



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:03 PM GMT

PDB ID : 3SKN
Title : Crystal structure of the RL42 TCR unliganded
Authors : Gras, S.; Wilmann, P.G.; Zhenjun, C.; Hanim, H.; Yu Chih, L.; Kjer-Nielsen, L.; Purcell, A.W.; Burrows, S.R.; Mccluskey, J.; Rossjohn, J.
Deposited on : 2011-06-22
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

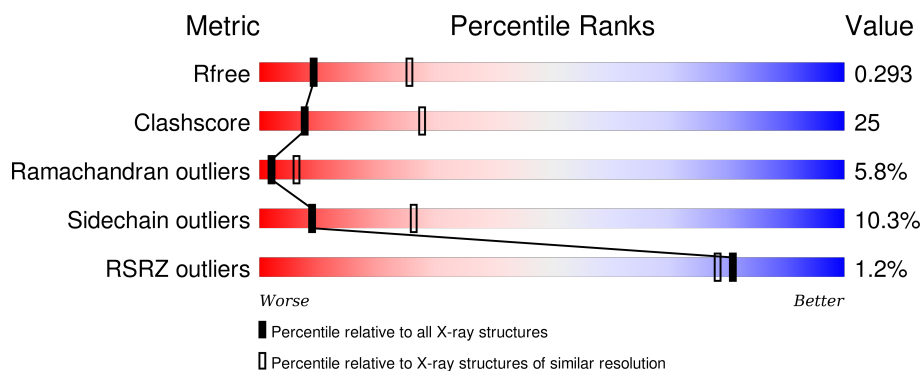
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	203	<div> <div>55%</div> <div>31%</div> <div>10%</div> <div>..</div> </div>
1	C	203	<div> <div>3%</div> <div>56%</div> <div>32%</div> <div>8%</div> <div>..</div> </div>
1	E	203	<div> <div>%</div> <div>58%</div> <div>31%</div> <div>8%</div> <div>.</div> </div>
1	G	203	<div> <div>2%</div> <div>55%</div> <div>35%</div> <div>7%</div> <div>.</div> </div>
2	B	244	<div> <div>56%</div> <div>33%</div> <div>9%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	244	<div><div><div>%</div><div><div></div><div>55%</div><div>35%</div><div>7%</div></div><div><div></div><div></div><div>..</div></div></div></div>
2	F	244	<div><div><div>2%</div><div><div></div><div>53%</div><div>39%</div><div>7%</div></div><div><div></div><div></div><div>.</div></div></div></div>
2	H	244	<div><div><div>%</div><div><div></div><div>54%</div><div>36%</div><div>7%</div></div><div><div></div><div></div><div>..</div></div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13825 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 RL42 T cell receptor, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1541	962	258	313	8			
1	C	197	Total	C	N	O	S	0	3	0
			1570	978	264	320	8			
1	E	197	Total	C	N	O	S	0	0	0
			1541	962	258	313	8			
1	G	197	Total	C	N	O	S	1	0	0
			1541	962	258	313	8			

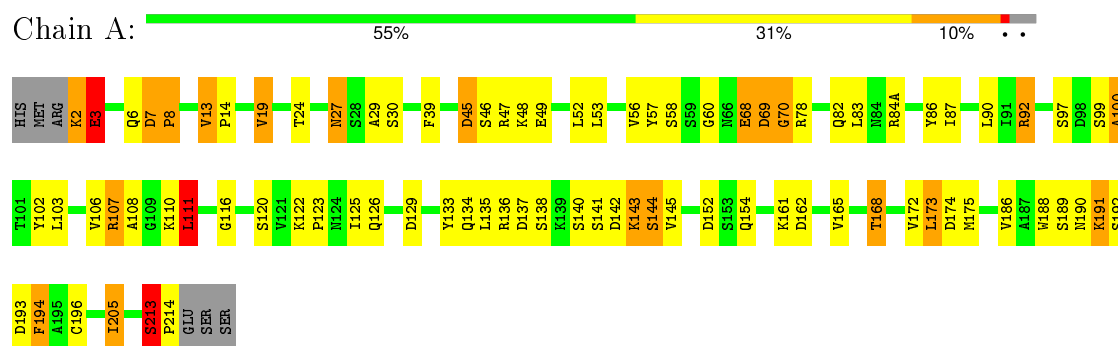
- Molecule 2 is a protein called RL42 T cell receptor, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	2	0	0
			1908	1205	331	363	9			
2	D	241	Total	C	N	O	S	2	0	0
			1908	1205	331	363	9			
2	F	241	Total	C	N	O	S	2	0	0
			1908	1205	331	363	9			
2	H	241	Total	C	N	O	S	2	0	0
			1908	1205	331	363	9			

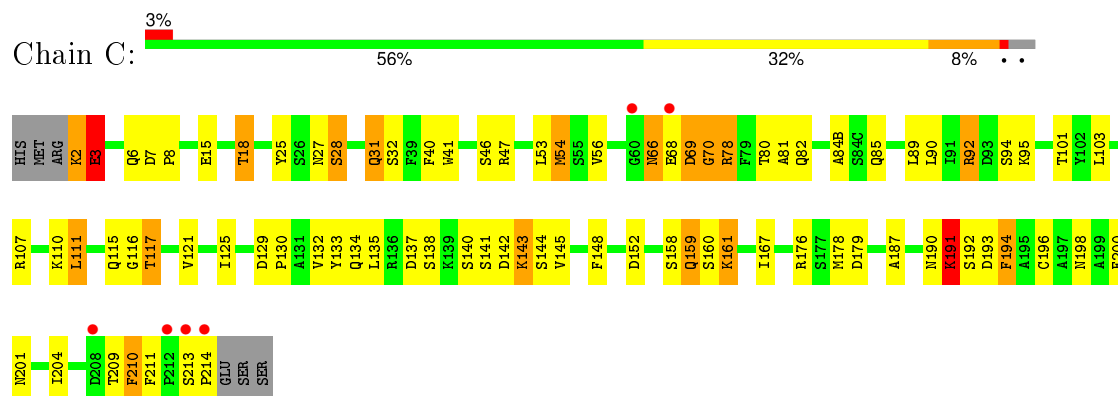
3 Residue-property plots [i](#)

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

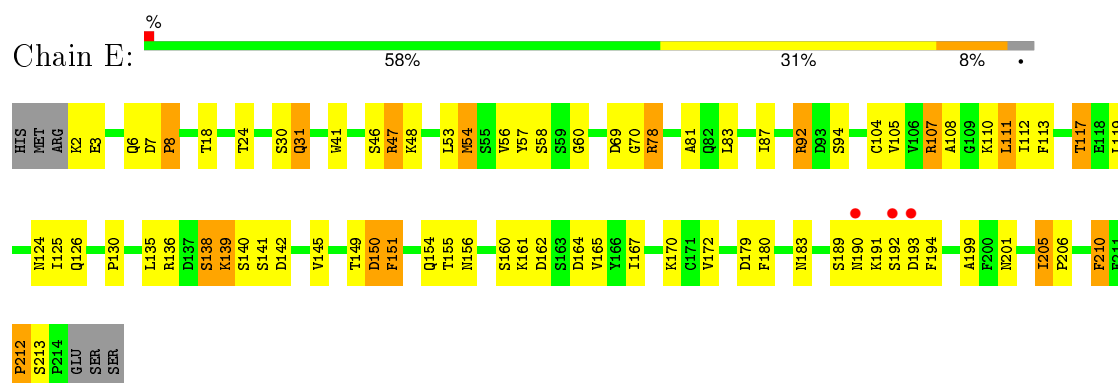
- Molecule 1: RL42 T cell receptor, alpha chain



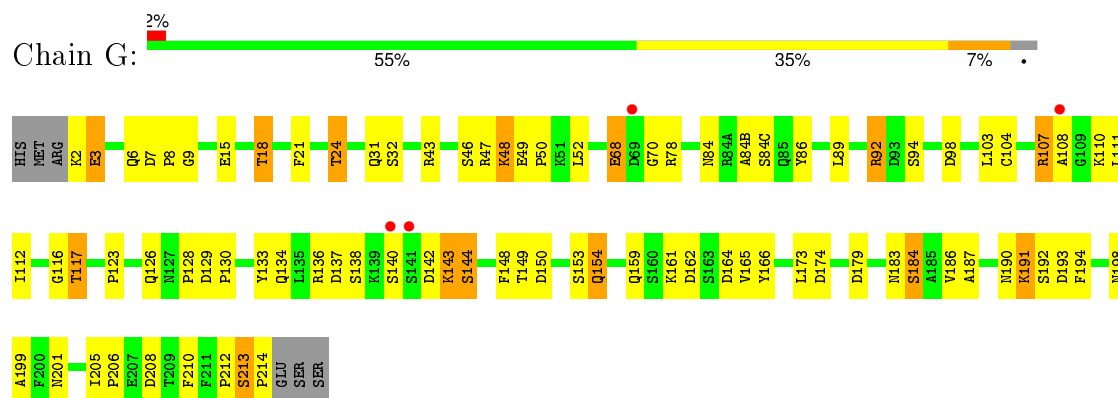
- Molecule 1: RL42 T cell receptor, alpha chain



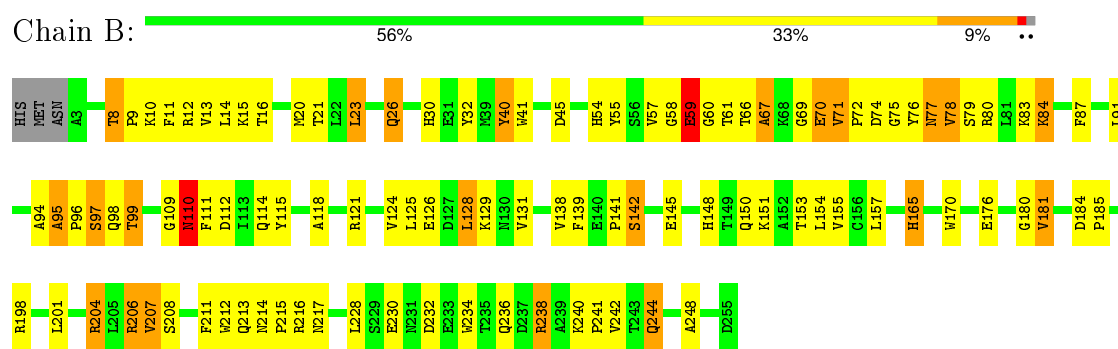
- Molecule 1: RL42 T cell receptor, alpha chain



