



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:03 AM UTC

PDB ID : 1UB6 / pdb_00001ub6
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

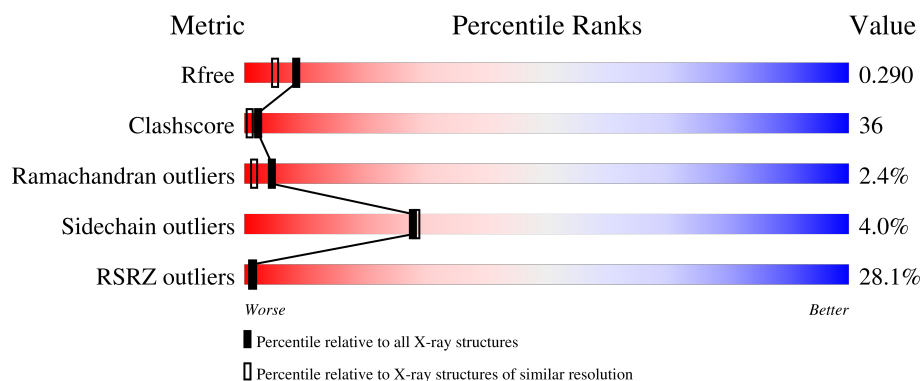
1 Overall quality at a glance

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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	27% 55% 39% 6%
1	H	208	25% 62% 33% 5%
2	B	213	36% 50% 46% .
2	L	213	25% 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			

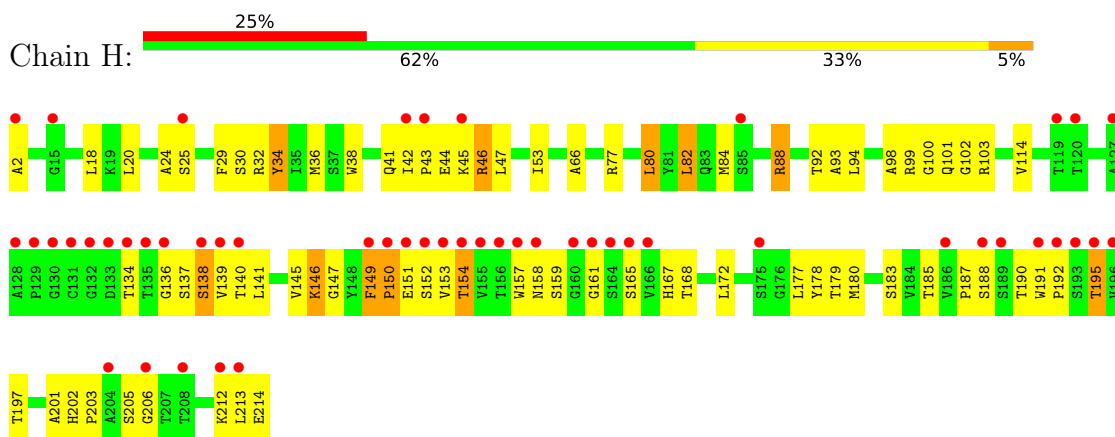
- Molecule 3 is water.

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

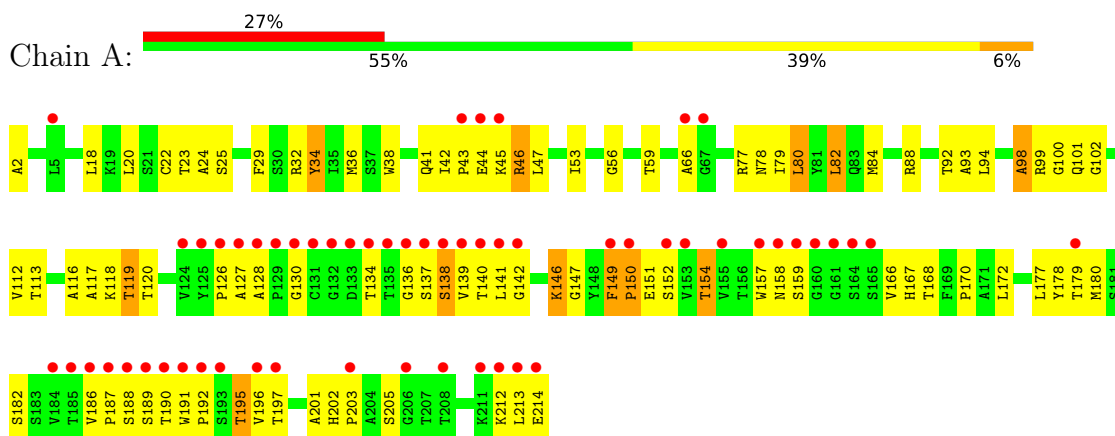
3 Residue-property plots [i](#)

