



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:36 PM UTC

PDB ID : 1C5D / pdb_00001c5d
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)

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

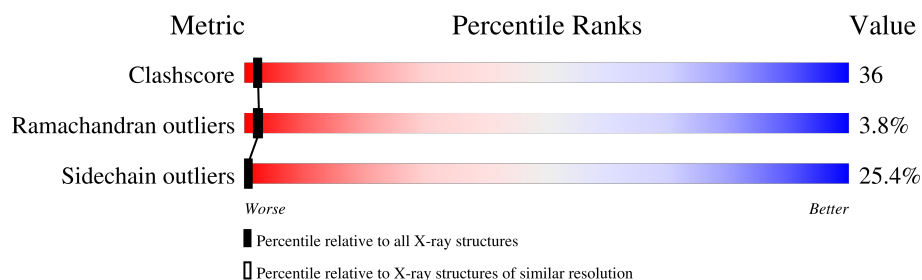
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 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	A	213	
1	L	213	
2	B	215	
2	H	215	

2 Entry composition

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 IMMUNOGENIC REGION OF THE HUMAN MUSCLE ACETYLCHOLINE RECEPTOR.

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

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

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

- Molecule 3 is water.

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

3 Residue-property plots [i](#)

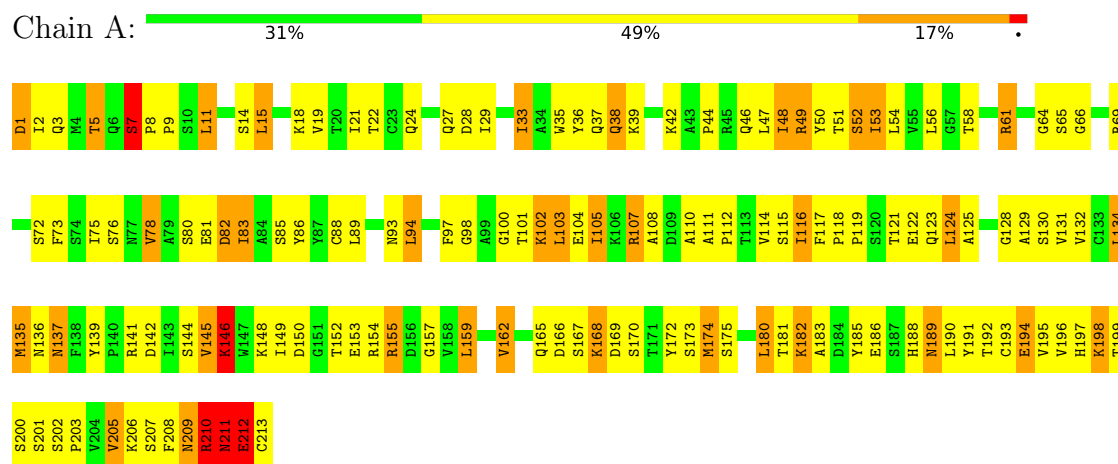
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: MONOCLONAL ANTIBODY AGAINST THE MAIN IMMUNOGENIC REGION OF THE HUMAN MUSCLE ACETYLCHOLINE RECEPTOR