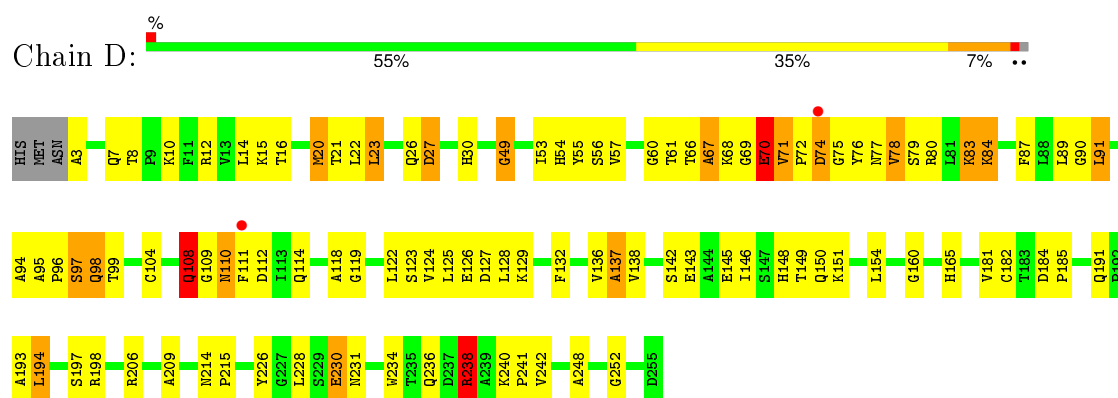
- Molecule 1: RL42 T cell receptor, alpha chain



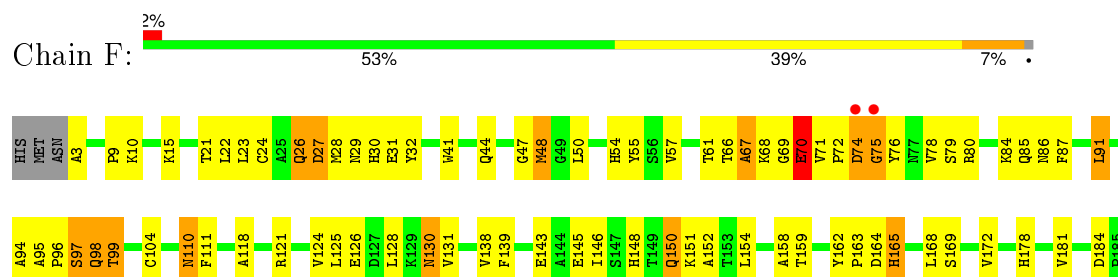
- Molecule 2: RL42 T cell receptor, beta chain



- Molecule 2: RL42 T cell receptor, beta chain

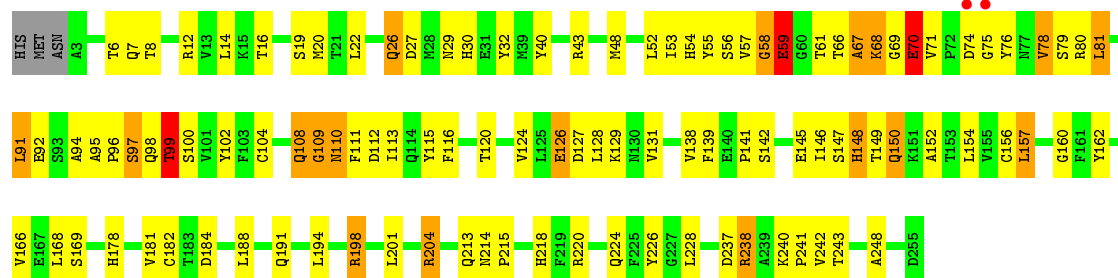


- Molecule 2: RL42 T cell receptor, beta chain





● Molecule 2: RL42 T cell receptor, beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.97Å 77.81Å 99.64Å 69.35° 72.20° 83.33°	Depositor
Resolution (Å)	45.49 – 2.90 71.38 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.8 (45.49-2.90) 86.9 (71.38-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.194 , 0.292 0.204 , 0.293	Depositor DCC
R_{free} test set	2195 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 55.5	EDS
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 43561 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13825	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/1574	0.53	0/2132
1	C	0.30	0/1603	0.49	0/2170
1	E	0.28	0/1574	0.47	0/2132
1	G	0.30	0/1574	0.49	0/2132
2	B	0.29	0/1959	0.49	0/2662
2	D	0.28	0/1959	0.47	0/2662
2	F	0.27	0/1959	0.48	0/2662
2	H	0.28	0/1959	0.49	0/2662
All	All	0.29	0/14161	0.49	0/19214

