Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 11:17 AM EDT

PDB ID	:	7U0C
Title	:	Crystal structure of broadly neutralizing antibody HEPC3.4
Authors	:	Flyak, A.I.; Bjorkman, P.J.
Deposited on	:	2022-02-17
Resolution	:	3.30 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:

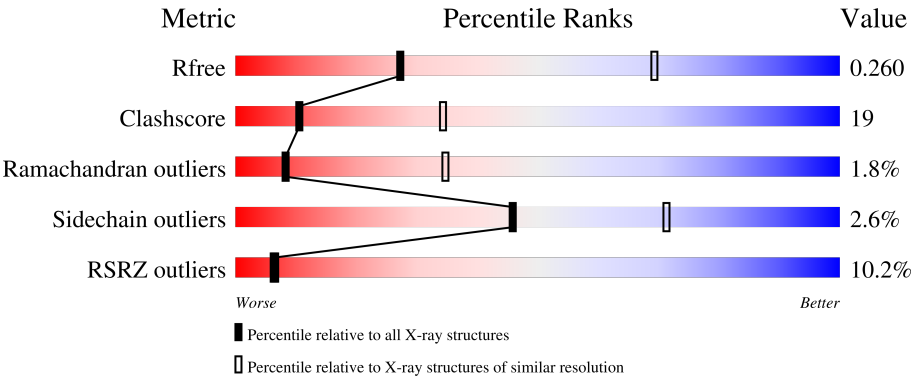
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	238	5% 59% 31% • 8%
1	C	238	13% 53% 32% • 12%
1	H	238	13% 60% 26% • 12%
2	B	214	3% 62% 31% • 5%
2	D	214	13% 58% 36% • 5%

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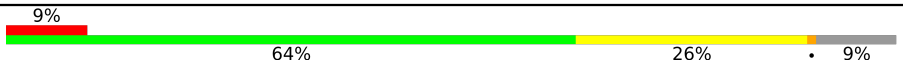
Mol	Chain	Length	Quality of chain
2	L	214	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9368 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 HEPC3.4 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1629	1028	279	315	7			
1	C	210	Total	C	N	O	S	0	0	0
			1567	991	267	302	7			
1	H	210	Total	C	N	O	S	0	0	0
			1570	991	269	303	7			

- Molecule 2 is a protein called HEPC3.4 Fab Light Chain.

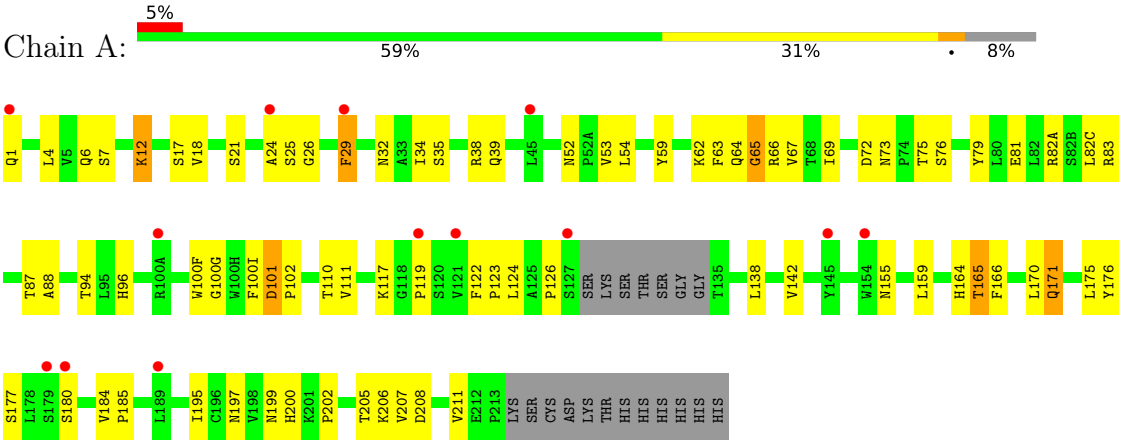
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	203	Total	C	N	O	S	0	0	0
			1561	973	269	315	4			
2	D	203	Total	C	N	O	S	0	0	0
			1555	970	266	315	4			
2	L	194	Total	C	N	O	S	0	0	0
			1486	926	255	301	4			

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.

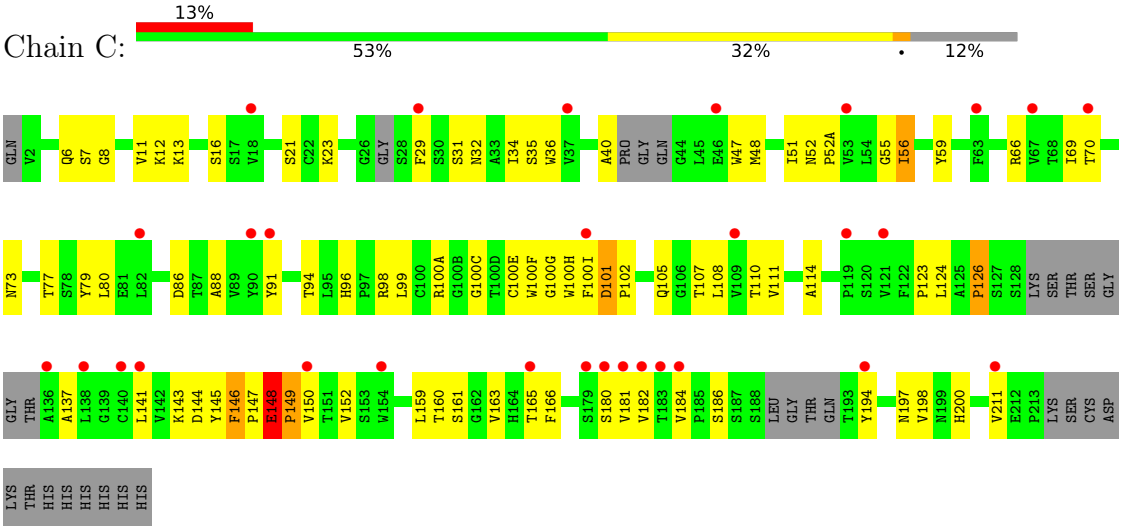
• Molecule 1: HEPC3.4 Fab Heavy Chain

Chain A:



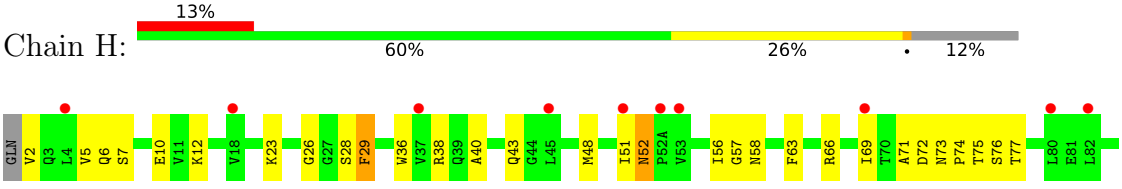
• Molecule 1: HEPC3.4 Fab Heavy Chain

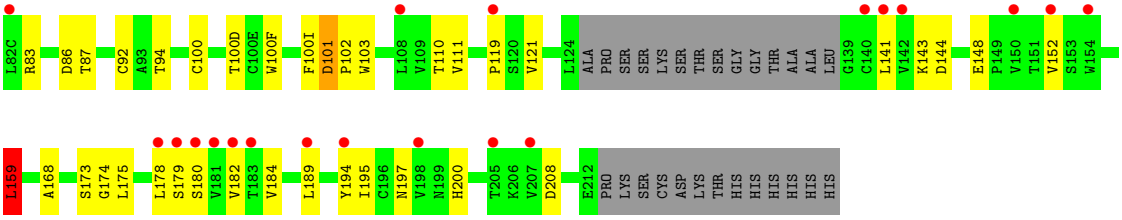
Chain C:



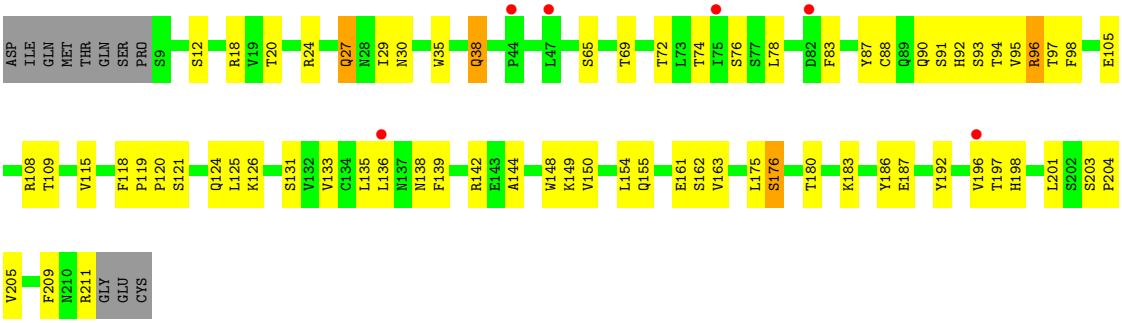
• Molecule 1: HEPC3.4 Fab Heavy Chain

Chain H:

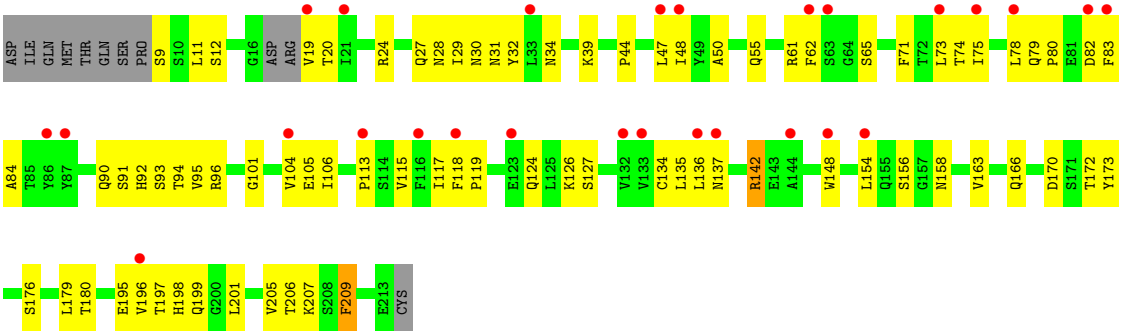




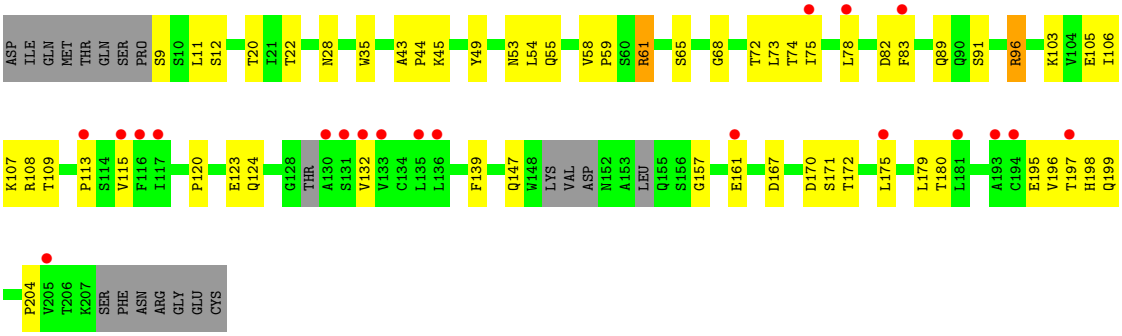
• Molecule 2: HEPC3.4 Fab Light Chain



• Molecule 2: HEPC3.4 Fab Light Chain



• Molecule 2: HEPC3.4 Fab Light Chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	263.79Å 263.79Å 207.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	79.70 – 3.30 79.70 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (79.70-3.30) 99.9 (79.70-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.215 , 0.260 0.215 , 0.260	Depositor DCC
R_{free} test set	2090 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	133.7	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 168.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9368	wwPDB-VP
Average B, all atoms (Å^2)	187.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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	0.44	0/1670	0.69	1/2280 (0.0%)
1	C	0.41	0/1604	0.70	1/2185 (0.0%)
1	H	0.40	0/1609	0.67	0/2194
2	B	0.48	1/1593 (0.1%)	0.70	0/2162
2	D	0.38	0/1586	0.65	0/2151
2	L	0.44	0/1514	0.62	0/2051
All	All	0.42	1/9576 (0.0%)	0.67	2/13023 (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	C	0	1
1	H	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	38	GLN	C-N	-5.76	1.20	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	146	PHE	C-N-CD	-5.88	107.67	120.60
1	A	171	GLN	CA-CB-CG	-5.38	101.57	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	148	GLU	Peptide
1	H	52	ASN	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	A	1629	0	1601	58	0
1	C	1567	0	1535	88	0
1	H	1570	0	1538	54	0
2	B	1561	0	1517	54	1
2	D	1555	0	1509	83	0
2	L	1486	0	1438	55	0
All	All	9368	0	9138	343	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 19.

