



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:20 PM UTC

PDB ID : 2F54 / pdb_00002f54
Title : Directed evolution of human T cell receptor CDR2 residues by phage display dramatically enhances affinity for cognate peptide-MHC without increasing apparent cross-reactivity
Authors : Rizkallah, P.J.; Jakobsen, B.K.; Dunn, S.M.; Sami, M.
Deposited on : 2005-11-25
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

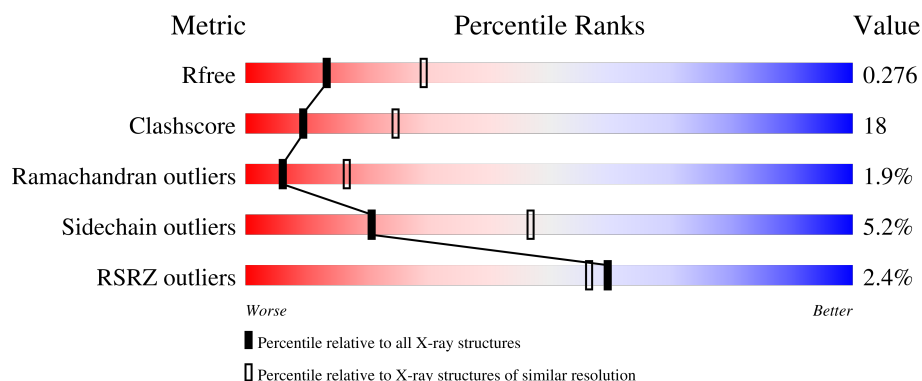
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	274	22% 65% 28% 7%
1	F	274	68% 27% 5%
2	B	100	69% 28% ..
2	G	100	3% 67% 30% .
3	C	9	22% 67% 22% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	9	78% 22%
4	D	206	7% 59% 35% 5%
4	K	206	4% 70% 24% 6%
5	E	241	2% 64% 30% 6%
5	L	241	76% 22%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13259 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 HLA class I histocompatibility antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2238	1398	408	423	9			
1	F	274	Total	C	N	O	S	0	0	0
			2238	1398	408	423	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			828	524	140	158	6			
2	G	100	Total	C	N	O	S	0	0	0
			828	524	140	158	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	cloning artifact	UNP P61769
B	67	CYS	TYR	engineered mutation	UNP P61769
B	91	CYS	LYS	engineered mutation	UNP P61769
G	0	MET	-	cloning artifact	UNP P61769
G	67	CYS	TYR	engineered mutation	UNP P61769
G	91	CYS	LYS	engineered mutation	UNP P61769

- Molecule 3 is a protein called Cancer/testis antigen 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			75	49	11	13	2			
3	H	9	Total	C	N	O	S	0	0	0
			75	49	11	13	2			

- Molecule 4 is a protein called T-cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	205	Total	C	N	O	S	0	0	0
			1567	975	262	323	7			
4	K	206	Total	C	N	O	S	0	0	0
			1576	981	264	324	7			

- Molecule 5 is a protein called T-cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	241	Total	C	N	O	S	0	0	0
			1902	1196	327	370	9			
5	L	241	Total	C	N	O	S	0	0	0
			1902	1196	327	370	9			

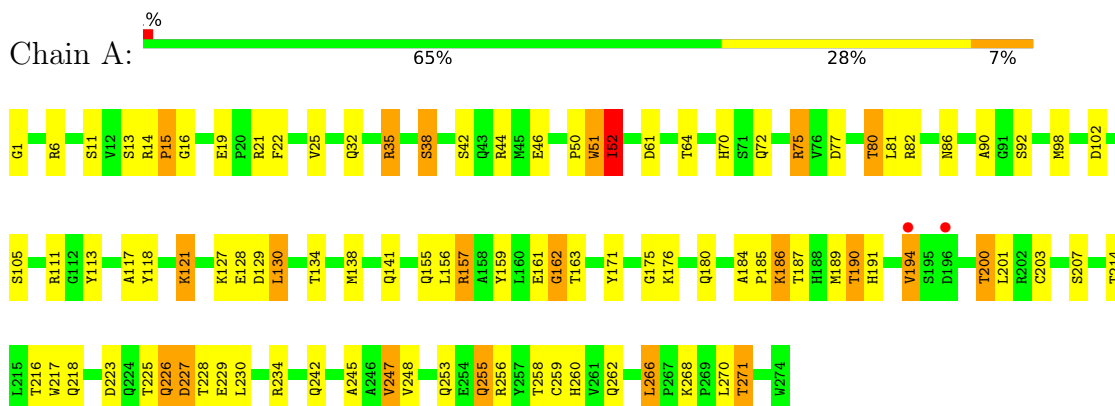
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	1	Total	O	0	0
			1	1		
6	C	1	Total	O	0	0
			1	1		
6	D	2	Total	O	0	0
			2	2		
6	E	1	Total	O	0	0
			1	1		
6	F	8	Total	O	0	0
			8	8		
6	G	1	Total	O	0	0
			1	1		
6	K	6	Total	O	0	0
			6	6		
6	L	4	Total	O	0	0
			4	4		

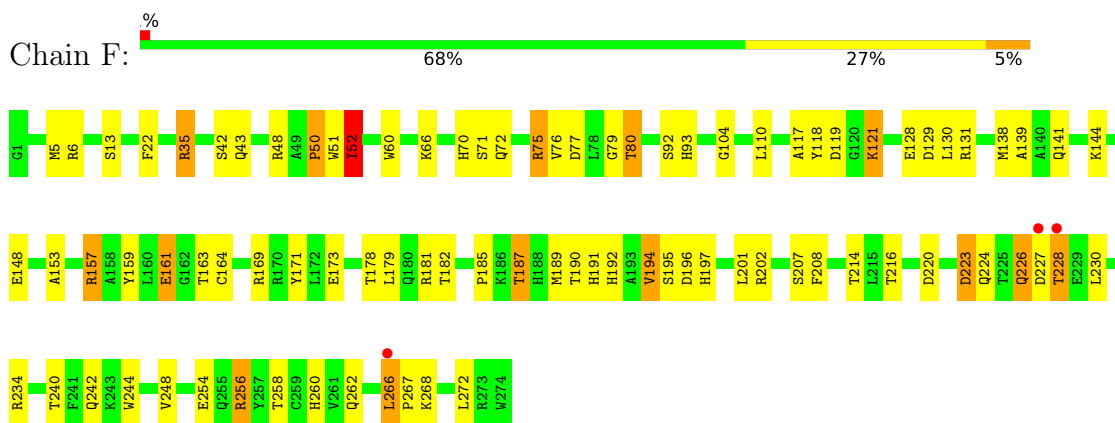
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

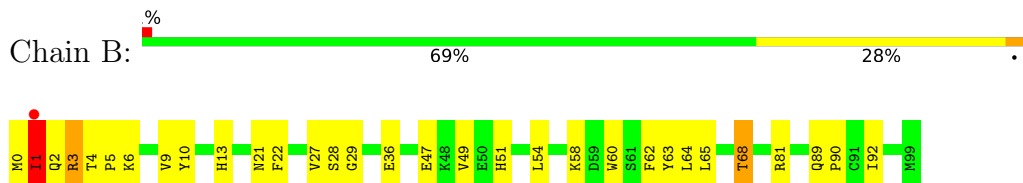
- Molecule 1: HLA class I histocompatibility antigen



