



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:53 PM UTC

PDB ID : 3D69 / pdb_00003d69
Title : Crystal Structure of the Fab Fragment of an Anti-Factor IX Antibody 10C12
Authors : Shi, X.L.; Huang, M.D.; Zeng, T.
Deposited on : 2008-05-19
Resolution : 3.77 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

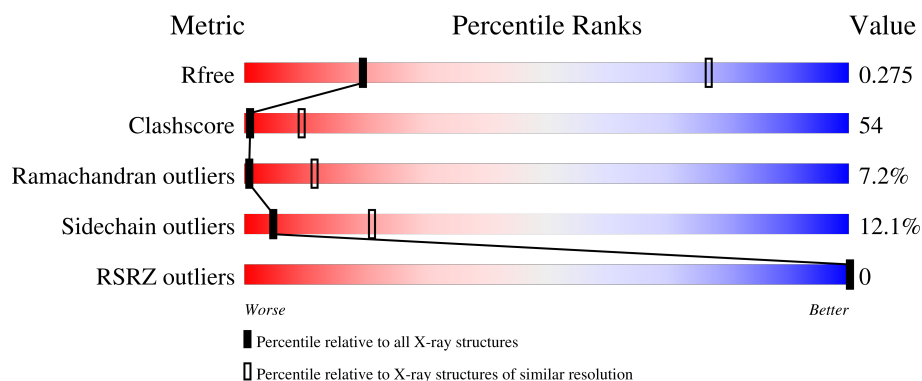
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.77 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	1085 (3.94-3.62)
Clashscore	190562	1029 (3.92-3.64)
Ramachandran outliers	187476	1064 (3.94-3.62)
Sidechain outliers	187428	1059 (3.94-3.62)
RSRZ outliers	180081	1084 (3.94-3.62)

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	216	29% 52% 16% ..
1	L	216	30% 57% 10% ..
2	B	224	28% 49% 19% ..
2	H	224	31% 53% 13% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6420 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 anti-factor IX antibody, 10C12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1576	989	259	323	5			
1	A	211	Total	C	N	O	S	0	0	0
			1576	989	259	323	5			

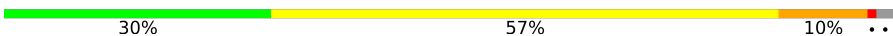
- Molecule 2 is a protein called anti-factor IX antibody, 10C12.

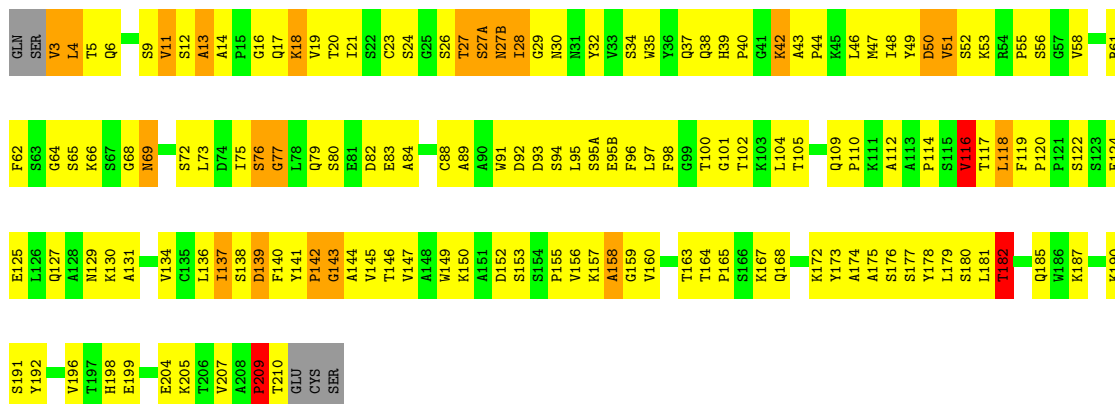
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1634	1031	280	315	8			
2	B	218	Total	C	N	O	S	0	0	0
			1634	1031	280	315	8			

3 Residue-property plots

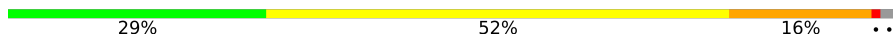
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

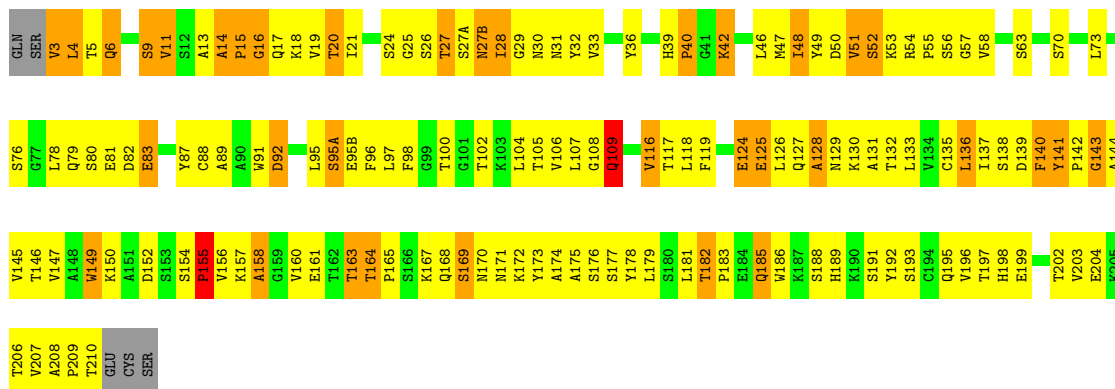
• Molecule 1: anti-factor IX antibody, 10C12

Chain L: 



• Molecule 1: anti-factor IX antibody, 10C12

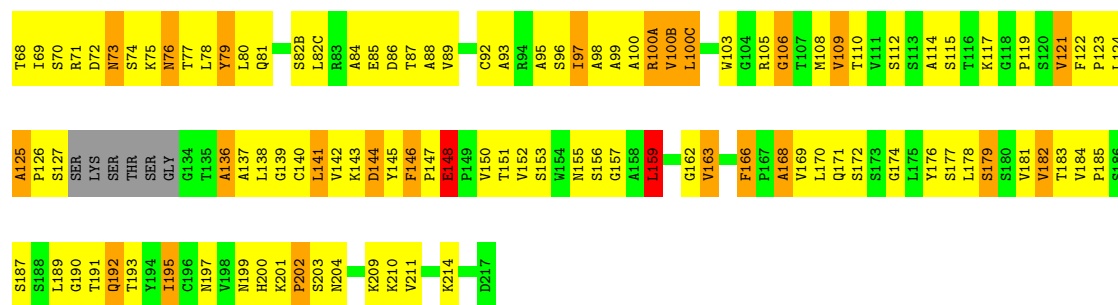
Chain A: 



• Molecule 2: anti-factor IX antibody, 10C12

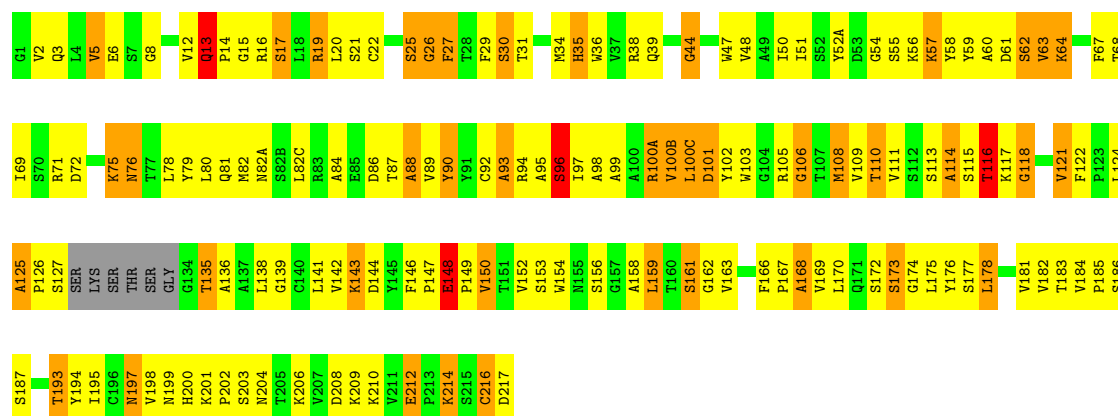
Chain H: 





- Molecule 2: anti-factor IX antibody, 10C12

Chain B: 28% 49% 19% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	159.61Å 159.61Å 65.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.26 – 3.77 41.26 – 3.77	Depositor EDS
% Data completeness (in resolution range)	82.2 (41.26-3.77) 82.2 (41.26-3.77)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.342 0.261 , 0.275	Depositor DCC
R_{free} test set	890 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å ²)	86.6	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 145.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.308 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6420	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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	0.62	0/1616	1.16	17/2206 (0.8%)
1	L	0.57	0/1616	1.08	7/2206 (0.3%)
2	B	0.56	0/1671	1.11	20/2271 (0.9%)
2	H	0.56	0/1671	1.07	11/2271 (0.5%)
All	All	0.58	0/6574	1.10	55/8954 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	L	0	1
All	All	0	2

