



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 08:30 PM GMT

PDB ID : 2F54
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 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/ValidationPDFNotes.html>

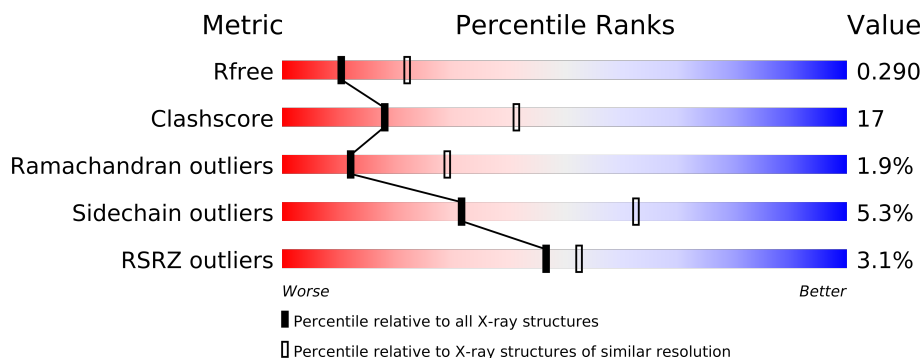
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	274	
1	F	274	
2	B	100	
2	G	100	
3	C	9	
3	H	9	
4	D	206	
4	K	206	
5	E	241	
5	L	241	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13259 atoms, of which 0 are hydrogen and 0 are deuterium.

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	UNP P61769
B	91	CYS	LYS	ENGINEERED	UNP P61769
G	0	MET	-	CLONING ARTIFACT	UNP P61769
G	67	CYS	TYR	ENGINEERED	UNP P61769
G	91	CYS	LYS	ENGINEERED	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.

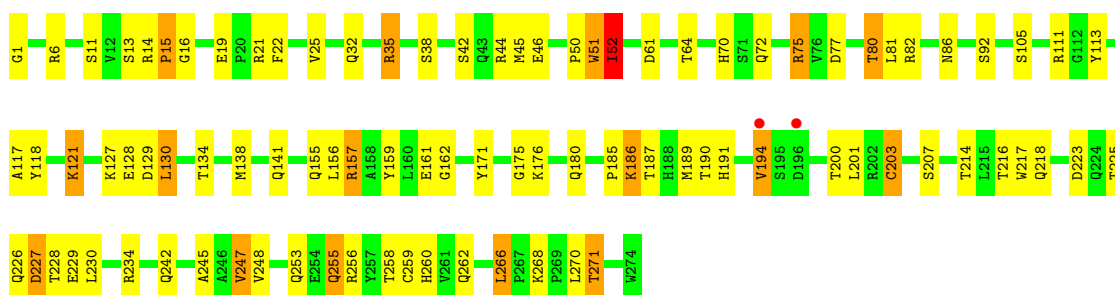
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	1	Total	O	0	0
			1	1		
6	C	1	Total	O	0	0
			1	1		
6	D	2	Total	O	0	0
			2	2		
6	E	1	Total	O	0	0
			1	1		
6	F	8	Total	O	0	0
			8	8		
6	G	1	Total	O	0	0
			1	1		
6	K	6	Total	O	0	0
			6	6		
6	L	4	Total	O	0	0
			4	4		

3 Residue-property plots

These plots are drawn for all protein, RNA 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.

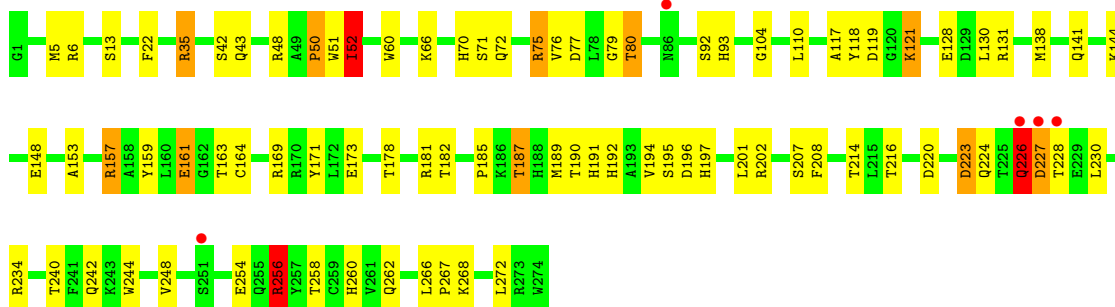
- Molecule 1: HLA class I histocompatibility antigen

Chain A: 



- Molecule 1: HLA class I histocompatibility antigen

Chain F: 



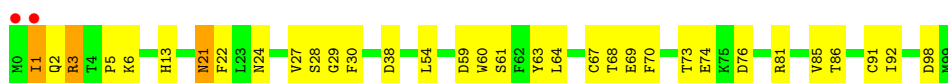
- Molecule 2: Beta-2-microglobulin

Chain B: 



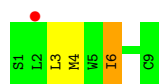
- Molecule 2: Beta-2-microglobulin

Chain G: 



- Molecule 3: Cancer/testis antigen 1B

Chain C: 



