



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:26 PM GMT

PDB ID : 1KB5
Title : MURINE T-CELL RECEPTOR VARIABLE DOMAIN/FAB COMPLEX
Authors : Housset, D.; Mazza, G.; Gregoire, C.; Piras, C.; Malissen, B.; Fontecilla-Camps, J.C.
Deposited on : 1997-04-06
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

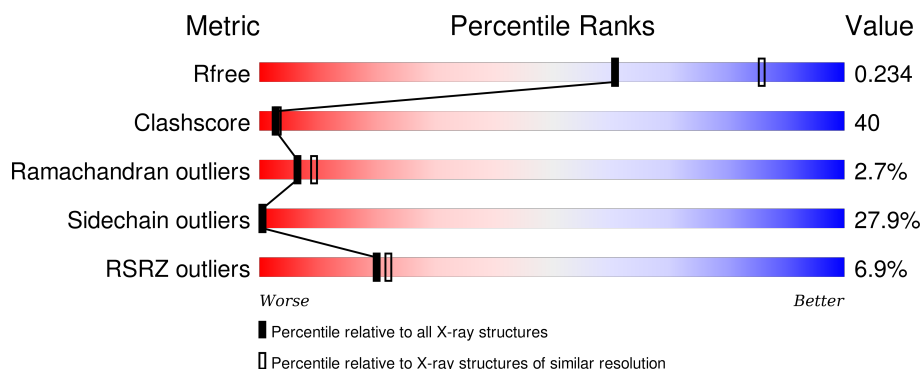
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 $\leq 5\%$. 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	115	<div> <div>5%</div> <div>29%</div> <div>49%</div> <div>19%</div> <div>•</div> </div>
2	B	117	<div> <div>8%</div> <div>26%</div> <div>46%</div> <div>24%</div> <div>•</div> </div>
3	L	214	<div> <div>5%</div> <div>31%</div> <div>52%</div> <div>15%</div> <div>•</div> </div>
4	H	219	<div> <div>10%</div> <div>40%</div> <div>43%</div> <div>16%</div> <div>•</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5438 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 KB5-C20 T-CELL ANTIGEN RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	S	0	0	0
			904	572	153	177	2			

- Molecule 2 is a protein called KB5-C20 T-CELL ANTIGEN RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	117	Total	C	N	O	S	0	0	0
			941	596	167	173	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	100	TRP	-	INSERTION	UNP P04214
B	101	GLY	TYR	CONFLICT	UNP P04214
B	102	ALA	ASN	CONFLICT	UNP P04214
B	104	ALA	-	INSERTION	UNP P04214
B	105	GLU	-	INSERTION	UNP P04214
B	105A	THR	PRO	CONFLICT	UNP P04214
B	109	GLY	ALA	CONFLICT	UNP P04214
B	110	SER	ALA	CONFLICT	UNP P04214

- Molecule 3 is a protein called ANTIBODY DESIRE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1661	1036	280	338	7			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	27	LYS	GLU	CONFLICT	UNP P01837
L	55	GLY	ALA	CONFLICT	UNP P01837

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	96	TYR	LEU	CONFLICT	UNP P01837
L	100	GLY	ALA	CONFLICT	UNP P01837
L	106	ILE	LEU	CONFLICT	UNP P01837

- Molecule 4 is a protein called ANTIBODY DESIRE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	219	Total	C	N	O	S	0	0	0
			1666	1052	270	337	7			

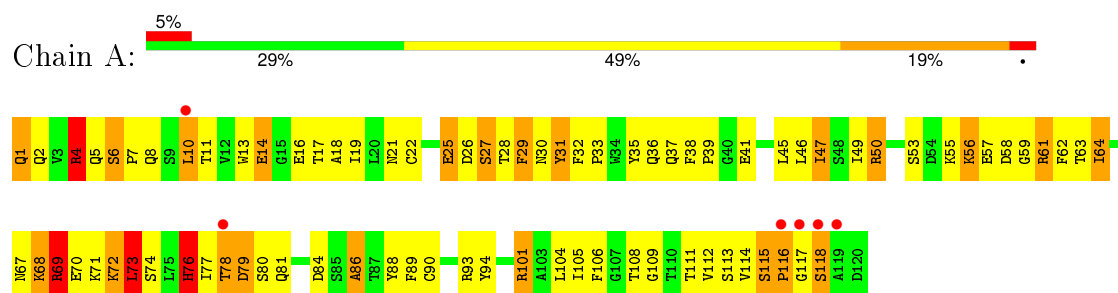
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total	O	0	0
			53	53		
5	B	54	Total	O	0	0
			54	54		
5	H	85	Total	O	0	0
			85	85		
5	L	74	Total	O	0	0
			74	74		

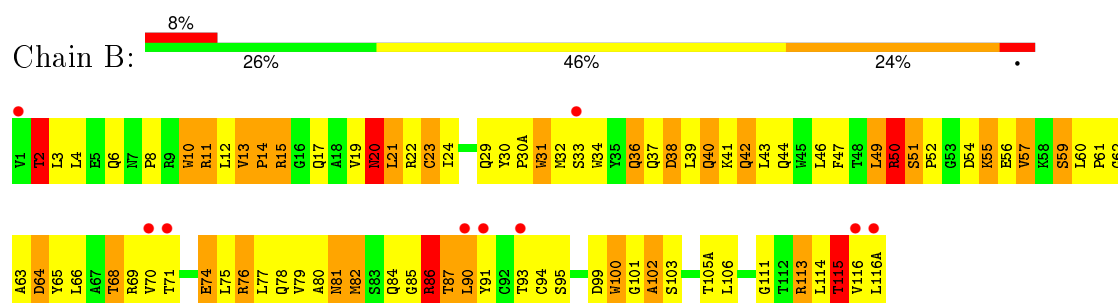
3 Residue-property plots [i](#)

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.

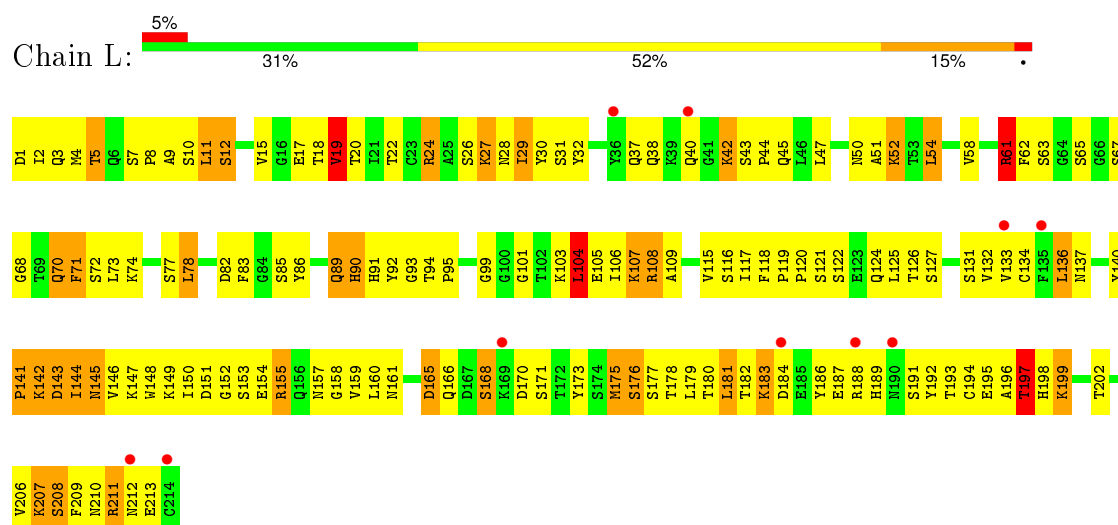
• Molecule 1: KB5-C20 T-CELL ANTIGEN RECEPTOR



