Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2023 – 02:53 PM EDT

PDB ID	:	1V7M
Title	:	Human Thrombopoietin Functional Domain Complexed To Neutralizing Antibody TN1 Fab
Authors	:	Feese, M.D.; Tamada, T.; Kato, Y.; Maeda, Y.; Hirose, M.; Matsukura, Y.; Shigematsu, H.; Kato, T.; Miyazaki, H.; Kuroki, R.
Deposited on	:	2003-12-18
Resolution	:	2.51 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:

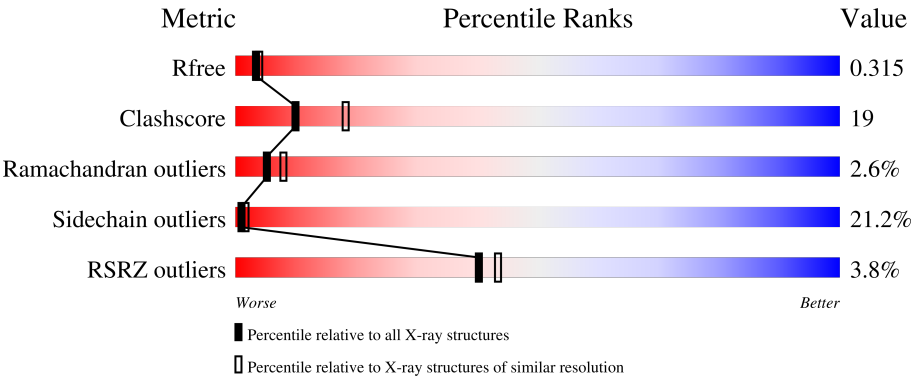
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	L	213	70% 23% 6%
1	M	213	62% 32% 5%
2	H	217	% 55% 35% 9%
2	I	217	% 61% 29% 9%
3	V	163	15% 45% 30% 12% 11%

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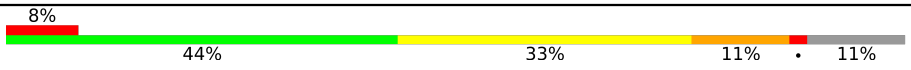
Mol	Chain	Length	Quality of chain
3	X	163	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8902 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 Monoclonal TN1 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1632	1015	277	332	8			
1	M	212	Total	C	N	O	S	0	0	0
			1632	1015	277	332	8			

- Molecule 2 is a protein called Monoclonal TN1 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1643	1038	273	324	8			
2	I	217	Total	C	N	O	S	0	0	0
			1643	1038	273	324	8			

- Molecule 3 is a protein called Thrombopoietin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V	145	Total	C	N	O	S	0	0	0
			1098	699	196	196	7			
3	X	145	Total	C	N	O	S	0	0	0
			1098	699	196	196	7			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	27	Total	O	0	0
			27	27		
4	H	35	Total	O	0	0
			35	35		
4	V	12	Total	O	0	0
			12	12		
4	M	36	Total	O	0	0
			36	36		

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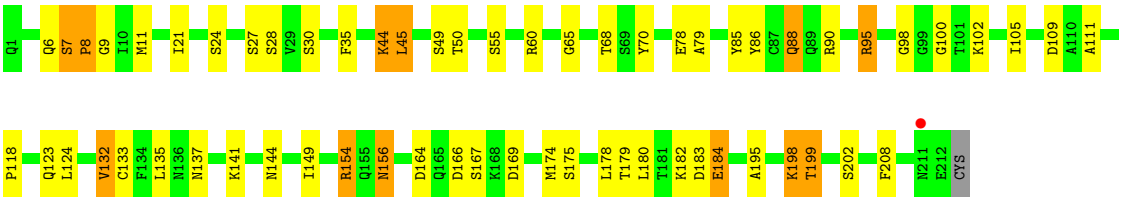
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	33	Total O 33 33	0	0
4	X	13	Total O 13 13	0	0

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.

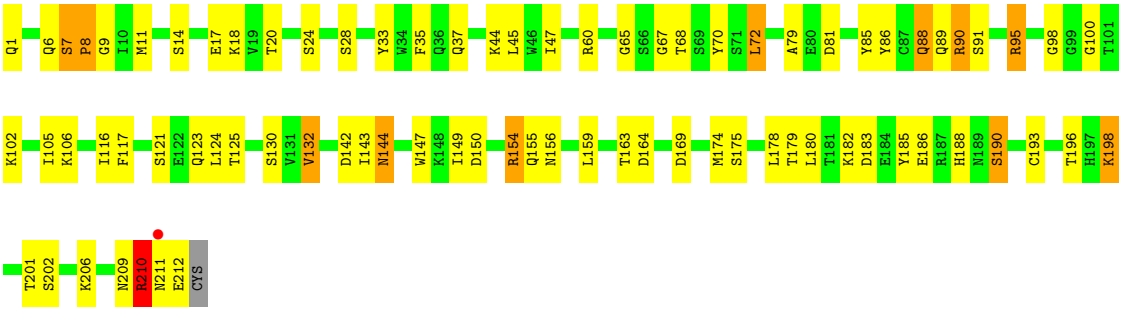
• Molecule 1: Monoclonal TN1 Fab Light Chain

Chain L:



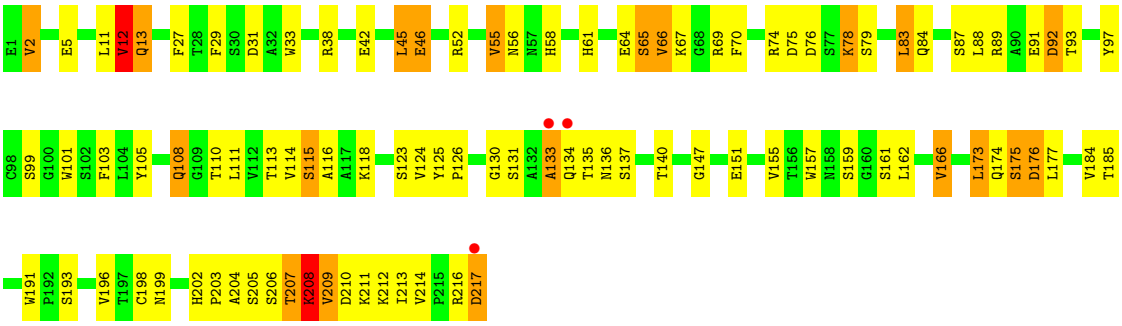
• Molecule 1: Monoclonal TN1 Fab Light Chain

Chain M:



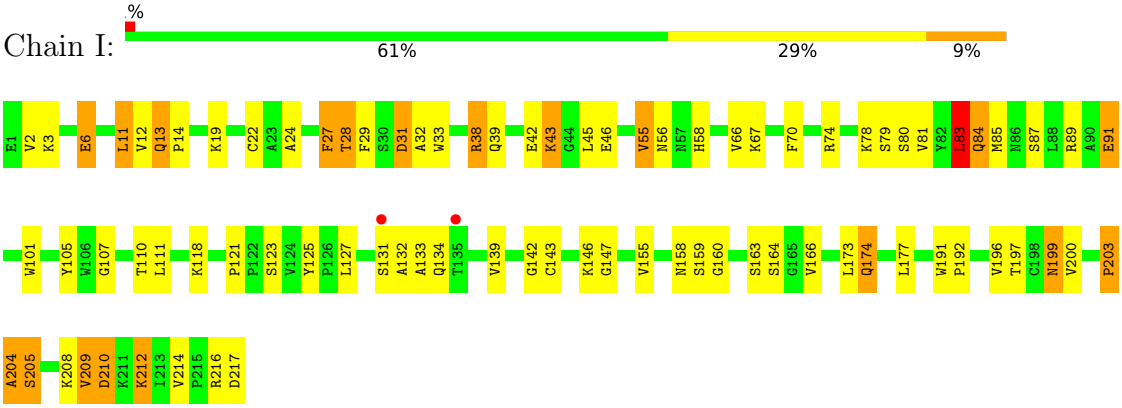
• Molecule 2: Monoclonal TN1 Fab Heavy Chain

Chain H:



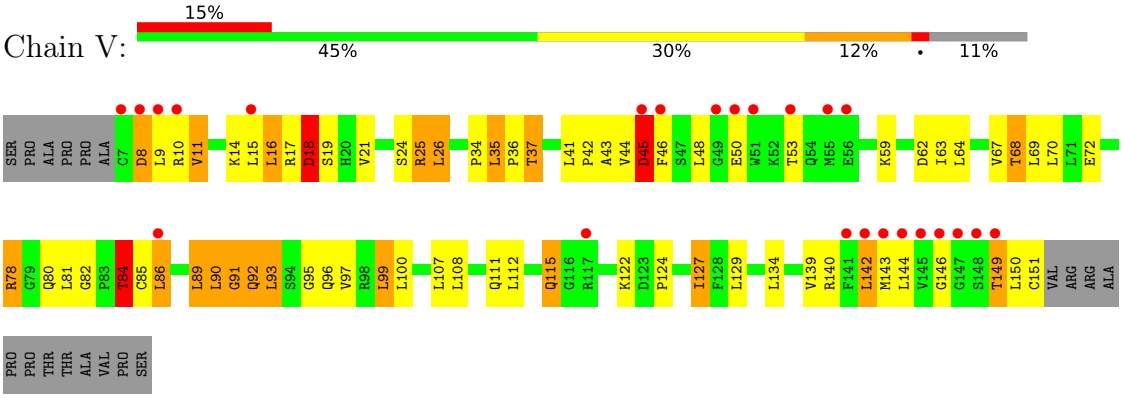
• Molecule 2: Monoclonal TN1 Fab Heavy Chain

Chain I:



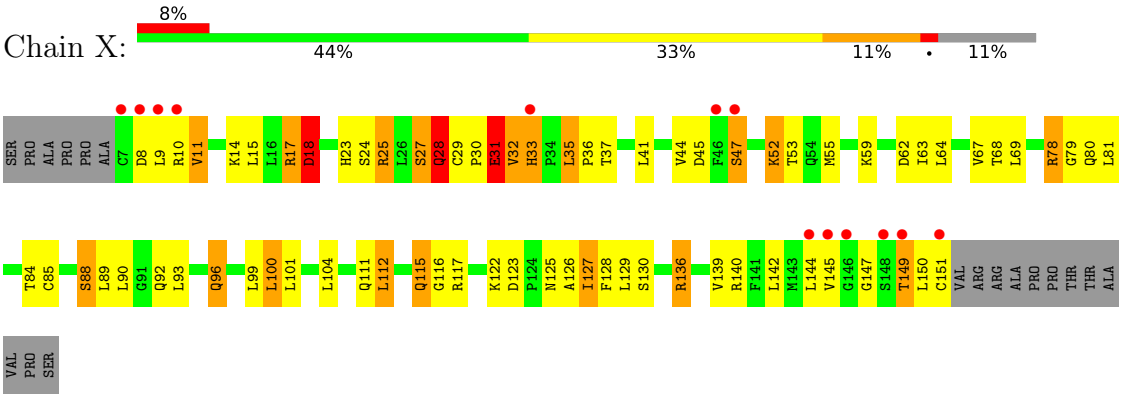
• Molecule 3: Thrombopoietin

Chain V:



• Molecule 3: Thrombopoietin

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	132.10Å 46.77Å 185.15Å 90.00° 90.48° 90.00°	Depositor
Resolution (Å)	45.28 – 2.51 45.28 – 2.51	Depositor EDS
% Data completeness (in resolution range)	92.9 (45.28-2.51) 92.8 (45.28-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.228 , 0.316 0.230 , 0.315	Depositor DCC
R_{free} test set	1852 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 35.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8902	wwPDB-VP
Average B, all atoms (Å^2)	49.0	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 46.04 % 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 1.2117e-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, 0.333 respectively for untwinned datasets, and 0.375, 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	L	0.91	1/1670 (0.1%)	1.07	9/2266 (0.4%)
1	M	0.98	1/1670 (0.1%)	1.11	10/2266 (0.4%)
2	H	0.98	1/1687 (0.1%)	1.13	14/2302 (0.6%)
2	I	0.96	2/1687 (0.1%)	1.05	4/2302 (0.2%)
3	V	0.79	0/1117	1.05	4/1515 (0.3%)
3	X	0.81	0/1117	1.01	3/1515 (0.2%)
All	All	0.92	5/8948 (0.1%)	1.08	44/12166 (0.4%)

