WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:43 PM GMT

PDB ID : 1C5D

Title : THE CRYSTAL STRUCTURE OF THE FAB FRAGMENT OF A RAT MONOCLONAL ANTIBODY AGAINST THE MAIN IMMUNOGENIC REGION OF THE HUMAN MUSCLE ACETYLCHOLINE RECEPTOR

Authors : Kontou, M.; Leonidas, D.D.; Vatzaki, E.H.; Tsantili, P.; Mamalaki, A.; Oikonomakos, N.G.; Acharya, K.R.; Tzartos, S.J.

Deposited on : 1999-11-17
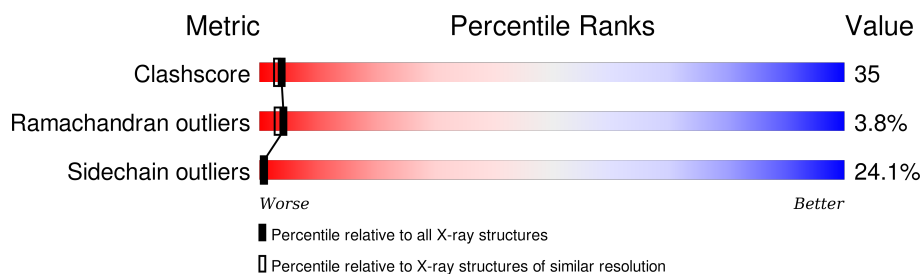
Resolution : 2.40 Å(reported)

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1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		35
Ramachandran outliers		3.8%
Sidechain outliers		24.1%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	213	31% 51% 15% •
1	L	213	51% 38% 10%
2	B	215	43% 40% 16% •
2	H	215	37% 48% 13% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6715 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 MONOCLONAL ANTIBODY AGAINST THE MAIN IM-MUNOGENIC REGION OF THE HUMAN MUSCLE ACETYLCHOLINE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total 1638	C 1022	N 276	O 332	S 8	0	0	0
1	A	213	Total 1638	C 1022	N 276	O 332	S 8	0	0	0

- Molecule 2 is a protein called MONOCLONAL ANTIBODY AGAINST THE MAIN IM-MUNOGENIC REGION OF THE HUMAN MUSCLE ACETYLCHOLINE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total 1609	C 1017	N 263	O 322	S 7	0	0	0
2	B	215	Total 1621	C 1023	N 267	O 324	S 7	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total 37	O 37	0	0
3	B	36	Total 36	O 36	0	0
3	H	41	Total 41	O 41	0	0
3	L	95	Total 95	O 95	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: MONOCLONAL ANTIBODY AGAINST THE MAIN IMMUNOGENIC REGION OF THE HUMAN MUSCLE ACETYLCHOLINE RECEPTOR
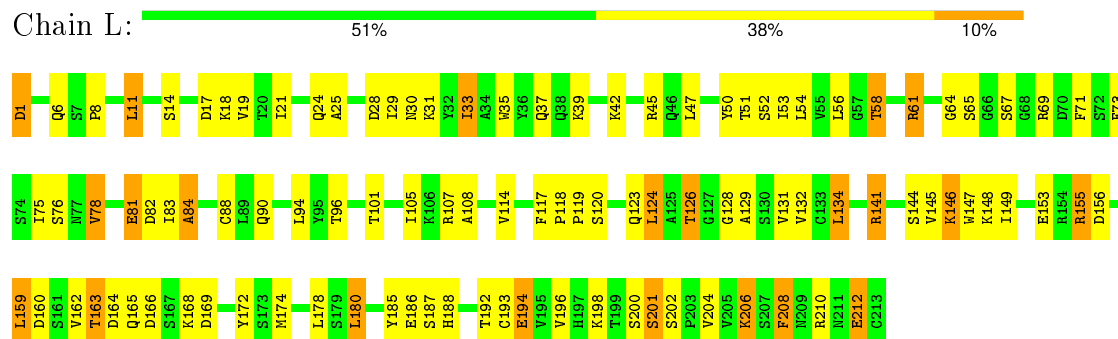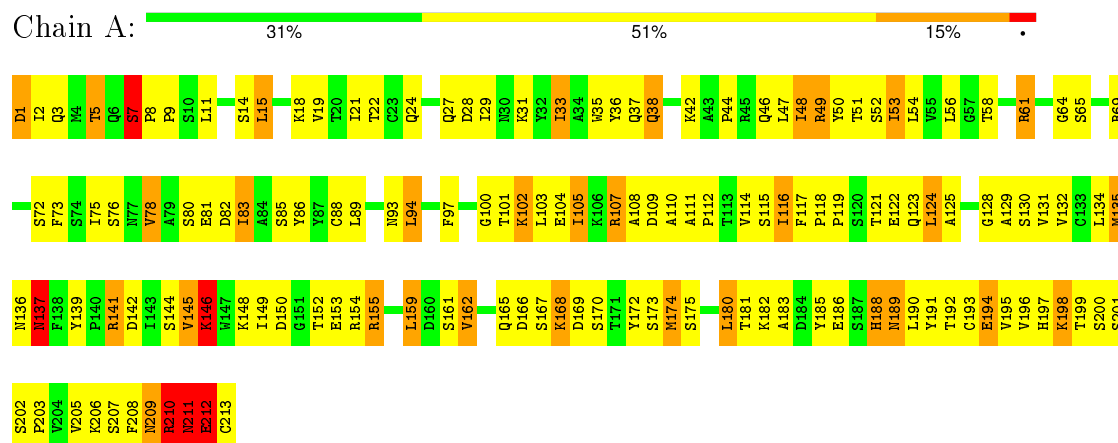
• Molecule 1: MONOCLONAL ANTIBODY AGAINST THE MAIN IMMUNOGENIC REGION OF THE HUMAN MUSCLE ACETYLCHOLINE RECEPTOR

• Molecule 2: MONOCLONAL ANTIBODY AGAINST THE MAIN IMMUNOGENIC REGION OF THE HUMAN MUSCLE ACETYLCHOLINE RECEPTOR

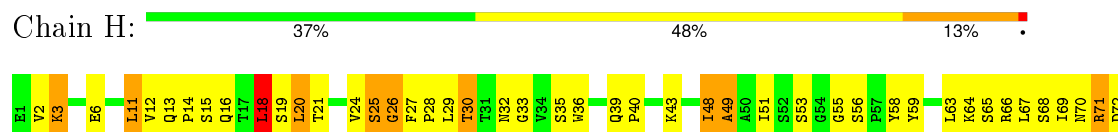T73 S74 K75 S76 Q77 V78 F79 L80 K81 M82 N83 S84 L85 Q86 T87 E88 D89 T90 A91 F94 R97 E98 D99 M102 Y103 T111 M112 V113 T114 V115 S116 S117 A118 Q119 T120 P123 Y126 P127 L128 C132 G133 D134 T135 T136 S137 S138 T139 V140 T141 L142 G143 V146