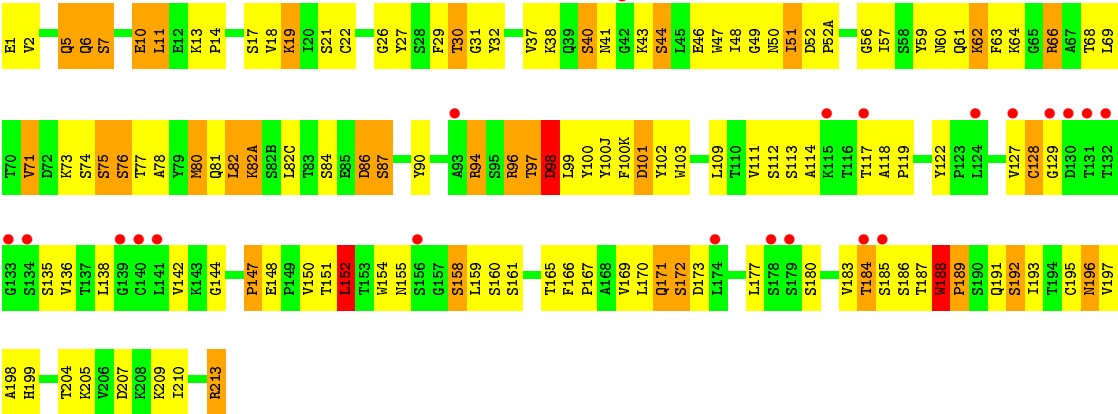
• Molecule 2: KB5-C20 T-CELL ANTIGEN RECEPTOR



• Molecule 3: ANTIBODY DESIRE-1



• Molecule 4: ANTIBODY DESIRE-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	187.31Å 80.95Å 52.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 24.31 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 73.0 (24.31-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.219 , (Not available) 0.219 , 0.234	Depositor DCC
R_{free} test set	1048 reflections (5.46%)	DCC
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 126.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 20606 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5438	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.78	1/927 (0.1%)	1.89	22/1256 (1.8%)
2	B	0.70	0/963	1.68	16/1310 (1.2%)
3	L	0.68	0/1700	1.52	21/2304 (0.9%)
4	H	0.67	0/1708	1.49	18/2328 (0.8%)
All	All	0.70	1/5298 (0.0%)	1.61	77/7198 (1.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	GLY	N-CA	-5.16	1.38	1.46

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ARG	CD-NE-CZ	19.98	151.57	123.60
2	B	115	THR	C-N-CA	19.09	169.42	121.70
1	A	116	PRO	C-N-CA	18.37	160.88	122.30
4	H	94	ARG	NE-CZ-NH2	11.72	126.16	120.30
2	B	86	ARG	CD-NE-CZ	11.72	140.00	123.60
1	A	93	ARG	NE-CZ-NH1	11.33	125.96	120.30
4	H	94	ARG	NE-CZ-NH1	-10.98	114.81	120.30
1	A	4	ARG	CD-NE-CZ	10.41	138.17	123.60
2	B	86	ARG	NE-CZ-NH1	10.02	125.31	120.30
4	H	66	ARG	CD-NE-CZ	9.65	137.12	123.60
1	A	76	HIS	CA-CB-CG	9.46	129.69	113.60
1	A	69	ARG	CD-NE-CZ	9.03	136.24	123.60
4	H	66	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	A	4	ARG	NE-CZ-NH1	8.26	124.43	120.30
3	L	61	ARG	CD-NE-CZ	8.12	134.97	123.60
1	A	61	ARG	CD-NE-CZ	8.02	134.82	123.60
1	A	61	ARG	NE-CZ-NH1	7.88	124.24	120.30
3	L	108	ARG	NE-CZ-NH1	7.86	124.23	120.30
4	H	189	PRO	N-CA-CB	7.51	112.32	103.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	104	LEU	CA-CB-CG	7.51	132.56	115.30
3	L	19	VAL	N-CA-CB	7.48	127.95	111.50
2	B	2	THR	N-CA-CB	7.45	124.45	110.30
1	A	4	ARG	NE-CZ-NH2	-7.13	116.74	120.30
3	L	91	HIS	CA-CB-CG	7.12	125.70	113.60
2	B	50	ARG	NE-CZ-NH1	-7.03	116.78	120.30
1	A	117	GLY	C-N-CA	6.92	138.99	121.70
3	L	141	PRO	N-CA-CB	6.77	111.42	103.30
4	H	152	LEU	CA-CB-CG	6.70	130.72	115.30
2	B	64	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	93	ARG	NE-CZ-NH2	-6.58	117.01	120.30
3	L	211	ARG	NE-CZ-NH1	-6.57	117.01	120.30
1	A	7	PRO	N-CA-CB	6.57	111.18	103.30
3	L	211	ARG	NE-CZ-NH2	6.55	123.57	120.30
3	L	95	PRO	N-CA-CB	6.50	111.11	103.30
3	L	29	ILE	CA-C-N	6.40	131.28	117.20
1	A	31	TYR	CB-CG-CD1	6.39	124.83	121.00
4	H	98	ASP	CB-CA-C	6.37	123.14	110.40
3	L	107	LYS	CA-CB-CG	6.28	127.22	113.40
1	A	73	LEU	CA-CB-CG	6.17	129.49	115.30
3	L	140	TYR	CA-C-O	-6.16	107.16	120.10
4	H	100(K)	PHE	C-N-CA	6.11	136.97	121.70
3	L	9	ALA	CB-CA-C	6.01	119.12	110.10
1	A	29	PHE	N-CA-C	-6.00	94.81	111.00
3	L	24	ARG	CD-NE-CZ	5.98	131.97	123.60
2	B	115	THR	N-CA-CB	5.98	121.66	110.30
4	H	52	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	29	PHE	CA-CB-CG	5.97	128.22	113.90
2	B	8	PRO	N-CA-CB	5.94	110.43	103.30
4	H	96	ARG	CA-CB-CG	5.94	126.47	113.40
2	B	10	TRP	CA-CB-CG	5.92	124.96	113.70
4	H	97	THR	C-N-CA	-5.86	107.06	121.70
4	H	86	ASP	CB-CG-OD2	5.78	123.50	118.30
2	B	42	GLN	CB-CA-C	5.66	121.71	110.40
1	A	116	PRO	N-CA-C	5.65	126.80	112.10
2	B	20	ASN	CB-CA-C	5.65	121.70	110.40
4	H	147	PRO	CA-N-CD	-5.58	103.68	111.50
1	A	79	ASP	CB-CG-OD2	-5.56	113.29	118.30
3	L	29	ILE	C-N-CA	-5.55	107.83	121.70
3	L	30	TYR	CB-CA-C	5.50	121.40	110.40
1	A	64	ILE	CB-CA-C	-5.49	100.61	111.60
2	B	91	TYR	N-CA-C	5.43	125.65	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	19	VAL	CA-CB-CG2	5.41	119.01	110.90
1	A	6	SER	CA-C-O	-5.38	108.81	120.10
3	L	108	ARG	CD-NE-CZ	5.37	131.12	123.60
3	L	8	PRO	N-CA-CB	5.29	109.64	103.30
3	L	197	THR	N-CA-CB	5.26	120.29	110.30
4	H	188	TRP	CA-C-O	-5.25	109.06	120.10
2	B	102	ALA	C-N-CA	5.20	134.70	121.70
3	L	95	PRO	CA-N-CD	-5.19	104.24	111.50
4	H	213	ARG	NE-CZ-NH1	-5.17	117.72	120.30
4	H	100	TYR	C-N-CA	5.17	134.62	121.70
4	H	147	PRO	N-CA-CB	5.16	109.49	103.30
2	B	40	GLN	C-N-CA	5.16	134.60	121.70
1	A	116	PRO	CA-C-O	5.12	132.49	120.20
2	B	74	GLU	CB-CG-CD	5.06	127.87	114.20
4	H	189	PRO	CA-N-CD	-5.05	104.43	111.50
2	B	100	TRP	C-N-CA	5.04	132.88	122.30