- Molecule 1: HLA class I histocompatibility antigen

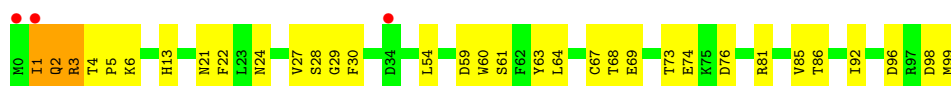


- Molecule 2: Beta-2-microglobulin

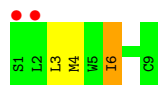


- Molecule 2: Beta-2-microglobulin

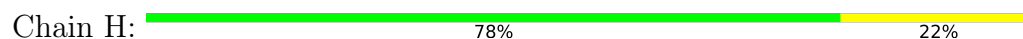




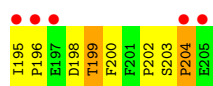
- Molecule 3: Cancer/testis antigen 1B



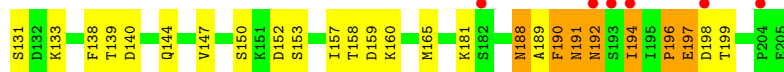
- Molecule 3: Cancer/testis antigen 1B



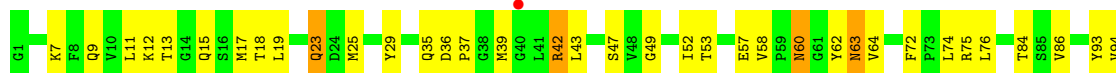
- Molecule 4: T-cell receptor alpha chain

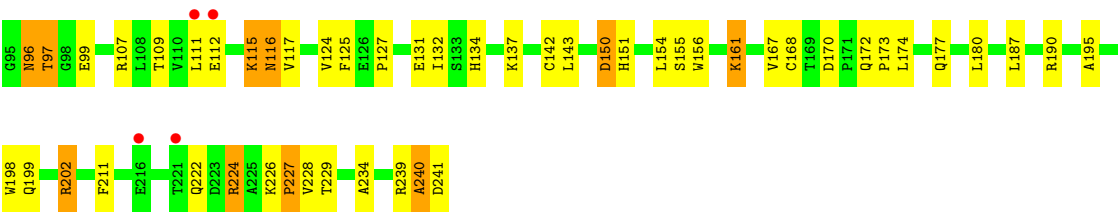


- Molecule 4: T-cell receptor alpha chain

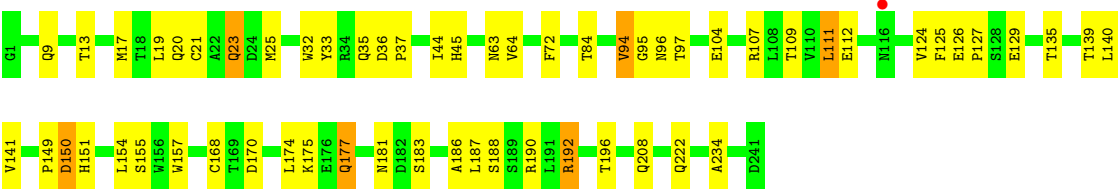


- Molecule 5: T-cell receptor beta chain





● Molecule 5: T-cell receptor beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.02Å 53.59Å 152.83Å 90.00° 96.04° 90.00°	Depositor
Resolution (Å)	50.66 – 2.70 50.66 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.66-2.70) 99.9 (50.66-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.221 , 0.286 (Not available) , 0.276	Depositor DCC
R_{free} test set	2740 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13259	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9909e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.14	1/2303 (0.0%)	0.87	3/3125 (0.1%)
1	F	1.07	2/2303 (0.1%)	0.90	3/3125 (0.1%)
2	B	1.13	2/850 (0.2%)	0.96	2/1149 (0.2%)
2	G	1.11	2/850 (0.2%)	0.95	1/1149 (0.1%)
3	C	0.96	0/76	0.84	0/101
3	H	1.15	0/76	0.99	0/101
4	D	0.95	1/1600 (0.1%)	0.90	4/2176 (0.2%)
4	K	1.02	1/1609 (0.1%)	0.95	4/2187 (0.2%)
5	E	1.01	0/1953	0.91	4/2659 (0.2%)
5	L	1.02	0/1953	0.86	6/2659 (0.2%)
All	All	1.05	9/13573 (0.1%)	0.90	27/18431 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	ILE	CA-CB	9.97	1.68	1.54
2	B	1	ILE	CA-CB	8.03	1.65	1.54
1	F	194	VAL	CA-CB	5.85	1.60	1.53
2	G	2	GLN	CA-C	5.78	1.59	1.52
1	F	228	THR	CA-CB	5.53	1.61	1.53
2	B	1	ILE	CA-C	5.47	1.59	1.52
4	K	93	PRO	CA-C	-5.19	1.46	1.52
4	D	162	VAL	N-CA	-5.17	1.40	1.46
1	A	184	ALA	CA-CB	-5.15	1.44	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	94	VAL	N-CA-C	-7.82	104.95	111.91
4	D	180	ASN	N-CA-C	-7.17	104.33	113.23
2	B	47	GLU	N-CA-C	7.01	118.71	111.14
5	E	94	VAL	N-CA-C	-6.95	105.72	111.91
5	L	129	GLU	N-CA-C	-6.58	104.11	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	240	ALA	N-CA-C	-6.28	101.95	110.68
5	E	93	TYR	N-CA-C	-6.18	102.38	110.53
4	K	1	GLN	N-CA-C	-6.06	100.69	110.32
1	F	179	LEU	N-CA-C	6.04	117.66	111.14
5	E	115	LYS	N-CA-C	-5.96	100.28	109.76
1	F	139	ALA	N-CA-C	-5.90	104.85	111.28
5	L	177	GLN	CA-C-N	5.85	125.72	119.28
5	L	177	GLN	C-N-CA	5.85	125.72	119.28
1	A	186	LYS	N-CA-C	-5.84	101.00	109.59
1	A	90	ALA	N-CA-C	5.79	117.68	111.36
4	K	165	MET	N-CA-C	-5.79	100.93	109.62
1	F	194	VAL	N-CA-C	5.74	114.63	106.53
4	D	203	SER	CA-C-N	5.73	127.00	119.84
4	D	203	SER	C-N-CA	5.73	127.00	119.84
4	D	104	GLY	N-CA-C	-5.71	102.74	112.51
2	B	92	ILE	CB-CA-C	-5.53	104.06	110.91
1	A	226	GLN	N-CA-C	-5.46	101.57	110.20
4	K	139	THR	N-CA-C	5.22	116.74	108.96
4	K	190	PHE	N-CA-C	-5.20	105.18	112.25
5	L	126	GLU	CA-C-N	5.14	125.07	119.78
5	L	126	GLU	C-N-CA	5.14	125.07	119.78
2	G	2	GLN	N-CA-CB	-5.04	102.86	110.77

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	2238	0	2090	77	1
1	F	2238	0	2090	78	1
2	B	828	0	791	24	0
2	G	828	0	791	30	0
3	C	75	0	79	5	0
3	H	75	0	79	3	0
4	D	1567	0	1499	76	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	1576	0	1512	60	0
5	E	1902	0	1799	87	0
5	L	1902	0	1799	51	0
6	A	6	0	0	2	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	1	0
6	E	1	0	0	0	0
6	F	8	0	0	4	0
6	G	1	0	0	0	0
6	K	6	0	0	0	0
6	L	4	0	0	0	0
All	All	13259	0	12529	462	1

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 18.