All (343) 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:H:100(F):TRP:CE3	2:L:96:ARG:HD2	1.59	1.38
1:H:100(F):TRP:CZ3	2:L:96:ARG:HD2	1.68	1.27
1:C:100(F):TRP:HZ3	2:D:92:HIS:N	1.48	1.10
1:C:100(F):TRP:CZ3	2:D:92:HIS:N	2.23	1.06
1:C:100(F):TRP:CH2	2:D:92:HIS:C	2.29	1.05
1:H:100(F):TRP:CE3	2:L:96:ARG:CD	2.44	1.01
1:C:100(F):TRP:CH2	2:D:92:HIS:O	2.18	0.96
2:L:89:GLN:HE21	2:L:96:ARG:NH2	1.63	0.95
2:L:89:GLN:NE2	2:L:96:ARG:NH2	2.15	0.94
1:H:100(F):TRP:CZ3	2:L:96:ARG:CD	2.52	0.90
1:H:6:GLN:NE2	1:H:92:CYS:SG	2.45	0.89
2:L:20:THR:HB	2:L:74:THR:HG23	1.58	0.84
2:L:89:GLN:NE2	2:L:96:ARG:HH22	1.74	0.82
1:A:12:LYS:NZ	1:A:17:SER:O	2.11	0.82
1:C:98:ARG:HH22	2:D:50:ALA:HA	1.44	0.81
1:C:145:TYR:HE2	1:C:148:GLU:HA	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100(F):TRP:HZ3	2:D:91:SER:C	1.84	0.80
1:C:101:ASP:OD2	2:D:55:GLN:NE2	2.14	0.80
2:D:197:THR:HG22	2:L:199:GLN:OE1	1.80	0.80
2:B:142:ARG:HE	2:B:163:VAL:HG11	1.48	0.79
1:A:32:ASN:OD1	1:A:73:ASN:ND2	2.16	0.79
2:B:20:THR:HB	2:B:74:THR:HG23	1.66	0.78
1:A:17:SER:HB3	1:A:82(A):ARG:HG3	1.66	0.77
1:A:63:PHE:HB3	1:A:67:VAL:HG21	1.65	0.77
2:B:97:THR:HG22	2:B:98:PHE:O	1.84	0.77
2:D:24:ARG:NH2	2:L:180:THR:O	2.16	0.76
1:C:32:ASN:OD1	1:C:73:ASN:ND2	2.19	0.76
2:D:20:THR:HG22	2:D:74:THR:HG23	1.66	0.76
1:C:100(F):TRP:HH2	2:D:92:HIS:C	1.87	0.76
2:L:115:VAL:HG11	2:L:196:VAL:HG11	1.67	0.75
1:C:35:SER:HB2	1:C:100(I):PHE:HE1	1.51	0.75
2:D:158:ASN:HB3	2:D:179:LEU:HD13	1.68	0.74
1:H:173:SER:O	1:H:175:LEU:N	2.19	0.74
1:A:126:PRO:HG3	1:A:138:LEU:HB3	1.70	0.73
1:H:195:ILE:HD11	1:H:208:ASP:HB3	1.70	0.73
1:A:101:ASP:HB3	1:A:102:PRO:HD3	1.71	0.71
2:D:117:ILE:HB	2:D:207:LYS:HG2	1.71	0.71
1:A:100(F):TRP:NE1	2:B:92:HIS:O	2.23	0.71
2:D:27:GLN:NE2	2:D:94:THR:OG1	2.23	0.71
2:D:135:LEU:HD21	2:D:137:ASN:HD22	1.56	0.70
1:C:100(F):TRP:HZ3	2:D:92:HIS:H	1.38	0.69
1:A:53:VAL:HG13	1:A:54:LEU:HD22	1.74	0.69
1:C:100(F):TRP:CZ2	2:D:93:SER:HA	2.27	0.69
1:A:59:TYR:HE1	1:A:69:ILE:HG12	1.58	0.69
2:L:103:LYS:NZ	2:L:105:GLU:OE2	2.23	0.68
2:D:32:TYR:HB3	2:D:91:SER:O	1.94	0.68
1:H:189:LEU:HB3	1:H:194:TYR:HE2	1.58	0.68
2:L:108:ARG:NH2	2:L:109:THR:O	2.27	0.67
2:D:47:LEU:HD23	2:D:48:ILE:HG13	1.75	0.67
2:L:197:THR:HG22	2:L:204:PRO:HB3	1.77	0.67
1:C:35:SER:HB2	1:C:100(I):PHE:CE1	2.30	0.66
2:B:65:SER:OG	2:B:72:THR:OG1	2.14	0.66
1:A:100(F):TRP:HE1	2:B:92:HIS:C	1.98	0.66
1:A:63:PHE:HB3	1:A:67:VAL:CG2	2.26	0.66
1:H:100(F):TRP:HE3	2:L:96:ARG:CD	2.07	0.66
1:C:100(F):TRP:CZ3	2:D:91:SER:C	2.65	0.65
2:D:124:GLN:O	2:D:127:SER:OG	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:40:ALA:HB3	1:H:43:GLN:HG2	1.77	0.65
1:C:40:ALA:HB2	1:C:88:ALA:HB2	1.78	0.65
2:D:195:GLU:HG2	2:D:206:THR:HB	1.79	0.65
2:L:106:ILE:HD11	2:L:171:SER:OG	1.98	0.64
1:A:124:LEU:HB3	2:B:118:PHE:CD1	2.33	0.64
1:C:52:ASN:ND2	1:C:100(C):GLY:O	2.31	0.63
2:D:19:VAL:HG22	2:D:75:ILE:HB	1.80	0.63
2:L:12:SER:HB3	2:L:107:LYS:HG3	1.81	0.63
1:H:51:ILE:HD13	1:H:71:ALA:HB2	1.81	0.62
1:A:35:SER:HB2	1:A:100(I):PHE:HE2	1.64	0.62
2:D:199:GLN:HA	2:L:199:GLN:HG3	1.80	0.62
2:B:29:ILE:HD13	2:B:90:GLN:HG2	1.81	0.62
1:A:94:THR:HB	1:A:102:PRO:HD2	1.82	0.62
1:C:94:THR:HB	1:C:102:PRO:HG2	1.82	0.61
2:L:9:SER:O	2:L:9:SER:OG	2.19	0.60
2:L:103:LYS:HE3	2:L:105:GLU:HG2	1.82	0.60
1:A:18:VAL:HG23	1:A:82(C):LEU:HD11	1.82	0.60
1:A:59:TYR:CE1	1:A:69:ILE:HG12	2.36	0.60
1:H:23:LYS:HG2	1:H:77:THR:HG22	1.83	0.60
1:H:66:ARG:NH2	1:H:86:ASP:OD2	2.31	0.60
1:C:184:VAL:HG11	1:C:194:TYR:CZ	2.38	0.59
1:H:29:PHE:CE1	1:H:94:THR:HG21	2.37	0.59
1:C:146:PHE:CD1	1:C:147:PRO:HA	2.37	0.59
1:C:181:VAL:HG21	2:D:135:LEU:HD11	1.85	0.59
1:C:100(F):TRP:HH2	2:D:93:SER:N	2.01	0.59
2:B:197:THR:HG22	2:B:204:PRO:HB3	1.86	0.58
1:C:34:ILE:HD12	1:C:34:ILE:O	2.03	0.58