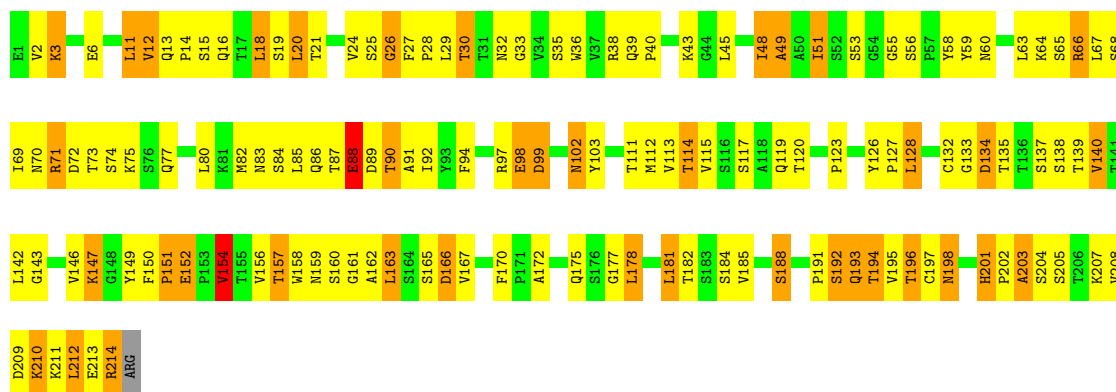


- Molecule 1: MONOCLONAL ANTIBODY AGAINST THE MAIN IMMUNOGENIC REGION OF THE HUMAN MUSCLE ACETYLCHOLINE RECEPTOR



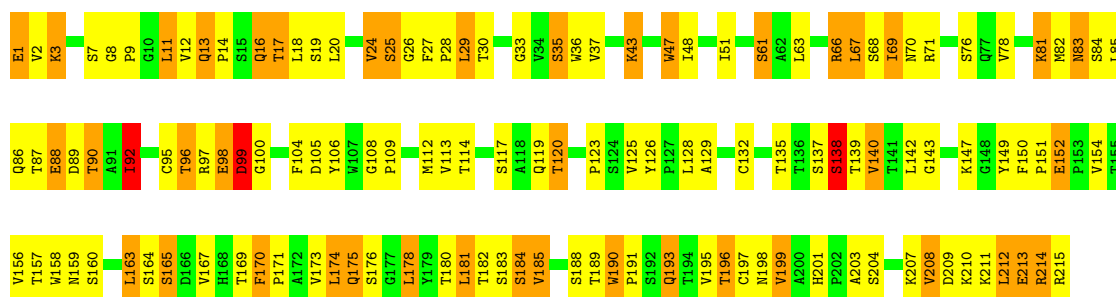
- Molecule 2: MONOCLONAL ANTIBODY AGAINST THE MAIN IMMUNOGENIC REGION OF THE HUMAN MUSCLE ACETYLCHOLINE RECEPTOR





