Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 07:49 pm BST

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
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 (i)) were used in the production of this report:

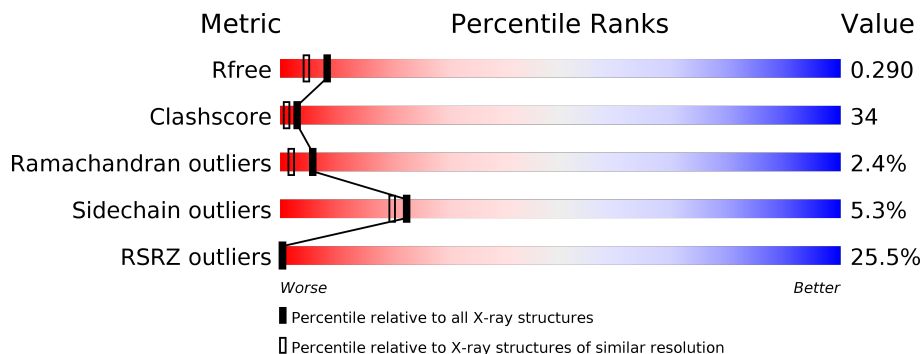|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (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	Percentile Ranks	Value
Rfree		0.290
Clashscore		34
Ramachandran outliers		2.4%
Sidechain outliers		5.3%
RSRZ outliers		25.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (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 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	208	25% 58% 37% 6%
1	H	208	18% 67% 27% 5%
2	B	213	35% 50% 46% 5%
2	L	213	23% 50% 46% •

2 Entry composition (i)

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 1541	C 972	N 259	O 302	S 8	0	0	0
1	A	208	Total 1541	C 972	N 259	O 302	S 8	0	0	0

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

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

- Molecule 3 is water.

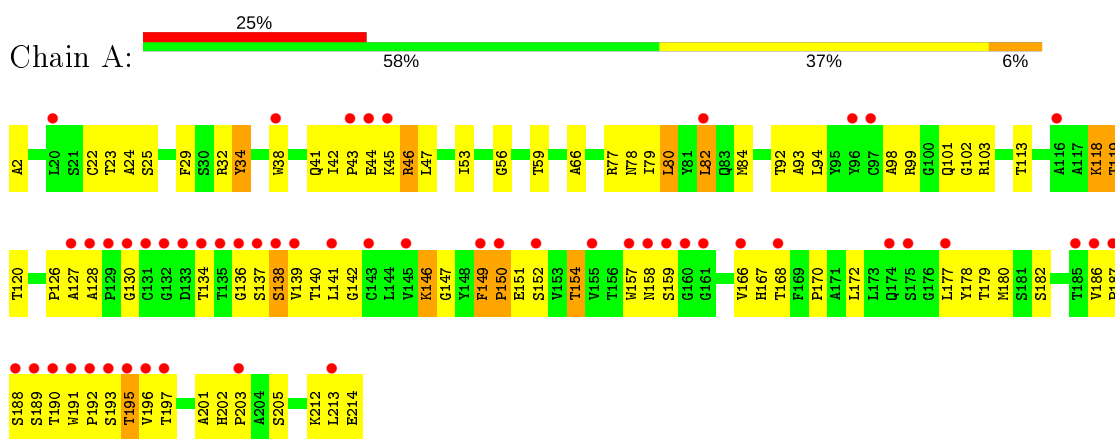| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	79	Total 79	O 79	0	0
3	L	122	Total 122	O 122	0	0
3	A	112	Total 112	O 112	0	0
3	B	125	Total 125	O 125	0	0