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	904	0	861	81	0
2	B	941	0	936	101	0
3	L	1661	0	1586	148	2
4	H	1666	0	1618	104	0
5	A	53	0	0	6	0
5	B	54	0	0	8	0
5	H	85	0	0	8	0
5	L	74	0	0	15	0
All	All	5438	0	5001	410	2

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 40.

All (410) 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:B:113:ARG:HH21	2:B:115:THR:HG21	1.25	1.00
3:L:119:PRO:HG2	4:H:213:ARG:HH12	1.29	0.95
4:H:199:HIS:HB3	4:H:204:THR:HB	1.51	0.93
2:B:22:ARG:HH21	2:B:74:GLU:HG3	1.34	0.92
1:A:11:THR:HG23	1:A:116:PRO:HG2	1.52	0.92
3:L:119:PRO:HD2	4:H:213:ARG:HH22	1.36	0.91
3:L:145:ASN:HB3	3:L:197:THR:HG22	1.51	0.91
1:A:4:ARG:HH22	1:A:25:GLU:HB2	1.35	0.91
3:L:187:GLU:HA	3:L:211:ARG:HD3	1.53	0.90
4:H:51:ILE:HG12	4:H:57:ILE:HG12	1.54	0.88
3:L:155:ARG:HD3	3:L:179:LEU:HD11	1.56	0.88
1:A:115:SER:N	1:A:116:PRO:HD3	1.90	0.87
2:B:21:LEU:HD23	2:B:77:LEU:HD23	1.59	0.84
2:B:80:ALA:O	2:B:81:ASN:HB2	1.76	0.83
2:B:13:VAL:HB	2:B:19:VAL:CG2	2.09	0.81
1:A:61:ARG:HD2	1:A:79:ASP:HB3	1.60	0.81
2:B:99:ASP:O	2:B:100:TRP:HB2	1.81	0.80
1:A:29:PHE:HE1	1:A:105:ILE:HD13	1.47	0.80
2:B:22:ARG:HH21	2:B:74:GLU:CG	1.94	0.79
2:B:22:ARG:NH2	2:B:74:GLU:HG3	1.97	0.78
3:L:28:ASN:ND2	3:L:68:GLY:HA2	2.00	0.76
3:L:122:SER:HA	3:L:125:LEU:HD12	1.66	0.76
3:L:141:PRO:HG2	3:L:199:LYS:HE2	1.66	0.76
3:L:42:LYS:NZ	3:L:43:SER:H	1.84	0.75
3:L:183:LYS:HD3	3:L:187:GLU:HG3	1.66	0.75
3:L:42:LYS:HZ2	3:L:42:LYS:HA	1.51	0.75
3:L:22:THR:HG22	3:L:72:SER:OG	1.86	0.75
1:A:61:ARG:NH1	1:A:79:ASP:O	2.18	0.75
3:L:147:LYS:HG2	3:L:154:GLU:HG3	1.69	0.74
4:H:87:SER:HA	4:H:109:LEU:O	1.87	0.74
2:B:36:GLN:HG2	2:B:46:LEU:HD21	1.69	0.73
3:L:28:ASN:HD22	3:L:68:GLY:HA2	1.50	0.73
3:L:187:GLU:HA	3:L:211:ARG:CD	2.18	0.73
1:A:104:LEU:HD12	2:B:106:LEU:HD23	1.69	0.73
2:B:66:LEU:HD23	2:B:78:GLN:HE21	1.53	0.72
3:L:150:ILE:HG13	3:L:192:TYR:CE1	2.25	0.72
3:L:155:ARG:HB2	3:L:155:ARG:HH11	1.54	0.72
3:L:83:PHE:HB3	3:L:106:ILE:CD1	2.20	0.72
1:A:1:GLN:HB3	1:A:4:ARG:HD3	1.70	0.72
3:L:183:LYS:HA	3:L:186:TYR:HB3	1.71	0.71
3:L:61:ARG:HG2	3:L:61:ARG:HH11	1.55	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:138:LEU:HD23	4:H:210:ILE:HG21	1.70	0.71
2:B:13:VAL:HB	2:B:19:VAL:HG23	1.72	0.71
3:L:11:LEU:HD13	3:L:104:LEU:HD23	1.72	0.70
1:A:4:ARG:NH2	1:A:25:GLU:HB2	2.06	0.70
3:L:119:PRO:HG2	4:H:213:ARG:NH1	2.05	0.70
1:A:5:GLN:HE22	1:A:90:CYS:H	1.39	0.69
3:L:27:LYS:HD3	5:L:229:HOH:O	1.91	0.69
3:L:12:SER:HA	3:L:105:GLU:O	1.93	0.69
4:H:30:THR:HA	4:H:52(A):PRO:HB2	1.75	0.68
1:A:5:GLN:NE2	1:A:90:CYS:H	1.92	0.68
3:L:193:THR:HG23	3:L:206:VAL:HG23	1.76	0.68
1:A:47:ILE:HG23	1:A:64:ILE:HD11	1.76	0.67
3:L:175:MET:HG2	3:L:176:SER:N	2.07	0.67
2:B:31:TRP:CZ3	2:B:50:ARG:HD2	2.29	0.67
2:B:79:VAL:HG21	2:B:82:MET:HE3	1.76	0.66
1:A:116:PRO:HB3	1:A:118:SER:HA	1.77	0.66
3:L:47:LEU:HA	3:L:58:VAL:HG21	1.76	0.66
3:L:144:ILE:HD12	3:L:198:HIS:HB2	1.78	0.66
4:H:94:ARG:NH1	4:H:102:TYR:HD2	1.94	0.66
3:L:86:TYR:O	3:L:101:GLY:HA2	1.96	0.66
4:H:187:THR:O	4:H:191:GLN:HB2	1.96	0.66
1:A:49:ILE:HG21	1:A:64:ILE:HG21	1.78	0.65
1:A:10:LEU:CD1	1:A:112:VAL:HG13	2.26	0.65
2:B:49:LEU:H	2:B:49:LEU:HD12	1.62	0.65
3:L:42:LYS:HZ2	3:L:42:LYS:CA	2.09	0.65
1:A:11:THR:HG23	1:A:116:PRO:CG	2.26	0.65
3:L:12:SER:HB2	3:L:105:GLU:HB3	1.79	0.65
3:L:136:LEU:HD23	3:L:196:ALA:HB2	1.78	0.65
1:A:49:ILE:HD12	1:A:56:LYS:HB2	1.80	0.64
4:H:51:ILE:HG21	4:H:71:VAL:HG23	1.80	0.64
4:H:155:ASN:HB2	4:H:159:LEU:HB2	1.78	0.64
3:L:83:PHE:HB3	3:L:106:ILE:HD11	1.76	0.64
2:B:113:ARG:NH2	2:B:115:THR:HG21	2.07	0.64
2:B:57:VAL:HG12	2:B:66:LEU:HA	1.79	0.63