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

Chain B: 39% 40% 20%



4 Data and refinement statistics

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

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	0.57	0/1671	1.14	10/2267 (0.4%)
1	L	0.59	0/1671	1.08	7/2267 (0.3%)
2	B	0.60	0/1663	1.12	15/2277 (0.7%)
2	H	0.62	0/1651	1.09	10/2263 (0.4%)
All	All	0.59	0/6656	1.11	42/9074 (0.5%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	SER	CA-C-N	-12.85	107.15	120.38
1	A	7	SER	C-N-CA	-12.85	107.15	120.38
2	B	190	TRP	N-CA-C	-8.85	98.93	110.07
2	B	170	PHE	N-CA-C	8.08	119.82	109.72
1	A	82	ASP	N-CA-C	-7.98	103.56	113.38
2	B	25	SER	N-CA-C	7.67	122.40	112.12
2	B	8	GLY	CA-C-N	7.42	127.69	119.90
2	B	8	GLY	C-N-CA	7.42	127.69	119.90
1	A	7	SER	N-CA-C	7.38	126.13	109.81
2	H	133	GLY	N-CA-C	-7.33	104.93	111.67
2	H	188	SER	N-CA-C	-7.23	103.65	114.64
2	B	33	GLY	N-CA-C	-7.16	101.58	112.89
2	H	201	HIS	CA-C-N	7.12	126.64	119.24
2	H	201	HIS	C-N-CA	7.12	126.64	119.24
1	L	182	LYS	N-CA-C	-6.80	103.89	111.71
1	A	205	VAL	N-CA-C	6.66	117.64	108.84
2	H	170	PHE	N-CA-C	6.65	118.03	109.65
1	L	132	VAL	N-CA-C	6.60	117.41	108.17
2	B	140	VAL	N-CA-C	6.53	117.70	108.36
1	A	98	GLY	N-CA-C	-6.46	103.91	112.82
1	L	200	SER	N-CA-C	6.43	120.94	112.13
2	H	154	VAL	N-CA-C	-6.28	99.15	108.45
1	L	189	ASN	N-CA-C	6.22	121.20	112.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	167	SER	N-CA-C	-6.20	105.68	113.18
1	A	52	SER	CA-C-N	-6.13	114.46	122.37
1	A	52	SER	C-N-CA	-6.13	114.46	122.37
2	B	99	ASP	N-CA-C	5.92	123.42	110.80
2	B	92	ILE	N-CA-C	-5.91	99.91	108.36
1	L	88	CYS	N-CA-C	-5.82	101.40	110.42
2	B	108	GLY	N-CA-C	-5.75	105.27	112.23
2	B	152	GLU	N-CA-C	-5.73	102.68	110.36
2	B	47	TRP	CA-C-N	-5.67	117.16	122.66
2	B	47	TRP	C-N-CA	-5.67	117.16	122.66
2	H	152	GLU	N-CA-C	-5.66	102.78	110.36
2	H	194	THR	N-CA-C	5.63	118.61	110.28
2	H	147	LYS	N-CA-C	5.46	117.48	109.24
2	H	60	ASN	N-CA-C	-5.21	102.15	109.96
2	B	109	PRO	N-CA-C	-5.21	107.24	114.27
2	B	48	ILE	N-CA-C	5.18	116.09	111.90
1	L	137	ASN	N-CA-C	5.13	117.43	111.02
1	A	39	LYS	N-CA-C	-5.11	104.25	110.13
1	A	66	GLY	N-CA-C	5.03	117.40	110.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1638	0	1595	167	0
1	L	1638	0	1595	87	0
2	B	1621	0	1585	121	0
2	H	1609	0	1572	107	0
3	A	37	0	0	1	0
3	B	36	0	0	1	0
3	H	41	0	0	3	0
3	L	95	0	0	3	0
All	All	6715	0	6347	467	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (467) 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:142:LEU:HD13	2:B:195:VAL:HG11	1.57	0.83
2:B:143:GLY:O	2:B:212:LEU:HD11	1.77	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
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:L:37:GLN:CB	1:L:47:LEU:HD21	2.17	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLU:HB2	1:A:205:VAL:CG1	2.16	0.74
2:B:17:THR:HB	2:B:83:ASN:HB3	1.70	0.73
2:B:96:THR:HG21	2:B:104:PHE:HA	1.70	0.72
2:B:142:LEU:CD1	2:B:195:VAL:HG11	2.19	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
1:A:36:TYR:CZ	1:A:46:GLN:HG3	2.25	0.70
2:B:2:VAL:HG13	2:B:27:PHE:CE1	2.27	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
2:B:181:LEU:HD23	2:B:181:LEU:C	2.18	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
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:L:166:ASP:HB3	1:L:169:ASP:OD1	1.95	0.67
1:L:200:SER:O	1:L:201:SER:CB	2.42	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:146:LYS:O	1:L:193:CYS:O	2.13	0.67
1:A:197:HIS:HB3	1:A:199:THR:HG22	1.76	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
2:B:66:ARG:NH2	2:B:89:ASP:OD2	2.29	0.64
2:H:36:TRP:HD1	2:H:69:ILE:HD12	1.62	0.64
2:H:128:LEU:HB2	2:H:143:GLY:C	2.22	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:PRO:O	2:B:113:VAL:HG22	1.98	0.64
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.78	0.64
1:A:102:LYS:HB2	1:A:102:LYS:HZ2	1.63	0.63
2:H:90:THR:HG22	2:H:115:VAL:HB	1.78	0.63
2:B:88:GLU:H	2:B:88:GLU:CD	2.06	0.63
1:L:117:PHE:HE1	1:L:134:LEU:HD22	1.63	0.63
1:L:160:ASP:HB3	1:L:174:MET:HE3	1.81	0.63
2:H:165:SER:O	2:H:166:ASP:HB2	1.98	0.63
2:B:28:PRO:HB2	2:B:30:THR:OG1	1.99	0.63
1:A:191:TYR:HE2	1:A:210:ARG:HG2	1.64	0.63
1:A:165:GLN:HG3	1:A:172:TYR:CZ	2.34	0.62
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
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	0.61
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:HA	2:H:193:GLN:OE1	2.00	0.61
1:A:210:ARG:HD2	1:A:210:ARG:O	2.01	0.60
2:H:39:GLN:C	2:H:91:ALA:HB1	2.27	0.60
1:L:33:ILE:HG22	1:L:51:THR:HA	1.83	0.60
1:L:155:ARG:NH1	1:L:155:ARG:HG2	2.15	0.60
2:B:96:THR:CG2	2:B:106:TYR:O	2.49	0.60
2:H:38:ARG:NH1	2:H:82:MET:HE1	2.16	0.60
2:B:164:SER:O	2:B:167:VAL:HG23	2.01	0.60
2:H:2:VAL:HG13	2:H:27:PHE:HD2	1.66	0.60
1:A:194:GLU:CB	1:A:205:VAL:HG13	2.22	0.60
2:B:123:PRO:HB3	2:B:149:TYR:HB3	1.83	0.60
2:B:189:THR:CB	2:B:193:GLN:HB2	2.31	0.60
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
2:B:128:LEU:C	2:B:212:LEU:HD21	2.27	0.59

Continued on next page...

Continued from previous page...