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

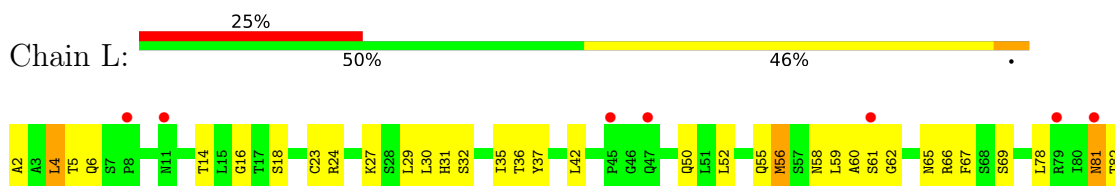
- Molecule 1: antibody 19G2, alpha chain

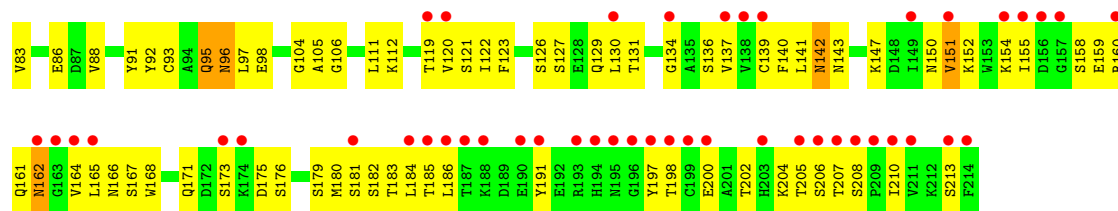


- Molecule 1: antibody 19G2, alpha chain

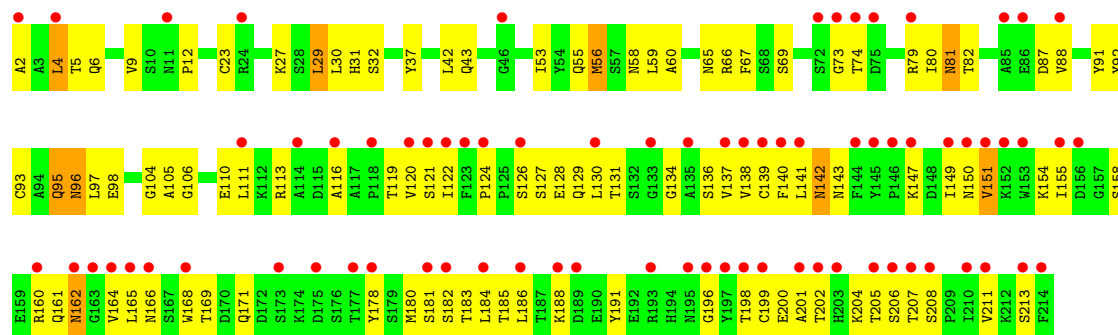


- Molecule 2: antibody 19G2, beta chain





● Molecule 2: antibody 19G2, beta chain



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) 88.8 (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 (4.67%)	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)	0.37 , 74.4	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	0.91	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

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	0.41	0/1579	0.89	4/2155 (0.2%)
1	H	0.38	0/1579	0.87	3/2155 (0.1%)
2	B	0.38	0/1669	0.86	1/2272 (0.0%)
2	L	0.40	0/1669	0.86	2/2272 (0.1%)
All	All	0.39	0/6496	0.87	10/8854 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ALA	N-CA-C	-6.39	105.64	113.50
1	H	98	ALA	N-CA-C	6.28	119.49	108.75
1	A	98	ALA	N-CA-C	6.04	119.33	109.06
1	H	34	TYR	N-CA-C	5.31	116.72	109.18
1	A	34	TYR	N-CA-C	5.25	116.64	109.18
1	H	100	GLY	N-CA-C	5.21	121.12	114.66
1	A	100	GLY	N-CA-C	5.17	121.08	114.66
2	B	142	ASN	N-CA-C	5.06	118.32	110.17
2	L	78	LEU	N-CA-C	-5.05	101.08	109.46
2	L	142	ASN	N-CA-C	5.02	118.25	110.17

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	116	0
1	H	1541	0	1521	83	0
2	B	1632	0	1580	133	0
2	L	1632	0	1580	133	0
3	A	112	0	0	52	0
3	B	125	0	0	55	0
3	H	79	0	0	19	0
3	L	122	0	0	46	0
All	All	6784	0	6202	456	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 36.