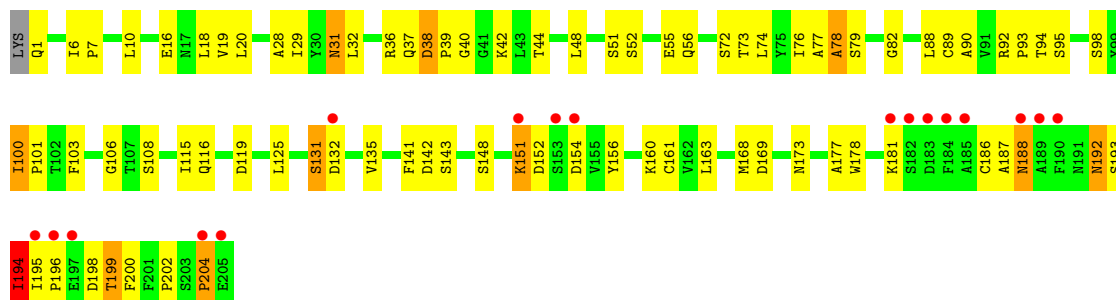
- Molecule 3: Cancer/testis antigen 1B

Chain H: 



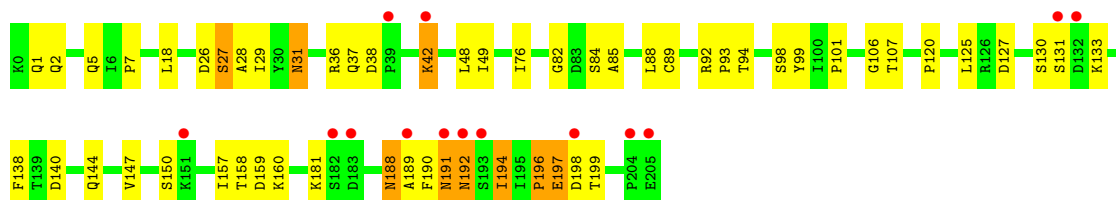
- Molecule 4: T-cell receptor alpha chain

Chain D: 



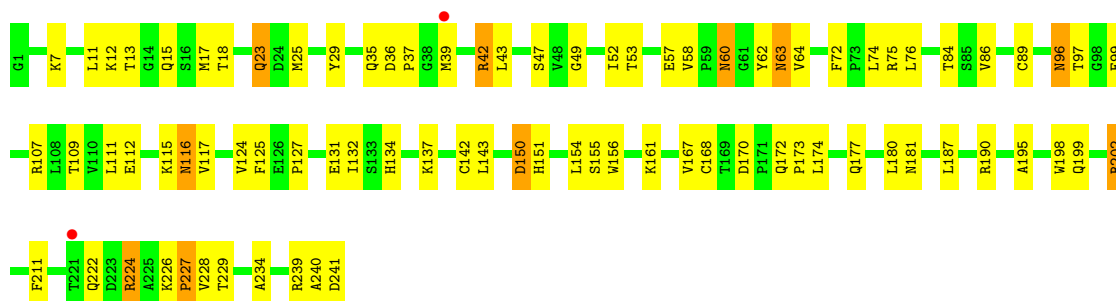
- Molecule 4: T-cell receptor alpha chain

Chain K: 



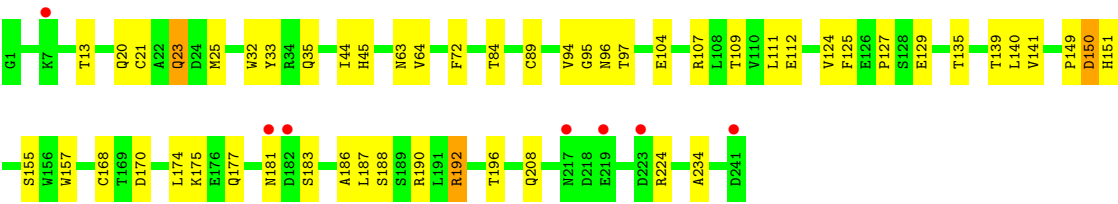
- Molecule 5: T-cell receptor beta chain

Chain E: 



- Molecule 5: T-cell receptor beta chain

Chain L: 



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) 100.0 (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 5.2.0005	Depositor
R, R_{free}	0.221 , 0.286 0.232 , 0.290	Depositor DCC
R_{free} test set	2740 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 14.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 53940 reflections (0.002%)	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.

