



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:02 AM UTC

PDB ID : 1BEY / pdb_00001bey
Title : ANTIBODY TO CAMPATH-1H HUMANIZED FAB
Authors : Cheetham, G.M.T.; Hale, G.; Waldmann, H.; Bloomer, A.C.
Deposited on : 1998-05-18
Resolution : 3.25 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

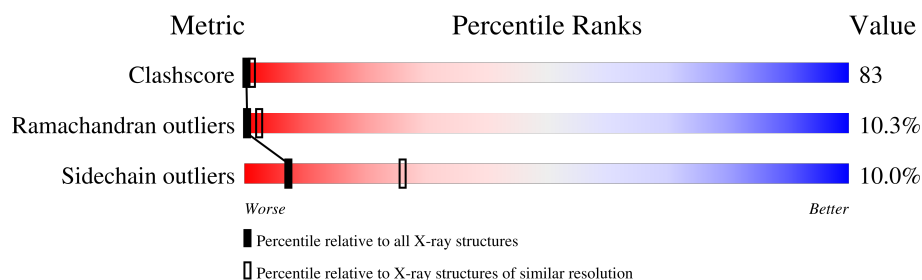
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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))
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	214	24% 51% 21% .
2	H	219	17% 60% 19% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3252 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 CAMPATH-1H ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1658	1034	283	335	6			

- Molecule 2 is a protein called CAMPATH-1H ANTIBODY.

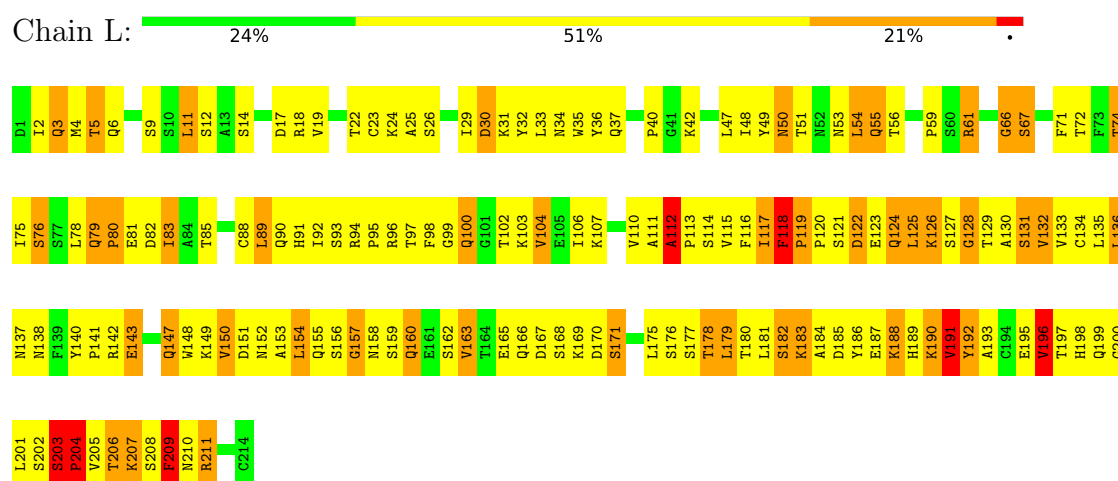
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	210	Total	C	N	O	S	0	0	0
			1594	1014	267	307	6			

3 Residue-property plots

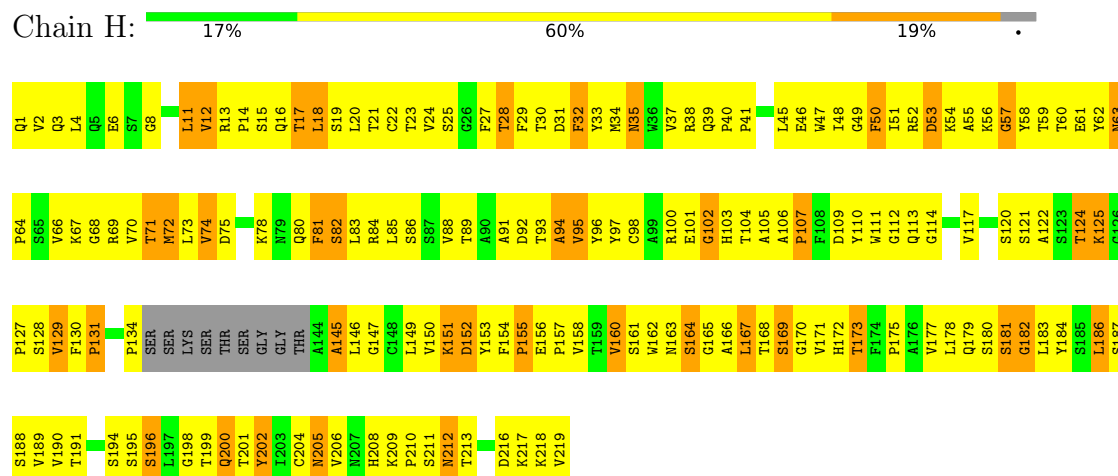
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: CAMPATH-1H ANTIBODY



• Molecule 2: CAMPATH-1H ANTIBODY



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	80.06 Å 80.06 Å 347.25 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 3.25	Depositor
% Data completeness (in resolution range)	90.9 (6.00-3.25)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.306	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3252	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

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	L	0.78	0/1692	1.48	33/2294 (1.4%)
2	H	0.86	1/1635 (0.1%)	1.38	21/2231 (0.9%)
All	All	0.82	1/3327 (0.0%)	1.43	54/4525 (1.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	173	THR	CA-CB	5.17	1.59	1.53

