Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:12 AM GMT

PDB ID	:	2FX8
Title	:	Crystal structure of hiv-1 neutralizing human fab 4e10 in complex with an aib-induced peptide encompassing the 4e10 epitope on gp41
Authors	:	Cardoso, R.M.F.; Brunel, F.M.; Ferguson, S.; Burton, D.R.; Dawson, P.E.; Wilson, I.A.
Deposited on	:	2006-02-03
Resolution	:	2.20 Å(reported)

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

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

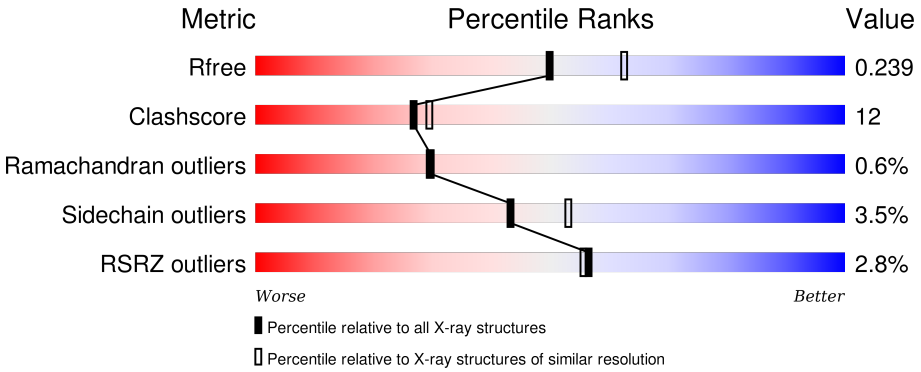
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	L	214	82% 17%
1	M	214	2% 74% 22%
1	N	214	73% 25%
1	O	214	73% 27%
2	H	227	4% 75% 22%

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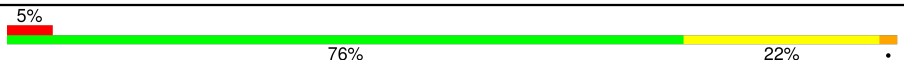
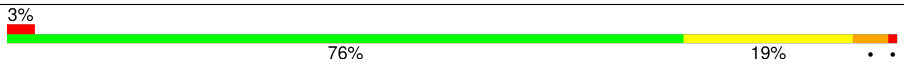
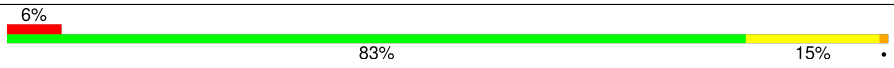
Mol	Chain	Length	Quality of chain
2	I	227	
2	J	227	
2	K	227	
3	P	12	
3	Q	12	
3	R	12	
3	S	12	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14340 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 Fab 4E10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1639	1017	284	334	4			
1	M	214	Total	C	N	O	S	0	0	0
			1639	1017	284	334	4			
1	N	214	Total	C	N	O	S	0	0	0
			1639	1017	284	334	4			
1	O	214	Total	C	N	O	S	0	0	0
			1639	1017	284	334	4			

- Molecule 2 is a protein called Fab 4E10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	227	Total	C	N	O	S	0	0	0
			1681	1063	287	326	5			
2	I	227	Total	C	N	O	S	0	0	0
			1681	1063	287	326	5			
2	J	227	Total	C	N	O	S	0	0	0
			1681	1063	287	326	5			
2	K	227	Total	C	N	O	S	0	0	0
			1681	1063	287	326	5			

- Molecule 3 is a protein called Fragment of HIV glycoprotein (GP41).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	12	Total	C	N	O	0	0	0
			115	75	22	18			
3	Q	12	Total	C	N	O	0	0	0
			115	75	22	18			
3	R	12	Total	C	N	O	0	0	0
			115	75	22	18			
3	S	12	Total	C	N	O	0	0	0
			115	75	22	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	681	ARG	TYR	ENGINEERED	UNP P05880
P	682	ARG	ILE	ENGINEERED	UNP P05880
Q	681	ARG	TYR	ENGINEERED	UNP P05880
Q	682	ARG	ILE	ENGINEERED	UNP P05880
R	681	ARG	TYR	ENGINEERED	UNP P05880
R	682	ARG	ILE	ENGINEERED	UNP P05880
S	681	ARG	TYR	ENGINEERED	UNP P05880
S	682	ARG	ILE	ENGINEERED	UNP P05880

- Molecule 4 is water.

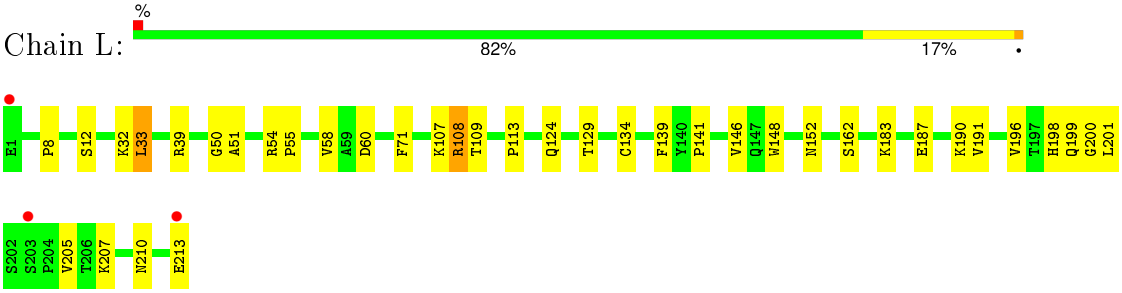
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	71	Total O 71 71	0	0
4	H	103	Total O 103 103	0	0
4	M	55	Total O 55 55	0	0
4	I	71	Total O 71 71	0	0
4	N	75	Total O 75 75	0	0
4	J	70	Total O 70 70	0	0
4	O	48	Total O 48 48	0	0
4	K	90	Total O 90 90	0	0
4	P	3	Total O 3 3	0	0
4	Q	5	Total O 5 5	0	0
4	R	5	Total O 5 5	0	0
4	S	4	Total O 4 4	0	0

