:HD11	3:L:148:PHE:HD2	1.80	0.47
1:A:140:PHE:C	1:A:141:LEU:HD12	2.35	0.47
1:E:95:LYS:NZ	2:F:105:ASP:HA	2.30	0.47
1:E:95:LYS:HZ1	2:F:105:ASP:HA	1.79	0.47
2:H:51:ILE:CD1	2:H:57:TYR:O	2.58	0.47
3:J:44:ARG:HH11	3:J:44:ARG:CG	2.23	0.47
3:K:91:PHE:HE1	3:K:166:LEU:HD13	1.80	0.47
1:A:89:LEU:O	1:A:90:ALA:HB2	2.15	0.46
1:C:67:ARG:HB2	1:C:82:SER:OG	2.15	0.46
2:D:139:ASN:OD1	2:D:139:ASN:N	2.48	0.46
3:J:174:ILE:O	3:J:176:PRO:HD3	2.15	0.46
1:A:13:VAL:HG22	1:A:17:GLU:HB2	1.97	0.46
2:B:6:GLN:HB2	2:B:111:GLN:OE1	2.15	0.46
3:I:95:LEU:O	3:I:96:ASN:HB2	2.15	0.46
1:C:95:LYS:HA	1:C:102:THR:O	2.16	0.46
1:C:140:PHE:C	1:C:141:LEU:HD12	2.35	0.46
1:G:200:GLU:HG3	1:G:211:VAL:HG12	1.98	0.46
3:I:69:LEU:HD13	3:I:109:GLU:HG2	1.96	0.46
3:J:44:ARG:NH2	3:L:44:ARG:NH2	2.63	0.46
1:C:13:VAL:CG2	1:C:17:GLU:HB2	2.46	0.46
1:E:88:ASP:OD1	4:E:222:GOL:O3	2.30	0.46
2:F:143:THR:C	2:F:144:LEU:HD12	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ARG:CZ	1:A:33:ARG:HB3	2.46	0.46
2:D:141:MET:HA	2:D:190:PRO:HA	1.97	0.46
1:G:216:ARG:HB3	1:G:216:ARG:HH21	1.81	0.46
2:H:205:HIS:NE2	2:H:207:ALA:HB3	2.30	0.46
3:K:98:GLN:O	3:K:99:THR:HB	2.15	0.46
1:C:37:ASN:HB2	1:C:57:ALA:HB2	1.98	0.46
1:E:216:ARG:NH2	1:E:216:ARG:HB3	2.31	0.46
3:I:91:PHE:HE2	3:I:97:ILE:CA	2.13	0.46
3:L:38:ILE:CD1	3:L:148:PHE:HD2	2.28	0.46
3:L:98:GLN:O	3:L:99:THR:HB	2.16	0.46
1:C:33:ARG:HB3	1:C:33:ARG:CZ	2.45	0.46
1:E:43:GLN:OE1	4:E:222:GOL:H11	2.16	0.46
1:E:93:TYR:OH	2:F:44:GLY:HA2	2.16	0.46
3:K:174:ILE:O	3:K:176:PRO:HD3	2.16	0.46
3:L:125:LYS:HB2	3:L:125:LYS:NZ	2.31	0.46
2:B:123:THR:HG23	2:B:151:TYR:HA	1.97	0.46
3:J:65:LEU:O	3:J:65:LEU:HD23	2.16	0.46
1:A:37:ASN:HB2	1:A:57:ALA:HB2	1.97	0.46
1:E:167:SER:HB2	2:F:175:VAL:CG2	2.46	0.46
3:I:119:SER:HB2	3:K:114:GLN:HB3	1.97	0.46
1:A:19:VAL:CG2	1:A:81:ILE:HD13	2.45	0.45
1:A:124:PRO:CD	2:B:219:ARG:HH12	2.25	0.45
1:A:216:ARG:HB3	1:A:216:ARG:NH2	2.31	0.45
1:C:54:ILE:HD13	1:C:70:GLY:CA	2.45	0.45
1:E:33:ARG:CZ	1:E:33:ARG:HB3	2.44	0.45
1:G:140:PHE:C	1:G:141:LEU:HD12	2.36	0.45
3:J:125:LYS:HB2	3:J:125:LYS:NZ	2.32	0.45
3:K:44:ARG:HG3	3:K:44:ARG:NH1	2.17	0.45
2:B:154:GLU:O	2:B:154:GLU:CG	2.64	0.45
1:G:13:VAL:CG2	1:G:17:GLU:HB2	2.45	0.45
3:L:7:ILE:O	3:L:11:VAL:HG13	2.16	0.45
1:A:95:LYS:HA	1:A:102:THR:O	2.15	0.45
1:A:128:GLU:O	1:A:132:SER:HB2	2.16	0.45
1:E:140:PHE:C	1:E:141:LEU:HD12	2.37	0.45
3:J:87:VAL:HB	3:J:88:PRO:HD3	1.98	0.45