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	0.91	1/2303 (0.0%)	0.66	0/3125
1	F	0.85	0/2303	0.67	1/3125 (0.0%)
2	B	0.89	0/850	0.71	0/1149
2	G	0.89	2/850 (0.2%)	0.70	0/1149
3	C	0.74	0/76	0.67	0/101
3	H	0.76	0/76	0.69	0/101
4	D	0.75	1/1600 (0.1%)	0.64	1/2176 (0.0%)
4	K	0.77	0/1609	0.65	0/2187
5	E	0.79	1/1953 (0.1%)	0.67	0/2659
5	L	0.83	2/1953 (0.1%)	0.61	0/2659
All	All	0.83	7/13573 (0.1%)	0.66	2/18431 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	89	CYS	CB-SG	-7.76	1.69	1.82
1	A	203	CYS	CB-SG	-7.76	1.69	1.82
5	L	89	CYS	CB-SG	-6.88	1.70	1.82
2	G	91	CYS	CB-SG	-6.08	1.72	1.82
2	G	1	ILE	CA-CB	5.72	1.68	1.54
4	D	89	CYS	CB-SG	-5.04	1.73	1.81
5	L	129	GLU	CG-CD	5.02	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	161	CYS	CA-CB-SG	5.20	123.36	114.00
1	F	256	ARG	NE-CZ-NH1	5.18	122.89	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2238	0	2090	72	1
1	F	2238	0	2090	77	1
2	B	828	0	791	23	0
2	G	828	0	791	29	0
3	C	75	0	79	5	0
3	H	75	0	79	3	0
4	D	1567	0	1499	72	0
4	K	1576	0	1512	57	0
5	E	1902	0	1799	84	0
5	L	1902	0	1799	45	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	439	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (439) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:80:THR:HG21	6:F:277:HOH:O	1.51	1.09
4:D:195:ILE:O	4:D:195:ILE:HD12	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:HH11	2:G:3:ARG:HG2	1.35	0.90
4:K:196:PRO:O	4:K:197:GLU:CG	2.22	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:3:ARG:HH11	2:B:3:ARG:HG2	1.39	0.86
4:D:37:GLN:HE22	5:E:35:GLN:HE22	1.20	0.85
4:K:188:ASN:HD22	4:K:188:ASN:C	1.79	0.84
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
5:E:42:ARG:HG3	5:E:42:ARG:HH11	1.44	0.81
4:K:192:ASN:C	4:K:194:ILE:H	1.83	0.80
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
1:A:51:TRP:O	1:A:52:ILE:HG22	1.82	0.79
1:A:157:ARG:HH11	1:A:157:ARG:HG3	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
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:188:ASN:C	4:D:188:ASN:HD22	1.87	0.76
4:D:28:ALA:HB1	4:D:94:THR:HG21	1.66	0.76
2:G:3:ARG:NH1	2:G:3:ARG:HG2	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:HA	1:A:255:GLN:HE21	1.53	0.72
4:D:31:ASN:HD22	4:D:31:ASN:C	1.90	0.72
4:D:18:LEU:HD11	4:D:76:ILE:HD12	1.72	0.72
5:E:150:ASP:OD2	5:E:173:PRO:HG3	1.91	0.71
1:A:72:GLN:HG3	5:E:49:GLY:HA2	1.73	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
5:E:60:ASN:HD22	5:E:60:ASN:N	1.88	0.70
1:A:13:SER:O	1:A:92:SER:HB2	1.91	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:CD1	4:D:195:ILE:O	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:K:192:ASN:C	4:K:194:ILE:N	2.46	0.67
4:D:115:ILE:HD12	4:D:141:PHE:O	1.95	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:CG	1:F:256:ARG:HH11	2.07	0.67
4:D:151:LYS:HD2	4:D:151:LYS:C	2.16	0.66
1:F:118:TYR:O	1:F:121:LYS:HG2	1.95	0.66
1:A:226:GLN:O	1:A:227:ASP:HB2	1.94	0.66
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
2:B:63:TYR:O	2:B:64:LEU:HD12	1.96	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:HH11	1:A:75:ARG:CG	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:HH11	5:E:224:ARG:HG3	1.64	0.63
2:B:3:ARG:NH1	2:B:3:ARG:HG2	2.10	0.63
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
5:E:202:ARG:HG3	5:E:202:ARG:NH1	2.15	0.61
4:D:90:ALA:HB2	4:D:103:PHE:CD1	2.34	0.61
1:A:226:GLN:O	1:A:227:ASP:CB	2.48	0.61
5:E:115:LYS:O	5:E:116:ASN:CG	2.39	0.61
2:G:54:LEU:HD13	2:G:64:LEU:HD11	1.83	0.61
5:L:170:ASP:OD2	5:L:188:SER:OG	2.17	0.61
4:D:6:ILE:HA	4:D:7:PRO:C	2.21	0.61
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
5:E:11:LEU:HD22	5:E:15:GLN:HE21	1.66	0.60
4:D:156:TYR:O	4:D:177:ALA:HA	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:266:LEU:HD13	1:F:267:PRO:CD	2.31	0.59
4:D:151:LYS:HD2	4:D:152:ASP:N	2.17	0.59
5:E:63:ASN:N	5:E:63:ASN:HD22	2.00	0.59
4:D:142:ASP:OD1	4:D:143:SER:N	2.36	0.59
4:K:26:ASP:O	4:K:27:SER:HB3	2.02	0.59
4:K:5:GLN:HE22	4:K:88:LEU:HA	1.66	0.59
5:L:124:VAL:HG23	5:L:234:ALA:HB3	1.83	0.59
1:F:75:ARG:HH11	1:F:75:ARG:HG2	1.67	0.59