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:112:MET:HE2	2:B:152:GLU:HB2	1.84	0.59
2:B:189:THR:HB	2:B:193:GLN:HB2	1.83	0.59
1:A:166:ASP:C	1:A:168:LYS:H	2.11	0.59
2:B:163:LEU:C	2:B:165:SER:H	2.11	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
2:H:181:LEU:C	2:H:181:LEU:HD23	2.28	0.58
1:A:5:THR:HG23	1:A:24:GLN:HB3	1.86	0.58
1:A:2:ILE:HD13	1:A:29:ILE:HG22	1.86	0.57
1:A:102:LYS:CB	1:A:102:LYS:NZ	2.67	0.57
2:H:128:LEU:HB2	2:H:143:GLY:O	2.04	0.57
1:A:155:ARG:HB3	1:A:155:ARG:CZ	2.34	0.57
2:B:97:ARG:HH11	2:B:99:ASP:HB3	1.68	0.57
2:B:159:ASN:HD21	2:B:195:VAL:HA	1.69	0.57
1:A:103:LEU:C	1:A:103:LEU:HD23	2.30	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
2:H:6:GLU:HB2	2:H:111:THR:HG23	1.87	0.56
2:H:85:LEU:HB3	2:H:115:VAL:HG21	1.86	0.56
2:H:115:VAL:HG12	2:H:115:VAL:O	2.06	0.56
1:L:160:ASP:HB3	1:L:174:MET:CE	2.35	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
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
2:B:29:LEU:O	2:B:71:ARG:NH1	2.38	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
1:A:54:LEU:HD22	1:A:58:THR:HG21	1.88	0.56
1:A:194:GLU:HB2	1:A:205:VAL:HG22	1.88	0.56
1:A:38:GLN:HG3	1:A:44:PRO:HA	1.88	0.56
2:B:82:MET:HE3	2:B:85:LEU:CD2	2.35	0.56
1:L:159:LEU:HD23	1:L:159:LEU:O	2.06	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:24:VAL:HB	2:H:29:LEU:HD11	1.87	0.55
2:B:214:ARG:H	2:B:214:ARG:HD3	1.70	0.55
2:H:38:ARG:HH12	2:H:82:MET:HE1	1.70	0.55
1:A:189:ASN:HD22	1:A:210:ARG:HB3	1.72	0.55
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:B:96:THR:HG23	2:B:106:TYR:O	2.07	0.55
1:L:17:ASP:O	1:L:78:VAL:HG22	2.06	0.55
2:H:167:VAL:HG22	2:H:185:VAL:HG23	1.89	0.55
2:H:123:PRO:HB3	2:H:149:TYR:HB3	1.88	0.55
1:A:124:LEU:HD12	1:A:182:LYS:CG	2.30	0.55
1:L:141:ARG:HG3	1:L:172:TYR:CD1	2.42	0.55
1:A:186:GLU:CA	1:A:210:ARG:HH21	2.17	0.55
1:A:144:SER:CB	1:A:146:LYS:HZ1	2.21	0.54
1:A:210:ARG:HD2	1:A:210:ARG:C	2.32	0.54
2:H:87:THR:C	2:H:89:ASP:H	2.15	0.54
1:A:119:PRO:HB2	1:A:124:LEU:CD2	2.37	0.54
2:B:18:LEU:HD11	2:B:20:LEU:HD21	1.89	0.54
1:L:180:LEU:HD12	1:L:180:LEU:N	2.22	0.54
2:H:13:GLN:HB2	2:H:16:GLN:CG	2.32	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:L:117:PHE:CE1	1:L:134:LEU:HD22	2.41	0.54
1:A:146:LYS:HG2	1:A:194:GLU:O	2.08	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
1:A:36:TYR:CE2	1:A:46:GLN:HG3	2.43	0.54
2:B:11:LEU:HD23	2:B:114:THR:O	2.08	0.54
1:L:147:TRP:O	1:L:153:GLU:HA	2.07	0.53
1:L:19:VAL:HG22	1:L:75:ILE:HB	1.90	0.53
1:A:123:GLN:HG2	1:A:128:GLY:O	2.08	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
1:A:102:LYS:HB2	1:A:102:LYS:NZ	2.23	0.53
2:H:98:GLU:HG3	2:H:103:TYR:CE2	2.43	0.53