All (456) 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
2:L:151:VAL:HG21	2:L:180:MET:HE1	1.68	0.76
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:151:VAL:HG21	2:B:180:MET:HE1	1.68	0.75
2:L:81:ASN:HD22	2:L:81:ASN:C	1.94	0.75
2:B:6:GLN:HB2	3:B:297:HOH:O	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:81:ASN:HD22	2:B:81:ASN:C	1.97	0.72
1:A:20:LEU:HG	1:A:84:MET:HE2	1.70	0.71
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:NH1	2:B:113:ARG:HB2	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
1:H:20:LEU:HG	1:H:84:MET:HE2	1.71	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:137:VAL:CG1	2:L:184:LEU:HB3	2.27	0.65
2:L:167:SER:HB3	3:L:316:HOH:O	1.95	0.65
1:H:141:LEU:HD21	1:H:191:TRP:CZ3	2.30	0.64
1:A:118:LYS:HD2	1:A:118:LYS:N	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:HD22	2:B:96:ASN:H	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
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
1:A:149:PHE:O	1:A:150:PRO:C	2.43	0.61
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:B:151:VAL:HG21	2:B:180:MET:CE	2.30	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:H:34:TYR:HB3	1:H:101:GLN:OE1	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: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
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
2:L:95:GLN:NE2	2:L:97:LEU:H	2.00	0.60
2:L:151:VAL:HG21	2:L:180:MET:CE	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:L:35:ILE:C	3:L:265:HOH:O	2.46	0.57
1:A:214:GLU:HG2	3:A:278:HOH:O	2.03	0.57
1:H:149:PHE:O	1:H:150:PRO:C	2.44	0.57
1:A:213:LEU:HD12	1:A:213:LEU:H	1.69	0.57
2:B:140:PHE:C	2:B:141:LEU:HD12	2.29	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:L:140:PHE:C	2:L:141:LEU:HD12	2.30	0.57
2:B:161:GLN:O	2:B:164:VAL:HG12	2.05	0.57
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:213:LEU:HD12	1:A:213:LEU:N	2.20	0.56
2:L:24:ARG:CZ	3:L:279:HOH:O	2.52	0.56
1:A:167:HIS:HB3	3:A:262:HOH:O	2.04	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:B:164:VAL:C	2:B:165:LEU:HD12	2.30	0.56
2:L:164:VAL:C	2:L:165:LEU:HD12	2.30	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:30:LEU:HD13	2:B:30:LEU:C	2.31	0.55
2:L:30:LEU:C	2:L:30:LEU:HD13	2.32	0.55
1:H:161:GLY:HA2	3:H:266:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:ARG:HD2	2:B:162:ASN:HB3	1.89	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:6:GLN:HE21	2:B:104:GLY:HA3	1.73	0.54
2:B:186:LEU:HD11	2:B:191:TYR:HB2	1.89	0.54
2:B:27:LYS:HE2	2:B:98:GLU:OE1	2.07	0.54
2:B:137:VAL:HG12	2:B:184:LEU:HB3	1.89	0.54
1:A:22:CYS:CB	3:A:301:HOH:O	2.47	0.54
1:A:195:THR:HB	1:A:212:LYS:HE3	1.90	0.54
1:H:42:ILE:HG22	1:H:44:GLU:H	1.73	0.54
2:B:147:LYS:HD3	2:B:147:LYS: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:A:168:THR:HG23	1:A:180:MET:HE1	1.91	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
2:L:6:GLN:HG2	2:L:93:CYS:SG	2.48	0.53
1:A:147:GLY:HA2	1:A:177:LEU:HD13	1.91	0.53
1:A:42:ILE:HG22	1:A:44:GLU:H	1.73	0.53
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: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
1:A:118:LYS:O	1:A:120:THR:HG23	2.08	0.53
2:L:86:GLU:HA	2:L:173:SER:O	2.08	0.53
1:A:149:PHE:O	1:A:178:TYR:HD2	1.92	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
2:L:160:ARG:HD2	2:L:162:ASN:HB3	1.89	0.52
1:A:92:THR:O	1:A:93:ALA:HB2	2.10	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
1:H:149:PHE:O	1:H:178:TYR:HD2	1.92	0.52
1:H:168:THR:HG23	1:H:180:MET:HE1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:5:THR:HG23	3:B:218:HOH:O	2.10	0.52
1:H:206:GLY:HA2	3:H:268:HOH:O	2.11	0.51
2:B:96:ASN:HD22	2:B:96:ASN:N	2.06	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
