Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:36 PM GMT

PDB ID	:	1UB6
Title	:	Crystal structure of Antibody 19G2 with sera ligand
Authors	:	Beuscher, A.B.; Wirsching, P.; Lerner, R.A.; Janda, K.; Stevens, R.C.
Deposited on	:	2003-03-30
Resolution	:	2.12 Å(reported)

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

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

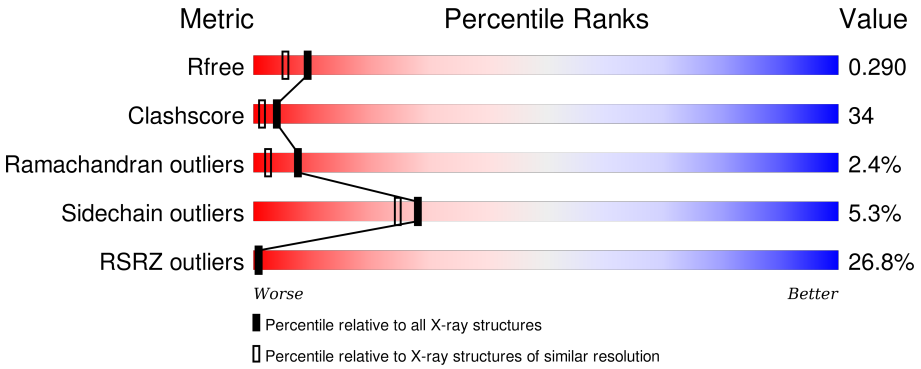
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.12 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (2.14-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	208	28% 58% 37% 6%
1	H	208	19% 67% 27% 5%
2	B	213	37% 50% 46% 5%
2	L	213	23% 50% 46% ·

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6784 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 antibody 19G2, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	208	Total	C	N	O	S	0	0	0
			1541	972	259	302	8			
1	A	208	Total	C	N	O	S	0	0	0
			1541	972	259	302	8			

- Molecule 2 is a protein called antibody 19G2, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1632	1022	272	332	6			
2	B	213	Total	C	N	O	S	0	0	0
			1632	1022	272	332	6			

- Molecule 3 is water.

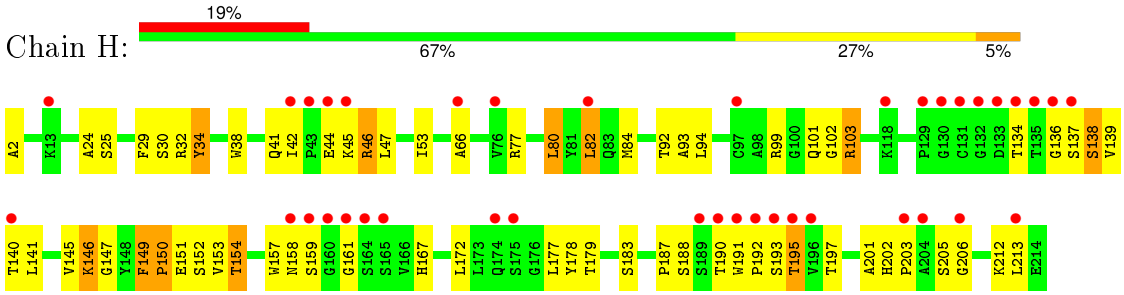
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total	O	0	0
			112	112		
3	B	125	Total	O	0	0
			125	125		
3	H	79	Total	O	0	0
			79	79		
3	L	122	Total	O	0	0
			122	122		

3 Residue-property plots (i)

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

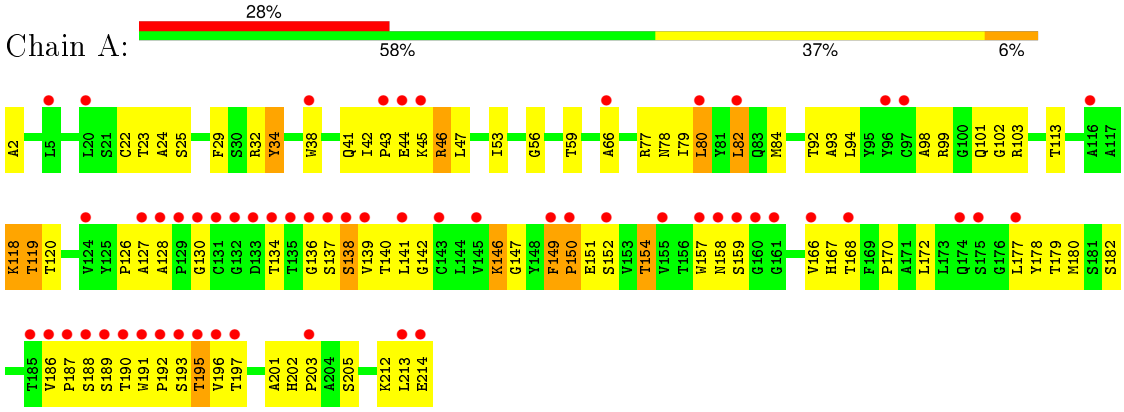
- Molecule 1: antibody 19G2, alpha chain

Chain H:



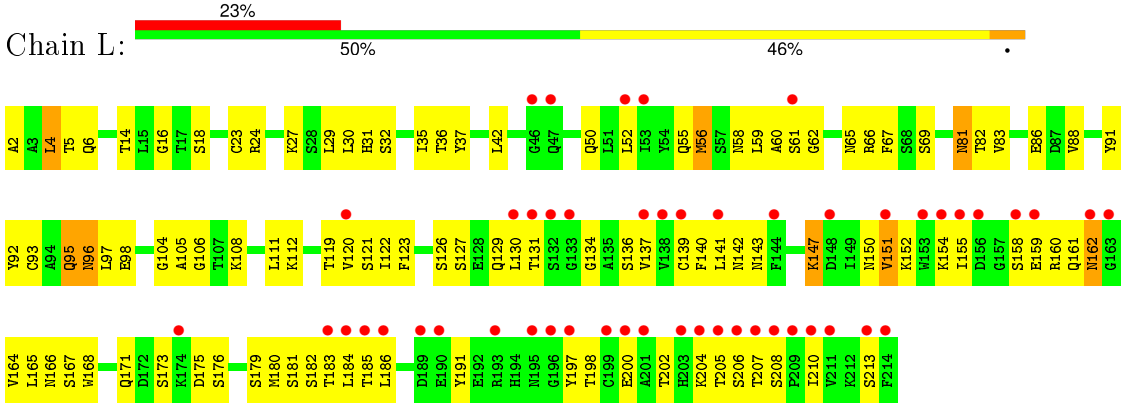
- Molecule 1: antibody 19G2, alpha chain

Chain A:



