



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:54 PM GMT

PDB ID : 1R3H
Title : Crystal Structure of T10
Authors : Rudolph, M.G.; Wilson, I.A.
Deposited on : 2003-10-02
Resolution : 2.50 Å(reported)

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

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

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

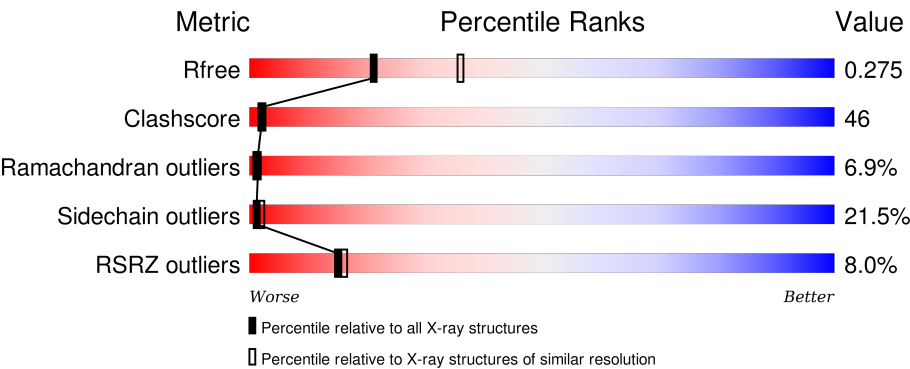
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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




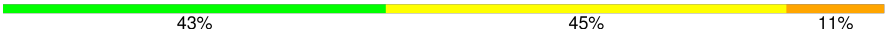

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	260	<div><div>10%</div><div>25%49%20%5%</div></div>
1	C	260	<div><div>15%</div><div>23%52%20%5%</div></div>
1	E	260	<div><div>9%</div><div>28%50%16%5%</div></div>
1	G	260	<div><div>7%</div><div>25%47%20%6%</div></div>
2	B	99	<div><div>%</div><div>38%49%12%</div></div>

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Mol	Chain	Length	Quality of chain
2	D	99	 3% 43% 49% 7%
2	F	99	 43% 45% 11%
2	H	99	 32% 51% 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11327 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 MHC H2-TL-T10-129.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			2019	1278	345	386	10			
1	C	248	Total	C	N	O	S	0	0	0
			2001	1263	344	384	10			
1	E	247	Total	C	N	O	S	0	0	0
			2005	1266	344	385	10			
1	G	245	Total	C	N	O	S	0	0	0
			1986	1256	341	379	10			

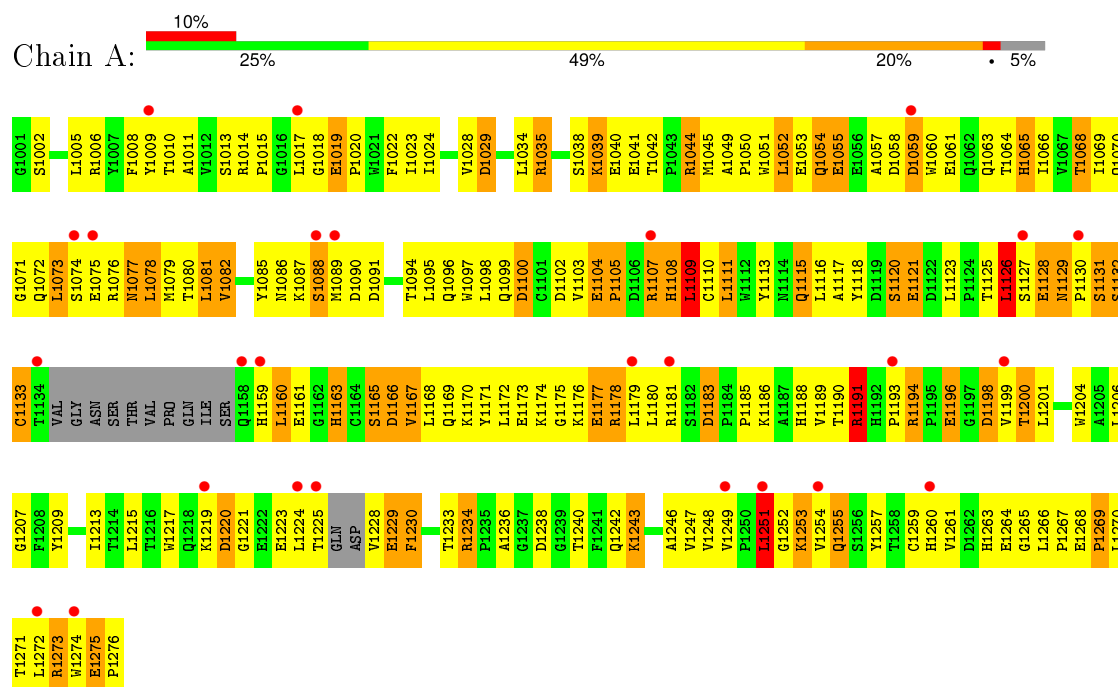
- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	D	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	F	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	H	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