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: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:B:136:SER:CB	2:B:185:THR:HG22	2.41	0.51
1:A:24:ALA:HB2	1:A:29:PHE:CZ	2.46	0.51
1:A:189:SER:N	3:A:308:HOH:O	2.44	0.51
2:B:201:ALA:HA	3:B:226:HOH:O	2.11	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
1:H:136:GLY:O	1:H:188:SER:HB2	2.12	0.50
2:L:56:MET:HE1	3:L:313:HOH:O	2.11	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:L:152:LYS:HA	3:L:322:HOH:O	2.11	0.50
2:B:129:GLN:HG2	2:B:134:GLY:O	2.12	0.50
2:B:206:SER:C	2:B:208:SER:H	2.20	0.50
1:H:146:LYS:HB3	1:H:179:THR:HG23	1.93	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:A:92:THR:HG23	1:A:113:THR:HA	1.94	0.50
1:H:203:PRO:C	1:H:205:SER:H	2.20	0.49
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:L:204:LYS:HE2	2:L:204:LYS:HA	1.94	0.49
2:B:82:THR:HG22	3:B:244:HOH:O	2.12	0.49
2:B:111:LEU:C	3:B:255:HOH:O	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:55:GLN:HB2	2:L:58:ASN:HD22	1.76	0.49
1:A:203:PRO:C	1:A:205:SER:H	2.21	0.49
2:B:88:VAL:HG12	2:B:111:LEU:HG	1.94	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:HE2	2:B:204:LYS:HA	1.93	0.49
2:L:210:ILE:C	3:L:227:HOH:O	2.55	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
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:H:32:ARG:NE	3:H:240:HOH:O	2.22	0.49
1:A:150:PRO:HG2	1:A:202:HIS:CE1	2.48	0.49
2:B:81:ASN:C	2:B:81:ASN:ND2	2.69	0.49
1:H:102:GLY:HA2	3:H:277:HOH:O	2.13	0.48
1:A:80:LEU:HD12	3:A:239:HOH:O	2.12	0.48
2:B:55:GLN:HB2	2:B:58:ASN:HD22	1.77	0.48
2:L:206:SER:C	2:L:208:SER:H	2.19	0.48
1:A:29:PHE:CD2	1:A:36:MET:HE2	2.48	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:L:129:GLN:HG2	2:L:134:GLY:O	2.14	0.48
2:L:204:LYS:HE2	2:L:204:LYS:CA	2.43	0.48
2:B:120:VAL:N	3:B:282:HOH:O	2.46	0.48
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
1:A:29:PHE:CE2	1:A:36:MET:HE2	2.49	0.48
2:B:74:THR:HB	3:B:290:HOH:O	2.13	0.48
2:B:119:THR:C	3:B:282:HOH:O	2.56	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:81:ASN:C	2:L:81:ASN:ND2	2.67	0.47
2:L:4:LEU:HD12	3:L:250:HOH:O	2.15	0.47
1:A:99:ARG:HD2	1:A:99:ARG:C	2.39	0.47
1:A:119:THR:HG23	3:A:296:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TRP:C	1:A:159:SER:H	2.21	0.47
2:B:141:LEU:HD12	2:B:141:LEU:N	2.29	0.47
2:L:96:ASN:HD22	2:L:96:ASN:N	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:H:99:ARG:HD2	1:H:99:ARG:C	2.40	0.47
2:L:127:SER:O	2:L:131:THR:HG23	2.15	0.47
1:A:46:ARG:HB2	3:B:329:HOH:O	2.14	0.47
1:A:128:ALA:HB2	3:A:290:HOH:O	2.13	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:66:ARG:HA	2:L:81:ASN:HD21	1.80	0.46
2:L:140:PHE:HB3	2:L:142: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:H:151:GLU:HB2	1:H:178:TYR:CE2	2.50	0.46
1:H:157:TRP:C	1:H:159:SER:H	2.22	0.46
1:A:192:PRO:HA	3:A:316:HOH:O	2.15	0.46
1:H:29:PHE:CD2	1:H:36:MET:HE2	2.50	0.46
2:L:180:MET:CE	2:L:182:SER:HB2	2.46	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: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:H:46:ARG:NH1	2:L:105:ALA:HB2	2.30	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: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
2:L:36:THR:CA	3:L:265:HOH:O	2.63	0.45
2:B:42:LEU:HD13	2:B:91:TYR:CZ	2.51	0.45
2:B:140:PHE:HB3	2:B:142:ASN:HD21	1.81	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
1:H:203:PRO:C	1:H:205:SER:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:GLN:HE22	2:B:92:TYR:HA	1.82	0.45
2:B:155:ILE:HG13	2:B:155:ILE:O	2.17	0.45
2:B:140:PHE:HB3	2:B:142:ASN:ND2	2.31	0.45
2:B:168:TRP:CD1	3:B:337:HOH:O	2.70	0.45
2:L:56:MET:O	2:L:69:SER:HB3	2.17	0.45