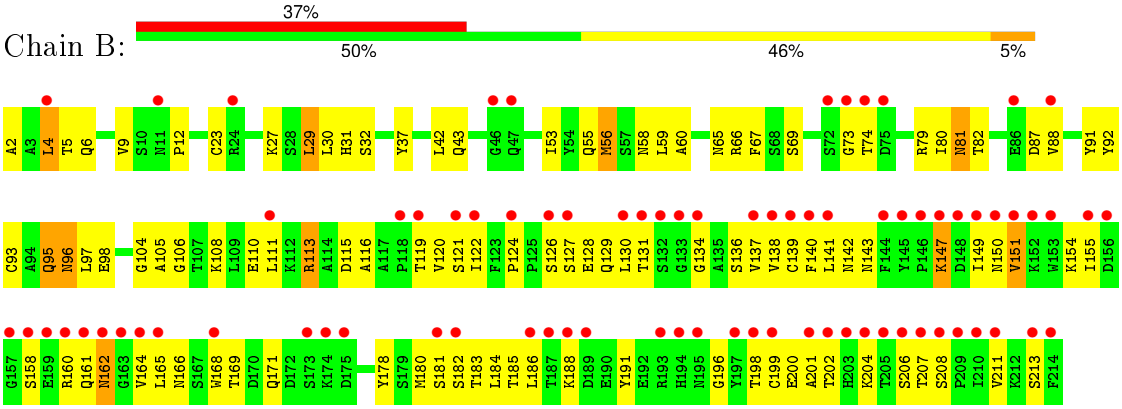
- Molecule 2: antibody 19G2, beta chain

Chain L:



• Molecule 2: antibody 19G2, beta chain

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	194.43Å 60.54Å 92.30Å 90.00° 117.30° 90.00°	Depositor
Resolution (Å)	19.43 – 2.12 19.43 – 2.12	Depositor EDS
% Data completeness (in resolution range)	89.0 (19.43-2.12) 89.0 (19.43-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 2.13Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.264 , 0.292 0.263 , 0.290	Depositor DCC
R_{free} test set	2350 reflections (4.87%)	DCC
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 73.9	EDS
Estimated twinning fraction	0.020 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 50364 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6784	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 5.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.33	0/1579	0.64	0/2155
1	H	0.31	0/1579	0.62	0/2155
2	B	0.33	0/1669	0.61	0/2272
2	L	0.34	0/1669	0.62	0/2272
All	All	0.33	0/6496	0.62	0/8854

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1541	0	1521	104	0
1	H	1541	0	1521	75	0
2	B	1632	0	1580	129	0
2	L	1632	0	1580	130	0
3	A	112	0	0	49	0
3	B	125	0	0	54	0
3	H	79	0	0	19	0
3	L	122	0	0	45	0
All	All	6784	0	6202	429	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 34.