4:D:48:LEU:CD1	5:E:97:THR:HG23	2.32	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
2:G:3:ARG:CG	2:G:3:ARG:HH11	2.13	0.59
1:A:111:ARG:HD2	1:A:128:GLU:HG3	1.84	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	1.85	0.58
5:L:111:LEU:HD12	5:L:111:LEU:N	2.18	0.58
5:E:240:ALA:C	5:E:241:ASP:OD1	2.42	0.58
4:K:31:ASN:HD22	4:K:31:ASN:C	2.06	0.57
4:D:29:ILE:O	4:D:29:ILE:HD12	2.04	0.57
1:A:194:VAL:HG21	1:A:200:THR:OG1	2.04	0.57
1:A:50:PRO:C	1:A:51:TRP:O	2.39	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:NH1	5:E:224:ARG:HG3	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
4:K:48:LEU:HD13	4:K:48:LEU:C	2.26	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:K:26:ASP:O	4:K:27:SER:CB	2.53	0.56
1:F:70:HIS:CD2	3:H:6:ILE:CD1	2.89	0.56
4:D:6:ILE:O	4:D:6:ILE:HD12	2.05	0.56
2:B:63:TYR:C	2:B:64:LEU:HD12	2.26	0.56
1:F:144:LYS:O	1:F:148:GLU:HG2	2.06	0.56
1:F:189:MET:HE2	1:F:201:LEU:HD22	1.88	0.56
3:C:6:ILE:H	3:C:6:ILE:HD13	1.71	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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
4:K:1:GLN:HE21	4:K:2:GLN:H	1.55	0.55
2:G:2:GLN:HG2	2:G:86:THR:HG22	1.89	0.55
1:F:93:HIS:HD2	1:F:119:ASP:OD1	1.88	0.55
5:E:172:GLN:CG	5:E:173:PRO:HD2	2.36	0.54
1:A:266:LEU:HD11	1:A:270:LEU:HD22	1.88	0.54
2:G:63:TYR:C	2:G:64:LEU:HD12	2.27	0.54
5:E:11:LEU:HD22	5:E:15:GLN:NE2	2.22	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
2:G:21:ASN:ND2	2:G:22:PHE:H	2.05	0.54
1:F:153:ALA:O	1:F:157:ARG:HB2	2.07	0.54
4:K:99:TYR:CE1	5:L:94:VAL:HG22	2.42	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
2:B:21:ASN:ND2	2:B:22:PHE:H	2.06	0.54
5:L:155:SER:HG	5:L:157:TRP:HZ3	1.49	0.53
4:D:20:LEU:HB2	4:D:74:LEU:HB3	1.90	0.53
4:K:188:ASN:C	4:K:188:ASN:ND2	2.52	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:O	5:E:174:LEU:HD12	2.08	0.53
1:A:51:TRP:CZ3	1:A:171:TYR:HB3	2.44	0.53
1:A:157:ARG:NH1	1:A:157:ARG:HG3	2.18	0.53
5:E:23:GLN:HE21	5:E:25:MET:H	1.57	0.53
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.44	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: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
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
4:D:125:LEU:N	4:D:125:LEU:HD12	2.24	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:5:PRO:HB3	2:G:30:PHE:HB3	1.92	0.52
1:A:258:THR:HG22	1:A:260:HIS:CD2	2.45	0.52
4:D:77:ALA:O	4:D:78:ALA:C	2.48	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
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
5:L:150:ASP:O	5:L:150:ASP:OD2	2.29	0.51
1:A:228:THR:HG22	1:A:230:LEU:CD1	2.40	0.51
1:A:14:ARG:O	1:A:16:GLY:N	2.43	0.51
2:B:13:HIS:H	2:B:21:ASN:HD21	1.57	0.51
1:F:207:SER:HA	1:F:240:THR:HB	1.93	0.51
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.46	0.51
5:L:20:GLN:NE2	5:L:20:GLN:HA	2.25	0.50
2:G:6:LYS:O	2:G:27:VAL:HA	2.12	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
5:E:224:ARG:HH11	5:E:224:ARG:CG	2.25	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:D:188:ASN:C	4:D:188:ASN:ND2	2.58	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
4:K:191:ASN:HD22	4:K:192:ASN:N	2.10	0.49
5:E:161:LYS:NZ	5:E:161:LYS:HB2	2.27	0.49
4:K:196:PRO:O	4:K:197:GLU:CB	2.60	0.49
5:E:174:LEU:HD12	5:E:174:LEU:C	2.31	0.49
1:F:224:GLN:HE21	1:F:226:GLN:CG	2.25	0.49
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.48	0.49
4:D:31:ASN:ND2	4:D:31:ASN:C	2.60	0.49
5:L:155:SER:OG	5:L:157:TRP:HZ3	1.93	0.49
1:A:259:CYS:O	1:A:271:THR:HA	2.12	0.49
1:F:66:LYS:O	1:F:70:HIS:HD2	1.96	0.49
1:F:266:LEU:HD22	1:F:267:PRO:HD2	1.94	0.49
1:F:169:ARG:O	1:F:173:GLU:HG2	2.12	0.49
1:F:5:MET:HE2	1:F:164:CYS:HB2	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
5:E:154:LEU:HD23	5:E:154:LEU:C	2.33	0.49
5:E:13:THR:HG21	5:E:112:GLU:HG2	1.96	0.48
1:A:190:THR:CG2	1:A:191:HIS:N	2.76	0.48
5:L:190:ARG:N	5:L:190:ARG:HD2	2.28	0.48
1:F:77:ASP:HA	1:F:80:THR:CG2	2.43	0.48
1:F:13:SER:OG	1:F:92:SER:HA	2.12	0.48
1:F:266:LEU:CD1	1:F:267:PRO:HD2	2.43	0.48
1:A:118:TYR:O	1:A:121:LYS:HG2	2.13	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: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:A:156:LEU:O	1:A:157:ARG:C	2.52	0.48
