



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:34 am 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

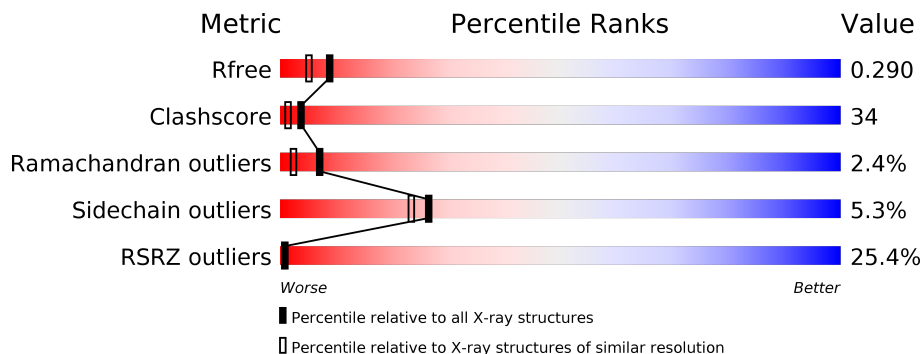
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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}	100719	4988 (2.14-2.10)
Clashscore	112137	5557 (2.14-2.10)
Ramachandran outliers	110173	5504 (2.14-2.10)
Sidechain outliers	110143	5505 (2.14-2.10)
RSRZ outliers	101464	5021 (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 $\leq 5\%$. 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	
1	H	208	
2	B	213	
2	L	213	

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			

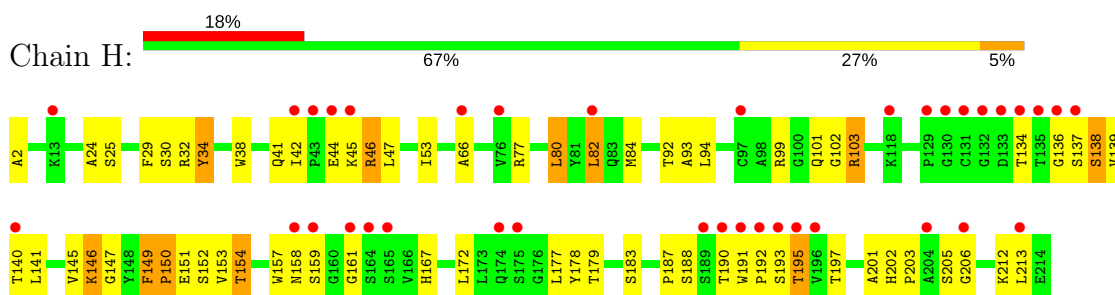
- Molecule 3 is water.

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		

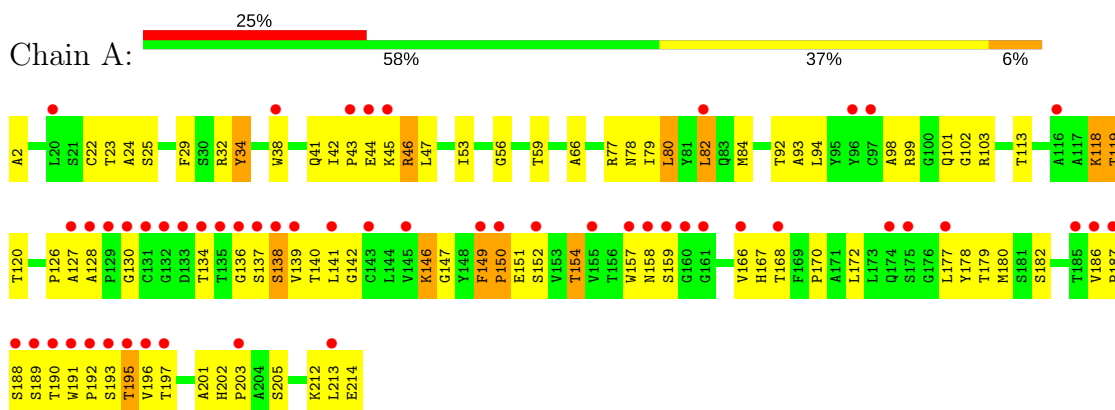
3 Residue-property plots

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.