All (429) 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:L:83:VAL:HB	3:L:290:HOH:O	1.68	0.93
2:L:83:VAL:HG23	3:L:328:HOH:O	1.71	0.90
1:A:23:THR:HA	3:A:295:HOH:O	1.71	0.90
2:B:80:ILE:HA	3:B:296:HOH:O	1.73	0.88
2:L:14:THR:HA	3:L:273:HOH:O	1.74	0.87
2:B:53:ILE:HA	3:B:321:HOH:O	1.78	0.83
2:L:59:LEU:HG	3:L:321:HOH:O	1.79	0.83
1:A:196:VAL:HA	3:A:241:HOH:O	1.79	0.83
1:A:150:PRO:HD2	3:A:299:HOH:O	1.78	0.81
1:A:177:LEU:HA	3:A:268:HOH:O	1.79	0.81
2:L:2:ALA:HB1	3:L:250:HOH:O	1.81	0.81
2:B:9:VAL:HG12	3:B:239:HOH:O	1.84	0.78
2:B:43:GLN:HG2	3:B:302:HOH:O	1.84	0.77
2:B:155:ILE:HG21	3:B:310:HOH:O	1.84	0.77
2:B:111:LEU:H	2:B:171:GLN:HE22	1.29	0.77
1:H:192:PRO:HA	3:H:249:HOH:O	1.85	0.77
1:A:197:THR:HB	1:A:212:LYS:HG2	1.67	0.76
1:H:197:THR:HB	1:H:212:LYS:HG2	1.68	0.76
1:A:22:CYS:HB3	3:A:301:HOH:O	1.84	0.76
1:A:126:PRO:HD2	3:B:303:HOH:O	1.87	0.75
2:B:82:THR:HG23	3:B:262:HOH:O	1.86	0.75
1:A:80:LEU:HB2	3:A:301:HOH:O	1.84	0.75
2:B:6:GLN:HB2	3:B:297:HOH:O	1.85	0.74
3:A:247:HOH:O	2:B:124:PRO:HD2	1.87	0.74
1:A:141:LEU:HD21	1:A:191:TRP:HZ3	1.52	0.74
2:L:30:LEU:HD22	3:L:265:HOH:O	1.88	0.74
1:H:141:LEU:HD21	1:H:191:TRP:HZ3	1.53	0.73
2:L:150:ASN:OD1	2:L:202:THR:HB	1.89	0.73
3:H:220:HOH:O	2:L:5:THR:HG22	1.88	0.73
2:B:200:GLU:HB2	3:B:273:HOH:O	1.89	0.72
1:H:150:PRO:HA	3:H:272:HOH:O	1.89	0.72
2:L:88:VAL:HG12	2:L:111:LEU:HD23	1.72	0.72
2:B:73:GLY:HA2	3:B:307:HOH:O	1.89	0.71
1:A:41:GLN:HB2	3:A:288:HOH:O	1.90	0.71
2:B:113:ARG:HB2	2:B:113:ARG:NH1	2.04	0.71
1:A:166:VAL:HA	3:A:286:HOH:O	1.90	0.71
2:L:181:SER:HB3	3:L:316:HOH:O	1.88	0.71
2:B:150:ASN:OD1	2:B:202:THR:HB	1.89	0.71
1:H:2:ALA:HA	1:H:25:SER:O	1.92	0.70
1:A:2:ALA:HA	1:A:25:SER:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:81:ASN:HD22	2:L:81:ASN:C	1.94	0.70
1:A:196:VAL:HG23	3:A:259:HOH:O	1.91	0.69
2:B:119:THR:HG23	3:B:286:HOH:O	1.93	0.69
2:B:120:VAL:HG11	3:B:336:HOH:O	1.92	0.69
2:B:67:PHE:HA	3:B:296:HOH:O	1.93	0.69
2:B:141:LEU:HA	3:B:282:HOH:O	1.91	0.68
2:L:30:LEU:CD2	3:L:265:HOH:O	2.40	0.68
2:B:113:ARG:HB2	2:B:113:ARG:HH11	1.59	0.68
2:B:81:ASN:HD22	2:B:81:ASN:C	1.97	0.68
2:L:30:LEU:HA	3:L:265:HOH:O	1.94	0.67
1:A:79:ILE:HG12	3:A:295:HOH:O	1.94	0.67
1:A:141:LEU:HB3	1:A:213:LEU:HD22	1.77	0.67
2:B:4:LEU:HD23	2:B:93:CYS:SG	2.35	0.67
2:L:105:ALA:HB3	3:L:272:HOH:O	1.95	0.66
1:A:141:LEU:HD21	1:A:191:TRP:CZ3	2.29	0.66
2:B:129:GLN:HG3	3:B:246:HOH:O	1.95	0.66
1:H:141:LEU:HB3	1:H:213:LEU:HD22	1.77	0.66
2:L:155:ILE:HD12	3:L:263:HOH:O	1.94	0.66
2:L:96:ASN:HD22	2:L:96:ASN:H	1.43	0.66
1:A:142:GLY:HA3	3:A:251:HOH:O	1.95	0.66
1:A:80:LEU:CB	3:A:301:HOH:O	2.42	0.65
2:B:130:LEU:HD22	3:B:268:HOH:O	1.96	0.65
2:B:128:GLU:HB2	3:B:303:HOH:O	1.96	0.65
2:B:150:ASN:HB2	3:B:327:HOH:O	1.95	0.65
1:A:172:LEU:HD11	2:B:166:ASN:O	1.96	0.65
1:A:187:PRO:HG2	1:A:190:THR:HG22	1.78	0.65
1:H:187:PRO:HG2	1:H:190:THR:HG22	1.78	0.65
1:A:149:PHE:O	1:A:151:GLU:N	2.29	0.65
2:B:196:GLY:HA3	3:B:281:HOH:O	1.96	0.65
1:H:149:PHE:O	1:H:151:GLU:N	2.30	0.65
2:L:167:SER:HB3	3:L:316:HOH:O	1.95	0.65
2:L:137:VAL:CG1	2:L:184:LEU:HB3	2.27	0.65
1:H:141:LEU:HD21	1:H:191:TRP:CZ3	2.30	0.64
1:A:118:LYS:N	1:A:118:LYS:HD2	2.11	0.64
2:B:154:LYS:HA	2:B:158:SER:O	1.97	0.64
2:B:199:CYS:HA	3:B:249:HOH:O	1.97	0.64
2:B:96:ASN:H	2:B:96:ASN:HD22	1.45	0.64
1:A:41:GLN:HB3	1:A:47:LEU:HD23	1.80	0.63
2:B:137:VAL:CG1	2:B:184:LEU:HB3	2.27	0.63
2:B:106:GLY:N	3:B:297:HOH:O	2.32	0.63
2:L:154:LYS:HA	2:L:158:SER:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PHE:HA	3:A:268:HOH:O	1.99	0.63
2:L:60:ALA:HB1	3:L:276:HOH:O	1.99	0.63
1:H:41:GLN:HB3	1:H:47:LEU:HD23	1.81	0.62
1:H:32:ARG:HB2	3:H:240:HOH:O	1.98	0.62
2:L:88:VAL:HG12	2:L:111:LEU:CD2	2.29	0.62
2:B:151:VAL:HG21	2:B:180:MET:CE	2.30	0.62
2:B:37:TYR:HB3	2:B:96:ASN:ND2	2.16	0.61
1:A:56:GLY:HA3	3:A:277:HOH:O	2.00	0.61
2:L:151:VAL:HG21	2:L:180:MET:CE	2.31	0.61
2:L:151:VAL:HG21	2:L:180:MET:HE1	1.82	0.61
1:A:38:TRP:CE2	1:A:82:LEU:HB2	2.35	0.61
2:B:80:ILE:HG23	3:B:296:HOH:O	2.00	0.60
2:B:198:THR:HA	2:B:213:SER:HB3	1.83	0.60
1:A:59:THR:HB	3:A:260:HOH:O	2.02	0.60
1:H:34:TYR:HB3	1:H:101:GLN:OE1	2.00	0.60
2:B:95:GLN:NE2	2:B:97:LEU:H	1.99	0.60
2:B:188:LYS:HE2	3:B:268:HOH:O	2.00	0.60
2:L:158:SER:HB3	3:L:293:HOH:O	2.00	0.60
1:A:34:TYR:HB3	1:A:101:GLN:OE1	2.01	0.60
1:H:206:GLY:HA2	3:H:227:HOH:O	2.01	0.60
2:L:95:GLN:NE2	2:L:97:LEU:H	2.00	0.60
2:B:60:ALA:N	3:B:321:HOH:O	2.35	0.60
2:B:6:GLN:NE2	2:B:106:GLY:H	1.99	0.59
2:L:52:LEU:HD23	3:L:268:HOH:O	2.01	0.59
2:L:86:GLU:HG2	3:L:319:HOH:O	2.01	0.59
2:L:6:GLN:NE2	2:L:106:GLY:H	2.00	0.59
1:H:38:TRP:CE2	1:H:82:LEU:HB2	2.37	0.59
2:L:198:THR:HA	2:L:213:SER:HB3	1.83	0.58
