



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:29 am 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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

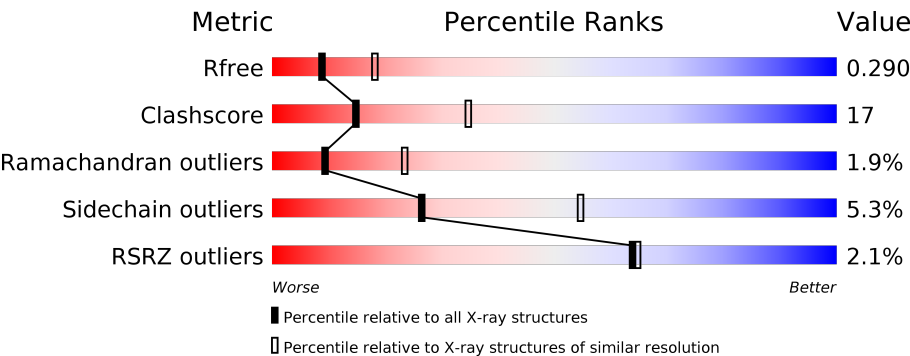
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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  $\geq 3$ , 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	274	<div> <div>%</div> <div>66% 28% 6%</div> </div>
1	F	274	<div> <div>%</div> <div>69% 26% . .</div> </div>
2	B	100	<div> <div>%</div> <div>70% 26% .</div> </div>
2	G	100	<div> <div>2%</div> <div>67% 30% .</div> </div>
3	C	9	<div> <div>67% 22% 11%</div> </div>
3	H	9	<div> <div>78% 22%</div> </div>

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Mol	Chain	Length	Quality of chain
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 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	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			

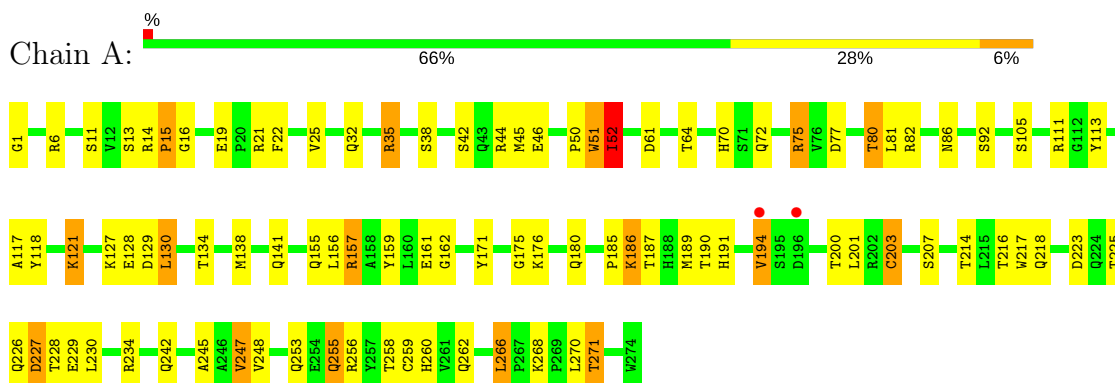
- Molecule 6 is water.