All (462) 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:F:80:THR:HG21	6:F:277:HOH:O	1.51	1.09
4:D:195:ILE:HD12	4:D:195:ILE:O	1.63	0.97
4:D:186:CYS:O	4:D:188:ASN:N	1.99	0.94
4:K:196:PRO:O	4:K:197:GLU:HG3	1.68	0.94
5:E:96:ASN:HD22	5:E:97:THR:N	1.67	0.91
5:E:96:ASN:HD22	5:E:97:THR:H	1.11	0.90
2:G:3:ARG:HG2	2:G:3:ARG:HH11	1.35	0.90
4:K:188:ASN:C	4:K:188:ASN:HD22	1.79	0.89
4:K:196:PRO:O	4:K:197:GLU:CG	2.22	0.87
2:B:3:ARG:HG2	2:B:3:ARG:HH11	1.39	0.86
4:K:192:ASN:C	4:K:194:ILE:H	1.83	0.85
4:D:37:GLN:HE22	5:E:35:GLN:HE22	1.20	0.85
4:K:1:GLN:HE22	4:K:26:ASP:H	1.21	0.84
5:E:132:ILE:HG21	5:E:199:GLN:HE21	1.40	0.84
4:K:192:ASN:O	4:K:194:ILE:N	2.11	0.83
4:K:158:THR:HG21	5:L:188:SER:OG	1.78	0.82
1:F:256:ARG:HG3	1:F:256:ARG:HH11	1.43	0.82
4:D:188:ASN:C	4:D:188:ASN:HD22	1.87	0.81
5:E:42:ARG:HG3	5:E:42:ARG:HH11	1.44	0.81
1:F:234:ARG:HE	1:F:242:GLN:HE21	1.30	0.80
5:E:96:ASN:ND2	5:E:97:THR:H	1.81	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:TRP:O	1:A:52:ILE:HG22	1.82	0.79
1:A:157:ARG:HG3	1:A:157:ARG:HH11	1.48	0.78
4:D:1:GLN:N	6:D:206:HOH:O	2.16	0.77
3:H:7:THR:HG23	5:L:96:ASN:HB3	1.66	0.77
4:D:16:GLU:O	4:D:79:SER:OG	2.03	0.77
4:D:31:ASN:C	4:D:31:ASN:HD22	1.90	0.77
5:E:132:ILE:HG21	5:E:199:GLN:NE2	2.00	0.77
4:K:1:GLN:NE2	4:K:26:ASP:H	1.82	0.77
4:D:28:ALA:HB1	4:D:94:THR:HG21	1.66	0.76
2:G:3:ARG:HG2	2:G:3:ARG:NH1	1.98	0.76
5:E:202:ARG:HG3	5:E:202:ARG:HH11	1.50	0.75
1:F:187:THR:HG23	1:F:272:LEU:HD11	1.68	0.75
1:F:266:LEU:HD13	1:F:267:PRO:HD2	1.69	0.73
1:A:255:GLN:HE21	1:A:255:GLN:HA	1.53	0.72
4:D:18:LEU:HD11	4:D:76:ILE:HD12	1.72	0.72
4:K:192:ASN:C	4:K:194:ILE:N	2.46	0.71
4:D:151:LYS:HD2	4:D:151:LYS:C	2.16	0.71
1:A:72:GLN:HG3	5:E:49:GLY:HA2	1.73	0.71
5:E:150:ASP:OD2	5:E:173:PRO:HG3	1.91	0.71
2:G:2:GLN:CG	2:G:86:THR:HG22	2.20	0.71
4:D:198:ASP:O	4:D:200:PHE:N	2.24	0.70
1:A:13:SER:O	1:A:92:SER:HB2	1.91	0.70
5:E:60:ASN:N	5:E:60:ASN:HD22	1.88	0.70
4:D:28:ALA:HB1	4:D:94:THR:CG2	2.21	0.70
1:F:70:HIS:CD2	3:H:6:ILE:HD11	2.26	0.70
4:K:127:ASP:HB3	4:K:130:SER:O	1.91	0.70
4:D:195:ILE:O	4:D:195:ILE:CD1	2.40	0.69
5:E:172:GLN:HG2	5:E:173:PRO:HD2	1.74	0.69
3:C:6:ILE:N	3:C:6:ILE:HD13	2.07	0.69
5:E:115:LYS:O	5:E:116:ASN:ND2	2.25	0.69
4:K:18:LEU:HD11	4:K:76:ILE:HD12	1.73	0.69
4:D:192:ASN:OD1	4:D:193:SER:N	2.21	0.67
1:F:191:HIS:CE1	1:F:254:GLU:OE1	2.47	0.67
4:D:115:ILE:HD12	4:D:141:PHE:O	1.95	0.67
5:L:17:MET:HE3	5:L:19:LEU:HD23	1.75	0.67
1:A:266:LEU:HD11	1:A:270:LEU:CD2	2.25	0.67
3:C:4:MET:SD	4:D:95:SER:HA	2.34	0.67
1:F:13:SER:O	1:F:92:SER:HB2	1.95	0.67
1:F:256:ARG:HH11	1:F:256:ARG:CG	2.07	0.67
1:A:226:GLN:O	1:A:227:ASP:HB2	1.94	0.66
1:F:118:TYR:O	1:F:121:LYS:HG2	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:81:ARG:HG2	2:G:92:ILE:CD1	2.25	0.66
5:E:23:GLN:NE2	5:E:25:MET:H	1.94	0.66
5:E:115:LYS:O	5:E:116:ASN:CG	2.39	0.66
2:B:63:TYR:O	2:B:64:LEU:HD12	1.96	0.65
4:D:6:ILE:HA	4:D:7:PRO:C	2.21	0.65
1:F:190:THR:HG21	2:G:98:ASP:OD2	1.96	0.65
1:A:266:LEU:CD1	1:A:268:LYS:O	2.45	0.65
1:A:72:GLN:HG3	5:E:49:GLY:CA	2.27	0.64
1:A:75:ARG:CG	1:A:75:ARG:HH11	2.09	0.64
1:F:227:ASP:OD2	1:F:248:VAL:HG22	1.98	0.64
4:K:1:GLN:HE22	4:K:26:ASP:N	1.95	0.64
5:L:20:GLN:HE21	5:L:20:GLN:HA	1.62	0.64
4:D:100:ILE:HD13	4:D:101:PRO:O	1.97	0.64
4:D:194:ILE:N	4:D:194:ILE:HD13	2.13	0.64
1:A:266:LEU:HD12	1:A:268:LYS:O	1.98	0.64
4:K:147:VAL:HA	4:K:194:ILE:HD12	1.80	0.64
5:E:84:THR:HG23	5:E:109:THR:HA	1.80	0.63
5:L:139:THR:OG1	5:L:192:ARG:HD3	1.98	0.63
5:E:224:ARG:HG3	5:E:224:ARG:HH11	1.64	0.63
2:B:3:ARG:HG2	2:B:3:ARG:NH1	2.10	0.63
5:E:240:ALA:C	5:E:241:ASP:OD1	2.42	0.62
4:K:48:LEU:HD13	4:K:49:ILE:N	2.15	0.62
1:F:51:TRP:O	1:F:52:ILE:HG22	1.99	0.62
4:D:90:ALA:HB2	4:D:103:PHE:CD1	2.34	0.61
4:D:188:ASN:C	4:D:188:ASN:ND2	2.58	0.61
5:E:202:ARG:HG3	5:E:202:ARG:NH1	2.15	0.61
1:A:50:PRO:C	1:A:51:TRP:O	2.39	0.61
1:A:226:GLN:O	1:A:227:ASP:CB	2.48	0.61
2:G:54:LEU:HD13	2:G:64:LEU:HD11	1.83	0.61
4:K:48:LEU:HD13	4:K:48:LEU:C	2.26	0.61
5:L:170:ASP:OD2	5:L:188:SER:OG	2.17	0.61
4:K:31:ASN:C	4:K:31:ASN:HD22	2.06	0.60
2:B:63:TYR:C	2:B:64:LEU:HD12	2.26	0.60
5:E:11:LEU:HD22	5:E:15:GLN:HE21	1.66	0.60
5:E:199:GLN:HA	5:E:239:ARG:O	2.02	0.60
1:F:5:MET:CE	1:F:164:CYS:HB2	2.32	0.60
4:D:156:TYR:O	4:D:177:ALA:HA	2.01	0.60
4:D:151:LYS:HD2	4:D:152:ASP:N	2.17	0.59
1:F:266:LEU:HD13	1:F:267:PRO:CD	2.31	0.59
4:D:142:ASP:OD1	4:D:143:SER:N	2.36	0.59
5:E:63:ASN:N	5:E:63:ASN:HD22	2.00	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:5:GLN:HE22	4:K:88:LEU:HA	1.66	0.59
4:K:26:ASP:O	4:K:27:SER:HB3	2.02	0.59
5:L:124:VAL:HG23	5:L:234:ALA:HB3	1.83	0.59
4:D:31:ASN:C	4:D:31:ASN:ND2	2.60	0.59
1:F:75:ARG:HG2	1:F:75:ARG:HH11	1.67	0.59
4:D:48:LEU:CD1	5:E:97:THR:HG23	2.32	0.59
2:G:63:TYR:C	2:G:64:LEU:HD12	2.27	0.59
1:F:75:ARG:HH11	1:F:75:ARG:CG	2.14	0.59
2:G:13:HIS:H	2:G:21:ASN:HD21	1.50	0.59
1:F:187:THR:CG2	1:F:272:LEU:HD11	2.31	0.59
1:A:111:ARG:HD2	1:A:128:GLU:HG3	1.84	0.59
2:G:3:ARG:HH11	2:G:3:ARG:CG	2.13	0.59
4:D:88:LEU:HD23	4:D:106:GLY:HA3	1.84	0.58
5:E:115:LYS:O	5:E:116:ASN:CB	2.51	0.58
1:A:189:MET:HE3	1:A:201:LEU:HB3	1.86	0.58
5:L:111:LEU:HD12	5:L:111:LEU:N	2.18	0.58
4:D:29:ILE:HD12	4:D:29:ILE:O	2.04	0.57
1:A:194:VAL:HG21	1:A:200:THR:OG1	2.04	0.57
1:A:185:PRO:HD2	1:A:266:LEU:HD23	1.85	0.57
4:D:36:ARG:NH2	4:D:82:GLY:O	2.29	0.57
1:A:75:ARG:HH11	1:A:75:ARG:HG2	1.68	0.57
5:E:12:LYS:HA	5:E:111:LEU:O	2.04	0.57
5:E:224:ARG:HG3	5:E:224:ARG:NH1	2.18	0.57
1:F:202:ARG:HD3	1:F:244:TRP:CE3	2.39	0.57
2:G:2:GLN:HG3	2:G:86:THR:HG22	1.86	0.57
5:L:155:SER:OG	5:L:157:TRP:CZ3	2.57	0.57
5:L:23:GLN:NE2	5:L:25:MET:H	2.02	0.56
1:A:22:PHE:H	1:A:38:SER:HG	1.54	0.56
4:D:77:ALA:O	4:D:78:ALA:C	2.48	0.56
2:G:54:LEU:CD1	2:G:64:LEU:HD11	2.36	0.56
4:D:202:PRO:O	4:D:204:PRO:HD3	2.04	0.56
4:D:6:ILE:O	4:D:6:ILE:HD12	2.05	0.56
1:F:70:HIS:CD2	3:H:6:ILE:CD1	2.89	0.56
4:K:26:ASP:O	4:K:27:SER:CB	2.53	0.56
5:L:17:MET:HE3	5:L:19:LEU:CD2	2.36	0.56
1:F:144:LYS:O	1:F:148:GLU:HG2	2.06	0.56
3:C:6:ILE:HD13	3:C:6:ILE:H	1.71	0.56
1:F:223:ASP:OD1	1:F:223:ASP:N	2.36	0.55
1:A:42:SER:CB	6:A:279:HOH:O	2.54	0.55
1:A:19:GLU:HG3	1:A:75:ARG:NH2	2.22	0.55
1:A:186:LYS:CE	1:A:207:SER:OG	2.54	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:196:PRO:HA	4:D:199:THR:HG23	1.87	0.55
1:F:157:ARG:O	1:F:161:GLU:HB2	2.07	0.55
1:F:93:HIS:HD2	1:F:119:ASP:OD1	1.88	0.55
2:G:2:GLN:HG2	2:G:86:THR:HG22	1.89	0.55
4:K:1:GLN:HE21	4:K:2:GLN:H	1.55	0.55
1:A:266:LEU:HD11	1:A:270:LEU:HD22	1.88	0.54
5:E:11:LEU:HD22	5:E:15:GLN:NE2	2.22	0.54
5:E:172:GLN:CG	5:E:173:PRO:HD2	2.36	0.54
1:A:77:ASP:HA	1:A:80:THR:HG23	1.89	0.54