3 Residue-property plots ⓘ

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.
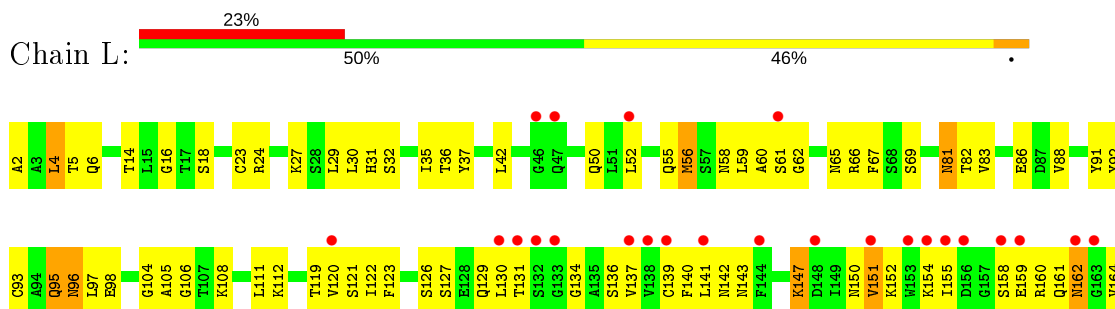
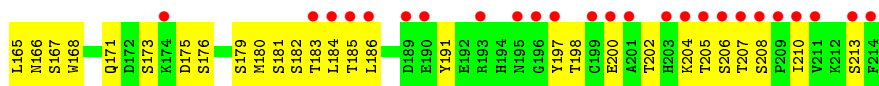- Molecule 1: antibody 19G2, alpha chain
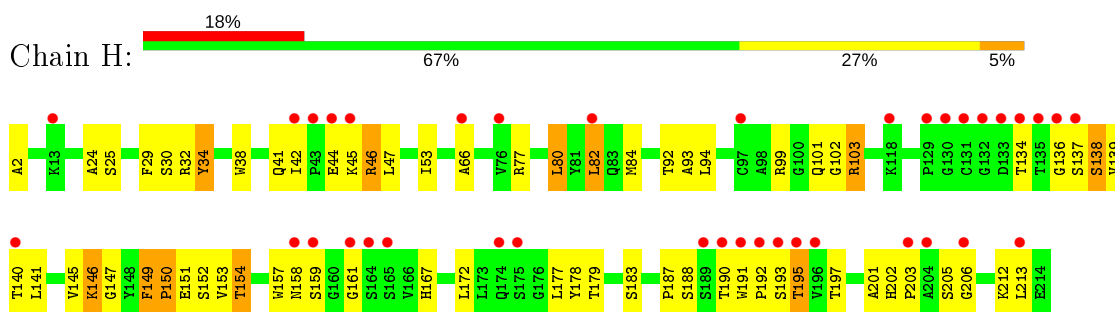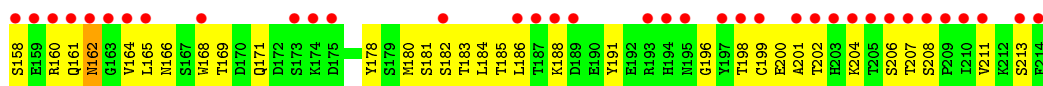

- Molecule 1: antibody 19G2, alpha chain

- Molecule 2: antibody 19G2, beta chain

L165 N166 S167 W168 Q171 D172 S173 K174 D175 S176 S179 M180 S181 S182 T183 L184 T185 L186 D189 E190 Y191 E192 R193 H194 N195 G196 Y197 T198 C199 E200 A201 T202 H203 K204 T205 S206 T207 S208 P209 I210 V211 K212 S213 F214

• Molecule 2: antibody 19G2, beta chain

Chain B:

35%

50%　　　　　　　　　　　　　　46%　　　　　　　　5%

A2 A3 L4 T5 Q6 V9 S10 N11 P12 C23 R24 K27 S28 L29 L30 H31 S32 Y37 L42 Q43 G46 Q47 I53 Y54 Q55 M56 S57 N58 L59 A60 N65 R66 F67 S68 S69 S72 G73 T74 D75 R79 I80 N81 T82 E86 D87 V88 Y91 Y92

C93 A94 Q95 N96 L97 E98 G104 A105 G106 T107 K108 L109 E110 L111 K112 R113 A114 D115 A116 A117 P118 T119 V120 S121 I122 F123 P124 P125 S126 S127 E128 Q129 L130 T131 S132 G133 G134 A135 S136 V137 V138 C139 F140 L141 N142 N143 P146 K147 D148 I149 N150 V151 K152 W153 K154 I155 D156 G157