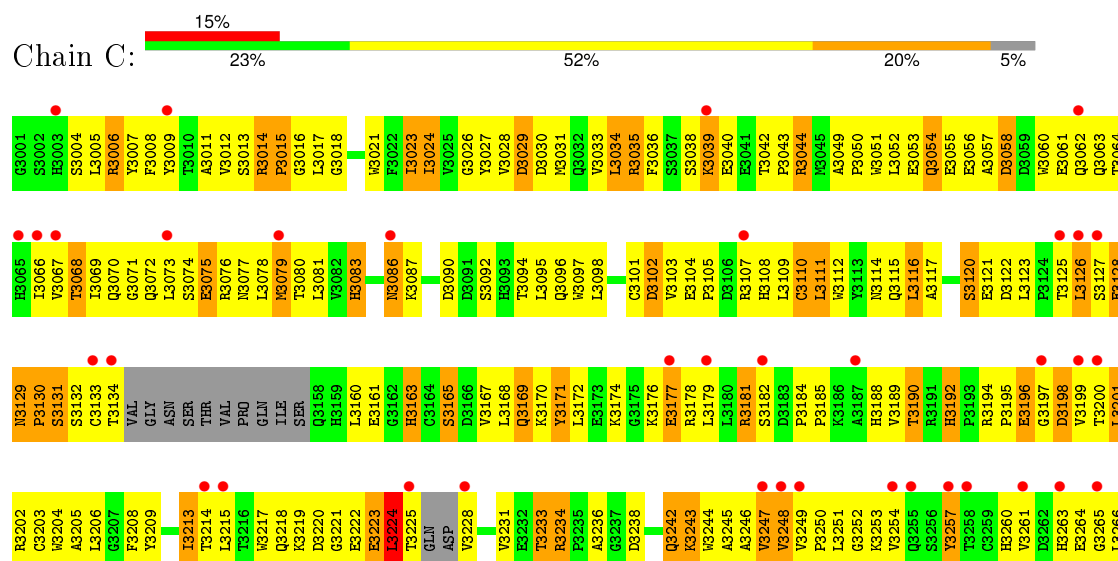
3 Residue-property plots

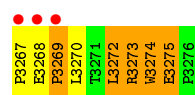
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: MHC H2-TL-T10-129