2:H:142:LEU:HD22	2:H:212:LEU:HD12	1.91	0.53
1:A:146:LYS:NZ	1:A:196:VAL:H	2.07	0.53
2:B:82:MET:HE3	2:B:85:LEU:HD23	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:202:PRO:C	2:H:204:SER:H	2.17	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
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:194:GLU:CG	1:A:205:VAL:HG22	2.39	0.52
2:H:86:GLN:O	2:H:89:ASP:HB2	2.09	0.52
1:A:202:SER:HB2	1:A:203:PRO:CD	2.40	0.52
2:B:128:LEU:O	2:B:212:LEU:HD21	2.10	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:8:PRO:HG3	1:L:11:LEU:HD22	1.91	0.51
1:L:123:GLN:O	1:L:126:THR:CB	2.56	0.51
1:L:124:LEU:C	1:L:126:THR:H	2.17	0.51
1:A:198:LYS:HD3	1:A:198:LYS:N	2.24	0.51
2:B:1:GLU:HA	2:B:1:GLU:OE1	2.11	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
1:L:149:ILE:HD11	1:L:178:LEU:HD21	1.93	0.51
1:L:118:PRO:HB3	1:L:208:PHE:CZ	2.45	0.51
1:A:146:LYS:HZ3	1:A:196:VAL:N	2.09	0.51
2:B:150:PHE:CE1	2:B:151:PRO:HB3	2.46	0.51
1:L:61:ARG:HG2	1:L:61:ARG:HH11	1.75	0.51
2:H:2:VAL:HG13	2:H:27:PHE:CD2	2.46	0.51
1:A:132:VAL:HG12	1:A:134:LEU:HD13	1.93	0.51
2:B:96:THR:HG22	2:B:106:TYR:O	2.11	0.51
1:A:15:LEU:HD13	1:A:78:VAL:O	2.10	0.50
2:B:28:PRO:C	2:B:30:THR:H	2.19	0.50
2:H:137:SER:C	2:H:139:THR:H	2.19	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:L:118:PRO:HB3	1:L:208:PHE:CE1	2.47	0.50
1:A:194:GLU:CA	1:A:205:VAL:HA	2.35	0.50
2:B:169:THR:HA	2:B:183:SER:HA	1.91	0.50
1:L:126:THR:HG22	1:L:128:GLY:H	1.77	0.50
1:A:117:PHE:CB	2:B:128:LEU:HD22	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:202:PRO:O	2:H:204:SER:N	2.45	0.50
1:A:19:VAL:HG22	1:A:75:ILE:HB	1.94	0.50
2:B:3:LYS:CG	2:B:25:SER:HB2	2.37	0.50
2:B:99:ASP:OD1	2:B:99:ASP:C	2.55	0.50
1:L:39:LYS:HD3	1:L:84:ALA:HB2	1.94	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:L:163:THR:HG23	1:L:164:ASP:N	2.27	0.49
1:A:18:LYS:HA	1:A:75:ILE:O	2.11	0.49
1:A:182:LYS:O	1:A:186:GLU:CG	2.61	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
1:A:145:VAL:HG13	1:A:146:LYS:N	2.22	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:L:124:LEU:C	1:L:126:THR:N	2.70	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
2:H:55:GLY:HA3	2:H:71:ARG:NH1	2.29	0.48
1:A:114:VAL:HG22	1:A:135:MET:CG	2.43	0.48
1:L:164:ASP:O	1:L:165:GLN:C	2.56	0.48
1:A:35:TRP:HB2	1:A:48:ILE:HB	1.94	0.48
1:A:49:ARG:HD3	1:A:53:ILE:HG13	1.96	0.48
1:L:155:ARG:HH11	1:L:155:ARG:CG	2.26	0.48
2:H:36:TRP:CD1	2:H:69:ILE:HD12	2.46	0.48
2:H:43:LYS:HE3	3:H:226:HOH:O	2.12	0.48
2:H:48:ILE:HB	2:H:67:LEU:HD11	1.96	0.47
1:A:136:ASN:ND2	1:A:173:SER:HB3	2.28	0.47
2:B:83:ASN:O	2:B:84:SER:HB2	2.14	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
2:H:73:THR:HG23	2:H:74:SER:N	2.28	0.47