4:D:19:VAL:HG13	4:D:73:THR:HG23	1.88	0.54
4:D:37:GLN:HE22	5:E:35:GLN:NE2	1.97	0.54
1:F:153:ALA:O	1:F:157:ARG:HB2	2.07	0.54
2:G:21:ASN:ND2	2:G:22:PHE:H	2.05	0.54
4:K:99:TYR:CE1	5:L:94:VAL:HG22	2.42	0.54
5:E:174:LEU:HD12	5:E:174:LEU:C	2.31	0.54
2:B:21:ASN:ND2	2:B:22:PHE:H	2.06	0.54
4:D:19:VAL:HG13	4:D:73:THR:CG2	2.38	0.54
4:K:42:LYS:HB3	5:L:104:GLU:O	2.07	0.54
4:D:20:LEU:HB2	4:D:74:LEU:HB3	1.90	0.53
5:L:155:SER:HG	5:L:157:TRP:HZ3	1.49	0.53
5:E:154:LEU:C	5:E:154:LEU:HD23	2.33	0.53
1:F:191:HIS:HE1	1:F:254:GLU:OE1	1.90	0.53
2:B:54:LEU:HD13	2:B:64:LEU:HD11	1.89	0.53
1:F:189:MET:CE	1:F:201:LEU:HD22	2.38	0.53
2:B:54:LEU:CD1	2:B:64:LEU:HD11	2.39	0.53
5:E:174:LEU:HD12	5:E:174:LEU:O	2.08	0.53
1:F:189:MET:HE2	1:F:201:LEU:HD22	1.91	0.53
1:A:51:TRP:CZ3	1:A:171:TYR:HB3	2.44	0.53
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.44	0.53
1:A:157:ARG:HG3	1:A:157:ARG:NH1	2.18	0.53
5:E:23:GLN:HE21	5:E:25:MET:H	1.57	0.53
1:F:266:LEU:CB	6:F:279:HOH:O	2.56	0.53
2:G:29:GLY:HA2	2:G:61:SER:CB	2.39	0.52
1:A:156:LEU:O	1:A:157:ARG:C	2.52	0.52
5:L:96:ASN:CG	5:L:97:THR:H	2.17	0.52
5:L:149:PRO:C	5:L:151:HIS:H	2.18	0.52
1:A:186:LYS:HE2	1:A:207:SER:OG	2.09	0.52
1:A:42:SER:HB2	6:A:279:HOH:O	2.08	0.52
2:G:29:GLY:HA2	2:G:61:SER:HB2	1.91	0.52
1:A:189:MET:HE2	1:A:201:LEU:HD22	1.91	0.52
4:D:125:LEU:HD12	4:D:125:LEU:N	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:11:LEU:HD11	5:E:17:MET:HB2	1.92	0.52
5:E:154:LEU:HD23	5:E:155:SER:N	2.24	0.52
1:A:258:THR:HG22	1:A:260:HIS:CD2	2.45	0.52
2:B:0:MET:C	2:B:2:GLN:H	2.18	0.52
2:G:5:PRO:HB3	2:G:30:PHE:HB3	1.92	0.52
1:F:224:GLN:CG	1:F:226:GLN:HB3	2.39	0.52
5:L:107:ARG:HD2	5:L:107:ARG:N	2.25	0.52
4:D:148:SER:OG	4:D:192:ASN:HB2	2.11	0.51
4:D:48:LEU:C	4:D:48:LEU:HD13	2.34	0.51
5:E:64:VAL:CG1	5:E:72:PHE:CE1	2.92	0.51
1:F:178:THR:O	1:F:181:ARG:HB3	2.11	0.51
1:F:182:THR:HG23	1:F:182:THR:O	2.09	0.51
1:A:51:TRP:O	1:A:52:ILE:CG2	2.58	0.51
2:G:73:THR:OG1	2:G:76:ASP:OD2	2.24	0.51
1:A:14:ARG:O	1:A:16:GLY:N	2.43	0.51
1:A:228:THR:HG22	1:A:230:LEU:CD1	2.40	0.51
4:D:98:SER:C	4:D:100:ILE:H	2.18	0.51
5:L:150:ASP:O	5:L:150:ASP:OD2	2.29	0.51
2:B:13:HIS:H	2:B:21:ASN:HD21	1.57	0.51
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.46	0.51
1:F:207:SER:HA	1:F:240:THR:HB	1.93	0.51
2:G:6:LYS:O	2:G:27:VAL:HA	2.12	0.50
5:L:20:GLN:HA	5:L:20:GLN:NE2	2.25	0.50
1:F:190:THR:CG2	1:F:191:HIS:N	2.75	0.50
2:G:68:THR:HG22	2:G:69:GLU:N	2.27	0.50
1:A:111:ARG:CD	1:A:128:GLU:HG3	2.41	0.50
1:F:159:TYR:CD1	1:F:163:THR:HB	2.47	0.50
4:D:38:ASP:O	4:D:39:PRO:C	2.54	0.50
5:E:224:ARG:HH11	5:E:224:ARG:CG	2.25	0.50
5:E:9:GLN:HG2	5:E:17:MET:HE2	1.94	0.50
1:F:234:ARG:HE	1:F:242:GLN:NE2	2.04	0.50
1:A:155:GLN:NE2	4:D:52:SER:OG	2.45	0.50
4:K:31:ASN:C	4:K:31:ASN:ND2	2.70	0.50
2:B:58:LYS:HD2	2:B:58:LYS:C	2.37	0.49
5:E:62:TYR:HB3	5:E:74:LEU:HD11	1.94	0.49
1:F:195:SER:O	1:F:197:HIS:N	2.45	0.49
5:E:17:MET:HE3	5:E:19:LEU:HD23	1.94	0.49
5:E:161:LYS:NZ	5:E:161:LYS:HB2	2.27	0.49
4:K:191:ASN:HD22	4:K:192:ASN:N	2.10	0.49
4:D:29:ILE:HD12	4:D:29:ILE:C	2.37	0.49
4:K:196:PRO:O	4:K:197:GLU:CB	2.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.48	0.49
1:F:224:GLN:HE21	1:F:226:GLN:CG	2.25	0.49
1:A:259:CYS:O	1:A:271:THR:HA	2.12	0.49
4:D:151:LYS:C	4:D:151:LYS:CD	2.85	0.49
5:L:155:SER:OG	5:L:157:TRP:HZ3	1.93	0.49
1:F:66:LYS:O	1:F:70:HIS:HD2	1.96	0.49
1:F:169:ARG:O	1:F:173:GLU:HG2	2.12	0.49
1:F:266:LEU:HD22	1:F:267:PRO:HD2	1.94	0.49
4:D:163:LEU:C	4:D:163:LEU:HD12	2.38	0.49
5:E:13:THR:HG21	5:E:112:GLU:CG	2.42	0.49
5:L:177:GLN:O	5:L:183:SER:HB2	2.11	0.49
4:D:20:LEU:HD12	4:D:74:LEU:HD23	1.94	0.49
1:A:175:GLY:O	1:A:176:LYS:C	2.55	0.48
1:A:190:THR:CG2	1:A:191:HIS:N	2.76	0.48
5:E:13:THR:HG21	5:E:112:GLU:HG2	1.96	0.48
5:L:190:ARG:N	5:L:190:ARG:HD2	2.28	0.48
1:F:13:SER:OG	1:F:92:SER:HA	2.12	0.48
1:F:77:ASP:HA	1:F:80:THR:CG2	2.43	0.48
1:A:118:TYR:O	1:A:121:LYS:HG2	2.13	0.48
1:F:266:LEU:CD1	1:F:267:PRO:HD2	2.43	0.48
1:F:51:TRP:O	1:F:52:ILE:CB	2.62	0.48
4:K:31:ASN:HD21	4:K:92:ARG:HG3	1.78	0.48
1:F:228:THR:HG22	1:F:230:LEU:HD13	1.96	0.48
4:D:18:LEU:HD12	4:D:18:LEU:C	2.39	0.48
4:K:131:SER:O	4:K:133:LYS:N	2.41	0.48
4:D:163:LEU:HD12	4:D:163:LEU:O	2.14	0.48
1:F:50:PRO:C	1:F:51:TRP:O	2.51	0.48
1:A:44:ARG:NH2	1:A:61:ASP:OD1	2.47	0.47
4:K:196:PRO:O	4:K:197:GLU:CD	2.57	0.47
4:D:178:TRP:CH2	5:E:143:LEU:HD11	2.50	0.47
2:G:63:TYR:O	2:G:64:LEU:HD12	2.14	0.47
1:A:82:ARG:O	1:A:86:ASN:N	2.48	0.47
5:L:174:LEU:HD12	5:L:174:LEU:O	2.15	0.47
5:L:21:CYS:HB2	5:L:32:TRP:CZ2	2.49	0.47
4:D:37:GLN:NE2	5:E:35:GLN:HE22	2.01	0.47
5:E:132:ILE:HG23	5:E:195:ALA:HB1	1.96	0.47
4:K:190:PHE:HB3	4:K:194:ILE:HD13	1.95	0.47
1:F:226:GLN:HG3	1:F:227:ASP:N	2.30	0.47
2:B:0:MET:C	2:B:2:GLN:N	2.73	0.47
1:A:253:GLN:HE21	1:A:256:ARG:HD3	1.79	0.46
1:F:266:LEU:HB2	6:F:279:HOH:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:7:LYS:HD3	5:E:7:LYS:N	2.29	0.46
2:G:24:ASN:ND2	2:G:67:CYS:HB3	2.31	0.46
4:K:125:LEU:HD12	4:K:125:LEU:N	2.30	0.46
5:L:9:GLN:HG2	5:L:17:MET:HE2	1.97	0.46
2:B:36:GLU:HG2	2:B:81:ARG:HH22	1.80	0.46
5:E:111:LEU:HD12	5:E:111:LEU:N	2.30	0.46
5:E:226:LYS:O	5:E:228:VAL:N	2.42	0.46
1:F:194:VAL:HG13	1:F:194:VAL:O	2.16	0.46
1:F:189:MET:HE3	1:F:201:LEU:HB3	1.96	0.46
1:F:190:THR:HG21	1:F:192:HIS:CE1	2.50	0.46
5:L:84:THR:HG23	5:L:109:THR:HA	1.98	0.46
4:D:92:ARG:HG2	4:D:101:PRO:HB3	1.98	0.46
4:D:168:MET:O	4:D:169:ASP:C	2.58	0.46
5:E:124:VAL:HG23	5:E:234:ALA:HB3	1.98	0.46
1:F:35:ARG:O	1:F:35:ARG:HD3	2.15	0.46
1:F:228:THR:CG2	1:F:230:LEU:HD13	2.45	0.46
1:A:194:VAL:CG2	1:A:200:THR:OG1	2.64	0.46
2:B:3:ARG:HB3	2:B:29:GLY:O	2.16	0.46
2:B:10:TYR:CD1	2:B:10:TYR:N	2.84	0.46
1:F:130:LEU:HB3	1:F:157:ARG:HG2	1.96	0.46
4:K:42:LYS:HG2	5:L:104:GLU:OE2	2.15	0.46
4:K:92:ARG:HG2	4:K:101:PRO:HB3	1.97	0.46
4:D:98:SER:OG	4:D:100:ILE:HG22	2.15	0.46
5:E:62:TYR:C	5:E:63:ASN:HD22	2.25	0.45
5:E:109:THR:HG22	5:E:111:LEU:HD11	1.98	0.45
1:F:138:MET:HA	1:F:141:GLN:HG2	1.97	0.45
2:B:81:ARG:HD3	2:B:90:PRO:HB3	1.97	0.45
4:D:194:ILE:HG12	4:D:196:PRO:HD3	1.97	0.45
5:L:170:ASP:HB2	5:L:187:LEU:HD12	1.97	0.45
5:E:58:VAL:HG23	5:E:58:VAL:O	2.17	0.45
5:E:76:LEU:HD12	5:E:76:LEU:N	2.32	0.45
4:K:188:ASN:HA	4:K:191:ASN:HB2	1.98	0.45
5:L:96:ASN:CG	5:L:97:THR:N	2.72	0.45
5:E:60:ASN:HD22	5:E:60:ASN:H	1.60	0.45
5:L:157:TRP:CZ3	5:L:208:GLN:HB3	2.52	0.45
5:E:52:ILE:CG1	5:E:53:THR:N	2.79	0.45
1:F:77:ASP:O	1:F:80:THR:HG23	2.16	0.45
1:A:218:GLN:HA	1:A:223:ASP:HA	1.97	0.45
5:E:107:ARG:HB3	5:E:151:HIS:NE2	2.32	0.45
1:A:11:SER:HA	1:A:21:ARG:O	2.17	0.45