3:L:3:GLN:HB3	3:L:26:SER:HB3	1.79	0.63
2:B:4:LEU:HD22	2:B:23:CYS:SG	2.39	0.63
3:L:170:ASP:O	3:L:171:SER:HB2	1.97	0.63
4:H:40:SER:O	4:H:43:LYS:HB2	1.99	0.63
2:B:66:LEU:HD23	2:B:78:GLN:NE2	2.13	0.63
2:B:113:ARG:HH21	2:B:115:THR:CG2	2.07	0.62
1:A:116:PRO:HB3	1:A:118:SER:CA	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:LEU:HD13	2:B:75:LEU:HD11	1.81	0.62
1:A:69:ARG:HG2	1:A:69:ARG:HH11	1.62	0.62
3:L:119:PRO:HD2	4:H:213:ARG:NH2	2.11	0.62
2:B:80:ALA:O	2:B:81:ASN:CB	2.46	0.62
3:L:42:LYS:HZ2	3:L:43:SER:H	1.46	0.62
2:B:101:GLY:O	2:B:103:SER:N	2.33	0.62
1:A:1:GLN:NE2	1:A:4:ARG:HB3	2.14	0.62
1:A:5:GLN:NE2	1:A:109:GLY:H	1.97	0.62
3:L:90:HIS:HD2	3:L:92:TYR:H	1.48	0.62
4:H:188:TRP:CG	4:H:189:PRO:HA	2.35	0.61
3:L:50:ASN:O	3:L:52:LYS:N	2.32	0.61
4:H:138:LEU:HB3	4:H:210:ILE:HD13	1.81	0.61
4:H:152:LEU:HB2	4:H:197:VAL:HG22	1.82	0.61
4:H:94:ARG:HH12	4:H:102:TYR:HD2	1.49	0.60
4:H:38:LYS:HB2	4:H:90:TYR:CE1	2.36	0.60
1:A:2:GLN:OE1	1:A:26:ASP:HB2	2.00	0.60
4:H:138:LEU:HD21	4:H:188:TRP:CD2	2.36	0.60
3:L:141:PRO:HG2	3:L:199:LYS:CE	2.31	0.60
2:B:22:ARG:HA	2:B:76:ARG:HA	1.84	0.60
4:H:10:GLU:HG3	4:H:18:VAL:HG21	1.84	0.60
1:A:45:LEU:HD12	1:A:46:LEU:N	2.16	0.60
1:A:101:ARG:NE	4:H:98:ASP:OD1	2.31	0.60
1:A:80:SER:HB3	1:A:114:VAL:CG1	2.32	0.59
1:A:13:TRP:O	1:A:16:GLU:HB2	2.02	0.59
4:H:50:ASN:O	4:H:57:ILE:HG23	2.03	0.59
3:L:159:VAL:HA	3:L:178:THR:O	2.02	0.59
1:A:18:ALA:O	1:A:76:HIS:HA	2.02	0.59
3:L:108:ARG:HG2	3:L:109:ALA:N	2.18	0.59
2:B:36:GLN:NE2	2:B:65:TYR:OH	2.35	0.59
1:A:101:ARG:HB2	4:H:98:ASP:OD1	2.03	0.59
4:H:1:GLU:O	4:H:26:GLY:HA3	2.03	0.59
3:L:115:VAL:CG1	3:L:207:LYS:HB2	2.33	0.58
1:A:80:SER:HB3	1:A:114:VAL:HG11	1.84	0.58
3:L:90:HIS:HE1	5:L:230:HOH:O	1.87	0.58
4:H:150:VAL:HG23	4:H:198:ALA:O	2.03	0.58
1:A:61:ARG:CD	1:A:79:ASP:HB3	2.31	0.58
4:H:41:ASN:HB3	4:H:43:LYS:HG3	1.85	0.57
1:A:50:ARG:HB3	5:B:137:HOH:O	2.04	0.57
3:L:108:ARG:HG2	3:L:109:ALA:H	1.69	0.57
1:A:116:PRO:HB3	1:A:118:SER:H	1.70	0.57
4:H:38:LYS:CB	4:H:48:ILE:HD11	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:117:ILE:HD11	3:L:132:VAL:HG11	1.87	0.56
3:L:42:LYS:HZ2	3:L:43:SER:N	2.02	0.56
2:B:32:MET:SD	5:B:134:HOH:O	2.57	0.56
3:L:70:GLN:HE21	3:L:71:PHE:N	2.03	0.56
3:L:2:ILE:HD13	3:L:29:ILE:CG2	2.35	0.56
4:H:154:TRP:O	4:H:155:ASN:HB2	2.04	0.56
4:H:7:SER:HB3	4:H:21:SER:H	1.70	0.56
4:H:86:ASP:HB2	4:H:111:VAL:HG21	1.88	0.56
3:L:83:PHE:HE1	3:L:168:SER:HG	1.51	0.56
2:B:31:TRP:HZ3	5:B:117:HOH:O	1.89	0.56
1:A:67:ASN:HB3	1:A:72:LYS:HB3	1.86	0.56
2:B:51:SER:O	2:B:54:ASP:HB2	2.05	0.56
3:L:3:GLN:HB2	5:L:237:HOH:O	2.06	0.56
1:A:115:SER:N	1:A:116:PRO:CD	2.67	0.56
3:L:144:ILE:HD11	3:L:196:ALA:HB1	1.89	0.55
3:L:193:THR:HG23	3:L:206:VAL:CG2	2.36	0.55
1:A:10:LEU:HD11	1:A:112:VAL:HG13	1.87	0.55
2:B:42:GLN:HB3	5:H:217:HOH:O	2.06	0.55
3:L:124:GLN:HG3	4:H:122:TYR:CZ	2.41	0.55
3:L:115:VAL:HG12	3:L:207:LYS:HB2	1.88	0.55
3:L:83:PHE:HB3	3:L:106:ILE:HD12	1.87	0.55
4:H:155:ASN:O	4:H:158:SER:HB3	2.07	0.55
2:B:55:LYS:HA	2:B:68:THR:HA	1.89	0.55
3:L:27:LYS:HE3	5:L:276:HOH:O	2.07	0.55
2:B:59:SER:O	4:H:56:GLY:HA2	2.06	0.55
4:H:18:VAL:HG11	4:H:109:LEU:CD1	2.37	0.55
3:L:86:TYR:HE2	3:L:104:LEU:HD12	1.72	0.55
1:A:1:GLN:HA	5:A:153:HOH:O	2.07	0.54
3:L:125:LEU:O	3:L:126:THR:C	2.46	0.54
1:A:29:PHE:CE1	1:A:105:ILE:HD13	2.37	0.54
4:H:18:VAL:HG11	4:H:109:LEU:HD13	1.88	0.54
4:H:43:LYS:HD2	5:H:247:HOH:O	2.06	0.54
3:L:181:LEU:HD23	5:L:231:HOH:O	2.07	0.54
2:B:49:LEU:N	2:B:49:LEU:HD12	2.22	0.54
4:H:38:LYS:HB2	4:H:48:ILE:HD11	1.89	0.54
3:L:148:TRP:O	3:L:154:GLU:HA	2.07	0.54
4:H:18:VAL:O	4:H:81:GLN:HG3	2.08	0.54