Continued on next page...

Continued from previous page...

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: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
2:H:66:ARG:NH1	2:H:82:MET:HE2	2.29	0.47
2:H:159:ASN:C	2:H:161:GLY:H	2.22	0.47
2:H:214:ARG:HD2	2:H:214:ARG:HA	1.53	0.47
1:A:2:ILE:HG12	1:A:27:GLN:HB2	1.96	0.47
1:A:122:GLU:O	1:A:125:ALA:HB3	2.15	0.47
1:A:189:ASN:ND2	1:A:210:ARG:HB3	2.29	0.47
2:B:12:VAL:HG12	2:B:13:GLN:N	2.30	0.47
1:L:120:SER:HB3	2:H:127:PRO:HD2	1.96	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:56:LEU:HD23	1:L:56:LEU:N	2.30	0.47
1:A:114:VAL:HG21	1:A:195:VAL:CG2	2.44	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:83:ILE:O	1:L:84:ALA:HB2	2.15	0.46
1:L:129:ALA:HB3	1:L:180:LEU:CD1	2.45	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:B:14:PRO:C	2:B:16:GLN:H	2.23	0.46
2:H:160:SER:N	2:H:198:ASN:OD1	2.40	0.46
2:H:152:GLU:OE2	2:H:172:ALA:HB3	2.16	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
1:A:83:ILE:HA	1:A:103:LEU:CD2	2.46	0.46
1:A:121:THR:HG23	1:A:122:GLU:N	2.30	0.46
2:H:98:GLU:O	2:H:102:ASN:O	2.34	0.46
1:A:149:ILE:O	1:A:152:THR:CG2	2.64	0.46
2:H:87:THR:C	2:H:89:ASP:N	2.73	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:L:212:GLU:O	2:H:132:CYS:HA	2.16	0.45
1:A:103:LEU:HD23	1:A:103:LEU:O	2.15	0.45
1:A:146:LYS:HZ3	1:A:195:VAL:C	2.24	0.45
1:A:209:ASN:O	1:A:210:ARG:CB	2.64	0.45
2:B:170:PHE:O	2:B:171:PRO:C	2.59	0.45
1:L:168:LYS:HE2	1:L:168:LYS:HB3	1.73	0.45
2:H:88:GLU:HA	3:H:224:HOH:O	2.15	0.45
2:H:127:PRO:HG3	2:H:210:LYS:HD3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ILE:HD13	1:A:29:ILE:CG2	2.45	0.45
2:B:104:PHE:N	2:B:104:PHE:CD1	2.84	0.45
1:A:89:LEU:HD13	1:A:97:PHE:CZ	2.51	0.45
1:A:146:LYS:O	1:A:193:CYS:O	2.34	0.45
2:H:3:LYS:HE3	2:H:3:LYS:HB2	1.81	0.45
1:L:61:ARG:NH2	1:L:82:ASP:OD1	2.42	0.45
1:A:14:SER:O	1:A:15:LEU:C	2.59	0.45
2:B:151:PRO:HD2	2:B:203:ALA:CB	2.46	0.45
2:H:202:PRO:C	2:H:204:SER:N	2.74	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:O	2:B:174:LEU:HG	2.17	0.45
2:B:201:HIS:HD1	2:B:204:SER:CB	2.29	0.45
2:H:208:VAL:HG22	2:H:209:ASP:N	2.32	0.45
1:A:7:SER:O	1:A:9:PRO:CD	2.64	0.45
1:A:200:SER:C	1:A:202:SER:H	2.25	0.45
1:L:1:ASP:OD1	1:L:1:ASP:N	2.45	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:22:THR:HA	1:A:72:SER:HA	1.97	0.45
1:A:132:VAL:CG1	1:A:134:LEU:HD13	2.47	0.45
1:L:94:LEU:HD12	1:L:94:LEU:HA	1.77	0.44
1:L:107:ARG:HG2	1:L:108:ALA:H	1.79	0.44
1:L:61:ARG:HH11	1:L:61:ARG:CG	2.31	0.44
2:B:123:PRO:CB	2:B:149:TYR:HB3	2.47	0.44
2:H:177:GLY:O	2:H:178:LEU:HD13	2.17	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:51:ILE:HA	2:H:56:SER:O	2.17	0.44
1:A:1:ASP:CG	2:B:61:SER:HB2	2.43	0.44
1:L:180:LEU:HD12	1:L:180:LEU:H	1.83	0.44
2:H:195:VAL:HG23	2:H:195:VAL:O	2.17	0.44
1:A:141:ARG:HH22	1:A:162:VAL:HB	1.82	0.44
1:A:180:LEU:CD1	1:A:185:TYR:HB2	2.48	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:B:163:LEU:HD11	2:B:195:VAL:HG23	1.99	0.44
1:L:162:VAL:HG23	3:L:276:HOH:O	2.16	0.44
2:H:24:VAL:CB	2:H:29:LEU:HD11	2.47	0.44
1:A:192:THR:HA	1:A:207:SER:OG	2.17	0.44
2:B:213:GLU:HA	2:B:213:GLU:OE1	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:35:TRP:CZ3	1:A:88:CYS:HB3	2.53	0.43
2:B:181:LEU:HD23	2:B:181:LEU:O	2.18	0.43
1:L:123:GLN:HG3	2:H:126:TYR:CZ	2.54	0.43
1:A:107:ARG:HG2	1:A:139:TYR:CD2	2.53	0.43
1:A:111:ALA:HA	1:A:199:THR:HG21	1.99	0.43
1:A:211:ASN:O	1:A:212:GLU:O	2.36	0.43
2:B:123:PRO:CA	2:B:149:TYR:HB3	2.48	0.43
