Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:29 PM GMT

PDB ID	:	1XF5
Title	:	Complex HCV core-Fab 19D9D6-Protein L mutant (H74C, Y64W)in space group P21212
Authors	:	Menez, R.; Housden, N.G.; Harrison, S.; Jolivet-Reynaud, C.; Gore, M.G.; Stura, E.A.
Deposited on	:	2004-09-14
Resolution	:	2.60 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:

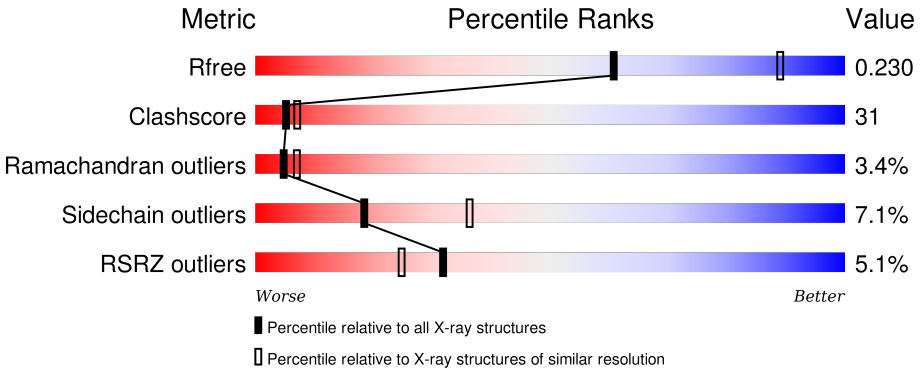
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	P	44	14% 23% 9% 64%
1	Q	44	11% 14% 82%
2	A	220	% 64% 29% 5%
2	C	220	5% 58% 35% 5%
3	B	218	3% 65% 28% 5%

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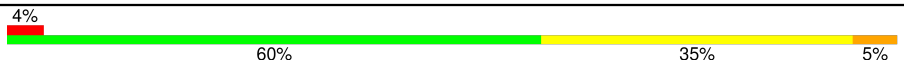
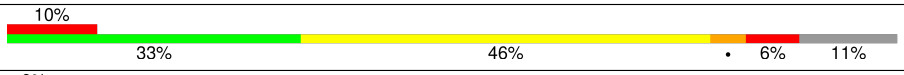
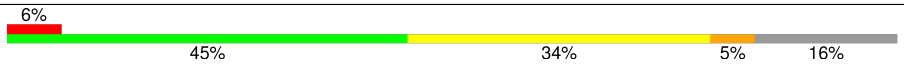
Mol	Chain	Length	Quality of chain
3	D	218	
4	L	80	
4	M	80	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8420 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 Capsid protein C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	P	16	Total	C	N	O	0	0	0
			115	74	23	18			
1	Q	8	Total	C	N	O	0	0	0
			59	40	9	10			

- Molecule 2 is a protein called Monoclonal antibody 19D9D6 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	220	Total	C	N	O	S	0	0	0
			1708	1063	291	346	8			
2	C	220	Total	C	N	O	S	3	0	0
			1708	1063	291	346	8			

- Molecule 3 is a protein called Monoclonal antibody 19D9D6 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	218	Total	C	N	O	S	0	0	0
			1660	1058	270	325	7			
3	D	218	Total	C	N	O	S	0	0	0
			1660	1058	270	325	7			

- Molecule 4 is a protein called Protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	71	Total	C	N	O	S	0	0	0
			547	346	87	112	2			
4	M	67	Total	C	N	O	S	0	0	0
			517	328	83	104	2			

- Molecule 5 is water.

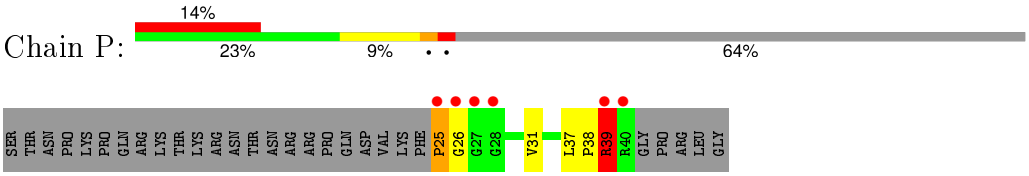
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	141	Total O 141 141	0	0
5	B	115	Total O 115 115	0	0
5	C	68	Total O 68 68	0	0
5	D	75	Total O 75 75	0	0
5	L	15	Total O 15 15	0	0
5	M	23	Total O 23 23	0	0
5	P	8	Total O 8 8	0	0
5	Q	1	Total O 1 1	0	0

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.

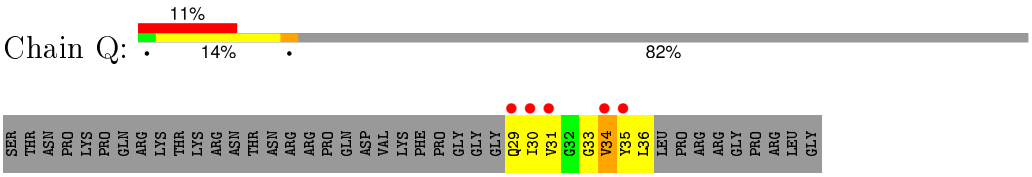
- Molecule 1: Capsid protein C

Chain P:



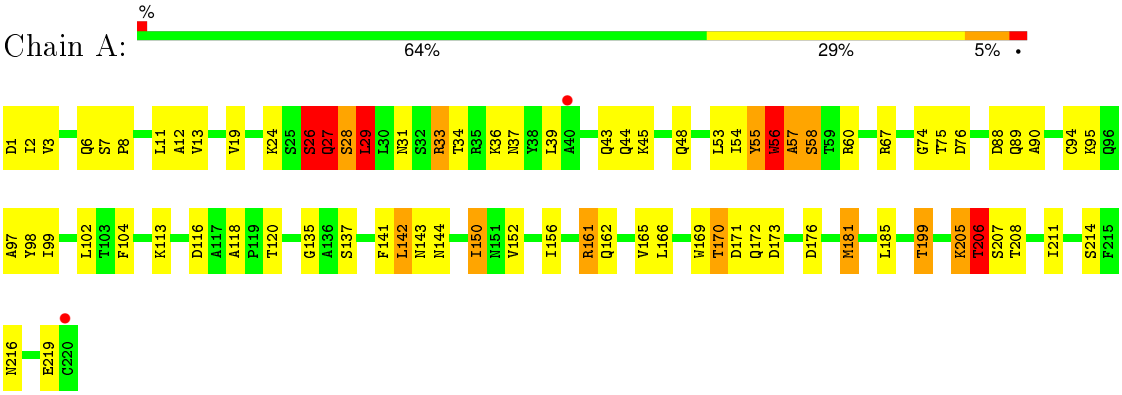
- Molecule 1: Capsid protein C

Chain Q:



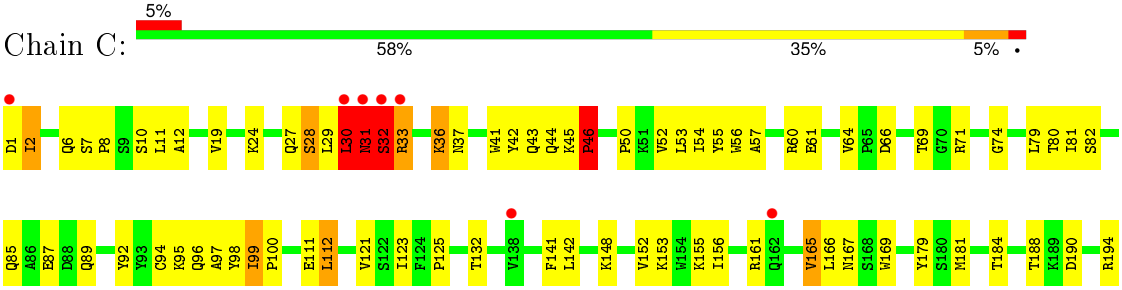
- Molecule 2: Monoclonal antibody 19D9D6 Light chain

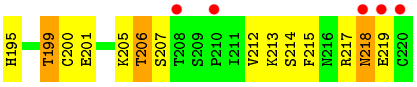
Chain A:



- Molecule 2: Monoclonal antibody 19D9D6 Light chain

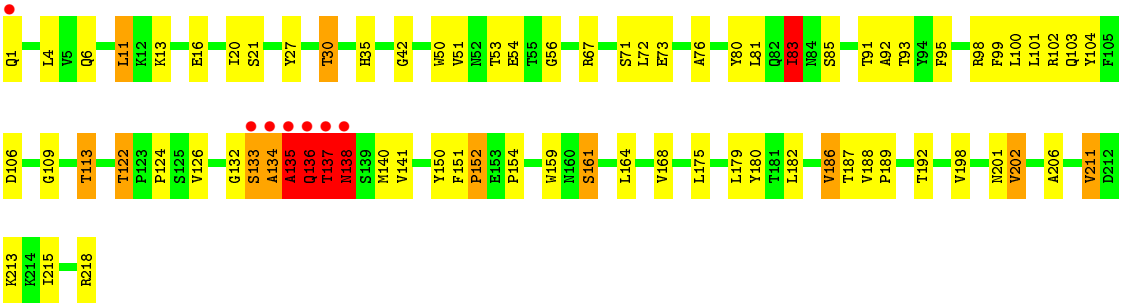
Chain C:





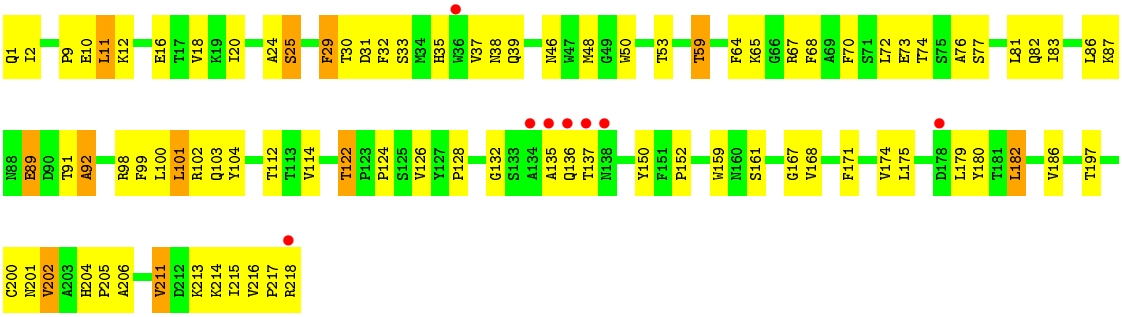
• Molecule 3: Monoclonal antibody 19D9D6 Heavy chain

Chain B:



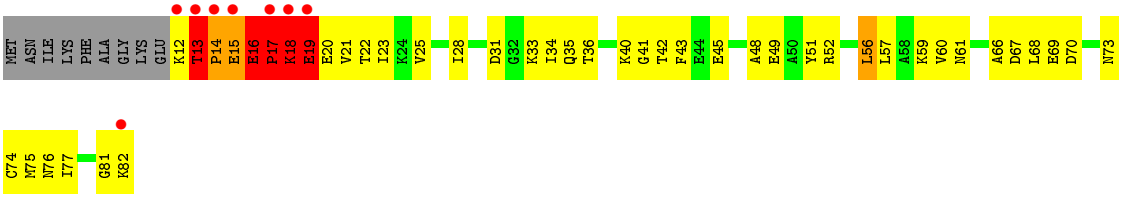
• Molecule 3: Monoclonal antibody 19D9D6 Heavy chain

Chain D:



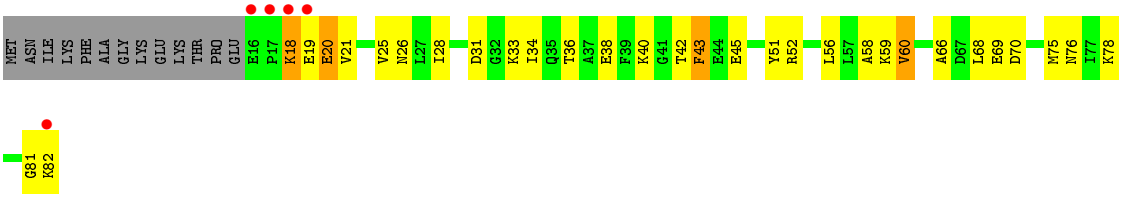
• Molecule 4: Protein L

Chain L:



• Molecule 4: Protein L

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	129.34Å 222.93Å 43.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.60 19.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.92-2.60) 97.8 (19.91-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.199 , 0.240 0.216 , 0.230	Depositor DCC
R_{free} test set	1951 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	45.6	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 39014 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8420	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	P	0.61	0/117	1.67	4/156 (2.6%)
1	Q	0.48	0/59	0.87	0/79
2	A	0.59	2/1745 (0.1%)	0.89	6/2366 (0.3%)
2	C	0.39	0/1745	0.78	6/2366 (0.3%)
3	B	0.46	0/1707	0.85	8/2335 (0.3%)
3	D	0.39	0/1707	0.64	0/2335
4	L	0.53	0/556	1.16	10/748 (1.3%)
4	M	0.42	0/525	0.63	0/705
All	All	0.47	2/8161 (0.0%)	0.84	34/11090 (0.3%)

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	A	0	9
3	B	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	55	TYR	C-N	-9.25	1.12	1.34
2	A	58	SER	CB-OG	-5.97	1.34	1.42

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	18	LYS	N-CA-C	13.11	146.41	111.00
2	A	27	GLN	C-N-CA	11.38	150.14	121.70
3	B	136	GLN	CA-C-N	-10.90	93.22	117.20
2	A	26	SER	C-N-CA	10.57	148.11	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	56	TRP	CA-C-N	-10.37	94.38	117.20
4	L	17	PRO	C-N-CA	8.75	143.57	121.70
1	P	25	PRO	N-CA-C	8.22	133.46	112.10
1	P	26	GLY	N-CA-C	-8.14	92.75	113.10
3	B	136	GLN	C-N-CA	7.18	139.66	121.70
2	C	33	ARG	CB-CA-C	7.17	124.74	110.40
2	C	30	LEU	N-CA-C	6.91	129.66	111.00
4	L	13	THR	N-CA-C	6.79	129.33	111.00
2	C	32	SER	C-N-CA	-6.70	104.95	121.70
4	L	17	PRO	CA-C-N	-6.63	102.61	117.20
2	C	33	ARG	CA-CB-CG	6.46	127.61	113.40
2	A	56	TRP	CB-CA-C	-6.45	97.50	110.40
1	P	25	PRO	CA-C-N	-5.97	104.26	116.20
2	C	30	LEU	CA-CB-CG	5.96	129.00	115.30
4	L	18	LYS	N-CA-CB	-5.94	99.92	110.60
3	B	136	GLN	O-C-N	5.85	132.06	122.70
4	L	17	PRO	N-CA-C	5.78	127.12	112.10
4	L	19	GLU	N-CA-C	5.65	126.25	111.00
2	A	29	LEU	CB-CA-C	5.56	120.77	110.20
3	B	83	ILE	CB-CA-C	-5.42	100.77	111.60
2	A	26	SER	N-CA-C	5.36	125.47	111.00
3	B	83	ILE	N-CA-CB	5.35	123.11	110.80
2	C	31	ASN	CA-C-N	-5.35	105.43	117.20
3	B	136	GLN	N-CA-C	5.34	125.42	111.00
3	B	135	ALA	C-N-CA	-5.24	108.60	121.70
4	L	15	GLU	N-CA-CB	5.16	119.88	110.60
4	L	18	LYS	CA-C-N	-5.12	105.94	117.20
1	P	39	ARG	C-N-CA	5.12	134.49	121.70
3	B	138	ASN	N-CA-C	-5.08	97.29	111.00
4	L	16	GLU	C-N-CA	-5.02	100.93	122.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	26	SER	Mainchain,Peptide
2	A	27	GLN	Sidechain,Mainchain,Peptide
2	A	28	SER	Mainchain
2	A	29	LEU	Mainchain
2	A	56	TRP	Mainchain
2	A	57	ALA	Mainchain
3	B	136	GLN	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	P	115	0	123	17	0
1	Q	59	0	62	14	0
2	A	1708	0	1655	84	0
2	C	1708	0	1658	119	0
3	B	1660	0	1615	77	0
3	D	1660	0	1615	97	0
4	L	547	0	520	69	0
4	M	517	0	499	33	0
5	A	141	0	0	8	0
5	B	115	0	0	5	0
5	C	68	0	0	3	1
5	D	75	0	0	0	1
5	L	15	0	0	3	0
5	M	23	0	0	3	0
5	P	8	0	0	2	0
5	Q	1	0	0	0	0
All	All	8420	0	7747	480	1

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 31.