K147 G148 Y149 F150 P151 E152 P153 V154 T155 V156 T157 W158 N159 S160 G161 A162 L163 S164 S165 D166 V167 A172 Q175 S176 G177 L178 L181 T182 S183 S184 V185 S188 S192 Q193 T194 V195 T196 C197 N198 H201 P202 A203 S204 S205 T206 K207 V208 D209 K210 K211 L212 E213 R214 ARG
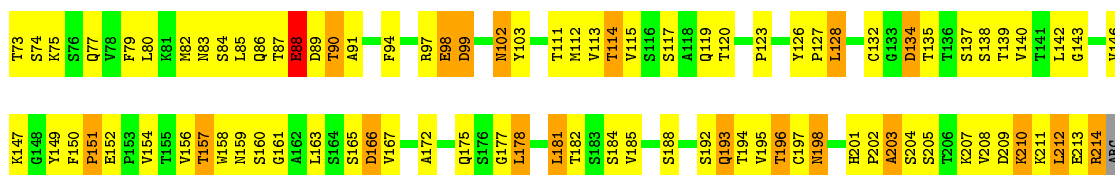
• Molecule 2: MONOCLONAL ANTIBODY AGAINST THE MAIN IMMUNOGENIC REGION OF THE HUMAN MUSCLE ACETYLCHOLINE RECEPTOR

Chain B:

43%   40%   16%   •

E1 V2 K3 S7 G8 P9 G10 L11 V12 Q13 P14 S15 Q16 T17 L18 S19 L20 V24 S25 G26 F27 P28 L29 T30 S35 W36 V37 K43 W47 I51 S61 A62 L63 R66 L67 S68 I69 N70 R71 S76 Q77 V78 K81 M82 N83 S84 L85 Q86 T87 E88

D89 T90 A91 I92 C95 T96 R97 E98 D99 G100 F104 D105 Y106 M112 V113 T114 S117 A118 Q119 T120 P123 S124 V125 Y126 P127 L128 A129 C132 T135 T136 S137 S138 T139 V140 T141 L142 G143 K147 G148 Y149 F150 P151 V154 T155 V156 T157 W158 N159 S160 L163

S164 S165 D166 V167 H168 T169 F170 P171 A172 V173 L174 Q175 S176 G177 L178 Y179 T180 L181 T182 S183 S184 V185 S188 T189 W190 P191 S192 Q193 T194 V195 T196 C197 N198 V199 A203 K207 V208 D209 K210 K211 L212 E213 R214 R215

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	79.71Å 110.08Å 199.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	76.1 (20.00-2.40)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.196 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6715	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.47	0/1671	0.73	1/2267 (0.0%)
1	L	0.50	0/1671	0.75	0/2267
2	B	0.48	0/1663	0.76	0/2277
2	H	0.51	0/1651	0.77	1/2263 (0.0%)
All	All	0.49	0/6656	0.75	2/9074 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	7	SER	N-CA-C	5.60	126.13	111.00
2	H	18	LEU	CA-CB-CG	5.47	127.88	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1638	0	1595	166	0
1	L	1638	0	1595	86	0
2	B	1621	0	1585	112	0
2	H	1609	0	1572	101	0
3	A	37	0	0	1	0
3	B	36	0	0	1	0
3	H	41	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	95	0	0	3	0
All	All	6715	0	6347	451	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 35.