1:H:48:MET:HG2	1:H:63:PHE:HE2	1.68	0.58
1:H:29:PHE:HE1	1:H:94:THR:HG21	1.69	0.58
2:D:79:GLN:O	2:D:82:ASP:HB2	2.02	0.58
1:A:166:PHE:CE2	2:B:176:SER:HB3	2.39	0.58
1:C:100(F):TRP:CZ2	2:D:92:HIS:O	2.57	0.57
2:L:113:PRO:HB3	2:L:139:PHE:HB3	1.86	0.57
1:C:100(H):TRP:HB3	2:D:34:ASN:ND2	2.18	0.57
1:A:123:PRO:HB3	1:A:211:VAL:HG22	1.87	0.57
2:B:119:PRO:HB3	2:B:209:PHE:CZ	2.39	0.57
2:L:22:THR:HG22	2:L:72:THR:HG22	1.86	0.57
1:H:2:VAL:HA	1:H:26:GLY:HA3	1.87	0.57
1:A:87:THR:HG23	1:A:110:THR:HA	1.86	0.57
1:A:195:ILE:HD11	1:A:208:ASP:HB3	1.87	0.56
1:C:52:ASN:HB3	1:C:55:GLY:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:103:TRP:CD1	2:L:43:ALA:HB1	2.41	0.56
1:A:25:SER:OG	1:A:26:GLY:N	2.38	0.56
2:B:27:GLN:HB2	2:B:94:THR:HG21	1.87	0.56
2:B:92:HIS:CD2	2:B:93:SER:H	2.23	0.56
2:D:39:LYS:HG2	2:D:84:ALA:HB2	1.88	0.56
2:B:97:THR:HG22	2:B:98:PHE:N	2.21	0.55
2:L:61:ARG:NH1	2:L:82:ASP:OD1	2.39	0.55
2:B:108:ARG:NH2	2:B:109:THR:O	2.39	0.55
1:C:100(F):TRP:HZ3	2:D:91:SER:CA	2.18	0.55
1:C:7:SER:HG	1:C:21:SER:HG	1.51	0.55
1:A:1:GLN:O	1:A:1:GLN:NE2	2.38	0.55
1:H:168:ALA:HA	1:H:178:LEU:HB3	1.87	0.55
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.87	0.55
1:C:29:PHE:CZ	1:C:102:PRO:HG3	2.42	0.55
2:L:198:HIS:CD2	2:L:199:GLN:H	2.23	0.55
2:D:11:LEU:O	2:D:104:VAL:HA	2.08	0.54
1:C:143:LYS:HG3	1:C:144:ASP:HB2	1.89	0.54
1:A:52:ASN:HD22	1:A:54:LEU:HD23	1.71	0.54
2:L:89:GLN:NE2	2:L:96:ARG:HH21	2.05	0.54
2:L:132:VAL:HB	2:L:179:LEU:HD23	1.90	0.54
1:A:200:HIS:CE1	1:A:202:PRO:HB2	2.43	0.54
2:B:186:TYR:CE2	2:B:192:TYR:CE1	2.96	0.54
1:C:99:LEU:HD11	1:C:100(A):ARG:NH2	2.23	0.54
1:A:18:VAL:CG2	1:A:82(C):LEU:HD11	2.38	0.53
2:D:170:ASP:OD1	2:D:172:THR:OG1	2.21	0.53
2:B:27:GLN:CB	2:B:94:THR:HG21	2.39	0.53
2:B:78:LEU:HD23	2:B:83:PHE:CE1	2.44	0.53
1:C:123:PRO:HB3	1:C:211:VAL:HG22	1.91	0.53
1:C:159:LEU:HD23	1:C:161:SER:H	1.73	0.53
1:H:38:ARG:HB2	1:H:48:MET:SD	2.49	0.53
1:H:100(I):PHE:HB2	1:H:103:TRP:CZ3	2.44	0.53
1:A:101:ASP:HB3	1:A:102:PRO:CD	2.38	0.52
1:A:171:GLN:NE2	1:A:177:SER:HB3	2.24	0.52
1:C:100(F):TRP:HZ2	2:D:93:SER:HA	1.70	0.52
2:D:166:GLN:HG3	2:D:173:TYR:CZ	2.43	0.52
1:H:23:LYS:HA	1:H:77:THR:HG22	1.90	0.52
2:B:144:ALA:HB2	2:B:198:HIS:HD2	1.74	0.52
1:C:148:GLU:HG2	1:C:149:PRO:N	2.25	0.52
1:A:119:PRO:HD2	1:A:205:THR:HG21	1.91	0.52
2:D:47:LEU:HD21	2:D:62:PHE:CD1	2.45	0.52
1:C:126:PRO:HB3	1:C:137:ALA:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASN:HA	1:A:195:ILE:HG23	1.92	0.52
1:C:32:ASN:O	1:C:51:ILE:CG2	2.57	0.52
2:D:158:ASN:HB3	2:D:179:LEU:CD1	2.37	0.52
2:L:132:VAL:O	2:L:179:LEU:HB3	2.10	0.51
1:A:171:GLN:HE21	1:A:177:SER:HB3	1.76	0.51
1:H:83:ARG:O	1:H:111:VAL:HG21	2.11	0.51
2:L:55:GLN:O	2:L:58:VAL:HG23	2.11	0.51
1:A:4:LEU:HD23	1:A:24:ALA:HA	1.93	0.51
2:B:186:TYR:CE2	2:B:192:TYR:HE1	2.28	0.50
1:C:100(F):TRP:CH2	2:D:92:HIS:N	2.78	0.50
1:A:17:SER:CB	1:A:82(A):ARG:HG3	2.36	0.50
2:D:27:GLN:CD	2:D:27:GLN:H	2.14	0.50
2:L:167:ASP:HB3	2:L:170:ASP:OD1	2.10	0.50
2:L:198:HIS:HD2	2:L:199:GLN:H	1.59	0.50
1:C:163:VAL:HA	1:C:182:VAL:HG12	1.92	0.50
2:D:78:LEU:HD21	2:D:83:PHE:CE1	2.46	0.50
2:B:187:GLU:O	2:B:211:ARG:NH2	2.45	0.50
2:D:199:GLN:HG3	2:L:199:GLN:HA	1.93	0.50
2:D:115:VAL:HG21	2:D:205:VAL:HG11	1.92	0.50
1:C:124:LEU:HB3	2:D:118:PHE:CD1	2.47	0.50
1:C:91:TYR:CE2	2:D:44:PRO:HD3	2.47	0.49
1:C:100(F):TRP:CZ3	2:D:91:SER:CA	2.94	0.49
1:C:100(F):TRP:CH2	2:D:93:SER:N	2.76	0.49
2:D:27:GLN:HE22	2:D:95:VAL:HG13	1.77	0.49
2:D:92:HIS:CG	2:D:93:SER:N	2.78	0.49
2:D:106:ILE:O	2:D:166:GLN:NE2	2.41	0.49
1:H:56:ILE:HG22	1:H:57:GLY:H	1.77	0.49
1:C:101:ASP:HB3	1:C:102:PRO:HD3	1.94	0.49
2:D:105:GLU:OE2	2:D:173:TYR:OH	2.27	0.49
2:D:61:ARG:NH1	2:D:82:ASP:OD2	2.45	0.49
2:D:12:SER:HB3	2:D:105:GLU:HB2	1.95	0.49
1:C:36:TRP:HD1	1:C:69:ILE:HD13	1.76	0.49
