Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 05:28 am BST

PDB ID	:	3T2N
Title	:	Human hepsin protease in complex with the Fab fragment of an inhibitory antibody
Authors	:	Koschubs, T.; Dengl, S.; Duerr, H.; Kaluza, K.; Georges, G.; Hartl, C.; Jennewein, S.; Lanzendoerfer, M.; Auer, J.; Stern, A.; Huang, K.-S.; Kostrewa, D.; Ries, S.; Hansen, S.; Kohnert, U.; Cramer, P.; Mundigl, O.
Deposited on	:	2011-07-22
Resolution	:	2.55 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 (i) symbol.

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

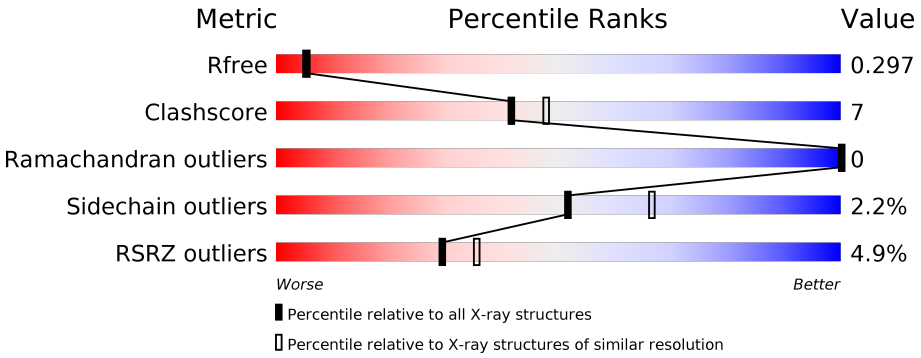
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	372	7% 75% 16% 9%
1	B	372	5% 75% 15% • 10%
2	H	225	3% 75% 15% • 10%
2	I	225	3% 79% 12% 9%
3	L	215	2% 81% 16% ••
3	M	215	4% 81% 16% ••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11749 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 Serine protease hepsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2605	1638	470	478	19			
1	B	335	Total	C	N	O	S	0	0	0
			2576	1622	464	471	19			

- Molecule 2 is a protein called Antibody, Fab fragment, Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	203	Total	C	N	O	S	0	0	0
			1535	980	250	299	6			
2	I	205	Total	C	N	O	S	0	0	0
			1547	987	252	302	6			

- Molecule 3 is a protein called Antibody, Fab fragment, Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1582	996	267	315	4			
3	M	212	Total	C	N	O	S	0	0	0
			1589	1000	268	317	4			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total	O	0	0
			64	64		
4	B	74	Total	O	0	0
			74	74		
4	H	46	Total	O	0	0
			46	46		
4	I	36	Total	O	0	0
			36	36		

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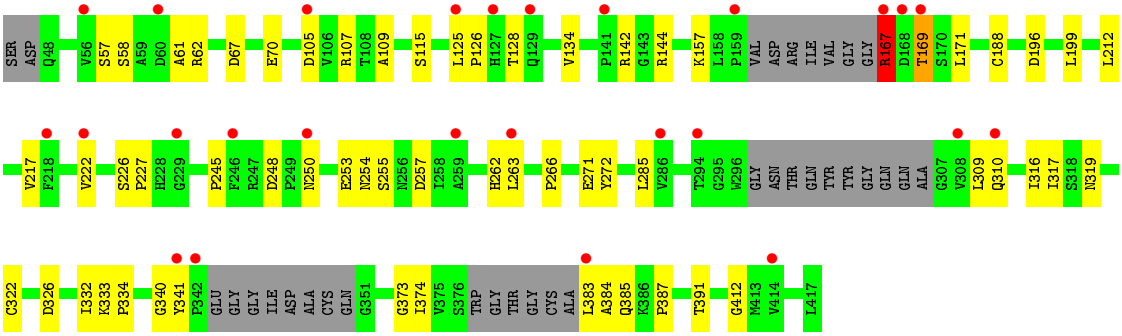
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	40	Total O 40 40	0	0
4	M	55	Total O 55 55	0	0

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 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.