All (480) 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:D:68:PHE:CD1	3:D:83:ILE:HD12	1.90	1.07
3:D:68:PHE:HD1	3:D:83:ILE:HD12	1.07	1.04
4:L:18:LYS:H	4:L:18:LYS:HD2	1.25	0.98
2:C:28:SER:OG	2:C:30:LEU:HB3	1.64	0.98
2:C:96:GLN:HE21	2:C:98:TYR:N	1.62	0.98
4:L:18:LYS:H	4:L:18:LYS:CD	1.75	0.96
3:D:161:SER:H	3:D:201:ASN:HD21	1.16	0.93
3:B:161:SER:H	3:B:201:ASN:HD21	1.17	0.90
2:C:30:LEU:HD12	2:C:31:ASN:HA	1.52	0.90
2:A:33:ARG:HG2	2:A:33:ARG:HH21	1.37	0.89
3:B:136:GLN:CD	3:B:137:THR:H	1.74	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:82:GLN:C	3:D:83:ILE:HD13	1.93	0.88
2:C:87:GLU:H	2:C:87:GLU:CD	1.73	0.88
3:B:135:ALA:O	3:B:136:GLN:NE2	2.05	0.88
2:A:199:THR:HB	2:A:214:SER:HB3	1.55	0.88
1:P:39:ARG:H	1:P:39:ARG:HD2	1.37	0.87
2:C:30:LEU:HD12	2:C:31:ASN:N	1.90	0.86
2:C:96:GLN:NE2	2:C:98:TYR:H	1.71	0.86
4:M:21:VAL:HG21	4:M:43:PHE:HB2	1.58	0.86
3:D:68:PHE:HD1	3:D:83:ILE:CD1	1.91	0.83
1:P:39:ARG:NH2	5:P:284:HOH:O	2.04	0.83
2:C:19:VAL:HG12	2:C:81:ILE:HB	1.58	0.82
3:D:124:PRO:HB3	3:D:150:TYR:HB3	1.62	0.82
2:C:19:VAL:HG13	2:C:81:ILE:HD13	1.61	0.82
2:C:60:ARG:CZ	2:C:66:ASP:HA	2.09	0.81
3:D:101:LEU:HD22	3:D:101:LEU:H	1.45	0.80
4:L:18:LYS:HA	4:L:18:LYS:HE3	1.64	0.80
1:P:39:ARG:H	1:P:39:ARG:CD	1.91	0.79
2:C:30:LEU:HD12	2:C:31:ASN:CA	2.12	0.79
3:D:202:VAL:HG13	3:D:211:VAL:HG13	1.64	0.79
3:D:102:ARG:HH11	3:D:102:ARG:HG3	1.48	0.78
2:A:150:ILE:CG2	2:A:181:MET:HE2	2.14	0.78
3:B:168:VAL:HG22	3:B:186:VAL:HG12	1.65	0.78
3:D:53:THR:HA	3:D:72:LEU:HD11	1.64	0.78
2:C:31:ASN:HB2	2:C:98:TYR:HE1	1.49	0.76
3:D:20:ILE:HD12	3:D:112:THR:HG21	1.66	0.76
4:L:20:GLU:HB3	5:L:91:HOH:O	1.85	0.76
2:C:96:GLN:HE21	2:C:98:TYR:H	0.85	0.76
4:L:28:ILE:HG12	4:L:34:ILE:HD12	1.68	0.75
2:C:85:GLN:HB3	2:C:87:GLU:OE2	1.87	0.74
2:A:24:LYS:NZ	5:A:297:HOH:O	2.21	0.73
4:L:18:LYS:HE3	4:L:18:LYS:CA	2.18	0.73
3:B:136:GLN:HA	3:B:136:GLN:NE2	2.04	0.73
3:B:161:SER:H	3:B:201:ASN:ND2	1.87	0.73
4:L:17:PRO:HA	4:L:18:LYS:HD2	1.71	0.72
1:Q:29:GLN:CG	3:D:33:SER:HB3	2.19	0.72
3:D:2:ILE:HG12	3:D:98:ARG:NH2	2.03	0.72
1:P:39:ARG:CD	1:P:39:ARG:N	2.52	0.71
1:P:39:ARG:HD2	1:P:39:ARG:N	2.05	0.71
3:B:168:VAL:HG22	3:B:186:VAL:CG1	2.21	0.70
2:C:2:ILE:CD1	2:C:2:ILE:H	2.04	0.70
3:D:197:THR:HB	3:D:214:LYS:HE3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:206:THR:HG22	5:A:256:HOH:O	1.91	0.69
3:D:82:GLN:O	3:D:83:ILE:HD13	1.91	0.69
2:C:166:LEU:HD21	3:D:174:VAL:HB	1.75	0.69
2:A:118:ALA:HA	2:A:206:THR:HG21	1.75	0.69
2:A:118:ALA:CA	2:A:206:THR:HG21	2.23	0.68
1:Q:29:GLN:HG2	3:D:33:SER:HB3	1.75	0.68
2:C:30:LEU:CD1	2:C:32:SER:H	2.06	0.67
4:M:42:THR:O	4:M:43:PHE:HB3	1.94	0.67
2:C:41:TRP:HD1	2:C:54:ILE:HD11	1.59	0.67
1:P:37:LEU:O	1:P:38:PRO:C	2.32	0.67
3:B:126:VAL:HG21	3:B:211:VAL:HG11	1.77	0.67
4:L:18:LYS:CA	4:L:18:LYS:CE	2.73	0.67
2:A:150:ILE:CG2	2:A:181:MET:CE	2.73	0.67
2:A:118:ALA:HB2	2:A:206:THR:CG2	2.25	0.66
2:A:142:LEU:HD11	2:A:152:VAL:HG22	1.77	0.66
1:P:39:ARG:NH2	5:P:325:HOH:O	2.27	0.66
2:C:81:ILE:N	2:C:81:ILE:HD12	2.10	0.66
4:L:21:VAL:HG22	4:L:22:THR:H	1.60	0.66
2:C:2:ILE:N	2:C:2:ILE:CD1	2.58	0.66
4:L:48:ALA:O	4:L:52:ARG:HG3	1.95	0.66
4:L:16:GLU:HB3	4:L:17:PRO:HD3	1.78	0.66
4:L:66:ALA:HB2	4:L:77:ILE:HD13	1.77	0.65
2:C:19:VAL:CG1	2:C:81:ILE:HB	2.26	0.65
2:A:150:ILE:HG23	2:A:181:MET:HE3	1.76	0.65
3:D:38:ASN:OD1	3:D:46:ASN:HB2	1.95	0.65
3:D:20:ILE:CD1	3:D:112:THR:HG21	2.26	0.65
4:L:21:VAL:HG22	4:L:22:THR:N	2.10	0.65
2:C:218:ASN:HD22	2:C:219:GLU:N	1.93	0.65
2:C:56:TRP:CZ2	3:D:102:ARG:HG2	2.32	0.65
2:A:33:ARG:CG	2:A:33:ARG:HH21	2.08	0.64
2:C:199:THR:HB	2:C:214:SER:HB3	1.80	0.64
4:M:19:GLU:HB2	4:M:40:LYS:HB3	1.80	0.64
2:A:36:LYS:HD2	2:A:56:TRP:CG	2.33	0.64
3:B:215:ILE:HD12	3:B:215:ILE:N	2.13	0.64
3:B:99:PHE:CZ	3:B:103:GLN:HA	2.33	0.64
4:M:26:ASN:ND2	4:M:36:THR:HG22	2.11	0.64
3:D:101:LEU:HD22	3:D:101:LEU:N	2.13	0.63
4:M:59:LYS:CE	5:M:103:HOH:O	2.46	0.63
3:B:93:THR:HA	3:B:113:THR:HA	1.80	0.63
3:B:138:ASN:HB2	3:B:140:MET:O	1.98	0.63
2:C:99:ILE:O	2:C:99:ILE:HG13	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:81:LEU:HD11	3:D:83:ILE:HD11	1.80	0.62
3:D:87:LYS:NZ	3:D:89:GLU:HG2	2.14	0.62
3:D:99:PHE:CZ	3:D:103:GLN:HA	2.33	0.62
2:A:150:ILE:HG23	2:A:181:MET:CE	2.29	0.62
4:M:19:GLU:HB2	4:M:40:LYS:HD3	1.82	0.62
2:A:11:LEU:HD13	2:A:19:VAL:CG2	2.30	0.62
2:A:55:TYR:O	2:A:56:TRP:C	2.38	0.62
4:L:42:THR:HG22	4:L:45:GLU:CG	2.29	0.62
4:M:18:LYS:HE2	4:M:20:GLU:O	2.00	0.62
3:D:70:PHE:CE2	3:D:81:LEU:HD23	2.35	0.62
1:Q:30:ILE:HG22	1:Q:31:VAL:H	1.65	0.62
2:A:3:VAL:N	2:A:26:SER:OG	2.27	0.61
2:C:199:THR:CB	2:C:214:SER:HB3	2.30	0.61
3:D:152:PRO:O	3:D:204:HIS:HE1	1.83	0.61
2:C:2:ILE:HD13	2:C:2:ILE:H	1.66	0.61
3:D:1:GLN:HG2	3:D:1:GLN:O	2.01	0.61
1:Q:30:ILE:HG22	1:Q:31:VAL:N	2.14	0.61
3:D:182:LEU:HD12	3:D:182:LEU:C	2.21	0.61
2:C:80:THR:C	2:C:81:ILE:HD12	2.21	0.61
4:L:42:THR:HG23	4:L:45:GLU:H	1.64	0.61
2:C:2:ILE:HD12	2:C:2:ILE:N	2.15	0.60
3:B:202:VAL:HG13	3:B:211:VAL:HG13	1.83	0.60
4:M:26:ASN:HD22	4:M:36:THR:HG22	1.66	0.60
3:D:102:ARG:NH1	3:D:102:ARG:HG3	2.17	0.60
2:A:3:VAL:H	2:A:26:SER:HG	1.48	0.60
2:C:121:VAL:HG22	2:C:142:LEU:HD22	1.84	0.60