1:A:128:GLU:O	1:A:130:LEU:HD22	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:98:SER:O	4:K:99:TYR:HB2	2.17	0.45
5:L:36:ASP:O	5:L:37:PRO:C	2.59	0.45
4:K:28:ALA:HB1	4:K:94:THR:CG2	2.47	0.45
1:A:258:THR:CG2	1:A:260:HIS:NE2	2.80	0.44
2:B:6:LYS:O	2:B:27:VAL:HA	2.17	0.44
4:K:18:LEU:C	4:K:18:LEU:HD12	2.41	0.44
4:K:48:LEU:CD1	5:L:97:THR:HG23	2.47	0.44
4:K:159:ASP:OD2	4:K:160:LYS:N	2.51	0.44
4:K:48:LEU:C	4:K:48:LEU:CD1	2.90	0.44
5:L:149:PRO:O	5:L:151:HIS:N	2.45	0.44
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.52	0.44
3:C:6:ILE:N	3:C:6:ILE:CD1	2.78	0.44
5:E:42:ARG:NH2	5:E:58:VAL:HG11	2.32	0.44
4:K:84:SER:O	4:K:85:ALA:HB2	2.17	0.44
5:L:23:GLN:HE21	5:L:25:MET:H	1.66	0.44
1:F:22:PHE:CD2	1:F:71:SER:HB3	2.53	0.44
1:F:190:THR:HG22	1:F:191:HIS:N	2.33	0.44
1:A:98:MET:SD	1:A:98:MET:C	3.01	0.44
4:D:38:ASP:OD1	4:D:38:ASP:N	2.49	0.44
5:L:44:ILE:HG22	5:L:45:HIS:CD2	2.52	0.44
4:D:98:SER:C	4:D:100:ILE:N	2.74	0.44
5:E:177:GLN:OE1	5:E:180:LEU:HD12	2.18	0.44
1:F:224:GLN:HG2	1:F:226:GLN:HB3	2.00	0.44
5:L:125:PHE:HB2	5:L:141:VAL:HG22	2.00	0.44
1:A:15:PRO:CD	1:A:92:SER:HB3	2.48	0.44
1:A:229:GLU:O	1:A:245:ALA:HA	2.18	0.44
2:B:0:MET:O	2:B:2:GLN:N	2.50	0.44
5:E:43:LEU:O	5:E:57:GLU:N	2.37	0.44
5:E:64:VAL:HG11	5:E:72:PHE:CE1	2.53	0.44
1:A:44:ARG:HA	1:A:64:THR:HG23	2.00	0.44
4:D:48:LEU:HD11	5:E:97:THR:HG23	2.00	0.44
5:E:64:VAL:HG11	5:E:72:PHE:CZ	2.52	0.44
5:E:97:THR:CG2	5:E:99:GLU:HB2	2.48	0.44
2:G:96:ASP:CB	2:G:99:MET:HE2	2.48	0.44
4:K:150:SER:HB2	4:K:157:ILE:CD1	2.48	0.44
2:B:54:LEU:HD11	2:B:62:PHE:CD1	2.53	0.43
5:E:170:ASP:HB2	5:E:187:LEU:HD12	2.00	0.43
1:A:138:MET:SD	1:A:141:GLN:HG3	2.58	0.43
5:E:117:VAL:HG12	5:E:227:PRO:HB2	2.01	0.43
4:K:140:ASP:OD1	4:K:140:ASP:N	2.51	0.43
4:D:93:PRO:HB2	4:D:95:SER:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:81:ARG:HG2	2:G:92:ILE:HD13	1.98	0.43
1:A:194:VAL:HG23	1:A:200:THR:H	1.83	0.43
4:D:125:LEU:N	4:D:125:LEU:CD1	2.82	0.43
5:E:18:THR:OG1	5:E:75:ARG:NH1	2.51	0.43
1:A:70:HIS:HE1	3:C:3:LEU:O	2.01	0.43
4:D:40:GLY:O	5:E:107:ARG:NH2	2.52	0.43
5:L:95:GLY:O	5:L:96:ASN:OD1	2.37	0.43
5:L:154:LEU:HD23	5:L:154:LEU:C	2.43	0.43
1:A:14:ARG:O	1:A:15:PRO:C	2.62	0.43
2:B:89:GLN:O	2:B:90:PRO:C	2.60	0.43
1:A:162:GLY:O	1:A:163:THR:C	2.60	0.43
2:B:51:HIS:HA	2:B:65:LEU:O	2.19	0.43
4:D:42:LYS:HE3	4:D:44:THR:OG1	2.19	0.43
1:F:266:LEU:HD12	1:F:268:LYS:O	2.18	0.43
4:D:119:ASP:OD1	5:E:134:HIS:NE2	2.52	0.42
1:F:75:ARG:CG	1:F:75:ARG:NH1	2.81	0.42
4:K:188:ASN:HD22	4:K:189:ALA:N	2.15	0.42
1:A:266:LEU:HD21	1:A:270:LEU:HD21	2.00	0.42
2:B:49:VAL:HA	2:B:68:THR:OG1	2.18	0.42
4:D:141:PHE:CZ	4:D:173:ASN:HB3	2.55	0.42
5:E:167:VAL:HA	5:E:190:ARG:O	2.19	0.42
1:F:51:TRP:O	1:F:52:ILE:CG2	2.65	0.42
1:F:52:ILE:HD12	1:F:60:TRP:CH2	2.54	0.42
2:G:5:PRO:CA	2:G:30:PHE:HB3	2.49	0.42
4:K:120:PRO:HB2	4:K:199:THR:HG22	2.01	0.42
1:A:156:LEU:O	1:A:159:TYR:N	2.53	0.42
2:B:5:PRO:HA	2:B:28:SER:O	2.19	0.42
2:G:59:ASP:O	2:G:60:TRP:HB2	2.19	0.42
4:D:48:LEU:O	4:D:56:GLN:OE1	2.38	0.42
4:D:194:ILE:N	4:D:194:ILE:CD1	2.81	0.42
5:E:96:ASN:ND2	5:E:97:THR:N	2.47	0.42
4:K:27:SER:O	4:K:29:ILE:N	2.53	0.42
4:K:28:ALA:HB1	4:K:94:THR:HG22	2.01	0.42
1:A:1:GLY:O	1:A:105:SER:HA	2.19	0.42
1:A:6:ARG:NH1	1:A:113:TYR:CD2	2.88	0.42
1:A:72:GLN:HG3	5:E:49:GLY:HA3	2.01	0.42
1:F:104:GLY:N	1:F:110:LEU:HD13	2.35	0.42
1:F:266:LEU:HB3	6:F:279:HOH:O	2.18	0.42
4:K:152:ASP:O	4:K:153:SER:C	2.63	0.42
5:L:175:LYS:HE2	5:L:183:SER:HB3	2.02	0.42
1:A:35:ARG:HD2	1:A:46:GLU:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:HE3	1:A:134:THR:OG1	2.19	0.42
4:D:6:ILE:HD12	4:D:6:ILE:C	2.44	0.42
1:F:5:MET:HE2	1:F:164:CYS:HB2	2.01	0.42
2:G:74:GLU:OE1	2:G:74:GLU:HA	2.20	0.42
5:L:135:THR:O	5:L:135:THR:HG22	2.18	0.42
5:E:86:VAL:HG22	5:E:107:ARG:HG3	2.02	0.42
5:E:211:PHE:O	5:E:229:THR:HG23	2.20	0.42
1:F:129:ASP:OD1	1:F:129:ASP:C	2.63	0.42
4:K:101:PRO:HG2	5:L:33:TYR:OH	2.20	0.42
4:K:190:PHE:O	4:K:194:ILE:HG23	2.19	0.42
5:L:170:ASP:HB2	5:L:187:LEU:CD1	2.50	0.42
5:L:174:LEU:CD1	5:L:186:ALA:HB3	2.50	0.42
1:A:50:PRO:O	1:A:51:TRP:O	2.37	0.42
1:F:185:PRO:HB3	1:F:208:PHE:HB3	2.01	0.42
5:E:115:LYS:C	5:E:116:ASN:HD22	2.27	0.41
1:F:42:SER:O	1:F:43:GLN:HB2	2.20	0.41
1:A:25:VAL:HG13	1:A:32:GLN:HG3	2.02	0.41
5:E:132:ILE:HG23	5:E:195:ALA:CB	2.50	0.41
1:F:5:MET:O	1:F:6:ARG:HD3	2.20	0.41
5:L:174:LEU:HD11	5:L:186:ALA:HB3	2.01	0.41
1:A:227:ASP:O	1:A:247:VAL:HG12	2.20	0.41
2:B:21:ASN:HD22	2:B:22:PHE:H	1.67	0.41
4:D:32:LEU:HD13	4:D:72:SER:HB2	2.01	0.41
4:D:154:ASP:OD1	4:D:181:LYS:HB2	2.21	0.41
5:E:127:PRO:HD2	5:E:198:TRP:CZ2	2.56	0.41
1:F:220:ASP:OD1	1:F:256:ARG:NH2	2.54	0.41
1:F:258:THR:HG22	1:F:260:HIS:NE2	2.36	0.41
2:G:29:GLY:HA2	2:G:61:SER:OG	2.19	0.41
4:D:119:ASP:CG	5:E:134:HIS:HE2	2.29	0.41
4:K:92:ARG:HA	4:K:93:PRO:HD3	1.90	0.41
1:A:102:ASP:OD2	1:A:113:TYR:OH	2.29	0.41
4:D:135:VAL:HG23	5:E:125:PHE:CE2	2.54	0.41
4:D:160:LYS:HE3	4:D:160:LYS:HB2	1.90	0.41
5:E:109:THR:HG22	5:E:111:LEU:CD1	2.50	0.41
5:E:142:CYS:HB2	5:E:156:TRP:CZ2	2.56	0.41
5:E:222:GLN:O	5:E:224:ARG:N	2.53	0.41
5:L:20:GLN:HE21	5:L:20:GLN:CA	2.26	0.41
1:A:266:LEU:HD12	1:A:268:LYS:C	2.46	0.41
1:F:214:THR:HB	1:F:262:GLN:HB2	2.03	0.41
4:K:5:GLN:NE2	4:K:89:CYS:H	2.17	0.41
1:A:186:LYS:HE3	1:A:207:SER:OG	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:131:SER:O	4:D:132:ASP:HB3	2.21	0.41
4:D:198:ASP:O	4:D:199:THR:C	2.64	0.41
1:F:51:TRP:CZ3	1:F:171:TYR:HB3	2.56	0.41
4:K:50:GLN:C	4:K:52:SER:H	2.29	0.41
1:A:266:LEU:HD21	1:A:270:LEU:CD2	2.50	0.41
1:F:216:THR:O	1:F:260:HIS:N	2.47	0.41
2:G:22:PHE:HA	2:G:69:GLU:HA	2.02	0.41
4:K:7:PRO:O	4:K:107:THR:HG23	2.19	0.41
4:K:191:ASN:HD22	4:K:191:ASN:C	2.28	0.41
5:L:13:THR:CG2	5:L:112:GLU:HG2	2.51	0.41
5:L:174:LEU:HD12	5:L:174:LEU:C	2.45	0.41
4:D:29:ILE:O	4:D:51:SER:HB3	2.21	0.41
5:E:29:TYR:HA	5:E:47:SER:O	2.21	0.41
4:K:1:GLN:OE1	4:K:26:ASP:HB3	2.21	0.41
4:K:36:ARG:NH2	4:K:82:GLY:O	2.52	0.41
1:A:214:THR:HB	1:A:262:GLN:HB2	2.02	0.40
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.69	0.40
5:E:36:ASP:HB2	5:E:39:MET:HG3	2.03	0.40
5:E:131:GLU:HG2	5:E:137:LYS:O	2.21	0.40
4:K:88:LEU:HD23	4:K:106:GLY:CA	2.50	0.40
4:K:198:ASP:N	4:K:198:ASP:OD1	2.54	0.40
5:E:11:LEU:HD11	5:E:17:MET:CB	2.51	0.40
1:A:216:THR:O	1:A:260:HIS:N	2.51	0.40
2:G:5:PRO:HA	2:G:28:SER:O	2.21	0.40
5:L:127:PRO:HG3	5:L:140:LEU:HD12	2.04	0.40
4:K:37:GLN:HE22	5:L:35:GLN:HE22	1.69	0.40
4:K:138:PHE:HB2	4:K:190:PHE:CE2	2.57	0.40
5:L:63:ASN:HD22	5:L:63:ASN:N	2.20	0.40
5:L:64:VAL:CG1	5:L:72:PHE:CE1	3.04	0.40
4:D:10:LEU:N	4:D:108:SER:O	2.46	0.40
1:F:76:VAL:O	1:F:79:GLY:N	2.55	0.40