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
3	X	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	184	GLU	CD-OE2	6.08	1.32	1.25
1	M	147	TRP	CB-CG	-5.46	1.40	1.50
2	H	208	LYS	CD-CE	5.18	1.64	1.51
2	I	55	VAL	CB-CG2	5.14	1.63	1.52
2	I	43	LYS	CD-CE	5.12	1.64	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	V	62	ASP	CB-CG-OD2	8.94	126.34	118.30
3	X	62	ASP	CB-CG-OD2	8.79	126.21	118.30
2	H	31	ASP	CB-CG-OD2	8.54	125.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	109	ASP	CB-CG-OD2	8.18	125.67	118.30
1	M	60	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	M	60	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	L	60	ARG	NE-CZ-NH1	7.39	124.00	120.30
3	X	8	ASP	CB-CG-OD2	7.38	124.94	118.30
1	M	142	ASP	CB-CG-OD2	7.36	124.93	118.30
1	M	169	ASP	CB-CG-OD2	7.35	124.91	118.30
3	V	8	ASP	CB-CG-OD2	7.32	124.88	118.30
2	H	76	ASP	CB-CG-OD2	7.09	124.69	118.30
2	I	210	ASP	CB-CG-OD2	6.99	124.59	118.30
2	H	217	ASP	CB-CG-OD2	6.94	124.55	118.30
2	H	52	ARG	NE-CZ-NH1	-6.88	116.86	120.30
2	H	75	ASP	CB-CG-OD2	6.84	124.46	118.30
1	M	164	ASP	CB-CG-OD2	6.81	124.43	118.30
2	I	31	ASP	CB-CG-OD2	6.80	124.42	118.30
1	L	60	ARG	NE-CZ-NH2	-6.76	116.92	120.30
2	I	83	LEU	CB-CG-CD2	6.72	122.42	111.00
1	L	169	ASP	CB-CG-OD2	6.63	124.27	118.30
1	M	90	ARG	NE-CZ-NH1	6.60	123.60	120.30
2	H	97	TYR	CB-CA-C	-6.57	97.26	110.40
1	M	95	ARG	NE-CZ-NH1	6.37	123.49	120.30
2	H	12	VAL	CB-CA-C	-6.37	99.31	111.40
1	L	164	ASP	CB-CG-OD2	6.30	123.97	118.30
1	M	183	ASP	CB-CG-OD2	6.24	123.92	118.30
1	M	150	ASP	CB-CG-OD2	6.17	123.85	118.30
1	L	95	ARG	NE-CZ-NH1	6.16	123.38	120.30
3	V	26	LEU	CA-CB-CG	6.10	129.33	115.30
2	I	217	ASP	CB-CG-OD2	6.04	123.74	118.30
3	V	45	ASP	CB-CG-OD2	6.03	123.72	118.30
2	H	208	LYS	CD-CE-NZ	5.82	125.08	111.70
2	H	45	LEU	CA-CB-CG	5.81	128.67	115.30
3	X	18	ASP	CB-CG-OD2	5.79	123.51	118.30
1	L	8	PRO	N-CA-C	-5.69	97.31	112.10
2	H	83	LEU	CB-CG-CD2	5.63	120.57	111.00
1	L	183	ASP	CB-CG-OD2	5.62	123.36	118.30
2	H	176	ASP	CB-CG-OD2	5.45	123.20	118.30
1	M	8	PRO	N-CA-C	-5.43	97.97	112.10
2	H	92	ASP	CB-CG-OD2	5.33	123.09	118.30
2	H	173	LEU	CA-CB-CG	5.21	127.29	115.30
2	H	55	VAL	CB-CA-C	-5.07	101.76	111.40
1	L	166	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	203	PRO	Peptide
3	X	33	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1632	0	1568	44	0
1	M	1632	0	1568	52	0
2	H	1643	0	1594	61	0
2	I	1643	0	1594	93	0
3	V	1098	0	1152	45	0
3	X	1098	0	1152	54	0
4	H	35	0	0	10	0
4	I	33	0	0	22	0
4	L	27	0	0	8	0
4	M	36	0	0	12	0
4	V	12	0	0	7	0
4	X	13	0	0	7	0
All	All	8902	0	8628	332	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 19.