1:A:10:LEU:O	1:A:10:LEU:HD12	2.06	0.54
1:A:4:ARG:NH1	5:A:136:HOH:O	2.39	0.54
3:L:183:LYS:CD	3:L:187:GLU:HG3	2.37	0.54
3:L:19:VAL:HG23	3:L:78:LEU:HD21	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PHE:HB3	1:A:73:LEU:HD21	1.90	0.54
2:B:79:VAL:HG21	2:B:82:MET:CE	2.38	0.53
3:L:195:GLU:HG2	3:L:206:VAL:HB	1.91	0.53
4:H:84:SER:HB2	5:H:231:HOH:O	2.07	0.53
2:B:62:GLY:HA2	2:B:84:GLN:OE1	2.08	0.53
4:H:68:THR:OG1	4:H:82(A):LYS:HE2	2.08	0.53
3:L:134:CYS:HB2	3:L:148:TRP:CH2	2.43	0.53
4:H:99:LEU:HB3	4:H:100(J):TYR:CD2	2.44	0.53
3:L:119:PRO:CG	4:H:213:ARG:HH12	2.11	0.53
2:B:17:GLN:NE2	5:B:129:HOH:O	2.41	0.53
2:B:85:GLY:H	2:B:116:VAL:HG21	1.73	0.53
3:L:42:LYS:NZ	3:L:43:SER:N	2.56	0.53
4:H:154:TRP:CZ3	4:H:210:ILE:HD11	2.44	0.53
4:H:1:GLU:HG2	4:H:2:VAL:H	1.74	0.53
1:A:62:PHE:CE1	1:A:77:ILE:HG23	2.43	0.53
4:H:196:ASN:HB3	4:H:207:ASP:OD1	2.09	0.53
3:L:207:LYS:HE2	5:L:245:HOH:O	2.09	0.52
4:H:11:LEU:HG	4:H:147:PRO:HG3	1.92	0.52
3:L:136:LEU:CD2	3:L:196:ALA:HB2	2.40	0.52
1:A:36:GLN:HG3	1:A:88:TYR:CE2	2.44	0.52
3:L:105:GLU:HG2	3:L:106:ILE:N	2.24	0.52
1:A:45:LEU:HD12	1:A:46:LEU:H	1.74	0.52
3:L:119:PRO:CD	4:H:213:ARG:HH22	2.15	0.52
3:L:31:SER:O	3:L:50:ASN:HA	2.10	0.52
2:B:11:ARG:HG3	5:B:165:HOH:O	2.09	0.52
4:H:138:LEU:HD21	4:H:188:TRP:CE2	2.45	0.52
3:L:210:ASN:HB2	3:L:213:GLU:HB2	1.91	0.52
4:H:59:TYR:HB2	4:H:64:LYS:HD2	1.93	0.51
3:L:150:ILE:HG23	5:L:255:HOH:O	2.10	0.51
3:L:184:ASP:O	3:L:188:ARG:HB2	2.10	0.51
3:L:28:ASN:HD22	3:L:68:GLY:CA	2.20	0.51
3:L:186:TYR:CE2	3:L:211:ARG:HG3	2.46	0.51
3:L:158:GLY:O	3:L:179:LEU:HA	2.11	0.51
2:B:37:GLN:OE1	2:B:43:LEU:HD13	2.10	0.51
3:L:186:TYR:HH	3:L:209:PHE:HE1	1.58	0.51
2:B:70:VAL:HG12	2:B:71:THR:HG23	1.93	0.51
1:A:114:VAL:O	1:A:115:SER:HB3	2.10	0.51
3:L:2:ILE:HB	3:L:90:HIS:CE1	2.46	0.51
2:B:84:GLN:O	2:B:86:ARG:NH1	2.44	0.51
5:L:268:HOH:O	4:H:61:GLN:HB2	2.10	0.51
1:A:76:HIS:HB3	5:A:124:HOH:O	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:THR:CB	2:B:106:LEU:HD11	2.41	0.50
3:L:136:LEU:HD21	3:L:146:VAL:HG22	1.94	0.50
4:H:142:VAL:CG2	4:H:197:VAL:HG21	2.42	0.50
3:L:125:LEU:CD2	3:L:183:LYS:HG3	2.42	0.50
2:B:85:GLY:H	2:B:116:VAL:CG2	2.25	0.50
3:L:19:VAL:HG12	3:L:20:THR:H	1.76	0.50
2:B:70:VAL:HB	2:B:74:GLU:HB3	1.94	0.49
2:B:22:ARG:NH2	2:B:74:GLU:CG	2.66	0.49
2:B:10:TRP:CD1	2:B:10:TRP:O	2.65	0.49
3:L:143:ASP:O	3:L:198:HIS:HD2	1.95	0.49
2:B:34:TRP:HE1	2:B:75:LEU:HG	1.77	0.49
3:L:108:ARG:NH2	5:L:236:HOH:O	2.45	0.49
3:L:18:THR:HG22	5:L:278:HOH:O	2.13	0.49
4:H:27:TYR:CZ	4:H:94:ARG:HD2	2.47	0.49
1:A:21:ASN:ND2	5:A:159:HOH:O	2.45	0.49
3:L:125:LEU:HD23	3:L:183:LYS:HG3	1.95	0.49
3:L:86:TYR:CE2	3:L:104:LEU:HD12	2.47	0.49
4:H:75:SER:O	4:H:76:SER:HB2	2.12	0.49
3:L:11:LEU:O	3:L:104:LEU:HA	2.12	0.48
1:A:45:LEU:HD23	2:B:105(A):THR:HG23	1.94	0.48
2:B:55:LYS:HB3	2:B:68:THR:HG23	1.95	0.48
1:A:8:GLN:NE2	1:A:108:THR:OG1	2.45	0.48
4:H:188:TRP:CD2	4:H:189:PRO:HA	2.48	0.48
2:B:6:GLN:HE22	2:B:111:GLY:HA2	1.77	0.48
3:L:210:ASN:HD22	3:L:213:GLU:HB2	1.78	0.48
2:B:37:GLN:HB2	2:B:43:LEU:CD1	2.43	0.48
3:L:37:GLN:HE22	3:L:82:ASP:HA	1.79	0.48
2:B:21:LEU:HD21	2:B:79:VAL:CG1	2.44	0.48
2:B:19:VAL:HG11	2:B:114:LEU:HD21	1.96	0.48
2:B:64:ASP:HB2	2:B:80:ALA:O	2.14	0.48
1:A:57:GLU:HG3	1:A:58:ASP:N	2.28	0.48
2:B:22:ARG:HG3	2:B:76:ARG:HD3	1.96	0.48
4:H:94:ARG:NH1	4:H:101:ASP:OD2	2.47	0.48
3:L:145:ASN:CB	3:L:197:THR:HG22	2.34	0.48
1:A:31:TYR:CE2	1:A:33:PRO:HG3	2.49	0.48
2:B:100:TRP:CE2	3:L:31:SER:HB2	2.48	0.47
3:L:50:ASN:ND2	5:L:216:HOH:O	2.41	0.47
3:L:119:PRO:CB	3:L:120:PRO:CD	2.92	0.47
1:A:78:THR:HB	5:A:171:HOH:O	2.14	0.47