2:C:98:TYR:CD2	2:C:99:ILE:HG23	2.36	0.60
2:A:118:ALA:HB2	2:A:206:THR:HG21	1.84	0.60
3:B:93:THR:HG22	3:B:113:THR:HB	1.83	0.60
4:L:51:TYR:OH	4:M:68:LEU:HD21	2.01	0.59
2:C:205:LYS:O	2:C:207:SER:N	2.35	0.59
4:L:18:LYS:N	4:L:18:LYS:CE	2.64	0.59
3:D:126:VAL:O	3:D:213:LYS:HE3	2.02	0.59
2:C:188:THR:HG23	5:C:233:HOH:O	2.02	0.59
2:C:169:TRP:CZ2	2:C:181:MET:HE2	2.38	0.59
2:A:97:ALA:HA	2:A:102:LEU:HD22	1.84	0.59
2:A:170:THR:HG21	5:A:277:HOH:O	2.02	0.59
4:L:16:GLU:CB	4:L:17:PRO:HD3	2.33	0.59
3:B:124:PRO:HB3	3:B:150:TYR:HB3	1.84	0.59
3:B:113:THR:HG21	5:B:329:HOH:O	2.01	0.59
2:A:67:ARG:NH1	2:A:88:ASP:OD1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:162:GLN:O	2:A:165:VAL:HG12	2.03	0.59
2:A:37:ASN:ND2	2:A:74:GLY:H	2.01	0.59
3:D:101:LEU:CD2	3:D:101:LEU:H	2.15	0.58
3:D:70:PHE:CD2	3:D:81:LEU:HD23	2.38	0.58
2:A:199:THR:CB	2:A:214:SER:HB3	2.31	0.58
3:B:215:ILE:H	3:B:215:ILE:HD12	1.69	0.58
2:C:199:THR:HG22	2:C:214:SER:CB	2.33	0.58
2:A:118:ALA:CB	2:A:206:THR:HG21	2.33	0.58
2:A:56:TRP:HZ2	5:A:310:HOH:O	1.86	0.58
2:C:97:ALA:CB	3:D:103:GLN:HB3	2.34	0.58
2:C:141:PHE:C	2:C:142:LEU:HD23	2.24	0.58
3:D:216:VAL:HG13	3:D:217:PRO:HD2	1.85	0.58
2:A:54:ILE:HD13	2:A:60:ARG:HA	1.85	0.57
3:D:10:GLU:HG2	3:D:18:VAL:CG2	2.34	0.57
1:P:37:LEU:O	1:P:38:PRO:O	2.22	0.57
4:L:28:ILE:HG23	4:L:34:ILE:HD11	1.87	0.57
3:D:218:ARG:HG3	3:D:218:ARG:O	2.05	0.57
2:C:10:SER:HB3	4:M:38:GLU:HB2	1.86	0.57
3:B:136:GLN:OE1	3:B:137:THR:HA	2.03	0.57
4:L:17:PRO:HA	4:L:18:LYS:HZ3	1.69	0.56
3:B:132:GLY:HA2	3:B:218:ARG:HD2	1.86	0.56
2:C:169:TRP:CE2	2:C:181:MET:HG3	2.40	0.56
3:D:159:TRP:CZ3	3:D:200:CYS:HB3	2.40	0.56
4:M:20:GLU:HG3	4:M:21:VAL:H	1.70	0.56
2:A:169:TRP:HE1	2:A:181:MET:CE	2.17	0.56
4:L:45:GLU:O	4:L:49:GLU:HG2	2.06	0.56
3:B:21:SER:HB3	3:B:80:TYR:CE1	2.40	0.56
3:B:198:VAL:HG12	3:B:215:ILE:HD13	1.87	0.56
2:C:99:ILE:HD12	2:C:100:PRO:O	2.06	0.56
3:D:126:VAL:HG21	3:D:202:VAL:HG11	1.87	0.56
3:D:161:SER:H	3:D:201:ASN:ND2	1.95	0.55
2:A:36:LYS:HD2	2:A:56:TRP:CD1	2.41	0.55
3:D:87:LYS:HZ2	3:D:89:GLU:HG2	1.69	0.55
3:D:10:GLU:HG2	3:D:18:VAL:HG23	1.89	0.55
2:C:165:VAL:HA	2:C:184:THR:O	2.07	0.55
3:B:93:THR:HG23	5:B:254:HOH:O	2.06	0.55
3:B:20:ILE:HD11	3:B:81:LEU:HD23	1.87	0.55
2:C:8:PRO:CG	2:C:11:LEU:HG	2.37	0.55
2:C:111:GLU:HG2	5:C:234:HOH:O	2.06	0.55
4:M:28:ILE:HA	4:M:34:ILE:HD13	1.88	0.55
2:A:170:THR:CG2	5:A:277:HOH:O	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:18:LYS:HA	4:L:18:LYS:CE	2.32	0.55
2:C:218:ASN:HD22	2:C:219:GLU:H	1.53	0.55
2:C:69:THR:CG2	2:C:71:ARG:HH11	2.20	0.55
4:L:43:PHE:HE1	4:M:51:TYR:CD2	2.25	0.55
4:L:51:TYR:HD1	4:M:43:PHE:HZ	1.54	0.54
2:A:211:ILE:HD11	5:A:256:HOH:O	2.07	0.54
1:P:25:PRO:HD2	1:P:37:LEU:CD1	2.38	0.54
2:C:69:THR:HG21	2:C:71:ARG:HH11	1.71	0.54
4:M:31:ASP:OD1	4:M:33:LYS:HG3	2.06	0.54
4:L:68:LEU:HD13	4:L:75:MET:HG2	1.89	0.54
3:B:113:THR:HG23	5:B:236:HOH:O	2.06	0.54
2:A:141:PHE:C	2:A:142:LEU:HD23	2.27	0.54
2:A:142:LEU:N	2:A:142:LEU:HD23	2.23	0.54
2:A:36:LYS:HE3	2:A:56:TRP:CE3	2.43	0.54
1:Q:31:VAL:HG12	3:D:99:PHE:CE1	2.43	0.54
3:D:122:THR:HG21	3:D:179:LEU:HD11	1.90	0.54
3:D:2:ILE:HG21	3:D:98:ARG:HH21	1.73	0.53
4:L:66:ALA:CB	4:L:77:ILE:HD13	2.37	0.53
4:M:52:ARG:HG2	5:M:94:HOH:O	2.07	0.53
3:D:83:ILE:HD13	3:D:83:ILE:N	2.23	0.53
1:Q:33:GLY:N	2:C:98:TYR:O	2.32	0.53
3:B:67:ARG:HD2	3:B:85:SER:HB2	1.89	0.53
4:L:17:PRO:HA	4:L:18:LYS:NZ	2.24	0.53
2:A:199:THR:HG22	2:A:214:SER:HB2	1.91	0.53
2:C:125:PRO:HB3	2:C:215:PHE:CZ	2.44	0.53
3:D:48:MET:HG2	3:D:64:PHE:CZ	2.44	0.52
3:B:136:GLN:CG	3:B:137:THR:H	2.19	0.52
4:L:28:ILE:HG23	4:L:34:ILE:CD1	2.39	0.52
2:C:12:ALA:HB3	4:M:36:THR:OG1	2.09	0.52
2:C:153:LYS:HD3	2:C:155:LYS:HE3	1.91	0.52
4:L:42:THR:CG2	4:L:45:GLU:H	2.22	0.52
2:C:148:LYS:HB3	2:C:179:TYR:CD1	2.44	0.52
4:L:42:THR:HG22	4:L:45:GLU:CD	2.30	0.52
3:B:73:GLU:HG2	3:B:76:ALA:HB3	1.92	0.52
3:B:161:SER:N	3:B:201:ASN:HD21	1.98	0.52
2:C:60:ARG:NH2	2:C:66:ASP:HB3	2.25	0.52
2:A:44:GLN:O	2:A:90:ALA:HB1	2.10	0.52
2:C:96:GLN:NE2	2:C:99:ILE:H	2.08	0.52
2:C:44:GLN:HE22	3:D:39:GLN:HE22	1.58	0.52
2:C:199:THR:HG22	2:C:214:SER:HB2	1.91	0.52
2:A:98:TYR:CD2	2:A:99:ILE:HG13	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:11:LEU:HG	3:B:152:PRO:HG3	1.91	0.52
2:C:28:SER:CB	2:C:30:LEU:HB3	2.40	0.52
2:C:148:LYS:HG2	5:C:260:HOH:O	2.08	0.52
4:L:18:LYS:H	4:L:18:LYS:CE	2.23	0.51
3:B:1:GLN:OE1	3:B:1:GLN:N	2.25	0.51
1:Q:29:GLN:OE1	3:D:33:SER:HA	2.10	0.51
4:L:42:THR:HG22	4:L:45:GLU:OE2	2.10	0.51
2:C:37:ASN:ND2	2:C:74:GLY:H	2.09	0.51
2:C:24:LYS:HG3	2:C:24:LYS:O	2.09	0.51
2:A:37:ASN:HD21	2:A:74:GLY:H	1.57	0.51
1:Q:36:LEU:N	1:Q:36:LEU:HD12	2.26	0.51
2:C:6:GLN:HG3	2:C:94:CYS:SG	2.50	0.51
2:C:217:ARG:HG2	2:C:217:ARG:HH11	1.74	0.51
3:D:2:ILE:HG12	3:D:98:ARG:HH22	1.76	0.51
2:A:36:LYS:HD2	2:A:56:TRP:CD2	2.46	0.51
3:B:98:ARG:NH1	3:B:106:ASP:OD2	2.44	0.51
3:B:189:PRO:HG2	3:B:192:THR:CG2	2.40	0.51
3:D:91:THR:O	3:D:92:ALA:HB2	2.10	0.51
3:D:126:VAL:HG21	3:D:211:VAL:CG1	2.42	0.50
2:C:36:LYS:HG2	2:C:56:TRP:CD1	2.46	0.50
4:L:25:VAL:HG22	4:L:75:MET:HB2	1.93	0.50
2:A:43:GLN:HB2	2:A:53:LEU:HD11	1.92	0.50
3:B:159:TRP:HZ3	3:B:215:ILE:HD11	1.76	0.50