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	112	ALA	CA-C-N	11.13	133.75	119.84
1	L	112	ALA	C-N-CA	11.13	133.75	119.84
2	H	57	GLY	N-CA-C	-11.12	98.19	112.65
1	L	128	GLY	N-CA-C	-10.19	101.81	115.36
1	L	136	LEU	N-CA-C	-9.44	96.26	110.14
1	L	85	THR	N-CA-C	-8.70	93.82	108.26
2	H	95	VAL	N-CA-C	-8.46	95.39	107.75
2	H	199	THR	N-CA-C	-8.43	101.14	112.26
1	L	169	LYS	N-CA-C	-8.17	101.18	112.12
1	L	124	GLN	N-CA-C	-8.11	102.44	111.28
1	L	118	PHE	CB-CA-C	-7.63	103.57	110.44
1	L	79	GLN	CA-C-N	7.55	129.27	119.84
1	L	79	GLN	C-N-CA	7.55	129.27	119.84
1	L	203	SER	CA-C-N	7.40	129.09	119.84
1	L	203	SER	C-N-CA	7.40	129.09	119.84
1	L	83	ILE	CB-CA-C	-6.97	105.41	113.22
2	H	74	VAL	N-CA-C	6.84	118.58	108.45
1	L	61	ARG	N-CA-C	-6.57	105.25	113.20
2	H	32	PHE	N-CA-C	6.53	119.02	108.32
1	L	103	LYS	N-CA-C	-6.52	102.12	110.53
2	H	200	GLN	N-CA-C	6.52	118.94	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	182	GLY	N-CA-C	-6.37	105.89	115.32
2	H	17	THR	N-CA-C	6.33	119.22	108.90
1	L	183	LYS	N-CA-C	6.29	117.99	110.19
2	H	121	SER	N-CA-C	-6.15	106.14	113.21
1	L	207	LYS	N-CA-C	-6.14	98.40	108.41
2	H	151	LYS	N-CA-C	6.07	119.71	109.76
2	H	102	GLY	N-CA-C	6.03	127.47	113.18
1	L	66	GLY	N-CA-C	6.00	121.79	111.47
2	H	181	SER	N-CA-C	-5.96	104.59	112.34
2	H	167	LEU	N-CA-C	5.96	117.91	108.67
1	L	118	PHE	CA-C-N	-5.92	114.28	120.38
1	L	118	PHE	C-N-CA	-5.92	114.28	120.38
1	L	74	THR	N-CA-C	5.80	118.92	109.24
2	H	145	ALA	N-CA-C	5.76	118.96	109.85
2	H	8	GLY	CA-C-N	5.62	125.55	119.76
2	H	8	GLY	C-N-CA	5.62	125.55	119.76
1	L	5	THR	N-CA-C	5.56	117.92	108.02
2	H	82	SER	N-CA-C	5.56	118.08	110.24
2	H	213	THR	N-CA-C	5.48	118.42	109.59
2	H	63	ASN	N-CA-C	-5.47	102.70	109.64
1	L	119	PRO	CA-C-N	5.46	126.67	119.84
1	L	119	PRO	C-N-CA	5.46	126.67	119.84
1	L	190	LYS	N-CA-C	5.46	122.44	110.80
1	L	196	VAL	N-CA-C	5.44	120.66	109.34
1	L	50	ASN	N-CA-C	5.37	118.53	111.28
1	L	178	THR	N-CA-C	5.30	117.85	109.96
2	H	68	GLY	N-CA-C	-5.29	108.19	114.48
1	L	131	SER	N-CA-C	5.28	117.12	108.52
1	L	176	SER	N-CA-C	-5.27	102.19	110.36
2	H	205	ASN	N-CA-C	5.11	116.91	109.71
1	L	42	LYS	N-CA-C	5.10	116.55	109.31
1	L	206	THR	N-CA-C	5.05	116.74	109.07
1	L	162	SER	N-CA-C	-5.01	100.13	110.80

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	L	1658	0	1622	309	0
2	H	1594	0	1569	241	0
All	All	3252	0	3191	533	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 83.