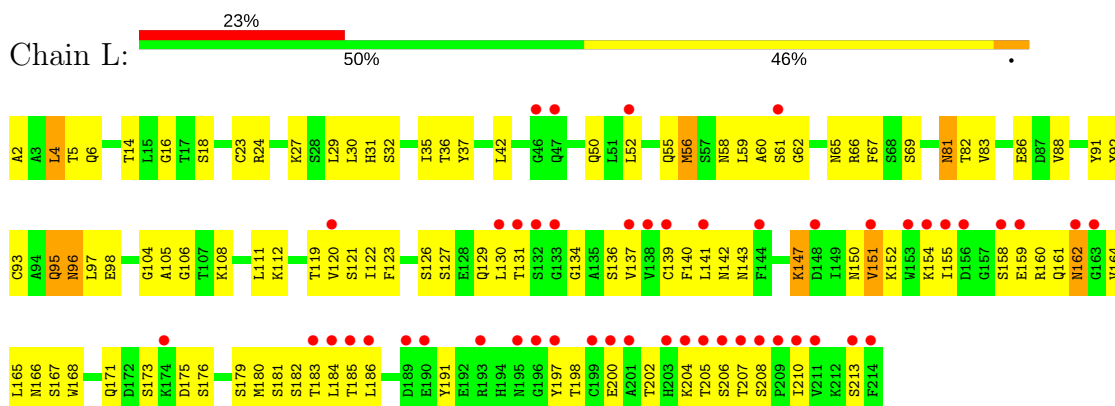
- Molecule 1: antibody 19G2, alpha chain



- Molecule 1: antibody 19G2, alpha chain

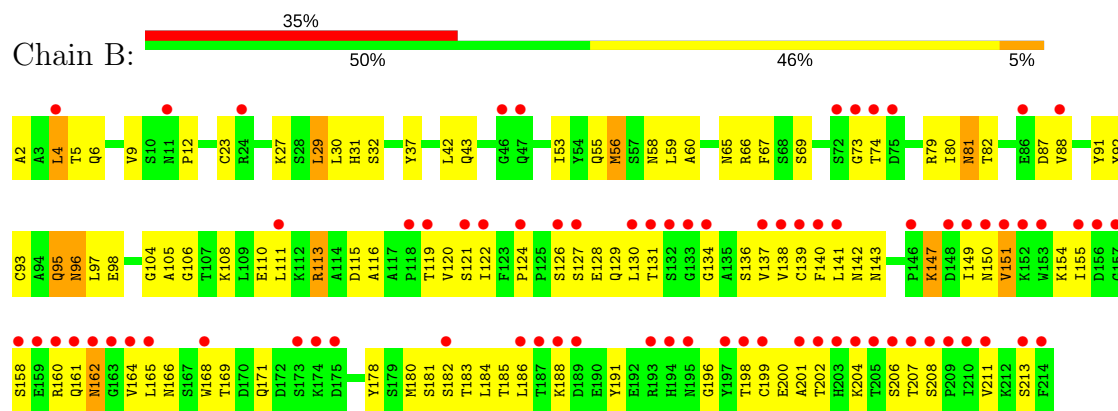


- Molecule 2: antibody 19G2, beta chain



● Molecule 2: antibody 19G2, beta chain

Chain B:



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h-2*1,-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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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%)	20	13
2	L	211/213 (99%)	200 (95%)	9 (4%)	2 (1%)	20	13
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

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%)	23	20
1	H	172/172 (100%)	164 (95%)	8 (5%)	30	28
2	B	187/187 (100%)	176 (94%)	11 (6%)	23	19
2	L	187/187 (100%)	178 (95%)	9 (5%)	30	27
All	All	718/718 (100%)	680 (95%)	38 (5%)	26	23

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, 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%) 1 1	17, 40, 85, 95	0
1	H	208/208 (100%)	1.19	37 (17%) 2 2	23, 45, 84, 96	0
2	B	213/213 (100%)	1.51	75 (35%) 0 0	22, 48, 80, 88	0
2	L	213/213 (100%)	1.13	49 (23%) 1 1	17, 41, 81, 87	0
All	All	842/842 (100%)	1.28	214 (25%) 1 1	17, 45, 82, 96	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	132	GLY	13.7
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	7.9
1	A	127	ALA	7.4
1	H	131	CYS	7.2
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	6.1
1	A	136	GLY	6.1
2	L	207	THR	6.1
1	H	137	SER	6.1
2	B	208	SER	6.1