All (1) 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)
1:A:129:ASP:OD2	1:F:226:GLN:NE2[2_546]	2.08	0.12

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	272/274 (99%)	247 (91%)	19 (7%)	6 (2%)	5	14
1	F	272/274 (99%)	246 (90%)	21 (8%)	5 (2%)	6	18
2	B	98/100 (98%)	96 (98%)	1 (1%)	1 (1%)	12	32
2	G	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	203/206 (98%)	173 (85%)	21 (10%)	9 (4%)	2	4
4	K	204/206 (99%)	185 (91%)	14 (7%)	5 (2%)	4	11
5	E	239/241 (99%)	224 (94%)	11 (5%)	4 (2%)	7	19
5	L	239/241 (99%)	223 (93%)	15 (6%)	1 (0%)	30	54
All	All	1639/1660 (99%)	1498 (91%)	110 (7%)	31 (2%)	6	17

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	PRO
4	D	187	ALA
4	D	194	ILE
4	D	199	THR
5	E	116	ASN
1	F	52	ILE
1	F	196	ASP
1	F	226	GLN
4	K	181	LYS
4	K	197	GLU
5	L	150	ASP
1	A	227	ASP
2	B	1	ILE
4	D	55	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	78	ALA
4	D	116	GLN
4	D	131	SER
4	D	192	ASN
4	D	204	PRO
5	E	150	ASP
1	A	51	TRP
4	K	192	ASN
4	K	27	SER
4	K	196	PRO
1	A	162	GLY
1	A	194	VAL
1	F	50	PRO
1	F	131	ARG
1	A	52	ILE
5	E	37	PRO
5	E	227	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	230/230 (100%)	211 (92%)	19 (8%)	10	26
1	F	230/230 (100%)	216 (94%)	14 (6%)	17	40
2	B	95/95 (100%)	90 (95%)	5 (5%)	20	46
2	G	95/95 (100%)	91 (96%)	4 (4%)	26	55
3	C	9/9 (100%)	8 (89%)	1 (11%)	6	15
3	H	9/9 (100%)	9 (100%)	0	100	100
4	D	180/181 (99%)	173 (96%)	7 (4%)	28	57
4	K	181/181 (100%)	173 (96%)	8 (4%)	25	53
5	E	208/208 (100%)	198 (95%)	10 (5%)	23	50
5	L	208/208 (100%)	201 (97%)	7 (3%)	32	62
All	All	1445/1446 (100%)	1370 (95%)	75 (5%)	21	47