All (451) 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)
1:A:212:GLU:HB2	2:B:132:CYS:HB2	1.33	1.09
1:A:194:GLU:HB2	1:A:205:VAL:HG13	1.37	1.06
2:H:28:PRO:HB2	2:H:30:THR:HG23	1.34	1.03
2:H:196:THR:HB	2:H:211:LYS:HA	1.41	1.02
2:H:40:PRO:HG2	2:H:43:LYS:HB2	1.41	1.01
1:A:124:LEU:HD12	1:A:182:LYS:HG3	1.46	0.96
2:H:13:GLN:HB2	2:H:16:GLN:HG3	1.52	0.91
2:B:11:LEU:HD12	2:B:120:THR:HG22	1.55	0.89
2:B:87:THR:O	2:B:90:THR:HG22	1.72	0.89
2:B:119:GLN:HG3	3:B:251:HOH:O	1.71	0.89
2:B:196:THR:HB	2:B:211:LYS:HA	1.55	0.88
1:A:186:GLU:HA	1:A:210:ARG:HH21	1.40	0.87
2:H:90:THR:HG22	2:H:115:VAL:H	1.37	0.87
1:A:146:LYS:HZ3	1:A:195:VAL:HA	1.38	0.86
2:H:142:LEU:HD13	2:H:195:VAL:HG21	1.59	0.85
1:A:196:VAL:HG22	1:A:203:PRO:HB3	1.56	0.84
2:B:143:GLY:O	2:B:212:LEU:HD11	1.77	0.83
2:B:142:LEU:HD13	2:B:195:VAL:HG11	1.57	0.83
2:H:87:THR:O	2:H:90:THR:HG23	1.78	0.83
1:A:145:VAL:O	1:A:146:LYS:HG2	1.78	0.83
2:B:147:LYS:CB	2:B:180:THR:HG23	2.09	0.82
2:B:2:VAL:HG13	2:B:27:PHE:CD1	2.14	0.82
2:B:147:LYS:HB2	2:B:180:THR:HG23	1.62	0.81
1:A:194:GLU:HA	1:A:205:VAL:HA	1.62	0.80
2:B:3:LYS:HG3	2:B:25:SER:HB2	1.62	0.80
1:A:112:PRO:HD3	1:A:197:HIS:ND1	1.99	0.77
2:B:98:GLU:O	2:B:100:GLY:N	2.16	0.77
1:A:146:LYS:NZ	1:A:195:VAL:HA	1.98	0.77
1:A:181:THR:HG22	1:A:183:ALA:H	1.48	0.76
1:A:145:VAL:HG13	1:A:146:LYS:H	1.48	0.76
1:L:200:SER:O	1:L:201:SER:HB3	1.83	0.76
1:A:81:GLU:HA	1:A:167:SER:OG	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:LEU:HD22	2:H:20:LEU:HD12	1.66	0.75
2:H:213:GLU:O	2:H:214:ARG:HB2	1.87	0.75
2:H:143:GLY:O	2:H:212:LEU:HD21	1.86	0.74
1:L:123:GLN:O	1:L:126:THR:HB	1.86	0.74
1:A:194:GLU:HB2	1:A:205:VAL:CG1	2.16	0.74
1:L:37:GLN:CB	1:L:47:LEU:HD21	2.17	0.74
2:B:17:THR:HB	2:B:83:ASN:HB3	1.70	0.73
2:B:142:LEU:CD1	2:B:195:VAL:HG11	2.19	0.72
2:B:96:THR:HG21	2:B:104:PHE:HA	1.70	0.72
2:B:87:THR:O	2:B:90:THR:CG2	2.38	0.71
1:A:211:ASN:O	1:A:212:GLU:HG2	1.90	0.70
1:A:7:SER:O	1:A:9:PRO:HD3	1.90	0.70
2:B:2:VAL:HG13	2:B:27:PHE:CE1	2.27	0.70
1:A:36:TYR:CZ	1:A:46:GLN:HG3	2.25	0.70
2:H:98:GLU:HG2	2:H:99:ASP:N	2.05	0.70
1:A:114:VAL:HG22	1:A:135:MET:HG2	1.74	0.69
1:L:18:LYS:HD3	3:L:242:HOH:O	1.92	0.69
2:H:90:THR:CG2	2:H:115:VAL:H	2.06	0.69
1:A:50:TYR:HB2	1:A:53:ILE:HG23	1.74	0.69
1:A:146:LYS:HZ3	1:A:195:VAL:CA	2.04	0.69
1:A:145:VAL:HG22	1:A:146:LYS:N	2.06	0.69
1:A:194:GLU:HG3	1:A:205:VAL:HG22	1.74	0.68
1:A:212:GLU:CB	2:B:132:CYS:HB2	2.18	0.68
1:L:47:LEU:HD12	1:L:58:THR:HG23	1.74	0.68
1:A:81:GLU:HA	1:A:167:SER:HG	1.58	0.68
2:B:157:THR:OG1	2:B:198:ASN:HB2	1.93	0.67
2:H:90:THR:HB	2:H:114:THR:HA	1.75	0.67
1:A:189:ASN:O	1:A:210:ARG:HB2	1.95	0.67
2:B:90:THR:HB	2:B:114:THR:HA	1.76	0.67
1:L:200:SER:O	1:L:201:SER:CB	2.42	0.67
1:L:166:ASP:HB3	1:L:169:ASP:OD1	1.95	0.67
1:A:197:HIS:HB3	1:A:199:THR:HG22	1.76	0.67
1:L:146:LYS:O	1:L:193:CYS:O	2.13	0.67
1:L:37:GLN:HB2	1:L:47:LEU:HD21	1.75	0.67
1:L:50:TYR:HB3	1:L:53:ILE:HD13	1.75	0.66
1:L:25:ALA:O	1:L:69:ARG:NH1	2.29	0.66
1:A:196:VAL:HG22	1:A:203:PRO:CB	2.26	0.66
2:H:14:PRO:O	2:H:15:SER:HB2	1.94	0.65
2:B:98:GLU:O	2:B:98:GLU:HG2	1.96	0.65
2:B:96:THR:CG2	2:B:104:PHE:HA	2.27	0.65
1:A:209:ASN:O	1:A:210:ARG:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:ARG:NH2	2:B:89:ASP:OD2	2.29	0.64
1:A:8:PRO:HD2	1:A:21:ILE:HG23	1.79	0.64
2:B:29:LEU:HD22	2:B:76:SER:HA	1.79	0.64
2:H:36:TRP:HD1	2:H:69:ILE:HD12	1.62	0.64
2:B:9:PRO:O	2:B:113:VAL:HG22	1.98	0.64
2:B:181:LEU:HD23	2:B:181:LEU:C	2.18	0.64
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.78	0.64
2:H:90:THR:HG22	2:H:115:VAL:HB	1.78	0.63
2:B:28:PRO:HB2	2:B:30:THR:OG1	1.99	0.63
1:L:117:PHE:HE1	1:L:134:LEU:HD22	1.63	0.63
2:H:165:SER:O	2:H:166:ASP:HB2	1.98	0.63
1:A:191:TYR:HE2	1:A:210:ARG:HG2	1.64	0.63
1:A:191:TYR:CE2	1:A:210:ARG:HG2	2.33	0.62
2:B:163:LEU:HD23	2:B:165:SER:OG	1.99	0.62
1:A:165:GLN:HG3	1:A:172:TYR:CZ	2.34	0.62
2:B:163:LEU:HD22	2:B:185:VAL:HG21	1.81	0.62
1:L:145:VAL:HG13	1:L:145:VAL:O	1.99	0.62
1:A:93:ASN:O	1:A:94:LEU:HB2	1.99	0.62
2:B:199:VAL:HB	2:B:208:VAL:HG13	1.82	0.61
1:L:21:ILE:HG12	1:L:101:THR:HG21	1.82	0.61
1:A:119:PRO:HB2	1:A:124:LEU:HD21	1.82	0.61
1:A:7:SER:HB3	1:A:8:PRO:HD3	1.82	0.61
1:A:149:ILE:O	1:A:152:THR:HG22	1.99	0.61
2:B:129:ALA:HB2	2:B:212:LEU:HD23	1.82	0.61
1:L:114:VAL:HA	1:L:134:LEU:O	2.01	0.61
2:B:137:SER:O	2:B:138:SER:HB2	2.01	0.61
1:L:107:ARG:HG2	1:L:108:ALA:N	2.15	0.61
2:H:193:GLN:OE1	2:H:193:GLN:HA	2.00	0.61
1:A:210:ARG:HD2	1:A:210:ARG:O	2.01	0.60
2:B:96:THR:CG2	2:B:106:TYR:O	2.49	0.60
1:L:155:ARG:NH1	1:L:155:ARG:HG2	2.15	0.60
1:L:33:ILE:HG22	1:L:51:THR:HA	1.83	0.60
2:B:164:SER:O	2:B:167:VAL:HG23	2.01	0.60
1:A:194:GLU:CB	1:A:205:VAL:HG13	2.22	0.60
2:B:189:THR:CB	2:B:193:GLN:HB2	2.31	0.60
2:H:2:VAL:HG13	2:H:27:PHE:HD2	1.66	0.60
2:B:123:PRO:HB3	2:B:149:TYR:HB3	1.83	0.60
2:H:128:LEU:HB2	2:H:143:GLY:C	2.22	0.59
1:A:121:THR:HG23	1:A:122:GLU:H	1.66	0.59
1:A:123:GLN:HE22	1:A:130:SER:HB2	1.65	0.59