3:L:69:LEU:HD13	3:L:109:GLU:HG2	1.97	0.45
1:A:86:ALA:HA	1:A:111:ILE:CD1	2.44	0.45
1:C:149:ILE:HD12	1:C:203:HIS:CB	2.39	0.45
1:G:24:LYS:HE2	1:G:76:ASP:OD2	2.16	0.45
1:G:128:GLU:O	1:G:132:SER:HB2	2.15	0.45
2:H:28:THR:HB	2:H:31:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:87:VAL:HB	3:K:88:PRO:HD3	1.98	0.45
1:A:37:ASN:HB2	1:A:57:ALA:CB	2.47	0.45
2:B:141:MET:CG	2:B:188:THR:CG2	2.94	0.45
1:E:13:VAL:HG22	1:E:17:GLU:HB2	1.97	0.45
2:F:31:ARG:HH12	3:K:26:ALA:HA	1.81	0.45
1:G:13:VAL:HG22	1:G:17:GLU:HB2	1.97	0.45
3:J:108:PHE:O	3:J:112:VAL:HG23	2.17	0.45
2:D:62:GLN:HE22	2:D:65:LYS:HD2	1.82	0.45
1:E:128:GLU:O	1:E:132:SER:HB2	2.16	0.45
1:G:33:ARG:CZ	1:G:33:ARG:HB3	2.45	0.45
3:J:53:VAL:HG22	3:J:148:PHE:HB3	1.99	0.45
2:B:154:GLU:O	2:B:154:GLU:CD	2.55	0.45
1:G:141:LEU:HD13	1:G:180:MET:HE2	1.99	0.45
1:A:13:VAL:CG2	1:A:17:GLU:HB2	2.47	0.45
1:A:95:LYS:HE2	1:A:95:LYS:HB3	1.85	0.45
1:C:13:VAL:HG22	1:C:17:GLU:HB2	1.98	0.45
2:D:154:GLU:OE1	2:D:181:TYR:CD2	2.70	0.45
1:G:138:VAL:HG21	2:H:130:LEU:HD11	1.99	0.45
3:K:94:ALA:HB2	3:K:169:LYS:CG	2.40	0.45
2:D:214:LYS:O	2:D:216:ILE:HD12	2.17	0.45
3:J:98:GLN:O	3:J:99:THR:HB	2.17	0.45
1:C:37:ASN:HB2	1:C:57:ALA:CB	2.47	0.44
1:C:99:ASN:O	1:C:100:LEU:HB2	2.17	0.44
3:I:43:ILE:HG12	3:I:51:LEU:HD11	1.99	0.44
2:H:193:THR:O	2:H:197:GLU:HB2	2.17	0.44
1:A:30:LEU:HD12	1:A:31:ASN:N	2.32	0.44
2:D:128:TYR:HA	2:D:129:PRO:HD3	1.83	0.44
2:D:141:MET:O	2:D:142:VAL:HB	2.17	0.44
3:J:44:ARG:NH1	3:J:44:ARG:CG	2.81	0.44
3:J:54:LYS:HB3	3:J:149:ILE:CD1	2.47	0.44
3:K:132:ILE:HD12	3:K:132:ILE:N	2.32	0.44
1:A:60:ARG:NH2	1:A:66:ASP:HA	2.32	0.44
2:D:193:THR:O	2:D:197:GLU:HB2	2.17	0.44
1:E:24:LYS:HE2	1:E:76:ASP:OD2	2.17	0.44
2:F:129:PRO:HB3	2:F:216:ILE:HD13	1.99	0.44
3:I:148:PHE:CE1	3:I:160:ILE:HG22	2.52	0.44
3:L:148:PHE:CE1	3:L:160:ILE:HG22	2.52	0.44
1:A:149:ILE:HD12	1:A:203:HIS:CB	2.39	0.44
2:B:193:THR:O	2:B:197:GLU:HB2	2.17	0.44
1:G:95:LYS:HA	1:G:102:THR:O	2.17	0.44
2:B:183:LEU:HD23	2:B:184:SER:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:TYR:OH	2:D:44:GLY:HA2	2.18	0.44
2:D:212:VAL:HG22	2:D:213:ASP:N	2.33	0.44
2:H:6:GLN:HB2	2:H:111:GLN:OE1	2.18	0.44
1:A:200:GLU:HG3	1:A:211:VAL:HG12	1.99	0.44
1:A:216:ARG:HB3	1:A:216:ARG:HH21	1.83	0.44
1:E:95:LYS:HA	1:E:102:THR:O	2.18	0.44
1:G:130:LEU:HD22	1:G:188:LYS:HG3	1.99	0.44
2:H:62:GLN:HE22	2:H:65:LYS:HD2	1.83	0.44