3:L:210:ASN:ND2	3:L:213:GLU:OE1	2.47	0.47
3:L:131:SER:HA	3:L:179:LEU:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:THR:OG1	2:B:106:LEU:HD11	2.14	0.47
2:B:116:VAL:HA	5:B:132:HOH:O	2.12	0.47
4:H:171:GLN:O	4:H:172:SER:C	2.52	0.47
3:L:195:GLU:HG3	3:L:206:VAL:HG23	1.97	0.47
4:H:18:VAL:HG22	4:H:19:LYS:N	2.28	0.47
4:H:135:SER:HA	4:H:184:THR:HA	1.96	0.47
4:H:29:PHE:HZ	4:H:71:VAL:HG22	1.79	0.47
3:L:3:GLN:HB3	3:L:26:SER:CB	2.45	0.47
3:L:206:VAL:O	3:L:207:LYS:HD3	2.13	0.47
3:L:5:THR:HG22	3:L:24:ARG:HD3	1.96	0.47
2:B:10:TRP:O	2:B:10:TRP:HD1	1.98	0.47
3:L:136:LEU:N	3:L:136:LEU:HD12	2.30	0.47
2:B:99:ASP:O	2:B:100:TRP:CB	2.55	0.47
4:H:46:GLU:OE2	4:H:62:LYS:HE2	2.14	0.47
3:L:106:ILE:H	3:L:166:GLN:HE22	1.63	0.47
3:L:10:SER:O	3:L:11:LEU:HB3	2.15	0.47
1:A:116:PRO:CB	1:A:118:SER:H	2.27	0.47
1:A:104:LEU:HD12	2:B:106:LEU:CD2	2.42	0.47
4:H:30:THR:O	4:H:32:TYR:N	2.48	0.47
1:A:62:PHE:CE1	1:A:77:ILE:HG12	2.50	0.47
3:L:44:PRO:HG2	4:H:103:TRP:CZ3	2.50	0.47
4:H:18:VAL:HG12	4:H:82(C):LEU:HD11	1.97	0.47
3:L:83:PHE:HE1	3:L:168:SER:OG	1.97	0.47
1:A:84:ASP:HB2	1:A:114:VAL:HG21	1.95	0.46
2:B:19:VAL:HG12	2:B:20:ASN:N	2.30	0.46
1:A:101:ARG:HD3	3:L:32:TYR:CZ	2.50	0.46
3:L:121:SER:OG	4:H:122:TYR:HB3	2.15	0.46
2:B:21:LEU:HD22	2:B:21:LEU:N	2.31	0.46
4:H:51:ILE:CG1	4:H:57:ILE:HG12	2.38	0.46
2:B:30:TYR:N	2:B:30(A):PRO:HD3	2.31	0.46
2:B:13:VAL:HA	2:B:14:PRO:HD3	1.77	0.46
1:A:116:PRO:HB3	1:A:118:SER:OG	2.16	0.46
4:H:60:ASN:HB3	4:H:63:PHE:HD2	1.81	0.46
1:A:116:PRO:HB3	1:A:118:SER:N	2.31	0.46
1:A:35:TYR:O	1:A:88:TYR:HA	2.16	0.46
2:B:14:PRO:HG2	2:B:17:GLN:HB2	1.98	0.45
2:B:13:VAL:HG11	2:B:82:MET:HG2	1.98	0.45
4:H:17:SER:O	4:H:81:GLN:NE2	2.49	0.45
2:B:87:THR:HB	2:B:113:ARG:HA	1.97	0.45
4:H:18:VAL:H	4:H:82(C):LEU:HD11	1.81	0.45
3:L:54:LEU:HD21	3:L:62:PHE:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:C	1:A:116:PRO:HD3	2.37	0.45
1:A:10:LEU:HD12	1:A:112:VAL:HG13	1.96	0.45
4:H:38:LYS:HB3	4:H:48:ILE:HD11	1.97	0.45
4:H:6:GLN:HB3	4:H:21:SER:O	2.16	0.45
3:L:210:ASN:HB3	3:L:213:GLU:H	1.82	0.45
4:H:184:THR:O	4:H:186:SER:N	2.50	0.45
1:A:29:PHE:HA	1:A:94:TYR:HA	1.98	0.45
1:A:14:GLU:HG3	1:A:81:GLN:HA	1.99	0.45
2:B:60:LEU:HB3	2:B:61:PRO:HD2	1.99	0.45
4:H:14:PRO:HA	4:H:82(C):LEU:O	2.17	0.44
4:H:22:CYS:HB3	4:H:78:ALA:HB3	1.99	0.44
3:L:89:GLN:HG2	3:L:90:HIS:O	2.18	0.44
4:H:2:VAL:HG13	4:H:27:TYR:CD2	2.52	0.44
2:B:21:LEU:CD2	2:B:77:LEU:HD23	2.38	0.44
4:H:43:LYS:HB3	4:H:44:SER:H	1.50	0.44
2:B:85:GLY:HA3	2:B:116:VAL:HG23	1.98	0.44
3:L:117:ILE:HG22	3:L:207:LYS:HB3	1.99	0.44
2:B:100:TRP:HH2	3:L:32:TYR:CD1	2.35	0.44
2:B:21:LEU:O	2:B:76:ARG:HB3	2.17	0.44
3:L:145:ASN:O	3:L:196:ALA:HA	2.17	0.44
3:L:61:ARG:CG	3:L:61:ARG:HH11	2.27	0.44
4:H:154:TRP:HZ3	4:H:210:ILE:HD11	1.80	0.44
4:H:142:VAL:HG22	4:H:197:VAL:HG21	2.00	0.44
4:H:32:TYR:O	4:H:52(A):PRO:HD2	2.18	0.44
2:B:13:VAL:HG23	2:B:14:PRO:HD2	1.99	0.44
4:H:138:LEU:HD23	4:H:210:ILE:CG2	2.44	0.44
2:B:62:GLY:O	2:B:63:ALA:HB2	2.18	0.44
1:A:27:SER:HA	1:A:71:LYS:HD3	1.99	0.44
4:H:136:VAL:HG13	4:H:138:LEU:CD1	2.48	0.43
3:L:142:LYS:HB2	3:L:173:TYR:CE2	2.53	0.43
2:B:87:THR:HG22	5:B:157:HOH:O	2.16	0.43
3:L:155:ARG:HH11	3:L:155:ARG:CB	2.28	0.43
2:B:37:GLN:HB2	2:B:43:LEU:HD12	2.00	0.43
2:B:6:GLN:NE2	2:B:111:GLY:HA2	2.33	0.43
3:L:131:SER:OG	3:L:180:THR:HG23	2.18	0.43
1:A:49:ILE:HG22	1:A:64:ILE:HD13	1.99	0.43
4:H:61:GLN:HB3	5:H:221:HOH:O	2.18	0.43
2:B:56:GLU:OE2	3:L:94:THR:N	2.40	0.43
3:L:143:ASP:O	3:L:198:HIS:CD2	2.72	0.43
1:A:10:LEU:C	1:A:10:LEU:HD12	2.39	0.43