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1541	0	1464	88	0
1	C	1570	0	1486	84	0
1	E	1541	0	1464	74	0
1	G	1541	0	1464	75	0
2	B	1908	0	1819	89	0
2	D	1908	0	1819	116	0
2	F	1908	0	1819	104	0
2	H	1908	0	1819	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13825	0	13154	679	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (679) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:99:THR:HG22	2:D:124:VAL:H	1.14	1.12
1:E:108:ALA:HB3	1:E:112:ILE:HD11	1.22	1.10
1:A:192:SER:N	1:A:193:ASP:HA	1.73	1.02
2:D:96:PRO:HA	2:D:97:SER:O	1.58	1.01
2:F:57:VAL:HG12	2:F:61:THR:HG21	1.44	0.99
2:D:55:TYR:HE2	2:D:68:LYS:HB2	1.28	0.99
1:G:192:SER:N	1:G:193:ASP:HA	1.78	0.98
1:E:192:SER:N	1:E:193:ASP:HA	1.78	0.98
2:F:96:PRO:HA	2:F:97:SER:O	1.62	0.97
2:D:110:ASN:HD22	2:D:110:ASN:H	1.13	0.96
1:A:30:SER:HA	1:A:108:ALA:HB2	1.49	0.94
1:G:78:ARG:HA	1:G:92:ARG:HD2	1.48	0.94
1:C:18:THR:HB	1:C:92:ARG:HA	1.48	0.93
1:E:78:ARG:HA	1:E:92:ARG:HD2	1.52	0.92
1:E:108:ALA:HB3	1:E:112:ILE:CD1	1.99	0.92
1:E:107:ARG:HG2	1:E:111:LEU:HD12	1.51	0.91
2:H:96:PRO:HA	2:H:97:SER:O	1.72	0.90
2:B:66:THR:HG22	2:B:67:ALA:H	1.36	0.89
2:D:83:LYS:O	2:D:84:LYS:HB3	1.72	0.89
1:C:192:SER:N	1:C:193:ASP:HA	1.87	0.87
2:H:66:THR:HG22	2:H:67:ALA:H	1.40	0.85
1:A:68:GLU:HG2	1:A:69:ASP:H	1.42	0.85
1:A:47:ARG:HD2	2:B:121:ARG:HH22	1.41	0.85
2:H:56:SER:HA	2:H:61:THR:HB	1.56	0.85
1:A:30:SER:HA	1:A:108:ALA:CB	2.08	0.83
1:G:18:THR:HB	1:G:92:ARG:HA	1.61	0.83
1:G:134:GLN:HE21	1:G:144:SER:HB2	1.41	0.82
2:D:14:LEU:HD11	2:D:20:MET:HG2	1.60	0.81
2:B:14:LEU:HD11	2:B:20:MET:HG2	1.61	0.81
2:H:55:TYR:HE2	2:H:68:LYS:HB2	1.44	0.81
2:D:99:THR:HG22	2:D:124:VAL:N	1.93	0.81
1:C:137:ASP:HB3	1:C:142:ASP:HA	1.62	0.81
1:A:30:SER:CA	1:A:108:ALA:HB2	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:SER:HB2	1:C:167:ILE:HG13	1.61	0.81
2:D:146:ILE:HD12	2:D:146:ILE:H	1.46	0.80
2:D:22:LEU:HD12	2:D:89:LEU:HD23	1.61	0.80
2:F:138:VAL:HG23	2:F:248:ALA:HB3	1.61	0.80
1:C:192:SER:H	1:C:193:ASP:HA	1.42	0.80
2:B:83:LYS:O	2:B:84:LYS:HB3	1.80	0.80
1:E:162:ASP:HB3	1:E:165:VAL:HG12	1.62	0.79
1:A:30:SER:CB	1:A:108:ALA:HB2	2.13	0.78
1:E:192:SER:H	1:E:193:ASP:HA	1.47	0.78
2:F:94:ALA:HA	2:F:98:GLN:HE22	1.48	0.78
2:D:194:LEU:HD12	2:D:194:LEU:H	1.50	0.77
1:A:205:ILE:H	1:A:205:ILE:HD12	1.49	0.76
2:D:69:GLY:O	2:D:70:GLU:HB3	1.84	0.76
2:D:55:TYR:CE2	2:D:68:LYS:HB2	2.17	0.76
2:F:66:THR:O	2:F:67:ALA:HB2	1.86	0.75
2:F:32:TYR:CE1	2:F:110:ASN:HA	2.22	0.75
2:D:132:PHE:CD2	2:D:198:ARG:HD3	2.22	0.75
2:B:96:PRO:HA	2:B:97:SER:O	1.87	0.75
2:D:99:THR:CG2	2:D:124:VAL:H	1.97	0.74
1:A:107:ARG:HA	1:A:111:LEU:HA	1.69	0.74
1:G:192:SER:H	1:G:193:ASP:HA	1.51	0.73
2:D:230:GLU:CD	2:D:231:ASN:HD22	1.92	0.72
2:B:214:ASN:HD21	2:B:216:ARG:NH2	1.87	0.71
2:H:53:ILE:O	2:H:71:VAL:HG22	1.90	0.71
2:B:54:HIS:CE1	2:B:71:VAL:HG21	2.25	0.71
2:D:3:ALA:HA	2:D:27:ASP:OD2	1.91	0.70
1:A:27:ASN:ND2	1:A:29:ALA:H	1.89	0.70
2:H:194:LEU:H	2:H:194:LEU:HD12	1.57	0.70
2:F:67:ALA:HB1	2:F:68:LYS:HG2	1.73	0.70
1:G:2:LYS:O	1:G:3:GLU:HB2	1.90	0.70
2:H:14:LEU:HD11	2:H:20:MET:HG2	1.73	0.70
2:H:58:GLY:O	2:H:59:GLU:HB3	1.92	0.70
1:A:57:TYR:CD2	1:G:179:ASP:HB2	2.27	0.70
1:A:107:ARG:NH1	2:B:111:PHE:HB2	2.07	0.69
1:A:136:ARG:HG3	1:A:142:ASP:OD1	1.93	0.69
2:D:94:ALA:HA	2:D:98:GLN:HE22	1.58	0.69
2:D:143:GLU:HA	2:D:146:ILE:HD13	1.73	0.69
1:A:107:ARG:HH11	1:A:107:ARG:HG3	1.58	0.69
2:B:12:ARG:HD2	2:B:13:VAL:H	1.58	0.69
2:H:26:GLN:HE21	2:H:27:ASP:N	1.91	0.69
2:H:32:TYR:CE1	2:H:57:VAL:HG13	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:TYR:CE2	1:C:85:GLN:HG2	2.28	0.69
2:D:78:VAL:HG13	2:D:79:SER:N	2.07	0.69
1:G:162:ASP:HB3	1:G:165:VAL:HG12	1.75	0.68
2:F:110:ASN:H	2:F:110:ASN:HD22	1.40	0.68
1:A:162:ASP:HB3	1:A:165:VAL:HG12	1.75	0.68
1:A:27:ASN:HD22	1:A:29:ALA:H	1.38	0.68
2:H:55:TYR:CE2	2:H:68:LYS:HB2	2.28	0.68
2:D:238:ARG:NH2	2:D:241:PRO:HG3	2.08	0.68
1:G:32:SER:HB2	1:G:107:ARG:HB2	1.76	0.68
2:D:110:ASN:ND2	2:D:110:ASN:H	1.89	0.67
2:D:15:LYS:HA	2:D:125:LEU:O	1.93	0.67
1:E:160:SER:HB2	1:E:167:ILE:HD11	1.76	0.67
1:A:137:ASP:HB3	1:A:142:ASP:HA	1.77	0.67
1:C:68:GLU:HG2	1:C:69:ASP:N	2.10	0.67
2:D:66:THR:HG22	2:D:67:ALA:H	1.60	0.67
1:A:162:ASP:HB3	1:A:165:VAL:CG1	2.25	0.66
2:B:11:PHE:HB3	2:B:165:HIS:CD2	2.29	0.66
1:C:111:LEU:HB2	2:D:111:PHE:HB2	1.78	0.66
2:H:30:HIS:CD2	2:H:108:GLN:HB3	2.29	0.66
2:F:66:THR:O	2:F:67:ALA:CB	2.43	0.66
2:H:14:LEU:HD11	2:H:20:MET:CG	2.25	0.66
1:G:43:ARG:HH12	1:G:98:ASP:HA	1.61	0.66
2:D:230:GLU:HG3	2:D:231:ASN:H	1.62	0.65
1:A:27:ASN:HD22	1:A:27:ASN:C	2.00	0.65
1:A:90:LEU:CD2	1:C:90:LEU:HD21	2.27	0.65
2:F:94:ALA:HA	2:F:98:GLN:NE2	2.12	0.65
1:E:210:PHE:CZ	1:E:212:PRO:HG3	2.32	0.64
2:F:213:GLN:HA	2:F:253:ARG:O	1.98	0.64
2:B:61:THR:HG22	2:B:66:THR:H	1.63	0.64
2:B:151:LYS:HD2	2:B:206:ARG:HH21	1.62	0.64
2:F:26:GLN:HG2	2:F:28:MET:H	1.62	0.64
2:F:95:ALA:O	2:F:98:GLN:HB2	1.97	0.64
2:F:143:GLU:HA	2:F:146:ILE:HD13	1.79	0.63
2:D:136:VAL:HG12	2:D:137:ALA:H	1.62	0.63
2:B:138:VAL:HG23	2:B:248:ALA:HB3	1.80	0.63
1:E:107:ARG:HD3	2:F:111:PHE:HB2	1.81	0.63
2:F:184:ASP:HB2	2:F:201:LEU:CD1	2.29	0.63
2:D:14:LEU:HD11	2:D:20:MET:CG	2.28	0.63
2:D:151:LYS:HD2	2:D:206:ARG:HD3	1.81	0.63
1:G:184:SER:OG	2:H:204:ARG:HD2	1.99	0.63
1:A:192:SER:N	1:A:193:ASP:CA	2.58	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:210:PHE:CE1	1:G:212:PRO:HG3	2.34	0.62
1:E:192:SER:N	1:E:193:ASP:CA	2.60	0.62
1:G:70:GLY:O	1:G:78:ARG:HB3	1.98	0.62
2:H:54:HIS:HE1	2:H:76:TYR:O	1.80	0.62
2:B:99:THR:HG22	2:B:124:VAL:HB	1.81	0.62
2:D:110:ASN:N	2:D:110:ASN:HD22	1.84	0.62
1:E:108:ALA:CB	1:E:112:ILE:HD11	2.13	0.61
1:A:173:LEU:HD21	2:B:180:GLY:C	2.20	0.61
2:H:226:TYR:HA	2:H:243:THR:HG23	1.81	0.61
1:G:198:ASN:HA	1:G:201:ASN:ND2	2.16	0.61
2:D:149:THR:O	2:D:150:GLN:HG2	2.01	0.61
1:G:166:TYR:HB3	2:H:188:LEU:HD21	1.83	0.61
2:F:99:THR:HB	2:F:124:VAL:H	1.66	0.61
2:B:153:THR:OG1	2:B:206:ARG:HG3	2.01	0.60
2:F:26:GLN:NE2	2:F:30:HIS:H	1.99	0.60
2:B:110:ASN:CG	2:B:111:PHE:H	2.04	0.60
1:E:18:THR:HG22	1:E:92:ARG:HA	1.83	0.60
1:E:205:ILE:HD12	1:E:205:ILE:H	1.67	0.60
1:C:132:VAL:HG12	1:C:196:CYS:HB3	1.82	0.60
1:E:149:THR:O	1:E:150:ASP:HB2	2.01	0.60
2:F:178:HIS:O	2:F:181:VAL:HG22	2.01	0.60
2:D:194:LEU:H	2:D:194:LEU:CD1	2.14	0.60
1:E:135:LEU:H	1:E:135:LEU:HD12	1.66	0.60
1:G:6:GLN:HE22	1:G:104:CYS:N	2.00	0.60
2:F:131:VAL:HG11	2:F:228:LEU:HD23	1.84	0.60
1:E:108:ALA:CB	1:E:112:ILE:CD1	2.76	0.60
2:F:110:ASN:ND2	2:F:110:ASN:H	1.99	0.60
1:G:52:LEU:HD22	2:H:113:ILE:HG23	1.84	0.59
1:G:15:GLU:O	1:G:94:SER:HB2	2.01	0.59
2:H:194:LEU:HD12	2:H:194:LEU:N	2.17	0.59
2:F:71:VAL:HB	2:F:72:PRO:HD3	1.83	0.59
2:D:95:ALA:O	2:D:98:GLN:HB2	2.02	0.59
1:E:41:TRP:HB2	1:E:54:MET:HB2	1.84	0.59
2:H:194:LEU:H	2:H:194:LEU:CD1	2.13	0.59
2:H:26:GLN:HE22	2:H:29:ASN:H	1.50	0.59
1:A:192:SER:H	1:A:193:ASP:HA	1.63	0.59
1:E:70:GLY:O	1:E:78:ARG:HB3	2.02	0.59
1:G:110:LYS:NZ	2:H:68:LYS:HG3	2.18	0.59
1:C:161:LYS:HE2	1:C:161:LYS:HA	1.84	0.59
1:A:134:GLN:HB2	1:A:196:CYS:SG	2.43	0.59
2:F:23:LEU:HD11	2:F:86:ASN:ND2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:191:GLN:HB3	2:D:194:LEU:HD13	1.84	0.59
2:B:15:LYS:HA	2:B:125:LEU:O	2.03	0.59
2:D:138:VAL:HG23	2:D:248:ALA:HB3	1.85	0.59
2:H:71:VAL:O	2:H:74:ASP:O	2.20	0.58
1:C:140:SER:O	1:C:141:SER:HB3	2.03	0.58
1:G:137:ASP:HB2	2:H:139:PHE:CE2	2.38	0.58
2:F:57:VAL:HG22	2:F:57:VAL:O	2.03	0.58
2:D:67:ALA:HB1	2:D:68:LYS:NZ	2.18	0.58
2:D:146:ILE:HG23	2:D:209:ALA:HB1	1.86	0.58
1:C:107:ARG:HG2	1:C:111:LEU:HD13	1.85	0.58
1:E:2:LYS:O	1:E:3:GLU:HB2	2.04	0.58
2:H:57:VAL:HG12	2:H:57:VAL:O	2.01	0.58
1:A:82:GLN:HE22	1:C:92:ARG:HE	1.50	0.58
2:D:69:GLY:O	2:D:70:GLU:CB	2.52	0.58
2:F:162:TYR:CD1	2:F:163:PRO:HA	2.39	0.58
2:H:52:LEU:O	2:H:69:GLY:HA3	2.02	0.58
1:A:143:LYS:O	1:A:144:SER:HB3	2.03	0.58
2:D:56:SER:HA	2:D:61:THR:HB	1.86	0.57
1:G:166:TYR:HB3	2:H:188:LEU:CD2	2.34	0.57
1:C:148:PHE:HB2	1:C:200:PHE:CE2	2.39	0.57
1:E:6:GLN:HG2	1:E:117:THR:HG22	1.85	0.57
1:A:194:PHE:CD2	1:A:194:PHE:O	2.57	0.57
2:B:83:LYS:O	2:B:84:LYS:CB	2.52	0.57
2:F:54:HIS:NE2	2:F:71:VAL:HG13	2.19	0.57
1:A:52:LEU:HD12	1:A:53:LEU:H	1.70	0.57
1:A:143:LYS:O	1:A:144:SER:CB	2.52	0.57
2:D:10:LYS:HZ2	2:D:118:ALA:HB3	1.69	0.57
1:G:205:ILE:HD12	1:G:205:ILE:O	2.03	0.57
2:F:96:PRO:HA	2:F:97:SER:C	2.24	0.57
2:D:194:LEU:HD12	2:D:194:LEU:N	2.19	0.57
2:F:26:GLN:HE21	2:F:29:ASN:N	2.03	0.57
1:A:2:LYS:O	1:A:3:GLU:HB2	2.04	0.57
2:B:110:ASN:ND2	2:B:111:PHE:H	2.03	0.56
1:E:151:PHE:HD1	1:E:155:THR:HB	1.70	0.56
2:F:214:ASN:HB3	2:F:217:ASN:ND2	2.20	0.56
2:F:168:LEU:HG	2:F:223:VAL:HG22	1.88	0.56
2:D:66:THR:O	2:D:67:ALA:HB3	2.05	0.56
2:B:11:PHE:HB3	2:B:165:HIS:HD2	1.69	0.56
2:H:69:GLY:O	2:H:70:GLU:HG3	2.04	0.56
1:C:68:GLU:CG	1:C:69:ASP:N	2.69	0.56
1:G:108:ALA:HB3	1:G:112:ILE:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:PHE:HB2	1:G:89:LEU:HB3	1.87	0.56
2:H:146:ILE:H	2:H:146:ILE:HD12	1.70	0.56
2:B:54:HIS:CE1	2:B:71:VAL:CG2	2.89	0.56
1:G:210:PHE:CZ	1:G:212:PRO:HG3	2.41	0.56
2:B:8:THR:HG22	2:B:9:PRO:HA	1.87	0.56
1:A:120:SER:OG	1:A:122:LYS:HE2	2.05	0.56
2:F:15:LYS:HA	2:F:125:LEU:O	2.05	0.56
1:E:107:ARG:HD3	2:F:111:PHE:CB	2.36	0.56
1:G:103:LEU:HD23	1:G:116:GLY:CA	2.36	0.56
2:B:66:THR:HG23	2:B:78:VAL:HG11	1.88	0.56
1:C:192:SER:N	1:C:193:ASP:CA	2.67	0.56
1:G:142:ASP:O	1:G:144:SER:N	2.39	0.56
1:G:173:LEU:HD23	1:G:174:ASP:N	2.21	0.56
2:D:215:PRO:HA	2:D:252:GLY:O	2.06	0.55
1:C:191:LYS:H	1:C:191:LYS:HZ1	1.53	0.55
1:G:6:GLN:HE22	1:G:104:CYS:H	1.51	0.55
2:F:110:ASN:CG	2:F:111:PHE:H	2.09	0.55
2:H:54:HIS:CD2	2:H:66:THR:HG22	2.41	0.55
2:F:97:SER:C	2:F:99:THR:H	2.08	0.55
1:A:134:GLN:O	2:B:142:SER:HB2	2.05	0.55
2:F:3:ALA:HA	2:F:27:ASP:OD2	2.05	0.55
1:E:205:ILE:CD1	1:E:205:ILE:H	2.19	0.55
2:H:69:GLY:C	2:H:70:GLU:HG3	2.27	0.55
2:D:136:VAL:HG12	2:D:137:ALA:N	2.21	0.55
1:E:205:ILE:HG22	1:E:206:PRO:HD2	1.89	0.55
1:A:173:LEU:HD21	2:B:180:GLY:O	2.07	0.55