1:A:54:LEU:HD22	1:A:58:THR:CG2	2.49	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:29:ILE:HD11	1:A:33:ILE:HG13	2.00	0.43
1:A:159:LEU:HD13	2:B:173:VAL:HG21	1.99	0.43
2:B:28:PRO:C	2:B:30:THR:N	2.75	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
1:A:197:HIS:C	1:A:198:LYS:HD3	2.44	0.43
2:B:170:PHE:HB2	2:B:182:THR:O	2.18	0.43
2:B:189:THR:OG1	2:B:193:GLN:HB2	2.18	0.43
2:H:13:GLN:O	2:H:14:PRO:C	2.62	0.43
1:A:8:PRO:O	1:A:101:THR:OG1	2.22	0.43
1:A:146:LYS:CG	1:A:194:GLU:O	2.67	0.43
1:L:35:TRP:CH2	1:L:88:CYS:HB3	2.53	0.43
1:L:78:VAL:HB	1:L:105:ILE:HD11	2.00	0.43
1:L:146:LYS:HE2	1:L:196:VAL:CG2	2.48	0.43
2:H:195:VAL:O	2:H:195:VAL:CG2	2.66	0.43
1:L:81:GLU:OE1	1:A:56:LEU:HD21	2.19	0.43
1:L:185:TYR:CZ	1:L:210:ARG:HG3	2.54	0.43
2:B:35:SER:O	2:B:95:CYS:HA	2.18	0.43
2:B:175:GLN:HE21	2:B:175:GLN:HB2	1.72	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:87:THR:C	2:B:89:ASP:N	2.76	0.42
2:B:164:SER:O	2:B:165:SER:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:LEU:HA	2:B:114:THR:O	2.19	0.42
1:A:50:TYR:HB2	1:A:53:ILE:CG2	2.45	0.42
2:B:195:VAL:O	2:B:195:VAL:HG13	2.20	0.42
1:L:119:PRO:HD3	1:L:131:VAL:HG22	2.01	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
2:B:43:LYS:HA	2:B:43:LYS:HD2	1.90	0.42
1:L:33:ILE:HD11	1:L:88:CYS:HB2	2.02	0.42
2:H:98:GLU:CG	2:H:99:ASP:N	2.81	0.42
1:A:145:VAL:HG22	1:A:146:LYS:H	1.82	0.42
2:B:99:ASP:O	2:B:99:ASP:CG	2.63	0.42
2:B:69:ILE:O	2:B:69:ILE:HG23	2.19	0.42
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
2:B:163:LEU:HD23	2:B:165:SER:CB	2.50	0.41
1:L:45:ARG:O	1:L:47:LEU:HD22	2.19	0.41
2:H:25:SER:HB3	2:H:26:GLY:H	1.61	0.41
2:H:210:LYS:HB2	2:H:210:LYS:HE2	1.68	0.41
1:A:146:LYS:HZ1	1:A:196:VAL:H	1.67	0.41
1:L:29:ILE:O	1:L:30:ASN:HB2	2.20	0.41
2:H:191:PRO:O	2:H:192:SER:C	2.64	0.41
1:L:145:VAL:O	1:L:145:VAL:CG1	2.67	0.41
1:L:148:LYS:HB2	1:L:192:THR:HB	2.03	0.41
2:H:48:ILE:O	2:H:48:ILE:HG12	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:A:166:ASP:C	1:A:168:LYS:N	2.77	0.41
1:L:50:TYR:O	1:L:52:SER:N	2.46	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:141:ARG:HG3	1:L:172:TYR:CE1	2.55	0.41
2:H:12:VAL:HG12	2:H:16:GLN:HB2	2.03	0.41
1:L:52:SER:HB3	1:L:64:GLY:O	2.20	0.41
2:H:162:ALA:O	2:H:163:LEU:C	2.64	0.41
1:A:35:TRP:CH2	1:A:88:CYS:HB3	2.55	0.41
1:A:116:ILE:HG13	1:A:117:PHE:N	2.36	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
1:A:11:LEU:HD13	1:A:19:VAL:HB	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ARG:C	1:A:157:GLY:H	2.29	0.41
2:B:12:VAL:HG11	2:B:85:LEU:CD1	2.50	0.41
1:L:90:GLN:HG3	1:L:96:THR:HB	2.03	0.41
2:H:70:ASN:HB2	3:H:249:HOH:O	2.21	0.41
2:H:72:ASP:OD1	2:H:74:SER:HB3	2.21	0.41
1:A:61:ARG:NH1	1:A:82:ASP:OD1	2.54	0.41
1:A:135:MET:SD	1:A:195:VAL:HG11	2.61	0.41
2:B:36:TRP:HE1	2:B:78:VAL:HG12	1.85	0.41
2:B:105:ASP:OD1	2:B:105:ASP:N	2.46	0.41
1:L:182:LYS:O	1:L:183:ALA:C	2.64	0.40
1:L:186:GLU:HA	1:L:210:ARG:CD	2.50	0.40
1:A:194:GLU:HB2	1:A:205:VAL:CB	2.51	0.40
1:A:149:ILE:HG23	1:A:191:TYR:CE1	2.56	0.40
2:H:2:VAL:CG1	2:H:27:PHE:CD2	3.05	0.40
1:A:117:PHE:CG	2:B:128:LEU:HD22	2.56	0.40
1:A:211:ASN:HB2	1:A:212:GLU:H	1.53	0.40
1:A:8:PRO:O	1:A:101:THR:HG23	2.21	0.40
1:A:197:HIS:CG	1:A:199:THR:HG22	2.55	0.40
2:B:63:LEU:O	2:B:67:LEU:HB2	2.22	0.40
2:B:214:ARG:O	2:B:215:ARG:CB	2.69	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	211/213 (99%)	179 (85%)	19 (9%)	13 (6%)	1	0
1	L	211/213 (99%)	194 (92%)	13 (6%)	4 (2%)	6	8
2	B	213/215 (99%)	186 (87%)	20 (9%)	7 (3%)	3	2
2	H	212/215 (99%)	180 (85%)	24 (11%)	8 (4%)	2	2
All	All	847/856 (99%)	739 (87%)	76 (9%)	32 (4%)	2	2