1:H:189:LEU:HB3	1:H:194:TYR:CE2	2.45	0.49
2:B:150:VAL:HG12	2:B:192:TYR:CD2	2.48	0.49
1:C:52:ASN:HD22	1:C:52(A):PRO:HD2	1.77	0.49
1:C:152:VAL:HG22	1:C:198:VAL:HG22	1.95	0.49
2:D:198:HIS:HB3	2:D:201:LEU:HG	1.95	0.49
2:B:150:VAL:HG12	2:B:192:TYR:HD2	1.78	0.48
1:A:38:ARG:HG2	1:A:39:GLN:N	2.29	0.48
2:D:156:SER:HB2	2:L:11:LEU:HD13	1.94	0.48
1:H:2:VAL:HG21	1:H:29:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:73:ASN:HB2	1:H:74:PRO:HD3	1.94	0.48
2:L:65:SER:OG	2:L:72:THR:OG1	2.31	0.48
2:L:161:GLU:HG3	2:L:175:LEU:HD21	1.95	0.48
2:B:118:PHE:HB2	2:B:133:VAL:HB	1.96	0.48
2:B:96:ARG:C	2:B:96:ARG:HE	2.17	0.48
2:D:31:ASN:HA	2:D:71:PHE:HE2	1.78	0.48
1:H:36:TRP:HD1	1:H:69:ILE:HD13	1.79	0.48
1:C:66:ARG:NH2	1:C:86:ASP:OD2	2.47	0.48
1:H:103:TRP:NE1	2:L:44:PRO:HD2	2.28	0.48
1:H:152:VAL:HG11	1:H:180:SER:HB3	1.96	0.48
1:C:96:HIS:HD1	1:C:100(H):TRP:HE1	1.60	0.48
1:C:124:LEU:HD11	1:C:141:LEU:HB2	1.95	0.48
1:C:145:TYR:CE2	1:C:148:GLU:HA	2.38	0.48
1:A:117:LYS:HD3	1:A:175:LEU:HD13	1.96	0.48
1:A:7:SER:HB3	1:A:21:SER:OG	2.14	0.47
1:C:59:TYR:CE1	1:C:69:ILE:HG13	2.49	0.47
2:L:83:PHE:CG	2:L:106:ILE:HG22	2.49	0.47
2:L:139:PHE:HB2	2:L:198:HIS:CE1	2.49	0.47
1:C:11:VAL:HG22	1:C:110:THR:OG1	2.14	0.47
1:C:32:ASN:O	1:C:51:ILE:HG22	2.12	0.47
1:C:36:TRP:CE2	1:C:80:LEU:HB2	2.48	0.47
1:C:159:LEU:O	1:C:161:SER:N	2.47	0.47
2:B:148:TRP:HB2	2:B:155:GLN:HB2	1.97	0.47
1:C:59:TYR:HE1	1:C:69:ILE:HG13	1.79	0.47
2:D:92:HIS:CG	2:D:93:SER:H	2.32	0.47
2:L:170:ASP:OD2	2:L:172:THR:OG1	2.28	0.47
1:H:141:LEU:HD21	1:H:143:LYS:HD2	1.97	0.47
1:A:66:ARG:HG3	1:A:82(A):ARG:HB3	1.97	0.47
1:A:62:LYS:HG2	1:A:63:PHE:CE2	2.49	0.47
1:H:6:GLN:HE22	1:H:92:CYS:H	1.63	0.47
1:H:87:THR:HG23	1:H:110:THR:HA	1.97	0.47
1:H:48:MET:HG2	1:H:63:PHE:CE2	2.49	0.47
2:B:18:ARG:HB2	2:B:76:SER:O	2.15	0.47
1:C:100(F):TRP:CZ3	2:D:91:SER:HA	2.49	0.47
2:L:147:GLN:HB2	2:L:195:GLU:HB3	1.96	0.47
1:A:29:PHE:CE1	1:A:76:SER:HB3	2.50	0.46
1:A:199:ASN:HB3	1:A:206:LYS:NZ	2.30	0.46
1:H:40:ALA:HB3	1:H:43:GLN:CG	2.45	0.46
1:A:170:LEU:HD12	1:A:176:TYR:CZ	2.50	0.46
1:C:40:ALA:HB2	1:C:88:ALA:CB	2.45	0.46
1:H:100(I):PHE:O	1:H:102:PRO:HD2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:ALA:HB2	2:B:198:HIS:CD2	2.51	0.46
2:B:29:ILE:HA	2:B:92:HIS:CE1	2.51	0.46
1:C:94:THR:HB	1:C:102:PRO:CG	2.45	0.46
1:A:66:ARG:CG	1:A:82(A):ARG:HB3	2.46	0.46
2:B:120:PRO:HD2	2:B:186:TYR:OH	2.15	0.46
2:B:161:GLU:HG2	2:B:175:LEU:HD21	1.97	0.46
2:D:113:PRO:HB3	2:D:136:LEU:HB3	1.97	0.46
1:H:119:PRO:HD3	1:H:200:HIS:CD2	2.51	0.46
2:L:75:ILE:HG21	2:L:78:LEU:HD12	1.98	0.46
2:B:131:SER:HA	2:B:180:THR:HA	1.97	0.46
2:L:198:HIS:CD2	2:L:199:GLN:N	2.84	0.46
2:B:126:LYS:HD2	2:B:126:LYS:HA	1.77	0.45
2:B:183:LYS:O	2:B:187:GLU:HG2	2.15	0.45
1:H:10:GLU:HB3	1:H:12:LYS:HE2	1.98	0.45
1:H:58:ASN:ND2	1:H:100(D):THR:HB	2.31	0.45
2:D:79:GLN:HB3	2:D:80:PRO:HD2	1.98	0.45
1:C:47:TRP:CG	2:D:96:ARG:NH2	2.84	0.45
1:C:186:SER:O	1:C:186:SER:OG	2.34	0.45
1:H:100(I):PHE:HB2	1:H:103:TRP:HZ3	1.81	0.45
1:A:72:ASP:OD1	1:A:75:THR:HG22	2.17	0.45
1:C:100(F):TRP:HZ3	2:D:91:SER:HA	1.81	0.45
2:D:29:ILE:HB	2:D:92:HIS:HB2	1.98	0.45
2:B:149:LYS:HG3	2:B:154:LEU:HD23	1.98	0.45
2:B:150:VAL:HG22	2:B:155:GLN:HE21	1.82	0.45
2:D:115:VAL:HG11	2:D:196:VAL:HG21	1.98	0.45
1:A:96:HIS:CE1	1:A:101:ASP:HB2	2.52	0.45
2:B:38:GLN:HE21	2:B:87:TYR:HE1	1.65	0.45
1:C:70:THR:OG1	1:C:79:TYR:HB2	2.17	0.45
2:D:27:GLN:HG2	2:D:28:ASN:H	1.81	0.45
2:L:45:LYS:HE3	2:L:45:LYS:HB3	1.81	0.45
1:A:66:ARG:HG3	1:A:82(A):ARG:CB	2.47	0.45
1:C:36:TRP:O	1:C:48:MET:HB2	2.17	0.45
2:B:35:TRP:CZ3	2:B:88:CYS:HB3	2.52	0.45
1:H:72:ASP:CG	1:H:75:THR:HG22	2.37	0.45
2:B:27:GLN:O	2:B:69:THR:HG22	2.17	0.44
2:B:29:ILE:HA	2:B:92:HIS:ND1	2.32	0.44
2:B:108:ARG:HH21	2:B:108:ARG:HG3	1.82	0.44