3:L:210:ASN:CB	3:L:213:GLU:HB2	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PHE:HB3	5:A:126:HOH:O	2.18	0.43
3:L:5:THR:HB	5:L:217:HOH:O	2.19	0.43
1:A:61:ARG:HA	1:A:78:THR:HG22	1.99	0.43
3:L:44:PRO:HG2	4:H:103:TRP:CH2	2.54	0.43
2:B:31:TRP:CE2	2:B:50:ARG:HG3	2.54	0.43
4:H:40:SER:O	4:H:41:ASN:HB3	2.19	0.43
3:L:210:ASN:HB2	5:L:244:HOH:O	2.18	0.43
1:A:58:ASP:O	1:A:59:GLY:C	2.56	0.43
3:L:118:PHE:HA	3:L:119:PRO:HD3	1.76	0.42
2:B:11:ARG:HB3	2:B:114:LEU:CD2	2.49	0.42
1:A:106:PHE:CE2	2:B:43:LEU:HD23	2.53	0.42
1:A:37:GLN:HE22	2:B:37:GLN:HE22	1.67	0.42
3:L:117:ILE:HD12	3:L:148:TRP:HZ3	1.83	0.42
3:L:38:GLN:NE2	3:L:42:LYS:O	2.43	0.42
3:L:71:PHE:N	3:L:71:PHE:CD1	2.87	0.42
3:L:142:LYS:HB2	3:L:173:TYR:CD2	2.54	0.42
2:B:14:PRO:O	2:B:15:ARG:HB2	2.19	0.42
2:B:60:LEU:HD13	2:B:65:TYR:HE2	1.84	0.42
2:B:22:ARG:HG3	2:B:76:ARG:CG	2.50	0.42
3:L:148:TRP:NE1	3:L:177:SER:OG	2.43	0.42
2:B:38:ASP:OD1	2:B:40:GLN:OE1	2.37	0.42
2:B:52:PRO:HB3	2:B:71:THR:HA	2.01	0.42
4:H:112:SER:OG	4:H:113:SER:N	2.52	0.42
3:L:178:THR:HG22	5:L:225:HOH:O	2.19	0.42
2:B:69:ARG:HD2	2:B:74:GLU:O	2.20	0.42
3:L:161:ASN:OD1	3:L:177:SER:HA	2.20	0.42
4:H:166:PHE:O	4:H:167:PRO:C	2.57	0.42
4:H:192:SER:O	4:H:193:ILE:HD13	2.20	0.42
1:A:35:TYR:OH	2:B:106:LEU:HB3	2.20	0.41
4:H:148:GLU:HB2	5:H:218:HOH:O	2.20	0.41
4:H:94:ARG:NH1	4:H:101:ASP:HB3	2.35	0.41
1:A:67:ASN:O	1:A:68:LYS:C	2.58	0.41
3:L:20:THR:HA	3:L:73:LEU:O	2.20	0.41
4:H:75:SER:HB2	4:H:77:THR:OG1	2.19	0.41
2:B:114:LEU:HA	2:B:114:LEU:HD23	1.94	0.41
4:H:29:PHE:CZ	4:H:71:VAL:HG22	2.55	0.41
4:H:154:TRP:HZ3	4:H:210:ILE:CD1	2.32	0.41
4:H:147:PRO:HB2	5:H:218:HOH:O	2.19	0.41
4:H:118:ALA:HB1	4:H:119:PRO:HD2	2.02	0.41
3:L:90:HIS:CD2	3:L:90:HIS:C	2.93	0.41
1:A:106:PHE:CZ	2:B:43:LEU:HD23	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ASN:O	1:A:22:CYS:HB2	2.20	0.41
2:B:38:ASP:O	2:B:41:LYS:HA	2.20	0.41
2:B:77:LEU:CD2	2:B:90:LEU:HD22	2.51	0.41
2:B:93:THR:HB	2:B:106:LEU:HD11	2.03	0.41
3:L:82:ASP:HA	5:L:288:HOH:O	2.19	0.41
3:L:149:LYS:HA	3:L:153:SER:O	2.21	0.41
3:L:155:ARG:HE	3:L:181:LEU:HD23	1.85	0.41
4:H:188:TRP:CD1	4:H:189:PRO:HA	2.55	0.41
3:L:151:ASP:OD2	3:L:189:HIS:HD2	2.04	0.41
2:B:90:LEU:CD1	2:B:114:LEU:HD12	2.51	0.41
4:H:47:TRP:O	4:H:60:ASN:HB2	2.20	0.41
3:L:148:TRP:CZ3	3:L:194:CYS:HB2	2.56	0.41
3:L:165:ASP:O	3:L:166:GLN:C	2.60	0.41
4:H:47:TRP:CZ2	4:H:49:GLY:HA2	2.56	0.41
2:B:22:ARG:HG3	2:B:76:ARG:CD	2.51	0.41
2:B:51:SER:HA	2:B:52:PRO:HD3	1.88	0.41
3:L:28:ASN:ND2	3:L:29:ILE:O	2.54	0.41
4:H:18:VAL:O	4:H:81:GLN:HA	2.20	0.41
4:H:37:VAL:HA	4:H:46:GLU:O	2.21	0.41
4:H:151:THR:HG22	4:H:151:THR:O	2.20	0.41
3:L:160:LEU:HD11	5:H:277:HOH:O	2.21	0.41
4:H:69:LEU:HD13	4:H:80:MET:HG3	2.02	0.41
2:B:10:TRP:CD2	2:B:113:ARG:HD3	2.56	0.41
3:L:144:ILE:HG13	3:L:145:ASN:N	2.34	0.41
1:A:2:GLN:HG3	1:A:29:PHE:CZ	2.56	0.41
1:A:38:PHE:CE1	1:A:86:ALA:HB2	2.57	0.41
3:L:186:TYR:OH	3:L:209:PHE:HE1	2.04	0.40
2:B:85:GLY:CA	2:B:116:VAL:HG23	2.52	0.40
4:H:5:GLN:HG3	5:H:237:HOH:O	2.21	0.40
3:L:146:VAL:HA	3:L:195:GLU:O	2.21	0.40
1:A:4:ARG:HH22	1:A:25:GLU:CB	2.19	0.40
3:L:208:SER:O	3:L:209:PHE:HB3	2.22	0.40
3:L:4:MET:HB2	3:L:99:GLY:HA2	2.04	0.40
1:A:1:GLN:O	1:A:4:ARG:NE	2.54	0.40
1:A:5:GLN:HE22	1:A:89:PHE:HA	1.87	0.40
1:A:17:THR:HG23	1:A:78:THR:HA	2.04	0.40
4:H:82:LEU:HB3	4:H:82(C):LEU:HD21	2.04	0.40
2:B:60:LEU:HB3	2:B:61:PRO:CD	2.51	0.40
4:H:188:TRP:CD1	4:H:191:GLN:O	2.75	0.40
3:L:108:ARG:HD3	3:L:109:ALA:O	2.22	0.40
2:B:41:LYS:NZ	5:B:135:HOH:O	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1:ASP:CB	3:L:157:ASN:ND2[3_558]	1.76	0.44
3:L:17:GLU:OE2	3:L:152:GLY:O[3_557]	2.06	0.14