3:K:53:VAL:HG22	3:K:148:PHE:HB3	1.98	0.44
3:K:158:CYS:HA	4:K:186:GOL:O3	2.18	0.44
2:B:128:TYR:HA	2:B:129:PRO:HD3	1.83	0.44
1:C:207:THR:O	1:C:209:PRO:HD3	2.18	0.44
2:D:140:SER:O	2:D:141:MET:HB2	2.17	0.44
1:E:207:THR:O	1:E:209:PRO:HD3	2.18	0.44
1:E:216:ARG:HB3	1:E:216:ARG:HH21	1.83	0.44
3:L:87:VAL:HB	3:L:88:PRO:HD3	1.98	0.44
2:B:176:LEU:HD13	2:B:181:TYR:CZ	2.52	0.44
2:B:194:TRP:CD1	2:B:195:PRO:HA	2.53	0.44
1:C:39:LEU:HD22	1:C:77:PHE:CG	2.53	0.44
1:E:200:GLU:HG3	1:E:211:VAL:HG12	1.99	0.43
3:L:80:THR:HG23	3:L:83:GLN:OE1	2.17	0.43
1:G:179:SER:OG	2:H:170:HIS:CE1	2.71	0.43
2:H:121:LYS:O	2:H:123:THR:HG23	2.18	0.43
2:H:214:LYS:O	2:H:216:ILE:HD12	2.18	0.43
3:J:69:LEU:HD13	3:J:109:GLU:HG2	1.99	0.43
2:F:111:GLN:H	2:F:111:GLN:NE2	2.16	0.43
2:F:193:THR:O	2:F:197:GLU:HB2	2.18	0.43
2:F:212:VAL:HG22	2:F:213:ASP:N	2.32	0.43
1:G:29:LEU:HD12	1:G:77:PHE:CE2	2.53	0.43
3:K:65:LEU:HD23	3:K:65:LEU:O	2.18	0.43
3:L:65:LEU:O	3:L:65:LEU:HD23	2.17	0.43
2:B:141:MET:HA	2:B:189:VAL:O	2.19	0.43
2:D:111:GLN:H	2:D:111:GLN:NE2	2.15	0.43
2:F:128:TYR:HA	2:F:129:PRO:HD3	1.85	0.43
3:K:7:ILE:O	3:K:11:VAL:HG13	2.18	0.43
3:K:125:LYS:HB2	3:K:125:LYS:NZ	2.32	0.43
1:C:72:GLY:HA3	1:C:77:PHE:HA	2.00	0.43
1:E:99:ASN:O	1:E:100:LEU:HB2	2.19	0.43
1:G:207:THR:O	1:G:209:PRO:HD3	2.18	0.43
1:A:39:LEU:HD22	1:A:77:PHE:CG	2.54	0.43
1:C:24:LYS:HE2	1:C:76:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:47:TRP:C	2:F:48:ILE:HD12	2.39	0.43
1:G:149:ILE:HD11	1:G:201:ALA:HB1	1.99	0.43
1:A:19:VAL:O	1:A:80:THR:HG23	2.19	0.43
2:B:129:PRO:HB3	2:B:216:ILE:HD13	2.00	0.43
2:B:141:MET:O	2:B:142:VAL:HB	2.19	0.43
1:C:216:ARG:HH21	1:C:216:ARG:HB3	1.84	0.43
2:D:57:TYR:HA	3:J:125:LYS:HD3	2.00	0.43
1:E:72:GLY:HA3	1:E:77:PHE:HA	2.01	0.43
3:J:67:ALA:O	3:J:70:SER:HB3	2.19	0.43
1:E:30:LEU:HD12	1:E:31:ASN:N	2.33	0.43
1:G:30:LEU:HD12	1:G:31:ASN:N	2.33	0.43
1:G:60:ARG:NH2	1:G:66:ASP:HA	2.33	0.43
1:A:24:LYS:HE2	1:A:76:ASP:OD2	2.18	0.43
1:A:72:GLY:HA3	1:A:77:PHE:HA	2.00	0.43
2:B:120:ALA:HB3	2:B:152:PHE:CE2	2.54	0.43
2:D:143:THR:HG22	2:D:188:THR:HG1	1.80	0.43
2:D:176:LEU:HD13	2:D:181:TYR:CZ	2.54	0.43
2:H:141:MET:CE	2:H:188:THR:CG2	2.97	0.43
3:I:132:ILE:HD12	3:I:132:ILE:N	2.34	0.43
1:E:141:LEU:HD13	1:E:180:MET:HE2	2.00	0.42
2:F:6:GLN:HB2	2:F:111:GLN:OE1	2.19	0.42
3:I:108:PHE:O	3:I:112:VAL:HG23	2.18	0.42
3:J:135:GLU:O	3:J:168:THR:HB	2.19	0.42
1:C:216:ARG:HB3	1:C:216:ARG:NH2	2.33	0.42