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	182	THR	N-CA-C	-8.35	99.58	109.93
1	A	182	THR	N-CA-C	-7.82	98.52	110.32
1	A	141	TYR	CA-C-N	-7.44	110.54	119.84
1	A	141	TYR	C-N-CA	-7.44	110.54	119.84
1	A	138	SER	N-CA-C	7.21	119.13	108.60
1	A	6	GLN	N-CA-C	-7.09	97.91	109.82
1	A	109	GLN	CA-C-N	6.93	127.34	119.93
1	A	109	GLN	C-N-CA	6.93	127.34	119.93
2	B	143	LYS	N-CA-C	6.91	119.67	108.76
1	L	147	VAL	N-CA-C	6.58	117.39	108.17
1	L	118	LEU	N-CA-C	6.35	118.79	108.63
2	B	148	GLU	N-CA-C	6.22	123.57	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	191	SER	N-CA-C	6.13	118.51	108.52
2	B	13	GLN	CA-C-N	6.07	127.43	119.84
2	B	13	GLN	C-N-CA	6.07	127.43	119.84
2	B	48	VAL	N-CA-C	6.02	117.14	111.48
2	H	93	ALA	N-CA-C	5.95	119.17	109.24
2	H	163	VAL	N-CA-C	5.95	116.85	108.17
1	A	139	ASP	N-CA-C	5.92	119.42	111.24
1	A	14	ALA	CA-C-N	5.91	127.23	119.84
1	A	14	ALA	C-N-CA	5.91	127.23	119.84
1	L	5	THR	N-CA-C	5.85	118.77	109.24
1	A	185	GLN	N-CA-C	-5.84	105.04	111.82
2	B	206	LYS	N-CA-C	-5.78	100.36	109.50
2	B	90	TYR	N-CA-C	5.74	118.02	108.20
2	H	79	TYR	N-CA-C	5.72	117.31	109.18
2	H	114	ALA	N-CA-C	5.69	117.64	110.24
2	H	148	GLU	N-CA-C	5.69	122.38	109.81
2	H	125	ALA	CA-C-N	5.67	125.58	119.85
2	H	125	ALA	C-N-CA	5.67	125.58	119.85
2	H	182	VAL	N-CA-C	5.64	118.26	108.90
2	B	35	HIS	N-CA-C	5.57	118.29	109.50
2	B	17	SER	N-CA-C	5.56	118.47	109.86
1	A	154	SER	CA-C-N	5.46	126.67	119.84
1	A	154	SER	C-N-CA	5.46	126.67	119.84
2	B	118	GLY	CA-C-N	5.46	126.61	120.66
2	B	118	GLY	C-N-CA	5.46	126.61	120.66
2	H	121	VAL	N-CA-C	5.39	116.97	109.80
2	B	144	ASP	N-CA-C	5.37	119.24	111.56
2	B	108	MET	N-CA-C	5.26	118.13	109.76
1	L	142	PRO	N-CA-C	-5.25	105.39	112.48
2	B	212	GLU	CA-C-N	5.22	125.38	119.90
2	B	212	GLU	C-N-CA	5.22	125.38	119.90
2	B	121	VAL	N-CA-C	5.17	120.09	109.34
2	H	166	PHE	N-CA-C	5.14	117.17	110.08
1	A	14	ALA	N-CA-C	5.14	117.74	110.24
2	B	93	ALA	N-CA-C	5.13	117.19	109.23
1	A	149	TRP	N-CA-C	5.12	117.67	110.14
2	B	125	ALA	CA-C-N	5.12	125.05	119.78
2	B	125	ALA	C-N-CA	5.12	125.05	119.78
2	B	114	ALA	N-CA-C	5.10	118.07	110.52
1	L	116	VAL	N-CA-C	5.10	115.62	108.89
1	A	92	ASP	N-CA-C	5.10	116.91	108.20
1	A	5	THR	N-CA-C	5.08	117.52	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	162	GLY	N-CA-C	-5.01	106.24	114.76

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	9	SER	Peptide
1	L	9	SER	Peptide

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	1576	0	1525	168	0
1	L	1576	0	1525	170	0
2	B	1634	0	1617	200	0
2	H	1634	0	1617	195	0
All	All	6420	0	6284	684	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 54.