2:C:218:ASN:ND2	2:C:219:GLU:N	2.58	0.50
2:C:89:GLN:HE21	2:C:112:LEU:HG	1.75	0.50
2:C:201:GLU:HG2	2:C:212:VAL:HG12	1.92	0.50
3:D:81:LEU:CD1	3:D:83:ILE:HD11	2.41	0.50
3:B:6:GLN:HE21	3:B:109:GLY:HA3	1.75	0.50
1:P:38:PRO:HD3	2:A:33:ARG:CB	2.42	0.50
4:L:31:ASP:OD1	4:L:33:LYS:HG3	2.12	0.50
2:C:56:TRP:O	2:C:57:ALA:HB3	2.12	0.50
2:C:97:ALA:HB1	3:D:103:GLN:HB3	1.94	0.50
2:A:2:ILE:N	2:A:2:ILE:HD12	2.26	0.50
3:B:132:GLY:O	3:B:134:ALA:N	2.44	0.50
3:B:136:GLN:HA	3:B:136:GLN:HE21	1.70	0.50
4:M:28:ILE:HG23	4:M:34:ILE:HD11	1.93	0.50
3:D:68:PHE:CD1	3:D:83:ILE:CD1	2.77	0.50
2:C:28:SER:OG	2:C:30:LEU:CB	2.47	0.49
2:C:19:VAL:CG1	2:C:81:ILE:HD13	2.36	0.49
3:D:11:LEU:HD12	3:D:152:PRO:HD3	1.94	0.49
2:A:67:ARG:HH12	2:A:88:ASP:CG	2.14	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:34:VAL:HG22	1:Q:34:VAL:O	2.12	0.49
3:B:133:SER:O	3:B:134:ALA:HB2	2.12	0.49
2:A:24:LYS:HA	2:A:75:THR:O	2.12	0.49
2:A:7:SER:HA	2:A:8:PRO:O	2.13	0.49
2:A:7:SER:HA	2:A:8:PRO:C	2.32	0.49
4:L:21:VAL:N	4:L:41:GLY:O	2.44	0.49
2:C:205:LYS:C	2:C:207:SER:H	2.15	0.49
3:D:9:PRO:HG3	3:D:205:PRO:HB2	1.94	0.49
1:Q:31:VAL:HG11	3:D:35:HIS:CE1	2.48	0.49
4:M:42:THR:O	4:M:43:PHE:CB	2.60	0.49
2:C:8:PRO:HG3	2:C:11:LEU:HG	1.94	0.49
2:C:195:HIS:O	2:C:217:ARG:NH2	2.44	0.49
2:A:170:THR:HG23	2:A:171:ASP:O	2.12	0.49
3:D:2:ILE:HD12	3:D:2:ILE:H	1.78	0.48
4:L:42:THR:HG21	5:L:90:HOH:O	2.12	0.48
1:P:25:PRO:HD2	1:P:37:LEU:HD11	1.94	0.48
1:P:38:PRO:HA	1:P:39:ARG:HD2	1.95	0.48
3:B:152:PRO:HD2	3:B:206:ALA:CB	2.43	0.48
3:B:93:THR:HG22	3:B:113:THR:CG2	2.44	0.48
2:C:142:LEU:HD11	2:C:152:VAL:HG22	1.94	0.48
2:A:135:GLY:HA3	5:A:266:HOH:O	2.13	0.48
3:D:30:THR:HG22	3:D:53:THR:O	2.13	0.48
4:L:23:ILE:HG21	4:L:75:MET:HE3	1.96	0.48
2:C:30:LEU:C	2:C:30:LEU:HD12	2.33	0.48
3:B:198:VAL:O	3:B:215:ILE:HD13	2.13	0.48
3:B:126:VAL:CG2	3:B:211:VAL:HG11	2.43	0.48
2:A:211:ILE:HD12	2:A:211:ILE:N	2.29	0.48
4:L:81:GLY:O	4:L:82:LYS:HB3	2.14	0.48
4:L:82:LYS:OXT	4:L:82:LYS:HD3	2.13	0.48
2:A:13:VAL:HG12	4:L:35:GLN:HG2	1.96	0.48
3:D:73:GLU:HG2	3:D:76:ALA:HB3	1.96	0.48
2:C:30:LEU:HD12	2:C:32:SER:H	1.77	0.48
3:B:93:THR:HG22	3:B:113:THR:CB	2.43	0.48
2:A:169:TRP:HE1	2:A:181:MET:HE2	1.78	0.48
2:C:148:LYS:HB3	2:C:179:TYR:CG	2.49	0.48
2:C:31:ASN:HB2	2:C:98:TYR:CE1	2.40	0.48
3:D:161:SER:N	3:D:201:ASN:HD21	1.98	0.47
3:B:42:GLY:HA2	5:B:298:HOH:O	2.14	0.47
1:P:37:LEU:C	1:P:38:PRO:O	2.52	0.47
2:C:87:GLU:N	2:C:87:GLU:CD	2.53	0.47
2:C:60:ARG:HH22	2:C:66:ASP:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:28:ILE:HD12	4:M:78:LYS:HG2	1.96	0.47
4:L:18:LYS:N	4:L:18:LYS:NZ	2.63	0.47
3:B:6:GLN:HE22	3:B:95:PHE:HA	1.79	0.47
2:A:39:LEU:C	2:A:39:LEU:HD13	2.35	0.47
2:C:153:LYS:CD	2:C:155:LYS:HE3	2.44	0.47
2:C:92:TYR:N	2:C:92:TYR:CD1	2.82	0.47
2:A:31:ASN:HB3	2:A:34:THR:OG1	2.14	0.47
2:A:137:SER:HA	2:A:185:LEU:O	2.15	0.47
2:C:28:SER:C	2:C:29:LEU:HD12	2.35	0.47
2:A:150:ILE:HG21	2:A:181:MET:HE2	1.92	0.47
2:A:118:ALA:CB	2:A:206:THR:CG2	2.93	0.47
3:B:126:VAL:HG21	3:B:211:VAL:CG1	2.44	0.47
4:L:18:LYS:N	4:L:18:LYS:CD	2.51	0.47
2:C:156:ILE:HD12	2:C:161:ARG:NH2	2.30	0.47
2:C:30:LEU:HD13	2:C:32:SER:H	1.78	0.46
4:M:20:GLU:OE2	4:M:20:GLU:HA	2.15	0.46
3:B:11:LEU:HB2	3:B:152:PRO:HG3	1.98	0.46
4:M:66:ALA:HA	4:M:76:ASN:O	2.14	0.46
3:D:24:ALA:O	3:D:25:SER:HB3	2.14	0.46
3:D:126:VAL:HG21	3:D:211:VAL:HG11	1.97	0.46
2:C:45:LYS:HB3	2:C:46:PRO:HD2	1.97	0.46
2:C:52:VAL:HG11	3:D:104:TYR:CD1	2.50	0.46
4:L:61:ASN:O	4:L:81:GLY:HA2	2.15	0.46
2:C:152:VAL:HG23	2:C:181:MET:HE3	1.97	0.46
2:A:143:ASN:HB3	2:A:144:ASN:ND2	2.30	0.46
2:A:169:TRP:HE1	2:A:181:MET:HE1	1.81	0.46
3:B:91:THR:O	3:B:92:ALA:HB2	2.16	0.46
2:A:12:ALA:O	2:A:113:LYS:HD2	2.15	0.46
2:C:96:GLN:NE2	2:C:98:TYR:N	2.43	0.46
1:P:38:PRO:HD3	2:A:33:ARG:HB2	1.97	0.46
2:A:205:LYS:C	2:A:207:SER:H	2.19	0.46
4:L:42:THR:HG22	4:L:45:GLU:CB	2.46	0.46
3:D:218:ARG:NH2	3:D:218:ARG:HB2	2.31	0.46
3:B:27:TYR:CE2	3:B:98:ARG:HD2	2.50	0.46
4:L:67:ASP:HB2	4:L:76:ASN:HB2	1.97	0.46
4:M:81:GLY:O	4:M:82:LYS:HB3	2.16	0.46
4:L:12:LYS:N	5:L:97:HOH:O	2.48	0.46
3:D:2:ILE:HD12	3:D:2:ILE:N	2.30	0.45
2:A:56:TRP:CH2	3:B:102:ARG:HG2	2.50	0.45
3:D:100:LEU:HD12	3:D:104:TYR:CZ	2.51	0.45
3:D:175:LEU:HD22	3:D:180:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:33:ARG:CG	2:A:33:ARG:NH2	2.74	0.45
2:A:29:LEU:O	2:A:37:ASN:HA	2.16	0.45
2:A:43:GLN:NE2	2:A:45:LYS:HE3	2.32	0.45
3:D:50:TRP:CE2	3:D:59:THR:HG21	2.52	0.45
3:D:2:ILE:HG12	3:D:98:ARG:HH21	1.78	0.45
2:C:8:PRO:HG2	2:C:11:LEU:HG	1.97	0.45
2:C:42:TYR:CE2	2:C:52:VAL:HG12	2.51	0.45
3:B:83:ILE:N	3:B:83:ILE:HD13	2.31	0.45
3:B:51:VAL:O	3:B:51:VAL:HG13	2.15	0.45
2:C:190:ASP:O	2:C:194:ARG:HG3	2.16	0.45
4:L:42:THR:HG22	4:L:45:GLU:HB2	1.98	0.45
2:C:42:TYR:OH	2:C:95:LYS:NZ	2.36	0.45
4:L:16:GLU:HB3	4:L:17:PRO:CD	2.44	0.45
2:C:27:GLN:O	2:C:29:LEU:HD12	2.16	0.45
3:D:37:VAL:HG13	3:D:46:ASN:O	2.16	0.45
2:A:67:ARG:NH1	2:A:88:ASP:OD2	2.44	0.45
3:B:189:PRO:HG2	3:B:192:THR:HG23	1.98	0.45
2:C:42:TYR:CE2	2:C:52:VAL:CG1	3.00	0.45
4:L:51:TYR:HD1	4:M:43:PHE:CZ	2.34	0.44
3:B:198:VAL:O	3:B:215:ILE:CD1	2.65	0.44
2:A:206:THR:O	2:A:206:THR:HG23	2.17	0.44
4:L:69:GLU:HG3	4:L:74:CYS:HB3	1.99	0.44