S158 E159 R160 Q161 N162 G163 V164 L165 N166 S167 W168 T169 D170 Q171 D172 S173 K174 D175 Y178 S179 M180 S181 S182 T183 L184 T185 L186 T187 K188 D189 E190 Y191 E192 R193 H194 N195 G196 Y197 T198 C199 E200 A201 T202 H203 K204 T205 S206 T207 S208 P209 I210 V211 K212 S213 F214

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 (4.67%)	wwPDB-VP
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 , 74.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h-2*l,-k,l	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.*

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[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 (i)

5.1 Standard geometry (i)

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 (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	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:155:ILE:HG21	3:B:310:HOH:O	1.84	0.77
2:B:43:GLN:HG2	3:B:302: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
1:A:141:LEU:HD21	1:A:191:TRP:HZ3	1.52	0.74
3:A:247:HOH:O	2:B:124:PRO:HD2	1.87	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
1:A:172:LEU:HD11	2:B:166:ASN: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: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: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
1:H:141:LEU:HD21	1:H:191:TRP:CZ3	2.30	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
1:A:56:GLY:HA3	3:A:277:HOH:O	2.00	0.61
2:B:37:TYR:HB3	2:B:96:ASN:ND2	2.16	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:198:THR:HA	2:B:213:SER:HB3	1.83	0.60
2:B:80:ILE:HG23	3:B:296:HOH:O	2.00	0.60
1:A:59:THR:HB	3:A:260:HOH:O	2.02	0.60
2:B:95:GLN:NE2	2:B:97:LEU:H	1.99	0.60
1:H:34:TYR:HB3	1:H:101:GLN:OE1	2.00	0.60
1:A:34:TYR:HB3	1:A:101:GLN:OE1	2.01	0.60
2:B:188:LYS:HE2	3:B:268:HOH:O	2.00	0.60
1:H:206:GLY:HA2	3:H:227:HOH:O	2.01	0.60
2:L:158:SER:HB3	3:L:293:HOH:O	2.00	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
1:H:38:TRP:CE2	1:H:82:LEU:HB2	2.37	0.59
2:L:6:GLN:NE2	2:L:106:GLY:H	2.00	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:A:214:GLU:HG2	3:A:278:HOH:O	2.03	0.57
1:H:153:VAL:HG12	3:H:262:HOH:O	2.04	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:A:213:LEU:N	1:A:213:LEU:HD12	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:141:LEU:HB3	1:H:213:LEU:CD2	2.36	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:B:31:HIS:CD2	2:B:32:SER:H	2.25	0.55
2:L:4:LEU:HD23	2:L:93:CYS:SG	2.47	0.55
1:H:45:LYS:O	1:H:46:ARG:HB3	2.07	0.55
2:L:186:LEU:HD11	2:L:191:TYR:HB2	1.88	0.55
2:L:31:HIS:CD2	2:L:32:SER:H	2.23	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:43:PRO:HG3	3:A:238:HOH:O	2.08	0.54
1:A:79:ILE:HA	3:A:295:HOH:O	2.06	0.54
2:B:186:LEU:HD11	2:B:191:TYR:HB2	1.89	0.54
2:B:6:GLN:HE21	2:B:104:GLY:HA3	1.73	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