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		

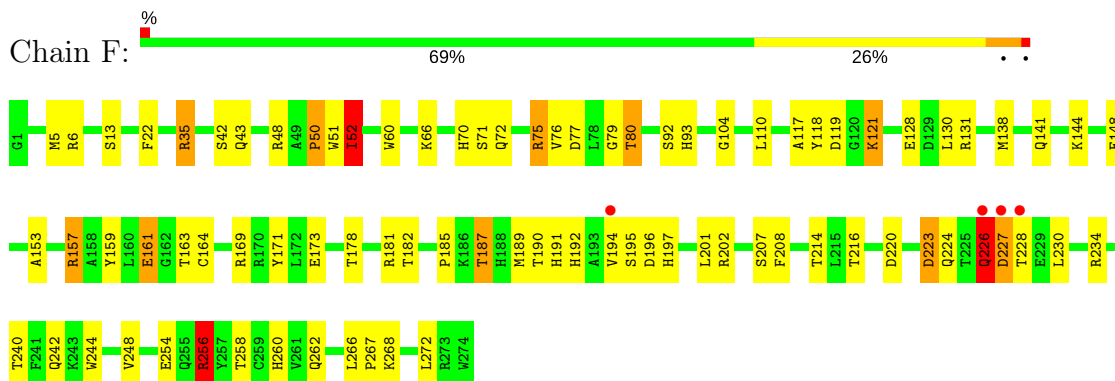
### 3 Residue-property plots

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

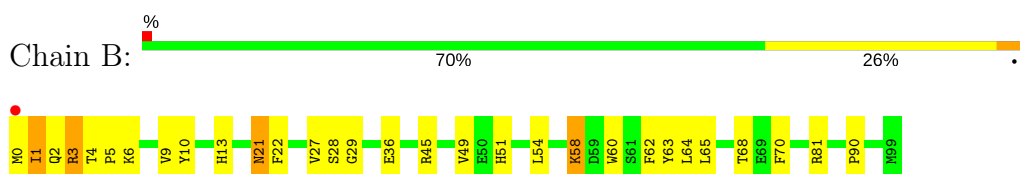
- Molecule 1: HLA class I histocompatibility antigen



- Molecule 1: HLA class I histocompatibility antigen



- Molecule 2: Beta-2-microglobulin

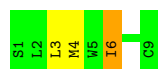


- Molecule 2: Beta-2-microglobulin

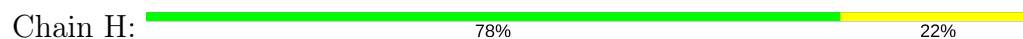




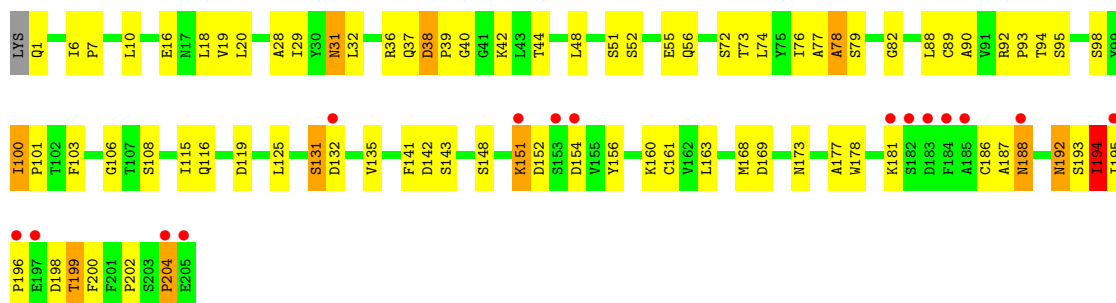
• Molecule 3: Cancer/testis antigen 1B



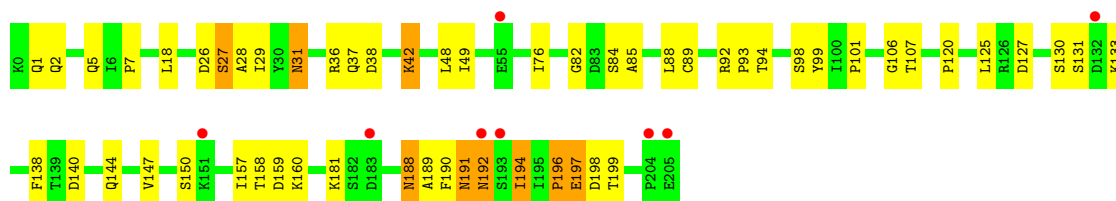
• Molecule 3: Cancer/testis antigen 1B



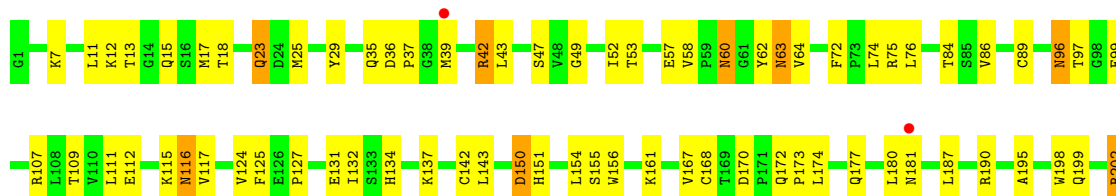
• Molecule 4: T-cell receptor alpha chain