All (533) 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:H:52:ARG:HD2	2:H:56:LYS:HG2	1.25	1.16
1:L:151:ASP:HA	1:L:191:VAL:HG23	1.34	1.07
1:L:187:GLU:HA	1:L:211:ARG:HH12	1.18	1.07
2:H:35:ASN:HB3	2:H:50:PHE:HB3	1.25	1.06
1:L:150:VAL:HG12	1:L:151:ASP:H	1.19	1.03
1:L:29:ILE:O	1:L:92:ILE:HD11	1.60	1.00
1:L:110:VAL:HG11	1:L:200:GLY:HA3	1.39	1.00
2:H:103:HIS:O	2:H:104:THR:HG22	1.62	1.00
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.44	0.99
1:L:89:LEU:HD12	1:L:90:GLN:N	1.78	0.98
2:H:17:THR:HG23	2:H:85:LEU:O	1.64	0.97
1:L:80:PRO:HA	1:L:106:ILE:HD12	1.45	0.96
1:L:29:ILE:C	1:L:92:ILE:HD11	1.91	0.96
1:L:195:GLU:HA	1:L:206:THR:HB	1.48	0.96
1:L:6:GLN:HB2	1:L:100:GLN:HE22	1.31	0.95
2:H:208:HIS:CE1	2:H:210:PRO:HG2	2.03	0.94
2:H:160:VAL:HG23	2:H:206:VAL:HA	1.51	0.92
1:L:55:GLN:HE21	1:L:55:GLN:HA	1.33	0.92
1:L:148:TRP:CE3	1:L:179:LEU:HD12	2.05	0.92
2:H:39:GLN:C	2:H:94:ALA:HB1	1.94	0.91
1:L:134:CYS:HB2	1:L:148:TRP:CZ2	2.07	0.90
1:L:119:PRO:HB3	1:L:209:PHE:CE2	2.06	0.90
2:H:28:THR:HB	2:H:30:THR:HG22	1.54	0.89
1:L:130:ALA:H	1:L:182:SER:HA	1.38	0.88
1:L:151:ASP:HA	1:L:191:VAL:CG2	2.03	0.88
2:H:204:CYS:O	2:H:216:ASP:HA	1.73	0.88
1:L:117:ILE:HG22	1:L:207:LYS:HB3	1.56	0.87
2:H:168:THR:HG22	2:H:169:SER:H	1.38	0.87
1:L:51:THR:HG22	1:L:71:PHE:HE2	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:135:LEU:HD21	2:H:189:VAL:HG11	1.57	0.85
1:L:150:VAL:HG12	1:L:151:ASP:N	1.92	0.85
2:H:127:PRO:HB3	2:H:153:TYR:CD2	2.13	0.84
1:L:150:VAL:HG13	1:L:192:TYR:CE1	2.13	0.83
2:H:201:THR:HA	2:H:218:LYS:NZ	1.94	0.83
1:L:31:LYS:HA	1:L:51:THR:HG21	1.62	0.82
2:H:127:PRO:HB3	2:H:153:TYR:HD2	1.45	0.81
2:H:52:ARG:NH1	2:H:59:THR:OG1	2.13	0.81
2:H:18:LEU:HD22	2:H:20:LEU:CD1	2.10	0.81
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.16	0.81
1:L:83:ILE:HD13	1:L:166:GLN:HB3	1.64	0.80
2:H:52:ARG:CD	2:H:56:LYS:HG2	2.11	0.80
1:L:49:TYR:O	1:L:53:ASN:HB2	1.81	0.80
1:L:31:LYS:HA	1:L:51:THR:CG2	2.11	0.80
2:H:18:LEU:HD11	2:H:117:VAL:HG11	1.63	0.80
2:H:22:CYS:HB3	2:H:81:PHE:HB3	1.64	0.80
1:L:132:VAL:HG12	1:L:148:TRP:CH2	2.17	0.79
1:L:128:GLY:C	1:L:183:LYS:HB2	2.07	0.79
1:L:37:GLN:CB	1:L:47:LEU:HD11	2.12	0.78
1:L:151:ASP:OD1	1:L:191:VAL:HG22	1.82	0.78
1:L:163:VAL:HB	1:L:175:LEU:HB3	1.64	0.78
1:L:208:SER:O	1:L:209:PHE:HB3	1.84	0.78
2:H:33:TYR:CD1	2:H:52:ARG:HA	2.18	0.78
1:L:93:SER:O	1:L:94:ARG:HG3	1.83	0.77
1:L:150:VAL:HG13	1:L:192:TYR:HE1	1.46	0.77
1:L:54:LEU:HD13	1:L:55:GLN:H	1.48	0.77
1:L:80:PRO:O	1:L:168:SER:HA	1.85	0.76
1:L:54:LEU:HD13	1:L:55:GLN:N	2.00	0.76
2:H:219:VAL:HG13	2:H:219:VAL:OXT	1.85	0.76
1:L:11:LEU:HD12	1:L:12:SER:N	2.01	0.75
1:L:34:ASN:OD1	2:H:107:PRO:HD2	1.86	0.75
2:H:35:ASN:HB3	2:H:50:PHE:CB	2.11	0.75
2:H:11:LEU:HD23	2:H:12:VAL:N	2.02	0.75
1:L:119:PRO:HB3	1:L:209:PHE:HE2	1.52	0.74
1:L:6:GLN:H	1:L:100:GLN:HE21	1.36	0.74
1:L:191:VAL:CG1	1:L:210:ASN:HA	2.18	0.74
1:L:24:LYS:HG2	1:L:25:ALA:N	2.03	0.74
1:L:134:CYS:HB2	1:L:148:TRP:HZ2	1.53	0.73
1:L:95:PRO:HD3	2:H:64:PRO:CD	2.17	0.73
1:L:114:SER:O	1:L:136:LEU:HA	1.87	0.73
2:H:160:VAL:HG23	2:H:206:VAL:CA	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2:ILE:HD11	1:L:93:SER:HB2	1.71	0.73
1:L:29:ILE:HA	1:L:92:ILE:CD1	2.19	0.72
2:H:48:ILE:HG23	2:H:66:VAL:HG21	1.69	0.72
1:L:95:PRO:HD3	2:H:64:PRO:HD3	1.70	0.72
1:L:121:SER:O	1:L:123:GLU:N	2.23	0.72
2:H:71:THR:O	2:H:71:THR:HG22	1.90	0.71
1:L:186:TYR:HD1	1:L:192:TYR:HE2	1.37	0.71
1:L:181:LEU:HD21	1:L:185:ASP:OD1	1.90	0.71
2:H:129:VAL:HA	2:H:149:LEU:O	1.90	0.71
1:L:80:PRO:HA	1:L:106:ILE:CD1	2.19	0.71
1:L:22:THR:HG22	1:L:72:THR:HG23	1.71	0.71
1:L:14:SER:HB2	1:L:17:ASP:OD1	1.91	0.71
1:L:89:LEU:HD12	1:L:90:GLN:H	1.53	0.70
2:H:32:PHE:CE1	2:H:102:GLY:HA2	2.26	0.70
2:H:170:GLY:C	2:H:190:VAL:HG23	2.17	0.70
2:H:161:SER:O	2:H:205:ASN:HB2	1.90	0.70
1:L:81:GLU:HA	1:L:168:SER:HB2	1.74	0.70
1:L:154:LEU:HG	1:L:155:GLN:N	2.06	0.70
1:L:55:GLN:HE21	1:L:55:GLN:CA	2.02	0.70
2:H:39:GLN:O	2:H:94:ALA:HB1	1.91	0.69
1:L:136:LEU:HD21	1:L:196:VAL:HG21	1.74	0.69
1:L:51:THR:HG21	1:L:67:SER:HB3	1.75	0.69
2:H:18:LEU:HD23	2:H:19:SER:H	1.58	0.68
1:L:33:LEU:HD13	1:L:71:PHE:CG	2.29	0.68
1:L:133:VAL:HG22	1:L:178:THR:OG1	1.94	0.68
1:L:33:LEU:C	1:L:33:LEU:HD23	2.19	0.68
1:L:191:VAL:HA	1:L:210:ASN:HA	1.75	0.67
1:L:156:SER:O	1:L:158:ASN:N	2.27	0.67
2:H:129:VAL:HG13	2:H:150:VAL:HG22	1.75	0.67
1:L:123:GLU:O	1:L:126:LYS:HB3	1.94	0.67
1:L:191:VAL:HG12	1:L:210:ASN:HA	1.75	0.67
2:H:190:VAL:HG22	2:H:190:VAL:O	1.94	0.67
1:L:55:GLN:HG3	1:L:56:THR:N	2.09	0.67
2:H:11:LEU:HB2	2:H:155:PRO:HG3	1.76	0.67
1:L:96:ARG:NH2	2:H:101:GLU:OE2	2.27	0.66
1:L:29:ILE:HD12	1:L:90:GLN:HB2	1.78	0.66
1:L:137:ASN:HD21	2:H:172:HIS:CD2	2.13	0.66
2:H:38:ARG:NH2	2:H:92:ASP:OD1	2.29	0.66
2:H:18:LEU:HD22	2:H:20:LEU:HD12	1.77	0.66
2:H:145:ALA:HB2	2:H:191:THR:HG22	1.78	0.66
1:L:24:LYS:HG2	1:L:25:ALA:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:19:VAL:HG21	1:L:78:LEU:HD13	1.78	0.66
1:L:33:LEU:HD23	1:L:33:LEU:O	1.95	0.65
2:H:49:GLY:C	2:H:72:MET:HE1	2.22	0.65
1:L:189:HIS:O	1:L:190:LYS:HG3	1.96	0.65
2:H:104:THR:HG23	2:H:105:ALA:N	2.10	0.65
1:L:75:ILE:O	1:L:76:SER:C	2.40	0.65
1:L:22:THR:CG2	1:L:72:THR:HG23	2.27	0.65
1:L:159:SER:O	1:L:160:GLN:HB2	1.96	0.65
1:L:29:ILE:CA	1:L:92:ILE:HD11	2.26	0.65
1:L:118:PHE:CZ	1:L:135:LEU:HD22	2.32	0.65
1:L:121:SER:O	1:L:124:GLN:N	2.29	0.65
1:L:29:ILE:HD11	1:L:90:GLN:HG2	1.78	0.64
2:H:125:LYS:HG3	2:H:153:TYR:HA	1.79	0.64
2:H:180:SER:C	2:H:182:GLY:N	2.54	0.64
1:L:6:GLN:HB2	1:L:100:GLN:NE2	2.07	0.64
2:H:52:ARG:HD2	2:H:56:LYS:CG	2.17	0.64
1:L:125:LEU:HD23	1:L:125:LEU:O	1.97	0.64
2:H:29:PHE:CZ	2:H:80:GLN:O	2.50	0.64
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.33	0.64
1:L:142:ARG:HE	1:L:163:VAL:HG21	1.62	0.63