3 Residue-property plots (i)

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

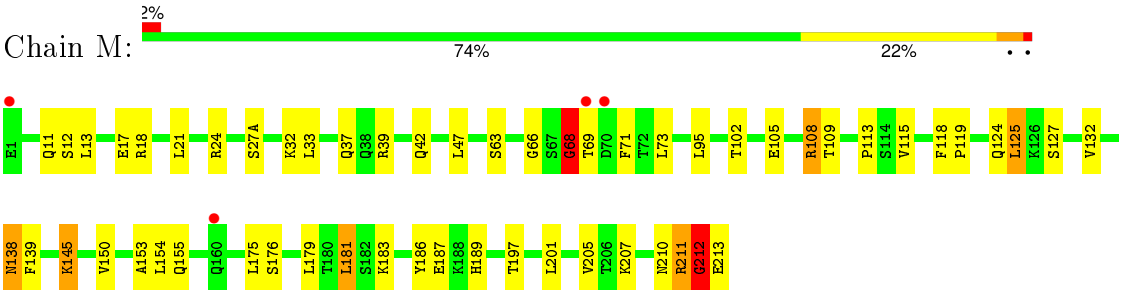
- Molecule 1: Fab 4E10

Chain L:



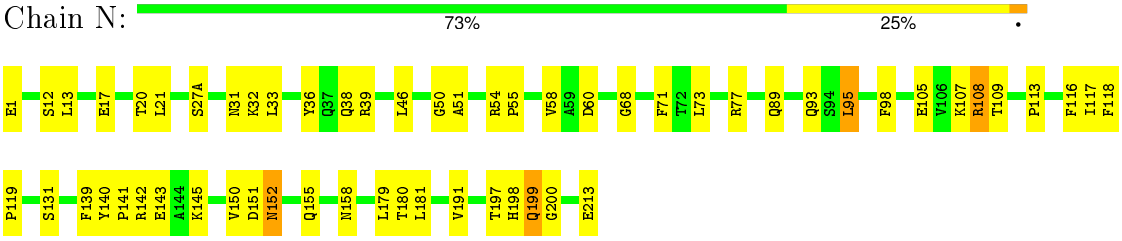
- Molecule 1: Fab 4E10

Chain M:



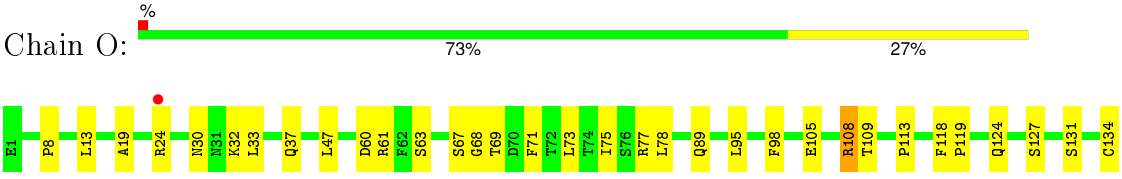
- Molecule 1: Fab 4E10

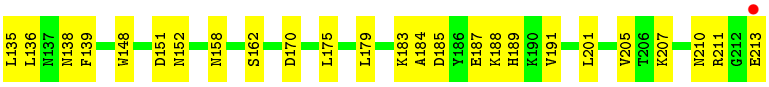
Chain N:



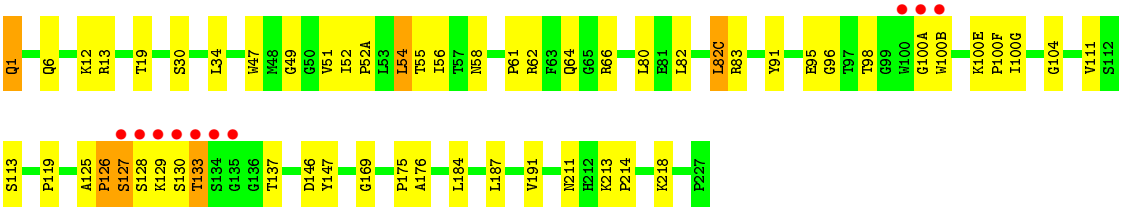
- Molecule 1: Fab 4E10

Chain O:

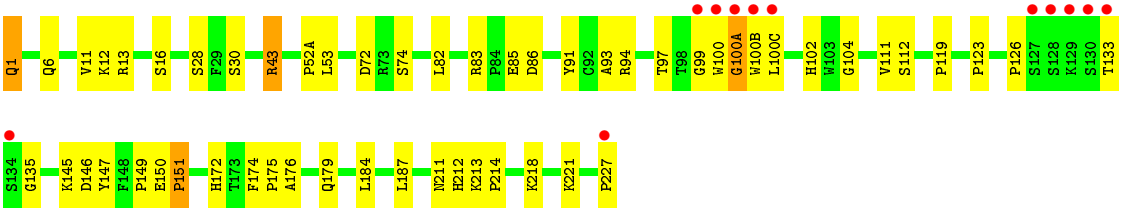




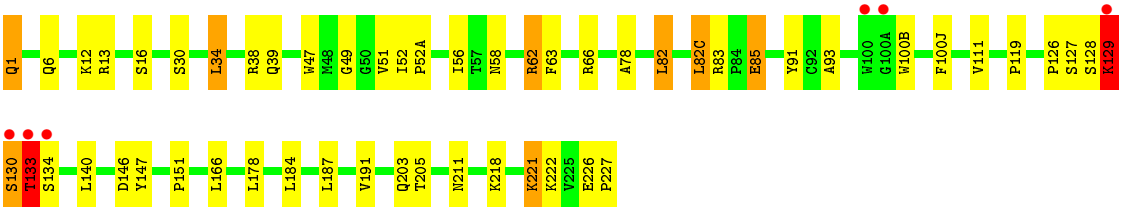
• Molecule 2: Fab 4E10



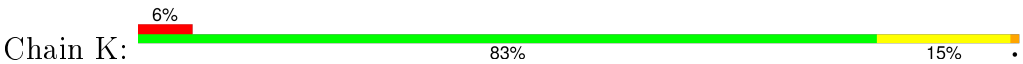
• Molecule 2: Fab 4E10

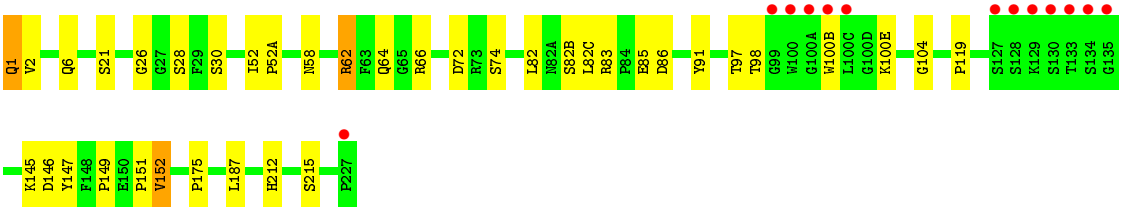


• Molecule 2: Fab 4E10

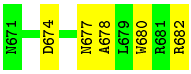


• Molecule 2: Fab 4E10





• Molecule 3: Fragment of HIV glycoprotein (GP41)

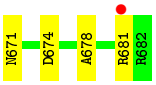


• Molecule 3: Fragment of HIV glycoprotein (GP41)