1:H:102:GLY:HA2	2:L:55:GLN:HE21	1.67	0.58
2:B:151:VAL:HG21	2:B:180:MET:HE1	1.85	0.58
2:L:155:ILE:HG13	3:L:293:HOH:O	2.02	0.58
2:L:119:THR:HG23	2:L:119:THR:O	2.04	0.58
1:A:141:LEU:HB3	1:A:213:LEU:CD2	2.34	0.57
1:H:153:VAL:HG12	3:H:262:HOH:O	2.04	0.57
1:A:214:GLU:HG2	3:A:278:HOH:O	2.03	0.57
1:A:213:LEU:H	1:A:213:LEU:HD12	1.69	0.57
1:A:195:THR:HA	3:A:313:HOH:O	2.03	0.57
2:L:37:TYR:HB3	2:L:96:ASN:ND2	2.19	0.57
2:B:161:GLN:O	2:B:164:VAL:HG12	2.05	0.57
1:A:149:PHE:O	1:A:150:PRO:C	2.43	0.57
1:H:141:LEU:HB3	1:H:213:LEU:CD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:N	1:A:213:LEU:HD12	2.20	0.56
2:L:119:THR:HG22	2:L:142:ASN:O	2.04	0.56
1:A:167:HIS:HB3	3:A:262:HOH:O	2.04	0.56
2:L:24:ARG:CZ	3:L:279:HOH:O	2.52	0.56
2:B:168:TRP:HB3	3:B:276:HOH:O	2.06	0.56
1:H:45:LYS:HG3	3:L:275:HOH:O	2.05	0.56
2:L:161:GLN:O	2:L:164:VAL:HG12	2.06	0.56
2:L:6:GLN:HE21	2:L:104:GLY:HA3	1.69	0.56
2:L:137:VAL:HG12	2:L:184:LEU:HB3	1.88	0.55
1:H:192:PRO:HG2	3:H:270:HOH:O	2.06	0.55
2:L:27:LYS:HE2	2:L:98:GLU:OE1	2.06	0.55
2:L:4:LEU:HD23	2:L:93:CYS:SG	2.47	0.55
2:B:31:HIS:CD2	2:B:32:SER:H	2.25	0.55
1:H:45:LYS:O	1:H:46:ARG:HB3	2.07	0.55
2:L:31:HIS:CD2	2:L:32:SER:H	2.23	0.55
2:L:186:LEU:HD11	2:L:191:TYR:HB2	1.88	0.55
2:B:160:ARG:HD2	2:B:162:ASN:HB3	1.89	0.54
1:H:161:GLY:HA2	3:H:266:HOH:O	2.07	0.54
1:H:213:LEU:HD12	1:H:213:LEU:H	1.72	0.54
1:A:154:THR:HG23	1:A:201:ALA:HB3	1.89	0.54
1:H:195:THR:HA	3:H:276:HOH:O	2.07	0.54
2:L:95:GLN:HE21	2:L:97:LEU:H	1.54	0.54
1:A:79:ILE:HA	3:A:295:HOH:O	2.06	0.54
2:B:6:GLN:HE21	2:B:104:GLY:HA3	1.73	0.54
1:A:43:PRO:HG3	3:A:238:HOH:O	2.08	0.54
2:B:186:LEU:HD11	2:B:191:TYR:HB2	1.89	0.54
2:B:137:VAL:HG12	2:B:184:LEU:HB3	1.89	0.54
2:B:27:LYS:HE2	2:B:98:GLU:OE1	2.07	0.54
1:A:195:THR:HB	1:A:212:LYS:HE3	1.90	0.54
1:A:22:CYS:CB	3:A:301:HOH:O	2.47	0.54
1:H:42:ILE:HG22	1:H:44:GLU:H	1.73	0.54
2:B:147:LYS:H	2:B:147:LYS:HD3	1.73	0.54
1:A:45:LYS:O	1:A:46:ARG:HB3	2.07	0.54
1:H:154:THR:HG23	1:H:201:ALA:HB3	1.88	0.53
1:H:213:LEU:HD12	1:H:213:LEU:N	2.22	0.53
2:B:149:ILE:HG12	3:B:226:HOH:O	2.08	0.53
1:A:147:GLY:HA2	1:A:177:LEU:HD13	1.91	0.53
2:L:6:GLN:HG2	2:L:93:CYS:SG	2.48	0.53
1:A:42:ILE:HG22	1:A:44:GLU:H	1.73	0.53
1:H:195:THR:HB	1:H:212:LYS:HE3	1.90	0.53
1:H:149:PHE:HB3	1:H:150:PRO:CD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LYS:HA	3:A:288:HOH:O	2.07	0.53
2:B:95:GLN:HE21	2:B:97:LEU:H	1.55	0.53
2:L:35:ILE:C	3:L:265:HOH:O	2.46	0.53
1:A:118:LYS:O	1:A:120:THR:HG23	2.08	0.53
1:A:149:PHE:O	1:A:178:TYR:HD2	1.92	0.53
1:H:149:PHE:O	1:H:150:PRO:C	2.44	0.53
2:L:86:GLU:HA	2:L:173:SER:O	2.08	0.53
2:B:140:PHE:C	2:B:141:LEU:HD12	2.29	0.53
2:L:61:SER:N	3:L:276:HOH:O	2.42	0.53
2:L:159:GLU:HG2	3:L:269:HOH:O	2.09	0.52
1:H:147:GLY:HA2	1:H:177:LEU:HD13	1.90	0.52
1:H:167:HIS:HE1	2:L:143:ASN:OD1	1.93	0.52
2:L:31:HIS:HD2	3:L:226:HOH:O	1.93	0.52
2:L:140:PHE:C	2:L:141:LEU:HD12	2.30	0.52
1:A:92:THR:O	1:A:93:ALA:HB2	2.10	0.52
2:L:160:ARG:HD2	2:L:162:ASN:HB3	1.89	0.52
1:A:149:PHE:HB3	1:A:150:PRO:CD	2.39	0.52
2:B:4:LEU:HD23	2:B:23:CYS:SG	2.50	0.52
2:B:168:TRP:CD1	2:B:180:MET:HG3	2.44	0.52
1:H:149:PHE:O	1:H:178:TYR:HD2	1.92	0.52
2:B:105:ALA:HB3	3:B:250:HOH:O	2.09	0.52
1:H:32:ARG:HD2	3:H:255:HOH:O	2.09	0.52
1:H:30:SER:HB2	3:H:229:HOH:O	2.10	0.52
2:L:147:LYS:HD3	2:L:147:LYS:H	1.73	0.52
2:B:204:LYS:HG2	3:B:279:HOH:O	2.09	0.52
2:B:164:VAL:C	2:B:165:LEU:HD12	2.30	0.52
2:B:5:THR:HG23	3:B:218:HOH:O	2.10	0.52
2:B:96:ASN:N	2:B:96:ASN:HD22	2.06	0.51
1:H:206:GLY:HA2	3:H:268:HOH:O	2.11	0.51
2:L:164:VAL:C	2:L:165:LEU:HD12	2.30	0.51
2:B:87:ASP:HA	3:B:311:HOH:O	2.10	0.51
2:B:27:LYS:HB2	3:B:233:HOH:O	2.10	0.51
2:L:186:LEU:CD1	2:L:191:TYR:HB2	2.41	0.51
2:B:30:LEU:C	2:B:30:LEU:HD13	2.31	0.51
2:B:136:SER:CB	2:B:185:THR:HG22	2.41	0.51
1:A:146:LYS:HB3	1:A:179:THR:HG23	1.92	0.51
1:A:158:ASN:O	1:A:159:SER:HB2	2.10	0.51
2:L:136:SER:CB	2:L:185:THR:HG22	2.41	0.51
1:H:158:ASN:O	1:H:159:SER:HB2	2.11	0.51
2:B:201:ALA:HA	3:B:226:HOH:O	2.11	0.51
1:A:24:ALA:HB2	1:A:29:PHE:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:SER:N	3:A:308:HOH:O	2.44	0.51
2:L:24:ARG:NH1	3:L:279:HOH:O	2.44	0.50
2:B:186:LEU:CD1	2:B:191:TYR:HB2	2.40	0.50
2:B:130:LEU:HD11	3:B:306:HOH:O	2.11	0.50
2:L:168:TRP:CD1	2:L:180:MET:HG3	2.46	0.50
1:H:136:GLY:O	1:H:188:SER:HB2	2.12	0.50
2:L:121:SER:O	2:L:139:CYS:HA	2.12	0.50
2:L:30:LEU:C	2:L:30:LEU:HD13	2.32	0.50
2:B:129:GLN:HG2	2:B:134:GLY:O	2.12	0.50
2:L:152:LYS:HA	3:L:322:HOH:O	2.11	0.50
1:A:136:GLY:O	1:A:188:SER:HB2	2.12	0.50
1:A:102:GLY:HA2	3:A:221:HOH:O	2.11	0.50
1:H:146:LYS:HB3	1:H:179:THR:HG23	1.93	0.50