All (684) 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:126:PRO:HB3	2:H:138:LEU:HB3	1.37	1.02
2:H:147:PRO:HB3	2:H:202:PRO:HG2	1.50	0.92
1:L:92:ASP:HB2	1:L:97:LEU:HD11	1.47	0.92
1:A:92:ASP:HB2	1:A:97:LEU:HD11	1.52	0.92
2:B:126:PRO:HB3	2:B:138:LEU:HB3	1.53	0.91
2:H:38:ARG:NH1	2:H:86:ASP:HA	1.86	0.90
2:H:153:SER:OG	2:H:197:ASN:HB2	1.72	0.89
2:H:2:VAL:O	2:H:3:GLN:HG2	1.71	0.89
2:H:15:GLY:HA2	2:H:82(B):SER:HA	1.52	0.89
2:H:12:VAL:HG21	2:H:82(C):LEU:HD22	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:109:GLN:HE21	1:L:172:LYS:HE3	1.39	0.86
1:L:136:LEU:CD1	2:H:181:VAL:HG11	2.06	0.86
2:B:87:THR:HG23	2:B:110:THR:HA	1.58	0.83
2:H:195:ILE:CG2	2:H:210:LYS:HA	2.09	0.82
2:H:96:SER:HB3	2:H:99:ALA:O	1.80	0.82
2:H:100(C):LEU:HD23	2:H:100(C):LEU:N	1.95	0.81
2:H:195:ILE:HG22	2:H:210:LYS:HA	1.62	0.81
1:A:14:ALA:HB1	1:A:15:PRO:HD2	1.63	0.81
2:B:19:ARG:HH11	2:B:19:ARG:HB3	1.46	0.81
2:H:122:PHE:HE2	2:H:143:LYS:HE2	1.43	0.81
1:A:83:GLU:HG3	1:A:105:THR:HA	1.62	0.81
1:A:145:VAL:HG12	1:A:198:HIS:HB2	1.61	0.81
1:L:136:LEU:HD13	2:H:181:VAL:HG11	1.62	0.80
2:H:78:LEU:HD12	2:H:79:TYR:H	1.45	0.80
1:L:18:LYS:HG2	1:L:76:SER:HB3	1.64	0.79
1:A:140:PHE:H	1:A:140:PHE:HD2	1.31	0.79
1:A:197:THR:CA	1:A:202:THR:HG23	2.13	0.78
1:L:32:TYR:OH	2:B:55:SER:HB2	1.83	0.78
1:L:167:LYS:HG2	1:L:173:TYR:HE2	1.48	0.78
2:H:145:TYR:CE1	2:H:176:TYR:HB2	2.18	0.78
2:B:193:THR:HG22	2:B:195:ILE:HD11	1.65	0.78
2:B:118:GLY:HA2	2:B:200:HIS:HD2	1.49	0.77
1:L:109:GLN:HB2	1:L:110:PRO:HD2	1.65	0.77
2:H:195:ILE:HG21	2:H:210:LYS:HG2	1.67	0.77
2:B:61:ASP:N	2:B:64:LYS:HE3	1.99	0.77
1:A:140:PHE:HE2	1:A:174:ALA:HA	1.50	0.77
1:A:197:THR:HA	1:A:202:THR:HG23	1.67	0.76
2:H:35:HIS:NE2	2:H:50:ILE:HD12	2.00	0.76
2:B:14:PRO:HD2	2:B:113:SER:HB3	1.67	0.76
1:L:167:LYS:HG2	1:L:173:TYR:CE2	2.21	0.76
2:B:82:MET:O	2:B:82(C):LEU:HD11	1.86	0.76
1:L:20:THR:O	1:L:21:ILE:HD12	1.84	0.76
2:B:122:PHE:HE2	2:B:143:LYS:HD3	1.49	0.76
2:H:201:LYS:HB3	2:H:202:PRO:HD3	1.68	0.76
2:B:122:PHE:CE2	2:B:143:LYS:HD3	2.20	0.76
1:L:143:GLY:HA3	1:L:173:TYR:CD1	2.22	0.75
1:L:92:ASP:HB2	1:L:97:LEU:CD1	2.17	0.75
2:H:78:LEU:HD12	2:H:79:TYR:N	2.00	0.75
2:B:17:SER:OG	2:B:82(A):ASN:HA	1.85	0.74
2:H:35:HIS:CE1	2:H:50:ILE:HD12	2.22	0.74
2:B:22:CYS:HB3	2:B:78:LEU:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:ALA:HA	2:B:178:LEU:HB3	1.67	0.74
2:B:100(C):LEU:N	2:B:100(C):LEU:HD23	2.02	0.74
1:L:119:PHE:HZ	2:H:138:LEU:HA	1.53	0.74
1:A:107:LEU:HA	1:A:141:TYR:OH	1.87	0.74
1:A:161:GLU:HA	1:A:161:GLU:OE1	1.88	0.74
2:B:194:TYR:C	2:B:195:ILE:HD12	2.13	0.74
1:L:168:GLN:HG2	1:L:172:LYS:O	1.88	0.73
1:L:52:SER:HB3	1:L:64:GLY:O	1.88	0.73
1:L:49:TYR:HB2	2:H:100(B):VAL:HG21	1.71	0.73
1:L:89:ALA:HB2	1:L:98:PHE:CE1	2.24	0.73
1:A:89:ALA:HB2	1:A:98:PHE:CD1	2.23	0.73
2:B:146:PHE:HB3	2:B:147:PRO:HD3	1.71	0.73
2:H:38:ARG:HH12	2:H:86:ASP:HA	1.51	0.72
2:H:108:MET:HE3	2:H:109:VAL:H	1.54	0.72
2:B:147:PRO:HB2	2:B:202:PRO:CB	2.19	0.72
1:A:51:VAL:HG12	1:A:52:SER:H	1.53	0.72
1:A:14:ALA:HB3	1:A:17:GLN:CD	2.14	0.72
2:H:97:ILE:HD12	2:B:98:ALA:HB2	1.70	0.72
2:H:100(A):ARG:HH11	2:H:100(A):ARG:HG2	1.54	0.72
1:A:104:LEU:C	1:A:104:LEU:HD23	2.14	0.72
1:L:49:TYR:HB2	2:H:100(B):VAL:CG2	2.20	0.72
1:L:18:LYS:O	1:L:19:VAL:HG23	1.90	0.72
2:H:156:SER:N	2:H:197:ASN:HD21	1.87	0.72
1:A:129:ASN:O	1:A:130:LYS:HG3	1.90	0.72
2:H:151:THR:CG2	2:H:199:ASN:HB3	2.20	0.71
2:H:59:TYR:OH	2:H:69:ILE:HG22	1.90	0.71
2:H:68:THR:HB	2:H:81:GLN:HB3	1.72	0.71
2:H:141:LEU:HD12	2:H:142:VAL:N	2.05	0.71
2:B:94:ARG:HH21	2:B:101:ASP:CG	1.98	0.71
1:L:140:PHE:CE1	1:L:145:VAL:HG13	2.26	0.71
2:B:156:SER:H	2:B:197:ASN:HD21	1.39	0.71
2:B:121:VAL:HG11	2:B:209:LYS:HB2	1.73	0.70
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.27	0.70
1:A:163:THR:HG23	1:A:176:SER:O	1.92	0.70
2:H:147:PRO:CB	2:H:202:PRO:HG2	2.21	0.70
2:B:35:HIS:CE1	2:B:50:ILE:HD12	2.26	0.70
1:L:48:ILE:HD12	1:L:73:LEU:CD1	2.22	0.70
2:B:195:ILE:HG23	2:B:209:LYS:O	1.91	0.70
2:B:13:GLN:HG3	2:B:113:SER:HA	1.74	0.69
2:H:87:THR:HG21	2:H:170:LEU:HD22	1.74	0.69
2:B:59:TYR:CZ	2:B:69:ILE:HG22	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:SER:HB3	1:A:206:THR:OG1	1.91	0.69
1:L:190:LYS:O	1:L:209:PRO:HD3	1.92	0.69
2:H:52(A):TYR:OH	1:A:53:LYS:HE3	1.93	0.69
2:B:178:LEU:O	2:B:178:LEU:HD12	1.93	0.69
1:L:18:LYS:HA	1:L:76:SER:HA	1.75	0.68
2:B:156:SER:H	2:B:197:ASN:ND2	1.91	0.68
2:H:60:ALA:C	2:H:62:SER:H	1.99	0.68
1:L:55:PRO:HD2	1:L:58:VAL:HG21	1.76	0.68
2:H:108:MET:HE3	2:H:109:VAL:N	2.08	0.68
2:H:125:ALA:HB1	2:H:214:LYS:HB2	1.74	0.68
2:H:189:LEU:HD12	2:H:190:GLY:H	1.58	0.68
2:B:100(A):ARG:HG2	2:B:100(A):ARG:HH11	1.58	0.68
2:H:126:PRO:HA	2:H:137:ALA:O	1.94	0.68
2:H:153:SER:HG	2:H:197:ASN:HB2	1.58	0.68
2:H:169:VAL:O	2:H:176:TYR:HA	1.93	0.67
1:L:27:THR:HG23	1:L:69:ASN:HD21	1.60	0.67
2:B:135:THR:HG22	2:B:186:SER:H	1.59	0.67
1:A:63:SER:O	1:A:73:LEU:HD12	1.95	0.67
2:B:19:ARG:HH11	2:B:19:ARG:CB	2.08	0.67
2:B:214:LYS:HG3	2:B:216:CYS:SG	2.34	0.67
2:H:156:SER:H	2:H:197:ASN:HD21	1.42	0.67
2:H:178:LEU:HD12	2:H:178:LEU:C	2.20	0.67
1:A:46:LEU:HD21	2:B:100(B):VAL:CG1	2.24	0.67
2:B:172:SER:C	2:B:174:GLY:H	2.01	0.67
2:H:136:ALA:HB3	2:H:184:VAL:H	1.59	0.66
1:L:51:VAL:HG12	1:L:52:SER:H	1.60	0.66
1:A:140:PHE:HD2	1:A:140:PHE:N	1.94	0.66
2:H:195:ILE:HG22	2:H:209:LYS:O	1.94	0.66
2:B:100(A):ARG:HG2	2:B:100(A):ARG:NH1	2.09	0.66
1:A:55:PRO:O	1:A:56:SER:C	2.37	0.66
1:L:48:ILE:HD11	1:L:62:PHE:O	1.96	0.66
1:A:27(B):ASN:O	1:A:29:GLY:N	2.29	0.66
2:H:4:LEU:HD23	2:H:24:ALA:HA	1.78	0.66
2:H:12:VAL:CG2	2:H:82(C):LEU:HD22	2.26	0.65
2:H:124:LEU:HB2	2:H:139:GLY:O	1.96	0.65
2:B:81:GLN:HA	2:B:81:GLN:OE1	1.96	0.65
1:L:190:LYS:C	1:L:190:LYS:HD3	2.20	0.65
1:A:4:LEU:HD22	1:A:25:GLY:HA3	1.76	0.65
2:H:87:THR:HG21	2:H:170:LEU:CD2	2.26	0.65
2:H:100(C):LEU:N	2:H:100(C):LEU:CD2	2.60	0.64
1:A:78:LEU:HD21	1:A:104:LEU:HD11	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.79	0.64
1:L:32:TYR:HB3	1:L:50:ASP:HA	1.78	0.64
2:B:2:VAL:HG13	2:B:27:PHE:HE1	1.63	0.64
1:A:141:TYR:HB3	1:A:142:PRO:HD3	1.79	0.64
2:B:126:PRO:O	2:B:127:SER:HB2	1.96	0.64
2:H:19:ARG:HB3	2:H:81:GLN:OE1	1.98	0.64
2:H:117:LYS:HE2	2:H:144:ASP:HB3	1.79	0.64
1:L:27(A):SER:HB3	1:L:94:SER:HB2	1.79	0.63
1:L:130:LYS:HD3	2:H:143:LYS:HZ2	1.63	0.63
1:A:11:VAL:HG21	1:A:21:ILE:HG12	1.79	0.63
1:L:42:LYS:HA	2:H:105:ARG:HD3	1.79	0.63
1:L:4:LEU:O	1:L:100:THR:HG23	1.97	0.63
1:L:16:GLY:HA2	1:L:77:GLY:HA2	1.81	0.63
1:L:109:GLN:NE2	1:L:172:LYS:HE3	2.13	0.63
1:L:157:LYS:O	1:L:158:ALA:C	2.41	0.63
2:B:2:VAL:HG12	2:B:3:GLN:N	2.13	0.63
2:H:13:GLN:HA	2:H:112:SER:O	1.99	0.63
1:A:124:GLU:O	1:A:127:GLN:N	2.32	0.63
1:L:51:VAL:HG12	1:L:52:SER:N	2.14	0.63
1:A:137:ILE:HB	1:A:175:ALA:O	1.98	0.63
2:H:122:PHE:CE2	2:H:143:LYS:HE2	2.32	0.62
2:B:121:VAL:HG12	2:B:209:LYS:HG3	1.80	0.62
1:L:116:VAL:HA	1:L:136:LEU:O	1.99	0.62
2:B:124:LEU:HD12	2:B:139:GLY:C	2.25	0.62
2:H:51:ILE:HD13	2:H:71:ARG:HG2	1.80	0.62
1:A:136:LEU:HD11	2:B:181:VAL:HG11	1.81	0.62
2:B:152:VAL:HG12	2:B:153:SER:N	2.15	0.62
1:L:44:PRO:HG2	2:H:103:TRP:CE3	2.33	0.62
2:B:51:ILE:HD11	2:B:54:GLY:HA2	1.82	0.62
1:L:136:LEU:HD22	2:H:166:PHE:CZ	2.35	0.62
2:B:61:ASP:C	2:B:63:VAL:H	2.08	0.62
2:B:195:ILE:HD12	2:B:195:ILE:N	2.15	0.61
1:A:150:LYS:HG2	1:A:155:PRO:HB3	1.81	0.61
1:L:27:THR:HG23	1:L:69:ASN:ND2	2.16	0.61
1:A:19:VAL:HG22	1:A:20:THR:N	2.14	0.61
2:B:61:ASP:CA	2:B:64:LYS:HE3	2.30	0.61