1:E:39:LEU:HD22	1:E:77:PHE:CG	2.54	0.42
1:G:56:TRP:O	1:G:57:ALA:HB3	2.19	0.42
3:I:67:ALA:O	3:I:70:SER:HB3	2.19	0.42
3:K:18:ILE:HD11	3:K:163:LEU:CD2	2.50	0.42
2:B:23:LYS:HE3	2:B:76:SER:O	2.19	0.42
1:C:130:LEU:HD22	1:C:188:LYS:HG3	2.00	0.42
1:E:175:ASP:OD1	1:E:177:THR:HG23	2.19	0.42
2:F:58:THR:H	3:K:125:LYS:CD	2.29	0.42
2:F:141:MET:HA	2:F:189:VAL:O	2.19	0.42
3:I:133:ILE:CG2	3:I:134:ASP:N	2.82	0.42
3:L:53:VAL:HG22	3:L:148:PHE:HB3	2.01	0.42
2:B:62:GLN:HE22	2:B:65:LYS:HD2	1.84	0.42
2:B:70:LEU:HD11	2:B:81:MET:HG2	2.01	0.42
2:B:140:SER:O	2:B:141:MET:HB3	2.19	0.42
2:D:172:PHE:HA	2:D:173:PRO:HD3	1.87	0.42
1:G:72:GLY:HA3	1:G:77:PHE:HA	2.00	0.42
1:E:153:TRP:O	1:E:159:GLU:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:TRP:CE2	1:G:79:LEU:HB2	2.55	0.42
3:I:87:VAL:HB	3:I:88:PRO:HD3	2.01	0.42
1:E:29:LEU:HD12	1:E:77:PHE:CE2	2.54	0.42
1:G:125:PRO:HD3	1:G:137:VAL:HG22	2.00	0.42
3:K:44:ARG:NH1	3:K:44:ARG:CG	2.77	0.42
1:A:130:LEU:HD22	1:A:188:LYS:HG3	2.01	0.42
2:F:141:MET:O	2:F:142:VAL:HB	2.20	0.42
2:F:183:LEU:HD23	2:F:184:SER:N	2.34	0.42
1:G:19:VAL:O	1:G:80:THR:HG23	2.20	0.42
2:H:23:LYS:HE3	2:H:76:SER:O	2.20	0.42
2:H:141:MET:HA	2:H:189:VAL:O	2.19	0.42
3:I:129:GLN:HB3	4:I:186:GOL:H32	2.01	0.42
1:C:42:TYR:CZ	1:C:52:LEU:HD13	2.54	0.42
1:G:37:ASN:HB2	1:G:57:ALA:CB	2.50	0.42
3:K:80:THR:HG23	3:K:83:GLN:OE1	2.20	0.42
1:G:10:SER:HA	1:G:108:LYS:O	2.20	0.42
1:G:17:GLU:O	1:G:84:VAL:HG12	2.20	0.42
1:G:153:TRP:O	1:G:159:GLU:HA	2.20	0.42
3:J:33:LYS:HG3	3:J:34:CYS:N	2.35	0.42
3:K:135:GLU:O	3:K:168:THR:HB	2.19	0.42
2:B:219:ARG:HG3	2:B:219:ARG:HH11	1.85	0.42
2:D:102:ASP:OD1	2:D:104:TYR:HB2	2.20	0.42
1:E:86:ALA:HA	1:E:111:ILE:CD1	2.47	0.42
1:G:93:TYR:OH	2:H:44:GLY:HA2	2.19	0.42
3:I:135:GLU:O	3:I:168:THR:HB	2.19	0.42
3:J:91:PHE:CE1	3:J:166:LEU:HD13	2.55	0.42
3:L:67:ALA:O	3:L:70:SER:HB3	2.19	0.42
1:C:153:TRP:O	1:C:159:GLU:HA	2.20	0.41
2:H:51:ILE:CD1	2:H:56:GLY:C	2.88	0.41
3:J:6:SER:O	3:J:9:THR:HB	2.20	0.41
3:J:80:THR:HG23	3:J:83:GLN:OE1	2.20	0.41
1:C:81:ILE:N	1:C:81:ILE:CD1	2.82	0.41
2:F:55:THR:HG22	3:K:61:ALA:CB	2.50	0.41
2:H:31:ARG:C	2:H:32:TYR:CD1	2.93	0.41
3:J:133:ILE:CG2	3:J:134:ASP:N	2.83	0.41
2:B:137:GLN:HG2	2:B:137:GLN:O	2.20	0.41
2:B:172:PHE:HA	2:B:173:PRO:HD3	1.86	0.41
1:C:30:LEU:HD12	1:C:31:ASN:N	2.34	0.41
1:E:33:ARG:CZ	1:E:33:ARG:CB	2.98	0.41
1:E:130:LEU:HD22	1:E:188:LYS:HG3	2.02	0.41