1:A:165:THR:HB	1:A:180:SER:HB2	1.99	0.44
1:C:165:THR:HG22	1:C:180:SER:OG	2.17	0.44
1:A:63:PHE:O	1:A:65:GLY:N	2.50	0.44
1:C:51:ILE:HG13	1:C:56:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52(A):PRO:HG2	1:C:100(E):CYS:SG	2.57	0.44
2:D:142:ARG:HG3	2:D:173:TYR:CE1	2.53	0.44
2:L:103:LYS:HB3	2:L:103:LYS:HE2	1.72	0.44
1:A:1:GLN:O	1:A:102:PRO:HG3	2.18	0.44
2:B:92:HIS:CG	2:B:93:SER:H	2.36	0.44
1:H:56:ILE:HG22	1:H:57:GLY:N	2.33	0.44
2:B:150:VAL:HG23	2:B:150:VAL:O	2.18	0.44
1:A:24:ALA:HB2	1:A:34:ILE:HD11	2.00	0.44
2:D:31:ASN:HA	2:D:71:PHE:CE2	2.53	0.44
1:A:39:GLN:O	1:A:88:ALA:HB1	2.18	0.43
2:D:207:LYS:HB2	2:D:207:LYS:HE2	1.61	0.43
1:H:121:VAL:HA	1:H:141:LEU:O	2.19	0.43
1:H:101:ASP:HB3	1:H:102:PRO:HD3	2.01	0.43
1:A:69:ILE:HA	1:A:79:TYR:O	2.18	0.43
2:B:12:SER:HA	2:B:105:GLU:HG2	2.01	0.43
1:C:166:PHE:CE1	2:D:176:SER:HB2	2.54	0.43
1:H:36:TRP:CD1	1:H:69:ILE:HD13	2.54	0.43
2:L:83:PHE:CD1	2:L:106:ILE:HG22	2.54	0.43
2:B:119:PRO:HB3	2:B:209:PHE:CE1	2.54	0.43
1:C:23:LYS:HG3	1:C:77:THR:HG22	2.00	0.43
2:D:166:GLN:HG3	2:D:173:TYR:CE2	2.54	0.43
2:L:54:LEU:HD21	2:L:59:PRO:O	2.18	0.43
1:A:66:ARG:NH2	1:A:81:GLU:OE2	2.45	0.43
1:C:99:LEU:HB2	2:D:32:TYR:CE1	2.54	0.43
1:C:55:GLY:O	1:C:56:ILE:HG22	2.18	0.43
1:H:5:VAL:HG23	1:H:23:LYS:HB3	2.01	0.43
2:L:35:TRP:CE3	2:L:73:LEU:HD22	2.54	0.43
1:C:47:TRP:CD2	2:D:96:ARG:NH2	2.82	0.43
1:H:52:ASN:ND2	1:H:100(D):THR:HA	2.34	0.42
1:H:72:ASP:OD1	1:H:74:PRO:HD2	2.19	0.42
1:H:100(I):PHE:O	1:H:102:PRO:CD	2.66	0.42
2:D:29:ILE:O	2:D:31:ASN:N	2.51	0.42
2:D:134:CYS:HB2	2:D:148:TRP:CZ2	2.54	0.42
1:C:6:GLN:HG2	1:C:105:GLN:OE1	2.20	0.42
1:C:12:LYS:O	1:C:111:VAL:HA	2.19	0.42
1:C:100(F):TRP:CH2	2:D:93:SER:HA	2.54	0.42
2:D:9:SER:HA	2:D:101:GLY:O	2.20	0.42
2:L:49:TYR:O	2:L:53:ASN:HB2	2.19	0.42
1:A:119:PRO:HB2	1:A:142:VAL:HG13	2.02	0.42
2:B:139:PHE:HD2	2:B:198:HIS:HE2	1.67	0.42
1:C:31:SER:HB3	1:C:73:ASN:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:VAL:O	1:A:111:VAL:HG23	2.20	0.42
2:L:28:ASN:OD1	2:L:68:GLY:HA2	2.20	0.42
2:D:20:THR:HA	2:D:73:LEU:O	2.19	0.42
1:A:83:ARG:O	1:A:111:VAL:HG21	2.19	0.42
1:C:8:GLY:H	1:C:107:THR:HG22	1.84	0.42
2:D:119:PRO:HB3	2:D:209:PHE:CE1	2.54	0.42
2:L:199:GLN:HE21	2:L:199:GLN:HB2	1.63	0.42
1:A:122:PHE:CE2	2:B:124:GLN:HG3	2.54	0.42
1:C:94:THR:CB	1:C:102:PRO:HG2	2.50	0.42
1:H:111:VAL:HG23	1:H:111:VAL:O	2.19	0.42
1:A:6:GLN:HE21	1:A:6:GLN:HB3	1.59	0.41
2:B:149:LYS:HE3	2:B:154:LEU:HD21	2.00	0.41
1:H:159:LEU:HD13	1:H:182:VAL:HG21	2.02	0.41
1:C:98:ARG:HH22	2:D:50:ALA:CA	2.24	0.41
1:C:100(F):TRP:CH2	2:D:93:SER:CA	3.02	0.41
2:B:201:LEU:HD13	2:B:205:VAL:HG23	2.02	0.41
1:H:184:VAL:HG13	1:H:189:LEU:HD23	2.02	0.41
2:L:91:SER:O	2:L:91:SER:OG	2.34	0.41
1:C:13:LYS:NZ	1:C:114:ALA:O	2.42	0.41
1:C:99:LEU:HB2	2:D:32:TYR:HE1	1.86	0.41
1:C:108:LEU:HD21	1:C:110:THR:HG23	2.01	0.41
2:B:121:SER:O	2:B:125:LEU:HD12	2.20	0.41
1:C:13:LYS:O	1:C:16:SER:HB2	2.21	0.41
1:C:56:ILE:HD12	1:C:56:ILE:HA	1.95	0.41
1:C:48:MET:HE3	1:C:48:MET:HB3	1.77	0.41
2:D:90:GLN:HE21	2:D:90:GLN:HB2	1.66	0.41
2:D:142:ARG:NH2	2:D:163:VAL:HG11	2.36	0.41
2:B:115:VAL:HA	2:B:135:LEU:O	2.20	0.41
2:L:59:PRO:HG2	2:L:61:ARG:NH2	2.36	0.41
1:A:184:VAL:HB	1:A:185:PRO:HD2	2.02	0.40
1:A:205:THR:HG22	1:A:207:VAL:HG23	2.02	0.40
2:D:154:LEU:HD23	2:D:154:LEU:HA	1.88	0.40
1:H:23:LYS:HG2	1:H:77:THR:CG2	2.49	0.40
1:H:58:ASN:HD21	1:H:100(D):THR:HB	1.87	0.40
1:C:150:VAL:HG23	1:C:200:HIS:HD2	1.87	0.40
2:B:97:THR:CG2	2:B:98:PHE:N	2.85	0.40
2:L:61:ARG:HH11	2:L:61:ARG:HD2	1.70	0.40
2:L:195:GLU:OE2	2:L:204:PRO:HB2	2.21	0.40
2:B:94:THR:HG22	2:B:95:VAL:HG13	2.02	0.40
2:B:136:LEU:HD11	2:B:196:VAL:HG11	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:ARG:NH2	2:B:180:THR:O[16_545]	2.08	0.12