1:A:92:THR:HG23	1:A:113:THR:HA	1.94	0.50
1:A:186:VAL:HG12	3:A:304:HOH:O	2.10	0.49
1:A:188:SER:HB3	3:A:308:HOH:O	2.12	0.49
2:L:111:LEU:H	2:L:171:GLN:HE22	1.59	0.49
2:B:82:THR:HG22	3:B:244:HOH:O	2.12	0.49
2:L:204:LYS:HA	2:L:204:LYS:HE2	1.94	0.49
2:L:55:GLN:HB2	2:L:58:ASN:HD22	1.76	0.49
2:B:88:VAL:HG12	2:B:111:LEU:HG	1.94	0.49
2:B:204:LYS:HE2	2:B:204:LYS:HA	1.93	0.49
2:B:204:LYS:CA	2:B:204:LYS:HE2	2.42	0.49
2:B:121:SER:O	2:B:139:CYS:HA	2.11	0.49
2:B:141:LEU:CD2	2:B:151:VAL:HG22	2.41	0.49
1:H:150:PRO:HG2	1:H:202:HIS:CE1	2.48	0.49
2:B:126:SER:HB2	3:B:303:HOH:O	2.13	0.49
1:A:32:ARG:HD3	3:A:305:HOH:O	2.13	0.49
2:L:112:LYS:HB3	3:L:273:HOH:O	2.12	0.49
1:A:213:LEU:HD23	3:A:290:HOH:O	2.13	0.49
1:A:150:PRO:HG2	1:A:202:HIS:CE1	2.48	0.49
1:H:32:ARG:NE	3:H:240:HOH:O	2.22	0.49
1:A:80:LEU:HD12	3:A:239:HOH:O	2.12	0.48
1:H:102:GLY:HA2	3:H:277:HOH:O	2.13	0.48
2:B:55:GLN:HB2	2:B:58:ASN:HD22	1.77	0.48
1:A:138:SER:H	1:A:187:PRO:HA	1.78	0.48
1:H:82:LEU:HD13	1:H:84:MET:HG3	1.96	0.48
2:L:16:GLY:N	3:L:290:HOH:O	2.46	0.48
2:B:120:VAL:N	3:B:282:HOH:O	2.46	0.48
2:L:204:LYS:CA	2:L:204:LYS:HE2	2.43	0.48
2:L:129:GLN:HG2	2:L:134:GLY:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:6:GLN:HE22	2:L:92:TYR:HA	1.79	0.48
2:L:141:LEU:CD2	2:L:151:VAL:HG22	2.43	0.48
1:A:166:VAL:HG22	3:A:286:HOH:O	2.13	0.48
1:A:170:PRO:HB2	3:A:267:HOH:O	2.13	0.48
2:B:74:THR:HB	3:B:290:HOH:O	2.13	0.48
2:L:200:GLU:HG3	3:L:227:HOH:O	2.12	0.48
1:A:167:HIS:HE1	2:B:143:ASN:OD1	1.96	0.48
1:H:24:ALA:HB2	1:H:29:PHE:CZ	2.49	0.48
2:L:4:LEU:HD12	3:L:250:HOH:O	2.15	0.47
1:A:119:THR:HG23	3:A:296:HOH:O	2.14	0.47
2:B:141:LEU:N	2:B:141:LEU:HD12	2.29	0.47
2:L:96:ASN:N	2:L:96:ASN:HD22	2.06	0.47
2:B:136:SER:HB3	2:B:185:THR:HG22	1.96	0.47
2:B:138:VAL:HB	3:B:254:HOH:O	2.15	0.47
2:L:141:LEU:HD12	2:L:141:LEU:N	2.30	0.47
1:A:128:ALA:HB2	3:A:290:HOH:O	2.13	0.47
1:A:46:ARG:HB2	3:B:329:HOH:O	2.14	0.47
2:L:127:SER:O	2:L:131:THR:HG23	2.15	0.47
1:H:138:SER:H	1:H:187:PRO:HA	1.78	0.47
2:L:136:SER:HB3	2:L:185:THR:HG22	1.97	0.47
1:H:183:SER:HB3	2:L:140:PHE:CE2	2.50	0.47
1:H:103:ARG:NH1	3:H:258:HOH:O	2.47	0.47
2:L:62:GLY:N	3:L:248:HOH:O	2.42	0.47
2:L:140:PHE:HB3	2:L:142:ASN:HD21	1.80	0.46
2:L:66:ARG:HA	2:L:81:ASN:HD21	1.80	0.46
2:B:127:SER:O	2:B:131:THR:HG23	2.15	0.46
1:H:92:THR:O	1:H:93:ALA:HB2	2.16	0.46
1:A:192:PRO:HA	3:A:316:HOH:O	2.15	0.46
1:H:151:GLU:HB2	1:H:178:TYR:CE2	2.50	0.46
1:A:177:LEU:HD23	3:A:268:HOH:O	2.15	0.46
2:L:180:MET:CE	2:L:182:SER:HB2	2.46	0.46
2:B:66:ARG:HA	2:B:81:ASN:HD21	1.81	0.46
2:L:83:VAL:CG1	2:L:111:LEU:HD11	2.45	0.46
2:L:140:PHE:HB3	2:L:142:ASN:ND2	2.30	0.46
1:A:151:GLU:HB2	1:A:178:TYR:CE2	2.50	0.46
1:H:46:ARG:NH1	2:L:105:ALA:HB2	2.30	0.46
2:B:110:GLU:HG3	3:B:256:HOH:O	2.16	0.46
1:A:32:ARG:NH2	3:A:276:HOH:O	2.49	0.46
2:B:59:LEU:HD13	3:B:232:HOH:O	2.14	0.46
2:B:180:MET:CE	2:B:182:SER:HB2	2.45	0.46
2:L:4:LEU:HD23	2:L:23:CYS:SG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:36:THR:CA	3:L:265:HOH:O	2.63	0.45
2:B:140:PHE:HB3	2:B:142:ASN:HD21	1.81	0.45
2:B:42:LEU:HD13	2:B:91:TYR:CZ	2.51	0.45
1:A:98:ALA:N	3:A:239:HOH:O	2.49	0.45
2:B:150:ASN:O	2:B:151:VAL:HB	2.17	0.45
2:B:155:ILE:HG13	2:B:155:ILE:O	2.17	0.45
2:B:6:GLN:HE22	2:B:92:TYR:HA	1.82	0.45
2:B:206:SER:C	2:B:208:SER:H	2.20	0.45
2:B:140:PHE:HB3	2:B:142:ASN:ND2	2.31	0.45
2:B:97:LEU:HG	2:B:98:GLU:HG3	1.98	0.45
2:L:56:MET:O	2:L:69:SER:HB3	2.17	0.45
2:B:122:ILE:HA	2:B:139:CYS:HB3	1.99	0.45
2:B:180:MET:HG2	2:B:181:SER:N	2.32	0.45
1:H:203:PRO:C	1:H:205:SER:H	2.20	0.45
1:A:82:LEU:HD13	1:A:84:MET:CG	2.47	0.45
2:B:111:LEU:C	3:B:255:HOH:O	2.55	0.45
2:B:122:ILE:HG13	2:B:139:CYS:HB3	1.99	0.45
2:B:56:MET:O	2:B:69:SER:HB3	2.17	0.45
2:B:126:SER:O	2:B:130:LEU:HG	2.17	0.45
2:L:202:THR:N	3:L:320:HOH:O	2.38	0.45
2:B:142:ASN:N	3:B:282:HOH:O	2.45	0.44
2:B:141:LEU:HD21	2:B:151:VAL:HG22	1.98	0.44
1:H:82:LEU:HD13	1:H:84:MET:CG	2.47	0.44
1:A:203:PRO:C	1:A:205:SER:H	2.21	0.44
2:L:210:ILE:C	3:L:227:HOH:O	2.55	0.44
2:B:151:VAL:HA	2:B:200:GLU:O	2.18	0.44
2:L:61:SER:HB2	3:L:256:HOH:O	2.17	0.44
2:L:155:ILE:O	2:L:155:ILE:HG13	2.17	0.44
2:L:97:LEU:HG	2:L:98:GLU:HG3	1.99	0.44
2:L:50:GLN:HG2	3:L:268:HOH:O	2.18	0.44
1:A:170:PRO:HB2	3:B:275:HOH:O	2.18	0.44
2:L:180:MET:HG2	2:L:181:SER:N	2.32	0.44
2:L:83:VAL:N	3:L:328:HOH:O	2.50	0.44
2:L:67:PHE:HB2	3:L:321:HOH:O	2.17	0.44
2:L:143:ASN:ND2	3:L:294:HOH:O	2.50	0.44
3:A:310:HOH:O	2:B:165:LEU:HD13	2.18	0.44
2:B:151:VAL:HG21	2:B:180:MET:SD	2.57	0.44
2:B:183:THR:HG22	2:B:185:THR:HG23	2.00	0.44
1:H:145:VAL:HG12	3:H:253:HOH:O	2.17	0.44
2:L:36:THR:N	3:L:265:HOH:O	2.51	0.43