2:F:141:MET:H	2:F:191:SER:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:ARG:CZ	1:G:33:ARG:CB	2.99	0.41
1:G:99:ASN:O	1:G:100:LEU:HB2	2.19	0.41
1:A:29:LEU:HD12	1:A:77:PHE:CE2	2.54	0.41
3:L:38:ILE:CD1	3:L:148:PHE:CD2	3.03	0.41
1:G:39:LEU:HD22	1:G:77:PHE:CG	2.55	0.41
1:G:53:LEU:HB3	1:G:54:ILE:CD1	2.43	0.41
1:G:81:ILE:HD12	1:G:81:ILE:H	1.85	0.41
2:H:169:VAL:O	2:H:170:HIS:HD2	2.02	0.41
2:H:194:TRP:CD1	2:H:195:PRO:HA	2.55	0.41
3:L:133:ILE:HG21	3:L:168:THR:HG21	2.02	0.41
1:A:207:THR:O	1:A:209:PRO:HD3	2.20	0.41
2:B:31:ARG:C	2:B:32:TYR:CD1	2.94	0.41
2:F:55:THR:HG22	3:K:61:ALA:HB2	2.03	0.41
2:F:151:TYR:O	2:F:152:PHE:HB2	2.19	0.41
1:A:10:SER:HA	1:A:108:LYS:O	2.21	0.41
2:F:122:THR:HG22	2:F:123:THR:N	2.36	0.41
2:H:140:SER:O	2:H:141:MET:HB2	2.21	0.41
2:H:151:TYR:CE2	2:H:156:VAL:HG13	2.54	0.41
2:H:151:TYR:O	2:H:152:PHE:HB2	2.20	0.41
2:H:183:LEU:HD23	2:H:184:SER:N	2.34	0.41
3:L:94:ALA:O	3:L:95:LEU:HD23	2.21	0.41
2:D:194:TRP:CD1	2:D:195:PRO:HA	2.56	0.41
1:G:89:LEU:O	1:G:90:ALA:HB2	2.20	0.41
1:G:155:ILE:HD12	1:G:197:TYR:CE1	2.56	0.41
2:H:31:ARG:HH12	3:L:63:ALA:HB1	1.86	0.41
3:I:52:THR:O	3:I:147:GLU:HA	2.20	0.41
3:J:94:ALA:O	3:J:95:LEU:HD23	2.21	0.41
1:A:153:TRP:O	1:A:159:GLU:HA	2.21	0.41
2:B:111:GLN:H	2:B:111:GLN:NE2	2.18	0.41
1:C:141:LEU:HD13	1:C:180:MET:HE2	2.03	0.41
2:D:137:GLN:O	2:D:137:GLN:HG2	2.21	0.41
2:D:141:MET:HA	2:D:189:VAL:O	2.19	0.41
2:D:153:PRO:HD2	2:D:207:ALA:HB1	2.03	0.41
1:E:89:LEU:O	1:E:90:ALA:HB2	2.21	0.41
1:E:165:LEU:HD21	2:F:177:GLN:OE1	2.20	0.41
1:G:37:ASN:CB	1:G:57:ALA:HB2	2.51	0.41
3:J:7:ILE:O	3:J:11:VAL:HG13	2.21	0.41
3:J:72:ALA:HB2	3:J:163:LEU:HD21	2.02	0.41
3:K:29:SER:OG	3:K:32:THR:OG1	2.12	0.41
3:L:135:GLU:O	3:L:168:THR:HB	2.21	0.41
1:A:33:ARG:CZ	1:A:33:ARG:CB	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ASN:ND2	1:A:217:ASN:OD1	2.40	0.41
2:B:141:MET:H	2:B:191:SER:H	1.69	0.41
2:D:141:MET:H	2:D:191:SER:H	1.68	0.41
1:E:195:ASN:O	1:E:215:ASN:HA	2.21	0.41
2:H:9:ALA:CB	2:H:155:PRO:HG2	2.51	0.41
2:H:102:ASP:OD1	2:H:104:TYR:HB2	2.20	0.41
3:L:6:SER:O	3:L:9:THR:HB	2.20	0.41
3:L:91:PHE:CE1	3:L:166:LEU:HD13	2.56	0.41
1:A:125:PRO:HD3	1:A:137:VAL:HG22	2.03	0.40
1:C:41:TRP:CE2	1:C:79:LEU:HB2	2.56	0.40
1:C:124:PRO:CD	2:D:219:ARG:HH12	2.29	0.40
2:D:70:LEU:HD11	2:D:81:MET:HG2	2.02	0.40
1:G:100:LEU:HD21	2:H:59:GLU:CD	2.33	0.40
3:I:80:THR:HG23	3:I:83:GLN:OE1	2.20	0.40