2:B:147:LYS:HD3	2:B:147:LYS:H	1.73	0.54
1:H:42:ILE:HG22	1:H:44:GLU:H	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:149:PHE:HB3	1:H:150:PRO:CD	2.39	0.53
1:H:195:THR:HB	1:H:212:LYS:HE3	1.90	0.53
1:A:118:LYS:O	1:A:120:THR:HG23	2.08	0.53
2:L:35:ILE:C	3:L:265:HOH:O	2.46	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
1:H:147:GLY:HA2	1:H:177:LEU:HD13	1.90	0.52
2:L:159:GLU:HG2	3:L:269:HOH:O	2.09	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
1:A:92:THR:O	1:A:93:ALA:HB2	2.10	0.52
2:L:140:PHE:C	2:L:141:LEU:HD12	2.30	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:105:ALA:HB3	3:B:250:HOH:O	2.09	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
1:H:30:SER:HB2	3:H:229:HOH:O	2.10	0.52
1:H:32:ARG:HD2	3:H:255:HOH:O	2.09	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:B:87:ASP:HA	3:B:311:HOH:O	2.10	0.51
2:L:164:VAL:C	2:L:165:LEU:HD12	2.30	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
1:A:158:ASN:O	1:A:159:SER:HB2	2.10	0.51
1:A:146:LYS:HB3	1:A:179:THR:HG23	1.92	0.51
2:B:136:SER:CB	2:B:185:THR:HG22	2.41	0.51
2:B:30:LEU:C	2:B:30:LEU:HD13	2.31	0.51
1:H:158:ASN:O	1:H:159:SER:HB2	2.11	0.51
2:L:136:SER:CB	2:L:185:THR:HG22	2.41	0.51
1:A:189:SER:N	3:A:308:HOH:O	2.44	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)
2:B:201:ALA:HA	3:B:226:HOH:O	2.11	0.51
2:B:186:LEU:CD1	2:B:191:TYR:HB2	2.40	0.50
2:L:24:ARG:NH1	3:L:279:HOH:O	2.44	0.50
2:B:130:LEU:HD11	3:B:306:HOH:O	2.11	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:168:TRP:CD1	2:L:180:MET:HG3	2.46	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
2:L:30:LEU:C	2:L:30:LEU:HD13	2.32	0.50
1:A:102:GLY:HA2	3:A:221:HOH:O	2.11	0.50
1:A:136:GLY:O	1:A:188:SER:HB2	2.12	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:B:82:THR:HG22	3:B:244:HOH:O	2.12	0.49
2:L:111:LEU:H	2:L:171:GLN:HE22	1.59	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:121:SER:O	2:B:139:CYS:HA	2.11	0.49
2:B:204:LYS:CA	2:B:204:LYS:HE2	2.42	0.49
2:B:204:LYS:HA	2:B:204:LYS:HE2	1.93	0.49
2:B:88:VAL:HG12	2:B:111:LEU:HG	1.94	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
1:A:32:ARG:HD3	3:A:305:HOH:O	2.13	0.49
2:B:126:SER:HB2	3:B:303:HOH:O	2.13	0.49
1:A:213:LEU:HD23	3:A:290:HOH:O	2.13	0.49
2:L:112:LYS:HB3	3:L:273:HOH:O	2.12	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:B:120:VAL:N	3:B:282:HOH:O	2.46	0.48
2:L:129:GLN:HG2	2:L:134:GLY:O	2.14	0.48
2:L:16:GLY:N	3:L:290:HOH:O	2.46	0.48
2:L:204:LYS:CA	2:L:204:LYS:HE2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:141:LEU:CD2	2:L:151:VAL:HG22	2.43	0.48
2:L:6:GLN:HE22	2:L:92:TYR:HA	1.79	0.48
2:B:74:THR:HB	3:B:290:HOH:O	2.13	0.48
1:A:167:HIS:HE1	2:B:143:ASN:OD1	1.96	0.48