• Molecule 4: T-cell receptor alpha chain

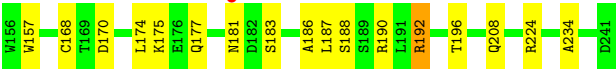
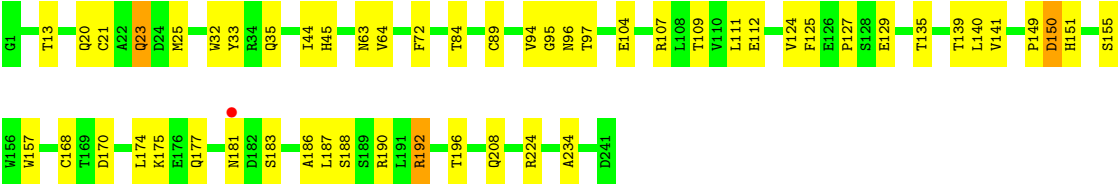


• Molecule 5: T-cell receptor beta chain





● 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	42.0	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13259	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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	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 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	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

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 17.

All (439) 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: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	Interatomic distance (Å)	Clash overlap (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:C	4:K:188:ASN:HD22	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
1:F:234:ARG:HE	1:F:242:GLN:HE21	1.30	0.80
4:K:192:ASN:C	4:K:194:ILE:H	1.83	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:HE21	1:A:255:GLN:HA	1.53	0.72
4:D:31:ASN:C	4:D:31:ASN:HD22	1.90	0.72
4:D:18:LEU:HD11	4:D:76:ILE:HD12	1.72	0.72
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:HD22	5:E:60:ASN:N	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
4:D:90:ALA:HB2	4:D:103:PHE:CD1	2.34	0.61
5:E:202:ARG:HG3	5:E:202:ARG:NH1	2.15	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
4:D:6:ILE:HA	4:D:7:PRO:C	2.21	0.61
5:L:170:ASP:OD2	5:L:188:SER:OG	2.17	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	5:E:63:ASN:N	2.00	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
1:A:111:ARG:HD2	1:A:128:GLU:HG3	1.84	0.59
2:G:3:ARG:CG	2:G:3:ARG:HH11	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	1.85	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:D:29:ILE:O	4:D:29:ILE:HD12	2.04	0.57
4:K:31:ASN:HD22	4:K:31:ASN:C	2.06	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
1:A:50:PRO:C	1:A:51:TRP:O	2.39	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: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
2:B:63:TYR:C	2:B:64:LEU:HD12	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:186:LYS:CE	1:A:207:SER:OG	2.54	0.55
1:A:19:GLU:HG3	1:A:75:ARG:NH2	2.22	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
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
2:G:63:TYR:C	2:G:64:LEU:HD12	2.27	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
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
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:157:ARG:NH1	1:A:157:ARG:HG3	2.18	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:29:GLY:HA2	2:G:61:SER:HB2	1.91	0.52
4:D:125:LEU:N	4:D:125:LEU:HD12	2.24	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
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
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:N	5:L:107:ARG:HD2	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
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
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: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
2:G:6:LYS:O	2:G:27:VAL:HA	2.12	0.50
5:L:20:GLN:NE2	5:L:20:GLN:HA	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
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
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
5:E:174:LEU:HD12	5:E:174:LEU:C	2.31	0.49
4:K:196:PRO:O	4:K:197:GLU:CB	2.60	0.49
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:31:ASN:ND2	4:D:31:ASN:C	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:13:THR:HG21	5:E:112:GLU:CG	2.42	0.49
1:F:5:MET:HE2	1:F:164:CYS:HB2	1.95	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
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: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:149:PRO:C	5:L:151:HIS:H	2.18	0.48
5:L:96:ASN:CG	5:L:97:THR:H	2.17	0.48
1:A:44:ARG:NH2	1:A:61:ASP:OD1	2.47	0.47
4:D:48:LEU:C	4:D:48:LEU:HD13	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
5:E:132:ILE:HG23	5:E:195:ALA:HB1	1.96	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
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:A:253:GLN:HE21	1:A:256:ARG:HD3	1.79	0.46
5:E:60:ASN:N	5:E:60:ASN:ND2	2.60	0.46
1:F:266:LEU:HB2	6:F:279:HOH:O	2.14	0.46
5:E:7:LYS:HD3	5:E:7:LYS:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
5:E:124:VAL:HG23	5:E:234:ALA:HB3	1.98	0.46