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	38	SER
1	A	52	ILE
1	A	75	ARG
1	A	80	THR
1	A	121	LYS
1	A	130	LEU
1	A	157	ARG
1	A	161	GLU
1	A	180	GLN
1	A	187	THR
1	A	190	THR
1	A	200	THR
1	A	225	THR
1	A	247	VAL
1	A	248	VAL
1	A	255	GLN
1	A	266	LEU
1	A	271	THR
2	B	1	ILE
2	B	3	ARG
2	B	4	THR
2	B	9	VAL
2	B	68	THR
3	C	6	ILE
4	D	31	ASN
4	D	38	ASP
4	D	48	LEU
4	D	100	ILE
4	D	151	LYS
4	D	188	ASN
4	D	194	ILE
5	E	23	GLN
5	E	42	ARG
5	E	60	ASN
5	E	63	ASN
5	E	96	ASN
5	E	97	THR
5	E	161	LYS
5	E	168	CYS
5	E	202	ARG
5	E	224	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	35	ARG
1	F	48	ARG
1	F	52	ILE
1	F	72	GLN
1	F	75	ARG
1	F	80	THR
1	F	121	LYS
1	F	128	GLU
1	F	157	ARG
1	F	161	GLU
1	F	187	THR
1	F	223	ASP
1	F	256	ARG
1	F	266	LEU
2	G	1	ILE
2	G	3	ARG
2	G	4	THR
2	G	85	VAL
4	K	31	ASN
4	K	38	ASP
4	K	42	LYS
4	K	48	LEU
4	K	144	GLN
4	K	188	ASN
4	K	191	ASN
4	K	194	ILE
5	L	23	GLN
5	L	111	LEU
5	L	168	CYS
5	L	181	ASN
5	L	192	ARG
5	L	196	THR
5	L	222	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	72	GLN
1	A	86	ASN
1	A	93	HIS
1	A	151	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	155	GLN
1	A	174	ASN
1	A	242	GLN
1	A	253	GLN
1	A	255	GLN
1	A	262	GLN
2	B	21	ASN
2	B	24	ASN
2	B	89	GLN
4	D	2	GLN
4	D	5	GLN
4	D	21	ASN
4	D	31	ASN
4	D	53	GLN
4	D	56	GLN
4	D	62	ASN
4	D	112	HIS
4	D	116	GLN
4	D	144	GLN
4	D	149	GLN
4	D	180	ASN
4	D	188	ASN
4	D	191	ASN
5	E	9	GLN
5	E	15	GLN
5	E	20	GLN
5	E	23	GLN
5	E	35	GLN
5	E	60	ASN
5	E	63	ASN
5	E	96	ASN
5	E	116	ASN
5	E	136	GLN
5	E	172	GLN
5	E	181	ASN
5	E	199	GLN
5	E	210	GLN
5	E	222	GLN
5	E	230	GLN
1	F	32	GLN
1	F	43	GLN
1	F	70	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	86	ASN
1	F	141	GLN
1	F	155	GLN
1	F	174	ASN
1	F	191	HIS
1	F	192	HIS
1	F	218	GLN
1	F	226	GLN
1	F	242	GLN
2	G	2	GLN
2	G	21	ASN
2	G	24	ASN
2	G	89	GLN
4	K	1	GLN
4	K	5	GLN
4	K	21	ASN
4	K	31	ASN
4	K	124	GLN
4	K	188	ASN
4	K	191	ASN
5	L	15	GLN
5	L	20	GLN
5	L	23	GLN
5	L	35	GLN
5	L	60	ASN
5	L	63	ASN
5	L	96	ASN
5	L	116	ASN
5	L	172	GLN
5	L	181	ASN
5	L	210	GLN
5	L	222	GLN
5	L	230	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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 ⓘ