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	113/115 (98%)	93 (82%)	15 (13%)	5 (4%)	3	3
2	B	115/117 (98%)	99 (86%)	12 (10%)	4 (4%)	4	6
3	L	212/214 (99%)	191 (90%)	19 (9%)	2 (1%)	21	37
4	H	217/219 (99%)	177 (82%)	33 (15%)	7 (3%)	5	6
All	All	657/665 (99%)	560 (85%)	79 (12%)	18 (3%)	6	9

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	SER
2	B	2	THR
2	B	102	ALA
3	L	51	ALA
4	H	127	VAL
1	A	118	SER
2	B	15	ARG
4	H	31	GLY
4	H	114	ALA
1	A	86	ALA
1	A	68	LYS
4	H	128	CYS
4	H	144	GLY
1	A	39	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	185	SER
2	B	14	PRO
4	H	129	GLY
3	L	93	GLY

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	98/98 (100%)	71 (72%)	27 (28%)	0	0
2	B	102/102 (100%)	67 (66%)	35 (34%)	0	0
3	L	188/188 (100%)	137 (73%)	51 (27%)	0	0
4	H	190/190 (100%)	142 (75%)	48 (25%)	1	1
All	All	578/578 (100%)	417 (72%)	161 (28%)	0	0

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	4	ARG
1	A	6	SER
1	A	10	LEU
1	A	14	GLU
1	A	19	ILE
1	A	25	GLU
1	A	27	SER
1	A	28	THR
1	A	30	ASN
1	A	41	GLU
1	A	47	ILE
1	A	50	ARG
1	A	53	SER
1	A	55	LYS
1	A	56	LYS
1	A	63	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	69	ARG
1	A	70	GLU
1	A	72	LYS
1	A	73	LEU
1	A	74	SER
1	A	76	HIS
1	A	78	THR
1	A	101	ARG
1	A	111	THR
1	A	113	SER
2	B	2	THR
2	B	3	LEU
2	B	11	ARG
2	B	12	LEU
2	B	13	VAL
2	B	20	ASN
2	B	21	LEU
2	B	23	CYS
2	B	24	ILE
2	B	29	GLN
2	B	31	TRP
2	B	33	SER
2	B	36	GLN
2	B	38	ASP
2	B	39	LEU
2	B	44	GLN
2	B	47	PHE
2	B	49	LEU
2	B	50	ARG
2	B	51	SER
2	B	55	LYS
2	B	57	VAL
2	B	59	SER
2	B	68	THR
2	B	76	ARG
2	B	81	ASN
2	B	82	MET
2	B	86	ARG
2	B	87	THR
2	B	90	LEU
2	B	94	CYS
2	B	95	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	113	ARG
2	B	115	THR
2	B	116(A)	LEU
3	L	5	THR
3	L	7	SER
3	L	11	LEU
3	L	12	SER
3	L	15	VAL
3	L	19	VAL
3	L	27	LYS
3	L	40	GLN
3	L	42	LYS
3	L	45	GLN
3	L	52	LYS
3	L	54	LEU
3	L	61	ARG
3	L	63	SER
3	L	65	SER
3	L	67	SER
3	L	70	GLN
3	L	71	PHE
3	L	74	LYS
3	L	77	SER
3	L	78	LEU
3	L	85	SER
3	L	89	GLN
3	L	90	HIS
3	L	103	LYS
3	L	104	LEU
3	L	107	LYS
3	L	116	SER
3	L	127	SER
3	L	133	VAL
3	L	136	LEU
3	L	137	ASN
3	L	142	LYS
3	L	143	ASP
3	L	144	ILE
3	L	145	ASN
3	L	155	ARG
3	L	165	ASP
3	L	168	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	175	MET
3	L	176	SER
3	L	181	LEU
3	L	182	THR
3	L	183	LYS
3	L	191	SER
3	L	197	THR
3	L	199	LYS
3	L	202	THR
3	L	207	LYS
3	L	208	SER
3	L	212	ASN
4	H	5	GLN
4	H	6	GLN
4	H	7	SER
4	H	10	GLU
4	H	11	LEU
4	H	13	LYS
4	H	19	LYS
4	H	30	THR
4	H	40	SER
4	H	44	SER
4	H	51	ILE
4	H	62	LYS
4	H	66	ARG
4	H	71	VAL
4	H	73	LYS
4	H	74	SER
4	H	75	SER
4	H	76	SER
4	H	80	MET
4	H	82	LEU
4	H	82(A)	LYS
4	H	87	SER
4	H	96	ARG
4	H	97	THR
4	H	98	ASP
4	H	101	ASP
4	H	117	THR
4	H	128	CYS
4	H	152	LEU
4	H	158	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	160	SER
4	H	161	SER
4	H	165	THR
4	H	169	VAL
4	H	170	LEU
4	H	171	GLN
4	H	172	SER
4	H	173	ASP
4	H	177	LEU
4	H	180	SER
4	H	183	VAL
4	H	184	THR
4	H	188	TRP
4	H	192	SER
4	H	195	CYS
4	H	196	ASN
4	H	205	LYS
4	H	209	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	8	GLN
1	A	37	GLN
1	A	95	GLN
2	B	29	GLN
2	B	36	GLN
2	B	37	GLN
2	B	40	GLN
2	B	44	GLN
2	B	78	GLN
3	L	28	ASN
3	L	70	GLN
3	L	90	HIS
3	L	145	ASN
3	L	189	HIS
3	L	210	ASN
4	H	3	GLN
4	H	5	GLN
4	H	81	GLN
4	H	164	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	171	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	115/115 (100%)	0.49	6 (5%)	31 35	30, 48, 65, 89	3 (2%)
2	B	117/117 (100%)	0.71	9 (7%)	16 18	35, 49, 72, 75	0
3	L	214/214 (100%)	0.24	10 (4%)	35 40	28, 44, 60, 75	2 (0%)
4	H	219/219 (100%)	0.57	21 (9%)	10 11	33, 50, 64, 84	0
All	All	665/665 (100%)	0.48	46 (6%)	20 22	28, 48, 66, 89	5 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	ALA	8.9
4	H	131	THR	7.7
2	B	116(A)	LEU	7.2
1	A	116	PRO	5.7
1	A	118	SER	5.2
4	H	133	GLY	5.1
4	H	130	ASP	5.0
3	L	212	ASN	4.8
2	B	1	VAL	4.5
1	A	117	GLY	4.5
4	H	132	THR	4.1
4	H	134	SER	4.0
3	L	214	CYS	3.7
2	B	93	THR	3.5
2	B	116	VAL	3.4
4	H	179	SER	3.3
4	H	129	GLY	3.2
4	H	156	SER	3.1
3	L	133	VAL	3.1
1	A	10	LEU	3.0
2	B	70	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	184	ASP	2.9
4	H	127	VAL	2.9
2	B	90	LEU	2.9
4	H	140	CYS	2.9
4	H	184	THR	2.8
4	H	185	SER	2.8
4	H	93	ALA	2.7
3	L	190	ASN	2.7
4	H	141	LEU	2.7
1	A	78	THR	2.7
3	L	36	TYR	2.6
4	H	139	GLY	2.5
2	B	91	TYR	2.5
3	L	169	LYS	2.4
4	H	42	GLY	2.2
3	L	135	PHE	2.2
3	L	40	GLN	2.1
4	H	124	LEU	2.1
4	H	178	SER	2.1
2	B	71	THR	2.1
2	B	33	SER	2.1
4	H	115	LYS	2.1
4	H	174	LEU	2.1
3	L	188	ARG	2.0
4	H	117	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.