2:F:158:ALA:O	2:F:200:ALA:HA	2.07	0.55
2:F:70:GLU:HG2	2:F:70:GLU:O	2.07	0.55
2:D:56:SER:OG	2:D:80:ARG:HD3	2.07	0.55
2:B:110:ASN:N	2:B:110:ASN:HD22	2.05	0.54
1:C:213:SER:N	1:C:214:PRO:CD	2.71	0.54
2:B:59:GLU:HG3	2:B:84:LYS:HB2	1.88	0.54
2:B:10:LYS:NZ	2:B:118:ALA:HB3	2.22	0.54
1:E:111:LEU:HD23	1:E:113:PHE:CE2	2.42	0.54
1:A:30:SER:OG	1:A:108:ALA:HB2	2.07	0.54
2:D:10:LYS:NZ	2:D:118:ALA:HB3	2.23	0.54
2:H:54:HIS:CE1	2:H:71:VAL:CG1	2.91	0.54
1:C:191:LYS:HA	1:C:193:ASP:OD1	2.06	0.54
1:C:84(B):ALA:HB2	1:E:57:TYR:CE1	2.43	0.54
2:D:68:LYS:HD2	2:D:68:LYS:N	2.23	0.54
2:F:168:LEU:HD23	2:F:169:SER:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:164:ASP:HB2	2:F:187:PRO:HG2	1.89	0.54
2:F:214:ASN:O	2:F:252:GLY:HA3	2.07	0.54
1:E:138:SER:O	1:E:140:SER:N	2.41	0.54
2:F:97:SER:O	2:F:99:THR:N	2.39	0.53
1:C:56:VAL:HG22	1:C:81:ALA:HB1	1.90	0.53
2:B:69:GLY:O	2:B:70:GLU:CB	2.56	0.53
1:C:107:ARG:HB3	2:D:111:PHE:HE1	1.73	0.53
2:F:54:HIS:HE2	2:F:71:VAL:HG13	1.74	0.53
1:A:135:LEU:HD22	2:B:155:VAL:HG23	1.89	0.53
2:B:141:PRO:HD2	2:B:212:TRP:CZ2	2.44	0.53
1:A:103:LEU:HD23	1:A:116:GLY:HA3	1.90	0.53
2:H:66:THR:O	2:H:67:ALA:HB3	2.08	0.53
2:D:165:HIS:HB3	2:D:226:TYR:HB2	1.90	0.53
1:G:107:ARG:HD3	2:H:111:PHE:HB3	1.90	0.53
1:C:194:PHE:H	1:C:194:PHE:HD2	1.55	0.53
1:E:165:VAL:HA	1:E:189:SER:HB2	1.90	0.53
2:B:32:TYR:CD1	2:B:110:ASN:HA	2.45	0.52
2:F:240:LYS:HG2	2:F:242:VAL:HG13	1.91	0.52
2:D:191:GLN:C	2:D:193:ALA:H	2.13	0.52
2:B:12:ARG:HD2	2:B:13:VAL:N	2.25	0.52
1:E:47:ARG:HG3	2:F:121:ARG:NH2	2.24	0.52
2:D:30:HIS:CD2	2:D:108:GLN:HB3	2.44	0.52
2:B:16:THR:HG23	2:B:95:ALA:HA	1.91	0.52
1:G:70:GLY:O	1:G:78:ARG:CB	2.57	0.52
1:E:58:SER:HA	1:E:83:LEU:HB3	1.90	0.52
2:D:12:ARG:HG2	2:D:20:MET:HE3	1.92	0.52
2:D:191:GLN:HB2	2:D:197:SER:HB2	1.89	0.52
1:A:190:ASN:O	1:A:191:LYS:C	2.48	0.52
1:G:134:GLN:HE21	1:G:144:SER:CB	2.18	0.52
1:C:133:TYR:HB3	2:D:142:SER:CB	2.40	0.52
2:H:168:LEU:HD23	2:H:169:SER:N	2.25	0.52
1:C:198:ASN:HA	1:C:201:ASN:ND2	2.25	0.52
2:B:71:VAL:O	2:B:74:ASP:O	2.29	0.51
2:B:94:ALA:O	2:B:95:ALA:HB2	2.09	0.51
2:H:26:GLN:HE22	2:H:29:ASN:N	2.07	0.51
2:F:66:THR:HG22	2:F:67:ALA:N	2.24	0.51
1:A:57:TYR:CG	1:G:179:ASP:HB2	2.45	0.51
1:C:70:GLY:O	1:C:78:ARG:CB	2.58	0.51
1:G:134:GLN:O	2:H:142:SER:HB2	2.10	0.51
1:C:167:ILE:HD13	1:C:187:ALA:CB	2.40	0.51
1:E:162:ASP:HB3	1:E:165:VAL:CG1	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LYS:HB2	1:A:49:GLU:OE1	2.10	0.51
2:H:19:SER:CB	2:H:92:GLU:HA	2.40	0.51
2:D:97:SER:O	2:D:99:THR:N	2.41	0.51
1:C:167:ILE:HD13	1:C:187:ALA:HB2	1.93	0.51
1:G:50:PRO:HB2	2:H:116:PHE:CD1	2.46	0.51
1:A:152:ASP:OD2	1:A:154:GLN:HG2	2.10	0.51
2:H:99:THR:HB	2:H:124:VAL:H	1.76	0.51
2:B:61:THR:HG22	2:B:66:THR:N	2.24	0.51
2:F:150:GLN:C	2:F:209:ALA:HB2	2.31	0.51
2:F:10:LYS:HZ2	2:F:118:ALA:HB3	1.76	0.51
2:H:78:VAL:HG13	2:H:79:SER:N	2.25	0.51
2:H:7:GLN:NE2	2:H:120:THR:N	2.58	0.51
1:C:6:GLN:CD	1:C:116:GLY:HA2	2.31	0.51
2:H:43:ARG:HB2	2:H:53:ILE:HD11	1.92	0.51
2:D:150:GLN:C	2:D:209:ALA:HB2	2.31	0.51
2:F:201:LEU:HD12	2:F:202:SER:H	1.76	0.51
2:D:78:VAL:CG1	2:D:79:SER:N	2.74	0.51
2:F:97:SER:O	2:F:99:THR:HG22	2.11	0.51
2:B:54:HIS:CE1	2:B:66:THR:HG22	2.46	0.51
1:G:110:LYS:HD2	2:H:68:LYS:HE2	1.93	0.51
2:D:97:SER:C	2:D:99:THR:H	2.15	0.50
2:H:12:ARG:HG2	2:H:20:MET:HE2	1.92	0.50
2:D:228:LEU:HD23	2:D:241:PRO:HB2	1.91	0.50
2:F:201:LEU:HD12	2:F:202:SER:N	2.26	0.50
1:E:135:LEU:N	1:E:135:LEU:HD12	2.25	0.50
1:E:56:VAL:HG22	1:E:81:ALA:HB1	1.93	0.50
1:C:135:LEU:HB2	1:C:145:VAL:HG23	1.93	0.50
2:F:55:TYR:CE2	2:F:67:ALA:HB3	2.47	0.50
2:F:95:ALA:H	2:F:98:GLN:HE21	1.58	0.50
1:A:111:LEU:HD23	1:A:111:LEU:O	2.11	0.50
1:G:149:THR:HG23	1:G:150:ASP:OD2	2.10	0.50
2:D:66:THR:O	2:D:67:ALA:CB	2.59	0.50
1:A:90:LEU:HD21	1:C:90:LEU:HD21	1.94	0.50
2:F:234:TRP:CZ2	2:F:236:GLN:HB2	2.47	0.50
2:B:181:VAL:HA	2:B:204:ARG:O	2.11	0.50
2:F:66:THR:HG22	2:F:67:ALA:H	1.76	0.50
2:D:12:ARG:HG2	2:D:20:MET:CE	2.42	0.50
2:B:30:HIS:O	2:B:84:LYS:HE3	2.11	0.50
1:E:47:ARG:HG3	2:F:121:ARG:HH22	1.77	0.50
2:H:154:LEU:N	2:H:154:LEU:HD12	2.26	0.50
1:A:39:PHE:HB2	1:A:56:VAL:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:147:SER:O	2:H:148:HIS:HB2	2.10	0.50
1:G:192:SER:N	1:G:193:ASP:CA	2.63	0.50
2:B:214:ASN:HB3	2:B:217:ASN:ND2	2.26	0.50
2:F:146:ILE:HG23	2:F:209:ALA:HB1	1.92	0.50
2:F:70:GLU:CG	2:F:70:GLU:O	2.58	0.50
1:C:15:GLU:O	1:C:94:SER:O	2.30	0.50
1:A:70:GLY:O	1:A:78:ARG:CB	2.60	0.50
2:H:128:LEU:O	2:H:131:VAL:HG23	2.12	0.50
1:C:135:LEU:HD12	2:D:142:SER:HB2	1.94	0.49
1:C:66:ASN:HD22	1:C:81:ALA:HB3	1.77	0.49
2:B:238:ARG:NH2	2:B:241:PRO:HG3	2.26	0.49
2:D:54:HIS:HE2	2:D:71:VAL:HG13	1.77	0.49
1:E:70:GLY:O	1:E:78:ARG:CB	2.60	0.49
1:E:135:LEU:HB2	1:E:145:VAL:HG23	1.94	0.49
2:H:80:ARG:HG3	2:H:80:ARG:O	2.13	0.49
2:F:85:GLN:CD	2:F:85:GLN:H	2.15	0.49
2:F:9:PRO:HD2	2:F:22:LEU:HD22	1.95	0.49
2:D:7:GLN:HE22	2:D:119:GLY:HA2	1.77	0.49
1:A:140:SER:O	1:A:141:SER:HB3	2.12	0.49
2:F:44:GLN:HB2	2:F:50:LEU:HD23	1.95	0.49
2:F:91:LEU:N	2:F:91:LEU:HD23	2.27	0.49
2:B:10:LYS:HZ2	2:B:118:ALA:HB3	1.78	0.49
1:C:84(B):ALA:HB2	1:E:57:TYR:CD1	2.47	0.49
2:H:19:SER:HB3	2:H:92:GLU:HA	1.94	0.49
2:H:126:GLU:OE1	2:H:127:ASP:HB2	2.12	0.49
1:E:112:ILE:N	1:E:112:ILE:HD12	2.26	0.49
2:B:54:HIS:ND1	2:B:66:THR:HG22	2.26	0.49
2:B:66:THR:HG22	2:B:67:ALA:N	2.15	0.49
1:A:107:ARG:HH11	1:A:107:ARG:CG	2.24	0.49
2:F:130:ASN:O	2:F:162:TYR:HD2	1.96	0.49
2:D:96:PRO:HA	2:D:97:SER:C	2.21	0.49
1:G:190:ASN:O	1:G:191:LYS:C	2.51	0.49
2:D:122:LEU:HD12	2:D:123:SER:H	1.78	0.48
1:C:132:VAL:HG11	1:C:196:CYS:O	2.13	0.48
1:A:175:MET:HE1	2:B:207:VAL:HA	1.94	0.48
2:D:74:ASP:CG	2:D:75:GLY:H	2.17	0.48
1:A:47:ARG:HD2	2:B:121:ARG:NH2	2.19	0.48
2:D:234:TRP:CZ2	2:D:236:GLN:HB2	2.48	0.48
2:B:40:TYR:CD2	2:B:40:TYR:N	2.80	0.48
2:H:66:THR:HG22	2:H:67:ALA:N	2.18	0.48
1:G:43:ARG:NH1	1:G:98:ASP:HA	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:MET:HA	1:E:54:MET:CE	2.44	0.48
2:D:53:ILE:HG22	2:D:54:HIS:CD2	2.47	0.48
1:C:70:GLY:O	1:C:78:ARG:HB3	2.13	0.48
2:F:131:VAL:HG11	2:F:228:LEU:CD2	2.42	0.48
1:C:6:GLN:NE2	1:C:116:GLY:HA2	2.29	0.48
2:F:154:LEU:HD12	2:F:154:LEU:N	2.28	0.48
2:H:54:HIS:CE1	2:H:71:VAL:HG11	2.49	0.48
1:A:145:VAL:HG12	1:A:188:TRP:HB3	1.93	0.48
2:H:81:LEU:HA	2:H:81:LEU:HD22	1.71	0.48
1:C:133:TYR:HB3	2:D:142:SER:HB3	1.96	0.48
2:D:54:HIS:NE2	2:D:71:VAL:HG13	2.28	0.48
1:A:6:GLN:O	1:A:7:ASP:C	2.52	0.48
2:B:184:ASP:HB2	2:B:201:LEU:HD12	1.96	0.48
2:H:238:ARG:NH2	2:H:241:PRO:HG3	2.29	0.48
2:D:66:THR:HG22	2:D:67:ALA:N	2.27	0.48
1:C:31:GLN:HE22	2:D:111:PHE:HZ	1.62	0.48
2:B:110:ASN:CG	2:B:111:PHE:N	2.67	0.48
2:D:238:ARG:HH22	2:D:241:PRO:HG3	1.79	0.48
1:E:160:SER:HB2	1:E:167:ILE:CD1	2.44	0.48
1:C:7:ASP:HB2	1:C:117:THR:HG21	1.96	0.48
1:E:190:ASN:O	1:E:192:SER:N	2.47	0.47
2:H:97:SER:C	2:H:99:THR:H	2.17	0.47
1:E:130:PRO:HB3	1:E:151:PHE:HB3	1.97	0.47
2:B:14:LEU:HD11	2:B:20:MET:CG	2.39	0.47
2:D:149:THR:HB	2:D:151:LYS:HE2	1.97	0.47
2:F:74:ASP:O	2:F:76:TYR:N	2.47	0.47
1:G:186:VAL:HG12	1:G:187:ALA:N	2.30	0.47
1:C:46:SER:HA	1:C:47:ARG:HA	1.54	0.47
2:B:128:LEU:HG	2:B:228:LEU:HD11	1.96	0.47
2:F:72:PRO:HA	2:F:74:ASP:O	2.14	0.47
1:C:125:ILE:HB	1:C:152:ASP:HA	1.97	0.47
2:B:66:THR:O	2:B:67:ALA:HB3	2.14	0.47
2:B:94:ALA:HA	2:B:98:GLN:HE22	1.80	0.47
1:C:40:PHE:HZ	1:C:107:ARG:HH21	1.63	0.47
1:G:6:GLN:NE2	1:G:104:CYS:H	2.12	0.47
2:H:156:CYS:O	2:H:157:LEU:HD12	2.15	0.47
2:H:160:GLY:HA2	2:H:198:ARG:HB3	1.95	0.47
1:E:107:ARG:HG2	1:E:111:LEU:CD1	2.36	0.47
2:D:57:VAL:HG12	2:D:61:THR:HG21	1.96	0.47
2:B:30:HIS:HE1	2:B:115:TYR:CE2	2.33	0.47
2:B:97:SER:C	2:B:99:THR:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:253:ARG:HB3	2:F:255:ASP:HB3	1.96	0.47
2:B:151:LYS:HD2	2:B:206:ARG:NH2	2.29	0.47
1:G:46:SER:HA	1:G:47:ARG:HA	1.54	0.47
1:G:112:ILE:N	1:G:112:ILE:HD12	2.29	0.47
2:F:44:GLN:HB2	2:F:50:LEU:CD2	2.45	0.47
2:H:228:LEU:HD23	2:H:241:PRO:HB2	1.97	0.47
2:F:47:GLY:O	2:F:48:MET:HB3	2.15	0.47
1:C:54:MET:HB3	1:C:54:MET:HE2	1.70	0.47
2:H:108:GLN:HE21	2:H:109:GLY:N	2.13	0.47
2:D:8:THR:OG1	2:D:23:LEU:HD12	2.15	0.47
1:C:6:GLN:HG2	1:C:117:THR:CG2	2.45	0.46
1:C:95:LYS:O	1:C:121:VAL:HG21	2.15	0.46
2:H:178:HIS:O	2:H:181:VAL:HG22	2.15	0.46
1:A:68:GLU:HG2	1:A:69:ASP:N	2.22	0.46
2:B:74:ASP:O	2:B:76:TYR:N	2.48	0.46
1:G:143:LYS:O	1:G:144:SER:CB	2.63	0.46
2:H:19:SER:HA	2:H:91:LEU:O	2.15	0.46
1:C:141:SER:C	1:C:143:LYS:H	2.19	0.46
2:B:242:VAL:O	2:B:244:GLN:HG2	2.15	0.46
1:G:126:GLN:O	1:G:128:PRO:HD3	2.16	0.46
2:D:214:ASN:HA	2:D:215:PRO:HD3	1.82	0.46
2:B:234:TRP:CZ2	2:B:241:PRO:HD3	2.50	0.46
2:B:240:LYS:HA	2:B:241:PRO:HD3	1.78	0.46
1:A:30:SER:O	1:A:84(A):ARG:NH2	2.48	0.46
1:E:141:SER:O	1:E:142:ASP:HB3	2.16	0.46
2:D:75:GLY:O	2:D:91:LEU:HA	2.16	0.46
1:G:84:ASN:OD1	1:G:84(B):ALA:HB3	2.15	0.46
2:H:110:ASN:CG	2:H:111:PHE:H	2.19	0.46
2:F:54:HIS:CE1	2:F:71:VAL:HG22	2.50	0.46
2:H:54:HIS:CE1	2:H:71:VAL:HG13	2.51	0.46
2:H:184:ASP:HB2	2:H:201:LEU:HD12	1.98	0.46
2:D:94:ALA:HA	2:D:98:GLN:NE2	2.28	0.46
2:H:26:GLN:NE2	2:H:29:ASN:H	2.11	0.46
2:F:172:VAL:HG12	2:F:172:VAL:O	2.14	0.46
2:H:16:THR:HG23	2:H:95:ALA:HA	1.98	0.45
1:A:125:ILE:HG13	1:A:152:ASP:HA	1.97	0.45
1:A:99:SER:O	1:A:100:ALA:HB2	2.16	0.45
2:H:58:GLY:O	2:H:59:GLU:CB	2.61	0.45
1:C:107:ARG:CB	2:D:111:PHE:HE1	2.29	0.45
2:B:41:TRP:HD1	2:B:87:PHE:CE2	2.33	0.45
2:F:24:CYS:HB2	2:F:41:TRP:CZ2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:78:ARG:HA	1:G:92:ARG:HH11	1.82	0.45
2:B:72:PRO:HA	2:B:74:ASP:HA	1.69	0.45
2:B:95:ALA:O	2:B:97:SER:O	2.34	0.45
1:C:32:SER:H	1:C:107:ARG:HB2	1.81	0.45
2:F:151:LYS:HA	2:F:209:ALA:N	2.31	0.45
2:F:131:VAL:O	2:F:238:ARG:NH2	2.48	0.45
2:F:26:GLN:HE21	2:F:29:ASN:H	1.62	0.45
2:F:69:GLY:O	2:F:70:GLU:CB	2.64	0.45
1:G:110:LYS:HZ3	2:H:68:LYS:HG3	1.81	0.45
2:H:127:ASP:OD1	2:H:129:LYS:HE3	2.16	0.45
2:B:32:TYR:CZ	2:B:57:VAL:HG23	2.51	0.45
2:H:160:GLY:O	2:H:198:ARG:NH1	2.50	0.45
1:C:142:ASP:O	1:C:143:LYS:C	2.55	0.45