1:A:141:LEU:HD13	1:A:180:MET:HE2	2.03	0.40
2:B:9:ALA:CB	2:B:155:PRO:HG2	2.51	0.40
1:C:33:ARG:CZ	1:C:33:ARG:CB	2.99	0.40
1:C:91:VAL:HG22	1:C:108:LYS:HA	2.02	0.40
1:E:125:PRO:HD3	1:E:137:VAL:HG22	2.03	0.40
2:F:31:ARG:C	2:F:32:TYR:CD1	2.95	0.40
1:G:170:ASP:O	1:G:171:GLN:C	2.59	0.40
1:G:195:ASN:ND2	1:G:217:ASN:OD1	2.42	0.40
2:H:38:LYS:HB2	2:H:48:ILE:HD11	2.02	0.40
2:H:111:GLN:NE2	2:H:111:GLN:H	2.19	0.40
3:L:108:PHE:O	3:L:112:VAL:HG23	2.21	0.40
1:A:86:ALA:O	1:A:111:ILE:HD11	2.20	0.40
1:C:217:ASN:C	1:C:218:GLU:HG2	2.41	0.40
2:F:9:ALA:CB	2:F:155:PRO:HG2	2.51	0.40
2:F:176:LEU:HD13	2:F:181:TYR:CZ	2.56	0.40
1:G:160:ARG:HH12	1:G:186:LEU:HD21	1.86	0.40
3:L:18:ILE:HD13	3:L:71:ALA:CB	2.47	0.40
3:L:43:ILE:HD13	3:L:136:CYS:CB	2.51	0.40
1:A:84:VAL:CG2	1:A:85:GLN:N	2.85	0.40
2:B:141:MET:N	2:B:191:SER:OG	2.55	0.40
1:C:125:PRO:HD3	1:C:137:VAL:HG22	2.02	0.40
1:C:126:SER:CB	2:D:128:TYR:HB3	2.52	0.40
1:C:136:SER:HG	1:C:185:THR:HG23	1.86	0.40
3:J:96:ASN:O	3:J:97:ILE:CG1	2.62	0.40
3:K:148:PHE:CE1	3:K:160:ILE:HG22	2.56	0.40
2:B:122:THR:CG2	2:B:208:SER:HB3	2.52	0.40
2:F:172:PHE:HA	2:F:173:PRO:HD3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:PHE:HA	1:G:124:PRO:HD3	1.89	0.40
2:H:122:THR:CG2	2:H:208:SER:HB3	2.51	0.40
3:I:44:ARG:HH12	3:K:134:ASP:HB2	1.85	0.40
3:I:53:VAL:HG22	3:I:148:PHE:HB3	2.02	0.40
3:J:94:ALA:HB2	3:J:169:LYS:CG	2.41	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	217/219 (99%)	193 (89%)	22 (10%)	2 (1%)	17	52
1	C	217/219 (99%)	193 (89%)	22 (10%)	2 (1%)	17	52
1	E	217/219 (99%)	193 (89%)	23 (11%)	1 (0%)	29	64
1	G	217/219 (99%)	194 (89%)	22 (10%)	1 (0%)	29	64
2	B	217/219 (99%)	198 (91%)	15 (7%)	4 (2%)	8	34
2	D	217/219 (99%)	198 (91%)	15 (7%)	4 (2%)	8	34
2	F	217/219 (99%)	197 (91%)	17 (8%)	3 (1%)	11	40
2	H	217/219 (99%)	198 (91%)	15 (7%)	4 (2%)	8	34
3	I	171/184 (93%)	147 (86%)	22 (13%)	2 (1%)	13	44
3	J	171/184 (93%)	146 (85%)	25 (15%)	0	100	100
3	K	171/184 (93%)	147 (86%)	22 (13%)	2 (1%)	13	44
3	L	171/184 (93%)	147 (86%)	22 (13%)	2 (1%)	13	44
All	All	2420/2488 (97%)	2151 (89%)	242 (10%)	27 (1%)	14	46

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	133	GLY
2	B	142	VAL
2	D	133	GLY
2	D	142	VAL
2	F	133	GLY
2	F	142	VAL
2	H	133	GLY
2	H	142	VAL
1	A	58	SER
2	B	134	SER
2	D	134	SER
2	F	134	SER
2	H	134	SER
1	C	58	SER
1	G	74	GLY
3	K	99	THR
1	A	74	GLY
3	I	99	THR
3	L	99	THR
1	C	74	GLY
1	E	74	GLY