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	274/274 (100%)	0.02	2 (0%) 84 83	4, 14, 28, 36	0
1	F	274/274 (100%)	-0.02	3 (1%) 78 76	4, 14, 27, 37	0
2	B	100/100 (100%)	-0.24	1 (1%) 79 78	6, 13, 25, 42	0
2	G	100/100 (100%)	0.19	3 (3%) 52 49	6, 13, 23, 42	0
3	C	9/9 (100%)	1.13	2 (22%) 2 2	2, 4, 6, 7	0
3	H	9/9 (100%)	0.28	0 100 100	2, 3, 6, 7	0
4	D	205/206 (99%)	0.59	14 (6%) 23 20	6, 20, 36, 45	0
4	K	206/206 (100%)	0.21	8 (3%) 43 39	6, 20, 37, 46	0
5	E	241/241 (100%)	0.23	5 (2%) 63 61	8, 17, 30, 48	0
5	L	241/241 (100%)	0.07	1 (0%) 88 87	9, 17, 29, 47	0
All	All	1659/1660 (99%)	0.15	39 (2%) 59 56	2, 16, 33, 48	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	1	ILE	5.3
4	D	204	PRO	3.8
2	B	1	ILE	3.7
4	K	193	SER	3.7
4	D	185	ALA	3.7
4	D	194	ILE	3.4
4	D	195	ILE	3.3
1	F	228	THR	3.2
5	E	216	GLU	3.2
4	D	55	GLU	3.2
4	D	196	PRO	3.2
1	F	227	ASP	3.1
4	K	198	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	197	GLU	2.9
2	G	0	MET	2.8
4	D	153	SER	2.8
4	D	187	ALA	2.8
5	E	221	THR	2.7
5	E	40	GLY	2.6
3	C	2	LEU	2.5
5	E	111	LEU	2.5
4	D	114	TYR	2.5
4	D	205	GLU	2.3
4	K	42	LYS	2.3
4	K	192	ASN	2.3
5	E	112	GLU	2.3
1	A	194	VAL	2.2
4	K	194	ILE	2.2
2	G	34	ASP	2.2
4	D	154	ASP	2.2
4	K	182	SER	2.2
4	K	55	GLU	2.1
4	D	188	ASN	2.1
1	A	196	ASP	2.1
3	C	1	SER	2.1
4	K	204	PRO	2.1
1	F	266	LEU	2.0
4	D	106	GLY	2.0
5	L	116	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.