2:D:191:GLN:HB2	2:D:197:SER:CB	2.46	0.45
1:A:82:GLN:HE22	1:C:92:ARG:NE	2.15	0.45
2:D:191:GLN:CB	2:D:194:LEU:HD13	2.47	0.45
1:G:130:PRO:HG3	1:G:206:PRO:HG2	1.98	0.45
2:H:97:SER:O	2:H:99:THR:N	2.44	0.45
2:D:14:LEU:HD12	2:D:122:LEU:HD11	1.98	0.45
1:A:135:LEU:HB2	1:A:145:VAL:HG23	1.99	0.45
2:D:90:GLY:C	2:D:91:LEU:HD23	2.37	0.45
2:B:170:TRP:O	2:B:176:GLU:HA	2.17	0.45
2:F:218:HIS:HE1	2:F:249:GLU:HB3	1.82	0.45
1:G:213:SER:HB3	1:G:214:PRO:HD3	1.98	0.45
1:A:57:TYR:CE2	1:G:179:ASP:HB2	2.52	0.45
1:A:137:ASP:HB2	2:B:139:PHE:CE2	2.52	0.45
1:C:68:GLU:CG	1:C:69:ASP:H	2.30	0.45
2:H:115:TYR:N	2:H:115:TYR:CD2	2.85	0.45
1:G:103:LEU:HD23	1:G:116:GLY:HA3	1.98	0.44
1:A:213:SER:HB3	1:A:214:PRO:HD3	1.98	0.44
2:F:225:PHE:CG	2:F:226:TYR:N	2.85	0.44
2:H:102:TYR:N	2:H:102:TYR:CD1	2.85	0.44
1:E:124:ASN:ND2	1:E:124:ASN:H	2.14	0.44
2:H:191:GLN:HB3	2:H:194:LEU:HD13	1.99	0.44
1:A:141:SER:O	1:A:142:ASP:HB3	2.18	0.44
1:A:123:PRO:HG3	1:A:172:VAL:HG21	1.98	0.44
2:H:218:HIS:CE1	2:H:220:ARG:HB2	2.52	0.44
2:D:146:ILE:HG23	2:D:209:ALA:CB	2.47	0.44
2:H:108:GLN:C	2:H:108:GLN:HE21	2.20	0.44
1:C:137:ASP:OD1	1:C:138:SER:N	2.50	0.44
2:B:95:ALA:N	2:B:124:VAL:HG11	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LYS:HG3	2:B:111:PHE:CZ	2.53	0.44
2:H:57:VAL:CG1	2:H:57:VAL:O	2.64	0.44
1:E:41:TRP:O	1:E:53:LEU:HB3	2.18	0.44
2:D:138:VAL:HG23	2:D:248:ALA:CB	2.46	0.44
1:E:136:ARG:HD3	1:E:142:ASP:OD1	2.17	0.44
2:H:240:LYS:HG2	2:H:242:VAL:HG13	1.99	0.44
2:H:76:TYR:CZ	2:H:98:GLN:OE1	2.71	0.44
1:C:25:TYR:CZ	1:C:85:GLN:HG2	2.53	0.44
2:F:85:GLN:NE2	2:F:85:GLN:H	2.15	0.44
1:C:41:TRP:CE2	1:C:89:LEU:HB2	2.53	0.44
1:E:78:ARG:O	1:E:92:ARG:HG3	2.18	0.44
2:H:14:LEU:HD11	2:H:20:MET:HG3	1.98	0.44
2:H:184:ASP:HB2	2:H:201:LEU:CD1	2.48	0.44
1:C:158:SER:O	1:C:159:GLN:O	2.36	0.44
1:G:133:TYR:CE1	2:H:145:GLU:HA	2.53	0.44
1:C:210:PHE:HD2	1:C:211:PHE:H	1.66	0.44
2:D:230:GLU:CD	2:D:231:ASN:ND2	2.66	0.44
2:F:151:LYS:HE2	2:F:206:ARG:NH2	2.33	0.44
1:C:134:GLN:HB2	1:C:196:CYS:SG	2.57	0.44
1:G:129:ASP:HA	1:G:130:PRO:HD2	1.67	0.44
1:G:48:LYS:HB2	1:G:49:GLU:H	1.61	0.44
1:C:130:PRO:O	1:C:209:THR:HA	2.18	0.44
2:D:95:ALA:N	2:D:124:VAL:HG11	2.33	0.44
1:A:191:LYS:C	1:A:193:ASP:HA	2.33	0.44
2:B:57:VAL:O	2:B:57:VAL:HG22	2.18	0.44
1:C:176:ARG:HD2	1:C:176:ARG:H	1.83	0.44
2:D:61:THR:HG22	2:D:66:THR:N	2.33	0.43
2:H:97:SER:O	2:H:99:THR:HG22	2.18	0.43
1:C:133:TYR:CE1	2:D:145:GLU:HA	2.53	0.43
1:G:48:LYS:H	1:G:48:LYS:HG2	1.56	0.43
2:B:32:TYR:CE2	2:B:109:GLY:O	2.72	0.43
1:A:2:LYS:O	1:A:3:GLU:CB	2.65	0.43
2:H:240:LYS:HA	2:H:241:PRO:HD3	1.72	0.43
2:H:138:VAL:HG23	2:H:248:ALA:HB3	2.00	0.43
2:D:67:ALA:HB1	2:D:68:LYS:HZ3	1.82	0.43
2:B:32:TYR:CE1	2:B:57:VAL:HG23	2.53	0.43
2:H:14:LEU:HD13	2:H:94:ALA:CB	2.48	0.43
2:D:136:VAL:O	2:D:137:ALA:HB2	2.17	0.43
1:A:39:PHE:CD1	1:A:87:ILE:HD11	2.54	0.43
1:G:68:GLU:O	1:G:70:GLY:HA2	2.18	0.43
1:A:107:ARG:HA	1:A:111:LEU:CA	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:PHE:CZ	1:G:205:ILE:HG22	2.53	0.43
1:E:105:VAL:HG22	1:E:113:PHE:CD1	2.53	0.43
1:G:32:SER:HB2	1:G:107:ARG:CB	2.46	0.43
2:D:15:LYS:O	2:D:16:THR:C	2.57	0.43
1:C:69:ASP:HA	1:C:70:GLY:HA2	1.86	0.43
2:F:145:GLU:HG2	2:F:151:LYS:O	2.18	0.43
1:E:145:VAL:HG23	1:E:145:VAL:O	2.19	0.43
2:D:214:ASN:O	2:D:252:GLY:HA3	2.18	0.43
2:B:69:GLY:O	2:B:70:GLU:HB2	2.19	0.43
2:F:9:PRO:HD2	2:F:22:LEU:CD2	2.48	0.43
1:G:140:SER:C	1:G:142:ASP:H	2.21	0.43
1:E:135:LEU:HB2	1:E:145:VAL:CG2	2.48	0.43
2:H:141:PRO:HB2	2:H:146:ILE:HD11	2.00	0.43
2:D:154:LEU:HD12	2:D:154:LEU:N	2.34	0.43
1:C:190:ASN:O	1:C:191:LYS:C	2.57	0.43
1:A:27:ASN:C	1:A:27:ASN:ND2	2.71	0.43
2:F:234:TRP:CZ2	2:F:241:PRO:HD3	2.54	0.43
2:B:80:ARG:HB2	2:B:87:PHE:HD1	1.83	0.43
1:A:13:VAL:HA	1:A:14:PRO:HD3	1.90	0.43
2:B:12:ARG:HG2	2:B:20:MET:CE	2.49	0.43
2:D:191:GLN:C	2:D:193:ALA:N	2.72	0.43
1:A:90:LEU:HD22	1:C:90:LEU:HD21	1.99	0.43
2:D:184:ASP:HA	2:D:185:PRO:HD3	1.85	0.43
2:B:97:SER:O	2:B:98:GLN:HB2	2.19	0.43
1:G:148:PHE:O	1:G:184:SER:HA	2.19	0.43
2:H:141:PRO:CG	2:H:152:ALA:HB1	2.49	0.43
2:D:110:ASN:ND2	2:D:110:ASN:N	2.56	0.42
1:A:46:SER:HA	1:A:47:ARG:HA	1.58	0.42
2:F:26:GLN:NE2	2:F:29:ASN:N	2.67	0.42
2:F:163:PRO:HB2	2:F:165:HIS:CE1	2.54	0.42
1:A:45:ASP:O	1:A:48:LYS:HG2	2.18	0.42
1:E:7:ASP:HA	1:E:8:PRO:HD3	1.63	0.42
2:H:112:ASP:CG	2:H:113:ILE:H	2.23	0.42
1:E:46:SER:HA	1:E:47:ARG:HA	1.57	0.42
2:D:143:GLU:HA	2:D:146:ILE:CD1	2.43	0.42
2:F:74:ASP:HB2	2:F:75:GLY:H	1.67	0.42
1:A:135:LEU:N	1:A:135:LEU:HD12	2.33	0.42
2:B:208:SER:O	2:B:211:PHE:N	2.52	0.42
2:D:160:GLY:O	2:D:198:ARG:HD2	2.20	0.42
1:A:106:VAL:O	1:A:111:LEU:HA	2.20	0.42
2:H:70:GLU:OE2	2:H:70:GLU:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:GLN:HA	2:D:49:GLY:CA	2.49	0.42
2:H:54:HIS:CE1	2:H:76:TYR:O	2.67	0.42
2:H:12:ARG:HG2	2:H:20:MET:CE	2.48	0.42
1:C:107:ARG:NH2	2:D:112:ASP:HB2	2.34	0.42
2:D:71:VAL:H	2:D:72:PRO:CD	2.32	0.42
1:A:13:VAL:HG11	1:A:19:VAL:HG11	2.01	0.42
2:H:95:ALA:O	2:H:98:GLN:HG3	2.20	0.42
1:C:191:LYS:HA	1:C:191:LYS:HE3	2.02	0.42
2:B:8:THR:OG1	2:B:23:LEU:HD12	2.19	0.42
2:D:240:LYS:HD3	2:D:242:VAL:CG1	2.49	0.42
2:B:77:ASN:H	2:B:77:ASN:ND2	2.17	0.42
2:F:228:LEU:HB2	2:F:241:PRO:O	2.20	0.42
1:C:103:LEU:HD23	1:C:116:GLY:HA3	2.00	0.42
2:D:67:ALA:CB	2:D:68:LYS:HD2	2.49	0.42
2:B:214:ASN:HA	2:B:215:PRO:HD3	1.90	0.42
2:F:240:LYS:HA	2:F:241:PRO:HD3	1.76	0.42
2:D:61:THR:HG22	2:D:66:THR:H	1.85	0.42
1:C:28:SER:HA	1:C:85:GLN:NE2	2.34	0.42
1:E:151:PHE:N	1:E:151:PHE:CD2	2.88	0.42
1:E:47:ARG:HD2	2:F:186:GLN:NE2	2.35	0.42
1:E:110:LYS:HG3	2:F:111:PHE:CZ	2.55	0.42
2:B:66:THR:CG2	2:B:67:ALA:N	2.81	0.42
2:H:69:GLY:O	2:H:70:GLU:CG	2.68	0.42
1:E:138:SER:O	1:E:139:LYS:C	2.58	0.42
1:A:102:TYR:O	1:A:116:GLY:HA2	2.20	0.42
2:B:184:ASP:HA	2:B:185:PRO:HD3	1.91	0.42
1:C:2:LYS:HB3	1:C:2:LYS:HE3	1.86	0.42
1:C:2:LYS:O	1:C:3[B]:GLU:CB	2.67	0.42
1:G:84(C):SER:HB2	1:G:86:TYR:CD2	2.55	0.42
2:B:129:LYS:HG3	2:B:236:GLN:HG3	2.02	0.42
2:B:26:GLN:OE1	2:B:30:HIS:HB2	2.20	0.41
1:C:129:ASP:HA	1:C:130:PRO:HD2	1.85	0.41
1:E:107:ARG:HA	1:E:111:LEU:HA	2.02	0.41
1:A:83:LEU:HD21	1:A:84(A):ARG:HG2	2.01	0.41
1:A:173:LEU:HD23	1:A:174:ASP:H	1.84	0.41
2:D:127:ASP:OD1	2:D:129:LYS:HE3	2.20	0.41
1:A:82:GLN:NE2	1:C:92:ARG:HE	2.14	0.41
1:G:183:ASN:O	1:G:184:SER:CB	2.68	0.41
1:G:7:ASP:O	1:G:117:THR:HB	2.20	0.41
2:D:78:VAL:HG21	2:D:87:PHE:CZ	2.55	0.41
1:E:180:PHE:CE2	2:F:151:LYS:HE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:PHE:CE2	1:G:205:ILE:HG22	2.56	0.41
1:C:134:GLN:C	2:D:142:SER:HB2	2.41	0.41
1:E:145:VAL:HG22	2:F:139:PHE:CD2	2.55	0.41
2:F:23:LEU:HD11	2:F:86:ASN:HD22	1.83	0.41
2:F:78:VAL:HG21	2:F:87:PHE:CZ	2.55	0.41
1:C:111:LEU:HD12	1:C:111:LEU:HA	1.91	0.41
2:D:112:ASP:O	2:D:114:GLN:HG3	2.20	0.41
1:G:103:LEU:HD23	1:G:116:GLY:HA2	2.02	0.41
2:F:27:ASP:CG	2:F:27:ASP:O	2.59	0.41
1:C:53:LEU:HG	1:C:54:MET:CG	2.50	0.41
1:G:84(C):SER:HB2	1:G:86:TYR:HD2	1.86	0.41
2:F:194:LEU:HA	2:F:194:LEU:HD12	1.95	0.41
1:G:6:GLN:NE2	1:G:104:CYS:N	2.65	0.41
2:F:211:PHE:O	2:F:217:ASN:ND2	2.50	0.41
1:E:154:GLN:NE2	1:G:24:THR:HG21	2.35	0.41
2:B:13:VAL:HG11	2:B:131:VAL:HG21	2.01	0.41
1:A:107:ARG:NH1	1:A:107:ARG:HG3	2.32	0.41
1:E:48:LYS:HE2	1:E:48:LYS:HB3	1.98	0.41
1:A:92:ARG:HH21	1:C:82:GLN:NE2	2.17	0.41
1:E:108:ALA:C	1:E:110:LYS:H	2.24	0.41
2:H:98:GLN:O	2:H:100:SER:N	2.54	0.41
1:A:69:ASP:HA	1:A:70:GLY:HA2	1.91	0.41
2:D:122:LEU:HD12	2:D:123:SER:N	2.35	0.41
1:C:66:ASN:HB3	1:C:68:GLU:H	1.72	0.41
2:F:239:ALA:O	2:F:240:LYS:C	2.59	0.41
1:E:125:ILE:HD13	1:E:125:ILE:N	2.36	0.41
2:F:61:THR:HG22	2:F:66:THR:N	2.36	0.41
2:H:20:MET:SD	2:H:22:LEU:HD21	2.61	0.41
2:F:152:ALA:O	2:F:206:ARG:HA	2.21	0.41
1:E:149:THR:O	1:E:150:ASP:CB	2.68	0.41
1:E:140:SER:O	1:E:141:SER:HB3	2.20	0.41
2:D:8:THR:OG1	2:D:23:LEU:HB2	2.21	0.41
1:E:48:LYS:HG2	1:E:48:LYS:H	1.71	0.41
1:E:87:ILE:HD11	1:E:104:CYS:SG	2.61	0.41
2:B:154:LEU:N	2:B:154:LEU:HD12	2.36	0.41
1:E:24:THR:CG2	1:G:154:GLN:HE22	2.34	0.41
2:H:166:VAL:HA	2:H:224:GLN:O	2.20	0.41
1:A:129:ASP:OD1	1:A:129:ASP:N	2.53	0.41
2:H:149:THR:C	2:H:150:GLN:HG2	2.41	0.41
2:H:66:THR:O	2:H:67:ALA:CB	2.69	0.41
2:H:95:ALA:O	2:H:97:SER:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:VAL:HG11	2:B:228:LEU:HD22	2.03	0.41
1:G:183:ASN:O	1:G:184:SER:HB2	2.20	0.41
1:E:2:LYS:HB3	1:E:2:LYS:HE3	1.94	0.41
2:D:76:TYR:CD1	2:D:91:LEU:HD22	2.56	0.41
1:G:186:VAL:CG1	1:G:187:ALA:N	2.83	0.41
1:A:58:SER:C	1:A:60:GLY:H	2.23	0.41
2:F:32:TYR:CE1	2:F:57:VAL:HG23	2.56	0.40
2:H:26:GLN:NE2	2:H:29:ASN:N	2.69	0.40
2:F:151:LYS:N	2:F:209:ALA:HB2	2.36	0.40
2:H:131:VAL:HG13	2:H:162:TYR:O	2.21	0.40
1:E:172:VAL:HG22	1:E:183:ASN:OD1	2.22	0.40
1:G:123:PRO:O	1:G:153:SER:OG	2.35	0.40
2:D:95:ALA:H	2:D:98:GLN:HE21	1.68	0.40
2:D:67:ALA:HB1	2:D:68:LYS:HD2	2.03	0.40
2:D:193:ALA:HB3	2:D:194:LEU:HD12	2.03	0.40
1:G:107:ARG:HD3	2:H:111:PHE:CB	2.52	0.40
1:C:110:LYS:O	1:C:111:LEU:O	2.40	0.40
2:F:128:LEU:HD23	2:F:228:LEU:HD11	2.04	0.40
1:C:53:LEU:HG	1:C:54:MET:HG3	2.02	0.40
2:F:80:ARG:NH2	2:F:84:LYS:HG3	2.35	0.40
1:E:31:GLN:HB2	1:E:31:GLN:HE21	1.54	0.40
1:A:189:SER:OG	1:A:190:ASN:N	2.54	0.40
1:C:80:THR:HB	1:C:90:LEU:HB3	2.04	0.40
1:A:48:LYS:HB2	1:A:49:GLU:H	1.72	0.40
2:H:91:LEU:HD23	2:H:91:LEU:N	2.36	0.40
1:A:7:ASP:HA	1:A:8:PRO:HD3	1.78	0.40
2:H:214:ASN:HA	2:H:215:PRO:HD3	1.79	0.40
1:A:168:THR:HG23	1:A:186:VAL:O	2.21	0.40
1:E:205:ILE:N	1:E:205:ILE:HD12	2.36	0.40
1:A:133:TYR:CD2	2:B:145:GLU:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	195/203 (96%)	157 (80%)	26 (13%)	12 (6%)	2	5
1	C	198/203 (98%)	163 (82%)	22 (11%)	13 (7%)	1	4
1	E	195/203 (96%)	150 (77%)	31 (16%)	14 (7%)	1	3
1	G	195/203 (96%)	150 (77%)	32 (16%)	13 (7%)	1	4
2	B	239/244 (98%)	206 (86%)	20 (8%)	13 (5%)	2	7
2	D	239/244 (98%)	191 (80%)	34 (14%)	14 (6%)	2	6
2	F	239/244 (98%)	198 (83%)	31 (13%)	10 (4%)	3	13
2	H	239/244 (98%)	187 (78%)	40 (17%)	12 (5%)	3	9
All	All	1739/1788 (97%)	1402 (81%)	236 (14%)	101 (6%)	2	6