2	D	152	PHE
2	H	152	PHE
3	I	97	ILE
2	B	152	PHE
3	K	97	ILE
3	L	97	ILE

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	193/193 (100%)	184 (95%)	9 (5%)	26	59
1	C	193/193 (100%)	183 (95%)	10 (5%)	23	55
1	E	193/193 (100%)	184 (95%)	9 (5%)	26	59
1	G	193/193 (100%)	185 (96%)	8 (4%)	30	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	186/186 (100%)	177 (95%)	9 (5%)	25 58
2	D	186/186 (100%)	175 (94%)	11 (6%)	19 50
2	F	186/186 (100%)	177 (95%)	9 (5%)	25 58
2	H	186/186 (100%)	177 (95%)	9 (5%)	25 58
3	I	145/151 (96%)	144 (99%)	1 (1%)	84 93
3	J	145/151 (96%)	142 (98%)	3 (2%)	53 79
3	K	145/151 (96%)	144 (99%)	1 (1%)	84 93
3	L	145/151 (96%)	143 (99%)	2 (1%)	67 86
All	All	2096/2120 (99%)	2015 (96%)	81 (4%)	32 65

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	39	LEU
1	A	76	ASP
1	A	87	GLU
1	A	89	LEU
1	A	109	LEU
1	A	113	ARG
1	A	149	ILE
1	A	184	LEU
2	B	11	LEU
2	B	71	THR
2	B	87	THR
2	B	111	GLN
2	B	114	LEU
2	B	134	SER
2	B	139	ASN
2	B	183	LEU
2	B	200	THR
1	C	11	LEU
1	C	39	LEU
1	C	76	ASP
1	C	81	ILE
1	C	87	GLU
1	C	89	LEU
1	C	109	LEU
1	C	113	ARG

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Mol	Chain	Res	Type
1	C	149	ILE
1	C	184	LEU
2	D	11	LEU
2	D	45	LEU
2	D	48	ILE
2	D	87	THR
2	D	111	GLN
2	D	114	LEU
2	D	134	SER
2	D	139	ASN
2	D	183	LEU
2	D	200	THR
2	D	216	ILE
1	E	11	LEU
1	E	39	LEU
1	E	76	ASP
1	E	87	GLU
1	E	89	LEU
1	E	109	LEU
1	E	113	ARG
1	E	149	ILE
1	E	184	LEU
2	F	11	LEU
2	F	45	LEU
2	F	87	THR
2	F	111	GLN
2	F	114	LEU
2	F	134	SER
2	F	139	ASN
2	F	183	LEU
2	F	200	THR
1	G	11	LEU
1	G	39	LEU
1	G	76	ASP
1	G	87	GLU
1	G	89	LEU
1	G	109	LEU
1	G	113	ARG
1	G	184	LEU
2	H	11	LEU
2	H	45	LEU
2	H	71	THR

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Mol	Chain	Res	Type
2	H	111	GLN
2	H	134	SER
2	H	139	ASN
2	H	183	LEU
2	H	200	THR
2	H	216	ILE
3	I	125	LYS
3	J	33	LYS
3	J	47	HIS
3	J	125	LYS
3	K	125	LYS
3	L	47	HIS
3	L	125	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	170	HIS
2	H	170	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	E	221	-	5,5,5	0.66	0	5,5,5	0.27	0
4	GOL	E	222	-	5,5,5	0.59	0	5,5,5	0.50	0
4	GOL	A	220	-	5,5,5	0.94	0	5,5,5	0.14	0
4	GOL	K	186	-	5,5,5	0.66	0	5,5,5	0.49	0
4	GOL	E	220	-	5,5,5	0.71	0	5,5,5	0.45	0
4	GOL	I	186	-	5,5,5	0.24	0	5,5,5	0.54	0
4	GOL	J	186	-	5,5,5	0.13	0	5,5,5	0.49	0
4	GOL	L	186	-	5,5,5	0.22	0	5,5,5	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	E	221	-	-	0/4/4/4	-