1:A:118:PRO:HB3	1:A:208:PHE:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:THR:HG23	1:A:205:VAL:CG1	2.33	0.59
1:A:182:LYS:O	1:A:186:GLU:HG2	2.03	0.59
2:B:189:THR:HB	2:B:193:GLN:HB2	1.83	0.59
2:B:88:GLU:CD	2:B:88:GLU:H	2.06	0.58
2:B:147:LYS:HB3	2:B:180:THR:HG23	1.85	0.58
2:H:11:LEU:HG	2:H:151:PRO:HG3	1.85	0.58
2:H:18:LEU:HD12	2:H:82:MET:H	1.69	0.58
1:A:5:THR:HG23	1:A:24:GLN:HB3	1.86	0.58
1:A:102:LYS:NZ	1:A:102:LYS:CB	2.67	0.57
1:A:2:ILE:HD13	1:A:29:ILE:HG22	1.86	0.57
2:H:128:LEU:HB2	2:H:143:GLY:O	2.04	0.57
2:B:159:ASN:HD21	2:B:195:VAL:HA	1.69	0.57
1:A:155:ARG:CZ	1:A:155:ARG:HB3	2.34	0.57
2:B:97:ARG:HH11	2:B:99:ASP:HB3	1.68	0.57
2:H:138:SER:O	2:H:188:SER:HA	2.05	0.57
2:B:13:GLN:HG3	2:B:117:SER:HA	1.87	0.57
1:A:49:ARG:HH21	1:A:50:TYR:HE2	1.53	0.57
2:B:24:VAL:HG22	2:B:27:PHE:CZ	2.40	0.56
1:L:160:ASP:HB3	1:L:174:MET:CE	2.35	0.56
2:H:115:VAL:HG12	2:H:115:VAL:O	2.06	0.56
2:H:85:LEU:HB3	2:H:115:VAL:HG21	1.86	0.56
2:H:6:GLU:HB2	2:H:111:THR:HG23	1.87	0.56
2:B:163:LEU:CD1	2:B:195:VAL:HG23	2.35	0.56
1:L:155:ARG:HG2	1:L:155:ARG:HH11	1.70	0.56
2:B:86:GLN:O	2:B:89:ASP:HB2	2.06	0.56
2:B:165:SER:HB2	2:B:185:VAL:HG22	1.88	0.56
2:B:29:LEU:O	2:B:71:ARG:NH1	2.38	0.56
1:L:6:GLN:HE21	1:L:21:ILE:CG2	2.19	0.56
1:A:118:PRO:HB3	1:A:208:PHE:CZ	2.41	0.56
1:A:194:GLU:HB2	1:A:205:VAL:HG22	1.88	0.56
1:A:54:LEU:HD22	1:A:58:THR:HG21	1.88	0.56
1:A:38:GLN:HG3	1:A:44:PRO:HA	1.88	0.56
1:L:159:LEU:O	1:L:159:LEU:HD23	2.06	0.56
2:H:39:GLN:C	2:H:91:ALA:HB1	2.27	0.56
1:L:132:VAL:HG21	2:H:128:LEU:HD11	1.87	0.56
2:H:48:ILE:O	2:H:49:ALA:O	2.23	0.56
1:L:123:GLN:HG3	2:H:126:TYR:CE2	2.42	0.55
2:B:214:ARG:H	2:B:214:ARG:HD3	1.70	0.55
2:H:24:VAL:HB	2:H:29:LEU:HD11	1.87	0.55
1:A:189:ASN:HD22	1:A:210:ARG:HB3	1.72	0.55
2:B:96:THR:HG23	2:B:106:TYR:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:NH2	1:A:110:ALA:HB2	2.22	0.55
2:B:18:LEU:HD11	2:B:20:LEU:CD2	2.37	0.55
2:H:167:VAL:HG22	2:H:185:VAL:HG23	1.89	0.55
1:L:17:ASP:O	1:L:78:VAL:HG22	2.06	0.55
1:A:124:LEU:HD12	1:A:182:LYS:CG	2.30	0.55
2:B:128:LEU:C	2:B:212:LEU:HD21	2.27	0.55
2:H:123:PRO:HB3	2:H:149:TYR:HB3	1.88	0.55
1:A:186:GLU:CA	1:A:210:ARG:HH21	2.17	0.55
1:L:141:ARG:HG3	1:L:172:TYR:CD1	2.42	0.55
1:A:144:SER:CB	1:A:146:LYS:HZ1	2.21	0.54
1:A:119:PRO:HB2	1:A:124:LEU:CD2	2.37	0.54
1:A:102:LYS:HB2	1:A:102:LYS:NZ	2.23	0.54
2:B:18:LEU:HD11	2:B:20:LEU:HD21	1.89	0.54
2:H:13:GLN:HB2	2:H:16:GLN:CG	2.32	0.54
1:L:180:LEU:HD12	1:L:180:LEU:N	2.22	0.54
1:A:166:ASP:C	1:A:168:LYS:H	2.11	0.54
1:A:194:GLU:HG3	1:A:203:PRO:HB2	1.88	0.54
2:B:163:LEU:HD22	2:B:185:VAL:CG2	2.37	0.54
1:A:146:LYS:HG2	1:A:194:GLU:O	2.08	0.54
2:B:163:LEU:C	2:B:165:SER:H	2.11	0.54
1:L:117:PHE:CE1	1:L:134:LEU:HD22	2.41	0.54
2:B:51:ILE:HB	2:B:69:ILE:HG12	1.88	0.54
1:A:129:ALA:HB3	1:A:180:LEU:HD12	1.89	0.54
2:B:11:LEU:HD23	2:B:114:THR:O	2.08	0.54
1:A:36:TYR:CE2	1:A:46:GLN:HG3	2.43	0.54
1:L:147:TRP:O	1:L:153:GLU:HA	2.07	0.53
1:A:123:GLN:HG2	1:A:128:GLY:O	2.08	0.53
1:L:19:VAL:HG22	1:L:75:ILE:HB	1.90	0.53
2:B:2:VAL:HG13	2:B:27:PHE:HD1	1.73	0.53
1:L:194:GLU:HA	1:L:204:VAL:O	2.09	0.53
1:A:83:ILE:HD11	1:A:105:ILE:HB	1.90	0.53
2:H:98:GLU:HG3	2:H:103:TYR:CE2	2.43	0.53
2:H:181:LEU:HD23	2:H:181:LEU:C	2.28	0.53
1:A:146:LYS:NZ	1:A:196:VAL:H	2.07	0.53
2:H:142:LEU:HD22	2:H:212:LEU:HD12	1.91	0.53
1:A:61:ARG:NH1	1:A:82:ASP:OD2	2.40	0.53
1:A:75:ILE:HG21	1:A:78:VAL:HG13	1.91	0.53
1:A:103:LEU:HD23	1:A:103:LEU:C	2.30	0.52
2:H:40:PRO:HA	2:H:91:ALA:HB2	1.90	0.52
2:B:213:GLU:HB3	2:B:214:ARG:HD3	1.90	0.52
2:H:40:PRO:HG2	2:H:43:LYS:CB	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:MET:HG3	1:A:175:SER:N	2.25	0.52
2:H:90:THR:HG22	2:H:115:VAL:N	2.16	0.52
2:H:213:GLU:O	2:H:214:ARG:CB	2.57	0.52
2:B:125:VAL:HG21	2:B:208:VAL:HG11	1.90	0.52
1:A:194:GLU:CG	1:A:205:VAL:HG22	2.39	0.52
2:H:40:PRO:HA	2:H:91:ALA:CB	2.40	0.52
2:H:201:HIS:CE1	2:H:203:ALA:HB3	2.44	0.52
1:A:202:SER:HB2	1:A:203:PRO:CD	2.40	0.52
2:H:86:GLN:O	2:H:89:ASP:HB2	2.09	0.52
2:B:128:LEU:O	2:B:212:LEU:HD21	2.10	0.52
1:L:160:ASP:HB3	1:L:174:MET:HE3	1.90	0.52
2:B:140:VAL:HG11	2:B:190:TRP:CZ3	2.44	0.52
1:L:188:HIS:O	1:L:210:ARG:NH1	2.42	0.52
1:L:123:GLN:O	1:L:126:THR:CB	2.56	0.51
1:A:198:LYS:N	1:A:198:LYS:HD3	2.24	0.51
2:B:1:GLU:HA	2:B:1:GLU:OE1	2.11	0.51
1:L:8:PRO:HG3	1:L:11:LEU:HD22	1.91	0.51
1:L:114:VAL:O	1:L:206:LYS:HD3	2.09	0.51
1:A:83:ILE:HA	1:A:103:LEU:HD22	1.92	0.51
2:H:21:THR:HG1	2:H:79:PHE:HD1	1.58	0.51
1:L:149:ILE:HD11	1:L:178:LEU:HD21	1.93	0.51
1:A:146:LYS:HZ3	1:A:196:VAL:N	2.09	0.51
1:L:118:PRO:HB3	1:L:208:PHE:CZ	2.45	0.51
2:B:150:PHE:CE1	2:B:151:PRO:HB3	2.46	0.51
2:B:96:THR:HG22	2:B:106:TYR:O	2.11	0.51
2:H:2:VAL:HG13	2:H:27:PHE:CD2	2.46	0.51
1:L:61:ARG:HG2	1:L:61:ARG:HH11	1.75	0.51
1:A:132:VAL:HG12	1:A:134:LEU:HD13	1.93	0.51
1:A:15:LEU:HD13	1:A:78:VAL:O	2.10	0.50
1:L:146:LYS:HE2	1:L:196:VAL:HG23	1.93	0.50
2:H:49:ALA:HA	2:H:58:TYR:O	2.12	0.50