1:L:187:GLU:HA	1:L:211:ARG:NH1	2.03	0.63
1:L:6:GLN:H	1:L:100:GLN:NE2	1.95	0.63
2:H:17:THR:CG2	2:H:85:LEU:O	2.43	0.63
1:L:163:VAL:CB	1:L:175:LEU:HB3	2.28	0.62
1:L:154:LEU:CD1	1:L:155:GLN:H	2.12	0.62
1:L:154:LEU:HD12	1:L:155:GLN:H	1.65	0.62
2:H:51:ILE:HD11	2:H:58:TYR:HB3	1.80	0.62
1:L:148:TRP:CZ3	1:L:179:LEU:HD12	2.35	0.62
1:L:186:TYR:HB3	1:L:187:GLU:OE1	1.99	0.62
2:H:39:GLN:C	2:H:94:ALA:CB	2.69	0.62
1:L:151:ASP:OD2	1:L:189:HIS:HB3	2.00	0.62
1:L:210:ASN:O	1:L:211:ARG:HB3	2.00	0.62
1:L:29:ILE:HA	1:L:92:ILE:HD12	1.80	0.62
1:L:36:TYR:CE1	1:L:89:LEU:HD23	2.34	0.62
1:L:115:VAL:C	1:L:116:PHE:CD1	2.78	0.62
1:L:158:ASN:HB3	1:L:179:LEU:HD23	1.81	0.62
2:H:164:SER:H	2:H:205:ASN:ND2	1.98	0.62
1:L:117:ILE:CG2	1:L:207:LYS:HB3	2.30	0.61
2:H:18:LEU:CD1	2:H:117:VAL:HG11	2.30	0.61
1:L:118:PHE:HZ	1:L:135:LEU:HD22	1.65	0.61
1:L:125:LEU:HG	1:L:183:LYS:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:150:VAL:HG22	2:H:206:VAL:HG21	1.83	0.61
1:L:50:ASN:O	1:L:51:THR:OG1	2.14	0.61
2:H:6:GLU:OE2	2:H:98:CYS:SG	2.59	0.61
2:H:158:VAL:HG23	2:H:208:HIS:HB2	1.82	0.61
1:L:187:GLU:C	1:L:189:HIS:H	2.08	0.61
2:H:186:LEU:HD12	2:H:186:LEU:C	2.25	0.61
1:L:95:PRO:HB2	2:H:63:ASN:ND2	2.15	0.61
1:L:29:ILE:HA	1:L:92:ILE:HD11	1.82	0.61
1:L:61:ARG:HB2	1:L:76:SER:HB2	1.82	0.61
2:H:38:ARG:HB3	2:H:96:TYR:CE1	2.37	0.60
1:L:186:TYR:HD1	1:L:192:TYR:CE2	2.19	0.60
1:L:187:GLU:O	1:L:189:HIS:N	2.35	0.60
2:H:201:THR:HA	2:H:218:LYS:HZ1	1.67	0.60
2:H:18:LEU:HD22	2:H:20:LEU:HD11	1.82	0.60
2:H:63:ASN:OD1	2:H:64:PRO:HD2	2.02	0.60
2:H:104:THR:CG2	2:H:105:ALA:N	2.65	0.60
2:H:204:CYS:HB3	2:H:217:LYS:O	2.02	0.59
2:H:27:PHE:CZ	2:H:100:ARG:HG3	2.36	0.59
2:H:179:GLN:O	2:H:182:GLY:N	2.30	0.59
1:L:115:VAL:HA	1:L:135:LEU:O	2.02	0.59
1:L:132:VAL:HG12	1:L:148:TRP:HH2	1.65	0.59
1:L:55:GLN:HG3	1:L:56:THR:O	2.02	0.59
2:H:103:HIS:O	2:H:104:THR:CG2	2.44	0.59
2:H:66:VAL:O	2:H:67:LYS:C	2.46	0.59
2:H:153:TYR:C	2:H:153:TYR:CD1	2.81	0.59
2:H:201:THR:HA	2:H:218:LYS:HZ2	1.68	0.59
1:L:187:GLU:OE1	1:L:187:GLU:N	2.36	0.58
1:L:154:LEU:CG	1:L:155:GLN:N	2.66	0.58
2:H:32:PHE:HE1	2:H:102:GLY:HA2	1.65	0.58
1:L:36:TYR:CD1	1:L:36:TYR:N	2.71	0.58
1:L:132:VAL:N	1:L:179:LEU:O	2.36	0.58
2:H:48:ILE:CG2	2:H:70:VAL:HG11	2.33	0.58
2:H:171:VAL:HG22	2:H:190:VAL:HB	1.84	0.58
1:L:93:SER:C	1:L:94:ARG:HG3	2.29	0.58
1:L:128:GLY:O	1:L:183:LYS:HB2	2.02	0.58
1:L:29:ILE:HD12	1:L:90:GLN:CB	2.33	0.58
2:H:168:THR:O	2:H:169:SER:C	2.47	0.58
1:L:91:HIS:N	1:L:91:HIS:ND1	2.52	0.58
1:L:118:PHE:CD1	1:L:118:PHE:N	2.71	0.58
1:L:198:HIS:ND1	1:L:199:GLN:N	2.51	0.58
1:L:209:PHE:C	1:L:211:ARG:H	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:116:PHE:O	1:L:118:PHE:CD1	2.56	0.57
1:L:154:LEU:CG	1:L:155:GLN:H	2.17	0.57
2:H:18:LEU:CD2	2:H:20:LEU:HD11	2.34	0.57
2:H:29:PHE:CE1	2:H:34:MET:HG3	2.40	0.57
1:L:135:LEU:CD2	2:H:189:VAL:HG11	2.30	0.57
1:L:130:ALA:N	1:L:182:SER:HA	2.14	0.57
2:H:200:GLN:HG2	2:H:201:THR:N	2.20	0.57
1:L:9:SER:O	1:L:102:THR:HA	2.05	0.57
1:L:35:TRP:C	1:L:36:TYR:CD1	2.82	0.57
2:H:2:VAL:HG11	2:H:27:PHE:HD2	1.70	0.57
1:L:191:VAL:O	1:L:192:TYR:C	2.48	0.57
2:H:33:TYR:CE1	2:H:52:ARG:HB3	2.40	0.57
2:H:52:ARG:O	2:H:58:TYR:HA	2.04	0.57
2:H:33:TYR:HE1	2:H:52:ARG:HB3	1.70	0.57
2:H:167:LEU:HD21	2:H:190:VAL:HG21	1.87	0.57
1:L:35:TRP:CH2	1:L:88:CYS:HB3	2.39	0.57
1:L:125:LEU:HG	1:L:183:LYS:CD	2.35	0.57
1:L:196:VAL:HG22	1:L:196:VAL:O	2.05	0.56
2:H:83:LEU:HD12	2:H:84:ARG:N	2.20	0.56
2:H:180:SER:C	2:H:182:GLY:H	2.12	0.56
1:L:6:GLN:N	1:L:100:GLN:NE2	2.53	0.56
1:L:94:ARG:HA	1:L:95:PRO:C	2.29	0.56
1:L:156:SER:OG	1:L:157:GLY:N	2.37	0.56
1:L:30:ASP:O	1:L:67:SER:HB2	2.06	0.56
2:H:120:SER:C	2:H:122:ALA:H	2.13	0.56
2:H:35:ASN:HA	2:H:50:PHE:HA	1.88	0.56
2:H:146:LEU:HD11	2:H:202:TYR:CD2	2.40	0.56
2:H:161:SER:O	2:H:205:ASN:ND2	2.34	0.56
1:L:93:SER:O	1:L:94:ARG:CG	2.53	0.56
2:H:24:VAL:CG1	2:H:25:SER:N	2.69	0.56
2:H:24:VAL:HG12	2:H:25:SER:N	2.21	0.56
1:L:166:GLN:HG2	1:L:171:SER:HA	1.88	0.55
1:L:188:LYS:C	1:L:189:HIS:ND1	2.65	0.55
2:H:18:LEU:HD21	2:H:117:VAL:HG11	1.88	0.55
2:H:153:TYR:O	2:H:154:PHE:HB2	2.05	0.55
2:H:200:GLN:CG	2:H:201:THR:H	2.20	0.55
1:L:153:ALA:O	1:L:154:LEU:HB2	2.07	0.55
2:H:33:TYR:HD1	2:H:52:ARG:HA	1.66	0.55
1:L:40:PRO:HB3	1:L:165:GLU:HG3	1.89	0.55
1:L:193:ALA:HB1	1:L:208:SER:HB3	1.88	0.55
2:H:4:LEU:O	2:H:112:GLY:HA2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:29:ILE:HG21	1:L:33:LEU:HB2	1.88	0.55
2:H:18:LEU:HB2	2:H:88:VAL:HG11	1.89	0.55
2:H:200:GLN:CG	2:H:201:THR:N	2.69	0.55
2:H:40:PRO:HA	2:H:94:ALA:HA	1.88	0.54
1:L:55:GLN:CG	1:L:56:THR:N	2.69	0.54
1:L:79:GLN:C	1:L:81:GLU:H	2.15	0.54
1:L:184:ALA:N	1:L:187:GLU:OE2	2.41	0.54
1:L:31:LYS:C	1:L:51:THR:HG23	2.32	0.54
1:L:112:ALA:HB1	1:L:201:LEU:HB2	1.88	0.54
2:H:18:LEU:CG	2:H:117:VAL:HG11	2.38	0.54
2:H:168:THR:HG22	2:H:169:SER:N	2.16	0.54
2:H:149:LEU:HD12	2:H:187:SER:HB3	1.90	0.54
2:H:160:VAL:HG11	2:H:188:SER:CB	2.37	0.54
1:L:6:GLN:HE21	1:L:99:GLY:HA3	1.73	0.54
1:L:61:ARG:HA	1:L:76:SER:OG	2.08	0.54
1:L:154:LEU:CD1	1:L:156:SER:H	2.21	0.54
2:H:164:SER:H	2:H:205:ASN:HD21	1.54	0.54
1:L:18:ARG:HH12	1:L:74:THR:HG21	1.72	0.54
1:L:83:ILE:HD13	1:L:166:GLN:CB	2.37	0.54
2:H:129:VAL:CG1	2:H:206:VAL:HG21	2.37	0.54
1:L:89:LEU:HD22	1:L:98:PHE:CZ	2.43	0.54
1:L:154:LEU:HG	1:L:156:SER:H	1.73	0.54
1:L:143:GLU:N	1:L:143:GLU:OE1	2.40	0.53
2:H:18:LEU:HB2	2:H:88:VAL:CG1	2.38	0.53
2:H:50:PHE:CD1	2:H:50:PHE:C	2.85	0.53
1:L:6:GLN:CB	1:L:100:GLN:HE22	2.11	0.53
1:L:22:THR:HG22	1:L:72:THR:CG2	2.38	0.53
1:L:140:TYR:HA	1:L:141:PRO:O	2.08	0.53
2:H:19:SER:C	2:H:20:LEU:HD12	2.34	0.53
1:L:111:ALA:O	1:L:112:ALA:C	2.52	0.53
1:L:150:VAL:HA	1:L:192:TYR:HD1	1.71	0.53
1:L:131:SER:HA	1:L:180:THR:HA	1.91	0.53
1:L:67:SER:HA	1:L:71:PHE:CE2	2.44	0.53