2:L:200:GLU:HG3	3:L:227:HOH:O	2.12	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:B:138:VAL:HB	3:B:254:HOH:O	2.15	0.47
2:B:136:SER:HB3	2:B:185:THR:HG22	1.96	0.47
2:L:96:ASN:HD22	2:L:96:ASN:N	2.06	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:103:ARG:NH1	3:H:258:HOH:O	2.47	0.47
1:H:183:SER:HB3	2:L:140:PHE:CE2	2.50	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:B:66:ARG:HA	2:B:81:ASN:HD21	1.81	0.46
2:L:180:MET:CE	2:L:182:SER:HB2	2.46	0.46
2:L:140:PHE:HB3	2:L:142:ASN:ND2	2.30	0.46
2:L:83:VAL:CG1	2:L:111:LEU:HD11	2.45	0.46
1:A:151:GLU:HB2	1:A:178:TYR:CE2	2.50	0.46
2:B:110:GLU:HG3	3:B:256:HOH:O	2.16	0.46
1:H:46:ARG:NH1	2:L:105:ALA:HB2	2.30	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:206:SER:C	2:B:208:SER:H	2.20	0.45
2:B:6:GLN:HE22	2:B:92:TYR:HA	1.82	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
1:A:82:LEU:HD13	1:A:84:MET:CG	2.47	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
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:141:LEU:HD21	2:B:151:VAL:HG22	1.98	0.44
2:B:142:ASN:N	3:B:282:HOH:O	2.45	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:B:151:VAL:HA	2:B:200:GLU:O	2.18	0.44
2:L:210:ILE:C	3:L:227:HOH:O	2.55	0.44
2:L:61:SER:HB2	3:L:256:HOH:O	2.17	0.44
1:A:170:PRO:HB2	3:B:275:HOH:O	2.18	0.44
2:L:155:ILE:O	2:L:155:ILE:HG13	2.17	0.44
2:L:50:GLN:HG2	3:L:268:HOH:O	2.18	0.44
2:L:97:LEU:HG	2:L:98:GLU:HG3	1.99	0.44
2:L:180:MET:HG2	2:L:181:SER:N	2.32	0.44
2:L:143:ASN:ND2	3:L:294:HOH:O	2.50	0.44
2:L:67:PHE:HB2	3:L:321:HOH:O	2.17	0.44
2:L:83:VAL:N	3:L:328: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
1:A:78:ASN:ND2	3:A:245:HOH:O	2.47	0.43
2:B:2:ALA:N	3:B:216:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:150:ASN:O	2:L:151:VAL:HB	2.18	0.43
2:L:206:SER:C	2:L:208:SER:H	2.19	0.43
2:L:36:THR:N	3:L:265:HOH:O	2.51	0.43
2:B:12:PRO:CB	3:B:255:HOH:O	2.66	0.43
2:B:206:SER:O	2:B:207:THR:HB	2.18	0.43
2:L:141:LEU:HD21	2:L:151:VAL:HG22	2.00	0.43
1:H:139:VAL:HG23	3:H:233:HOH:O	2.18	0.43
2:L:151:VAL:HA	2:L:200:GLU:O	2.18	0.43
1:A:45:LYS:O	1:A:46:ARG:CB	2.66	0.43
2:B:119:THR:C	3:B:282:HOH:O	2.56	0.43
1:H:172:LEU:HD11	2:L:166:ASN:O	2.18	0.43
2:L:81:ASN:ND2	2:L:81:ASN:C	2.67	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:CD1	2.49	0.43
2:L:206:SER:O	2:L:207:THR:HB	2.18	0.43
2:L:83:VAL:HG11	2:L:111:LEU:HD11	2.00	0.43
1:A:166:VAL:HB	3:A:224:HOH:O	2.17	0.43
1:H:191:TRP:N	1:H:192:PRO:HD2	2.34	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:A:213:LEU:H	1:A:213:LEU:CD1	2.31	0.42
1:H:141:LEU:HD11	1:H:191:TRP:CZ3	2.54	0.42
1:H:136:GLY:HA2	1:H:188:SER:HB2	2.01	0.42
1:H:202:HIS:ND1	1:H:205:SER:CB	2.83	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
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
1:H:167:HIS:CE1	2:L:179:SER:OG	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:99:ARG:HD2	1:H:99:ARG:C	2.40	0.42