1:A:194:GLU:CA	1:A:205:VAL:HA	2.35	0.50
1:L:118:PRO:HB3	1:L:208:PHE:CE1	2.47	0.50
2:B:169:THR:HA	2:B:183:SER:HA	1.91	0.50
1:A:117:PHE:CB	2:B:128:LEU:HD22	2.42	0.50
1:L:126:THR:HG22	1:L:128:GLY:H	1.77	0.50
1:A:210:ARG:HD2	1:A:210:ARG:C	2.32	0.50
2:H:87:THR:C	2:H:89:ASP:H	2.15	0.50
2:H:202:PRO:O	2:H:204:SER:N	2.45	0.50
2:B:3:LYS:CG	2:B:25:SER:HB2	2.37	0.50
1:A:19:VAL:HG22	1:A:75:ILE:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:39:LYS:HD3	1:L:84:ALA:HB2	1.94	0.49
1:L:163:THR:HG23	1:L:164:ASP:N	2.27	0.49
1:L:1:ASP:OD1	1:L:1:ASP:N	2.45	0.49
2:H:146:VAL:HG11	2:H:154:VAL:HG21	1.94	0.49
2:H:6:GLU:OE2	2:H:94:PHE:HA	2.11	0.49
1:A:182:LYS:O	1:A:186:GLU:CG	2.61	0.49
1:A:18:LYS:HA	1:A:75:ILE:O	2.11	0.49
1:A:145:VAL:HG13	1:A:146:LYS:N	2.22	0.49
2:H:28:PRO:O	2:H:32:ASN:HB2	2.12	0.49
2:H:87:THR:O	2:H:89:ASP:N	2.45	0.49
2:H:59:TYR:CE1	2:H:69:ILE:HG22	2.48	0.49
2:H:157:THR:OG1	2:H:198:ASN:OD1	2.29	0.49
2:H:48:ILE:CG2	2:H:63:LEU:HD12	2.43	0.49
1:A:11:LEU:CD1	1:A:19:VAL:HB	2.43	0.49
2:B:174:LEU:HA	2:B:178:LEU:O	2.13	0.49
1:A:136:ASN:HB3	1:A:137:ASN:OD1	2.12	0.49
1:A:209:ASN:HB3	1:A:212:GLU:OE2	2.13	0.48
1:L:186:GLU:HA	1:L:210:ARG:HD2	1.95	0.48
1:L:29:ILE:HD11	1:L:71:PHE:CE1	2.48	0.48
1:L:37:GLN:HB3	1:L:47:LEU:HD21	1.94	0.48
2:H:48:ILE:HG22	2:H:63:LEU:HD12	1.95	0.48
1:A:166:ASP:HB3	1:A:169:ASP:OD1	2.14	0.48
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.49	0.48
1:A:114:VAL:HG22	1:A:135:MET:CG	2.43	0.48
2:H:55:GLY:HA3	2:H:71:ARG:NH1	2.29	0.48
1:A:49:ARG:HD3	1:A:53:ILE:HG13	1.96	0.48
1:A:35:TRP:HB2	1:A:48:ILE:HB	1.94	0.48
2:H:36:TRP:CD1	2:H:69:ILE:HD12	2.46	0.48
1:L:155:ARG:HH11	1:L:155:ARG:CG	2.26	0.48
2:H:43:LYS:HE3	3:H:226:HOH:O	2.12	0.48
2:B:83:ASN:O	2:B:84:SER:HB2	2.14	0.47
1:A:102:LYS:HB2	1:A:102:LYS:HZ2	1.79	0.47
2:H:48:ILE:HB	2:H:67:LEU:HD11	1.96	0.47
2:H:202:PRO:C	2:H:204:SER:H	2.17	0.47
1:A:136:ASN:ND2	1:A:173:SER:HB3	2.28	0.47
1:A:212:GLU:HG3	2:B:132:CYS:SG	2.54	0.47
2:B:137:SER:O	2:B:138:SER:CB	2.62	0.47
1:L:124:LEU:C	1:L:126:THR:H	2.17	0.47
2:H:73:THR:HG23	2:H:74:SER:N	2.28	0.47
1:A:123:GLN:NE2	1:A:130:SER:HB2	2.30	0.47
1:A:189:ASN:HA	1:A:210:ARG:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:SER:HB3	1:A:8:PRO:CD	2.44	0.47
1:A:189:ASN:ND2	1:A:210:ARG:HB3	2.29	0.47
2:H:214:ARG:HA	2:H:214:ARG:HD2	1.53	0.47
1:A:122:GLU:O	1:A:125:ALA:HB3	2.15	0.47
1:A:2:ILE:HG12	1:A:27:GLN:HB2	1.96	0.47
2:B:12:VAL:HG12	2:B:13:GLN:N	2.30	0.47
1:A:123:GLN:HE22	1:A:130:SER:CB	2.27	0.47
1:A:146:LYS:NZ	1:A:196:VAL:N	2.63	0.47
1:L:120:SER:HB3	2:H:127:PRO:HD2	1.96	0.47
1:A:114:VAL:HG21	1:A:195:VAL:CG2	2.44	0.47
1:L:56:LEU:HD23	1:L:56:LEU:N	2.30	0.47
2:H:90:THR:O	2:H:91:ALA:HB2	2.15	0.47
2:B:167:VAL:HG22	2:B:185:VAL:HG23	1.97	0.47
1:L:129:ALA:HB3	1:L:180:LEU:CD1	2.45	0.46
1:L:83:ILE:O	1:L:84:ALA:HB2	2.15	0.46
1:A:33:ILE:HG22	1:A:51:THR:HA	1.97	0.46
1:A:189:ASN:O	1:A:209:ASN:O	2.34	0.46
2:H:160:SER:N	2:H:198:ASN:OD1	2.40	0.46
1:A:209:ASN:CB	1:A:212:GLU:OE2	2.63	0.46
2:B:167:VAL:HA	2:B:184:SER:O	2.16	0.46
2:H:152:GLU:OE2	2:H:172:ALA:HB3	2.16	0.46
1:A:121:THR:HG23	1:A:122:GLU:N	2.30	0.46
1:A:83:ILE:HA	1:A:103:LEU:CD2	2.46	0.46
1:A:149:ILE:O	1:A:152:THR:CG2	2.64	0.46
2:H:98:GLU:O	2:H:102:ASN:O	2.34	0.46
2:H:137:SER:C	2:H:139:THR:H	2.19	0.46
1:L:180:LEU:HD13	1:L:185:TYR:HB2	1.98	0.45
1:A:188:HIS:ND1	1:A:188:HIS:N	2.64	0.45
1:A:209:ASN:O	1:A:210:ARG:CB	2.64	0.45
1:A:103:LEU:HD23	1:A:103:LEU:O	2.15	0.45
1:L:212:GLU:O	2:H:132:CYS:HA	2.16	0.45
2:H:88:GLU:HA	3:H:224:HOH:O	2.15	0.45
2:B:104:PHE:N	2:B:104:PHE:CD1	2.84	0.45
1:A:2:ILE:HD13	1:A:29:ILE:CG2	2.45	0.45
2:H:127:PRO:HG3	2:H:210:LYS:HD3	1.98	0.45
1:L:168:LYS:HE2	1:L:168:LYS:HB3	1.73	0.45
1:A:146:LYS:O	1:A:193:CYS:O	2.34	0.45
1:A:89:LEU:HD13	1:A:97:PHE:CZ	2.51	0.45
2:H:3:LYS:HB2	2:H:3:LYS:HE3	1.81	0.45
2:B:28:PRO:C	2:B:30:THR:H	2.19	0.45
2:B:99:ASP:C	2:B:99:ASP:OD1	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:PRO:HD2	2:B:203:ALA:CB	2.46	0.45
1:L:61:ARG:NH2	1:L:82:ASP:OD1	2.42	0.45
1:A:5:THR:CG2	1:A:24:GLN:HB3	2.46	0.45
2:B:18:LEU:O	2:B:81:LYS:HA	2.17	0.45
2:B:174:LEU:HG	2:B:174:LEU:O	2.17	0.45
1:A:7:SER:O	1:A:9:PRO:CD	2.64	0.45
2:H:208:VAL:HG22	2:H:209:ASP:N	2.32	0.45
1:A:86:TYR:O	1:A:100:GLY:HA2	2.17	0.45
2:B:37:VAL:HG22	2:B:47:TRP:HA	1.99	0.45
1:A:132:VAL:CG1	1:A:134:LEU:HD13	2.47	0.45
1:A:22:THR:HA	1:A:72:SER:HA	1.97	0.45
1:L:107:ARG:HG2	1:L:108:ALA:H	1.79	0.44
1:L:94:LEU:HD12	1:L:94:LEU:HA	1.77	0.44
2:B:123:PRO:CB	2:B:149:TYR:HB3	2.47	0.44
1:L:61:ARG:CG	1:L:61:ARG:HH11	2.31	0.44
1:A:194:GLU:CB	1:A:205:VAL:HG22	2.46	0.44
2:B:2:VAL:HA	2:B:26:GLY:HA3	1.99	0.44
2:H:177:GLY:O	2:H:178:LEU:HD13	2.17	0.44
2:H:51:ILE:HA	2:H:56:SER:O	2.17	0.44
1:A:192:THR:HG23	1:A:205:VAL:HG13	1.99	0.44
2:B:87:THR:O	2:B:89:ASP:N	2.50	0.44
2:H:195:VAL:HG23	2:H:195:VAL:O	2.17	0.44
2:B:163:LEU:HD11	2:B:195:VAL:HG23	1.99	0.44