1:L:83:ILE:HG21	1:L:166:GLN:HB3	1.91	0.53
1:L:110:VAL:CG1	1:L:200:GLY:HA3	2.26	0.53
2:H:128:SER:O	2:H:151:LYS:N	2.28	0.53
2:H:155:PRO:HG2	2:H:210:PRO:HB3	1.91	0.53
2:H:50:PHE:C	2:H:50:PHE:HD1	2.17	0.52
1:L:189:HIS:O	1:L:190:LYS:CG	2.57	0.52
1:L:208:SER:O	1:L:209:PHE:CB	2.55	0.52
1:L:32:TYR:CD1	1:L:32:TYR:N	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:182:GLY:O	2:H:183:LEU:HD23	2.10	0.52
1:L:31:LYS:HA	1:L:51:THR:HG23	1.90	0.52
1:L:110:VAL:HG11	1:L:200:GLY:CA	2.27	0.52
1:L:170:ASP:O	1:L:171:SER:HB2	2.10	0.52
2:H:18:LEU:HD23	2:H:19:SER:N	2.24	0.52
2:H:162:TRP:CD1	2:H:162:TRP:N	2.76	0.52
1:L:29:ILE:O	1:L:92:ILE:CD1	2.47	0.52
1:L:121:SER:O	1:L:122:ASP:C	2.53	0.52
1:L:150:VAL:HG11	1:L:189:HIS:CD2	2.45	0.52
2:H:127:PRO:CB	2:H:153:TYR:HD2	2.20	0.52
2:H:204:CYS:CB	2:H:217:LYS:O	2.57	0.52
1:L:150:VAL:CG1	1:L:151:ASP:N	2.65	0.52
2:H:83:LEU:HD12	2:H:84:ARG:H	1.75	0.52
1:L:136:LEU:HD21	1:L:196:VAL:CG2	2.39	0.51
1:L:190:LYS:O	1:L:210:ASN:HA	2.10	0.51
2:H:146:LEU:HD22	2:H:219:VAL:HG22	1.92	0.51
1:L:6:GLN:HA	1:L:23:CYS:CB	2.40	0.51
1:L:125:LEU:HD23	1:L:183:LYS:HZ3	1.75	0.51
2:H:171:VAL:HA	2:H:190:VAL:HB	1.92	0.51
1:L:51:THR:HG22	1:L:71:PHE:CE2	2.31	0.51
1:L:132:VAL:HG12	1:L:132:VAL:O	2.10	0.51
2:H:38:ARG:HD2	2:H:46:GLU:OE1	2.11	0.51
2:H:48:ILE:HG21	2:H:70:VAL:HG11	1.92	0.51
2:H:13:ARG:O	2:H:14:PRO:C	2.51	0.51
2:H:28:THR:CB	2:H:30:THR:HG22	2.33	0.51
1:L:125:LEU:O	1:L:125:LEU:CD2	2.59	0.51
2:H:100:ARG:NH2	2:H:110:TYR:CG	2.79	0.51
2:H:153:TYR:C	2:H:153:TYR:HD1	2.17	0.51
2:H:211:SER:O	2:H:212:ASN:HB2	2.10	0.51
1:L:2:ILE:O	1:L:3:GLN:C	2.54	0.51
2:H:13:ARG:HB2	2:H:16:GLN:HG2	1.93	0.51
2:H:62:TYR:CD1	2:H:72:MET:HE3	2.45	0.51
2:H:104:THR:CG2	2:H:105:ALA:H	2.24	0.51
1:L:47:LEU:O	1:L:48:ILE:HG13	2.11	0.51
1:L:132:VAL:CG1	1:L:148:TRP:CH2	2.90	0.51
2:H:103:HIS:O	2:H:105:ALA:N	2.39	0.51
1:L:151:ASP:OD1	1:L:191:VAL:CG2	2.55	0.51
1:L:134:CYS:HB3	1:L:177:SER:HB3	1.94	0.50
1:L:150:VAL:O	1:L:152:ASN:N	2.42	0.50
1:L:34:ASN:ND2	1:L:50:ASN:H	2.10	0.50
1:L:110:VAL:HG13	1:L:140:TYR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:154:LEU:HG	1:L:155:GLN:H	1.71	0.50
1:L:181:LEU:O	1:L:182:SER:O	2.30	0.50
2:H:146:LEU:HD22	2:H:219:VAL:CG2	2.40	0.50
1:L:47:LEU:C	1:L:48:ILE:HG13	2.36	0.50
1:L:79:GLN:O	1:L:82:ASP:N	2.43	0.50
2:H:72:MET:O	2:H:73:LEU:HB3	2.12	0.50
1:L:133:VAL:HA	1:L:178:THR:HA	1.94	0.50
2:H:18:LEU:CD1	2:H:96:TYR:HE2	2.25	0.50
1:L:94:ARG:HH11	2:H:61:GLU:CD	2.19	0.49
2:H:29:PHE:HZ	2:H:80:GLN:O	1.95	0.49
1:L:90:GLN:CD	1:L:90:GLN:C	2.79	0.49
1:L:31:LYS:HG2	1:L:32:TYR:CE1	2.47	0.49
1:L:79:GLN:O	1:L:81:GLU:N	2.45	0.49
1:L:31:LYS:O	1:L:50:ASN:HA	2.12	0.49
1:L:191:VAL:HG12	1:L:210:ASN:CA	2.41	0.49
2:H:93:THR:O	2:H:94:ALA:HB2	2.13	0.49
1:L:29:ILE:CD1	1:L:90:GLN:HG2	2.43	0.49
1:L:138:ASN:HD21	2:H:172:HIS:CE1	2.31	0.49
1:L:196:VAL:HG13	1:L:205:VAL:O	2.13	0.49
2:H:34:MET:HB3	2:H:81:PHE:CZ	2.48	0.48
2:H:134:PRO:HB3	2:H:145:ALA:O	2.12	0.48
1:L:95:PRO:HB3	2:H:63:ASN:CG	2.38	0.48
2:H:134:PRO:HD3	2:H:146:LEU:HD23	1.95	0.48
2:H:157:PRO:HD2	2:H:157:PRO:O	2.14	0.48
2:H:124:THR:O	2:H:125:LYS:HB2	2.13	0.48
1:L:14:SER:HB2	1:L:17:ASP:CG	2.39	0.48
1:L:125:LEU:CD2	1:L:183:LYS:NZ	2.76	0.48
2:H:201:THR:CA	2:H:218:LYS:HZ2	2.26	0.48
2:H:208:HIS:NE2	2:H:210:PRO:HG2	2.27	0.48
2:H:73:LEU:N	2:H:73:LEU:HD23	2.29	0.48
1:L:112:ALA:CB	1:L:201:LEU:HB2	2.43	0.48
1:L:22:THR:HG22	1:L:72:THR:OG1	2.14	0.47
2:H:152:ASP:OD1	2:H:179:GLN:NE2	2.47	0.47
1:L:66:GLY:O	1:L:67:SER:CB	2.62	0.47
1:L:118:PHE:HD1	1:L:118:PHE:H	1.62	0.47
1:L:125:LEU:CG	1:L:183:LYS:HD3	2.44	0.47
1:L:115:VAL:HG12	1:L:116:PHE:N	2.28	0.47
1:L:134:CYS:O	1:L:177:SER:N	2.48	0.47
1:L:187:GLU:C	1:L:189:HIS:N	2.68	0.47
2:H:33:TYR:CE1	2:H:52:ARG:CB	2.97	0.47
1:L:156:SER:O	1:L:157:GLY:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:THR:HG23	2:H:86:SER:HA	1.96	0.47
2:H:211:SER:O	2:H:212:ASN:CB	2.63	0.47
1:L:55:GLN:CA	1:L:55:GLN:NE2	2.76	0.47
1:L:114:SER:O	1:L:136:LEU:CA	2.59	0.47
1:L:50:ASN:C	1:L:51:THR:HG1	2.15	0.47
1:L:137:ASN:HD21	2:H:172:HIS:HD2	1.60	0.47
1:L:193:ALA:CB	1:L:208:SER:HB3	2.45	0.47
2:H:35:ASN:HD21	2:H:101:GLU:HB2	1.80	0.47
2:H:37:VAL:HB	2:H:97:TYR:HB2	1.95	0.47
2:H:56:LYS:C	2:H:57:GLY:O	2.51	0.47
1:L:186:TYR:O	1:L:211:ARG:NH1	2.48	0.47
1:L:33:LEU:HD23	1:L:34:ASN:O	2.15	0.47
2:H:145:ALA:HA	2:H:191:THR:HA	1.97	0.47
2:H:160:VAL:CG2	2:H:206:VAL:HG22	2.45	0.47
1:L:95:PRO:CB	2:H:63:ASN:ND2	2.78	0.46
1:L:112:ALA:HB1	1:L:201:LEU:HD22	1.97	0.46
2:H:162:TRP:CD1	2:H:162:TRP:H	2.33	0.46
2:H:177:VAL:O	2:H:184:TYR:HA	2.15	0.46
1:L:118:PHE:O	1:L:119:PRO:C	2.58	0.46
2:H:204:CYS:N	2:H:217:LYS:O	2.49	0.46
1:L:61:ARG:O	1:L:75:ILE:HA	2.15	0.46
1:L:138:ASN:N	1:L:138:ASN:HD22	2.13	0.46
1:L:160:GLN:OE1	2:H:177:VAL:HG21	2.15	0.46
2:H:211:SER:OG	2:H:212:ASN:N	2.49	0.46
2:H:34:MET:O	2:H:51:ILE:HG22	2.15	0.46
2:H:147:GLY:HA2	2:H:189:VAL:HA	1.98	0.46
1:L:120:PRO:HG3	1:L:132:VAL:CG2	2.46	0.46
2:H:129:VAL:HG11	2:H:206:VAL:HG21	1.98	0.46
1:L:115:VAL:HG21	1:L:196:VAL:HG11	1.96	0.46
2:H:14:PRO:O	2:H:15:SER:HB3	2.14	0.46
2:H:62:TYR:CD2	2:H:70:VAL:HG23	2.51	0.46
2:H:167:LEU:HD21	2:H:190:VAL:CG2	2.46	0.46
2:H:186:LEU:C	2:H:186:LEU:CD1	2.88	0.46
1:L:112:ALA:HB1	1:L:201:LEU:HD13	1.98	0.46
1:L:154:LEU:CG	1:L:156:SER:H	2.29	0.46
2:H:80:GLN:O	2:H:81:PHE:HB2	2.16	0.46
2:H:131:PRO:HD3	2:H:217:LYS:HG2	1.96	0.46
1:L:137:ASN:OD1	1:L:138:ASN:ND2	2.49	0.46
1:L:150:VAL:HG13	1:L:192:TYR:CD1	2.50	0.46
1:L:188:LYS:HB3	1:L:189:HIS:CE1	2.51	0.46
1:L:203:SER:O	1:L:204:PRO:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:62:TYR:CD1	2:H:62:TYR:N	2.81	0.45
1:L:120:PRO:HG3	1:L:132:VAL:HG23	1.97	0.45
2:H:38:ARG:HB3	2:H:96:TYR:CD1	2.52	0.45
2:H:125:LYS:CG	2:H:153:TYR:HA	2.44	0.45