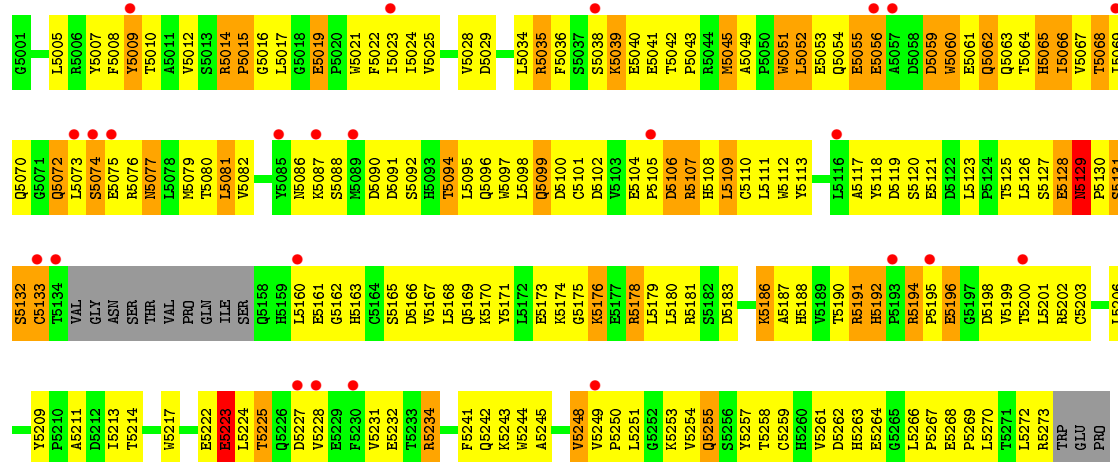


• Molecule 1: MHC H2-TL-T10-129

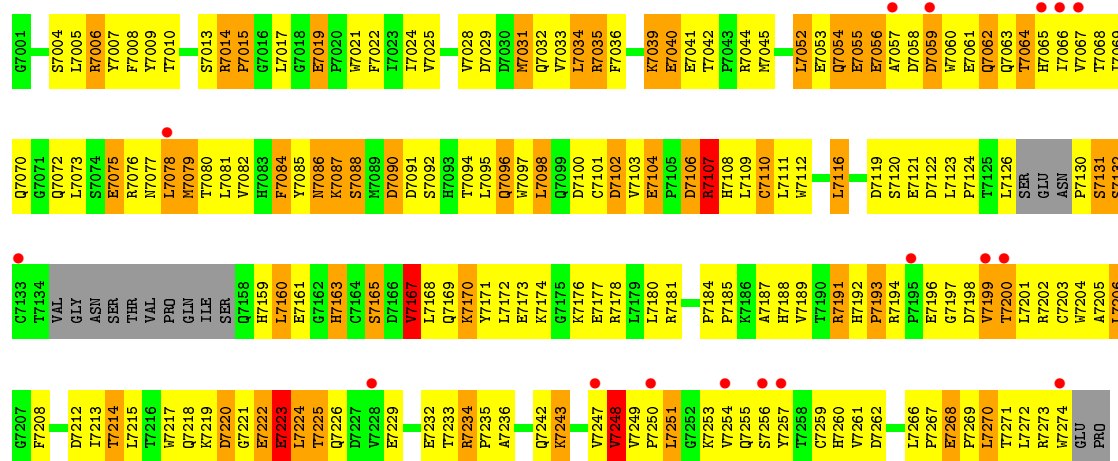




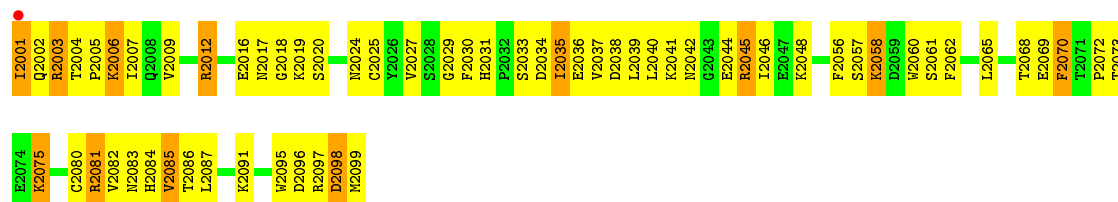
• Molecule 1: MHC H2-TL-T10-129



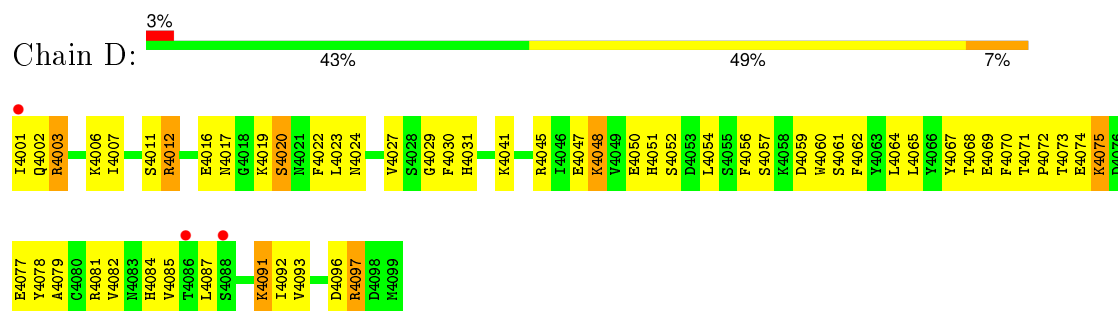
• Molecule 1: MHC H2-TL-T10-129



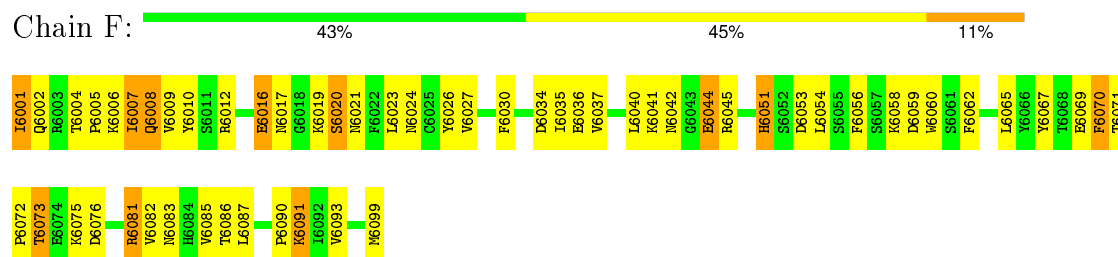
• Molecule 2: Beta-2-microglobulin



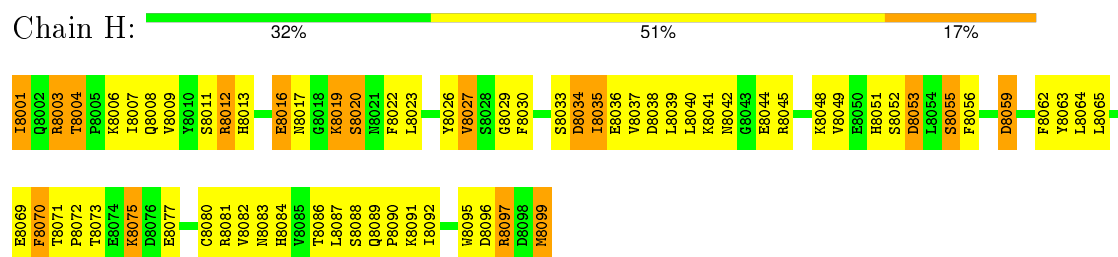
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.16Å 70.05Å 139.22Å 90.00° 106.79° 90.00°	Depositor
Resolution (Å)	46.00 – 2.50 45.10 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.5 (46.00-2.50) 90.2 (45.10-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.272 0.238 , 0.275	Depositor DCC
R_{free} test set	2191 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.2	EDS
Estimated twinning fraction	0.407 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 46904 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11327	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.20% 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	0.39	0/2078	0.68	1/2830 (0.0%)
1	C	0.38	0/2058	0.68	0/2803
1	E	0.37	0/2062	0.69	1/2809 (0.0%)
1	G	0.39	0/2043	0.71	0/2784
2	B	0.30	0/852	0.67	0/1152
2	D	0.31	0/852	0.63	0/1152
2	F	0.32	0/852	0.66	0/1152
2	H	0.32	0/852	0.67	0/1152
All	All	0.36	0/11649	0.68	2/15834 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1191	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	E	5009	TYR	CA-CB-CG	5.82	124.47	113.40

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	2019	0	1901	245	0
1	C	2001	0	1871	221	0
1	E	2005	0	1891	181	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1986	0	1866	177	0
2	B	829	0	791	61	0
2	D	829	0	791	41	0
2	F	829	0	791	55	0
2	H	829	0	791	76	0
All	All	11327	0	10693	1011	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 46.