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	8	PRO
1	A	144	SER
2	B	59	GLU
2	B	67	ALA
2	B	70	GLU
2	B	97	SER
1	C	8	PRO
1	C	111	LEU
1	C	159	GLN
2	D	67	ALA
2	D	70	GLU
2	D	84	LYS
2	D	97	SER
1	E	138	SER
1	E	191	LYS
2	F	67	ALA
2	F	70	GLU
2	F	97	SER
1	G	8	PRO
1	G	213	SER
2	H	59	GLU
2	H	67	ALA
2	H	70	GLU

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Mol	Chain	Res	Type
2	H	97	SER
1	A	107	ARG
1	A	191	LYS
2	B	75	GLY
2	B	84	LYS
2	B	148	HIS
1	C	3[A]	GLU
1	C	3[B]	GLU
1	C	179	ASP
2	D	98	GLN
2	D	148	HIS
1	E	8	PRO
1	E	30	SER
1	E	94	SER
1	E	139	LYS
1	E	150	ASP
1	E	151	PHE
2	F	75	GLY
2	F	98	GLN
1	G	3	GLU
1	G	9	GLY
1	G	138	SER
1	G	143	LYS
1	G	144	SER
1	G	184	SER
2	H	75	GLY
2	H	99	THR
2	H	110	ASN
2	H	148	HIS
1	A	100	ALA
1	A	138	SER
2	B	58	GLY
2	B	110	ASN
1	C	66	ASN
1	C	78	ARG
1	C	144	SER
1	C	191	LYS
2	D	108	GLN
2	D	137	ALA
1	E	126	GLN
1	E	199	ALA
2	F	48	MET