2:H:18:LEU:CD1	2:H:96:TYR:CE2	3.00	0.45
1:L:124:GLN:HA	2:H:130:PHE:CE1	2.50	0.45
2:H:13:ARG:C	2:H:14:PRO:O	2.57	0.45
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.51	0.45
2:H:209:LYS:O	2:H:210:PRO:C	2.60	0.45
1:L:31:LYS:CA	1:L:51:THR:HG23	2.47	0.45
1:L:175:LEU:C	1:L:175:LEU:HD12	2.42	0.45
1:L:54:LEU:HD12	1:L:55:GLN:O	2.17	0.45
1:L:190:LYS:O	1:L:210:ASN:CA	2.64	0.45
2:H:201:THR:CA	2:H:218:LYS:NZ	2.72	0.45
1:L:127:SER:C	1:L:129:THR:H	2.21	0.44
2:H:69:ARG:HH22	2:H:92:ASP:CG	2.25	0.44
2:H:81:PHE:CG	2:H:81:PHE:O	2.70	0.44
1:L:4:MET:SD	1:L:25:ALA:CB	3.06	0.44
2:H:155:PRO:HG2	2:H:210:PRO:CB	2.48	0.44
2:H:163:ASN:O	2:H:165:GLY:N	2.50	0.44
2:H:195:SER:O	2:H:196:SER:HB3	2.17	0.44
1:L:118:PHE:N	1:L:118:PHE:HD1	2.11	0.44
1:L:154:LEU:O	1:L:155:GLN:HG2	2.17	0.44
2:H:51:ILE:HB	2:H:60:THR:HG22	1.98	0.44
2:H:104:THR:C	2:H:106:ALA:N	2.75	0.44
1:L:112:ALA:HA	1:L:113:PRO:HD2	1.47	0.44
2:H:18:LEU:CD2	2:H:20:LEU:CD1	2.87	0.44
2:H:63:ASN:OD1	2:H:64:PRO:CD	2.65	0.44
2:H:73:LEU:C	2:H:74:VAL:HG13	2.43	0.44
2:H:146:LEU:HD11	2:H:202:TYR:CE2	2.52	0.44
1:L:138:ASN:N	1:L:138:ASN:ND2	2.66	0.44
2:H:66:VAL:HG21	2:H:70:VAL:HG11	1.99	0.44
2:H:178:LEU:HD13	2:H:184:TYR:CZ	2.53	0.44
1:L:156:SER:C	1:L:158:ASN:N	2.76	0.44
1:L:196:VAL:CG1	1:L:205:VAL:O	2.66	0.44
2:H:102:GLY:HA3	2:H:109:ASP:OD2	2.18	0.44
2:H:113:GLN:HB2	2:H:114:GLY:H	1.51	0.44
1:L:80:PRO:O	1:L:168:SER:CA	2.61	0.44
1:L:191:VAL:HG13	1:L:210:ASN:HA	1.98	0.44
2:H:52:ARG:HG3	2:H:52:ARG:HH11	1.82	0.44
2:H:165:GLY:O	2:H:167:LEU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:37:VAL:HG21	2:H:111:TRP:CH2	2.53	0.43
2:H:130:PHE:HB2	2:H:149:LEU:HB3	2.01	0.43
2:H:162:TRP:HZ3	2:H:219:VAL:HG11	1.83	0.43
1:L:6:GLN:N	1:L:100:GLN:HE21	2.08	0.43
1:L:6:GLN:HG3	1:L:99:GLY:HA3	2.01	0.43
1:L:106:ILE:H	1:L:166:GLN:NE2	2.17	0.43
2:H:147:GLY:HA3	2:H:189:VAL:HG22	2.00	0.43
2:H:52:ARG:O	2:H:53:ASP:O	2.36	0.43
1:L:32:TYR:HB2	1:L:92:ILE:HG13	2.01	0.43
1:L:75:ILE:O	1:L:75:ILE:HG22	2.18	0.43
1:L:97:THR:C	1:L:98:PHE:HD1	2.26	0.43
1:L:83:ILE:HD12	1:L:167:ASP:O	2.18	0.43
2:H:52:ARG:NH1	2:H:52:ARG:HG3	2.33	0.43
1:L:25:ALA:O	1:L:26:SER:C	2.61	0.43
1:L:163:VAL:HG12	1:L:175:LEU:CB	2.48	0.43
2:H:62:TYR:HE1	2:H:72:MET:HG3	1.83	0.43
1:L:125:LEU:HD23	1:L:183:LYS:NZ	2.34	0.42
1:L:131:SER:HB3	1:L:180:THR:OG1	2.19	0.42
1:L:79:GLN:C	1:L:81:GLU:N	2.76	0.42
1:L:149:LYS:O	1:L:192:TYR:HA	2.19	0.42
2:H:18:LEU:CD2	2:H:19:SER:N	2.81	0.42
2:H:106:ALA:HB1	2:H:107:PRO:HA	2.00	0.42
1:L:94:ARG:NH1	2:H:61:GLU:OE2	2.33	0.42
2:H:30:THR:HG23	2:H:31:ASP:OD1	2.19	0.42
2:H:40:PRO:HA	2:H:93:THR:O	2.18	0.42
1:L:97:THR:C	1:L:98:PHE:CD1	2.98	0.42
1:L:190:LYS:O	1:L:210:ASN:C	2.63	0.42
2:H:209:LYS:N	2:H:210:PRO:HD2	2.34	0.42
1:L:22:THR:HA	1:L:72:THR:HA	2.01	0.42
1:L:153:ALA:O	1:L:154:LEU:CB	2.68	0.42
1:L:183:LYS:C	1:L:185:ASP:H	2.27	0.42
1:L:35:TRP:HB2	1:L:48:ILE:HB	2.01	0.42
2:H:18:LEU:CD2	2:H:117:VAL:HG11	2.49	0.42
2:H:69:ARG:HD2	2:H:86:SER:O	2.19	0.42
2:H:182:GLY:C	2:H:183:LEU:HD23	2.45	0.42
1:L:209:PHE:C	1:L:211:ARG:N	2.76	0.42
2:H:89:THR:O	2:H:91:ALA:N	2.53	0.42
2:H:219:VAL:OXT	2:H:219:VAL:CG1	2.57	0.42
2:H:96:TYR:HD2	2:H:117:VAL:HG21	1.85	0.42
1:L:54:LEU:CD1	1:L:55:GLN:N	2.79	0.42
2:H:22:CYS:SG	2:H:81:PHE:HD2	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:125:LYS:HB3	2:H:154:PHE:N	2.34	0.42
1:L:6:GLN:HA	1:L:23:CYS:HB3	2.01	0.41
2:H:28:THR:HB	2:H:30:THR:CG2	2.38	0.41
2:H:66:VAL:HG23	2:H:70:VAL:CG2	2.49	0.41
2:H:124:THR:HA	2:H:154:PHE:O	2.20	0.41
1:L:89:LEU:CD1	1:L:90:GLN:N	2.67	0.41
1:L:95:PRO:CB	2:H:63:ASN:CG	2.93	0.41
1:L:140:TYR:HA	1:L:141:PRO:C	2.46	0.41
1:L:127:SER:C	1:L:129:THR:N	2.74	0.41
1:L:147:GLN:OE1	1:L:147:GLN:HA	2.19	0.41
2:H:53:ASP:HB2	2:H:54:LYS:H	1.63	0.41
2:H:163:ASN:O	2:H:164:SER:C	2.62	0.41
1:L:55:GLN:CG	1:L:56:THR:H	2.33	0.41
1:L:163:VAL:HG12	1:L:175:LEU:HB2	2.01	0.41
1:L:187:GLU:CA	1:L:211:ARG:HH12	2.09	0.41
2:H:2:VAL:HG12	2:H:3:GLN:N	2.35	0.41
2:H:162:TRP:CZ2	2:H:190:VAL:HG12	2.56	0.41
1:L:33:LEU:HD13	1:L:71:PHE:CD2	2.54	0.41
1:L:90:GLN:CD	1:L:90:GLN:O	2.64	0.41
1:L:210:ASN:O	1:L:211:ARG:CB	2.68	0.41
2:H:11:LEU:HD23	2:H:11:LEU:C	2.46	0.41
1:L:131:SER:HB3	1:L:180:THR:HG23	2.01	0.41
1:L:140:TYR:CD1	1:L:141:PRO:HA	2.56	0.41
1:L:202:SER:O	1:L:203:SER:O	2.38	0.41
1:L:47:LEU:O	1:L:48:ILE:CG1	2.68	0.41
1:L:188:LYS:C	1:L:189:HIS:HD1	2.27	0.41
2:H:55:ALA:C	2:H:57:GLY:H	2.26	0.41
2:H:157:PRO:O	2:H:157:PRO:CD	2.69	0.41
1:L:49:TYR:H	1:L:49:TYR:HD1	1.68	0.41
1:L:180:THR:O	1:L:180:THR:HG22	2.20	0.41
2:H:1:GLN:HB3	2:H:2:VAL:H	1.57	0.41
1:L:4:MET:O	1:L:99:GLY:HA2	2.21	0.41
1:L:107:LYS:HB2	1:L:107:LYS:HE3	1.86	0.41
1:L:115:VAL:O	1:L:116:PHE:CD1	2.74	0.41
1:L:137:ASN:OD1	1:L:138:ASN:CG	2.63	0.41
1:L:191:VAL:HA	1:L:209:PHE:O	2.21	0.41
1:L:208:SER:HB2	1:L:209:PHE:H	1.69	0.41
2:H:21:THR:CG2	2:H:80:GLN:HG2	2.51	0.41
1:L:18:ARG:NH1	1:L:74:THR:HG21	2.34	0.41
1:L:142:ARG:HH21	1:L:163:VAL:HG22	1.85	0.41
2:H:34:MET:HB3	2:H:81:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100:ARG:NH1	2:H:109:ASP:OD1	2.54	0.41
2:H:75:ASP:OD2	2:H:78:LYS:HG3	2.21	0.40
1:L:141:PRO:HB2	1:L:143:GLU:OE1	2.21	0.40
1:L:190:LYS:O	1:L:191:VAL:HG13	2.21	0.40
2:H:13:ARG:HB2	2:H:16:GLN:CG	2.51	0.40
2:H:95:VAL:O	2:H:95:VAL:HG23	2.20	0.40
1:L:126:LYS:HB2	1:L:126:LYS:HE3	1.82	0.40
1:L:184:ALA:HA	1:L:187:GLU:OE2	2.21	0.40
1:L:186:TYR:HA	1:L:192:TYR:OH	2.22	0.40
2:H:66:VAL:HG23	2:H:70:VAL:HG22	2.04	0.40
2:H:120:SER:C	2:H:122:ALA:N	2.77	0.40
2:H:168:THR:CG2	2:H:169:SER:H	2.19	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	L	212/214 (99%)	132 (62%)	54 (26%)	26 (12%)	0	1
2	H	206/219 (94%)	146 (71%)	43 (21%)	17 (8%)	0	4
All	All	418/433 (96%)	278 (66%)	97 (23%)	43 (10%)	0	2