1:F:228:THR:CG2	1:F:230:LEU:HD13	2.45	0.46
1:F:35:ARG:O	1:F:35:ARG:HD3	2.15	0.46
1:A:194:VAL:CG2	1:A:200:THR:OG1	2.64	0.46
2:B:10:TYR:N	2:B:10:TYR:CD1	2.84	0.46
2:B:3:ARG:HB3	2:B:29:GLY:O	2.16	0.46
1:F:130:LEU:HB3	1:F:157:ARG:HG2	1.96	0.46
4:K:92:ARG:HG2	4:K:101:PRO:HB3	1.97	0.46
4:K:42:LYS:HG2	5:L:104:GLU:OE2	2.15	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
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:O	5:E:58:VAL:HG23	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
1:A:22:PHE:H	1:A:38:SER:HG	1.58	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
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: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
1:F:189:MET:HE3	1:F:201:LEU:HB3	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:159:ASP:OD2	4:K:160:LYS:N	2.51	0.44
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
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: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
2:B:58:LYS:C	2:B:58:LYS:HD2	2.37	0.44
4:D:151:LYS:CD	4:D:151:LYS:C	2.85	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:229:GLU:O	1:A:245:ALA:HA	2.18	0.44
1:A:15:PRO:CD	1:A:92:SER:HB3	2.48	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:175:GLY:O	1:A:176:LYS:C	2.55	0.44
1:A:44:ARG:HA	1:A:64: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
4:D:48:LEU:HD11	5:E:97:THR:HG23	2.00	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
2:G:81:ARG:HG2	2:G:92:ILE:HD13	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:18:LEU:C	4:D:18:LEU:HD12	2.39	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
1:F:50:PRO:C	1:F:51:TRP:O	2.51	0.43
5:L:95:GLY:O	5:L:96:ASN:OD1	2.37	0.43
4:K:196:PRO:O	4:K:197:GLU:CD	2.57	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
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:194:ILE:CD1	4:D:194:ILE:N	2.81	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:K:28:ALA:HB1	4:K:94:THR:HG22	2.01	0.42
1:A:6:ARG:NH1	1:A:113:TYR:CD2	2.88	0.42
1:A:1:GLY:O	1:A:105:SER:HA	2.19	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: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
5:L:175:LYS:HE2	5:L:183:SER:HB3	2.02	0.42
5:L:96:ASN:CG	5:L:97:THR:N	2.72	0.42
1:A:127:LYS:HE3	1:A:134:THR:OG1	2.19	0.42
1:A:35:ARG:HD2	1:A:46:GLU:HB2	2.01	0.42
2:G:74:GLU:HA	2:G:74:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:135:THR:O	5:L:135:THR:HG22	2.18	0.42
5:E:211:PHE:O	5:E:229:THR:HG23	2.20	0.42
5:E:86:VAL:HG22	5:E:107:ARG:HG3	2.02	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
4:K:101:PRO:HG2	5:L:33:TYR:OH	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
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: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
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:K:92:ARG:HA	4:K:93:PRO:HD3	1.90	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
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
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
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
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
4:D:131:SER:O	4:D:132:ASP:HB3	2.21	0.41
1:F:51:TRP:CZ3	1:F:171:TYR:HB3	2.56	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
4:K:7:PRO:O	4:K:107:THR:HG23	2.19	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
5:L:13:THR:CG2	5:L:112:GLU:HG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:234:ARG:HE	1:A:242:GLN:HE21	1.69	0.40
1:A:214:THR:HB	1:A:262:GLN:HB2	2.02	0.40
5:E:131:GLU:HG2	5:E:137:LYS:O	2.21	0.40
5:E:36:ASP:HB2	5:E:39:MET:HG3	2.03	0.40
4:K:198:ASP:OD1	4:K:198:ASP:N	2.54	0.40
4:K:88:LEU:HD23	4:K:106:GLY:CA	2.50	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:138:PHE:HB2	4:K:190:PHE:CE2	2.57	0.40
4:K:37:GLN:HE22	5:L:35:GLN:HE22	1.69	0.40
4:K:48:LEU:C	4:K:48:LEU:CD1	2.90	0.40
5:L:63:ASN:N	5:L:63:ASN:HD22	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 [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	272/274 (99%)	247 (91%)	19 (7%)	6 (2%)	8	20
1	F	272/274 (99%)	246 (90%)	21 (8%)	5 (2%)	10	25
2	B	98/100 (98%)	96 (98%)	1 (1%)	1 (1%)	18	43
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%)	3	6
4	K	204/206 (99%)	185 (91%)	14 (7%)	5 (2%)	6	17
5	E	239/241 (99%)	224 (94%)	11 (5%)	4 (2%)	11	27
5	L	239/241 (99%)	223 (93%)	15 (6%)	1 (0%)	38	66
All	All	1639/1660 (99%)	1498 (91%)	110 (7%)	31 (2%)	9	23