3:D:48:MET:HG2	3:D:64:PHE:CE2	2.53	0.44
3:D:70:PHE:HE2	3:D:81:LEU:HD23	1.82	0.44
4:L:43:PHE:CE1	4:M:51:TYR:HD2	2.35	0.44
2:C:7:SER:HA	2:C:8:PRO:C	2.37	0.44
2:A:95:LYS:HB2	2:A:104:PHE:CD2	2.53	0.44
2:A:89:GLN:NE2	2:A:172:GLN:HG2	2.32	0.44
3:B:56:GLY:HA2	3:B:72:LEU:HD11	1.99	0.44
2:A:27:GLN:C	2:A:75:THR:HG22	2.37	0.44
4:L:21:VAL:CG2	4:L:22:THR:H	2.29	0.44
2:C:199:THR:HG22	2:C:214:SER:HB3	2.00	0.44
2:C:141:PHE:O	2:C:142:LEU:HD23	2.18	0.44
3:B:13:LYS:HB2	3:B:16:GLU:CD	2.38	0.44
2:C:166:LEU:HD21	3:D:174:VAL:CB	2.43	0.44
3:B:134:ALA:HB1	3:B:135:ALA:H	1.43	0.44
4:L:22:THR:OG1	4:L:40:LYS:HD3	2.17	0.44
2:A:211:ILE:H	2:A:211:ILE:HD12	1.83	0.44
1:Q:30:ILE:CG2	1:Q:31:VAL:H	2.31	0.44
1:P:31:VAL:HG21	3:B:50:TRP:CE2	2.53	0.44
2:C:199:THR:CG2	2:C:214:SER:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:166:LEU:HD23	2:C:167:ASN:N	2.33	0.43
4:M:58:ALA:O	4:M:59:LYS:C	2.56	0.43
3:B:151:PHE:CE1	3:B:152:PRO:HB3	2.53	0.43
2:A:48:GLN:HB3	5:A:252:HOH:O	2.19	0.43
3:D:168:VAL:HG22	3:D:186:VAL:HG23	1.99	0.43
2:C:60:ARG:HD3	2:C:64:VAL:O	2.18	0.43
3:B:159:TRP:CZ2	3:B:186:VAL:HG22	2.53	0.43
4:L:21:VAL:CG2	4:L:22:THR:N	2.78	0.43
3:B:30:THR:CG2	3:B:53:THR:O	2.66	0.43
3:B:30:THR:HG23	3:B:53:THR:O	2.19	0.43
3:D:128:PRO:CB	3:D:215:ILE:HD13	2.48	0.43
3:D:32:PHE:CG	3:D:98:ARG:HD3	2.54	0.43
2:A:24:LYS:HG2	2:A:76:ASP:OD2	2.18	0.43
2:C:166:LEU:C	2:C:166:LEU:HD23	2.38	0.43
3:D:10:GLU:HG2	3:D:18:VAL:HG21	2.01	0.43
2:C:95:LYS:HE2	2:C:95:LYS:HB3	1.75	0.43
3:D:102:ARG:NH1	3:D:102:ARG:CG	2.80	0.43
2:A:28:SER:HA	2:A:74:GLY:O	2.19	0.43
3:B:71:SER:HB2	5:B:303:HOH:O	2.18	0.43
4:L:23:ILE:HG21	4:L:75:MET:CE	2.48	0.43
2:A:116:ASP:OD1	2:A:205:LYS:HD2	2.19	0.43
4:M:60:VAL:O	4:M:60:VAL:CG2	2.65	0.43
3:D:64:PHE:HB3	3:D:68:PHE:CD2	2.53	0.43
2:A:118:ALA:HB2	2:A:206:THR:HG23	2.00	0.43
2:C:97:ALA:HB3	3:D:103:GLN:HB3	2.01	0.43
3:B:93:THR:CG2	3:B:113:THR:HG22	2.49	0.43
4:L:68:LEU:CD1	4:L:75:MET:HG2	2.49	0.43
3:B:122:THR:HG21	3:B:179:LEU:HD21	2.01	0.43
1:Q:33:GLY:C	1:Q:35:TYR:H	2.22	0.43
3:D:32:PHE:HE1	3:D:101:LEU:HD21	1.84	0.43
3:D:126:VAL:CG2	3:D:211:VAL:HG11	2.49	0.43
2:A:67:ARG:NH1	2:A:88:ASP:CG	2.71	0.43
3:D:18:VAL:HG12	3:D:86:LEU:HD11	2.01	0.43
3:D:64:PHE:O	3:D:65:LYS:HB2	2.19	0.43
2:C:55:TYR:C	2:C:57:ALA:N	2.72	0.43
2:C:31:ASN:C	2:C:31:ASN:OD1	2.58	0.42
3:B:161:SER:N	3:B:201:ASN:ND2	2.60	0.42
3:D:11:LEU:HD23	3:D:12:LYS:N	2.33	0.42
3:D:182:LEU:C	3:D:182:LEU:CD1	2.88	0.42
4:L:18:LYS:HZ2	4:L:18:LYS:N	2.17	0.42
2:C:41:TRP:CD1	2:C:54:ILE:HD11	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:124:PRO:CB	3:B:150:TYR:HB3	2.49	0.42
2:A:216:ASN:HB2	2:A:219:GLU:OE2	2.19	0.42
4:L:76:ASN:HD22	4:L:76:ASN:HA	1.68	0.42
2:A:6:GLN:HG3	2:A:94:CYS:SG	2.59	0.42
2:A:173:ASP:HB3	2:A:176:ASP:OD2	2.19	0.42
4:L:43:PHE:CE1	4:M:51:TYR:CD2	3.06	0.42
4:L:16:GLU:CB	4:L:17:PRO:CD	2.98	0.42
4:L:18:LYS:HB3	4:L:19:GLU:H	1.20	0.42
4:M:59:LYS:HE3	5:M:103:HOH:O	2.18	0.42
1:Q:30:ILE:CG2	1:Q:31:VAL:N	2.81	0.42
2:C:121:VAL:O	2:C:213:LYS:HE3	2.19	0.42
3:D:218:ARG:CZ	3:D:218:ARG:HB2	2.49	0.42
3:B:141:VAL:HG12	3:B:188:VAL:O	2.20	0.42
4:M:69:GLU:O	4:M:70:ASP:HB2	2.20	0.42
3:D:11:LEU:C	3:D:11:LEU:CD2	2.88	0.42
1:P:25:PRO:HD2	1:P:37:LEU:HD12	2.02	0.42
3:D:152:PRO:HD2	3:D:206:ALA:CB	2.50	0.42
3:D:171:PHE:N	3:D:171:PHE:CD1	2.88	0.42
4:L:56:LEU:HD23	4:L:59:LYS:HD3	2.00	0.42
2:C:56:TRP:CH2	3:D:102:ARG:HG2	2.55	0.41
3:D:11:LEU:HD23	3:D:11:LEU:C	2.39	0.41
4:M:42:THR:HG23	4:M:45:GLU:OE2	2.20	0.41
2:C:132:THR:HG22	2:C:132:THR:O	2.20	0.41
4:L:70:ASP:O	4:L:73:ASN:ND2	2.53	0.41
4:L:60:VAL:HG23	4:L:61:ASN:OD1	2.20	0.41
3:B:175:LEU:HB2	3:B:180:TYR:CE1	2.55	0.41
2:A:56:TRP:CZ2	3:B:102:ARG:HG2	2.56	0.41
3:D:67:ARG:NH1	3:D:87:LYS:HE3	2.35	0.41
3:B:71:SER:OG	3:B:80:TYR:HB2	2.20	0.41
2:A:156:ILE:HD12	2:A:161:ARG:HB2	2.02	0.41
2:C:81:ILE:CD1	2:C:81:ILE:N	2.79	0.41
4:M:19:GLU:OE2	4:M:40:LYS:HD2	2.21	0.41
2:C:123:ILE:HD12	2:C:200:CYS:SG	2.60	0.41
4:L:28:ILE:HA	4:L:34:ILE:HD13	2.02	0.41
3:B:213:LYS:HA	3:B:213:LYS:HD3	1.72	0.41
2:C:218:ASN:HD22	2:C:218:ASN:N	2.18	0.41
4:L:82:LYS:C	4:L:82:LYS:HD3	2.40	0.41
3:D:167:GLY:O	3:D:186:VAL:HA	2.21	0.41
4:L:13:THR:HA	4:L:14:PRO:HD2	1.79	0.41
4:L:66:ALA:HB2	4:L:77:ILE:CD1	2.49	0.41
3:B:93:THR:HG22	3:B:113:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:73:GLU:O	3:D:74:THR:HB	2.20	0.41
3:B:179:LEU:HA	3:B:179:LEU:HD23	1.87	0.41
2:C:43:GLN:HB2	2:C:53:LEU:HD11	2.02	0.41
3:D:29:PHE:CD2	3:D:77:SER:HA	2.56	0.41
3:B:35:HIS:N	3:B:35:HIS:CD2	2.89	0.41
2:C:60:ARG:O	2:C:61:GLU:C	2.60	0.41
3:B:124:PRO:CA	3:B:150:TYR:HB3	2.51	0.41
2:C:30:LEU:C	2:C:30:LEU:CD1	2.90	0.40
2:C:85:GLN:CB	2:C:87:GLU:OE2	2.65	0.40
2:C:206:THR:O	2:C:207:SER:HB2	2.22	0.40
1:Q:31:VAL:HG23	1:Q:31:VAL:O	2.21	0.40
3:B:30:THR:HG22	3:B:54:GLU:HA	2.02	0.40
4:M:25:VAL:HG22	4:M:75:MET:HB3	2.02	0.40
4:L:21:VAL:HG11	4:L:43:PHE:HA	2.04	0.40
2:C:218:ASN:ND2	2:C:219:GLU:HG3	2.36	0.40
3:B:100:LEU:HD12	3:B:104:TYR:CZ	2.56	0.40
1:P:38:PRO:HD3	2:A:33:ARG:HB3	2.03	0.40
2:C:212:VAL:O	2:C:212:VAL:HG23	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:285:HOH:O	5:D:278:HOH:O[1_554]	2.06	0.14