2:B:97:LEU:HG	2:B:98:GLU:HG3	1.98	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
2:B:56:MET:O	2:B:69:SER:HB3	2.17	0.45
2:B:122:ILE:HG13	2:B:139:CYS:HB3	1.99	0.45
2:L:202:THR:N	3:L:320:HOH:O	2.38	0.45
2:B:126:SER:O	2:B:130:LEU:HG	2.17	0.45
1:H:82:LEU:HD13	1:H:84:MET:CG	2.47	0.44
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
2:L:61:SER:HB2	3:L:256:HOH:O	2.17	0.44
2:B:151:VAL:HA	2:B:200:GLU:O	2.18	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:155:ILE:HG13	2:L:155:ILE:O	2.17	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: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
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
1:H:29:PHE:CE2	1:H:36:MET:HE2	2.53	0.44
2:L:205:THR:C	2:L:207:THR:H	2.26	0.44
2:B:151:VAL:HG21	2:B:180:MET:SD	2.57	0.44
1:H:145:VAL:HG12	3:H:253:HOH:O	2.17	0.44
2:B:183:THR:HG22	2:B:185:THR:HG23	2.00	0.44
1:H:18:LEU:HB3	1:H:84:MET:HE3	2.00	0.43
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
1:A:42:ILE:O	1:A:43:PRO:C	2.61	0.43
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
2:L:141:LEU:HD21	2:L:151:VAL:HG22	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:186:LEU:C	2:L:186:LEU:HD12	2.43	0.43
1:H:172:LEU:HD11	2:L:166:ASN:O	2.18	0.43
1:A:45:LYS:O	1:A:46:ARG:CB	2.66	0.43
2:B:205:THR:C	2:B:207:THR:H	2.26	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
2:B:30:LEU:N	3:B:307:HOH:O	2.50	0.43
2:L:183:THR:HG22	2:L:185:THR:HG23	2.00	0.43
1:A:202:HIS:CE1	3:A:299:HOH:O	2.71	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:H:88:ARG:C	1:H:114:VAL:HG11	2.44	0.43
1:A:118:LYS:N	1:A:118:LYS:CD	2.80	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
2:L:122:ILE:HA	2:L:139:CYS:HB3	2.00	0.42
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
1:A:157:TRP:NE1	3:A:240:HOH:O	2.52	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: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:L:42:LEU:HD13	2:L:91:TYR:CZ	2.53	0.42
1:A:203:PRO:C	1:A:205:SER:N	2.75	0.42
2:B:165:LEU:HD12	2:B:165:LEU:N	2.34	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
2:B:29:LEU:N	3:B:307:HOH:O	2.52	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:HE2	2:B:204:LYS:N	2.34	0.42
1:H:134:THR:HG23	1:H:134:THR:O	2.19	0.42
2:L:205:THR:HG22	3:L:262:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:120:VAL:HA	2:L:140:PHE:O	2.19	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: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:B:160:ARG:NH1	3:B:310:HOH:O	2.53	0.42
2:L:142:ASN:HB3	2:L:143:ASN:OD1	2.20	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:200:GLU:HG3	2:B:211:VAL:HG12	2.02	0.41
1:H:165:SER:HB2	1:H:185:THR:HG1	1.84	0.41
2:B:113:ARG:HH11	2:B:113:ARG:CB	2.28	0.41
1:H:2:ALA:N	3:H:216:HOH:O	2.53	0.41
2:L:204:LYS:HE2	2:L:204:LYS:N	2.35	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
2:B:186:LEU:C	2:B:186:LEU:HD12	2.45	0.41
1:A:84:MET:HE1	1:A:112:VAL:HG21	2.02	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:167:HIS:C	3:A:319:HOH:O	2.62	0.41
1:A:191:TRP:N	1:A:192:PRO:HD2	2.35	0.41
1:H:213:LEU:O	1:H:214:GLU:C	2.64	0.41
2:L:59:LEU:HD13	3:L:259:HOH:O	2.19	0.41
1:A:23:THR:HG22	3:A:295:HOH:O	2.21	0.41
1:A:130:GLY:HA3	3:A:244:HOH:O	2.20	0.41
1:A:139:VAL:HG22	1:A:140:THR:N	2.35	0.41
1:H:187:PRO:O	1:H:190:THR:HG22	2.20	0.41
1:A:213:LEU:O	1:A:214:GLU:C	2.64	0.41
1:H:138:SER:HA	1:H:187:PRO:HA	2.03	0.41
1:H:140:THR:O	2:L:123:PHE:HZ	2.04	0.41
1:H:202:HIS:ND1	1:H:205:SER:HB2	2.35	0.41
2:L:162:ASN:ND2	3:L:334:HOH:O	2.53	0.41
1:A:18:LEU:HB3	1:A:84:MET:HE3	2.02	0.41
1:A:53:ILE:O	1:A:53:ILE:HG23	2.20	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
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