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Mol	Chain	Res	Type	RSRZ
2	L	209	PRO	6.0
1	A	128	ALA	5.9
1	H	129	PRO	5.8
1	H	191	TRP	5.8
1	A	191	TRP	5.7
1	H	135	THR	5.4
1	H	136	GLY	5.4
2	B	133	GLY	5.4
1	A	138	SER	5.3
2	L	155	ILE	5.2
1	A	192	PRO	5.2
2	B	202	THR	4.9
2	B	149	ILE	4.8
2	L	156	ASP	4.8
2	B	204	LYS	4.8
1	H	161	GLY	4.8
2	B	132	SER	4.8
2	B	205	THR	4.7
1	H	175	SER	4.7
1	A	196	VAL	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	197	TYR	4.4
2	B	161	GLN	4.4
2	B	206	SER	4.4
1	A	133	ASP	4.4
2	B	141	LEU	4.2
2	L	139	CYS	4.2
1	H	195	THR	4.1
1	H	159	SER	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
2	L	211	VAL	4.0
1	A	159	SER	4.0
1	H	130	GLY	4.0
2	B	156	ASP	4.0

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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
2	B	159	GLU	3.8
1	A	189	SER	3.8
2	B	158	SER	3.8
2	L	205	THR	3.8
2	L	137	VAL	3.8
1	A	193	SER	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
1	A	141	LEU	3.7
2	B	150	ASN	3.7
2	L	200	GLU	3.7
2	B	47	GLN	3.6
2	L	159	GLU	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
2	B	189	ASP	3.5
1	A	213	LEU	3.5
1	H	193	SER	3.5
1	H	206	GLY	3.5
2	B	122	ILE	3.4
1	A	197	THR	3.4
1	A	203	PRO	3.4
2	L	210	ILE	3.4
2	L	162	ASN	3.4
2	L	47	GLN	3.3
2	B	119	THR	3.3
1	A	186	VAL	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
2	B	162	ASN	3.0
1	H	213	LEU	3.0
1	A	187	PRO	3.0
1	H	45	LYS	3.0
2	B	72	SER	3.0
2	B	88	VAL	2.9
2	B	187	THR	2.9
1	A	45	LYS	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	24	ARG	2.8
2	B	137	VAL	2.8
1	H	42	ILE	2.8
2	B	195	ASN	2.8
2	B	155	ILE	2.8
1	H	190	THR	2.8
2	L	196	GLY	2.8
2	L	154	LYS	2.8
2	B	139	CYS	2.8
2	B	152	LYS	2.8
1	A	152	SER	2.8
2	B	134	GLY	2.7
1	A	143	CYS	2.7
2	B	173	SER	2.7
2	B	182	SER	2.7
1	H	82	LEU	2.7
2	B	148	ASP	2.7
1	A	160	GLY	2.7
2	B	151	VAL	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	201	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	174	GLN	2.7
2	B	203	HIS	2.7
2	L	213	SER	2.6
1	A	38	TRP	2.6
1	H	174	GLN	2.6
2	B	118	PRO	2.6
2	L	120	VAL	2.6
1	H	189	SER	2.6
2	B	174	LYS	2.6
1	A	129	PRO	2.6
2	B	121	SER	2.6
1	H	158	ASN	2.5
2	L	204	LYS	2.5
1	A	161	GLY	2.5
2	B	111	LEU	2.5
2	L	203	HIS	2.5
2	B	213	SER	2.5
2	B	175	ASP	2.5
2	B	214	PHE	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	97	CYS	2.4
1	A	149	PHE	2.4
2	B	188	LYS	2.4
2	L	141	LEU	2.4
2	B	126	SER	2.4
2	L	132	SER	2.4
2	L	133	GLY	2.4
2	L	183	THR	2.4
2	B	131	THR	2.4
1	A	155	VAL	2.3
2	L	163	GLY	2.3
2	L	185	THR	2.3
2	B	74	THR	2.3
2	B	160	ARG	2.3
2	B	164	VAL	2.3
2	B	127	SER	2.3
1	A	177	LEU	2.2
1	A	185	THR	2.2
1	A	188	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	151	VAL	2.2
2	B	138	VAL	2.2
2	L	174	LYS	2.2
2	L	158	SER	2.2
1	A	20	LEU	2.2
2	L	199	CYS	2.2
2	B	11	ASN	2.2
1	H	140	THR	2.2
2	B	4	LEU	2.2
1	A	96	TYR	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
2	L	130	LEU	2.1
1	A	168	THR	2.1
1	H	97	CYS	2.1
2	B	168	TRP	2.0
1	H	13	LYS	2.0
1	H	66	ALA	2.0
1	H	204	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 ⓘ

There are no such residues in this entry.