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Mol	Chain	Res	Type
2	F	243	THR
1	G	208	ASP
2	H	68	LYS
1	C	143	LYS
1	C	204	ILE
2	D	109	GLY
1	E	179	ASP
2	F	74	ASP
2	F	148	HIS
1	G	68	GLU
1	G	191	LYS
1	G	199	ALA
2	H	182	CYS
1	A	143	LYS
2	B	95	ALA
2	B	112	ASP
2	D	71	VAL
2	D	74	ASP
2	D	238	ARG
1	E	60	GLY
1	E	78	ARG
1	G	111	LEU
2	H	58	GLY
1	A	111	LEU
2	D	60	GLY
2	F	240	LYS
1	A	7	ASP
1	A	213	SER
2	B	71	VAL
2	D	49	GLY
2	H	109	GLY
2	B	60	GLY
1	E	213	SER
1	A	70	GLY
1	C	70	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	177/183 (97%)	157 (89%)	20 (11%)	7	22
1	C	180/183 (98%)	163 (91%)	17 (9%)	11	32
1	E	177/183 (97%)	159 (90%)	18 (10%)	9	27
1	G	177/183 (97%)	164 (93%)	13 (7%)	17	45
2	B	205/208 (99%)	174 (85%)	31 (15%)	3	11
2	D	205/208 (99%)	185 (90%)	20 (10%)	10	30
2	F	205/208 (99%)	187 (91%)	18 (9%)	12	35
2	H	205/208 (99%)	184 (90%)	21 (10%)	9	27
All	All	1531/1564 (98%)	1373 (90%)	158 (10%)	9	26