2:L:82:THR:HG22	3:L:245:HOH:O	2.18	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
1:H:134:THR:O	1:H:134:THR:HG23	2.19	0.42
2:L:205:THR:HG22	3:L:262:HOH:O	2.19	0.42
1:A:139:VAL:HG22	1:A:140:THR:N	2.35	0.42
1:A:141:LEU:HD11	1:A:191:TRP:CZ3	2.55	0.42
2:B:37:TYR:HB3	2:B:96:ASN:HD22	1.85	0.42
2:L:120:VAL:HA	2:L:140:PHE:O	2.19	0.42
1:A:187:PRO:O	1:A:190:THR:HG22	2.20	0.42
2:B:160:ARG:NH1	3:B:310:HOH:O	2.53	0.42
2:B:147:LYS:HB3	2:B:178:TYR:CD2	2.55	0.42
2:L:151:VAL:HG21	2:L:180:MET:SD	2.59	0.42
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:200:GLU:HG3	2:B:211:VAL:HG12	2.02	0.41
2:L:142:ASN:HB3	2:L:143:ASN:OD1	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:A:136:GLY:HA2	1:A:188:SER:HB2	2.02	0.41
2:B:120:VAL:HA	2:B:140:PHE:O	2.20	0.41
1:H:193:SER:O	1:H:195:THR:OG1	2.36	0.41
1:H:2:ALA:N	3:H:216:HOH:O	2.53	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
1:H:139:VAL:HG22	1:H:140:THR:N	2.35	0.41
2:L:136:SER:HB2	2:L:185:THR:HG22	2.02	0.41
1:A:191:TRP:N	1:A:192:PRO:HD2	2.35	0.41
1:A:130:GLY:HA3	3:A:244:HOH:O	2.20	0.41
1:A:23:THR:HG22	3:A:295:HOH:O	2.21	0.41
1:A:53:ILE:O	1:A:53:ILE:HG23	2.20	0.41
2:L:59:LEU:HD13	3:L:259:HOH:O	2.19	0.41
1:H:187:PRO:O	1:H:190:THR:HG22	2.20	0.41
1:H:140:THR:O	2:L:123:PHE:HZ	2.04	0.41
2:L:162:ASN:ND2	3:L:334:HOH:O	2.53	0.41
2:B:73:GLY:CA	3:B:307:HOH:O	2.57	0.41
2:B:95:GLN:HE22	2:B:98:GLU:H	1.69	0.41
1:H:138:SER:HA	1:H:187:PRO:HA	2.03	0.41
1:H:202:HIS:ND1	1:H:205:SER:HB2	2.35	0.41
2:B:116:ALA:HB1	3:B:263:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:ASN:HB3	2:B:143:ASN:OD1	2.21	0.41
3:A:262:HOH:O	2:B:169:THR:HG21	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:53:ILE:O	1:H:53:ILE:HG23	2.22	0.40
1:H:38:TRP:NE1	1:H:80:LEU:HD13	2.36	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:B:149:ILE:HG22	3:B:337:HOH:O	2.21	0.40
2:L:81:ASN:HA	3:L:218:HOH:O	2.21	0.40
1:A:168:THR:HG23	1:A:180:MET:CE	2.51	0.40
1:A:138:SER:HA	1:A:186:VAL:O	2.22	0.40
2:B:82:THR:O	2:B:82:THR:HG22	2.21	0.40
2:L:18:SER:HA	3:L:328:HOH:O	2.21	0.40
2:L:197:TYR:O	2:L:213:SER:HB2	2.22	0.40
2:L:95:GLN:HE22	2:L:98:GLU:H	1.69	0.40
1:A:149:PHE:HB3	1:A:150:PRO:HD2	2.04	0.40
2:B:136:SER:HB2	2:B:185:THR:HG22	2.03	0.40
2:L:147:LYS:CD	2:L:147:LYS:H	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	3	1
1	H	206/208 (99%)	184 (89%)	14 (7%)	8 (4%)	3	1
2	B	211/213 (99%)	200 (95%)	9 (4%)	2 (1%)	17	12
2	L	211/213 (99%)	200 (95%)	9 (4%)	2 (1%)	17	12
All	All	834/842 (99%)	769 (92%)	45 (5%)	20 (2%)	6	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%)	20	17
1	H	172/172 (100%)	164 (95%)	8 (5%)	26	24
2	B	187/187 (100%)	176 (94%)	11 (6%)	19	16
2	L	187/187 (100%)	178 (95%)	9 (5%)	25	23
All	All	718/718 (100%)	680 (95%)	38 (5%)	22	20