All (332) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:11:LEU:HG	4:I:227:HOH:O	1.20	1.32
3:X:85:CYS:HA	4:X:173:HOH:O	1.17	1.30
1:M:8:PRO:HD2	4:M:241:HOH:O	1.17	1.27
2:I:209:VAL:HG12	4:I:231:HOH:O	1.19	1.27
2:H:209:VAL:HG23	4:H:228:HOH:O	1.18	1.26
2:H:155:VAL:HB	4:H:235:HOH:O	1.09	1.25
1:L:8:PRO:HD2	4:L:219:HOH:O	1.35	1.23
2:H:206:SER:HB3	4:H:247:HOH:O	1.06	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:66:VAL:HB	4:I:228:HOH:O	1.39	1.18
2:I:196:VAL:O	2:I:212:LYS:HD2	1.42	1.16
2:I:191:TRP:NE1	2:I:212:LYS:HE2	1.65	1.11
1:M:188:HIS:O	1:M:210:ARG:NH1	1.86	1.08
2:I:191:TRP:HE1	2:I:212:LYS:HE2	0.87	1.01
1:L:7:SER:O	1:L:8:PRO:C	1.96	0.99
2:I:212:LYS:HD3	2:I:212:LYS:N	1.76	0.98
2:I:212:LYS:HD3	2:I:212:LYS:H	1.27	0.97
1:M:212:GLU:HG2	2:I:132:ALA:HB2	1.47	0.96
2:I:191:TRP:HE1	2:I:212:LYS:CE	1.77	0.95
2:I:196:VAL:O	2:I:212:LYS:CD	2.14	0.95
2:I:209:VAL:CG1	4:I:231:HOH:O	1.85	0.91
1:L:149:ILE:HD12	1:L:154:ARG:HD2	1.53	0.90
2:I:209:VAL:CB	4:I:231:HOH:O	2.15	0.89
3:V:11:VAL:O	3:V:15:LEU:HB2	1.74	0.88
2:H:12:VAL:HB	4:H:237:HOH:O	1.74	0.88
3:X:78:ARG:HG2	3:X:78:ARG:HH11	1.38	0.87
2:I:33:TRP:H	3:X:111:GLN:NE2	1.74	0.85
1:M:8:PRO:CD	4:M:241:HOH:O	1.89	0.85
3:X:23:HIS:HE1	3:X:125:ASN:ND2	1.76	0.83
2:I:191:TRP:NE1	2:I:212:LYS:CE	2.41	0.82
1:M:212:GLU:CG	2:I:132:ALA:HB2	2.08	0.82
3:X:23:HIS:CE1	3:X:125:ASN:ND2	2.48	0.81
3:X:30:PRO:O	3:X:31:GLU:HB2	1.80	0.80
2:I:212:LYS:CE	2:I:212:LYS:O	2.31	0.79
2:H:130:GLY:O	2:H:133:ALA:HA	1.82	0.79
1:L:7:SER:O	1:L:9:GLY:N	2.15	0.79
3:V:84:THR:OG1	3:V:85:CYS:N	2.13	0.78
1:M:37:GLN:HE22	2:I:39:GLN:HE22	1.29	0.78
2:I:27:PHE:HE2	2:I:32:ALA:HB2	1.49	0.77
3:X:68:THR:HG22	3:X:101:LEU:HD11	1.66	0.77
3:V:41:LEU:HD11	3:V:127:ILE:HG22	1.67	0.77
1:L:7:SER:CA	4:L:219:HOH:O	2.33	0.76
1:L:8:PRO:HG2	1:L:11:MET:HE2	1.67	0.76
1:M:7:SER:CA	4:M:241:HOH:O	2.34	0.75
2:I:13:GLN:NE2	2:I:14:PRO:O	2.19	0.75
1:L:8:PRO:HG2	1:L:11:MET:CE	2.16	0.75
2:I:133:ALA:O	4:I:222:HOH:O	2.05	0.75
2:H:66:VAL:HG13	2:H:70:PHE:HB2	1.70	0.74
2:H:159:SER:H	2:H:199:ASN:HD21	1.36	0.73
3:X:78:ARG:HG2	3:X:78:ARG:NH1	2.00	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:66:VAL:HG13	2:I:70:PHE:HB2	1.71	0.72
3:X:88:SER:HB3	4:X:173:HOH:O	1.88	0.72
3:V:41:LEU:HA	4:V:175:HOH:O	1.87	0.72
1:M:159:LEU:HD11	2:I:174:GLN:HG2	1.72	0.71
1:L:154:ARG:CZ	1:L:156:ASN:HD21	2.04	0.71
3:X:23:HIS:HE1	3:X:125:ASN:HD21	1.39	0.71
2:I:2:VAL:HG11	2:I:105:TYR:CD1	2.25	0.70
2:H:89:ARG:HH11	2:H:89:ARG:CG	2.05	0.70
3:X:11:VAL:O	3:X:15:LEU:HB2	1.91	0.70
2:I:127:LEU:HB2	2:I:142:GLY:HA3	1.74	0.69
1:M:144:ASN:O	4:M:227:HOH:O	2.09	0.69
1:L:8:PRO:CD	4:L:219:HOH:O	2.09	0.69
2:I:191:TRP:CD1	2:I:212:LYS:HE3	2.28	0.69
3:V:95:GLY:O	3:V:99:LEU:HD23	1.93	0.69
3:X:68:THR:HG22	3:X:101:LEU:CD1	2.23	0.69
2:I:155:VAL:HG13	2:I:155:VAL:O	1.92	0.68
3:X:27:SER:O	3:X:29:CYS:N	2.27	0.68
1:M:7:SER:O	1:M:8:PRO:C	2.31	0.67
3:X:78:ARG:HH11	3:X:78:ARG:CG	2.07	0.67
3:V:16:LEU:O	3:V:19:SER:OG	2.12	0.66
2:H:89:ARG:HH11	2:H:89:ARG:HG2	1.60	0.66
3:V:36:PRO:HG3	4:V:170:HOH:O	1.95	0.66
2:I:33:TRP:HE1	2:I:56:ASN:HD22	1.42	0.66
1:L:154:ARG:NH2	1:L:156:ASN:HD21	1.94	0.66
3:V:18:ASP:HB3	3:V:96:GLN:OE1	1.96	0.66
3:V:139:VAL:O	4:V:169:HOH:O	2.14	0.66
2:I:66:VAL:CG1	4:I:228:HOH:O	2.44	0.65
1:L:6:GLN:HE21	1:L:98:GLY:HA3	1.62	0.65
3:V:90:LEU:HD11	3:V:127:ILE:HD11	1.77	0.65
2:H:147:GLY:HA2	2:H:177:LEU:HB3	1.77	0.65
2:I:212:LYS:HE2	2:I:212:LYS:O	1.97	0.64
1:M:88:GLN:NE2	1:M:90:ARG:HD2	2.13	0.64
2:I:159:SER:H	2:I:199:ASN:HD21	1.45	0.64
1:L:7:SER:HB3	4:L:219:HOH:O	1.98	0.64
3:X:149:THR:O	3:X:150:LEU:HG	1.98	0.64
3:X:90:LEU:CD2	3:X:127:ILE:HD11	2.28	0.63
2:I:33:TRP:HE1	2:I:56:ASN:ND2	1.97	0.63
1:L:149:ILE:HD12	1:L:154:ARG:CD	2.25	0.63
2:I:191:TRP:CD1	2:I:212:LYS:CE	2.81	0.63
3:V:64:LEU:HD23	3:V:108:LEU:HD12	1.81	0.63
1:M:47:ILE:HD12	1:M:72:LEU:HD12	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2:VAL:HG11	2:H:105:TYR:CE1	2.34	0.62
2:H:101:TRP:HA	3:V:111:GLN:NE2	2.14	0.62
1:L:88:GLN:NE2	1:L:90:ARG:HE	1.96	0.62
2:I:66:VAL:CG1	2:I:70:PHE:HB2	2.28	0.62
2:I:91:GLU:N	2:I:91:GLU:OE2	2.31	0.62
2:I:160:GLY:HA2	4:I:237:HOH:O	1.99	0.62
1:L:35:PHE:CE2	1:L:45:LEU:HD23	2.35	0.62
2:I:196:VAL:C	2:I:212:LYS:HD2	2.19	0.61
3:X:90:LEU:HD22	3:X:127:ILE:HD11	1.82	0.61
1:M:123:GLN:HG3	2:I:125:TYR:CE2	2.35	0.61
1:M:88:GLN:HE22	1:M:90:ARG:HH11	1.46	0.61
3:V:45:ASP:HA	4:V:168:HOH:O	2.00	0.61
2:I:80:SER:O	4:I:242:HOH:O	2.16	0.61
1:M:7:SER:N	4:M:241:HOH:O	2.34	0.61
1:M:121:SER:O	1:M:125:THR:HG23	2.01	0.60
2:I:212:LYS:H	2:I:212:LYS:CD	2.08	0.60
2:H:46:GLU:OE2	4:H:239:HOH:O	2.16	0.60
3:X:147:GLY:HA3	4:X:164:HOH:O	2.00	0.60
1:L:154:ARG:CZ	1:L:156:ASN:ND2	2.63	0.60
3:X:67:VAL:HG21	3:X:100:LEU:HD13	1.82	0.60
2:H:206:SER:CB	4:H:247:HOH:O	1.87	0.60
2:H:217:ASP:OXT	3:X:140:ARG:NH1	2.35	0.60