Chain Q:

• Molecule 3: Fragment of HIV glycoprotein (GP41)

Chain R:



• Molecule 3: Fragment of HIV glycoprotein (GP41)

Chain S:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.45Å 113.25Å 149.96Å 90.00° 94.15° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 49.86 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.00-2.20) 95.0 (49.86-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.283 0.234 , 0.239	Depositor DCC
R_{free} test set	4314 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	5 of 86299 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14340	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.82 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.9291e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: AIB

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	L	0.37	0/1672	0.64	0/2266
1	M	0.35	0/1672	0.72	5/2266 (0.2%)
1	N	0.37	0/1672	0.68	0/2266
1	O	0.35	0/1672	0.61	0/2266
2	H	0.37	0/1724	0.69	0/2355
2	I	0.37	0/1724	0.67	0/2355
2	J	0.36	0/1724	0.76	6/2355 (0.3%)
2	K	0.36	0/1724	0.71	2/2355 (0.1%)
3	P	0.47	0/113	0.54	0/152
3	Q	0.42	0/113	0.43	0/152
3	R	0.47	0/113	0.52	0/152
3	S	0.42	0/113	0.46	0/152
All	All	0.37	0/14036	0.68	13/19092 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	133	THR	O-C-N	8.96	137.04	122.70
2	J	130	SER	O-C-N	8.65	136.54	122.70
1	M	212	GLY	O-C-N	8.24	135.88	122.70
2	K	28	SER	O-C-N	7.73	135.07	122.70
1	M	68	GLY	O-C-N	7.31	134.39	122.70
2	J	130	SER	CA-C-N	-7.08	101.62	117.20
2	J	129	LYS	O-C-N	6.96	133.83	122.70
2	J	133	THR	CA-C-N	-6.71	102.43	117.20
2	K	28	SER	CA-C-N	-6.50	102.91	117.20
1	M	212	GLY	CA-C-N	-6.27	103.41	117.20
1	M	68	GLY	CA-C-N	-5.67	104.72	117.20
1	M	212	GLY	C-N-CA	-5.67	107.53	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	129	LYS	CA-C-N	-5.39	105.33	117.20

There are no chirality outliers.

There are no planarity outliers.

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	L	1639	0	1589	27	0
1	M	1639	0	1589	47	0
1	N	1639	0	1589	56	0
1	O	1639	0	1589	34	0
2	H	1681	0	1666	45	0
2	I	1681	0	1666	46	0
2	J	1681	0	1666	58	0
2	K	1681	0	1666	28	0
3	P	115	0	106	6	0
3	Q	115	0	106	2	0
3	R	115	0	106	3	0
3	S	115	0	106	3	0
4	H	103	0	0	1	0
4	I	71	0	0	3	0
4	J	70	0	0	0	0
4	K	90	0	0	0	0
4	L	71	0	0	1	0
4	M	55	0	0	0	0
4	N	75	0	0	0	0
4	O	48	0	0	2	0
4	P	3	0	0	0	0
4	Q	5	0	0	0	0
4	R	5	0	0	0	0
4	S	4	0	0	0	0
All	All	14340	0	13444	329	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 12.