1:L:12:SER:O	1:L:13:ALA:HB2	2.01	0.61
1:A:78:LEU:HD22	1:A:104:LEU:HD21	1.82	0.61
2:B:149:PRO:O	2:B:150:VAL:HG23	2.00	0.61
1:L:157:LYS:O	1:L:159:GLY:N	2.33	0.61
2:B:5:VAL:HG23	2:B:5:VAL:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:165:PRO:HA	1:L:175:ALA:HB2	1.83	0.61
2:H:151:THR:HG22	2:H:199:ASN:HB3	1.82	0.61
1:A:149:TRP:HZ2	1:A:177:SER:HG	1.46	0.61
2:H:60:ALA:O	2:H:64:LYS:HG3	2.01	0.60
2:B:63:VAL:O	2:B:64:LYS:C	2.44	0.60
1:L:160:VAL:CG2	1:L:179:LEU:HD13	2.31	0.60
1:A:131:ALA:HB3	1:A:181:LEU:HB2	1.84	0.60
1:L:182:THR:OG1	1:L:185:GLN:HG3	2.01	0.60
1:L:20:THR:C	1:L:21:ILE:HD12	2.26	0.60
1:L:92:ASP:OD1	1:L:94:SER:HB3	2.02	0.60
2:B:118:GLY:HA2	2:B:200:HIS:CD2	2.32	0.60
2:H:59:TYR:CZ	2:H:69:ILE:HG22	2.36	0.60
2:H:189:LEU:C	2:H:191:THR:H	2.09	0.60
1:L:49:TYR:O	1:L:53:LYS:HB2	2.02	0.59
2:H:34:MET:O	2:H:50:ILE:HG13	2.02	0.59
1:A:127:GLN:C	1:A:129:ASN:H	2.10	0.59
2:B:124:LEU:HD21	2:B:141:LEU:HB2	1.83	0.59
1:L:27(B):ASN:HB3	1:L:92:ASP:HA	1.85	0.59
1:A:125:GLU:HG3	2:B:122:PHE:CE2	2.38	0.59
1:A:196:VAL:CG2	1:A:203:VAL:HB	2.32	0.59
1:L:91:TRP:CZ2	1:L:95(A):SER:HA	2.38	0.59
2:H:202:PRO:C	2:H:204:ASN:H	2.10	0.59
1:A:197:THR:HG23	1:A:202:THR:OG1	2.03	0.59
2:B:198:VAL:HG12	2:B:199:ASN:N	2.17	0.59
2:H:87:THR:HG23	2:H:110:THR:HA	1.85	0.59
1:A:4:LEU:O	1:A:100:THR:HG23	2.02	0.59
2:H:97:ILE:HD12	2:B:98:ALA:CB	2.33	0.59
1:L:79:GLN:O	1:L:82:ASP:N	2.30	0.59
1:L:125:GLU:HG3	2:H:122:PHE:CE2	2.38	0.58
1:A:196:VAL:HG23	1:A:196:VAL:O	2.02	0.58
1:A:202:THR:HG22	1:A:203:VAL:H	1.68	0.58
2:B:51:ILE:HG22	2:B:69:ILE:HD11	1.83	0.58
1:L:19:VAL:CG1	1:L:20:THR:N	2.66	0.58
2:H:124:LEU:HD12	2:H:139:GLY:C	2.28	0.58
2:B:100(A):ARG:HG3	2:B:100(B):VAL:HG23	1.85	0.58
1:A:42:LYS:HE3	2:B:105:ARG:HE	1.68	0.58
1:A:136:LEU:CD1	2:B:181:VAL:HG11	2.33	0.58
1:L:145:VAL:HG12	1:L:198:HIS:CD2	2.39	0.58
1:A:109:GLN:HG2	1:A:141:TYR:CD2	2.38	0.58
1:L:6:GLN:NE2	1:L:101:GLY:C	2.61	0.58
2:H:97:ILE:CG2	2:H:98:ALA:N	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HA	1:A:82:ASP:OD2	2.04	0.58
2:B:82(C):LEU:HD12	2:B:82(C):LEU:N	2.17	0.58
1:L:137:ILE:HG12	1:L:175:ALA:O	2.04	0.58
1:A:108:GLY:N	1:A:141:TYR:OH	2.34	0.58
2:B:117:LYS:HE2	2:B:118:GLY:H	1.66	0.58
1:L:3:VAL:HG12	1:L:4:LEU:H	1.69	0.57
1:L:131:ALA:HB3	1:L:181:LEU:O	2.03	0.57
2:H:70:SER:O	2:H:78:LEU:HD12	2.04	0.57
1:A:140:PHE:N	1:A:140:PHE:CD2	2.66	0.57
1:L:112:ALA:HB3	1:L:140:PHE:HA	1.87	0.57
2:H:147:PRO:HB3	2:H:202:PRO:CG	2.29	0.57
2:H:182:VAL:HG22	2:H:183:THR:N	2.18	0.57
2:H:156:SER:H	2:H:197:ASN:ND2	2.03	0.57
1:A:147:VAL:HG11	1:A:177:SER:HB2	1.86	0.57
2:B:105:ARG:O	2:B:106:GLY:O	2.23	0.57
1:L:37:GLN:HB2	1:L:47:MET:CG	2.35	0.57
1:L:38:GLN:O	1:L:84:ALA:HB1	2.05	0.57
1:L:95:LEU:O	1:L:95(B):GLU:HG3	2.05	0.56
1:L:104:LEU:HD23	1:L:104:LEU:C	2.29	0.56
2:H:86:ASP:O	2:H:87:THR:C	2.47	0.56
1:A:31:ASN:ND2	1:A:91:TRP:O	2.38	0.56
1:A:55:PRO:O	1:A:57:GLY:N	2.38	0.56
1:A:79:GLN:O	1:A:82:ASP:N	2.37	0.56
1:L:116:VAL:HB	1:L:205:LYS:HG3	1.86	0.56
2:H:155:ASN:O	2:H:156:SER:OG	2.21	0.56
2:B:114:ALA:HB3	2:B:146:PHE:CD1	2.40	0.56
2:B:185:PRO:C	2:B:187:SER:N	2.62	0.56
1:A:167:LYS:HE2	1:A:171:ASN:O	2.04	0.56
1:L:28:ILE:C	1:L:30:ASN:H	2.12	0.56
1:L:190:LYS:O	1:L:209:PRO:CD	2.54	0.56
1:A:4:LEU:HA	1:A:24:SER:O	2.06	0.56
1:A:156:VAL:HG22	1:A:158:ALA:H	1.71	0.56
2:B:61:ASP:O	2:B:63:VAL:N	2.38	0.56
1:A:208:ALA:HB1	1:A:209:PRO:HD2	1.86	0.56
2:B:59:TYR:OH	2:B:69:ILE:HG22	2.06	0.56
2:B:201:LYS:HB2	2:B:202:PRO:HD3	1.87	0.56
1:L:136:LEU:HD11	2:H:181:VAL:HG11	1.85	0.56
2:H:182:VAL:CG2	2:H:183:THR:N	2.69	0.56
2:B:159:LEU:HD11	2:B:161:SER:HB2	1.88	0.56
2:B:195:ILE:HG23	2:B:209:LYS:C	2.31	0.56
1:L:124:GLU:O	1:L:127:GLN:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:97:ILE:HG22	2:H:98:ALA:N	2.21	0.55
2:H:147:PRO:HG2	2:H:202:PRO:HB2	1.87	0.55
1:A:118:LEU:HD21	1:A:207:VAL:HG22	1.88	0.55
2:B:185:PRO:C	2:B:187:SER:H	2.13	0.55
1:L:160:VAL:HG23	1:L:179:LEU:HD13	1.88	0.55
2:H:152:VAL:HG12	2:H:153:SER:N	2.20	0.55
1:A:14:ALA:O	1:A:16:GLY:N	2.35	0.55
2:B:148:GLU:HA	2:B:148:GLU:OE1	2.06	0.55
1:L:92:ASP:CB	1:L:97:LEU:HD11	2.30	0.55
2:B:139:GLY:HA2	2:B:154:TRP:CH2	2.42	0.55
1:L:14:ALA:O	1:L:17:GLN:HG2	2.07	0.55
2:B:195:ILE:HG13	2:B:210:LYS:HA	1.89	0.55
2:H:123:PRO:CB	2:H:211:VAL:HG22	2.37	0.55
2:H:60:ALA:C	2:H:62:SER:N	2.66	0.54
1:A:89:ALA:HB2	1:A:98:PHE:CE1	2.43	0.54
1:L:140:PHE:HE1	1:L:145:VAL:HG13	1.70	0.54
1:L:19:VAL:HG12	1:L:20:THR:N	2.23	0.54
2:H:51:ILE:HG22	2:H:69:ILE:HD11	1.90	0.54
2:B:3:GLN:HA	2:B:3:GLN:OE1	2.07	0.54
2:B:172:SER:C	2:B:174:GLY:N	2.65	0.54
2:B:216:CYS:O	2:B:217:ASP:CG	2.50	0.54
1:L:61:ARG:HD2	1:L:76:SER:O	2.06	0.54
1:A:140:PHE:HE2	1:A:174:ALA:CA	2.19	0.54
2:B:84:ALA:HA	2:B:111:VAL:HG11	1.90	0.54
2:B:100(C):LEU:N	2:B:100(C):LEU:CD2	2.68	0.54
2:B:97:ILE:HG23	2:B:98:ALA:N	2.22	0.54
2:H:126:PRO:HB3	2:H:138:LEU:CB	2.26	0.54
1:A:135:CYS:HB2	1:A:149:TRP:CH2	2.43	0.54
1:A:164:THR:HG22	1:A:165:PRO:HD2	1.88	0.54
2:B:147:PRO:CB	2:B:202:PRO:HB3	2.38	0.54
2:H:168:ALA:HA	2:H:177:SER:O	2.08	0.54
2:H:115:SER:O	2:H:146:PHE:HB3	2.08	0.53
2:B:198:VAL:HG12	2:B:199:ASN:H	1.73	0.53
1:A:150:LYS:HD3	1:A:204:GLU:OE2	2.08	0.53
1:A:152:ASP:OD2	1:A:189:HIS:HB3	2.08	0.53
1:L:163:THR:OG1	1:L:175:ALA:HB1	2.08	0.53
1:A:36:TYR:HE2	2:B:103:TRP:HE1	1.57	0.53
2:B:52(A):TYR:HA	2:B:71:ARG:NH1	2.23	0.53
1:A:79:GLN:O	1:A:80:SER:C	2.52	0.53
1:A:182:THR:HG23	1:A:185:GLN:OE1	2.09	0.53
1:L:83:GLU:HG3	1:L:105:THR:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ILE:HG23	1:A:33:VAL:HG21	1.89	0.53
1:A:87:TYR:OH	2:B:44:GLY:HA2	2.08	0.53
2:B:38:ARG:NH1	2:B:86:ASP:HA	2.23	0.53
2:B:117:LYS:HG3	2:B:118:GLY:N	2.24	0.53
2:B:139:GLY:HA2	2:B:154:TRP:HH2	1.73	0.53
2:B:184:VAL:HG11	2:B:194:TYR:CE2	2.43	0.53
2:H:121:VAL:HG12	2:H:122:PHE:N	2.24	0.53
1:L:142:PRO:O	1:L:144:ALA:N	2.42	0.52
1:A:3:VAL:O	1:A:4:LEU:HB2	2.08	0.52
2:H:29:PHE:CD2	2:H:76:ASN:HA	2.45	0.52
1:A:118:LEU:C	1:A:118:LEU:HD12	2.34	0.52
2:B:61:ASP:C	2:B:63:VAL:N	2.67	0.52
1:L:109:GLN:CD	1:L:141:TYR:CD2	2.87	0.52
1:A:140:PHE:CE2	1:A:174:ALA:HA	2.38	0.52
1:L:92:ASP:CG	1:L:94:SER:HB3	2.34	0.52
1:A:19:VAL:CG2	1:A:20:THR:N	2.72	0.52
1:L:145:VAL:HG12	1:L:198:HIS:HD2	1.74	0.52
2:H:63:VAL:O	2:H:64:LYS:C	2.53	0.52
2:H:155:ASN:ND2	2:H:193:THR:O	2.43	0.52
2:B:2:VAL:HG13	2:B:27:PHE:CE1	2.44	0.52
1:L:55:PRO:O	1:L:56:SER:C	2.53	0.52
1:A:133:LEU:HB2	1:A:179:LEU:HB3	1.91	0.52
1:L:119:PHE:HE1	2:H:125:ALA:O	1.93	0.52
1:L:181:LEU:HD11	1:L:192:TYR:CE2	2.45	0.52
2:B:20:LEU:HG	2:B:82:MET:HE2	1.92	0.52
2:B:38:ARG:HA	2:B:89:VAL:O	2.10	0.52
2:H:75:LYS:O	2:H:77:THR:N	2.44	0.51
1:A:51:VAL:HG12	1:A:52:SER:N	2.23	0.51
2:H:3:GLN:HB2	2:H:25:SER:HB3	1.91	0.51
1:L:129:ASN:O	1:L:130:LYS:HG2	2.10	0.51
2:H:87:THR:O	2:H:88:ALA:HB2	2.10	0.51
1:L:21:ILE:HG13	1:L:102:THR:HG21	1.93	0.51
2:H:72:ASP:O	2:H:75:LYS:N	2.44	0.51
2:B:117:LYS:CD	2:B:118:GLY:H	2.22	0.51
2:B:201:LYS:O	2:B:204:ASN:N	2.39	0.51
1:A:92:ASP:HB2	1:A:97:LEU:CD1	2.32	0.51
2:B:6:GLU:CD	2:B:92:CYS:HB3	2.36	0.51
1:A:4:LEU:CD1	1:A:28:ILE:HD11	2.41	0.51
2:H:2:VAL:C	2:H:3:GLN:HG2	2.36	0.51
2:B:56:LYS:C	2:B:57:LYS:HG2	2.36	0.51
2:B:117:LYS:CG	2:B:118:GLY:H	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:48:ILE:HD12	1:L:73:LEU:HD12	1.91	0.50
2:H:82(C):LEU:N	2:H:82(C):LEU:HD12	2.26	0.50
2:B:152:VAL:CG1	2:B:153:SER:N	2.74	0.50