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 (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 carbohydrates 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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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%)	1.30	53 (25%)	0	0	17, 40, 85, 95	0
1	H	208/208 (100%)	1.19	38 (18%)	1	1	23, 45, 84, 96	0
2	B	213/213 (100%)	1.50	75 (35%)	0	0	22, 48, 80, 88	0
2	L	213/213 (100%)	1.12	49 (23%)	0	0	17, 41, 81, 87	0
All	All	842/842 (100%)	1.28	215 (25%)	0	0	17, 45, 82, 96	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	132	GLY	13.6
1	H	134	THR	12.5
1	A	130	GLY	10.3
1	A	134	THR	10.2
1	H	43	PRO	9.0
1	A	43	PRO	8.7
1	A	131	CYS	8.3
1	H	133	ASP	7.8
1	A	127	ALA	7.4
1	H	131	CYS	7.1
1	A	137	SER	7.0
1	H	164	SER	7.0
2	L	195	ASN	6.6
2	L	208	SER	6.5
1	A	132	GLY	6.3
2	L	206	SER	6.3
1	A	135	THR	6.2
1	A	136	GLY	6.1
2	L	207	THR	6.1
2	B	208	SER	6.0
1	H	137	SER	6.0

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Mol	Chain	Res	Type	RSRZ
2	L	209	PRO	6.0
1	A	128	ALA	5.9
1	H	191	TRP	5.8
1	H	129	PRO	5.8
1	A	191	TRP	5.6
1	H	135	THR	5.4
1	A	138	SER	5.4
1	H	136	GLY	5.4
2	B	133	GLY	5.4
2	L	155	ILE	5.2
1	A	192	PRO	5.1
2	B	202	THR	4.9
1	H	161	GLY	4.8
2	B	149	ILE	4.8
2	B	204	LYS	4.8
2	L	156	ASP	4.8
2	B	132	SER	4.8
1	H	175	SER	4.7
1	A	196	VAL	4.7
2	B	205	THR	4.7
2	B	165	LEU	4.6
2	B	46	GLY	4.6
1	A	190	THR	4.6
1	H	192	PRO	4.6
2	B	161	GLN	4.4
2	B	206	SER	4.4
2	B	197	TYR	4.4
1	A	133	ASP	4.4
2	B	141	LEU	4.2
2	L	139	CYS	4.2
1	H	159	SER	4.2
1	H	195	THR	4.1
2	B	163	GLY	4.1
2	B	153	TRP	4.1
2	B	198	THR	4.1
2	B	186	LEU	4.1
1	H	44	GLU	4.0
1	H	76	VAL	4.0
1	A	159	SER	4.0
2	L	211	VAL	4.0
1	H	130	GLY	4.0
2	B	156	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	210	ILE	3.9
2	B	211	VAL	3.9
1	A	157	TRP	3.9
1	A	189	SER	3.8
2	B	159	GLU	3.8
1	A	193	SER	3.8
2	B	158	SER	3.8
2	L	205	THR	3.8
2	L	137	VAL	3.8
2	L	153	TRP	3.8
2	B	199	CYS	3.7
2	B	207	THR	3.7
2	B	130	LEU	3.7
2	L	200	GLU	3.7
2	B	150	ASN	3.7
1	A	141	LEU	3.7
2	L	159	GLU	3.7
2	B	47	GLN	3.6
2	B	193	ARG	3.6
1	A	44	GLU	3.6
2	L	138	VAL	3.6
2	L	61	SER	3.6
2	L	193	ARG	3.5
2	L	131	THR	3.5
1	A	145	VAL	3.5
1	H	193	SER	3.5
2	B	189	ASP	3.5