5:L:96:ASN:CG	5:L:97:THR:H	2.17	0.48
5:L:149:PRO:C	5:L:151:HIS:H	2.18	0.48
1:A:44:ARG:NH2	1:A:61:ASP:OD1	2.47	0.47
4:D:48:LEU:HD13	4:D:48:LEU:C	2.34	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
2:B:0:MET:C	2:B:2:GLN:H	2.18	0.47
4:D:37:GLN:NE2	5:E:35:GLN:HE22	2.01	0.47
4:K:190:PHE:HB3	4:K:194:ILE:HD13	1.95	0.47
5:E:132:ILE:HG23	5:E:195:ALA:HB1	1.96	0.47
1:F:226:GLN:HG3	1:F:227:ASP:N	2.30	0.47
1:A:189:MET:HE2	1:A:201:LEU:HD22	1.97	0.47
1:F:266:LEU:HB2	6:F:279:HOH:O	2.14	0.46
5:E:60:ASN:N	5:E:60:ASN:ND2	2.60	0.46
1:A:253:GLN:HE21	1:A:256:ARG:HD3	1.79	0.46
5:E:7:LYS:HD3	5:E:7:LYS:N	2.29	0.46
4:K:125:LEU:HD12	4:K:125:LEU:N	2.30	0.46
2:G:24:ASN:ND2	2:G:67:CYS:HB3	2.31	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
2:B:36:GLU:HG2	2:B:81:ARG:HH22	1.80	0.46
1:F:194:VAL:HG13	1:F:194:VAL:O	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:190:THR:HG21	1:F:192:HIS:CE1	2.50	0.46
4:D:98:SER:C	4:D:100:ILE:H	2.18	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
1:F:228:THR:CG2	1:F:230:LEU:HD13	2.45	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
2:B:3:ARG:HB3	2:B:29:GLY:O	2.16	0.46
4:K:92:ARG:HG2	4:K:101:PRO:HB3	1.97	0.46
1:A:194:VAL:CG2	1:A:200:THR:OG1	2.64	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
2:B:10:TYR:N	2:B:10:TYR:CD1	2.84	0.46
4:D:98:SER:OG	4:D:100:ILE:HG22	2.15	0.46
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
5:L:170:ASP:HB2	5:L:187:LEU:HD12	1.97	0.45
4:D:194:ILE:HG12	4:D:196:PRO:HD3	1.97	0.45
2:B:81:ARG:HD3	2:B:90:PRO:HB3	1.97	0.45
4:K:188:ASN:HA	4:K:191:ASN:HB2	1.98	0.45
5:E:58:VAL:O	5:E:58:VAL:HG23	2.17	0.45
5:E:76:LEU:HD12	5:E:76:LEU:N	2.32	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
1:A:22:PHE:H	1:A:38:SER:HG	1.58	0.45
1:F:77:ASP:O	1:F:80:THR:HG23	2.16	0.45
4:D:38:ASP:O	4:D:39:PRO:C	2.54	0.45
5:E:52:ILE:CG1	5:E:53:THR:N	2.79	0.45
1:F:189:MET:HE3	1:F:201:LEU:HB3	1.97	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:128:GLU:O	1:A:130:LEU:HD22	2.16	0.45
4:K:31:ASN:C	4:K:31:ASN:ND2	2.70	0.45
4:K:98:SER:O	4:K:99:TYR:HB2	2.17	0.45
1:A:11:SER:HA	1:A:21:ARG:O	2.17	0.45
4:K:28:ALA:HB1	4:K:94:THR:CG2	2.47	0.45
4:K:188:ASN:HD22	4:K:189:ALA:N	2.15	0.44
4:K:48:LEU:CD1	5:L:97:THR:HG23	2.47	0.44
1:A:258:THR:CG2	1:A:260:HIS:NE2	2.80	0.44
4:K:159:ASP:OD2	4:K:160:LYS:N	2.51	0.44
2:B:6:LYS:O	2:B:27:VAL:HA	2.17	0.44
5:L:149:PRO:O	5:L:151:HIS:N	2.45	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:42:ARG:NH2	5:E:58:VAL:HG11	2.32	0.44
3:C:6:ILE:N	3:C:6:ILE:CD1	2.78	0.44
5:L:23:GLN:HE21	5:L:25:MET:H	1.66	0.44
4:K:84:SER:O	4:K:85:ALA:HB2	2.17	0.44
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.52	0.44
1:F:190:THR:HG22	1:F:191:HIS:N	2.33	0.44
1:F:22:PHE:CD2	1:F:71:SER:HB3	2.53	0.44
4:D:29:ILE:C	4:D:29:ILE:HD12	2.37	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:163:LEU:C	4:D:163:LEU:HD12	2.38	0.44
4:D:151:LYS:CD	4:D:151:LYS:C	2.85	0.44
1:F:224:GLN:HG2	1:F:226:GLN:HB3	2.00	0.44
2:B:58:LYS:C	2:B:58:LYS:HD2	2.37	0.44
5:E:177:GLN:OE1	5:E:180:LEU:HD12	2.18	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
5:E:64:VAL:HG11	5:E:72:PHE:CE1	2.53	0.44
2:B:0:MET:O	2:B:2:GLN:N	2.50	0.44
1:A:229:GLU:O	1:A:245:ALA:HA	2.18	0.44
5:E:43:LEU:O	5:E:57:GLU:N	2.37	0.44
4:D:48:LEU:HD11	5:E:97:THR:HG23	2.00	0.44
5:E:97:THR:CG2	5:E:99:GLU:HB2	2.48	0.44
5:E:64:VAL:HG11	5:E:72:PHE:CZ	2.52	0.44
1:A:44:ARG:HA	1:A:64:THR:HG23	2.00	0.44
4:K:150:SER:HB2	4:K:157:ILE:CD1	2.48	0.44
1:A:175:GLY:O	1:A:176:LYS:C	2.55	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
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
1:A:138:MET:SD	1:A:141:GLN:HG3	2.58	0.43
4:D:93:PRO:HB2	4:D:95:SER:O	2.18	0.43
2:G:81:ARG:HG2	2:G:92:ILE:HD13	1.98	0.43
4:D:18:LEU:HD12	4:D:18:LEU:C	2.39	0.43
1:A:194:VAL:HG23	1:A:200:THR:H	1.83	0.43
4:D:125:LEU:CD1	4:D:125:LEU:N	2.82	0.43
5:E:18:THR:OG1	5:E:75:ARG:NH1	2.51	0.43
5:L:95:GLY:O	5:L:96:ASN:OD1	2.37	0.43
1:F:50:PRO:C	1:F:51:TRP:O	2.51	0.43
4:D:40:GLY:O	5:E:107:ARG:NH2	2.52	0.43