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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
1:H:42:ILE:O	1:H:43:PRO:C	2.62	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:117:ALA:C	1:A:118:LYS:HD2	2.46	0.40
2:L:81:ASN:HA	3:L:218:HOH:O	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:18:SER:HA	3:L:328:HOH:O	2.21	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:138:SER:HA	1:A:186:VAL:O	2.22	0.40
1:A:142:GLY:C	3:A:293:HOH:O	2.64	0.40
1:A:168:THR:HG23	1:A:180:MET:CE	2.51	0.40
2:B:82:THR:HG22	2:B:82:THR:O	2.21	0.40
2:L:147:LYS:H	2:L:147:LYS:CD	2.35	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

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%)	2	0
1	H	206/208 (99%)	184 (89%)	14 (7%)	8 (4%)	2	0
2	B	211/213 (99%)	200 (95%)	9 (4%)	2 (1%)	14	10
2	L	211/213 (99%)	200 (95%)	9 (4%)	2 (1%)	14	10
All	All	834/842 (99%)	769 (92%)	45 (5%)	20 (2%)	4	1

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%)	164 (95%)	8 (5%)	23	23
1	H	172/172 (100%)	165 (96%)	7 (4%)	27	27
2	B	187/187 (100%)	180 (96%)	7 (4%)	30	31
2	L	187/187 (100%)	180 (96%)	7 (4%)	30	31
All	All	718/718 (100%)	689 (96%)	29 (4%)	28	28

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	77	ARG
1	H	80	LEU
1	H	82	LEU
1	H	88	ARG
1	H	94	LEU
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
1	A	77	ARG
1	A	80	LEU
1	A	82	LEU
1	A	88	ARG
1	A	94	LEU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	167	HIS
1	H	174	GLN
2	L	6	GLN
2	L	31	HIS
2	L	43	GLN
2	L	50	GLN
2	L	55	GLN
2	L	58	ASN
2	L	65	ASN
2	L	81	ASN