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	P	14/44 (32%)	10 (71%)	4 (29%)	0	100 100
1	Q	6/44 (14%)	2 (33%)	3 (50%)	1 (17%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	218/220 (99%)	203 (93%)	9 (4%)	6 (3%)	6 10
2	C	218/220 (99%)	194 (89%)	18 (8%)	6 (3%)	6 10
3	B	216/218 (99%)	197 (91%)	14 (6%)	5 (2%)	8 14
3	D	216/218 (99%)	193 (89%)	15 (7%)	8 (4%)	4 5
4	L	69/80 (86%)	61 (88%)	2 (3%)	6 (9%)	1 1
4	M	65/80 (81%)	55 (85%)	7 (11%)	3 (5%)	3 3
All	All	1022/1124 (91%)	915 (90%)	72 (7%)	35 (3%)	5 7

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	133	SER
4	L	16	GLU
4	L	17	PRO
4	L	18	LYS
4	L	19	GLU
2	C	31	ASN
2	C	46	PRO
2	C	206	THR
3	D	135	ALA
3	D	136	GLN
3	D	137	THR
2	A	27	GLN
2	A	56	TRP
3	B	135	ALA
4	L	14	PRO
2	C	82	SER
3	D	29	PHE
3	D	132	GLY
4	M	43	PHE
2	A	26	SER
2	A	57	ALA
2	A	58	SER
3	B	134	ALA
3	B	137	THR
4	M	18	LYS
3	B	161	SER
2	C	28	SER
3	D	16	GLU
3	D	25	SER