2:I:200:VAL:HB	4:I:241:HOH:O	2.02	0.59
3:X:115:GLN:HG3	3:X:116:GLY:N	2.17	0.59
2:H:101:TRP:HZ2	3:V:68:THR:CG2	2.15	0.59
2:H:33:TRP:HE1	2:H:56:ASN:ND2	2.01	0.59
2:I:155:VAL:O	2:I:155:VAL:CG1	2.51	0.59
1:M:211:ASN:HA	1:M:212:GLU:OE1	2.03	0.59
1:M:33:TYR:CD1	1:M:90:ARG:HD3	2.38	0.58
1:L:88:GLN:HE22	1:L:90:ARG:HE	1.49	0.58
2:H:216:ARG:HH22	3:X:136:ARG:NH1	2.02	0.58
2:I:91:GLU:CD	2:I:91:GLU:H	2.07	0.58
1:L:7:SER:CB	4:L:219:HOH:O	2.52	0.57
2:I:66:VAL:HG13	2:I:70:PHE:CG	2.39	0.57
2:I:212:LYS:CD	2:I:212:LYS:O	2.52	0.57
2:I:84:GLN:HG2	4:I:223:HOH:O	2.04	0.57
3:V:25:ARG:HB2	3:V:89:LEU:HD21	1.86	0.57
1:M:7:SER:HB3	4:M:241:HOH:O	2.03	0.57
2:I:11:LEU:HA	4:I:227:HOH:O	2.04	0.57
3:V:10:ARG:O	3:V:10:ARG:HD3	2.05	0.57
2:I:196:VAL:HG22	2:I:212:LYS:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:65:GLY:HA3	1:M:70:TYR:HA	1.86	0.57
2:I:127:LEU:HB2	2:I:142:GLY:CA	2.34	0.57
2:I:209:VAL:HB	4:I:231:HOH:O	1.95	0.57
2:H:69:ARG:NH2	2:H:92:ASP:OD2	2.37	0.56
3:X:25:ARG:HB3	3:X:89:LEU:HD21	1.87	0.56
3:V:42:PRO:HG2	3:V:70:LEU:HB2	1.86	0.56
1:M:8:PRO:HG3	1:M:11:MET:CE	2.35	0.56
2:H:191:TRP:CD1	2:H:196:VAL:HG13	2.41	0.56
2:I:80:SER:C	4:I:242:HOH:O	2.42	0.56
1:M:185:TYR:CZ	1:M:210:ARG:HD2	2.40	0.56
3:V:59:LYS:HA	4:V:165:HOH:O	2.05	0.56
3:X:52:LYS:HA	3:X:59:LYS:HZ1	1.70	0.56
1:M:8:PRO:HG3	1:M:11:MET:HE2	1.87	0.56
3:X:23:HIS:CE1	3:X:125:ASN:HD22	2.23	0.56
2:H:101:TRP:CZ2	3:V:68:THR:CG2	2.89	0.56
3:V:82:GLY:O	3:V:84:THR:HG22	2.07	0.55
2:I:158:ASN:ND2	2:I:197:THR:H	2.05	0.55
2:H:101:TRP:HZ2	3:V:68:THR:HG23	1.71	0.55
2:I:147:GLY:HA2	2:I:177:LEU:HB3	1.87	0.55
2:H:207:THR:O	2:H:207:THR:HG22	2.05	0.55
2:I:74:ARG:HA	4:I:242:HOH:O	2.05	0.54
2:H:166:VAL:HG12	2:H:184:VAL:HG23	1.89	0.54
3:X:31:GLU:OE2	3:X:31:GLU:HA	2.07	0.54
1:L:8:PRO:CG	1:L:11:MET:CE	2.85	0.54
3:X:44:VAL:HG12	3:X:44:VAL:O	2.08	0.53
2:I:196:VAL:H	2:I:212:LYS:HE3	1.71	0.53
2:I:66:VAL:HG13	2:I:70:PHE:CB	2.38	0.53
3:V:93:LEU:O	3:V:97:VAL:HG23	2.08	0.53
2:H:175:SER:O	2:H:175:SER:OG	2.27	0.53
3:X:63:ILE:HG22	3:X:104:LEU:HD11	1.91	0.53
3:V:86:LEU:HD22	3:V:90:LEU:HD22	1.91	0.52
1:M:143:ILE:HG12	4:M:227:HOH:O	2.08	0.52
2:H:33:TRP:H	3:V:111:GLN:NE2	2.07	0.52
2:H:155:VAL:HG13	2:H:155:VAL:O	2.09	0.52
2:I:27:PHE:CE2	2:I:32:ALA:HB2	2.37	0.52
2:I:196:VAL:HG22	2:I:212:LYS:HG3	1.91	0.52
2:H:209:VAL:CG2	4:H:228:HOH:O	2.04	0.52
3:V:63:ILE:O	3:V:67:VAL:HG23	2.08	0.52
1:L:6:GLN:HE22	1:L:86:TYR:HA	1.73	0.52
1:L:123:GLN:HG3	2:H:125:TYR:CE2	2.45	0.52
3:V:89:LEU:O	3:V:91:GLY:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:47:ILE:CD1	1:M:72:LEU:HD12	2.40	0.52
2:I:81:VAL:CA	4:I:242:HOH:O	2.58	0.52
2:I:11:LEU:CG	4:I:227:HOH:O	2.04	0.52
1:M:6:GLN:HE21	1:M:98:GLY:HA3	1.74	0.51
1:L:6:GLN:HE21	1:L:98:GLY:CA	2.22	0.51
2:I:58:HIS:CD2	2:I:74:ARG:HD3	2.46	0.51
2:I:83:LEU:HD13	2:I:85:MET:HG3	1.92	0.51
1:L:35:PHE:CZ	1:L:45:LEU:HD23	2.46	0.51
1:L:65:GLY:HA3	1:L:70:TYR:HA	1.93	0.51
2:H:99:SER:HA	2:H:105:TYR:O	2.11	0.51
2:I:139:VAL:HA	4:I:249:HOH:O	2.10	0.50
1:L:49:SER:O	1:L:50:THR:HB	2.11	0.50
1:M:7:SER:C	4:M:241:HOH:O	2.49	0.50
1:M:88:GLN:NE2	1:M:90:ARG:HH11	2.10	0.50
1:L:8:PRO:CG	1:L:11:MET:HE1	2.42	0.50
1:M:14:SER:N	1:M:17:GLU:OE1	2.45	0.50
2:H:61:HIS:HD2	4:H:236:HOH:O	1.94	0.50
2:H:191:TRP:HD1	2:H:196:VAL:HG13	1.76	0.50
3:X:64:LEU:HD23	3:X:112:LEU:HD22	1.94	0.49
2:I:158:ASN:HD21	2:I:196:VAL:HA	1.77	0.49
2:H:124:VAL:HB	2:H:208:LYS:HE2	1.93	0.49
2:I:121:PRO:HA	4:I:248:HOH:O	2.10	0.49
2:H:176:ASP:O	2:H:177:LEU:HD23	2.13	0.49
2:I:196:VAL:HG13	2:I:212:LYS:HE3	1.94	0.49
1:M:6:GLN:NE2	1:M:100:GLY:H	2.11	0.49
1:M:8:PRO:CG	1:M:11:MET:CE	2.90	0.49
3:V:89:LEU:HG	3:V:92:GLN:HE22	1.77	0.49
3:X:139:VAL:O	4:X:172:HOH:O	2.20	0.49
2:H:99:SER:OG	2:H:103:PHE:HA	2.12	0.48
1:L:135:LEU:HD23	1:L:195:ALA:HB2	1.96	0.48
2:I:196:VAL:H	2:I:212:LYS:CE	2.27	0.48
3:V:134:LEU:O	3:V:139:VAL:HG23	2.13	0.48
3:V:142:LEU:HG	3:V:142:LEU:O	2.12	0.48
3:V:18:ASP:CB	3:V:96:GLN:OE1	2.61	0.48
2:I:191:TRP:CD1	2:I:196:VAL:HG13	2.48	0.48
1:M:116:ILE:HD12	1:M:193:CYS:HB2	1.96	0.47
2:H:29:PHE:CD2	2:H:79:SER:HA	2.49	0.47
2:H:93:THR:HG23	2:H:113:THR:HA	1.95	0.47
1:M:124:LEU:O	1:M:182:LYS:HE2	2.14	0.47
2:I:22:CYS:HB3	2:I:81:VAL:HG12	1.96	0.47
3:X:14:LYS:HE3	3:X:18:ASP:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:141:LYS:HD2	4:L:233:HOH:O	2.13	0.47
3:V:64:LEU:CD2	3:V:108:LEU:HD12	2.42	0.47
2:H:42:GLU:OE1	2:H:42:GLU:N	2.36	0.47
2:H:5:GLU:HG3	2:H:108:GLN:HE21	1.80	0.47
2:H:33:TRP:HE1	2:H:56:ASN:HD22	1.62	0.47
2:H:130:GLY:O	2:H:133:ALA:CA	2.57	0.47
1:M:8:PRO:CG	1:M:11:MET:HE2	2.45	0.47
3:X:35:LEU:HD22	3:X:122:LYS:O	2.15	0.47
3:X:36:PRO:HG2	3:X:80:GLN:HB3	1.95	0.47
1:L:7:SER:N	4:L:219:HOH:O	2.45	0.46
1:M:144:ASN:OD1	1:M:144:ASN:N	2.49	0.46
2:I:66:VAL:HG13	2:I:70:PHE:CD2	2.49	0.46
3:X:90:LEU:HD21	3:X:127:ILE:HD11	1.96	0.46