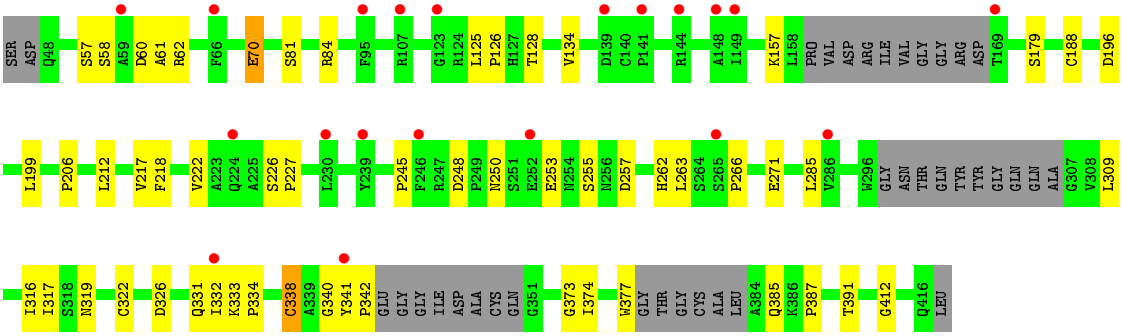
- Molecule 1: Serine protease hepsin

Chain A:



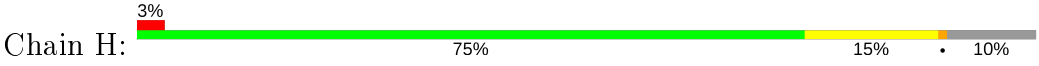
- Molecule 1: Serine protease hepsin

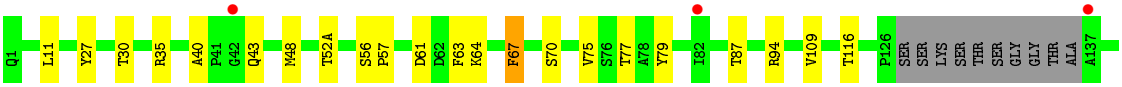
Chain B:

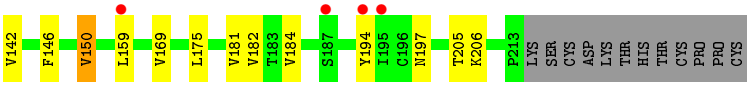


- Molecule 2: Antibody, Fab fragment, Heavy Chain

Chain H:

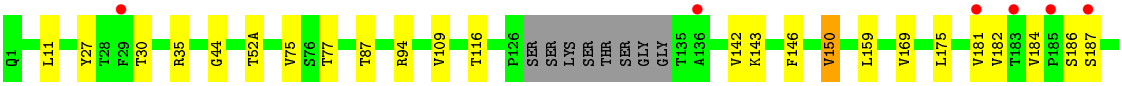






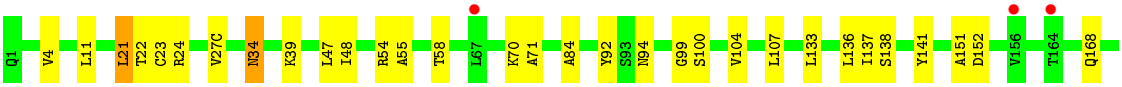
- Molecule 2: Antibody, Fab fragment, Heavy Chain

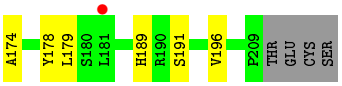
Chain I:



- Molecule 3: Antibody, Fab fragment, Light Chain

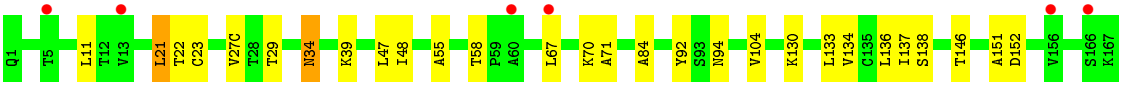
Chain L:





- Molecule 3: Antibody, Fab fragment, Light Chain

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	62.98Å 66.58Å 108.33Å 88.71° 94.30° 104.53°	Depositor
Resolution (Å)	47.33 – 2.55 47.33 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.33-2.55) 79.2 (47.33-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 2.54Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.242 , 0.275 0.257 , 0.297	Depositor DCC
R_{free} test set	2772 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	11749	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.52	0/2665	0.75	3/3615 (0.1%)
1	B	0.54	1/2637 (0.0%)	0.74	0/3579
2	H	0.56	0/1575	0.78	0/2148
2	I	0.50	0/1587	0.77	0/2165
3	L	0.55	0/1623	0.74	0/2222
3	M	0.59	0/1630	0.75	1/2232 (0.0%)
All	All	0.54	1/11717 (0.0%)	0.75	4/15961 (0.0%)

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
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	206	PRO	N-CD	-5.43	1.40	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	107	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	A	107	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	167	ARG	CD-NE-CZ	5.99	131.99	123.60
3	M	209	PRO	C-N-CA	5.32	135.00	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	ARG	Sidechain
1	B	257	ASP	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2605	0	2536	43	0
1	B	2576	0	2500	37	0
2	H	1535	0	1502	22	0
2	I	1547	0	1514	16	0
3	L	1582	0	1541	25	0
3	M	1589	0	1548	27	0
4	A	64	0	0	0	0
4	B	74	0	0	0	0
4	H	46	0	0	0	0
4	I	36	0	0	0	0
4	L	40	0	0	1	0
4	M	55	0	0	1	0
All	All	11749	0	11141	158	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 7.