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Mol	Chain	Res	Type
2	A	206	THR
4	L	13	THR
3	D	92	ALA
4	M	20	GLU
1	Q	34	VAL
2	C	50	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	P	11/37 (30%)	10 (91%)	1 (9%)	12 22
1	Q	6/37 (16%)	6 (100%)	0	100 100
2	A	195/195 (100%)	182 (93%)	13 (7%)	20 40
2	C	195/195 (100%)	182 (93%)	13 (7%)	20 40
3	B	187/187 (100%)	169 (90%)	18 (10%)	10 20
3	D	187/187 (100%)	177 (95%)	10 (5%)	28 53
4	L	54/63 (86%)	48 (89%)	6 (11%)	8 13
4	M	51/63 (81%)	49 (96%)	2 (4%)	39 68
All	All	886/964 (92%)	823 (93%)	63 (7%)	18 36

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	39	ARG
2	A	1	ASP
2	A	33	ARG
2	A	120	THR
2	A	142	LEU
2	A	150	ILE
2	A	161	ARG
2	A	166	LEU
2	A	170	THR

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Mol	Chain	Res	Type
2	A	181	MET
2	A	199	THR
2	A	205	LYS
2	A	206	THR
2	A	208	THR
3	B	4	LEU
3	B	11	LEU
3	B	30	THR
3	B	83	ILE
3	B	101	LEU
3	B	113	THR
3	B	122	THR
3	B	136	GLN
3	B	137	THR
3	B	138	ASN
3	B	152	PRO
3	B	154	PRO
3	B	164	LEU
3	B	182	LEU
3	B	186	VAL
3	B	187	THR
3	B	202	VAL
3	B	211	VAL
4	L	15	GLU
4	L	18	LYS
4	L	19	GLU
4	L	36	THR
4	L	56	LEU
4	L	57	LEU
2	C	1	ASP
2	C	2	ILE
2	C	30	LEU
2	C	32	SER
2	C	33	ARG
2	C	36	LYS
2	C	46	PRO
2	C	79	LEU
2	C	99	ILE
2	C	112	LEU
2	C	165	VAL
2	C	199	THR
2	C	218	ASN

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Mol	Chain	Res	Type
3	D	11	LEU
3	D	31	ASP
3	D	59	THR
3	D	89	GLU
3	D	101	LEU
3	D	114	VAL
3	D	122	THR
3	D	182	LEU
3	D	202	VAL
3	D	211	VAL
4	M	56	LEU
4	M	60	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	37	ASN
2	A	85	GLN
2	A	163	ASN
2	A	167	ASN
2	A	196	ASN
3	B	6	GLN
3	B	39	GLN
3	B	201	ASN
4	L	35	GLN
4	L	76	ASN
2	C	37	ASN
2	C	43	GLN
2	C	85	GLN
2	C	89	GLN
2	C	96	GLN
2	C	216	ASN
2	C	218	ASN
3	D	39	GLN
3	D	46	ASN
3	D	138	ASN
3	D	201	ASN
3	D	204	HIS
4	M	26	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	P	16/44 (36%)	1.93	6 (37%) 0 0	38, 57, 94, 96	0
1	Q	8/44 (18%)	2.78	5 (62%) 0 0	104, 109, 111, 111	0
2	A	220/220 (100%)	-0.16	2 (0%) 85 83	17, 32, 52, 75	0
2	C	220/220 (100%)	0.15	12 (5%) 29 21	26, 45, 73, 90	1 (0%)
3	B	218/218 (100%)	-0.15	7 (3%) 51 44	15, 29, 48, 93	0
3	D	218/218 (100%)	0.14	8 (3%) 45 37	23, 46, 71, 97	0
4	L	71/80 (88%)	0.72	8 (11%) 7 4	29, 45, 124, 137	0
4	M	67/80 (83%)	0.28	5 (7%) 17 12	26, 37, 88, 113	0
All	All	1038/1124 (92%)	0.11	53 (5%) 32 25	15, 38, 74, 137	1 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	13	THR	8.6
3	B	137	THR	6.8
2	C	220	CYS	6.4
1	P	27	GLY	6.4
1	P	26	GLY	6.3
4	M	17	PRO	6.2
1	P	25	PRO	6.1
4	L	14	PRO	5.9
4	M	18	LYS	5.8
3	D	135	ALA	5.3
3	D	134	ALA	5.2
1	P	40	ARG	5.2
4	M	19	GLU	5.1
3	B	136	GLN	5.0
4	L	12	LYS	4.8
3	B	135	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
4	L	17	PRO	4.6
4	L	18	LYS	4.4
1	Q	29	GLN	4.4
1	P	39	ARG	4.4
4	M	16	GLU	4.3
2	C	30	LEU	4.0
1	Q	30	ILE	4.0
3	B	138	ASN	4.0
3	D	136	GLN	3.9
1	Q	35	TYR	3.8
4	L	19	GLU	3.4
1	P	28	GLY	3.4
3	D	138	ASN	3.1
3	D	218	ARG	3.1
3	B	133	SER	3.1
2	A	220	CYS	3.0
4	L	82	LYS	2.9
1	Q	31	VAL	2.9
2	C	219	GLU	2.9
2	C	218	ASN	2.8
2	C	32	SER	2.7
2	C	162	GLN	2.6
3	B	134	ALA	2.5
4	L	15	GLU	2.4
3	D	137	THR	2.4
3	D	36	TRP	2.4
1	Q	34	VAL	2.4
3	B	1	GLN	2.4
2	C	208	THR	2.4
2	C	1	ASP	2.3
2	C	138	VAL	2.2
4	M	82	LYS	2.2
2	C	210	PRO	2.2
2	C	31	ASN	2.1
3	D	178	ASP	2.1
2	A	40	ALA	2.0
2	C	33	ARG	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.