1:M:7:SER:CB	4:M:241:HOH:O	2.56	0.46
3:X:45:ASP:HB2	3:X:47:SER:HB2	1.98	0.46
2:I:11:LEU:CA	4:I:227:HOH:O	2.62	0.46
2:I:158:ASN:HD21	2:I:197:THR:N	2.13	0.46
2:I:28:THR:O	2:I:31:ASP:HB2	2.16	0.46
1:M:6:GLN:HE22	1:M:86:TYR:HA	1.79	0.46
2:H:202:HIS:HB3	2:H:206:SER:HB2	1.97	0.46
1:L:7:SER:C	4:L:219:HOH:O	2.54	0.46
2:H:64:GLU:C	2:H:66:VAL:H	2.19	0.46
1:M:117:PHE:HB2	1:M:132:VAL:HG13	1.96	0.46
2:H:12:VAL:O	2:H:114:VAL:HA	2.16	0.45
2:H:140:THR:HG23	2:H:185:THR:HG22	1.98	0.45
2:H:151:GLU:HG3	4:H:226:HOH:O	2.16	0.45
1:M:144:ASN:N	4:M:227:HOH:O	2.49	0.45
3:X:96:GLN:HG3	4:X:167:HOH:O	2.15	0.45
2:H:157:TRP:CZ3	2:H:198:CYS:HB3	2.52	0.45
3:V:78:ARG:HH21	3:V:91:GLY:HA3	1.81	0.45
1:L:135:LEU:CD2	1:L:195:ALA:HB2	2.46	0.45
1:M:190:SER:HB2	1:M:209:ASN:ND2	2.31	0.45
3:V:59:LYS:CA	4:V:165:HOH:O	2.61	0.45
2:I:6:GLU:OE1	2:I:107:GLY:HA3	2.17	0.45
2:I:38:ARG:HD3	2:I:46:GLU:HG3	1.97	0.45
3:V:59:LYS:HB2	3:V:142:LEU:HD13	1.97	0.45
2:I:208:LYS:HB2	4:I:241:HOH:O	2.17	0.45
2:H:89:ARG:CG	2:H:89:ARG:NH1	2.72	0.45
2:H:212:LYS:HE2	2:H:212:LYS:HB2	1.71	0.45
3:V:81:LEU:HD23	4:V:170:HOH:O	2.16	0.45
2:I:81:VAL:HA	4:I:242:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:23:HIS:CE1	3:X:125:ASN:HD21	2.21	0.45
2:H:91:GLU:H	2:H:91:GLU:CD	2.20	0.44
2:I:191:TRP:CG	2:I:192:PRO:HA	2.51	0.44
3:X:35:LEU:CD1	3:X:81:LEU:HD21	2.47	0.44
1:L:7:SER:O	1:L:8:PRO:O	2.35	0.44
1:M:149:ILE:CD1	1:M:154:ARG:HG3	2.47	0.44
3:V:37:THR:HB	3:V:80:GLN:NE2	2.33	0.44
3:V:8:ASP:HB3	3:V:10:ARG:HB3	1.99	0.44
1:M:89:GLN:OE1	1:M:91:SER:OG	2.31	0.44
3:X:63:ILE:HG22	3:X:104:LEU:CD1	2.48	0.44
3:V:35:LEU:N	3:V:122:LYS:O	2.47	0.44
3:V:115:GLN:HE21	3:V:115:GLN:HB3	1.63	0.43
1:L:8:PRO:HG2	1:L:11:MET:HE1	1.95	0.43
1:L:111:ALA:N	1:L:199:THR:HG21	2.34	0.43
1:L:118:PRO:HB3	1:L:208:PHE:CZ	2.53	0.43
3:X:45:ASP:C	3:X:47:SER:H	2.20	0.43
3:X:88:SER:CB	4:X:173:HOH:O	2.57	0.43
2:I:29:PHE:CD2	2:I:79:SER:HA	2.52	0.43
1:L:154:ARG:NH2	1:L:156:ASN:ND2	2.63	0.43
2:I:212:LYS:O	2:I:212:LYS:NZ	2.52	0.43
2:I:191:TRP:HD1	2:I:196:VAL:HG13	1.83	0.43
2:I:159:SER:H	2:I:199:ASN:ND2	2.14	0.43
1:M:35:PHE:HA	1:M:44:LYS:O	2.19	0.43
1:M:88:GLN:HE22	1:M:90:ARG:NH1	2.15	0.43
2:I:33:TRP:H	3:X:111:GLN:HE22	1.60	0.43
2:H:78:LYS:HB3	2:H:78:LYS:HE3	1.70	0.43
3:X:52:LYS:HD2	3:X:59:LYS:NZ	2.34	0.43
3:X:126:ALA:O	3:X:130:SER:HB2	2.19	0.43
1:M:7:SER:O	1:M:9:GLY:N	2.51	0.42
3:V:21:VAL:O	3:V:24:SER:OG	2.33	0.42
1:M:196:THR:N	4:M:227:HOH:O	2.52	0.42
1:M:212:GLU:CD	4:M:239:HOH:O	2.58	0.42
2:I:2:VAL:O	2:I:2:VAL:HG13	2.19	0.42
2:I:196:VAL:O	2:I:212:LYS:HD3	2.13	0.42
1:L:11:MET:HE3	1:L:21:ILE:HG12	2.02	0.42
2:H:116:ALA:O	2:H:118:LYS:HE3	2.19	0.42
3:V:34:PRO:HA	3:V:124:PRO:HD3	2.02	0.42
1:L:85:TYR:O	1:L:100:GLY:HA2	2.20	0.42
3:V:14:LYS:HD2	3:V:14:LYS:HA	1.88	0.42
1:M:149:ILE:HD11	1:M:154:ARG:HG3	2.02	0.42
2:I:158:ASN:HD21	2:I:197:THR:H	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:79:ALA:C	1:M:81:ASP:H	2.23	0.41
3:X:115:GLN:CG	3:X:116:GLY:N	2.83	0.41
1:M:8:PRO:CG	1:M:11:MET:HE3	2.50	0.41
2:I:24:ALA:HB1	2:I:27:PHE:HE1	1.85	0.41
3:X:125:ASN:O	3:X:128:PHE:HB2	2.20	0.41
1:L:135:LEU:N	1:L:135:LEU:HD12	2.35	0.41
3:X:28:GLN:O	3:X:30:PRO:HD3	2.20	0.41
1:L:132:VAL:HG23	1:L:133:CYS:N	2.36	0.41
2:H:13:GLN:HE21	2:H:13:GLN:HB2	1.64	0.41
3:V:142:LEU:O	3:V:142:LEU:CG	2.69	0.41
2:I:101:TRP:HA	3:X:111:GLN:NE2	2.36	0.41
3:X:25:ARG:CB	3:X:25:ARG:HH11	2.33	0.41
1:L:6:GLN:NE2	1:L:100:GLY:H	2.19	0.41
1:L:35:PHE:HA	1:L:44:LYS:O	2.21	0.41
2:H:13:GLN:HA	2:H:115:SER:O	2.20	0.41
2:H:125:TYR:HA	2:H:126:PRO:HD3	1.84	0.41
1:M:85:TYR:O	1:M:100:GLY:HA2	2.21	0.41
2:I:203:PRO:O	2:I:204:ALA:HB2	2.20	0.41
1:L:8:PRO:CG	1:L:11:MET:HE2	2.42	0.41
3:X:79:GLY:HA3	4:X:166:HOH:O	2.20	0.41
3:X:123:ASP:OD1	3:X:125:ASN:HB2	2.20	0.41
2:H:55:VAL:HG22	4:H:222:HOH:O	2.19	0.40
3:X:127:ILE:HG12	3:X:128:PHE:N	2.36	0.40
2:H:58:HIS:CD2	2:H:74:ARG:HD3	2.57	0.40
2:H:89:ARG:HB3	2:H:91:GLU:OE1	2.21	0.40
2:I:2:VAL:HG11	2:I:105:TYR:CE1	2.56	0.40
3:X:29:CYS:HA	3:X:30:PRO:HD2	1.91	0.40
3:X:88:SER:O	3:X:92:GLN:OE1	2.39	0.40
2:H:66:VAL:CG1	2:H:70:PHE:HB2	2.48	0.40
2:H:211:LYS:HD3	2:H:213:ILE:HG23	2.03	0.40
2:H:212:LYS:HA	2:H:212:LYS:HD3	1.82	0.40
1:M:123:GLN:HG3	2:I:125:TYR:CZ	2.57	0.40
2:I:191:TRP:HD1	2:I:212:LYS:HE3	1.83	0.40
1:L:78:GLU:O	1:L:79:ALA:C	2.59	0.40
3:V:41:LEU:HA	3:V:42:PRO:HD3	1.94	0.40
3:V:78:ARG:HH21	3:V:91:GLY:CA	2.34	0.40
2:I:203:PRO:O	2:I:204:ALA:CB	2.69	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	210/213 (99%)	201 (96%)	7 (3%)	2 (1%)	15 28
1	M	210/213 (99%)	197 (94%)	9 (4%)	4 (2%)	8 13
2	H	215/217 (99%)	197 (92%)	13 (6%)	5 (2%)	6 10
2	I	215/217 (99%)	202 (94%)	9 (4%)	4 (2%)	8 13
3	V	143/163 (88%)	116 (81%)	20 (14%)	7 (5%)	2 2
3	X	143/163 (88%)	113 (79%)	22 (15%)	8 (6%)	2 1
All	All	1136/1186 (96%)	1026 (90%)	80 (7%)	30 (3%)	5 8