2:H:6:GLU:OE2	2:H:92:CYS:HB3	2.11	0.50
1:A:14:ALA:HB3	1:A:17:GLN:HG3	1.93	0.50
1:A:104:LEU:C	1:A:104:LEU:CD2	2.84	0.50
2:B:173:SER:OG	2:B:175:LEU:HD12	2.11	0.50
1:L:37:GLN:HB2	1:L:47:MET:HG3	1.91	0.50
2:B:6:GLU:OE1	2:B:6:GLU:N	2.44	0.50
2:H:95:ALA:HB1	2:H:100:ALA:HA	1.92	0.50
1:A:78:LEU:CD2	1:A:104:LEU:HD21	2.41	0.50
1:A:208:ALA:HB1	1:A:209:PRO:CD	2.41	0.50
1:A:136:LEU:HD13	2:B:166:PHE:HZ	1.76	0.50
1:A:168:GLN:HG2	1:A:172:LYS:O	2.12	0.50
1:L:150:LYS:HA	1:L:155:PRO:HA	1.92	0.50
2:B:39:GLN:C	2:B:88:ALA:HB1	2.37	0.50
2:H:100(A):ARG:HG2	2:H:100(A):ARG:NH1	2.22	0.50
1:A:79:GLN:N	1:A:82:ASP:OD2	2.41	0.50
2:B:153:SER:CB	2:B:197:ASN:HD22	2.25	0.50
1:L:4:LEU:HA	1:L:24:SER:O	2.11	0.50
1:L:39:HIS:O	1:L:40:PRO:C	2.54	0.50
1:A:18:LYS:HA	1:A:76:SER:HA	1.94	0.50
1:A:39:HIS:HB3	1:A:40:PRO:HD2	1.94	0.50
1:L:178:TYR:OH	2:H:179:SER:OG	2.26	0.50
1:A:189:HIS:HB2	1:A:192:TYR:CE1	2.47	0.50
1:A:4:LEU:HD13	1:A:28:ILE:HD11	1.93	0.49
1:A:197:THR:HA	1:A:202:THR:HA	1.94	0.49
1:L:198:HIS:O	1:L:199:GLU:HB2	2.12	0.49
2:B:60:ALA:O	2:B:61:ASP:C	2.54	0.49
2:B:117:LYS:CG	2:B:118:GLY:N	2.75	0.49
1:L:119:PHE:N	1:L:134:VAL:O	2.43	0.49
2:B:153:SER:OG	2:B:197:ASN:HB2	2.12	0.49
2:B:156:SER:N	2:B:197:ASN:HD21	2.08	0.49
2:B:162:GLY:O	2:B:182:VAL:HA	2.12	0.49
2:B:200:HIS:CD2	2:B:203:SER:HB3	2.46	0.49
1:L:27(B):ASN:O	1:L:29:GLY:N	2.46	0.49
1:L:125:GLU:HA	2:H:122:PHE:CZ	2.48	0.49
2:H:153:SER:CB	2:H:197:ASN:HD22	2.25	0.49
1:A:152:ASP:N	1:A:191:SER:O	2.43	0.49
1:L:47:MET:O	1:L:48:ILE:HG13	2.12	0.49
1:L:53:LYS:HE3	2:B:52(A):TYR:OH	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:178:TYR:HH	2:H:179:SER:HG	1.51	0.49
1:A:91:TRP:HH2	2:B:58:TYR:HD2	1.60	0.49
1:L:18:LYS:HA	1:L:75:ILE:O	2.13	0.49
1:A:18:LYS:HG2	1:A:76:SER:HB3	1.95	0.49
1:A:48:ILE:HG23	1:A:51:VAL:O	2.12	0.49
1:A:150:LYS:HA	1:A:155:PRO:HA	1.95	0.49
2:H:126:PRO:CA	2:H:137:ALA:O	2.59	0.49
1:A:104:LEU:HD23	1:A:104:LEU:O	2.12	0.49
1:A:96:PHE:HB3	2:B:47:TRP:CG	2.47	0.49
2:B:16:ARG:O	2:B:82(C):LEU:HD13	2.12	0.49
2:B:100(A):ARG:HH11	2:B:100(A):ARG:CG	2.25	0.49
1:L:149:TRP:C	1:L:150:LYS:HG3	2.37	0.49
1:A:14:ALA:HB3	1:A:17:GLN:CG	2.42	0.49
1:A:14:ALA:CB	1:A:15:PRO:HD2	2.33	0.49
1:A:140:PHE:CE2	1:A:173:TYR:C	2.91	0.49
2:B:22:CYS:O	2:B:78:LEU:N	2.32	0.49
2:B:82(C):LEU:N	2:B:82(C):LEU:CD1	2.76	0.49
1:L:89:ALA:HB1	1:L:96:PHE:CE2	2.48	0.48
1:A:117:THR:O	1:A:117:THR:HG22	2.13	0.48
1:L:95:LEU:O	1:L:95(A):SER:C	2.56	0.48
2:B:61:ASP:H	2:B:64:LYS:HE3	1.72	0.48
1:L:11:VAL:HG21	1:L:21:ILE:HD11	1.96	0.48
2:H:6:GLU:N	2:H:6:GLU:OE1	2.46	0.48
2:H:189:LEU:HD12	2:H:190:GLY:N	2.27	0.48
1:L:79:GLN:O	1:L:80:SER:C	2.56	0.48
1:L:16:GLY:CA	1:L:77:GLY:HA2	2.43	0.48
1:L:124:GLU:O	1:L:127:GLN:N	2.45	0.48
1:A:129:ASN:HA	1:A:183:PRO:HG2	1.93	0.48
2:H:3:GLN:HB2	2:H:25:SER:CB	2.43	0.48
1:L:122:SER:HB3	2:H:123:PRO:O	2.13	0.48
1:A:27:THR:O	1:A:30:ASN:ND2	2.46	0.48
2:B:147:PRO:HB2	2:B:202:PRO:CG	2.43	0.48
2:B:142:VAL:HB	2:B:178:LEU:HD12	1.95	0.48
2:B:147:PRO:CB	2:B:202:PRO:CB	2.89	0.48
2:H:72:ASP:O	2:H:73:ASN:C	2.57	0.48
1:A:25:GLY:O	1:A:26:SER:HB3	2.12	0.48
1:L:35:TRP:CE3	1:L:88:CYS:HB3	2.49	0.48
2:H:159:LEU:HD13	2:H:159:LEU:O	2.14	0.48
2:B:36:TRP:NE1	2:B:80:LEU:HB2	2.29	0.48
2:B:63:VAL:HG23	2:B:64:LYS:N	2.29	0.48
2:B:72:ASP:CG	2:B:75:LYS:NZ	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:ALA:HA	2:B:111:VAL:CG1	2.43	0.48
2:H:29:PHE:HB3	2:H:76:ASN:OD1	2.13	0.47
1:A:46:LEU:CD2	2:B:101:ASP:HA	2.44	0.47
2:B:60:ALA:C	2:B:62:SER:N	2.71	0.47
2:H:201:LYS:HB3	2:H:202:PRO:CD	2.41	0.47
1:A:83:GLU:CG	1:A:105:THR:HA	2.41	0.47
1:A:165:PRO:HA	1:A:175:ALA:HB2	1.96	0.47
1:L:196:VAL:HG23	1:L:196:VAL:O	2.15	0.47
1:L:4:LEU:HD23	1:L:23:CYS:SG	2.54	0.47
1:L:21:ILE:CG1	1:L:102:THR:HG21	2.45	0.47
2:H:145:TYR:CD1	2:H:145:TYR:C	2.93	0.47
2:H:156:SER:N	2:H:197:ASN:ND2	2.60	0.47
1:A:202:THR:HG22	1:A:203:VAL:N	2.30	0.47
2:B:35:HIS:CD2	2:B:95:ALA:HB2	2.49	0.47
1:L:143:GLY:CA	1:L:173:TYR:CD1	2.95	0.47
1:A:47:MET:O	1:A:48:ILE:HD12	2.14	0.47
2:B:5:VAL:O	2:B:5:VAL:CG2	2.61	0.47
2:B:117:LYS:HG3	2:B:118:GLY:H	1.80	0.47
1:L:43:ALA:HB1	1:L:44:PRO:CD	2.44	0.47
1:L:119:PHE:CZ	2:H:138:LEU:HA	2.41	0.47
2:H:121:VAL:HG22	2:H:142:VAL:HG22	1.97	0.47
1:A:196:VAL:HG22	1:A:203:VAL:HB	1.96	0.47
2:H:6:GLU:OE2	2:H:92:CYS:N	2.41	0.47
2:H:202:PRO:O	2:H:204:ASN:N	2.48	0.47
2:B:35:HIS:HD2	2:B:95:ALA:HB2	1.79	0.47
2:B:138:LEU:O	2:B:182:VAL:HG12	2.15	0.47
1:L:27(B):ASN:O	1:L:28:ILE:C	2.58	0.47
2:H:75:LYS:O	2:H:76:ASN:C	2.57	0.47
1:A:54:ARG:HB3	1:A:58:VAL:HB	1.96	0.47
2:B:60:ALA:O	2:B:62:SER:N	2.48	0.47
2:H:209:LYS:HD3	2:H:210:LYS:N	2.29	0.47
1:A:124:GLU:O	1:A:125:GLU:C	2.57	0.47
2:B:2:VAL:CG1	2:B:3:GLN:N	2.77	0.47
2:B:159:LEU:CD1	2:B:161:SER:HB2	2.45	0.47
2:B:19:ARG:HH11	2:B:19:ARG:CG	2.27	0.47
2:H:39:GLN:CD	2:H:45:LEU:HD23	2.40	0.46
1:L:163:THR:HG23	1:L:176:SER:O	2.15	0.46
2:H:121:VAL:CG1	2:H:122:PHE:N	2.79	0.46
1:A:197:THR:N	1:A:202:THR:HG23	2.31	0.46
2:B:17:SER:HB3	2:B:82:MET:O	2.16	0.46
2:B:117:LYS:CE	2:B:118:GLY:H	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:SER:O	2:H:18:LEU:HB2	2.14	0.46
1:A:42:LYS:CE	2:B:105:ARG:HE	2.28	0.46
1:A:198:HIS:O	1:A:199:GLU:HB2	2.16	0.46
2:B:96:SER:HA	2:B:101:ASP:OD2	2.15	0.46
2:B:168:ALA:CA	2:B:178:LEU:HB3	2.40	0.46
1:L:3:VAL:O	1:L:4:LEU:HB2	2.13	0.46
2:H:5:VAL:O	2:H:5:VAL:CG2	2.64	0.46
1:A:49:TYR:CE1	1:A:53:LYS:HB2	2.51	0.46
1:A:118:LEU:HD12	1:A:119:PHE:N	2.30	0.46
2:B:72:ASP:CG	2:B:75:LYS:HZ1	2.23	0.46
2:H:125:ALA:CB	2:H:214:LYS:HD2	2.46	0.46
2:H:148:GLU:OE1	2:H:148:GLU:HA	2.15	0.46
2:H:171:GLN:O	2:H:174:GLY:N	2.43	0.46
2:B:125:ALA:HB1	2:B:214:LYS:HB2	1.97	0.46
1:L:118:LEU:HD21	1:L:207:VAL:HG22	1.98	0.46
2:H:47:TRP:CZ2	2:H:49:ALA:HA	2.51	0.46
2:H:152:VAL:CG1	2:H:153:SER:N	2.79	0.46
1:L:177:SER:C	1:L:178:TYR:CD2	2.93	0.46
2:B:13:GLN:H	2:B:13:GLN:HE21	1.63	0.46
2:B:214:LYS:C	2:B:216:CYS:H	2.24	0.46
1:A:168:GLN:O	1:A:171:ASN:N	2.49	0.46
2:B:115:SER:O	2:B:116:THR:C	2.58	0.46
1:L:138:SER:OG	1:L:139:ASP:N	2.49	0.46
1:A:13:ALA:HB3	1:A:78:LEU:HD13	1.98	0.46
2:H:52(A):TYR:HA	2:H:71:ARG:NH1	2.30	0.45
1:L:12:SER:O	1:L:13:ALA:CB	2.64	0.45
1:L:52:SER:HB3	1:L:64:GLY:C	2.42	0.45
2:H:52(A):TYR:CG	2:H:53:ASP:N	2.83	0.45
1:A:78:LEU:HD22	1:A:106:VAL:HG22	1.98	0.45
1:A:95:LEU:O	1:A:95(A):SER:C	2.59	0.45
1:A:195:GLN:HE21	1:A:202:THR:HG21	1.81	0.45
1:L:49:TYR:CB	2:H:100(B):VAL:HG21	2.44	0.45
1:L:109:GLN:HB2	1:L:110:PRO:CD	2.43	0.45
1:L:137:ILE:CG2	1:L:196:VAL:HG11	2.46	0.45
2:H:145:TYR:HE1	2:H:176:TYR:HB2	1.75	0.45
2:B:52(A):TYR:HD1	2:B:52(A):TYR:H	1.63	0.45
1:L:39:HIS:ND1	1:L:84:ALA:HB2	2.31	0.45
1:L:198:HIS:ND1	1:L:199:GLU:HG2	2.32	0.45
1:L:129:ASN:O	1:L:129:ASN:CG	2.59	0.45
2:H:126:PRO:CB	2:H:137:ALA:O	2.65	0.45
1:A:13:ALA:HB3	1:A:78:LEU:CD1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:21:ILE:O	1:L:72:SER:HA	2.17	0.45
2:H:138:LEU:HG	2:H:182:VAL:HG13	1.99	0.45
2:H:195:ILE:CG2	2:H:210:LYS:HG2	2.43	0.45
1:A:157:LYS:O	1:A:160:VAL:HG23	2.17	0.45
2:H:124:LEU:HB2	2:H:139:GLY:C	2.41	0.45
2:H:156:SER:CA	2:H:197:ASN:HD21	2.30	0.45
1:A:46:LEU:HD11	1:A:49:TYR:HB3	1.98	0.45
1:A:88:CYS:SG	1:A:88:CYS:O	2.75	0.45
2:H:108:MET:HE3	2:H:109:VAL:O	2.17	0.45
1:A:163:THR:OG1	1:A:175:ALA:HB1	2.17	0.45
1:A:206:THR:HG22	1:A:207:VAL:N	2.32	0.45
2:H:36:TRP:HD1	2:H:69:ILE:HD12	1.82	0.45
2:H:178:LEU:C	2:H:178:LEU:CD1	2.88	0.45
1:A:46:LEU:HD22	2:B:101:ASP:HA	1.99	0.45