1:L:124:LEU:C	1:L:126:THR:N	2.70	0.44
1:L:180:LEU:HD12	1:L:180:LEU:H	1.83	0.44
1:A:180:LEU:CD1	1:A:185:TYR:HB2	2.48	0.44
1:A:141:ARG:HH22	1:A:162:VAL:HB	1.82	0.44
1:A:192:THR:HA	1:A:207:SER:OG	2.17	0.44
1:A:102:LYS:HB3	1:A:102:LYS:HZ3	1.81	0.44
2:B:213:GLU:HA	2:B:213:GLU:OE1	2.18	0.44
2:H:24:VAL:CB	2:H:29:LEU:HD11	2.47	0.44
1:L:162:VAL:HG23	3:L:276:HOH:O	2.16	0.44
2:H:67:LEU:HD22	2:H:80:LEU:HD11	2.00	0.44
1:A:35:TRP:CE2	1:A:73:PHE:HB2	2.53	0.44
1:L:200:SER:HB2	1:L:202:SER:O	2.18	0.44
2:B:92:ILE:CD1	2:B:112:MET:HG2	2.48	0.44
1:A:1:ASP:OD2	2:B:61:SER:HB2	2.18	0.44
2:B:181:LEU:HD23	2:B:181:LEU:O	2.18	0.43
1:A:35:TRP:CZ3	1:A:88:CYS:HB3	2.53	0.43
1:A:211:ASN:O	1:A:212:GLU:O	2.36	0.43
1:A:111:ALA:HA	1:A:199:THR:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:123:GLN:HG3	2:H:126:TYR:CZ	2.54	0.43
2:B:123:PRO:CA	2:B:149:TYR:HB3	2.48	0.43
1:A:107:ARG:HG2	1:A:139:TYR:CD2	2.53	0.43
1:A:123:GLN:HB2	2:B:126:TYR:CE1	2.54	0.43
1:A:212:GLU:O	1:A:213:CYS:O	2.35	0.43
1:A:54:LEU:HD22	1:A:58:THR:CG2	2.49	0.43
1:A:29:ILE:HD11	1:A:33:ILE:HG13	2.00	0.43
1:L:164:ASP:O	1:L:165:GLN:C	2.56	0.43
1:A:159:LEU:HD13	2:B:173:VAL:HG21	1.99	0.43
1:A:7:SER:HB2	3:A:226:HOH:O	2.18	0.43
1:A:150:ASP:HA	1:A:190:LEU:HB3	1.99	0.43
2:B:189:THR:OG1	2:B:193:GLN:HB2	2.18	0.43
2:B:69:ILE:O	2:B:69:ILE:HG23	2.19	0.43
2:B:170:PHE:HB2	2:B:182:THR:O	2.18	0.43
1:A:146:LYS:CG	1:A:194:GLU:O	2.67	0.43
1:A:8:PRO:O	1:A:101:THR:OG1	2.22	0.43
2:H:195:VAL:CG2	2:H:195:VAL:O	2.66	0.43
1:L:146:LYS:HE2	1:L:196:VAL:CG2	2.48	0.43
1:L:35:TRP:CH2	1:L:88:CYS:HB3	2.53	0.43
1:A:102:LYS:CB	1:A:102:LYS:HZ3	2.31	0.43
1:L:78:VAL:HB	1:L:105:ILE:HD11	2.00	0.43
1:L:185:TYR:CZ	1:L:210:ARG:HG3	2.54	0.43
1:L:81:GLU:OE1	1:A:56:LEU:HD21	2.19	0.43
2:B:175:GLN:HB2	2:B:175:GLN:HE21	1.72	0.43
2:B:35:SER:O	2:B:95:CYS:HA	2.18	0.43
2:H:159:ASN:C	2:H:161:GLY:H	2.22	0.43
1:A:52:SER:HB3	1:A:64:GLY:O	2.19	0.42
2:H:86:GLN:HB2	2:H:88:GLU:OE2	2.19	0.42
2:B:96:THR:HG21	2:B:104:PHE:CA	2.44	0.42
1:L:18:LYS:CD	3:L:242:HOH:O	2.61	0.42
1:L:141:ARG:HG3	1:L:172:TYR:CG	2.54	0.42
2:B:11:LEU:HA	2:B:114:THR:O	2.19	0.42
2:B:195:VAL:HG13	2:B:195:VAL:O	2.20	0.42
1:A:50:TYR:HB2	1:A:53:ILE:CG2	2.45	0.42
2:H:33:GLY:HA3	2:H:98:GLU:OE1	2.20	0.42
1:A:18:LYS:HB2	1:A:76:SER:HA	2.02	0.42
1:L:119:PRO:HD3	1:L:131:VAL:HG22	2.01	0.42
2:B:43:LYS:HA	2:B:43:LYS:HD2	1.90	0.42
1:A:145:VAL:HG22	1:A:146:LYS:H	1.82	0.42
2:H:98:GLU:CG	2:H:99:ASP:N	2.81	0.42
1:L:33:ILE:HD11	1:L:88:CYS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:PRO:C	2:B:16:GLN:H	2.23	0.42
2:B:163:LEU:HD23	2:B:165:SER:CB	2.50	0.41
2:H:18:LEU:CD2	2:H:20:LEU:HD12	2.44	0.41
2:H:158:TRP:CH2	2:H:197:CYS:HB3	2.55	0.41
2:B:158:TRP:CH2	2:B:197:CYS:HB3	2.54	0.41
1:A:146:LYS:HZ1	1:A:196:VAL:H	1.67	0.41
1:L:45:ARG:O	1:L:47:LEU:HD22	2.19	0.41
2:H:210:LYS:HB2	2:H:210:LYS:HE2	1.68	0.41
2:H:25:SER:HB3	2:H:26:GLY:H	1.61	0.41
1:L:29:ILE:O	1:L:30:ASN:HB2	2.20	0.41
2:H:140:VAL:HG23	2:H:142:LEU:HG	2.02	0.41
1:A:165:GLN:HE21	1:A:170:SER:CA	2.33	0.41
1:L:145:VAL:O	1:L:145:VAL:CG1	2.67	0.41
2:H:48:ILE:O	2:H:48:ILE:HG12	2.20	0.41
1:L:148:LYS:HB2	1:L:192:THR:HB	2.03	0.41
1:A:119:PRO:HG3	1:A:130:SER:N	2.35	0.41
2:B:98:GLU:O	2:B:98:GLU:CG	2.65	0.41
1:L:50:TYR:O	1:L:52:SER:N	2.46	0.41
2:H:87:THR:C	2:H:89:ASP:N	2.73	0.41
2:H:12:VAL:HG12	2:H:16:GLN:HB2	2.03	0.41
1:L:141:ARG:HG3	1:L:172:TYR:CE1	2.55	0.41
1:A:116:ILE:HG13	1:A:117:PHE:N	2.36	0.41
1:L:52:SER:HB3	1:L:64:GLY:O	2.20	0.41
1:A:35:TRP:CH2	1:A:88:CYS:HB3	2.55	0.41
2:H:18:LEU:HD12	2:H:82:MET:N	2.33	0.41
2:H:20:LEU:HD11	2:H:113:VAL:HG21	2.02	0.41
2:H:150:PHE:HA	2:H:151:PRO:HA	1.79	0.41
2:B:12:VAL:HG11	2:B:85:LEU:CD1	2.50	0.41
1:A:11:LEU:HD13	1:A:19:VAL:HB	2.02	0.41
2:B:170:PHE:O	2:B:171:PRO:C	2.59	0.41
1:A:135:MET:SD	1:A:195:VAL:HG11	2.61	0.41
1:A:146:LYS:HZ3	1:A:195:VAL:C	2.24	0.41
1:A:61:ARG:NH1	1:A:82:ASP:OD1	2.54	0.41
2:H:72:ASP:OD1	2:H:74:SER:HB3	2.21	0.41
1:L:90:GLN:HG3	1:L:96:THR:HB	2.03	0.41
2:B:105:ASP:N	2:B:105:ASP:OD1	2.46	0.41
2:H:70:ASN:HB2	3:H:249:HOH:O	2.21	0.41
2:B:36:TRP:HE1	2:B:78:VAL:HG12	1.85	0.41
1:A:194:GLU:HB2	1:A:205:VAL:CB	2.51	0.40
1:L:186:GLU:HA	1:L:210:ARG:CD	2.50	0.40
1:A:149:ILE:HG23	1:A:191:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2:VAL:CG1	2:H:27:PHE:CD2	3.05	0.40
1:A:14:SER:O	1:A:15:LEU:C	2.59	0.40
1:A:211:ASN:HB2	1:A:212:GLU:H	1.53	0.40
1:A:117:PHE:CG	2:B:128:LEU:HD22	2.56	0.40
1:A:200:SER:C	1:A:202:SER:H	2.25	0.40
1:A:197:HIS:CG	1:A:199:THR:HG22	2.55	0.40
1:A:8:PRO:O	1:A:101:THR:HG23	2.21	0.40
2:B:214:ARG:O	2:B:215:ARG:CB	2.69	0.40
2:B:63:LEU:O	2:B:67:LEU:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	211/213 (99%)	179 (85%)	19 (9%)	13 (6%)	2	0
1	L	211/213 (99%)	194 (92%)	13 (6%)	4 (2%)	10	12
2	B	213/215 (99%)	186 (87%)	20 (9%)	7 (3%)	5	4
2	H	212/215 (99%)	180 (85%)	24 (11%)	8 (4%)	4	3
All	All	847/856 (99%)	739 (87%)	76 (9%)	32 (4%)	4	3