All (158) 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:B:317:ILE:HD11	1:B:340:GLY:HA2	1.52	0.92
2:I:181:VAL:HG11	3:M:136:LEU:HD13	1.54	0.89
1:A:383:LEU:HG	1:A:383:LEU:O	1.76	0.85
2:H:75:VAL:HG13	2:H:77:THR:HG22	1.66	0.77
2:H:181:VAL:HG11	3:L:136:LEU:HD13	1.66	0.76
1:A:383:LEU:HD21	3:L:54:ARG:H	1.51	0.74
2:I:75:VAL:HG13	2:I:77:THR:HG22	1.70	0.73
1:A:169:THR:HG22	1:A:222:VAL:HG21	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:47:LEU:HD22	3:L:58:THR:HG22	1.76	0.67
1:A:317:ILE:HD11	1:A:340:GLY:HA2	1.77	0.67
2:I:181:VAL:CG1	3:M:136:LEU:HD13	2.24	0.67
2:H:67:PHE:N	2:H:67:PHE:CD1	2.63	0.65
3:M:47:LEU:HD22	3:M:58:THR:HG22	1.77	0.65
1:B:338:CYS:SG	1:B:387:PRO:HB2	2.37	0.65
2:H:61:ASP:OD1	2:H:64:LYS:NZ	2.28	0.64
3:M:134:VAL:HG12	3:M:136:LEU:HD21	1.78	0.64
1:A:105:ASP:O	1:A:109:ALA:HB3	1.99	0.63
3:L:100:SER:HB2	4:L:225:HOH:O	1.97	0.62
2:H:61:ASP:HA	2:H:64:LYS:HD2	1.80	0.62
1:B:196:ASP:O	1:B:262:HIS:HD2	1.83	0.62
1:A:169:THR:HG22	1:A:222:VAL:CG2	2.31	0.60
1:A:196:ASP:O	1:A:262:HIS:HD2	1.84	0.60
1:B:84:ARG:HB2	1:B:125:LEU:HD21	1.83	0.60
3:M:151:ALA:O	3:M:191:SER:O	2.21	0.59
3:L:151:ALA:O	3:L:191:SER:O	2.20	0.59
3:M:23:CYS:HB3	3:M:71:ALA:HB3	1.84	0.59
3:L:23:CYS:HB3	3:L:71:ALA:HB3	1.84	0.58
3:L:168:GLN:HE21	3:L:174:ALA:HB2	1.68	0.58
3:M:168:GLN:HE21	3:M:174:ALA:HB2	1.68	0.58
1:B:222:VAL:CG2	1:B:309:LEU:HB3	2.34	0.58
1:A:383:LEU:HD21	3:L:54:ARG:N	2.19	0.57
3:M:11:LEU:HD12	3:M:21:LEU:HD22	1.86	0.57
1:A:322:CYS:HB2	1:A:332:ILE:HD11	1.86	0.57
1:B:341:TYR:CD2	3:M:29:THR:HG21	2.40	0.57
1:A:105:ASP:O	1:A:109:ALA:CB	2.53	0.57
1:B:322:CYS:HB2	1:B:332:ILE:HD11	1.87	0.57
2:H:181:VAL:CG1	3:L:136:LEU:HD13	2.33	0.57
3:L:11:LEU:HD12	3:L:21:LEU:HD22	1.87	0.56
1:A:222:VAL:CG2	1:A:309:LEU:HB3	2.37	0.55
3:L:55:ALA:HB3	3:L:58:THR:HG23	1.89	0.55
1:A:142:ARG:HG2	1:A:144:ARG:HG3	1.89	0.55
3:M:152:ASP:OD2	3:M:189:HIS:HD2	1.91	0.54
3:M:55:ALA:HB3	3:M:58:THR:HG23	1.89	0.54
1:A:333:LYS:HB3	1:A:334:PRO:HD2	1.90	0.54
1:A:128:THR:HG21	1:A:134:VAL:HG11	1.89	0.54
2:I:197:ASN:HB3	2:I:206:LYS:HE2	1.90	0.53
3:M:134:VAL:CG1	3:M:136:LEU:HD21	2.38	0.53
1:B:333:LYS:HB3	1:B:334:PRO:HD2	1.90	0.53
3:M:138:SER:HB2	3:M:168:GLN:HE22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:146:PHE:HB2	2:H:175:LEU:HD23	1.90	0.52
2:H:27:TYR:CZ	2:H:94:ARG:HD2	2.44	0.52
1:A:373:GLY:HA2	1:A:391:THR:O	2.10	0.52
2:H:197:ASN:HB3	2:H:206:LYS:HE2	1.91	0.52
2:H:67:PHE:H	2:H:67:PHE:HD1	1.56	0.52
1:A:167:ARG:O	1:A:310:GLN:HA	2.10	0.52
1:B:385:GLN:HB3	3:M:29:THR:HG23	1.92	0.51