1:A:70:HIS:HE1	3:C:3:LEU:O	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:K:196:PRO:O	4:K:197:GLU:CD	2.57	0.43
1:F:266:LEU:HD12	1:F:268:LYS:O	2.18	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:75:ARG:CG	1:F:75:ARG:NH1	2.81	0.42
4:D:119:ASP:OD1	5:E:134:HIS:NE2	2.52	0.42
4:D:141:PHE:CZ	4:D:173:ASN:HB3	2.55	0.42
1:A:266:LEU:HD21	1:A:270:LEU:HD21	2.00	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
5:E:167:VAL:HA	5:E:190:ARG:O	2.19	0.42
2:B:49:VAL:HA	2:B:68:THR:OG1	2.18	0.42
1:A:156:LEU:O	1:A:159:TYR:N	2.53	0.42
2:G:59:ASP:O	2:G:60:TRP:HB2	2.19	0.42
2:B:5:PRO:HA	2:B:28:SER:O	2.19	0.42
4:D:48:LEU:O	4:D:56:GLN:OE1	2.38	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:D:194:ILE:CD1	4:D:194:ILE:N	2.81	0.42
4:K:28:ALA:HB1	4:K:94:THR:HG22	2.01	0.42
1:A:72:GLN:HG3	5:E:49:GLY:HA3	2.01	0.42
2:B:0:MET:C	2:B:2:GLN:N	2.73	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
5:L:96:ASN:CG	5:L:97:THR:N	2.72	0.42
1:F:266:LEU:HB3	6:F:279:HOH:O	2.18	0.42
5:L:175:LYS:HE2	5:L:183:SER:HB3	2.02	0.42
1:F:104:GLY:N	1:F:110:LEU:HD13	2.35	0.42
1:A:35:ARG:HD2	1:A:46:GLU:HB2	2.01	0.42
1:A:127:LYS:HE3	1:A:134:THR:OG1	2.19	0.42
5:L:135:THR:O	5:L:135:THR:HG22	2.18	0.42
2:G:74:GLU:HA	2:G:74:GLU:OE1	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
4:K:101:PRO:HG2	5:L:33:TYR:OH	2.20	0.42
5:L:174:LEU:CD1	5:L:186:ALA:HB3	2.50	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:42:SER:O	1:F:43:GLN:HB2	2.20	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
1:A:25:VAL:HG13	1:A:32:GLN:HG3	2.02	0.41
5:L:174:LEU:HD11	5:L:186:ALA:HB3	2.01	0.41
1:F:220:ASP:OD1	1:F:256:ARG:NH2	2.54	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
2:G:29:GLY:HA2	2:G:61:SER:OG	2.19	0.41
5:E:127:PRO:HD2	5:E:198:TRP:CZ2	2.56	0.41
1:F:258:THR:HG22	1:F:260:HIS:NE2	2.36	0.41
4:D:154:ASP:OD1	4:D:181:LYS:HB2	2.21	0.41
4:D:32:LEU:HD13	4:D:72:SER:HB2	2.01	0.41
4:K:92:ARG:HA	4:K:93:PRO:HD3	1.90	0.41
5:L:20:GLN:HE21	5:L:20:GLN:CA	2.26	0.41
5:E:109:THR:HG22	5:E:111:LEU:CD1	2.50	0.41
5:E:222:GLN:O	5:E:224:ARG:N	2.53	0.41
4:D:135:VAL:HG23	5:E:125:PHE:CE2	2.54	0.41
5:E:142:CYS:HB2	5:E:156:TRP:CZ2	2.56	0.41
4:D:160:LYS:HE3	4:D:160:LYS:HB2	1.90	0.41
4:K:5:GLN:NE2	4:K:89:CYS:H	2.17	0.41
4:D:168:MET:O	4:D:169:ASP:C	2.58	0.41
1:F:214:THR:HB	1:F:262:GLN:HB2	2.03	0.41
1:F:51:TRP:CZ3	1:F:171:TYR:HB3	2.56	0.41
1:A:186:LYS:HE3	1:A:207:SER:OG	2.21	0.41
4:D:131:SER:O	4:D:132:ASP:HB3	2.21	0.41
1:A:266:LEU:HD21	1:A:270:LEU:CD2	2.50	0.41
5:E:62:TYR:C	5:E:63:ASN:HD22	2.25	0.41
2:G:22:PHE:HA	2:G:69:GLU:HA	2.02	0.41
1:F:216:THR:O	1:F:260:HIS:N	2.47	0.41
4:K:7:PRO:O	4:K:107:THR:HG23	2.19	0.41
5:L:13:THR:CG2	5:L:112:GLU:HG2	2.51	0.41
4:K:1:GLN:OE1	4:K:26:ASP:HB3	2.21	0.41
4:D:29:ILE:O	4:D:51:SER:HB3	2.21	0.41
4:K:36:ARG:NH2	4:K:82:GLY:O	2.52	0.41
5:E:29:TYR:HA	5:E:47:SER:O	2.21	0.41
4:K:88:LEU:HD23	4:K:106:GLY:CA	2.50	0.40
5:E:131:GLU:HG2	5:E:137:LYS:O	2.21	0.40
4:K:198:ASP:OD1	4:K:198:ASP:N	2.54	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
1:A:214:THR:HB	1:A:262:GLN:HB2	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:11:LEU:HD11	5:E:17:MET:CB	2.51	0.40
2:G:5:PRO:HA	2:G:28:SER:O	2.21	0.40
1:A:216:THR:O	1:A:260:HIS:N	2.51	0.40
5:L:127:PRO:HG3	5:L:140:LEU:HD12	2.04	0.40
4:K:138:PHE:HB2	4:K:190:PHE:CE2	2.57	0.40
4:K:48:LEU:C	4:K:48:LEU:CD1	2.90	0.40
5:L:64:VAL:CG1	5:L:72:PHE:CE1	3.04	0.40
5:L:63:ASN:N	5:L:63:ASN:HD22	2.20	0.40
4:K:37:GLN:HE22	5:L:35:GLN:HE22	1.69	0.40
1:F:76:VAL:O	1:F:79:GLY:N	2.55	0.40
4:D:10:LEU:N	4:D:108:SER:O	2.46	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	Distance(Å)	Clash(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%)	10	25
1	F	272/274 (99%)	246 (90%)	21 (8%)	5 (2%)	13	31
2	B	98/100 (98%)	96 (98%)	1 (1%)	1 (1%)	22	51
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%)	4	8
4	K	204/206 (99%)	185 (91%)	14 (7%)	5 (2%)	9	21
5	E	239/241 (99%)	224 (94%)	11 (5%)	4 (2%)	14	33
5	L	239/241 (99%)	223 (93%)	15 (6%)	1 (0%)	43	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1639/1660 (99%)	1498 (91%)	110 (7%)	31 (2%)	12	29