All (329) 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)
1:N:151:ASP:O	1:N:152:ASN:ND2	1.71	1.24
2:J:119:PRO:HB3	2:J:147:TYR:HB3	1.43	0.97
1:N:116:PHE:HD1	2:J:130:SER:HB2	1.30	0.96
1:N:93:GLN:HE22	2:K:64:GLN:HE22	1.07	0.95
2:K:30:SER:HA	2:K:52(A):PRO:HB2	1.51	0.92
1:N:38:GLN:HE22	2:J:39:GLN:NE2	1.68	0.92
2:J:130:SER:C	2:J:134:SER:H	1.74	0.91
1:N:116:PHE:HD1	2:J:130:SER:CB	1.84	0.91
1:N:38:GLN:HE22	2:J:39:GLN:HE22	0.96	0.90
2:J:1:GLN:NE2	2:J:1:GLN:H1	1.68	0.90
2:J:129:LYS:NZ	2:J:130:SER:HB3	1.88	0.89
1:N:116:PHE:CD1	2:J:130:SER:CB	2.56	0.88
1:N:116:PHE:CD1	2:J:130:SER:HB2	2.10	0.87
2:I:43:ARG:HB3	2:I:43:ARG:HH21	1.40	0.87
1:N:151:ASP:C	1:N:152:ASN:HD22	1.78	0.86
2:I:211:ASN:HD21	2:I:218:LYS:HE3	1.40	0.85
1:N:117:ILE:O	2:J:129:LYS:HB2	1.75	0.85
2:I:119:PRO:HB3	2:I:147:TYR:HB3	1.58	0.84
1:N:93:GLN:NE2	2:K:64:GLN:HE22	1.75	0.84
1:N:38:GLN:NE2	2:J:39:GLN:HE22	1.76	0.83
2:J:1:GLN:NE2	2:J:1:GLN:N	2.26	0.83
2:J:1:GLN:HE21	2:J:1:GLN:H1	1.26	0.80
2:H:61:PRO:HA	2:H:64:GLN:HG3	1.64	0.79
1:O:37:GLN:HB2	1:O:47:LEU:HD11	1.66	0.78
2:K:62:ARG:HH11	2:K:62:ARG:HB2	1.49	0.78
2:I:211:ASN:ND2	2:I:218:LYS:HE3	1.99	0.76
2:J:30:SER:HA	2:J:52(A):PRO:HB2	1.65	0.76
1:M:39:ARG:HD2	1:M:42:GLN:NE2	2.01	0.76
1:N:150:VAL:HG12	1:N:155:GLN:NE2	2.05	0.72
2:K:62:ARG:NH1	2:K:62:ARG:HB2	2.04	0.72
2:K:119:PRO:HB3	2:K:147:TYR:HB3	1.71	0.72
1:N:93:GLN:HE22	2:K:64:GLN:NE2	1.85	0.72
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.72	0.71
2:K:83:ARG:HG2	2:K:86:ASP:OD2	1.90	0.71
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.73	0.70
2:K:1:GLN:NE2	2:K:1:GLN:H3	1.89	0.70
2:H:130:SER:OG	2:H:137:THR:O	2.09	0.70
1:N:198:HIS:CD2	1:N:200:GLY:H	2.09	0.70
1:L:207:LYS:HE3	2:H:133:THR:OG1	1.92	0.70
2:I:30:SER:HA	2:I:52(A):PRO:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:30:SER:HA	2:H:52(A):PRO:HB2	1.73	0.69
2:J:129:LYS:HZ3	2:J:130:SER:HB3	1.58	0.69
2:K:2:VAL:HG22	2:K:26:GLY:O	1.91	0.69
1:M:138:ASN:HD22	1:M:138:ASN:N	1.91	0.69
1:N:113:PRO:HB3	1:N:139:PHE:HB3	1.74	0.69
2:K:149:PRO:O	2:K:212:HIS:HE1	1.77	0.68
1:M:138:ASN:HD22	1:M:138:ASN:H	1.40	0.68
2:J:129:LYS:HZ2	2:J:130:SER:HB3	1.58	0.67
1:O:184:ALA:O	1:O:188:LYS:HG3	1.95	0.66
2:J:130:SER:C	2:J:134:SER:N	2.47	0.66
2:J:47:TRP:CZ2	2:J:49:GLY:HA2	2.31	0.66
2:H:130:SER:O	2:H:133:THR:HG22	1.96	0.66
2:H:1:GLN:NE2	2:H:1:GLN:H3	1.93	0.66
1:L:190:LYS:HD2	1:L:210:ASN:HB3	1.78	0.65
1:L:207:LYS:CE	2:H:133:THR:OG1	2.44	0.65
1:N:108:ARG:HD3	1:N:109:THR:O	1.97	0.64
2:H:187:LEU:C	2:H:187:LEU:HD12	2.18	0.64
1:N:54:ARG:CZ	1:N:60:ASP:HA	2.27	0.64
1:M:187:GLU:HA	1:M:211:ARG:NE	2.11	0.64
1:M:181:LEU:HD12	1:M:181:LEU:N	2.12	0.64
1:L:146:VAL:HG22	1:L:196:VAL:HG22	1.79	0.64
2:I:1:GLN:H3	2:I:1:GLN:NE2	1.96	0.64
1:L:124:GLN:HG2	1:L:129:THR:O	1.97	0.63
1:L:198:HIS:CD2	1:L:200:GLY:H	2.16	0.63
4:I:247:HOH:O	3:P:682:ARG:HD2	1.98	0.63
1:M:113:PRO:HB3	1:M:139:PHE:HB3	1.79	0.63
1:M:212:GLY:O	1:M:213:GLU:HG2	1.98	0.63
2:K:97:THR:HG21	2:K:100(B):TRP:O	1.98	0.63
1:O:19:ALA:HB3	1:O:75:ILE:HB	1.78	0.63
2:K:98:THR:HG21	2:K:100(E):LYS:HE2	1.78	0.63
1:M:108:ARG:HD3	1:M:109:THR:O	1.98	0.63
1:O:201:LEU:HD13	1:O:205:VAL:HG23	1.80	0.63
1:M:145:LYS:HB3	1:M:197:THR:HB	1.81	0.62
2:J:130:SER:O	2:J:133:THR:HG22	2.00	0.62
2:J:66:ARG:NH2	2:J:82:LEU:HD21	2.15	0.62
1:M:32:LYS:HE3	3:Q:674:ASP:OD1	2.00	0.62
1:M:39:ARG:HD2	1:M:42:GLN:HE22	1.64	0.62
2:I:43:ARG:CB	2:I:43:ARG:HH21	2.11	0.61
1:M:37:GLN:HB2	1:M:47:LEU:HD11	1.81	0.61
2:I:123:PRO:HD3	2:I:221:LYS:HE2	1.84	0.60
2:J:130:SER:O	2:J:134:SER:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:33:LEU:HD13	1:O:71:PHE:CG	2.37	0.59
2:J:6:GLN:HE22	2:J:91:TYR:HA	1.66	0.59
1:N:32:LYS:HE3	3:R:674:ASP:OD1	2.02	0.59