2:I:27:TYR:CZ	2:I:94:ARG:HD2	2.45	0.51
1:B:222:VAL:HG22	1:B:309:LEU:HB3	1.93	0.51
2:I:146:PHE:HB2	2:I:175:LEU:HD23	1.92	0.51
3:M:137:ILE:HG12	3:M:196:VAL:HG21	1.92	0.51
3:M:92:TYR:O	3:M:94:ASN:N	2.41	0.51
1:A:326:ASP:O	2:H:35:ARG:NH2	2.43	0.51
1:B:373:GLY:HA2	1:B:391:THR:O	2.11	0.51
1:B:341:TYR:O	1:B:342:PRO:C	2.48	0.50
3:M:22:THR:HB	3:M:70:LYS:HD2	1.92	0.50
2:I:30:THR:HA	2:I:52(A):THR:HG22	1.93	0.50
1:B:57:SER:HB2	1:B:62:ARG:HG2	1.94	0.50
1:B:212:LEU:HD12	1:B:412:GLY:HA2	1.94	0.50
1:B:128:THR:HG21	1:B:134:VAL:HG11	1.93	0.50
1:B:157:LYS:HB2	1:B:271:GLU:HA	1.94	0.50
1:B:326:ASP:O	2:I:35:ARG:NH2	2.44	0.50
1:A:125:LEU:N	1:A:126:PRO:HD2	2.27	0.50
2:I:87:THR:HA	2:I:109:VAL:O	2.12	0.50
3:L:22:THR:HB	3:L:70:LYS:HD2	1.93	0.50
3:L:152:ASP:OD2	3:L:189:HIS:HD2	1.95	0.49
1:A:57:SER:HB2	1:A:62:ARG:HG2	1.94	0.49
3:L:138:SER:HB2	3:L:168:GLN:HE22	1.77	0.49
1:B:317:ILE:HD12	1:B:387:PRO:HB3	1.95	0.49
2:I:143:LYS:NZ	3:M:130:LYS:HD2	2.27	0.49
1:A:245:PRO:HA	1:A:248:ASP:O	2.12	0.48
2:H:184:VAL:HG11	2:H:194:TYR:CE1	2.47	0.48
2:H:87:THR:HA	2:H:109:VAL:O	2.13	0.48
3:L:107:LEU:HD23	3:L:141:TYR:HE1	1.78	0.48
2:I:184:VAL:HG11	2:I:194:TYR:CE1	2.48	0.48
1:A:383:LEU:O	1:A:384:ALA:HB2	2.13	0.48
2:H:11:LEU:HD11	2:H:146:PHE:HZ	1.78	0.48
2:H:30:THR:HA	2:H:52(A):THR:HG22	1.94	0.48
2:H:70:SER:OG	2:H:79:TYR:HB2	2.13	0.48
1:A:212:LEU:HD12	1:A:412:GLY:HA2	1.94	0.48
1:A:341:TYR:HE2	1:A:385:GLN:HE21	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:137:ILE:HG12	3:L:196:VAL:HG21	1.95	0.47
1:B:245:PRO:HA	1:B:248:ASP:O	2.15	0.47
3:L:133:LEU:HD12	3:L:179:LEU:HD23	1.97	0.47
1:B:81:SER:HB2	1:B:84:ARG:HD3	1.96	0.47
1:B:285:LEU:HG	1:B:316:ILE:HD13	1.97	0.47
3:L:92:TYR:O	3:L:94:ASN:N	2.43	0.47
2:I:11:LEU:HD11	2:I:146:PHE:HZ	1.80	0.46
1:B:341:TYR:HE2	1:B:385:GLN:HE21	1.63	0.46
2:H:142:VAL:HG11	2:H:150:VAL:HG11	1.97	0.46
1:A:222:VAL:HG23	1:A:309:LEU:HB3	1.97	0.46
1:B:196:ASP:HB3	1:B:266:PRO:HA	1.98	0.46
1:A:222:VAL:HG22	1:A:309:LEU:HB3	1.98	0.46
3:L:47:LEU:HA	3:L:58:THR:HG21	1.98	0.46
1:B:317:ILE:CD1	1:B:340:GLY:HA2	2.36	0.46
1:A:115:SER:HB2	1:B:70:GLU:O	2.15	0.46
1:B:253:GLU:HG3	1:B:255:SER:H	1.81	0.45
3:L:39:LYS:HG2	3:L:84:ALA:HB2	1.98	0.45
1:A:196:ASP:HB3	1:A:266:PRO:HA	1.99	0.45
1:A:253:GLU:HG3	1:A:255:SER:N	2.31	0.45
1:B:222:VAL:HG23	1:B:309:LEU:HB3	1.97	0.45
1:A:157:LYS:HB2	1:A:271:GLU:HA	1.98	0.45
1:B:199:LEU:HD21	1:B:374:ILE:HD11	1.98	0.45
1:B:125:LEU:N	1:B:126:PRO:HD2	2.32	0.44
1:B:199:LEU:CD2	1:B:374:ILE:HD11	2.46	0.44
1:A:67:ASP:OD2	1:A:70:GLU:HB2	2.17	0.44