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
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%)	212 (92%)	18 (8%)	18	40
1	F	230/230 (100%)	215 (94%)	15 (6%)	24	51
2	B	95/95 (100%)	87 (92%)	8 (8%)	16	34
2	G	95/95 (100%)	89 (94%)	6 (6%)	25	53
3	C	9/9 (100%)	8 (89%)	1 (11%)	9	20
3	H	9/9 (100%)	9 (100%)	0	100	100
4	D	180/181 (99%)	174 (97%)	6 (3%)	50	81
4	K	181/181 (100%)	174 (96%)	7 (4%)	43	76
5	E	208/208 (100%)	199 (96%)	9 (4%)	40	72
5	L	208/208 (100%)	202 (97%)	6 (3%)	55	85
All	All	1445/1446 (100%)	1369 (95%)	76 (5%)	32	62

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	45	MET
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	186	LYS
1	A	187	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	21	ASN

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Mol	Chain	Res	Type
2	B	45	ARG
2	B	58	LYS
2	B	70	PHE
3	C	6	ILE
4	D	31	ASN
4	D	38	ASP
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	168	CYS
5	E	181	ASN
5	E	202	ARG
5	E	224	ARG
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	226	GLN
1	F	227	ASP
1	F	256	ARG
2	G	1	ILE
2	G	3	ARG
2	G	21	ASN
2	G	38	ASP
2	G	70	PHE
2	G	85	VAL
4	K	31	ASN
4	K	38	ASP