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	201	SER
1	L	212	GLU
2	H	49	ALA
1	A	211	ASN
1	A	212	GLU
2	B	99	ASP

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Mol	Chain	Res	Type
2	B	165	SER
2	B	213	GLU
1	L	84	ALA
2	H	84	SER
2	H	88	GLU
2	H	163	LEU
2	H	203	ALA
1	A	137	ASN
1	A	194	GLU
1	A	209	ASN
1	A	210	ARG
2	B	138	SER
2	H	134	ASP
1	A	108	ALA
2	B	88	GLU
2	B	176	SER
1	L	194	GLU
2	H	151	PRO
1	A	94	LEU
1	A	145	VAL
1	A	146	LYS
1	A	28	ASP
2	H	26	GLY
1	A	7	SER
1	A	83	ILE
2	B	191	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/187 (100%)	137 (73%)	50 (27%)	0	0
1	L	187/187 (100%)	155 (83%)	32 (17%)	2	3
2	B	187/187 (100%)	140 (75%)	47 (25%)	1	1
2	H	186/187 (100%)	135 (73%)	51 (27%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	747/748 (100%)	567 (76%)	180 (24%)	1 1

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	11	LEU
1	L	14	SER
1	L	24	GLN
1	L	28	ASP
1	L	31	LYS
1	L	33	ILE
1	L	42	LYS
1	L	54	LEU
1	L	58	THR
1	L	61	ARG
1	L	65	SER
1	L	67	SER
1	L	73	PHE
1	L	76	SER
1	L	78	VAL
1	L	81	GLU
1	L	124	LEU
1	L	126	THR
1	L	134	LEU
1	L	141	ARG
1	L	144	SER
1	L	146	LYS
1	L	155	ARG
1	L	156	ASP
1	L	159	LEU
1	L	163	THR
1	L	180	LEU
1	L	187	SER
1	L	198	LYS
1	L	206	LYS
1	L	208	PHE
2	H	3	LYS
2	H	11	LEU
2	H	18	LEU
2	H	19	SER
2	H	20	LEU