2:L:150:ASN:O	2:L:151:VAL:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:206:SER:C	2:L:208:SER:H	2.19	0.43
2:B:2:ALA:N	3:B:216:HOH:O	2.50	0.43
1:A:78:ASN:ND2	3:A:245:HOH:O	2.47	0.43
2:B:12:PRO:CB	3:B:255:HOH:O	2.66	0.43
2:L:141:LEU:HD21	2:L:151:VAL:HG22	2.00	0.43
2:B:206:SER:O	2:B:207:THR:HB	2.18	0.43
2:L:151:VAL:HA	2:L:200:GLU:O	2.18	0.43
1:H:139:VAL:HG23	3:H:233:HOH:O	2.18	0.43
2:B:119:THR:C	3:B:282:HOH:O	2.56	0.43
1:A:45:LYS:O	1:A:46:ARG:CB	2.66	0.43
2:L:81:ASN:ND2	2:L:81:ASN:C	2.67	0.43
1:H:172:LEU:HD11	2:L:166:ASN:O	2.18	0.43
2:B:30:LEU:N	3:B:307:HOH:O	2.50	0.43
1:H:44:GLU:O	1:H:45:LYS:HB2	2.17	0.43
2:L:165:LEU:HD12	2:L:165:LEU:N	2.34	0.43
1:A:202:HIS:CE1	3:A:299:HOH:O	2.71	0.43
2:L:183:THR:HG22	2:L:185:THR:HG23	2.00	0.43
2:L:83:VAL:HG11	2:L:111:LEU:HD11	2.00	0.43
2:L:83:VAL:HG11	2:L:111:LEU:CD1	2.49	0.43
2:L:206:SER:O	2:L:207:THR:HB	2.18	0.43
1:H:191:TRP:N	1:H:192:PRO:HD2	2.34	0.43
1:A:166:VAL:HB	3:A:224:HOH:O	2.17	0.43
1:A:118:LYS:CD	1:A:118:LYS:N	2.80	0.43
1:A:157:TRP:C	1:A:159:SER:H	2.21	0.43
1:A:182:SER:N	3:A:320:HOH:O	2.51	0.43
1:A:2:ALA:N	3:A:297:HOH:O	2.51	0.43
1:A:99:ARG:HD2	1:A:99:ARG:C	2.39	0.43
1:A:44:GLU:O	1:A:45:LYS:HB2	2.18	0.42
1:A:82:LEU:HD13	1:A:84:MET:HG3	2.00	0.42
2:L:122:ILE:HA	2:L:139:CYS:HB3	2.00	0.42
1:H:141:LEU:HD11	1:H:191:TRP:CZ3	2.54	0.42
1:A:213:LEU:H	1:A:213:LEU:CD1	2.31	0.42
1:H:202:HIS:ND1	1:H:205:SER:CB	2.83	0.42
1:H:136:GLY:HA2	1:H:188:SER:HB2	2.01	0.42
2:L:122:ILE:HG13	2:L:139:CYS:HB3	2.00	0.42
2:L:126:SER:O	2:L:130:LEU:HG	2.19	0.42
2:B:165:LEU:HD12	2:B:165:LEU:N	2.34	0.42
2:L:42:LEU:HD13	2:L:91:TYR:CZ	2.53	0.42
1:H:167:HIS:CE1	2:L:179:SER:OG	2.72	0.42
2:B:29:LEU:N	3:B:307:HOH:O	2.52	0.42
1:H:45:LYS:O	1:H:46:ARG:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:82:THR:HG22	3:L:245:HOH:O	2.18	0.42
1:H:99:ARG:HD2	1:H:99:ARG:C	2.40	0.42
1:A:101:GLN:HG3	3:A:220:HOH:O	2.20	0.42
2:B:204:LYS:N	2:B:204:LYS:HE2	2.34	0.42
2:L:205:THR:HG22	3:L:262:HOH:O	2.19	0.42
1:H:134:THR:O	1:H:134:THR:HG23	2.19	0.42
1:A:141:LEU:HD11	1:A:191:TRP:CZ3	2.55	0.42
2:L:120:VAL:HA	2:L:140:PHE:O	2.19	0.42
2:B:37:TYR:HB3	2:B:96:ASN:HD22	1.85	0.42
1:A:139:VAL:HG22	1:A:140:THR:N	2.35	0.42
2:B:160:ARG:NH1	3:B:310:HOH:O	2.53	0.42
2:L:151:VAL:HG21	2:L:180:MET:SD	2.59	0.42
1:A:187:PRO:O	1:A:190:THR:HG22	2.20	0.42
2:B:147:LYS:HB3	2:B:178:TYR:CD2	2.55	0.42
2:L:142:ASN:HB3	2:L:143:ASN:OD1	2.20	0.41
2:B:200:GLU:HG3	2:B:211:VAL:HG12	2.02	0.41
1:A:127:ALA:CB	3:A:293:HOH:O	2.67	0.41
1:A:134:THR:HG23	1:A:134:THR:O	2.20	0.41
2:B:113:ARG:CB	2:B:113:ARG:HH11	2.28	0.41
1:H:157:TRP:C	1:H:159:SER:H	2.22	0.41
1:H:193:SER:O	1:H:195:THR:OG1	2.36	0.41
2:B:120:VAL:HA	2:B:140:PHE:O	2.20	0.41
1:H:2:ALA:N	3:H:216:HOH:O	2.53	0.41
1:A:136:GLY:HA2	1:A:188:SER:HB2	2.02	0.41
2:L:204:LYS:N	2:L:204:LYS:HE2	2.35	0.41
2:B:79:ARG:HB3	3:B:316:HOH:O	2.19	0.41
2:L:136:SER:HB2	2:L:185:THR:HG22	2.02	0.41
1:H:139:VAL:HG22	1:H:140:THR:N	2.35	0.41
1:A:191:TRP:N	1:A:192:PRO:HD2	2.35	0.41
1:A:23:THR:HG22	3:A:295:HOH:O	2.21	0.41
2:L:59:LEU:HD13	3:L:259:HOH:O	2.19	0.41
1:A:53:ILE:O	1:A:53:ILE:HG23	2.20	0.41
1:A:130:GLY:HA3	3:A:244:HOH:O	2.20	0.41
1:H:187:PRO:O	1:H:190:THR:HG22	2.20	0.41
1:H:202:HIS:ND1	1:H:205:SER:HB2	2.35	0.41
2:B:73:GLY:CA	3:B:307:HOH:O	2.57	0.41
1:H:138:SER:HA	1:H:187:PRO:HA	2.03	0.41
2:B:95:GLN:HE22	2:B:98:GLU:H	1.69	0.41
2:L:162:ASN:ND2	3:L:334:HOH:O	2.53	0.41
1:H:140:THR:O	2:L:123:PHE:HZ	2.04	0.41
2:B:142:ASN:HB3	2:B:143:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:262:HOH:O	2:B:169:THR:HG21	2.21	0.41
2:B:116:ALA:HB1	3:B:263:HOH:O	2.21	0.41
1:A:193:SER:O	1:A:195:THR:OG1	2.37	0.40
1:H:203:PRO:C	1:H:205:SER:N	2.75	0.40
1:H:206:GLY:CA	3:H:268:HOH:O	2.68	0.40
1:H:38:TRP:NE1	1:H:80:LEU:HD13	2.36	0.40
1:H:53:ILE:O	1:H:53:ILE:HG23	2.22	0.40
2:L:175:ASP:O	2:L:176:SER:HB2	2.21	0.40
1:A:202:HIS:ND1	1:A:205:SER:HB2	2.37	0.40
2:L:81:ASN:HA	3:L:218:HOH:O	2.21	0.40
2:B:149:ILE:HG22	3:B:337:HOH:O	2.21	0.40
2:L:18:SER:HA	3:L:328:HOH:O	2.21	0.40
2:B:82:THR:O	2:B:82:THR:HG22	2.21	0.40
1:A:138:SER:HA	1:A:186:VAL:O	2.22	0.40
2:L:95:GLN:HE22	2:L:98:GLU:H	1.69	0.40
2:L:197:TYR:O	2:L:213:SER:HB2	2.22	0.40
1:A:168:THR:HG23	1:A:180:MET:CE	2.51	0.40
1:A:149:PHE:HB3	1:A:150:PRO:HD2	2.04	0.40
2:L:147:LYS:CD	2:L:147:LYS:H	2.35	0.40
2:B:136:SER:HB2	2:B:185:THR:HG22	2.03	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	206/208 (99%)	185 (90%)	13 (6%)	8 (4%)	4 1
1	H	206/208 (99%)	184 (89%)	14 (7%)	8 (4%)	4 1
2	B	211/213 (99%)	200 (95%)	9 (4%)	2 (1%)	21 14
2	L	211/213 (99%)	200 (95%)	9 (4%)	2 (1%)	21 14
All	All	834/842 (99%)	769 (92%)	45 (5%)	20 (2%)	7 2