2:I:142:VAL:HG11	2:I:150:VAL:HG11	2.00	0.44
2:I:159:LEU:HD21	2:I:182:VAL:HG21	2.00	0.44
1:A:105:ASP:HB2	1:A:144:ARG:HH11	1.83	0.44
1:A:285:LEU:HG	1:A:316:ILE:HD13	1.98	0.44
1:A:383:LEU:CG	1:A:383:LEU:O	2.52	0.44
3:L:24:ARG:HB2	3:L:70:LYS:HD3	2.00	0.44
3:M:186:TRP:O	3:M:209:PRO:HG3	2.17	0.44
1:A:199:LEU:CD2	1:A:374:ILE:HD11	2.48	0.43
1:B:253:GLU:HG3	1:B:255:SER:N	2.32	0.43
2:H:48:MET:HG2	2:H:63:PHE:CZ	2.53	0.43
1:A:142:ARG:CG	1:A:144:ARG:HG3	2.49	0.43
1:A:254:ASN:O	1:A:257:ASP:HB2	2.17	0.43
1:A:317:ILE:HD12	1:A:387:PRO:HB3	2.01	0.43
2:H:40:ALA:O	2:H:43:GLN:HB2	2.18	0.43
1:B:179:SER:HB3	1:B:218:PHE:HB3	2.01	0.43
1:B:217:VAL:HG21	1:B:263:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:VAL:HG21	1:B:263:LEU:HD22	2.00	0.43
2:I:44:GLY:HA3	4:M:216:HOH:O	2.19	0.42
3:M:133:LEU:HD12	3:M:179:LEU:HD23	2.01	0.42
1:B:226:SER:HA	1:B:227:PRO:HD3	1.90	0.42
3:M:133:LEU:O	3:M:178:TYR:HA	2.19	0.42
3:M:39:LYS:HG2	3:M:84:ALA:HB2	2.01	0.42
2:H:159:LEU:HD21	2:H:182:VAL:HG21	2.00	0.42
1:A:226:SER:HA	1:A:227:PRO:HD3	1.92	0.42
1:A:171:LEU:HD22	1:A:272:TYR:CD1	2.55	0.42
2:H:56:SER:HA	2:H:57:PRO:HD3	1.97	0.42
3:L:133:LEU:O	3:L:178:TYR:HA	2.19	0.42
1:B:331:GLN:HB2	1:B:331:GLN:HE21	1.69	0.42
3:M:34:ASN:HA	3:M:48:ILE:O	2.20	0.42
3:M:47:LEU:HA	3:M:58:THR:HG21	2.02	0.42
2:H:116:THR:HA	2:H:146:PHE:O	2.20	0.42
1:A:57:SER:O	1:A:61:ALA:HA	2.19	0.41
1:A:217:VAL:HG21	1:A:263:LEU:CD2	2.50	0.41
3:L:27(C):VAL:HG11	3:L:71:ALA:HB2	2.01	0.41
1:A:217:VAL:HG21	1:A:263:LEU:HD22	2.03	0.41
1:B:57:SER:O	1:B:61:ALA:HA	2.21	0.41
3:L:34:ASN:HA	3:L:48:ILE:O	2.20	0.41
3:M:152:ASP:OD2	3:M:189:HIS:CD2	2.72	0.41
3:M:146:THR:HB	3:M:197:THR:HB	2.02	0.41
1:A:199:LEU:HD21	1:A:374:ILE:HD11	2.02	0.41
3:L:4:VAL:O	3:L:99:GLY:HA2	2.22	0.40
3:M:27(C):VAL:HG11	3:M:71:ALA:HB2	2.02	0.40
2:I:116:THR:HA	2:I:146:PHE:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/372 (88%)	319 (97%)	10 (3%)	0	100	100
1	B	325/372 (87%)	316 (97%)	9 (3%)	0	100	100
2	H	199/225 (88%)	193 (97%)	6 (3%)	0	100	100
2	I	201/225 (89%)	194 (96%)	7 (4%)	0	100	100
3	L	209/215 (97%)	203 (97%)	6 (3%)	0	100	100
3	M	210/215 (98%)	200 (95%)	10 (5%)	0	100	100
All	All	1473/1624 (91%)	1425 (97%)	48 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/302 (93%)	275 (98%)	5 (2%)	59	74
1	B	276/302 (91%)	268 (97%)	8 (3%)	42	57
2	H	172/191 (90%)	168 (98%)	4 (2%)	50	65
2	I	173/191 (91%)	169 (98%)	4 (2%)	50	65
3	L	175/179 (98%)	172 (98%)	3 (2%)	60	75
3	M	176/179 (98%)	172 (98%)	4 (2%)	50	65
All	All	1252/1344 (93%)	1224 (98%)	28 (2%)	52	66