2:B:101:ASP:HB2	2:B:102:TYR:CD2	2.52	0.45
1:A:132:THR:CG2	2:B:141:LEU:HD21	2.47	0.45
2:B:178:LEU:HD12	2:B:178:LEU:C	2.42	0.45
2:B:75:LYS:O	2:B:76:ASN:C	2.60	0.44
2:H:185:PRO:C	2:H:187:SER:H	2.25	0.44
1:A:4:LEU:HD22	1:A:25:GLY:CA	2.44	0.44
1:L:55:PRO:HD2	1:L:58:VAL:CG2	2.44	0.44
1:L:92:ASP:C	1:L:94:SER:N	2.75	0.44
2:H:192:GLN:OE1	2:H:193:THR:N	2.50	0.44
1:L:11:VAL:CG2	1:L:21:ILE:HD11	2.47	0.44
1:A:49:TYR:O	1:A:50:ASP:C	2.58	0.44
1:L:27(B):ASN:ND2	1:L:97:LEU:CD1	2.80	0.44
1:L:49:TYR:O	1:L:50:ASP:C	2.59	0.44
1:L:119:PHE:HB2	1:L:134:VAL:HB	2.00	0.44
2:H:100(B):VAL:C	2:H:100(C):LEU:HD23	2.42	0.44
1:A:136:LEU:HG	2:B:181:VAL:HG11	2.00	0.44
1:L:140:PHE:CE1	1:L:145:VAL:CG1	2.98	0.44
2:H:97:ILE:CD1	2:B:98:ALA:CB	2.96	0.44
2:H:136:ALA:CB	2:H:184:VAL:O	2.66	0.44
2:H:189:LEU:C	2:H:191:THR:N	2.75	0.44
1:A:189:HIS:HB2	1:A:192:TYR:HE1	1.83	0.44
2:B:29:PHE:HD2	2:B:76:ASN:HA	1.82	0.44
2:B:108:MET:HE3	2:B:109:VAL:O	2.17	0.44
1:L:79:GLN:O	1:L:82:ASP:HB2	2.17	0.44
1:L:109:GLN:CB	1:L:110:PRO:HD2	2.43	0.44
1:L:137:ILE:O	1:L:174:ALA:HA	2.18	0.44
1:A:183:PRO:O	1:A:186:TRP:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:GLY:O	2:B:20:LEU:HD23	2.18	0.44
2:B:147:PRO:HB2	2:B:202:PRO:HG2	1.99	0.44
1:L:4:LEU:CD1	1:L:97:LEU:HB2	2.48	0.44
1:L:16:GLY:C	1:L:77:GLY:HA2	2.43	0.44
2:H:168:ALA:HA	2:H:178:LEU:HB3	1.98	0.44
1:A:142:PRO:O	1:A:144:ALA:N	2.51	0.44
2:H:36:TRP:NE1	2:H:80:LEU:HB2	2.33	0.43
1:A:136:LEU:HD22	1:A:136:LEU:HA	1.76	0.43
1:L:137:ILE:HG21	1:L:196:VAL:HG11	2.00	0.43
2:H:145:TYR:CZ	2:H:150:VAL:HG21	2.54	0.43
2:H:151:THR:HG23	2:H:199:ASN:HB3	2.00	0.43
2:H:163:VAL:HG13	2:H:181:VAL:O	2.18	0.43
1:A:145:VAL:HG12	1:A:198:HIS:CD2	2.53	0.43
1:L:50:ASP:O	1:L:53:LYS:HG3	2.18	0.43
1:L:131:ALA:O	1:L:180:SER:HA	2.18	0.43
2:H:51:ILE:HG22	2:H:69:ILE:CD1	2.48	0.43
1:A:19:VAL:CG1	1:A:78:LEU:HD11	2.49	0.43
2:B:163:VAL:HA	2:B:181:VAL:O	2.18	0.43
1:L:190:LYS:C	1:L:190:LYS:CD	2.90	0.43
1:A:143:GLY:HA3	1:A:173:TYR:CD1	2.52	0.43
1:A:168:GLN:HG3	1:A:170:ASN:OD1	2.19	0.43
2:B:78:LEU:HD12	2:B:79:TYR:H	1.83	0.43
2:B:168:ALA:HA	2:B:177:SER:O	2.18	0.43
2:B:29:PHE:CD2	2:B:76:ASN:HA	2.54	0.43
1:A:6:GLN:OE1	1:A:87:TYR:HA	2.18	0.43
1:A:11:VAL:HG22	1:A:102:THR:HG21	2.00	0.43
2:B:3:GLN:HB2	2:B:25:SER:O	2.18	0.43
2:B:57:LYS:C	2:B:58:TYR:HD1	2.26	0.43
2:H:123:PRO:HB3	2:H:211:VAL:HG22	2.01	0.43
2:H:147:PRO:HB2	2:H:200:HIS:CE1	2.54	0.43
2:H:126:PRO:HB3	2:H:137:ALA:O	2.19	0.43
1:A:125:GLU:O	1:A:126:LEU:C	2.61	0.43
2:B:87:THR:O	2:B:88:ALA:HB2	2.19	0.43
1:L:104:LEU:C	1:L:104:LEU:CD2	2.90	0.43
2:H:156:SER:CA	2:H:197:ASN:ND2	2.82	0.43
2:B:12:VAL:HG23	2:B:12:VAL:O	2.19	0.43
2:B:34:MET:HB3	2:B:78:LEU:HD22	2.01	0.43
1:L:50:ASP:CG	2:H:100(A):ARG:HH21	2.26	0.43
2:H:55:SER:HB2	1:A:32:TYR:OH	2.18	0.42
1:A:136:LEU:CG	2:B:181:VAL:HG11	2.49	0.42
1:A:175:ALA:C	2:B:166:PHE:HE2	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:PRO:O	2:B:187:SER:N	2.52	0.42
1:A:128:ALA:O	1:A:129:ASN:C	2.60	0.42
1:A:177:SER:OG	1:A:178:TYR:N	2.52	0.42
2:B:198:VAL:CG1	2:B:199:ASN:N	2.83	0.42
2:H:57:LYS:HD3	2:H:69:ILE:HG23	2.01	0.42
1:A:14:ALA:HB3	1:A:17:GLN:OE1	2.19	0.42
1:A:168:GLN:O	1:A:169:SER:C	2.62	0.42
1:L:125:GLU:HG3	2:H:143:LYS:NZ	2.34	0.42
2:H:27:PHE:CE2	2:H:29:PHE:HA	2.54	0.42
2:H:72:ASP:O	2:H:74:SER:N	2.53	0.42
2:H:124:LEU:HD12	2:H:140:CYS:N	2.35	0.42
1:A:127:GLN:C	1:A:129:ASN:N	2.77	0.42
2:B:63:VAL:HG11	2:B:67:PHE:CD2	2.55	0.42
2:B:90:TYR:N	2:B:90:TYR:CD1	2.88	0.42
1:L:28:ILE:C	1:L:30:ASN:N	2.77	0.42
1:L:48:ILE:HD11	1:L:62:PHE:C	2.45	0.42
1:L:114:PRO:HB2	1:L:137:ILE:HG22	2.02	0.42
1:A:136:LEU:HD13	2:B:166:PHE:CZ	2.55	0.42
2:H:172:SER:C	2:H:174:GLY:H	2.26	0.42
1:A:27(B):ASN:O	1:A:28:ILE:C	2.63	0.42
1:A:146:THR:HB	1:A:197:THR:HB	2.02	0.42
2:H:209:LYS:HD3	2:H:210:LYS:H	1.84	0.42
1:A:170:ASN:O	1:A:171:ASN:HB2	2.19	0.42
1:L:48:ILE:HD12	1:L:73:LEU:HD11	2.01	0.42
2:H:108:MET:CE	2:H:109:VAL:O	2.68	0.42
1:L:143:GLY:CA	1:L:173:TYR:HD1	2.33	0.41
2:H:77:THR:HG22	2:H:78:LEU:N	2.35	0.41
2:H:147:PRO:CB	2:H:202:PRO:CG	2.95	0.41
1:A:175:ALA:C	2:B:166:PHE:CE2	2.98	0.41
2:H:32:TYR:CE1	2:H:97:ILE:HB	2.56	0.41
2:H:95:ALA:O	2:H:96:SER:C	2.61	0.41
2:H:105:ARG:O	2:H:106:GLY:O	2.38	0.41
2:H:202:PRO:C	2:H:204:ASN:N	2.74	0.41
1:A:198:HIS:O	1:A:198:HIS:ND1	2.53	0.41
2:B:35:HIS:HB2	2:B:93:ALA:O	2.20	0.41
1:L:49:TYR:C	1:L:49:TYR:CD2	2.98	0.41
2:H:3:GLN:HB2	2:H:25:SER:OG	2.20	0.41
1:A:116:VAL:HA	1:A:136:LEU:O	2.19	0.41
2:B:96:SER:HB3	2:B:99:ALA:O	2.19	0.41
2:H:72:ASP:OD2	2:H:75:LYS:HG3	2.20	0.41
2:H:97:ILE:HG22	2:H:98:ALA:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:138:LEU:HD12	2:H:138:LEU:C	2.45	0.41
2:B:170:LEU:HD13	2:B:176:TYR:CZ	2.55	0.41
1:L:39:HIS:CE1	1:L:84:ALA:HB2	2.56	0.41
2:H:155:ASN:C	2:H:157:GLY:H	2.28	0.41
1:A:42:LYS:HE3	2:B:105:ARG:HH21	1.86	0.41
1:A:51:VAL:CG1	1:A:52:SER:H	2.28	0.41
1:A:145:VAL:HG12	1:A:198:HIS:CB	2.42	0.41
2:B:56:LYS:C	2:B:57:LYS:CG	2.94	0.41
2:B:166:PHE:HB3	2:B:167:PRO:HD2	2.02	0.41
1:L:27(B):ASN:O	1:L:30:ASN:N	2.54	0.41
2:H:38:ARG:HA	2:H:89:VAL:O	2.20	0.41
2:H:70:SER:OG	2:H:79:TYR:HB2	2.20	0.41
1:A:48:ILE:HA	1:A:53:LYS:O	2.19	0.41
2:B:182:VAL:HG22	2:B:183:THR:N	2.34	0.41
1:L:125:GLU:HG3	2:H:143:LYS:HZ3	1.86	0.41
2:B:67:PHE:CD1	2:B:82:MET:HA	2.55	0.41
2:B:72:ASP:CG	2:B:75:LYS:HE3	2.46	0.41
1:A:79:GLN:C	1:A:81:GLU:N	2.75	0.41
1:A:141:TYR:O	1:A:143:GLY:N	2.54	0.41
2:B:2:VAL:HA	2:B:26:GLY:HA3	2.02	0.41
1:L:46:LEU:HD12	1:L:47:MET:H	1.86	0.41
1:L:48:ILE:HG22	1:L:51:VAL:O	2.21	0.41
1:L:119:PHE:HA	1:L:120:PRO:HD3	1.83	0.41
1:L:164:THR:O	1:L:165:PRO:C	2.63	0.41
1:L:175:ALA:O	2:H:166:PHE:HE2	2.03	0.41
2:H:12:VAL:O	2:H:12:VAL:HG23	2.20	0.41
2:H:125:ALA:HB3	2:H:214:LYS:HD2	2.03	0.41
2:H:184:VAL:HB	2:H:185:PRO:CD	2.51	0.41
1:A:92:ASP:OD1	1:A:92:ASP:C	2.63	0.41
2:B:95:ALA:HA	2:B:100(B):VAL:O	2.20	0.41
2:B:96:SER:OG	2:B:97:ILE:N	2.54	0.41
2:B:122:PHE:CD2	2:B:143:LYS:HD3	2.56	0.41
2:B:217:ASP:OD1	2:B:217:ASP:C	2.64	0.41
1:L:92:ASP:O	1:L:93:ASP:C	2.63	0.41
1:L:127:GLN:C	1:L:129:ASN:H	2.28	0.41
2:B:97:ILE:CG2	2:B:98:ALA:N	2.83	0.41
2:H:6:GLU:CD	2:H:106:GLY:HA2	2.47	0.40
2:H:51:ILE:CD1	2:H:71:ARG:HG2	2.50	0.40
1:A:19:VAL:HG12	1:A:78:LEU:HD11	2.04	0.40
2:B:69:ILE:O	2:B:69:ILE:HG23	2.22	0.40
2:B:148:GLU:CB	2:B:149:PRO:HD3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:LEU:C	2:B:178:LEU:CD1	2.94	0.40
2:H:75:LYS:C	2:H:77:THR:N	2.76	0.40
2:H:168:ALA:CA	2:H:178:LEU:HB3	2.51	0.40
1:A:141:TYR:CB	1:A:142:PRO:HD3	2.51	0.40
1:A:143:GLY:HA3	1:A:173:TYR:CG	2.57	0.40
2:B:15:GLY:O	2:B:16:ARG:C	2.64	0.40
2:B:19:ARG:CG	2:B:19:ARG:NH1	2.83	0.40
2:B:135:THR:HB	2:B:184:VAL:O	2.21	0.40
2:B:158:ALA:O	2:B:159:LEU:C	2.64	0.40
2:B:184:VAL:HB	2:B:185:PRO:CD	2.51	0.40
1:L:46:LEU:HD12	1:L:47:MET:N	2.35	0.40
1:L:152:ASP:HB3	1:L:153:SER:H	1.65	0.40
1:L:28:ILE:O	1:L:66:LYS:HE3	2.21	0.40
1:L:142:PRO:HB2	1:L:198:HIS:CE1	2.57	0.40
2:B:95:ALA:O	2:B:96:SER:O	2.40	0.40
2:B:172:SER:O	2:B:174:GLY:N	2.54	0.40
2:H:153:SER:OG	2:H:197:ASN:ND2	2.45	0.40
2:B:29:PHE:C	2:B:31:THR:H	2.29	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	209/216 (97%)	151 (72%)	41 (20%)	17 (8%)	1	10
1	L	209/216 (97%)	147 (70%)	51 (24%)	11 (5%)	1	16
2	B	214/224 (96%)	160 (75%)	36 (17%)	18 (8%)	0	9
2	H	214/224 (96%)	156 (73%)	43 (20%)	15 (7%)	1	12
All	All	846/880 (96%)	614 (73%)	171 (20%)	61 (7%)	1	11