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	149	PHE
1	A	149	PHE
1	H	66	ALA
1	H	137	SER
1	H	138	SER
1	A	66	ALA
1	A	137	SER
1	A	138	SER
2	B	162	ASN
1	H	152	SER
1	H	195	THR
2	L	151	VAL
2	L	162	ASN
1	A	152	SER
1	A	195	THR
2	B	151	VAL
1	H	46	ARG
1	H	150	PRO
1	A	46	ARG
1	A	150	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	172/172 (100%)	162 (94%)	10 (6%)	25 21
1	H	172/172 (100%)	164 (95%)	8 (5%)	32 29
2	B	187/187 (100%)	176 (94%)	11 (6%)	24 20
2	L	187/187 (100%)	178 (95%)	9 (5%)	31 28
All	All	718/718 (100%)	680 (95%)	38 (5%)	28 25

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	34	TYR
1	H	77	ARG
1	H	80	LEU
1	H	82	LEU
1	H	94	LEU
1	H	103	ARG
1	H	146	LYS
1	H	154	THR
2	L	4	LEU
2	L	29	LEU
2	L	56	MET
2	L	65	ASN
2	L	81	ASN
2	L	95	GLN
2	L	96	ASN
2	L	108	LYS
2	L	147	LYS
1	A	34	TYR
1	A	77	ARG
1	A	80	LEU
1	A	82	LEU
1	A	94	LEU
1	A	103	ARG
1	A	118	LYS
1	A	119	THR
1	A	146	LYS
1	A	154	THR
2	B	4	LEU
2	B	29	LEU
2	B	56	MET
2	B	65	ASN
2	B	81	ASN
2	B	95	GLN
2	B	96	ASN
2	B	108	LYS
2	B	113	ARG
2	B	115	ASP
2	B	147	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	167	HIS