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	169	THR
1	A	188	CYS
1	A	250	ASN
1	A	319	ASN
1	B	58	SER
1	B	60	ASP

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Mol	Chain	Res	Type
1	B	70	GLU
1	B	188	CYS
1	B	250	ASN
1	B	319	ASN
1	B	338	CYS
1	B	377	TRP
2	H	67	PHE
2	H	150	VAL
2	H	169	VAL
2	H	205	THR
2	I	150	VAL
2	I	169	VAL
2	I	186	SER
2	I	187	SER
3	L	21	LEU
3	L	34	ASN
3	L	104	VAL
3	M	21	LEU
3	M	34	ASN
3	M	67	LEU
3	M	104	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	ASN
1	A	262	HIS
1	B	256	ASN
1	B	262	HIS
2	H	1	GLN
2	H	43	GLN
2	H	199	ASN
2	I	43	GLN
2	I	199	ASN
3	L	53	ASN
3	L	79	GLN
3	L	168	GLN
3	L	189	HIS
3	M	79	GLN
3	M	168	GLN
3	M	189	HIS

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	A	339/372 (91%)	0.59	26 (7%)	13	17	25, 48, 72, 93	1 (0%)
1	B	335/372 (90%)	0.64	20 (5%)	21	25	28, 49, 72, 102	1 (0%)
2	H	203/225 (90%)	0.46	7 (3%)	45	52	25, 45, 68, 88	0
2	I	205/225 (91%)	0.43	7 (3%)	45	52	25, 44, 67, 88	0
3	L	211/215 (98%)	0.28	4 (1%)	66	73	24, 44, 61, 79	0
3	M	212/215 (98%)	0.34	9 (4%)	36	42	30, 43, 58, 64	0
All	All	1505/1624 (92%)	0.48	73 (4%)	29	35	24, 46, 69, 102	2 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	VAL	6.1
1	B	123	GLY	5.2
1	A	383	LEU	4.7
1	B	239	TYR	4.0
2	H	137	ALA	3.7
1	B	59	ALA	3.6
2	I	187	SER	3.6
3	M	156	VAL	3.5
1	B	230	LEU	3.5
1	A	125	LEU	3.4
1	A	250	ASN	3.4
2	H	159	LEU	3.4
1	A	159	PRO	3.4
1	A	141	PRO	3.3
1	A	168	ASP	3.3
1	B	224	GLN	3.3
1	A	56	VAL	3.2
1	A	286	VAL	3.2
3	M	67	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	252	GLU	3.2
2	H	195	ILE	3.2
2	I	185	PRO	3.1
3	M	203	VAL	3.1
1	B	95	PHE	2.9
2	H	194	TYR	2.9
1	B	148	ALA	2.9
2	I	136	ALA	2.8
1	B	265	SER	2.8
1	A	105	ASP	2.8
3	M	5	THR	2.7
1	A	218	PHE	2.7
2	H	187	SER	2.6
2	H	42	GLY	2.6
1	B	66	PHE	2.6
2	I	29	PHE	2.6
1	A	229	GLY	2.6
1	B	332	ILE	2.5
1	A	127	HIS	2.5
1	B	141	PRO	2.5
2	I	183	THR	2.4
1	B	107	ARG	2.4
1	A	167	ARG	2.4
1	A	129	GLN	2.4
1	A	263	LEU	2.4
3	M	13	VAL	2.3
3	M	60	ALA	2.3
3	L	164	THR	2.3
3	L	67	LEU	2.3
3	L	181	LEU	2.3
1	A	60	ASP	2.3
2	H	82	ILE	2.3
3	M	166	SER	2.3
1	B	149	ILE	2.3
1	A	414	VAL	2.2
2	I	181	VAL	2.2
1	A	259	ALA	2.2
1	B	144	ARG	2.2
1	A	308	VAL	2.2
3	L	156	VAL	2.2
1	B	169	THR	2.2
3	M	178	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	342	PRO	2.2
1	B	246	PHE	2.2
1	B	139	ASP	2.1
1	A	169	THR	2.1
1	B	286	VAL	2.1
1	B	341	TYR	2.1
3	M	175	ALA	2.1
1	A	294	THR	2.0
2	I	194	TYR	2.0
1	A	341	TYR	2.0
1	A	246	PHE	2.0
1	A	310	GLN	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 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.