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	28	ILE
1	L	42	LYS
1	L	158	ALA
2	H	106	GLY
1	A	28	ILE
1	A	158	ALA
2	B	64	LYS
2	B	96	SER
2	B	136	ALA
1	L	68	GLY
1	L	143	GLY
1	L	187	LYS
2	H	73	ASN
2	H	76	ASN
2	H	192	GLN
2	H	203	SER
1	A	52	SER
1	A	124	GLU
1	A	188	SER
2	B	62	SER
2	B	76	ASN
2	B	106	GLY
2	B	116	THR
2	B	159	LEU
1	L	13	ALA
1	L	209	PRO
2	H	84	ALA
2	H	159	LEU
1	A	15	PRO
1	A	51	VAL
1	A	83	GLU
1	A	125	GLU
1	A	169	SER
2	B	26	GLY
2	B	27	PHE
2	B	44	GLY
2	B	63	VAL
2	B	88	ALA
2	B	173	SER
1	L	77	GLY
2	H	16	ARG
2	H	136	ALA
2	H	144	ASP

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Mol	Chain	Res	Type
1	A	128	ALA
1	A	143	GLY
2	B	168	ALA
2	B	214	LYS
1	L	18	LYS
1	L	51	VAL
2	H	168	ALA
2	H	202	PRO
1	A	16	GLY
1	A	95(B)	GLU
2	H	64	LYS
2	H	119	PRO
1	A	40	PRO
1	A	95(A)	SER
2	B	30	SER
2	B	150	VAL
2	H	146	PHE
1	A	155	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	179/184 (97%)	160 (89%)	19 (11%)	6	26
1	L	179/184 (97%)	157 (88%)	22 (12%)	4	21
2	B	180/185 (97%)	154 (86%)	26 (14%)	3	17
2	H	180/185 (97%)	160 (89%)	20 (11%)	6	24
All	All	718/738 (97%)	631 (88%)	87 (12%)	5	21