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Mol	Chain	Res	Type
1	H	174	GLN
2	L	6	GLN
2	L	31	HIS
2	L	50	GLN
2	L	55	GLN
2	L	58	ASN
2	L	65	ASN
2	L	81	ASN
2	L	95	GLN
2	L	96	ASN
2	L	142	ASN
2	L	166	ASN
2	L	171	GLN
2	L	195	ASN
1	A	167	HIS
1	A	174	GLN
2	B	6	GLN
2	B	31	HIS
2	B	50	GLN
2	B	58	ASN
2	B	65	ASN
2	B	81	ASN
2	B	95	GLN
2	B	96	ASN
2	B	142	ASN
2	B	166	ASN
2	B	171	GLN
2	B	195	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	208/208 (100%)	1.40	58 (27%)	1	1	17, 40, 85, 95	0
1	H	208/208 (100%)	1.29	39 (18%)	2	2	23, 45, 84, 96	0
2	B	213/213 (100%)	1.61	79 (37%)	0	0	22, 48, 80, 88	0
2	L	213/213 (100%)	1.22	50 (23%)	1	1	17, 41, 81, 87	0
All	All	842/842 (100%)	1.38	226 (26%)	1	1	17, 45, 82, 96	0

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	132	GLY	14.2
1	H	134	THR	13.0
1	A	130	GLY	10.8
1	A	134	THR	10.6
1	H	43	PRO	9.3
1	A	43	PRO	9.0
1	A	131	CYS	8.6
1	H	133	ASP	8.2
1	A	127	ALA	7.8
1	H	131	CYS	7.4
1	A	137	SER	7.3
1	H	164	SER	7.2
2	L	195	ASN	6.8
2	L	208	SER	6.8
1	A	132	GLY	6.6
2	L	206	SER	6.5
1	A	136	GLY	6.4
1	A	135	THR	6.4
2	L	207	THR	6.3
1	H	137	SER	6.3
2	B	208	SER	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	128	ALA	6.3
2	L	209	PRO	6.2
1	H	191	TRP	6.0
1	H	129	PRO	6.0
1	A	191	TRP	6.0
1	H	135	THR	5.7
1	H	136	GLY	5.6
2	B	133	GLY	5.6
1	A	138	SER	5.6
2	L	155	ILE	5.5
1	A	192	PRO	5.4
2	B	149	ILE	5.1
2	B	202	THR	5.1
1	H	161	GLY	5.0
2	L	156	ASP	5.0
1	A	196	VAL	5.0
2	B	132	SER	5.0
2	B	204	LYS	5.0
2	B	205	THR	4.9
1	H	175	SER	4.9
2	B	165	LEU	4.9
2	B	46	GLY	4.8
1	A	190	THR	4.8
1	H	192	PRO	4.8
1	A	133	ASP	4.6
2	B	206	SER	4.6
2	B	197	TYR	4.6
2	B	161	GLN	4.6
2	B	141	LEU	4.4
1	H	195	THR	4.3
2	L	139	CYS	4.3
2	B	163	GLY	4.3
2	B	153	TRP	4.3
1	H	159	SER	4.3
2	B	198	THR	4.3
1	H	76	VAL	4.3
2	B	186	LEU	4.3
2	L	211	VAL	4.3
2	B	210	ILE	4.2
1	H	130	GLY	4.2
1	H	44	GLU	4.2
2	B	211	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	159	SER	4.2
2	B	156	ASP	4.1
2	L	137	VAL	4.1
1	A	157	TRP	4.1
2	L	205	THR	4.0
1	A	189	SER	4.0
2	B	158	SER	4.0
2	L	153	TRP	4.0
1	A	193	SER	4.0
2	B	159	GLU	3.9
2	B	130	LEU	3.9
2	B	199	CYS	3.9
2	B	207	THR	3.9
1	A	141	LEU	3.9
2	L	138	VAL	3.8
2	B	150	ASN	3.8
2	B	47	GLN	3.8
2	L	200	GLU	3.8
2	L	159	GLU	3.8
2	B	193	ARG	3.7
2	L	61	SER	3.7
1	A	44	GLU	3.7
1	A	145	VAL	3.7
2	L	131	THR	3.7
2	B	122	ILE	3.7
2	L	193	ARG	3.7
1	A	213	LEU	3.7
1	H	206	GLY	3.6
2	B	189	ASP	3.6
2	L	210	ILE	3.6
1	H	193	SER	3.6
1	A	197	THR	3.6
1	A	186	VAL	3.6
1	A	203	PRO	3.5
2	B	119	THR	3.5
1	A	139	VAL	3.5
2	L	162	ASN	3.5
2	L	184	LEU	3.5
2	L	214	PHE	3.5
2	B	209	PRO	3.5
2	B	157	GLY	3.5
2	L	47	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
2	L	189	ASP	3.4
2	L	197	TYR	3.4
1	A	166	VAL	3.4
1	A	195	THR	3.2
2	B	88	VAL	3.2
1	H	213	LEU	3.2
1	A	150	PRO	3.2
2	B	162	ASN	3.1
1	A	187	PRO	3.1
2	B	187	THR	3.1
2	B	72	SER	3.1
2	L	46	GLY	3.1
1	H	45	LYS	3.1
1	A	82	LEU	3.1
1	A	45	LYS	3.1
2	B	73	GLY	3.1
2	L	52	LEU	3.0
2	B	137	VAL	3.0
1	H	42	ILE	3.0
2	B	86	GLU	3.0
2	B	155	ILE	3.0
2	B	195	ASN	2.9
2	B	24	ARG	2.9
2	L	196	GLY	2.9
1	H	190	THR	2.9
1	H	82	LEU	2.9
2	B	139	CYS	2.9
2	B	151	VAL	2.9
2	B	134	GLY	2.9
1	A	152	SER	2.9
1	A	143	CYS	2.9
2	L	154	LYS	2.9
2	B	173	SER	2.9
2	B	182	SER	2.9
1	A	160	GLY	2.9
2	B	152	LYS	2.9
2	L	201	ALA	2.9
2	B	148	ASP	2.9
1	A	175	SER	2.8
2	B	124	PRO	2.8
2	L	120	VAL	2.8
1	A	158	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	118	LYS	2.8
1	A	38	TRP	2.8
2	L	213	SER	2.8
1	A	174	GLN	2.8
2	B	203	HIS	2.8
1	H	174	GLN	2.7
2	B	118	PRO	2.7
1	H	189	SER	2.7
1	A	129	PRO	2.7
2	B	121	SER	2.7
2	B	174	LYS	2.7
2	B	111	LEU	2.6
1	H	196	VAL	2.6
1	A	161	GLY	2.6
1	H	158	ASN	2.6
2	B	214	PHE	2.6
2	L	204	LYS	2.6
2	B	213	SER	2.6
2	B	175	ASP	2.6
2	L	203	HIS	2.6
1	A	149	PHE	2.6
1	H	165	SER	2.6
1	A	97	CYS	2.5
2	L	141	LEU	2.5
1	A	155	VAL	2.5
2	B	194	HIS	2.5
2	L	190	GLU	2.5
2	B	126	SER	2.5
2	L	133	GLY	2.5
2	B	188	LYS	2.5
2	L	183	THR	2.5
2	B	131	THR	2.5
2	L	132	SER	2.5
2	L	163	GLY	2.5
2	B	164	VAL	2.5
2	L	185	THR	2.5
2	B	74	THR	2.5
2	L	151	VAL	2.4
2	B	138	VAL	2.4
2	B	160	ARG	2.4
1	A	177	LEU	2.4
1	A	185	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	127	SER	2.4
1	A	188	SER	2.4
1	A	20	LEU	2.3
2	L	158	SER	2.3
2	B	4	LEU	2.3
2	L	199	CYS	2.3
1	H	140	THR	2.3
2	L	174	LYS	2.3
2	L	186	LEU	2.3
2	B	201	ALA	2.3
2	B	11	ASN	2.3
1	A	96	TYR	2.3
2	B	140	PHE	2.3
2	L	148	ASP	2.2
2	L	130	LEU	2.2
2	B	146	PRO	2.2
1	A	168	THR	2.2
1	H	66	ALA	2.2
1	H	204	ALA	2.2
1	A	116	ALA	2.2
1	H	97	CYS	2.2
2	B	168	TRP	2.2
2	L	144	PHE	2.2
1	H	13	LYS	2.1
2	B	75	ASP	2.1
1	H	203	PRO	2.1
1	A	66	ALA	2.1
1	H	160	GLY	2.1
1	A	80	LEU	2.1
1	A	5	LEU	2.0
2	B	144	PHE	2.0
2	B	145	TYR	2.0
2	B	147	LYS	2.0
1	A	124	VAL	2.0
1	A	214	GLU	2.0
2	B	181	SER	2.0
2	L	53	ILE	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.