2:I:176:ALA:HB2	2:I:187:LEU:HD23	1.85	0.59
2:J:146:ASP:HB3	2:J:184:LEU:HD13	1.84	0.59
1:M:210:ASN:HB2	1:M:213:GLU:HG3	1.83	0.59
1:L:201:LEU:HD13	1:L:205:VAL:HG23	1.85	0.59
2:I:146:ASP:HB3	2:I:184:LEU:HD13	1.85	0.59
2:J:13:ARG:HH11	2:J:13:ARG:HG3	1.67	0.58
1:N:17:GLU:O	1:N:77:ARG:HA	2.04	0.58
1:O:24:ARG:HG3	1:O:24:ARG:HH11	1.68	0.58
2:I:212:HIS:CE1	2:I:214:PRO:HB2	2.37	0.58
2:I:28:SER:HA	4:I:292:HOH:O	2.04	0.58
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.39	0.58
2:K:187:LEU:HD12	2:K:187:LEU:C	2.24	0.58
2:J:126:PRO:HG2	2:J:227:PRO:HA	1.86	0.58
2:J:83:ARG:HB3	2:J:85:GLU:OE2	2.03	0.58
2:I:83:ARG:HG2	2:I:86:ASP:OD2	2.03	0.58
2:J:130:SER:C	2:J:133:THR:HG22	2.24	0.57
1:O:162:SER:OG	2:K:175:PRO:HD2	2.04	0.57
2:J:187:LEU:C	2:J:187:LEU:HD12	2.24	0.57
2:I:97:THR:OG1	2:I:100(B):TRP:HA	2.05	0.57
1:O:108:ARG:HD3	1:O:109:THR:O	2.04	0.57
2:J:62:ARG:HD2	2:J:63:PHE:CZ	2.39	0.57
1:N:179:LEU:HG	1:N:181:LEU:HD11	1.87	0.57
2:K:212:HIS:HD2	2:K:215:SER:OG	1.86	0.56
2:I:1:GLN:N	2:I:1:GLN:NE2	2.53	0.56
1:N:1:GLU:HG2	1:N:95:LEU:CD1	2.35	0.56
2:H:96:GLY:O	2:H:100(G):ILE:HG12	2.05	0.56
1:N:1:GLU:HG2	1:N:95:LEU:HD13	1.87	0.56
1:O:183:LYS:O	1:O:187:GLU:HG3	2.05	0.56
2:I:176:ALA:HA	2:I:187:LEU:HB3	1.88	0.56
1:N:55:PRO:HG2	1:N:58:VAL:CG2	2.36	0.56
1:L:54:ARG:CZ	1:L:60:ASP:HA	2.36	0.56
2:H:54:LEU:HD23	2:H:56:ILE:HD12	1.88	0.56
2:H:6:GLN:HE22	2:H:91:TYR:HA	1.71	0.56
1:O:8:PRO:HB2	4:O:241:HOH:O	2.06	0.56
2:K:6:GLN:HE21	2:K:104:GLY:HA3	1.71	0.56
2:I:43:ARG:NH2	2:I:43:ARG:HB3	2.17	0.55
2:J:119:PRO:CB	2:J:147:TYR:HB3	2.28	0.55
1:L:108:ARG:HD3	1:L:109:THR:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:151:ASP:H	1:N:191:VAL:HG13	1.71	0.55
2:H:1:GLN:N	2:H:1:GLN:CD	2.60	0.55
2:H:82:LEU:HD22	2:H:82(C):LEU:CD1	2.37	0.55
1:M:212:GLY:O	1:M:213:GLU:CG	2.55	0.55
1:N:179:LEU:HG	1:N:181:LEU:CD1	2.37	0.55
1:N:150:VAL:CG1	1:N:155:GLN:NE2	2.70	0.54
2:J:38:ARG:NH1	2:J:62:ARG:NH2	2.55	0.54
2:I:126:PRO:HG2	2:I:227:PRO:HG3	1.88	0.54
3:P:678:AIB:O	3:P:682:ARG:HG2	2.08	0.54
2:H:66:ARG:NH1	2:H:83:ARG:HH21	2.05	0.54
1:N:54:ARG:NH1	1:N:60:ASP:HA	2.23	0.54
1:L:213:GLU:HA	1:L:213:GLU:OE2	2.07	0.54
1:M:124:GLN:O	1:M:127:SER:HB3	2.08	0.53
2:H:128:SER:C	2:H:130:SER:N	2.61	0.53
2:J:38:ARG:NH1	2:J:62:ARG:HH22	2.06	0.53
2:H:82:LEU:HD22	2:H:82(C):LEU:HD12	1.91	0.53
1:L:162:SER:OG	2:H:175:PRO:HD2	2.08	0.53
1:M:21:LEU:HD22	1:M:102:THR:HG21	1.89	0.53
1:M:33:LEU:HD13	1:M:71:PHE:CD2	2.44	0.53
2:H:214:PRO:HA	4:H:323:HOH:O	2.08	0.53
1:M:138:ASN:ND2	1:M:138:ASN:N	2.52	0.53
3:R:678:AIB:HB22	3:R:681:ARG:HB2	1.92	0.52
2:H:129:LYS:C	2:H:133:THR:H	2.13	0.52
1:N:145:LYS:HB3	1:N:197:THR:HB	1.90	0.52
1:N:180:THR:C	1:N:181:LEU:HD12	2.29	0.52
1:M:24:ARG:HG3	1:M:24:ARG:HH11	1.73	0.52
1:L:210:ASN:O	1:L:213:GLU:HG2	2.09	0.52
1:N:55:PRO:HG2	1:N:58:VAL:HG21	1.91	0.52
3:R:671:ASN:HB3	3:R:674:ASP:OD2	2.10	0.52
2:J:128:SER:HA	2:J:133:THR:HB	1.91	0.52
1:M:189:HIS:O	1:M:211:ARG:NH2	2.41	0.52
1:L:12:SER:HB3	1:L:107:LYS:HB2	1.92	0.52
1:M:115:VAL:HG12	1:M:207:LYS:HG3	1.93	0.51
2:I:72:ASP:OD1	2:I:74:SER:HB2	2.11	0.51
1:N:150:VAL:HG13	1:N:150:VAL:O	2.10	0.51
2:I:100(A):GLY:O	2:I:100(B):TRP:HB2	2.09	0.51
1:O:24:ARG:HG3	1:O:24:ARG:NH1	2.25	0.51
2:H:13:ARG:HD3	2:H:113:SER:HA	1.93	0.51
2:H:1:GLN:NE2	2:H:1:GLN:N	2.59	0.51
2:I:6:GLN:HE21	2:I:104:GLY:HA3	1.76	0.51
1:L:141:PRO:O	1:L:198:HIS:HE1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:67:SER:HA	1:O:71:PHE:CE1	2.47	0.50
2:I:126:PRO:CG	2:I:227:PRO:HG3	2.40	0.50
2:J:211:ASN:HD21	2:J:218:LYS:NZ	2.10	0.50
2:H:211:ASN:HD22	2:H:218:LYS:HG2	1.76	0.50
2:J:12:LYS:O	2:J:111:VAL:HA	2.11	0.50
1:O:32:LYS:HE3	3:S:674:ASP:OD1	2.12	0.50
1:O:211:ARG:HH11	1:O:211:ARG:HG2	1.76	0.50
2:H:34:LEU:C	2:H:34:LEU:HD13	2.32	0.50