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Mol	Chain	Res	Type
4	K	42	LYS
4	K	144	GLN
4	K	188	ASN
4	K	191	ASN
4	K	194	ILE
5	L	23	GLN
5	L	168	CYS
5	L	181	ASN
5	L	192	ARG
5	L	196	THR
5	L	224	ARG

Some 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	43	GLN
1	A	86	ASN
1	A	93	HIS
1	A	151	HIS
1	A	155	GLN
1	A	174	ASN
1	A	191	HIS
1	A	242	GLN
1	A	253	GLN
1	A	255	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	50	GLN
4	D	53	GLN
4	D	62	ASN
4	D	80	GLN
4	D	112	HIS
4	D	116	GLN
4	D	144	GLN
4	D	149	GLN
4	D	188	ASN

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Mol	Chain	Res	Type
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	222	GLN
1	F	32	GLN
1	F	43	GLN
1	F	70	HIS
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	226	GLN
1	F	242	GLN
1	F	253	GLN
2	G	2	GLN
2	G	21	ASN
2	G	24	ASN
2	G	89	GLN
4	K	1	GLN
4	K	2	GLN
4	K	5	GLN
4	K	21	ASN
4	K	31	ASN
4	K	112	HIS
4	K	144	GLN
4	K	149	GLN
4	K	188	ASN
4	K	191	ASN
5	L	9	GLN

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Mol	Chain	Res	Type
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	116	ASN
5	L	172	GLN
5	L	181	ASN
5	L	210	GLN
5	L	222	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	0.17	2 (0%) 84 89	4, 14, 28, 36	0
1	F	274/274 (100%)	0.18	5 (1%) 65 71	4, 14, 27, 37	0
2	B	100/100 (100%)	-0.03	1 (1%) 79 83	6, 13, 25, 42	0
2	G	100/100 (100%)	0.04	2 (2%) 62 68	6, 13, 23, 42	0
3	C	9/9 (100%)	0.70	1 (11%) 6 6	2, 4, 6, 7	0
3	H	9/9 (100%)	0.54	0 100 100	2, 3, 6, 7	0
4	D	205/206 (99%)	0.55	17 (8%) 11 12	6, 20, 36, 45	0
4	K	206/206 (100%)	0.32	14 (6%) 17 19	7, 20, 37, 46	0
5	E	241/241 (100%)	0.16	2 (0%) 83 87	8, 17, 30, 48	0
5	L	241/241 (100%)	0.15	7 (2%) 49 55	9, 17, 29, 47	0
All	All	1659/1660 (99%)	0.22	51 (3%) 47 52	2, 16, 33, 48	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	205	GLU	6.7
4	K	193	SER	6.1
2	G	0	MET	5.3
4	D	197	GLU	5.2
4	K	205	GLU	4.9
5	L	181	ASN	4.5
4	D	204	PRO	4.1
4	K	192	ASN	4.0
4	K	183	ASP	3.9
4	K	204	PRO	3.9
2	G	1	ILE	3.6
4	K	151	LYS	3.5
4	D	132	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
4	K	132	ASP	3.4
1	F	228	THR	3.4
4	D	188	ASN	3.4
2	B	0	MET	3.4
1	A	196	ASP	3.3
1	F	227	ASP	3.2
1	A	194	VAL	3.2
4	K	39	PRO	3.1
1	F	226	GLN	3.0
4	D	153	SER	3.0
4	D	196	PRO	2.9
5	E	39	MET	2.9
4	D	185	ALA	2.8
5	L	182	ASP	2.8
4	D	183	ASP	2.6
4	D	182	SER	2.6
4	D	154	ASP	2.6
4	K	182	SER	2.4
5	L	219	GLU	2.4
4	K	189	ALA	2.3
4	K	131	SER	2.3
4	D	151	LYS	2.3
4	D	184	PHE	2.3
5	E	221	THR	2.3
4	K	198	ASP	2.3
1	F	251	SER	2.2
5	L	7	LYS	2.2
4	D	190	PHE	2.2
4	K	191	ASN	2.2
5	L	223	ASP	2.1
3	C	2	LEU	2.1
4	D	195	ILE	2.1
5	L	241	ASP	2.1
1	F	86	ASN	2.1
4	D	181	LYS	2.0
4	K	42	LYS	2.0
5	L	217	ASN	2.0
4	D	189	ALA	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.