4	GOL	E	222	-	-	0/4/4/4	-
4	GOL	A	220	-	-	0/4/4/4	-
4	GOL	K	186	-	-	0/4/4/4	-
4	GOL	E	220	-	-	0/4/4/4	-
4	GOL	I	186	-	-	0/4/4/4	-
4	GOL	J	186	-	-	0/4/4/4	-
4	GOL	L	186	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	222	GOL	7	0
4	A	220	GOL	5	0
4	K	186	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	186	GOL	2	0
4	J	186	GOL	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	219/219 (100%)	-0.13	2 (0%)	84	69	13, 39, 68, 100	0
1	C	219/219 (100%)	-0.13	1 (0%)	91	81	12, 39, 68, 99	0
1	E	219/219 (100%)	-0.02	3 (1%)	75	56	11, 39, 68, 100	0
1	G	219/219 (100%)	-0.05	2 (0%)	84	69	14, 40, 69, 99	0
2	B	219/219 (100%)	-0.19	3 (1%)	75	56	11, 34, 72, 101	0
2	D	219/219 (100%)	-0.15	3 (1%)	75	56	11, 33, 72, 102	0
2	F	219/219 (100%)	0.01	6 (2%)	54	31	11, 34, 72, 102	0
2	H	219/219 (100%)	-0.06	3 (1%)	75	56	11, 33, 73, 102	0
3	I	173/184 (94%)	-0.12	3 (1%)	70	49	14, 37, 63, 97	0
3	J	173/184 (94%)	-0.15	3 (1%)	70	49	13, 36, 62, 97	0
3	K	173/184 (94%)	-0.05	6 (3%)	44	23	13, 36, 62, 97	0
3	L	173/184 (94%)	-0.14	3 (1%)	70	49	15, 37, 63, 97	0
All	All	2444/2488 (98%)	-0.10	38 (1%)	72	51	11, 37, 69, 102	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	219	CYS	4.8
2	F	137	GLN	4.7
2	D	137	GLN	4.3
3	I	4	ALA	3.9
1	A	219	CYS	3.9
1	G	1	ASP	3.9
3	J	176	PRO	3.7
2	H	137	GLN	3.7
2	F	138	THR	3.6
3	K	176	PRO	3.6
2	B	139	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
3	K	91	PHE	3.5
3	I	5	ALA	3.5
2	B	137	GLN	3.4
2	D	138	THR	3.4
3	L	5	ALA	3.3
3	K	4	ALA	3.3
2	B	138	THR	3.1
1	E	1	ASP	3.0
1	C	219	CYS	2.9
3	L	176	PRO	2.8
2	F	139	ASN	2.8
2	F	136	ALA	2.6
1	A	1	ASP	2.6
3	J	175	ALA	2.6
2	H	218	PRO	2.4
3	I	123	ASP	2.4
3	K	5	ALA	2.3
2	H	138	THR	2.3
3	K	175	ALA	2.3
2	F	142	VAL	2.2
1	E	214	PHE	2.2
3	K	98	GLN	2.2
1	G	219	CYS	2.1
2	D	139	ASN	2.1
3	J	5	ALA	2.1
2	F	134	SER	2.1
3	L	101	VAL	2.1

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)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å^2)	Q<0.9
4	GOL	A	220	6/6	0.66	0.52	49,54,55,56	0
4	GOL	L	186	6/6	0.84	0.36	40,43,45,46	0
4	GOL	I	186	6/6	0.85	0.31	31,34,36,38	0
4	GOL	E	222	6/6	0.85	0.26	57,58,58,58	0
4	GOL	K	186	6/6	0.86	0.29	41,45,47,48	0
4	GOL	E	221	6/6	0.91	0.31	52,53,54,54	0
4	GOL	E	220	6/6	0.92	0.21	49,50,51,52	0
4	GOL	J	186	6/6	0.94	0.31	39,41,42,44	0

6.5 Other polymers (i)

There are no such residues in this entry.