1:O:185:ASP:HA	1:O:188:LYS:HD2	1.93	0.50
1:M:211:ARG:NH2	1:M:211:ARG:HB3	2.25	0.50
2:J:221:LYS:HB2	2:J:221:LYS:NZ	2.26	0.50
1:N:116:PHE:CD1	2:J:130:SER:OG	2.65	0.49
1:O:63:SER:O	1:O:73:LEU:HD12	2.12	0.49
1:N:151:ASP:OD1	1:N:191:VAL:HG12	2.12	0.49
2:J:128:SER:C	2:J:130:SER:N	2.65	0.49
2:H:128:SER:C	2:H:130:SER:H	2.15	0.49
1:M:33:LEU:HD13	1:M:71:PHE:CG	2.46	0.49
1:N:142:ARG:HG2	1:N:142:ARG:HH21	1.77	0.49
1:O:175:LEU:C	1:O:175:LEU:HD23	2.33	0.49
3:P:678:AIB:HB21	3:P:682:ARG:HH12	1.78	0.49
2:J:166:LEU:HD21	2:J:191:VAL:HG21	1.93	0.49
2:K:152:VAL:HG23	2:K:212:HIS:HB2	1.95	0.49
2:I:83:ARG:HG3	2:I:85:GLU:HB3	1.95	0.49
1:O:61:ARG:HD2	1:O:77:ARG:O	2.13	0.49
1:M:27(A):SER:HA	1:M:68:GLY:O	2.12	0.49
2:K:1:GLN:NE2	2:K:1:GLN:N	2.59	0.48
2:I:12:LYS:HB3	2:I:16:SER:OG	2.13	0.48
1:N:213:GLU:HA	1:N:213:GLU:OE2	2.12	0.48
2:I:133:THR:C	2:I:135:GLY:H	2.14	0.48
1:M:186:TYR:CZ	1:M:211:ARG:HG3	2.49	0.48
2:J:82:LEU:HD22	2:J:82(C):LEU:CD1	2.44	0.48
1:L:183:LYS:O	1:L:187:GLU:HG3	2.13	0.48
1:M:212:GLY:C	1:M:213:GLU:HG2	2.33	0.48
1:L:108:ARG:CD	1:L:109:THR:O	2.61	0.48
2:I:99:GLY:O	2:I:100:TRP:HB2	2.12	0.48
1:L:191:VAL:HG22	1:L:210:ASN:OD1	2.13	0.48
1:O:191:VAL:HG22	1:O:210:ASN:OD1	2.13	0.48
1:L:32:LYS:HE3	3:P:674:ASP:OD1	2.14	0.48
1:M:145:LYS:NZ	1:M:145:LYS:HB2	2.28	0.48
2:H:169:GLY:O	2:H:191:VAL:HA	2.13	0.48
2:J:126:PRO:HB3	2:J:140:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:113:PRO:HB3	1:O:139:PHE:HB3	1.94	0.48
2:I:1:GLN:N	2:I:1:GLN:CD	2.67	0.47
1:O:151:ASP:OD2	1:O:189:HIS:HB3	2.14	0.47
1:N:155:GLN:HB3	1:N:158:ASN:HB2	1.96	0.47
2:J:127:SER:C	2:J:129:LYS:H	2.16	0.47
1:L:207:LYS:HE2	2:H:133:THR:OG1	2.13	0.47
2:I:86:ASP:HB2	2:I:111:VAL:HG21	1.97	0.47
2:K:6:GLN:HE22	2:K:91:TYR:HA	1.79	0.47
1:N:33:LEU:HD22	1:N:71:PHE:CG	2.48	0.47
1:O:89:GLN:HB2	1:O:98:PHE:CD1	2.50	0.47
2:J:62:ARG:HD2	2:J:63:PHE:CE1	2.50	0.47
1:N:181:LEU:HD12	1:N:181:LEU:N	2.29	0.47
1:O:13:LEU:HD12	1:O:78:LEU:HD11	1.97	0.47
1:L:134:CYS:HB2	1:L:148:TRP:CZ2	2.50	0.47
1:N:199:GLN:HB3	1:N:199:GLN:HE21	1.56	0.47
2:J:128:SER:C	2:J:130:SER:H	2.18	0.47
1:N:143:GLU:H	1:N:143:GLU:CD	2.18	0.46
2:I:213:LYS:HB3	2:I:214:PRO:HD3	1.97	0.46
1:M:24:ARG:HA	1:M:69:THR:O	2.15	0.46
2:I:145:LYS:NZ	2:I:179:GLN:OE1	2.48	0.46
1:M:39:ARG:HG2	1:M:39:ARG:HH11	1.79	0.46
1:M:132:VAL:HB	1:M:179:LEU:HB3	1.97	0.46
2:H:126:PRO:O	2:H:127:SER:HB2	2.16	0.46
2:K:72:ASP:OD1	2:K:74:SER:HB3	2.16	0.46
1:O:33:LEU:HD13	1:O:71:PHE:CD2	2.51	0.46
1:M:150:VAL:O	1:M:153:ALA:HB3	2.16	0.46
1:O:134:CYS:HB2	1:O:148:TRP:CH2	2.50	0.46
2:I:119:PRO:CB	2:I:147:TYR:HB3	2.39	0.45
1:M:11:GLN:HG2	1:M:13:LEU:HD21	1.97	0.45
1:N:12:SER:O	1:N:13:LEU:HD23	2.15	0.45
2:J:129:LYS:HG2	2:J:130:SER:N	2.31	0.45
1:L:8:PRO:HB2	4:L:245:HOH:O	2.17	0.45
2:H:187:LEU:C	2:H:187:LEU:CD1	2.85	0.45
1:N:20:THR:C	1:N:21:LEU:HD12	2.37	0.45
2:J:1:GLN:HA	2:J:100(B):TRP:CE2	2.52	0.45
2:K:83:ARG:HG3	2:K:85:GLU:HB2	1.98	0.45
2:I:211:ASN:HD21	2:I:218:LYS:CE	2.21	0.44
1:O:201:LEU:HD13	1:O:205:VAL:CG2	2.45	0.44
1:M:125:LEU:HD12	1:M:183:LYS:HG3	1.99	0.44
1:L:39:ARG:HG2	1:L:39:ARG:HH11	1.83	0.44
1:N:21:LEU:N	1:N:21:LEU:HD12	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:31:ASN:HD21	1:N:68:GLY:H	1.65	0.44
2:I:149:PRO:HD2	2:I:214:PRO:HB3	2.00	0.44
2:I:13:ARG:HA	2:I:112:SER:O	2.18	0.44
2:H:98:THR:HG21	2:H:100(E):LYS:HE2	1.99	0.44
1:N:150:VAL:HA	1:N:191:VAL:O	2.17	0.43
2:H:12:LYS:O	2:H:111:VAL:HA	2.18	0.43
2:H:6:GLN:HE21	2:H:104:GLY:HA3	1.84	0.43
2:K:66:ARG:HD2	2:K:82(B):SER:HB2	1.99	0.43
2:H:95:GLU:OE1	2:H:100(F):PRO:HB2	2.18	0.43
1:O:207:LYS:HE2	4:O:226:HOH:O	2.17	0.43
3:Q:679:LEU:HD22	3:Q:682:ARG:HH21	1.83	0.43
2:H:213:LYS:HB3	2:H:214:PRO:HD3	2.00	0.43
1:M:201:LEU:HD13	1:M:205:VAL:HG23	1.99	0.43