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	67	SER
1	L	122	ASP
1	L	150	VAL
1	L	160	GLN
1	L	204	PRO
1	L	209	PHE

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Mol	Chain	Res	Type
2	H	53	ASP
2	H	81	PHE
2	H	166	ALA
2	H	175	PRO
2	H	196	SER
2	H	212	ASN
1	L	59	PRO
1	L	117	ILE
1	L	157	GLY
1	L	171	SER
1	L	182	SER
1	L	188	LYS
1	L	192	TYR
2	H	94	ALA
2	H	125	LYS
2	H	164	SER
2	H	169	SER
2	H	198	GLY
2	H	202	TYR
1	L	3	GLN
1	L	76	SER
1	L	154	LEU
1	L	30	ASP
1	L	80	PRO
1	L	143	GLU
1	L	211	ARG
1	L	112	ALA
1	L	126	LYS
1	L	196	VAL
1	L	203	SER
2	H	71	THR
2	H	152	ASP
2	H	194	SER
1	L	104	VAL
2	H	124	THR
2	H	131	PRO
1	L	191	VAL

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	L	191/191 (100%)	173 (91%)	18 (9%)	8	29
2	H	180/187 (96%)	161 (89%)	19 (11%)	6	24
All	All	371/378 (98%)	334 (90%)	37 (10%)	7	26