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	215/238 (90%)	200 (93%)	10 (5%)	5 (2%)	6 29
1	C	200/238 (84%)	186 (93%)	7 (4%)	7 (4%)	3 21
1	H	206/238 (87%)	191 (93%)	9 (4%)	6 (3%)	4 24
2	B	201/214 (94%)	185 (92%)	14 (7%)	2 (1%)	15 46
2	D	199/214 (93%)	182 (92%)	16 (8%)	1 (0%)	29 61
2	L	186/214 (87%)	172 (92%)	13 (7%)	1 (0%)	29 61
All	All	1207/1356 (89%)	1116 (92%)	69 (6%)	22 (2%)	8 35

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	THR
1	C	56	ILE
1	C	148	GLU
1	C	149	PRO
1	C	160	THR
2	D	30	ASN
1	H	7	SER
1	H	101	ASP
1	H	174	GLY
1	H	28	SER
1	A	64	GLN
1	H	159	LEU
1	A	100(G)	GLY

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Mol	Chain	Res	Type
1	A	101	ASP
2	B	30	ASN
2	B	138	ASN
1	C	101	ASP
1	H	144	ASP
2	L	157	GLY
1	C	100(G)	GLY
1	C	126	PRO
1	A	65	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/200 (92%)	178 (97%)	5 (3%)	44	71
1	C	177/200 (88%)	176 (99%)	1 (1%)	86	91
1	H	177/200 (88%)	170 (96%)	7 (4%)	31	61
2	B	178/188 (95%)	172 (97%)	6 (3%)	37	65
2	D	177/188 (94%)	172 (97%)	5 (3%)	43	70
2	L	169/188 (90%)	165 (98%)	4 (2%)	49	73
All	All	1061/1164 (91%)	1033 (97%)	28 (3%)	46	71