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

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Mol	Chain	Res	Type
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%)	15	33
1	F	230/230 (100%)	215 (94%)	15 (6%)	20	44
2	B	95/95 (100%)	87 (92%)	8 (8%)	13	29
2	G	95/95 (100%)	89 (94%)	6 (6%)	21	46
3	C	9/9 (100%)	8 (89%)	1 (11%)	7	16
3	H	9/9 (100%)	9 (100%)	0	100	100
4	D	180/181 (99%)	174 (97%)	6 (3%)	43	73
4	K	181/181 (100%)	174 (96%)	7 (4%)	37	68
5	E	208/208 (100%)	199 (96%)	9 (4%)	33	64
5	L	208/208 (100%)	202 (97%)	6 (3%)	48	77
All	All	1445/1446 (100%)	1369 (95%)	76 (5%)	26	54

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	274/274 (100%)	0.02	2 (0%) 87 88	4, 14, 28, 36	0
1	F	274/274 (100%)	0.10	4 (1%) 74 75	4, 14, 27, 37	0
2	B	100/100 (100%)	-0.15	1 (1%) 82 82	6, 13, 25, 42	0
2	G	100/100 (100%)	-0.09	2 (2%) 65 66	6, 13, 23, 42	0
3	C	9/9 (100%)	0.49	0 100 100	2, 4, 6, 7	0
3	H	9/9 (100%)	0.46	0 100 100	2, 3, 6, 7	0
4	D	205/206 (99%)	0.43	15 (7%) 16 13	6, 20, 36, 45	0
4	K	206/206 (100%)	0.23	8 (3%) 40 39	7, 20, 37, 46	0
5	E	241/241 (100%)	0.05	2 (0%) 86 86	8, 17, 30, 48	0
5	L	241/241 (100%)	0.03	1 (0%) 92 93	9, 17, 29, 47	0
All	All	1659/1660 (99%)	0.10	35 (2%) 64 65	2, 16, 33, 48	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	K	193	SER	7.0
4	D	205	GLU	5.7
4	K	205	GLU	4.6
1	A	196	ASP	4.5
1	F	227	ASP	4.4
4	D	197	GLU	4.3
1	F	228	THR	4.0
2	G	0	MET	3.8
4	D	132	ASP	3.7
1	F	226	GLN	3.6
4	D	153	SER	3.6
4	D	182	SER	3.6
4	K	192	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
4	D	204	PRO	3.5
4	D	154	ASP	3.4
4	D	151	LYS	3.2
5	L	181	ASN	3.1
4	D	196	PRO	3.1
4	D	188	ASN	3.0
1	A	194	VAL	2.8
4	K	204	PRO	2.8
4	D	183	ASP	2.7
4	K	132	ASP	2.7
2	B	0	MET	2.7
4	D	185	ALA	2.7
5	E	181	ASN	2.6
5	E	39	MET	2.6
2	G	1	ILE	2.5
4	K	151	LYS	2.4
4	K	183	ASP	2.3
4	D	181	LYS	2.2
1	F	194	VAL	2.1
4	D	195	ILE	2.1
4	D	184	PHE	2.1
4	K	55	GLU	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.