2:J:93:ALA:HB1	2:J:100(J):PHE:HB3	2.00	0.43
2:I:43:ARG:HD2	2:I:43:ARG:HA	1.86	0.43
2:H:176:ALA:HA	2:H:187:LEU:HB3	2.01	0.43
2:I:11:VAL:HG21	2:I:149:PRO:HG3	2.00	0.43
2:J:56:ILE:HD11	3:S:679:LEU:HD21	2.00	0.43
2:H:213:LYS:HB2	2:H:213:LYS:HE3	1.88	0.43
2:J:222:LYS:HE2	2:J:226:GLU:CG	2.47	0.43
1:M:33:LEU:HD23	1:M:33:LEU:C	2.39	0.43
1:M:17:GLU:HG2	1:M:18:ARG:H	1.83	0.43
1:M:175:LEU:HD23	1:M:176:SER:N	2.34	0.43
1:M:138:ASN:ND2	2:I:172:HIS:NE2	2.64	0.43
2:H:100(E):LYS:HG3	3:P:677:ASN:ND2	2.34	0.43
2:I:94:ARG:HD3	4:I:269:HOH:O	2.19	0.43
2:K:98:THR:CG2	2:K:100(E):LYS:HB3	2.48	0.43
1:O:210:ASN:O	1:O:213:GLU:HG2	2.18	0.43
2:J:129:LYS:NZ	2:J:130:SER:CB	2.72	0.42
2:J:1:GLN:CD	2:J:1:GLN:N	2.72	0.42
2:H:51:VAL:HG22	2:H:52:ILE:N	2.34	0.42
2:I:52(A):PRO:O	2:I:53:LEU:C	2.58	0.42
1:O:24:ARG:HA	1:O:69:THR:O	2.19	0.42
2:I:1:GLN:CD	2:I:1:GLN:H1	2.22	0.42
1:O:118:PHE:HA	1:O:119:PRO:HD3	1.90	0.42
1:N:140:TYR:CG	1:N:141:PRO:HA	2.55	0.42
2:H:146:ASP:HB3	2:H:184:LEU:HD13	2.00	0.42
1:M:211:ARG:HH21	1:M:211:ARG:CB	2.33	0.42
1:M:12:SER:O	1:M:13:LEU:HD23	2.19	0.42
2:K:1:GLN:CD	2:K:1:GLN:N	2.73	0.42
1:M:66:GLY:HA3	1:M:71:PHE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:142:ARG:HG2	1:N:142:ARG:NH2	2.34	0.42
2:H:100(E):LYS:HB2	3:P:680:TRP:CH2	2.54	0.42
1:M:175:LEU:C	1:M:175:LEU:HD23	2.40	0.42
2:J:51:VAL:HG22	2:J:52:ILE:N	2.35	0.42
1:M:150:VAL:HG23	1:M:155:GLN:CG	2.50	0.41
1:N:12:SER:HB3	1:N:107:LYS:HB2	2.02	0.41
2:H:19:THR:HA	2:H:80:LEU:O	2.20	0.41
1:O:158:ASN:ND2	1:O:179:LEU:HD11	2.35	0.41
2:I:6:GLN:HE22	2:I:91:TYR:HA	1.85	0.41
2:I:93:ALA:HA	2:I:102:HIS:O	2.20	0.41
1:N:55:PRO:HG2	1:N:58:VAL:HG23	2.02	0.41
1:L:50:GLY:O	1:L:51:ALA:HB3	2.20	0.41
2:H:125:ALA:HA	2:H:126:PRO:HD3	1.97	0.41
2:I:150:GLU:OE1	2:I:151:PRO:HA	2.19	0.41
1:M:118:PHE:HA	1:M:119:PRO:HD3	1.93	0.41
1:N:50:GLY:O	1:N:51:ALA:HB3	2.21	0.41
1:O:135:LEU:C	1:O:136:LEU:HD12	2.40	0.41
1:M:108:ARG:CD	1:M:109:THR:O	2.68	0.41
2:H:54:LEU:O	2:H:55:THR:OG1	2.34	0.41
1:N:36:TYR:CE2	1:N:46:LEU:HD13	2.54	0.41
1:O:124:GLN:HE22	1:O:131:SER:CB	2.33	0.41
1:O:138:ASN:ND2	1:O:170:ASP:OD2	2.54	0.41
2:I:187:LEU:C	2:I:187:LEU:HD12	2.41	0.41
2:J:12:LYS:HB3	2:J:16:SER:OG	2.21	0.41
1:N:118:PHE:HA	1:N:119:PRO:HD3	1.92	0.41
2:J:34:LEU:HD22	2:J:78:ALA:CB	2.50	0.41
1:N:89:GLN:HB2	1:N:98:PHE:CD1	2.56	0.41
1:M:186:TYR:CE2	1:M:211:ARG:HD2	2.56	0.40
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.56	0.40
1:M:63:SER:O	1:M:73:LEU:HD12	2.21	0.40
1:N:39:ARG:HH11	1:N:39:ARG:HG2	1.84	0.40
2:J:130:SER:HB3	2:J:133:THR:H	1.37	0.40
2:K:6:GLN:HA	2:K:21:SER:O	2.21	0.40
1:L:108:ARG:HD3	1:L:109:THR:N	2.36	0.40
2:H:100(A):GLY:HA2	2:H:100(B):TRP:CE3	2.56	0.40
2:J:203:GLN:OE1	2:J:205:THR:N	2.53	0.40
2:I:174:PHE:HA	2:I:175:PRO:HD3	1.97	0.40
2:K:145:LYS:HG2	2:K:146:ASP:N	2.37	0.40
2:I:213:LYS:N	2:I:214:PRO:CD	2.84	0.40
1:N:131:SER:HA	1:N:179:LEU:O	2.21	0.40
2:J:211:ASN:ND2	2:J:218:LYS:NZ	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:55:PRO:HG2	1:L:58:VAL:HG23	2.04	0.40
2:K:52:ILE:HG13	3:S:672:TRP:CZ2	2.57	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	L	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
1	M	212/214 (99%)	200 (94%)	9 (4%)	3 (1%)	14	10
1	N	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
1	O	212/214 (99%)	198 (93%)	12 (6%)	2 (1%)	21	19
2	H	225/227 (99%)	209 (93%)	13 (6%)	3 (1%)	15	11
2	I	225/227 (99%)	212 (94%)	12 (5%)	1 (0%)	39	42
2	J	225/227 (99%)	209 (93%)	15 (7%)	1 (0%)	39	42
2	K	225/227 (99%)	215 (96%)	10 (4%)	0	100	100
3	P	9/12 (75%)	9 (100%)	0	0	100	100
3	Q	9/12 (75%)	9 (100%)	0	0	100	100
3	R	9/12 (75%)	9 (100%)	0	0	100	100
3	S	9/12 (75%)	9 (100%)	0	0	100	100
All	All	1784/1812 (98%)	1688 (95%)	86 (5%)	10 (1%)	30	29