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

Mol	Chain	Res	Type
1	A	12	LYS
1	A	29	PHE
1	A	159	LEU
1	A	164	HIS
1	A	197	ASN
2	B	27	GLN
2	B	91	SER
2	B	96	ARG
2	B	162	SER

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Mol	Chain	Res	Type
2	B	176	SER
2	B	203	SER
1	C	197	ASN
2	D	65	SER
2	D	126	LYS
2	D	142	ARG
2	D	180	THR
2	D	209	PHE
1	H	29	PHE
1	H	76	SER
1	H	100	CYS
1	H	148	GLU
1	H	159	LEU
1	H	179	SER
1	H	197	ASN
2	L	61	ARG
2	L	96	ARG
2	L	123	GLU
2	L	124	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	92	HIS
1	C	52	ASN
2	D	27	GLN
2	D	90	GLN
1	H	58	ASN
2	L	89	GLN
2	L	198	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	A	219/238 (92%)	0.60	13 (5%) 22 22	128, 187, 249, 275	0
1	C	210/238 (88%)	0.74	30 (14%) 2 2	142, 192, 263, 290	0
1	H	210/238 (88%)	0.69	30 (14%) 2 2	123, 189, 277, 330	0
2	B	203/214 (94%)	0.76	6 (2%) 50 49	118, 153, 198, 243	0
2	D	203/214 (94%)	0.71	27 (13%) 3 3	152, 197, 251, 282	0
2	L	194/214 (90%)	0.77	20 (10%) 6 6	122, 189, 252, 283	0
All	All	1239/1356 (91%)	0.71	126 (10%) 6 6	118, 184, 255, 330	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	GLN	8.3
1	H	194	TYR	6.0
1	C	165	THR	5.1
2	L	197	THR	4.9
1	H	182	VAL	4.6
2	L	116	PHE	4.4
2	L	115	VAL	4.3
1	H	179	SER	4.2
2	D	62	PHE	4.2
1	C	18	VAL	4.1
1	C	90	TYR	4.1
1	H	152	VAL	4.1
1	H	207	VAL	4.1
1	C	211	VAL	4.0
1	H	183	THR	3.9
1	H	154	TRP	3.9
2	D	137	ASN	3.8
1	A	119	PRO	3.7
2	D	75	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	82	LEU	3.6
1	C	109	VAL	3.5
1	C	180	SER	3.5
1	C	37	VAL	3.5
1	C	181	VAL	3.5
2	D	87	TYR	3.5
1	H	181	VAL	3.4
1	C	179	SER	3.4
1	H	53	VAL	3.4
2	L	193	ALA	3.3
2	L	181	LEU	3.3
2	D	63	SER	3.3
2	L	131	SER	3.2
1	H	141	LEU	3.2
2	D	47	LEU	3.2
2	L	133	VAL	3.1
1	C	29	PHE	3.1
1	A	180	SER	3.1
2	D	123	GLU	3.1
1	A	24	ALA	3.1
2	L	136	LEU	3.1
2	L	175	LEU	3.0
1	H	69	ILE	3.0
1	A	154	TRP	3.0
2	D	21	ILE	3.0
2	D	83	PHE	3.0
1	A	45	LEU	2.9
1	H	140	CYS	2.9
1	C	138	LEU	2.9
1	H	142	VAL	2.9
2	L	113	PRO	2.9
1	C	194	TYR	2.9
2	D	104	VAL	2.9
1	C	140	CYS	2.8
1	H	82	LEU	2.8
2	L	194	CYS	2.8
2	D	136	LEU	2.8
1	A	127	SER	2.8
2	L	161	GLU	2.8
1	A	189	LEU	2.7
1	C	141	LEU	2.7
2	L	135	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	184	VAL	2.7
1	H	51	ILE	2.7
1	H	119	PRO	2.7
1	H	189	LEU	2.6
1	H	198	VAL	2.6
2	D	19	VAL	2.6
2	D	33	LEU	2.5
2	B	47	LEU	2.5
2	D	144	ALA	2.5
1	C	150	VAL	2.5
1	H	82(C)	LEU	2.5
1	C	183	THR	2.5
1	A	145	TYR	2.5
2	D	113	PRO	2.5
1	A	179	SER	2.5
2	D	78	LEU	2.4
1	C	100(I)	PHE	2.4
2	D	48	ILE	2.4
1	H	178	LEU	2.4
2	L	130	ALA	2.4
2	L	117	ILE	2.4
1	A	29	PHE	2.3
1	A	100(A)	ARG	2.3
1	C	182	VAL	2.3
1	C	67	VAL	2.3
1	C	70	THR	2.3
1	C	154	TRP	2.3
2	B	82	ASP	2.3
2	D	116	PHE	2.3
2	D	196	VAL	2.3
2	L	83	PHE	2.3
1	C	91	TYR	2.2
2	D	82	ASP	2.2
2	B	44	PRO	2.2
2	D	86	TYR	2.2
2	D	148	TRP	2.2
2	D	132	VAL	2.2
2	D	118	PHE	2.2
2	D	73	LEU	2.2
1	C	63	PHE	2.2
1	H	18	VAL	2.2
1	H	37	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	119	PRO	2.2
1	H	80	LEU	2.2
2	D	154	LEU	2.1
1	C	136	ALA	2.1
2	D	133	VAL	2.1
1	C	53	VAL	2.1
2	L	205	VAL	2.1
2	B	136	LEU	2.1
1	A	121	VAL	2.1
1	H	150	VAL	2.1
1	H	205	THR	2.1
1	H	4	LEU	2.1
1	H	108	LEU	2.1
1	H	52(A)	PRO	2.1
2	L	75	ILE	2.1
1	H	45	LEU	2.1
1	C	46	GLU	2.1
1	H	180	SER	2.1
1	C	121	VAL	2.0
2	B	196	VAL	2.0
2	B	75	ILE	2.0
2	L	78	LEU	2.0
2	L	132	VAL	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.