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	7	SER
2	H	65	SER
2	H	134	GLN
2	H	137	SER
2	H	204	ALA
3	V	84	THR
3	V	90	LEU
3	V	149	THR
1	M	7	SER
2	I	204	ALA
3	X	28	GLN
3	X	84	THR
3	V	18	ASP
3	V	43	ALA
3	V	146	GLY
1	M	67	GLY
1	M	198	LYS
3	X	31	GLU
3	X	149	THR
2	I	203	PRO

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Mol	Chain	Res	Type
2	I	205	SER
3	X	27	SER
3	X	32	VAL
1	L	198	LYS
1	M	210	ARG
2	I	43	LYS
3	X	17	ARG
2	H	133	ALA
3	V	91	GLY
3	X	145	VAL

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	185/186 (100%)	156 (84%)	29 (16%)	2 4
1	M	185/186 (100%)	153 (83%)	32 (17%)	2 3
2	H	185/185 (100%)	148 (80%)	37 (20%)	1 2
2	I	185/185 (100%)	146 (79%)	39 (21%)	1 2
3	V	124/138 (90%)	86 (69%)	38 (31%)	0 0
3	X	124/138 (90%)	90 (73%)	34 (27%)	0 0
All	All	988/1018 (97%)	779 (79%)	209 (21%)	1 2

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	24	SER
1	L	27	SER
1	L	28	SER
1	L	30	SER
1	L	44	LYS
1	L	45	LEU
1	L	55	SER
1	L	68	THR

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Mol	Chain	Res	Type
1	L	88	GLN
1	L	95	ARG
1	L	102	LYS
1	L	105	ILE
1	L	124	LEU
1	L	132	VAL
1	L	137	ASN
1	L	144	ASN
1	L	154	ARG
1	L	156	ASN
1	L	167	SER
1	L	174	MET
1	L	175	SER
1	L	178	LEU
1	L	179	THR
1	L	180	LEU
1	L	182	LYS
1	L	184	GLU
1	L	198	LYS
1	L	199	THR
1	L	202	SER
2	H	2	VAL
2	H	11	LEU
2	H	12	VAL
2	H	13	GLN
2	H	27	PHE
2	H	38	ARG
2	H	45	LEU
2	H	46	GLU
2	H	65	SER
2	H	66	VAL
2	H	67	LYS
2	H	78	LYS
2	H	83	LEU
2	H	84	GLN
2	H	87	SER
2	H	88	LEU
2	H	108	GLN
2	H	110	THR
2	H	111	LEU
2	H	115	SER
2	H	123	SER