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Mol	Chain	Res	Type
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	41	GLN
1	A	167	HIS
1	A	174	GLN
2	B	6	GLN
2	B	31	HIS
2	B	43	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	1.26	57 (27%) 1 1	17, 40, 85, 95	0
1	H	208/208 (100%)	1.27	51 (24%) 2 2	23, 45, 84, 96	0
2	B	213/213 (100%)	1.56	76 (35%) 1 1	22, 48, 80, 88	0
2	L	213/213 (100%)	1.16	53 (24%) 2 2	17, 41, 81, 87	0
All	All	842/842 (100%)	1.31	237 (28%) 1 1	17, 45, 82, 96	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	132	GLY	6.3
2	L	195	ASN	6.2
1	A	127	ALA	6.1
2	B	149	ILE	5.9
2	B	72	SER	5.8
1	H	191	TRP	5.7
1	A	191	TRP	5.5
1	A	157	TRP	5.3
1	H	43	PRO	5.1
1	A	43	PRO	5.1
1	H	136	GLY	5.1
1	A	150	PRO	4.9
2	B	198	THR	4.9
2	B	88	VAL	4.7
1	A	141	LEU	4.6
1	A	134	THR	4.6
2	B	73	GLY	4.6
1	A	135	THR	4.5
2	B	199	CYS	4.5
2	L	163	GLY	4.5
1	A	186	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	197	TYR	4.4
1	H	135	THR	4.4
1	A	137	SER	4.3
2	L	174	LYS	4.2
2	B	210	ILE	4.2
2	B	202	THR	4.2
2	L	197	TYR	4.2
2	L	203	HIS	4.2
1	A	149	PHE	4.2
1	A	196	VAL	4.2
1	A	139	VAL	4.2
1	A	136	GLY	4.1
1	A	138	SER	4.1
1	A	132	GLY	4.1
1	H	129	PRO	4.1
1	H	133	ASP	4.0
2	L	213	SER	4.0
2	L	210	ILE	4.0
1	A	190	THR	3.9
1	A	197	THR	3.9
2	L	139	CYS	3.9
1	H	196	VAL	3.8
1	A	142	GLY	3.8
2	L	196	GLY	3.8
1	A	133	ASP	3.8
2	L	214	PHE	3.8
2	L	200	GLU	3.7
1	A	159	SER	3.7
2	B	74	THR	3.7
2	L	162	ASN	3.7
1	A	131	CYS	3.6
1	A	152	SER	3.6
2	L	47	GLN	3.6
2	L	155	ILE	3.6
2	B	146	PRO	3.6
2	B	46	GLY	3.6
2	L	156	ASP	3.6
2	B	123	PHE	3.6
2	B	196	GLY	3.6
2	B	214	PHE	3.6
1	A	129	PRO	3.6
1	H	192	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	173	SER	3.5
1	A	155	VAL	3.5
1	A	45	LYS	3.5
1	A	185	THR	3.5
2	L	209	PRO	3.5
2	B	126	SER	3.5
2	B	189	ASP	3.5
2	L	81	ASN	3.5
1	A	160	GLY	3.4
2	B	205	THR	3.4
2	B	175	ASP	3.4
2	B	166	ASN	3.4
2	L	154	LYS	3.4
2	B	165	LEU	3.4
2	L	190	GLU	3.3
2	L	207	THR	3.3
2	L	61	SER	3.3
2	L	173	SER	3.3
2	L	151	VAL	3.2
2	B	145	TYR	3.2
1	H	119	THR	3.2
1	A	187	PRO	3.2
1	A	158	ASN	3.1
2	L	119	THR	3.1
2	L	185	THR	3.1
2	L	184	LEU	3.1
1	H	139	VAL	3.0
2	B	163	GLY	3.0
1	A	128	ALA	3.0
1	H	213	LEU	3.0
1	H	130	GLY	3.0
1	H	206	GLY	3.0
1	A	130	GLY	3.0
2	L	134	GLY	3.0
1	H	149	PHE	3.0
2	L	193	ARG	2.9
2	L	208	SER	2.9
2	B	213	SER	2.9
2	L	130	LEU	2.9
2	B	195	ASN	2.9
2	B	144	PHE	2.9
2	B	120	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	147	LYS	2.9