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	VAL
1	L	4	LEU
1	L	11	VAL

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Mol	Chain	Res	Type
1	L	26	SER
1	L	27	THR
1	L	27(A)	SER
1	L	27(B)	ASN
1	L	34	SER
1	L	50	ASP
1	L	65	SER
1	L	69	ASN
1	L	76	SER
1	L	116	VAL
1	L	117	THR
1	L	137	ILE
1	L	139	ASP
1	L	146	THR
1	L	156	VAL
1	L	182	THR
1	L	204	GLU
1	L	209	PRO
1	L	210	THR
2	H	2	VAL
2	H	5	VAL
2	H	11	VAL
2	H	17	SER
2	H	19	ARG
2	H	21	SER
2	H	25	SER
2	H	28	THR
2	H	85	GLU
2	H	97	ILE
2	H	100(A)	ARG
2	H	100(B)	VAL
2	H	100(C)	LEU
2	H	109	VAL
2	H	127	SER
2	H	141	LEU
2	H	148	GLU
2	H	159	LEU
2	H	179	SER
2	H	195	ILE
1	A	3	VAL
1	A	4	LEU
1	A	9	SER

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Mol	Chain	Res	Type
1	A	11	VAL
1	A	20	THR
1	A	27	THR
1	A	27(A)	SER
1	A	27(B)	ASN
1	A	42	LYS
1	A	48	ILE
1	A	70	SER
1	A	109	GLN
1	A	116	VAL
1	A	136	LEU
1	A	140	PHE
1	A	155	PRO
1	A	163	THR
1	A	164	THR
1	A	210	THR
2	B	5	VAL
2	B	13	GLN
2	B	19	ARG
2	B	21	SER
2	B	25	SER
2	B	30	SER
2	B	57	LYS
2	B	68	THR
2	B	75	LYS
2	B	96	SER
2	B	100(A)	ARG
2	B	100(B)	VAL
2	B	100(C)	LEU
2	B	101	ASP
2	B	110	THR
2	B	116	THR
2	B	135	THR
2	B	148	GLU
2	B	161	SER
2	B	169	VAL
2	B	178	LEU
2	B	193	THR
2	B	197	ASN
2	B	208	ASP
2	B	212	GLU
2	B	216	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	39	HIS
1	L	69	ASN
1	L	79	GLN
1	L	109	GLN
1	L	168	GLN
2	H	39	GLN
2	H	82(A)	ASN
2	H	164	HIS
2	H	197	ASN
2	H	200	HIS
1	A	30	ASN
1	A	31	ASN
1	A	38	GLN
1	A	39	HIS
1	A	129	ASN
1	A	168	GLN
1	A	195	GLN
2	B	13	GLN
2	B	35	HIS
2	B	39	GLN
2	B	155	ASN
2	B	171	GLN
2	B	197	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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	211/216 (97%)	-1.25	0 100 100	39, 78, 115, 137	0
1	L	211/216 (97%)	-1.19	0 100 100	36, 85, 139, 190	0
2	B	218/224 (97%)	-1.15	0 100 100	29, 85, 136, 199	0
2	H	218/224 (97%)	-1.11	0 100 100	29, 91, 157, 190	0
All	All	858/880 (97%)	-1.17	0 100 100	29, 83, 141, 199	0

There are no RSRZ outliers to report.

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.