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
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 ⓘ

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%)	139 (74%)	48 (26%)	0	0
1	L	187/187 (100%)	151 (81%)	36 (19%)	1	2
2	B	187/187 (100%)	138 (74%)	49 (26%)	0	0
2	H	186/187 (100%)	129 (69%)	57 (31%)	0	0
All	All	747/748 (100%)	557 (75%)	190 (25%)	0	1

All (190) 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	28	ASP
1	L	31	LYS
1	L	33	ILE
1	L	42	LYS
1	L	54	LEU
1	L	55	VAL
1	L	56	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	89	LEU
1	L	94	LEU
1	L	105	ILE
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	153	GLU
1	L	155	ARG
1	L	159	LEU
1	L	162	VAL
1	L	163	THR
1	L	180	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	187	SER
1	L	198	LYS
1	L	206	LYS
2	H	3	LYS
2	H	11	LEU
2	H	12	VAL
2	H	18	LEU
2	H	19	SER
2	H	20	LEU
2	H	21	THR
2	H	30	THR
2	H	35	SER
2	H	45	LEU
2	H	48	ILE
2	H	51	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	92	ILE
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	140	VAL
2	H	147	LYS
2	H	154	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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	11	LEU
1	A	15	LEU
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	103	LEU
1	A	104	GLU
1	A	105	ILE
1	A	107	ARG
1	A	115	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	116	ILE
1	A	124	LEU
1	A	131	VAL
1	A	134	LEU
1	A	135	MET
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	162	VAL
1	A	168	LYS
1	A	174	MET
1	A	180	LEU
1	A	182	LYS
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	24	VAL
2	B	29	LEU
2	B	35	SER
2	B	43	LYS
2	B	61	SER
2	B	66	ARG
2	B	67	LEU
2	B	68	SER
2	B	69	ILE
2	B	70	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	81	LYS
2	B	83	ASN
2	B	90	THR
2	B	92	ILE
2	B	96	THR
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
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

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	24	GLN
1	L	137	ASN
2	H	13	GLN
2	H	77	GLN
2	H	86	GLN
1	A	27	GLN
1	A	37	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	38	GLN
1	A	165	GLN
1	A	189	ASN
2	B	39	GLN
2	B	77	GLN
2	B	83	ASN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.