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	211	ARG
2	I	100(A)	GLY

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Mol	Chain	Res	Type
1	O	30	ASN
2	H	127	SER
2	H	133	THR
2	J	133	THR
1	O	68	GLY
1	M	68	GLY
2	H	126	PRO
1	M	212	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	L	184/184 (100%)	180 (98%)	4 (2%)	60 72
1	M	184/184 (100%)	176 (96%)	8 (4%)	35 43
1	N	184/184 (100%)	177 (96%)	7 (4%)	40 49
1	O	184/184 (100%)	178 (97%)	6 (3%)	45 56
2	H	186/186 (100%)	181 (97%)	5 (3%)	52 64
2	I	186/186 (100%)	181 (97%)	5 (3%)	52 64
2	J	186/186 (100%)	175 (94%)	11 (6%)	24 27
2	K	186/186 (100%)	179 (96%)	7 (4%)	40 49
3	P	11/11 (100%)	11 (100%)	0	100 100
3	Q	11/11 (100%)	11 (100%)	0	100 100
3	R	11/11 (100%)	11 (100%)	0	100 100
3	S	11/11 (100%)	11 (100%)	0	100 100
All	All	1524/1524 (100%)	1471 (96%)	53 (4%)	43 53

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	33	LEU
1	L	108	ARG

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Mol	Chain	Res	Type
1	L	152	ASN
1	L	199	GLN
2	H	1	GLN
2	H	54	LEU
2	H	58	ASN
2	H	62	ARG
2	H	82(C)	LEU
1	M	95	LEU
1	M	105	GLU
1	M	108	ARG
1	M	125	LEU
1	M	138	ASN
1	M	145	LYS
1	M	154	LEU
1	M	181	LEU
2	I	1	GLN
2	I	43	ARG
2	I	82	LEU
2	I	100(C)	LEU
2	I	151	PRO
1	N	27(A)	SER
1	N	73	LEU
1	N	95	LEU
1	N	105	GLU
1	N	108	ARG
1	N	152	ASN
1	N	199	GLN
2	J	1	GLN
2	J	34	LEU
2	J	58	ASN
2	J	62	ARG
2	J	82	LEU
2	J	82(C)	LEU
2	J	85	GLU
2	J	129	LYS
2	J	151	PRO
2	J	178	LEU
2	J	221	LYS
1	O	60	ASP
1	O	95	LEU
1	O	105	GLU
1	O	108	ARG

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Mol	Chain	Res	Type
1	O	127	SER
1	O	152	ASN
2	K	1	GLN
2	K	58	ASN
2	K	62	ARG
2	K	82	LEU
2	K	82(C)	LEU
2	K	151	PRO
2	K	152	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	93	GLN
1	L	152	ASN
1	L	160	GLN
1	L	198	HIS
1	L	199	GLN
2	H	1	GLN
2	H	6	GLN
2	H	58	ASN
2	H	82(A)	ASN
2	H	211	ASN
1	M	31	ASN
1	M	42	GLN
1	M	138	ASN
1	M	147	GLN
1	M	160	GLN
1	M	199	GLN
2	I	1	GLN
2	I	6	GLN
2	I	58	ASN
2	I	211	ASN
1	N	31	ASN
1	N	42	GLN
1	N	155	GLN
1	N	158	ASN
1	N	160	GLN
1	N	198	HIS
1	N	199	GLN
2	J	1	GLN
2	J	3	GLN

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Mol	Chain	Res	Type
2	J	6	GLN
2	J	39	GLN
2	J	58	ASN
2	J	64	GLN
2	J	82(A)	ASN
2	J	211	ASN
1	O	147	GLN
1	O	152	ASN
1	O	199	GLN
2	K	1	GLN
2	K	6	GLN
2	K	58	ASN
2	K	64	GLN
2	K	82(A)	ASN
2	K	212	HIS
3	P	677	ASN
3	R	677	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	AIB	P	678	3	1,5,6	0.98	0	1,7,9	0.48	0
3	AIB	Q	678	3	1,5,6	0.98	0	1,7,9	0.78	0
3	AIB	R	678	3	1,5,6	1.06	0	1,7,9	0.65	0
3	AIB	S	678	3	1,5,6	1.11	0	1,7,9	0.51	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
3	AIB	P	678	3	-	0/2/3/6	0/0/0/0
3	AIB	Q	678	3	-	0/2/3/6	0/0/0/0
3	AIB	R	678	3	-	0/2/3/6	0/0/0/0
3	AIB	S	678	3	-	0/2/3/6	0/0/0/0

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	678	AIB	2	0
3	R	678	AIB	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	L	214/214 (100%)	-0.14	3 (1%) 78 77	16, 28, 40, 62	0
1	M	214/214 (100%)	0.02	4 (1%) 70 68	20, 35, 47, 65	0
1	N	214/214 (100%)	-0.11	0 100 100	13, 27, 45, 69	0
1	O	214/214 (100%)	0.06	2 (0%) 85 85	19, 36, 51, 76	0
2	H	227/227 (100%)	0.07	10 (4%) 38 37	18, 26, 48, 82	0
2	I	227/227 (100%)	0.24	12 (5%) 30 29	19, 30, 54, 83	0
2	J	227/227 (100%)	0.05	6 (2%) 59 58	17, 28, 46, 79	0
2	K	227/227 (100%)	0.26	13 (5%) 27 27	17, 29, 57, 83	0
3	P	11/12 (91%)	0.17	0 100 100	17, 25, 57, 62	0
3	Q	11/12 (91%)	0.36	0 100 100	26, 31, 58, 58	0
3	R	11/12 (91%)	0.15	1 (9%) 11 11	20, 22, 60, 66	0
3	S	11/12 (91%)	0.25	0 100 100	25, 31, 55, 55	0
All	All	1808/1812 (99%)	0.06	51 (2%) 56 55	13, 30, 51, 83	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	130	SER	15.1
2	K	100(A)	GLY	12.4
2	I	133	THR	11.6
2	K	100(B)	TRP	11.0
2	H	133	THR	10.6
2	K	133	THR	10.3
2	I	100(A)	GLY	9.4
2	I	130	SER	8.7
2	K	100	TRP	8.7
2	J	133	THR	8.1
2	I	100	TRP	7.7

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Mol	Chain	Res	Type	RSRZ
2	H	129	LYS	7.4
2	K	134	SER	6.8
2	J	100	TRP	6.5
2	I	100(B)	TRP	6.3
2	H	100	TRP	6.1
2	I	134	SER	6.0
2	K	129	LYS	5.9
2	H	130	SER	5.5
2	J	134	SER	5.3
1	O	213	GLU	4.9
2	K	130	SER	4.8
2	I	128	SER	4.4
2	H	134	SER	4.2
2	K	100(C)	LEU	4.0
2	K	127	SER	3.8
2	H	127	SER	3.4
2	I	127	SER	3.3
1	L	203	SER	3.2
2	I	129	LYS	3.1
1	M	70	ASP	3.0
2	J	129	LYS	2.8
2	K	128	SER	2.7
2	I	100(C)	LEU	2.7
2	K	99	GLY	2.6
1	L	1	GLU	2.5
1	L	213	GLU	2.5
2	I	99	GLY	2.4
3	R	681	ARG	2.4
2	J	100(A)	GLY	2.4
2	H	135	GLY	2.4
2	I	227	PRO	2.4
2	H	100(A)	GLY	2.3
2	K	227	PRO	2.2
2	H	128	SER	2.1
2	K	135	GLY	2.1
2	H	100(B)	TRP	2.1
1	M	160	GLN	2.1
1	M	69	THR	2.0
1	O	24	ARG	2.0
1	M	1	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	AIB	S	678	6/7	0.91	0.12	-	35,36,38,39	0
3	AIB	R	678	6/7	0.92	0.11	-	30,31,33,34	0
3	AIB	Q	678	6/7	0.92	0.14	-	37,37,38,39	0
3	AIB	P	678	6/7	0.86	0.13	-	29,31,34,35	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.