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Mol	Chain	Res	Type
2	H	25	SER
2	H	30	THR
2	H	35	SER
2	H	48	ILE
2	H	53	SER
2	H	64	LYS
2	H	65	SER
2	H	66	ARG
2	H	68	SER
2	H	71	ARG
2	H	75	LYS
2	H	77	GLN
2	H	83	ASN
2	H	88	GLU
2	H	90	THR
2	H	97	ARG
2	H	98	GLU
2	H	99	ASP
2	H	102	ASN
2	H	112	MET
2	H	114	THR
2	H	117	SER
2	H	119	GLN
2	H	120	THR
2	H	128	LEU
2	H	134	ASP
2	H	135	THR
2	H	147	LYS
2	H	156	VAL
2	H	157	THR
2	H	166	ASP
2	H	175	GLN
2	H	178	LEU
2	H	181	LEU
2	H	182	THR
2	H	184	SER
2	H	192	SER
2	H	193	GLN
2	H	194	THR
2	H	196	THR
2	H	198	ASN
2	H	205	SER

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Mol	Chain	Res	Type
2	H	207	LYS
2	H	210	LYS
2	H	212	LEU
2	H	214	ARG
1	A	1	ASP
1	A	3	GLN
1	A	5	THR
1	A	7	SER
1	A	15	LEU
1	A	31	LYS
1	A	33	ILE
1	A	38	GLN
1	A	42	LYS
1	A	48	ILE
1	A	49	ARG
1	A	53	ILE
1	A	61	ARG
1	A	65	SER
1	A	69	ARG
1	A	78	VAL
1	A	80	SER
1	A	85	SER
1	A	102	LYS
1	A	104	GLU
1	A	105	ILE
1	A	107	ARG
1	A	109	ASP
1	A	115	SER
1	A	116	ILE
1	A	124	LEU
1	A	131	VAL
1	A	135	MET
1	A	137	ASN
1	A	141	ARG
1	A	142	ASP
1	A	146	LYS
1	A	148	LYS
1	A	153	GLU
1	A	154	ARG
1	A	155	ARG
1	A	159	LEU
1	A	161	SER

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Mol	Chain	Res	Type
1	A	162	VAL
1	A	168	LYS
1	A	174	MET
1	A	180	LEU
1	A	188	HIS
1	A	189	ASN
1	A	198	LYS
1	A	201	SER
1	A	206	LYS
1	A	210	ARG
1	A	211	ASN
1	A	212	GLU
2	B	1	GLU
2	B	3	LYS
2	B	7	SER
2	B	11	LEU
2	B	13	GLN
2	B	16	GLN
2	B	17	THR
2	B	19	SER
2	B	29	LEU
2	B	35	SER
2	B	43	LYS
2	B	61	SER
2	B	66	ARG
2	B	68	SER
2	B	70	ASN
2	B	83	ASN
2	B	90	THR
2	B	92	ILE
2	B	96	THR
2	B	97	ARG
2	B	98	GLU
2	B	99	ASP
2	B	120	THR
2	B	135	THR
2	B	138	SER
2	B	139	THR
2	B	154	VAL
2	B	156	VAL
2	B	160	SER
2	B	163	LEU

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Mol	Chain	Res	Type
2	B	174	LEU
2	B	175	GLN
2	B	178	LEU
2	B	181	LEU
2	B	184	SER
2	B	185	VAL
2	B	188	SER
2	B	193	GLN
2	B	196	THR
2	B	199	VAL
2	B	207	LYS
2	B	208	VAL
2	B	209	ASP
2	B	210	LYS
2	B	212	LEU
2	B	214	ARG
2	B	215	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	24	GLN
1	L	37	GLN
1	L	136	ASN
1	L	137	ASN
2	H	77	GLN
2	H	86	GLN
1	A	27	GLN
1	A	38	GLN
1	A	165	GLN
1	A	189	ASN
2	B	39	GLN
2	B	86	GLN
2	B	159	ASN
2	B	175	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.