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	3	GLU
1	A	13	VAL
1	A	19	VAL
1	A	24	THR
1	A	27	ASN
1	A	45	ASP
1	A	68	GLU
1	A	69	ASP
1	A	86	TYR
1	A	92	ARG
1	A	97	SER
1	A	111	LEU
1	A	126	GLN
1	A	161	LYS
1	A	168	THR
1	A	173	LEU
1	A	194	PHE
1	A	205	ILE
1	A	213	SER
2	B	8	THR
2	B	21	THR
2	B	23	LEU
2	B	26	GLN
2	B	40	TYR

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Mol	Chain	Res	Type
2	B	45	ASP
2	B	55	TYR
2	B	59	GLU
2	B	77	ASN
2	B	78	VAL
2	B	79	SER
2	B	91	LEU
2	B	99	THR
2	B	110	ASN
2	B	114	GLN
2	B	126	GLU
2	B	128	LEU
2	B	142	SER
2	B	150	GLN
2	B	157	LEU
2	B	165	HIS
2	B	181	VAL
2	B	198	ARG
2	B	204	ARG
2	B	206	ARG
2	B	207	VAL
2	B	213	GLN
2	B	230	GLU
2	B	232	ASP
2	B	238	ARG
2	B	244	GLN
1	C	2	LYS
1	C	3[A]	GLU
1	C	3[B]	GLU
1	C	18	THR
1	C	27	ASN
1	C	28	SER
1	C	31	GLN
1	C	54	MET
1	C	69	ASP
1	C	92	ARG
1	C	101	THR
1	C	117	THR
1	C	161	LYS
1	C	178	MET
1	C	191	LYS
1	C	194	PHE

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Mol	Chain	Res	Type
1	C	210	PHE
2	D	20	MET
2	D	21	THR
2	D	23	LEU
2	D	26	GLN
2	D	27	ASP
2	D	70	GLU
2	D	77	ASN
2	D	78	VAL
2	D	83	LYS
2	D	91	LEU
2	D	104	CYS
2	D	108	GLN
2	D	110	ASN
2	D	126	GLU
2	D	128	LEU
2	D	181	VAL
2	D	182	CYS
2	D	194	LEU
2	D	230	GLU
2	D	238	ARG
1	E	31	GLN
1	E	47	ARG
1	E	54	MET
1	E	69	ASP
1	E	92	ARG
1	E	107	ARG
1	E	111	LEU
1	E	117	THR
1	E	119	LEU
1	E	156	ASN
1	E	161	LYS
1	E	164	ASP
1	E	170	LYS
1	E	194	PHE
1	E	201	ASN
1	E	205	ILE
1	E	210	PHE
1	E	212	PRO
2	F	21	THR
2	F	26	GLN
2	F	27	ASP

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Mol	Chain	Res	Type
2	F	31	GLU
2	F	70	GLU
2	F	79	SER
2	F	91	LEU
2	F	99	THR
2	F	104	CYS
2	F	110	ASN
2	F	126	GLU
2	F	130	ASN
2	F	150	GLN
2	F	159	THR
2	F	165	HIS
2	F	228	LEU
2	F	230	GLU
2	F	238	ARG
1	G	18	THR
1	G	24	THR
1	G	31	GLN
1	G	48	LYS
1	G	92	ARG
1	G	107	ARG
1	G	117	THR
1	G	136	ARG
1	G	154	GLN
1	G	159	GLN
1	G	161	LYS
1	G	164	ASP
1	G	194	PHE
2	H	6	THR
2	H	8	THR
2	H	26	GLN
2	H	40	TYR
2	H	48	MET
2	H	59	GLU
2	H	70	GLU
2	H	78	VAL
2	H	81	LEU
2	H	91	LEU
2	H	99	THR
2	H	104	CYS
2	H	108	GLN
2	H	126	GLU

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Mol	Chain	Res	Type
2	H	150	GLN
2	H	157	LEU
2	H	198	ARG
2	H	204	ARG
2	H	213	GLN
2	H	237	ASP
2	H	238	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	82	GLN
1	A	85	GLN
2	B	77	ASN
2	B	98	GLN
2	B	110	ASN
2	B	148	HIS
2	B	165	HIS
2	B	224	GLN
2	B	231	ASN
2	B	236	GLN
2	B	244	GLN
1	C	27	ASN
1	C	31	GLN
1	C	66	ASN
1	C	82	GLN
1	C	85	GLN
1	C	127	ASN
1	C	190	ASN
1	C	201	ASN
2	D	26	GLN
2	D	44	GLN
2	D	77	ASN
2	D	98	GLN
2	D	110	ASN
2	D	224	GLN
2	D	231	ASN
2	D	236	GLN
1	E	31	GLN
1	E	85	GLN
1	E	124	ASN

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Mol	Chain	Res	Type
2	F	26	GLN
2	F	44	GLN
2	F	98	GLN
2	F	114	GLN
2	F	224	GLN
1	G	6	GLN
1	G	134	GLN
1	G	154	GLN
1	G	201	ASN
2	H	18	GLN
2	H	26	GLN
2	H	54	HIS
2	H	77	ASN
2	H	98	GLN
2	H	108	GLN
2	H	114	GLN
2	H	148	HIS
2	H	178	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	197/203 (97%)	-0.49	0 100 100	18, 44, 101, 168	0
1	C	197/203 (97%)	-0.04	6 (3%) 54 47	17, 50, 147, 181	0
1	E	197/203 (97%)	-0.13	3 (1%) 76 74	15, 64, 133, 197	0
1	G	197/203 (97%)	-0.29	4 (2%) 68 64	24, 54, 127, 159	0
2	B	241/244 (98%)	-0.39	0 100 100	25, 48, 87, 119	2 (0%)
2	D	241/244 (98%)	-0.29	2 (0%) 87 86	27, 55, 108, 129	2 (0%)
2	F	241/244 (98%)	-0.16	4 (1%) 73 70	22, 61, 114, 186	2 (0%)
2	H	241/244 (98%)	-0.33	2 (0%) 87 86	26, 56, 100, 143	2 (0%)
All	All	1752/1788 (97%)	-0.27	21 (1%) 81 78	15, 54, 120, 197	8 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	193	ASP	6.9
1	G	141	SER	3.5
1	C	208	ASP	3.4
1	G	69	ASP	3.3
2	F	74	ASP	3.2
2	D	111	PHE	3.0
1	E	190	ASN	2.8
1	E	192	SER	2.8
1	C	213	SER	2.6
1	C	212	PRO	2.5
2	F	248	ALA	2.5
1	C	68	GLU	2.5
2	D	74	ASP	2.4
2	F	75	GLY	2.4
1	G	108	ALA	2.4
2	F	255	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	74	ASP	2.2
1	G	140	SER	2.2
1	C	60	GLY	2.1
1	C	214	PRO	2.1
2	H	75	GLY	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.