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	11	LEU
1	L	54	LEU
1	L	55	GLN
1	L	89	LEU
1	L	100	GLN
1	L	104	VAL
1	L	118	PHE
1	L	125	LEU
1	L	132	VAL
1	L	147	GLN
1	L	163	VAL
1	L	179	LEU
1	L	191	VAL
1	L	196	VAL
1	L	197	THR
1	L	204	PRO
1	L	209	PHE
2	H	11	LEU
2	H	12	VAL
2	H	18	LEU
2	H	23	THR
2	H	28	THR
2	H	35	ASN
2	H	41	PRO
2	H	45	LEU
2	H	50	PHE
2	H	72	MET
2	H	82	SER
2	H	107	PRO
2	H	129	VAL

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Mol	Chain	Res	Type
2	H	155	PRO
2	H	156	GLU
2	H	160	VAL
2	H	173	THR
2	H	181	SER
2	H	186	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	34	ASN
1	L	37	GLN
1	L	38	GLN
1	L	50	ASN
1	L	53	ASN
1	L	55	GLN
1	L	100	GLN
1	L	124	GLN
1	L	138	ASN
1	L	158	ASN
1	L	166	GLN
2	H	39	GLN
2	H	172	HIS
2	H	205	ASN
2	H	212	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 oligosaccharides 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.