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Mol	Chain	Res	Type
2	H	131	SER
2	H	135	THR
2	H	136	ASN
2	H	161	SER
2	H	162	LEU
2	H	166	VAL
2	H	173	LEU
2	H	174	GLN
2	H	175	SER
2	H	193	SER
2	H	205	SER
2	H	207	THR
2	H	208	LYS
2	H	209	VAL
2	H	210	ASP
2	H	214	VAL
3	V	9	LEU
3	V	11	VAL
3	V	16	LEU
3	V	17	ARG
3	V	18	ASP
3	V	25	ARG
3	V	26	LEU
3	V	35	LEU
3	V	37	THR
3	V	44	VAL
3	V	45	ASP
3	V	46	PHE
3	V	48	LEU
3	V	50	GLU
3	V	53	THR
3	V	68	THR
3	V	69	LEU
3	V	72	GLU
3	V	78	ARG
3	V	84	THR
3	V	86	LEU
3	V	89	LEU
3	V	92	GLN
3	V	93	LEU
3	V	99	LEU
3	V	100	LEU

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Mol	Chain	Res	Type
3	V	107	LEU
3	V	112	LEU
3	V	115	GLN
3	V	127	ILE
3	V	129	LEU
3	V	140	ARG
3	V	142	LEU
3	V	143	MET
3	V	144	LEU
3	V	149	THR
3	V	150	LEU
3	V	151	CYS
1	M	1	GLN
1	M	18	LYS
1	M	20	THR
1	M	24	SER
1	M	28	SER
1	M	45	LEU
1	M	68	THR
1	M	72	LEU
1	M	88	GLN
1	M	95	ARG
1	M	102	LYS
1	M	105	ILE
1	M	106	LYS
1	M	130	SER
1	M	132	VAL
1	M	144	ASN
1	M	154	ARG
1	M	155	GLN
1	M	156	ASN
1	M	163	THR
1	M	174	MET
1	M	175	SER
1	M	178	LEU
1	M	179	THR
1	M	180	LEU
1	M	186	GLU
1	M	190	SER
1	M	198	LYS
1	M	201	THR
1	M	202	SER

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Mol	Chain	Res	Type
1	M	206	LYS
1	M	210	ARG
2	I	3	LYS
2	I	6	GLU
2	I	11	LEU
2	I	12	VAL
2	I	13	GLN
2	I	19	LYS
2	I	27	PHE
2	I	28	THR
2	I	38	ARG
2	I	42	GLU
2	I	45	LEU
2	I	55	VAL
2	I	67	LYS
2	I	78	LYS
2	I	83	LEU
2	I	84	GLN
2	I	87	SER
2	I	89	ARG
2	I	91	GLU
2	I	110	THR
2	I	111	LEU
2	I	118	LYS
2	I	123	SER
2	I	131	SER
2	I	134	GLN
2	I	143	CYS
2	I	146	LYS
2	I	163	SER
2	I	164	SER
2	I	166	VAL
2	I	173	LEU
2	I	174	GLN
2	I	199	ASN
2	I	205	SER
2	I	209	VAL
2	I	210	ASP
2	I	212	LYS
2	I	214	VAL
2	I	216	ARG
3	X	9	LEU

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Mol	Chain	Res	Type
3	X	10	ARG
3	X	11	VAL
3	X	17	ARG
3	X	18	ASP
3	X	24	SER
3	X	25	ARG
3	X	28	GLN
3	X	31	GLU
3	X	32	VAL
3	X	33	HIS
3	X	35	LEU
3	X	37	THR
3	X	41	LEU
3	X	47	SER
3	X	52	LYS
3	X	53	THR
3	X	55	MET
3	X	69	LEU
3	X	78	ARG
3	X	88	SER
3	X	93	LEU
3	X	96	GLN
3	X	99	LEU
3	X	100	LEU
3	X	112	LEU
3	X	115	GLN
3	X	117	ARG
3	X	127	ILE
3	X	129	LEU
3	X	136	ARG
3	X	142	LEU
3	X	144	LEU
3	X	151	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	88	GLN
1	L	156	ASN
1	L	160	ASN
2	H	13	GLN

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Mol	Chain	Res	Type
2	H	56	ASN
2	H	58	HIS
2	H	61	HIS
2	H	108	GLN
2	H	158	ASN
2	H	199	ASN
3	V	20	HIS
3	V	92	GLN
3	V	105	GLN
3	V	111	GLN
3	V	115	GLN
3	V	132	GLN
3	V	133	HIS
1	M	6	GLN
1	M	36	GLN
1	M	37	GLN
1	M	88	GLN
1	M	155	GLN
1	M	188	HIS
1	M	209	ASN
2	I	56	ASN
2	I	58	HIS
2	I	84	GLN
2	I	158	ASN
2	I	199	ASN
3	X	23	HIS
3	X	28	GLN
3	X	105	GLN
3	X	111	GLN
3	X	125	ASN
3	X	132	GLN

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)

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	212/213 (99%)	-0.45	1 (0%) 91 91	26, 39, 57, 75	0
1	M	212/213 (99%)	-0.40	1 (0%) 91 91	26, 39, 60, 77	0
2	H	217/217 (100%)	-0.33	3 (1%) 75 77	26, 41, 62, 86	0
2	I	217/217 (100%)	-0.30	2 (0%) 84 86	29, 42, 62, 79	0
3	V	145/163 (88%)	0.83	24 (16%) 1 1	30, 75, 112, 118	0
3	X	145/163 (88%)	0.55	13 (8%) 9 9	32, 66, 101, 116	0
All	All	1148/1186 (96%)	-0.10	44 (3%) 40 43	26, 44, 93, 118	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	V	144	LEU	14.8
3	X	7	CYS	9.8
3	V	7	CYS	7.9
3	V	145	VAL	6.7
3	V	46	PHE	6.2
3	V	141	PHE	6.0
3	X	8	ASP	5.3
3	V	146	GLY	5.0
3	X	145	VAL	4.9
3	X	151	CYS	4.9
3	V	149	THR	4.8
3	V	143	MET	4.4
2	H	133	ALA	4.0
3	X	9	LEU	3.8
3	X	46	PHE	3.6
3	V	15	LEU	3.4
3	V	55	MET	3.3
3	V	8	ASP	3.1
1	M	211	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
3	X	47	SER	3.0
2	I	135	THR	3.0
2	H	134	GLN	2.8
3	V	9	LEU	2.8
3	X	144	LEU	2.8
3	V	86	LEU	2.7
3	V	148	SER	2.6
3	V	53	THR	2.6
3	X	148	SER	2.6
3	X	149	THR	2.5
3	X	33	HIS	2.4
3	V	147	GLY	2.4
3	V	51	TRP	2.4
3	V	10	ARG	2.4
3	X	146	GLY	2.3
1	L	211	ASN	2.3
3	V	56	GLU	2.2
3	V	142	LEU	2.2
2	I	131	SER	2.2
3	V	49	GLY	2.2
3	V	117	ARG	2.1
3	X	10	ARG	2.1
2	H	217	ASP	2.1
3	V	50	GLU	2.1
3	V	45	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.