2	B	122	ILE	3.5
1	A	213	LEU	3.5
1	H	206	GLY	3.5
1	A	197	THR	3.4
1	A	203	PRO	3.4
1	A	186	VAL	3.4
2	L	210	ILE	3.4
2	B	119	THR	3.4
2	L	162	ASN	3.3
2	L	47	GLN	3.3
2	B	209	PRO	3.3
2	L	184	LEU	3.3
2	L	189	ASP	3.3
2	L	197	TYR	3.3
2	B	157	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	L	214	PHE	3.3
1	A	139	VAL	3.3
1	A	166	VAL	3.2
1	A	195	THR	3.1
1	A	150	PRO	3.0
1	H	213	LEU	3.0
2	B	162	ASN	3.0
1	H	45	LYS	3.0
1	A	187	PRO	3.0
2	B	72	SER	3.0
2	B	187	THR	2.9
1	A	45	LYS	2.9
2	B	88	VAL	2.9
2	B	86	GLU	2.9
2	L	46	GLY	2.9
2	B	73	GLY	2.9
1	A	82	LEU	2.9
2	L	52	LEU	2.9
2	B	195	ASN	2.8
2	B	24	ARG	2.8
2	B	137	VAL	2.8
1	H	42	ILE	2.8
2	B	155	ILE	2.8
1	H	190	THR	2.8
2	L	154	LYS	2.8
2	L	196	GLY	2.8
2	B	139	CYS	2.8
1	A	152	SER	2.8
2	B	152	LYS	2.7
2	B	173	SER	2.7
1	H	82	LEU	2.7
2	B	134	GLY	2.7
2	B	148	ASP	2.7
2	B	182	SER	2.7
1	A	143	CYS	2.7
2	B	151	VAL	2.7
1	A	160	GLY	2.7
1	H	118	LYS	2.7
1	A	158	ASN	2.7
1	A	175	SER	2.7
2	B	124	PRO	2.7
2	L	213	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	L	201	ALA	2.7
2	B	203	HIS	2.6
1	A	174	GLN	2.6
1	A	38	TRP	2.6
1	H	174	GLN	2.6
1	H	189	SER	2.6
2	B	174	LYS	2.6
1	A	129	PRO	2.6
2	B	118	PRO	2.6
2	L	120	VAL	2.6
2	B	121	SER	2.5
2	L	204	LYS	2.5
1	H	158	ASN	2.5
1	A	161	GLY	2.5
2	B	111	LEU	2.5
2	B	213	SER	2.5
2	B	175	ASP	2.5
2	B	214	PHE	2.5
2	L	203	HIS	2.5
1	H	196	VAL	2.4
1	H	165	SER	2.4
2	L	190	GLU	2.4
2	B	194	HIS	2.4
1	A	149	PHE	2.4
2	L	141	LEU	2.4
1	A	97	CYS	2.4
2	B	188	LYS	2.4
1	A	155	VAL	2.4
2	L	133	GLY	2.4
2	L	183	THR	2.4
2	B	126	SER	2.4
2	B	131	THR	2.4
2	L	132	SER	2.3
2	L	163	GLY	2.3
2	L	185	THR	2.3
2	B	160	ARG	2.3
2	B	74	THR	2.3
2	B	127	SER	2.3
1	A	177	LEU	2.3
1	A	185	THR	2.3
2	B	164	VAL	2.3
1	A	188	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	138	VAL	2.2
2	L	151	VAL	2.2
2	L	158	SER	2.2
2	L	174	LYS	2.2
2	B	11	ASN	2.2
1	A	20	LEU	2.2
2	L	199	CYS	2.2
2	B	4	LEU	2.2
1	A	96	TYR	2.2
1	H	140	THR	2.2
2	L	186	LEU	2.1
2	B	140	PHE	2.1
2	B	201	ALA	2.1
2	L	148	ASP	2.1
2	B	146	PRO	2.1
1	H	97	CYS	2.1
2	L	130	LEU	2.0
1	H	204	ALA	2.0
1	A	168	THR	2.0
2	B	168	TRP	2.0
1	H	13	LYS	2.0
1	H	203	PRO	2.0
1	H	66	ALA	2.0
1	A	116	ALA	2.0
2	L	144	PHE	2.0
2	B	75	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.