1	H	134	THR	2.9
1	H	175	SER	2.9
1	A	66	ALA	2.9
2	L	194	HIS	2.9
2	B	207	THR	2.8
2	B	164	VAL	2.8
2	B	122	ILE	2.8
1	H	151	GLU	2.8
2	B	85	ALA	2.8
2	B	141	LEU	2.8
2	B	138	VAL	2.8
1	H	140	THR	2.8
1	H	212	LYS	2.8
2	B	118	PRO	2.8
1	A	153	VAL	2.8
2	B	133	GLY	2.7
1	H	131	CYS	2.7
2	B	11	ASN	2.7
2	B	86	GLU	2.7
2	B	168	TRP	2.7
1	H	127	ALA	2.7
2	L	205	THR	2.7
1	H	150	PRO	2.7
1	H	42	ILE	2.7
2	L	206	SER	2.7
2	B	181	SER	2.7
1	H	15	GLY	2.7
1	H	161	GLY	2.7
1	H	154	THR	2.7
1	H	195	THR	2.7
2	B	121	SER	2.7
2	B	206	SER	2.7
2	B	75	ASP	2.7
1	H	186	VAL	2.6
2	L	199	CYS	2.6
2	B	162	ASN	2.6
1	A	126	PRO	2.6
1	H	2	ALA	2.6
1	A	211	LYS	2.5
2	B	193	ARG	2.5
2	L	198	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	165	SER	2.5
2	B	130	LEU	2.5
2	B	208	SER	2.5
2	L	165	LEU	2.5
1	A	67	GLY	2.5
1	H	164	SER	2.5
1	H	189	SER	2.5
1	H	208	THR	2.5
1	A	179	THR	2.5
2	B	111	LEU	2.5
2	L	157	GLY	2.5
2	L	149	ILE	2.5
2	B	135	ALA	2.4
1	H	166	VAL	2.4
2	L	120	VAL	2.4
2	L	164	VAL	2.4
1	H	193	SER	2.4
2	B	79	ARG	2.4
2	B	4	LEU	2.4
2	B	186	LEU	2.4
1	H	153	VAL	2.4
2	B	151	VAL	2.4
1	A	189	SER	2.4
2	L	191	TYR	2.4
2	B	114	ALA	2.4
2	B	116	ALA	2.4
2	B	184	LEU	2.4
2	L	137	VAL	2.4
1	H	45	LYS	2.4
1	H	120	THR	2.4
2	L	187	THR	2.4
1	A	161	GLY	2.3
1	A	213	LEU	2.3
2	B	160	ARG	2.3
1	H	157	TRP	2.3
1	A	164	SER	2.3
2	L	181	SER	2.3
2	L	211	VAL	2.3
2	L	160	ARG	2.3
2	B	178	TYR	2.3
1	A	214	GLU	2.2
1	H	25	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	155	ILE	2.2
2	B	137	VAL	2.2
2	L	11	ASN	2.2
2	B	152	LYS	2.2
1	H	204	ALA	2.2
2	L	186	LEU	2.2
1	H	188	SER	2.2
1	A	184	VAL	2.2
1	A	212	LYS	2.2
2	L	188	LYS	2.2
1	A	188	SER	2.2
2	B	153	TRP	2.2
2	B	150	ASN	2.2
2	B	177	THR	2.2
2	B	156	ASP	2.2
1	H	160	GLY	2.2
1	A	193	SER	2.2
2	B	24	ARG	2.2
2	B	182	SER	2.2
1	A	203	PRO	2.1
2	L	8	PRO	2.1
1	A	124	VAL	2.1
2	L	138	VAL	2.1
1	H	128	ALA	2.1
1	A	140	THR	2.1
1	A	192	PRO	2.1
1	A	206	GLY	2.1
2	B	203	HIS	2.1
2	B	211	VAL	2.1
2	B	2	ALA	2.1
2	B	188	LYS	2.1
1	H	85	SER	2.1
1	H	152	SER	2.1
1	A	165	SER	2.1
1	H	156	THR	2.1
2	B	124	PRO	2.1
2	B	201	ALA	2.1
1	H	138	SER	2.1
1	H	158	ASN	2.1
1	A	125	TYR	2.1
2	L	45	PRO	2.1
1	H	155	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	140	PHE	2.1
1	A	44	GLU	2.0
1	A	5	LEU	2.0
2	L	79	ARG	2.0
2	B	139	CYS	2.0
1	A	208	THR	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 oligosaccharides 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.