All (1011) 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:C:3201:LEU:HD11	1:C:3254:VAL:HG13	1.27	1.10
2:F:6007:ILE:HD12	2:F:6027:VAL:HG22	1.18	1.09
1:A:1201:LEU:HD11	1:A:1254:VAL:HG13	1.35	1.06
1:C:3104:GLU:H	1:C:3109:LEU:HB3	1.26	1.01
1:C:3014:ARG:HH21	1:C:3018:GLY:HA3	1.26	1.00
1:E:5198:ASP:HA	1:E:5251:LEU:HB2	1.37	1.00
1:A:1185:PRO:HD2	1:A:1266:LEU:HD21	1.45	0.99
1:C:3201:LEU:CD1	1:C:3254:VAL:HG13	1.96	0.94
2:H:8083:ASN:HD21	2:H:8090:PRO:HG3	1.29	0.93
1:G:7189:VAL:HG23	1:G:7272:LEU:HD13	1.51	0.92
2:H:8020:SER:HA	2:H:8071:THR:HG22	1.51	0.92
2:B:2035:ILE:HD13	2:B:2084:HIS:HD2	1.34	0.90
2:B:2035:ILE:HD13	2:B:2084:HIS:CD2	2.07	0.90
1:A:1110:CYS:HB3	1:A:1133:CYS:H	1.38	0.89
1:C:3178:ARG:HA	1:C:3181:ARG:HD3	1.53	0.89
1:A:1170:LYS:HG3	1:A:1174:LYS:HE2	1.55	0.88
1:E:5261:VAL:HB	1:E:5270:LEU:HB3	1.53	0.88
1:G:7206:LEU:HD22	1:G:7242:GLN:HG2	1.53	0.88
1:C:3265:GLY:O	1:C:3267:PRO:HD3	1.73	0.88
2:H:8037:VAL:HG22	2:H:8082:VAL:HG13	1.55	0.87
1:A:1014:ARG:HH21	1:A:1018:GLY:HA3	1.37	0.87
1:E:5194:ARG:HD3	1:E:5196:GLU:OE2	1.76	0.86
2:B:2035:ILE:HD12	2:B:2083:ASN:O	1.74	0.86
1:E:5061:GLU:HA	1:E:5064:THR:HG22	1.57	0.85
1:E:5066:ILE:O	1:E:5070:GLN:HG3	1.77	0.85
1:G:7170:LYS:HE3	1:G:7170:LYS:HA	1.59	0.85
1:E:5225:THR:O	1:E:5228:VAL:HG12	1.76	0.84
1:A:1095:LEU:HD21	1:A:1116:LEU:HD23	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1103:VAL:HG11	1:A:1165:SER:HB3	1.60	0.84
1:G:7078:LEU:O	1:G:7082:VAL:HG23	1.77	0.83
1:A:1199:VAL:HG23	1:A:1251:LEU:HB2	1.59	0.83
2:F:6007:ILE:HG13	2:F:6082:VAL:HG21	1.61	0.83
1:G:7249:VAL:HG21	1:G:7254:VAL:HG22	1.61	0.83
1:A:1249:VAL:HG11	1:A:1254:VAL:HG22	1.60	0.83
2:H:8081:ARG:HB2	2:H:8092:ILE:HD13	1.60	0.83
1:A:1120:SER:HB2	2:B:2031:HIS:CE1	2.14	0.82
1:E:5199:VAL:HG23	1:E:5251:LEU:HA	1.62	0.82
1:E:5127:SER:O	1:E:5128:GLU:HG2	1.79	0.81
1:A:1249:VAL:CG1	1:A:1254:VAL:HG22	2.09	0.81
1:A:1108:HIS:O	1:A:1109:LEU:HD13	1.80	0.81
1:A:1228:VAL:HG13	1:A:1228:VAL:O	1.80	0.80
1:G:7060:TRP:O	1:G:7064:THR:HG23	1.81	0.80
1:A:1059:ASP:H	1:A:1170:LYS:HZ3	1.27	0.80
1:G:7076:ARG:O	1:G:7080:THR:HG23	1.80	0.80
2:H:8006:LYS:HE2	2:H:8029:GLY:HA3	1.63	0.79
1:C:3063:GLN:O	1:C:3067:VAL:HG23	1.82	0.79
1:A:1118:TYR:O	1:A:1121:GLU:HG3	1.83	0.79
1:A:1263:HIS:CD2	1:A:1265:GLY:H	2.01	0.79
1:A:1128:GLU:HG2	1:A:1129:ASN:H	1.48	0.79
1:C:3202:ARG:HG3	1:C:3246:ALA:HB2	1.63	0.78
1:C:3076:ARG:O	1:C:3080:THR:HG23	1.83	0.78
1:A:1005:LEU:HB2	1:A:1168:LEU:HD13	1.64	0.78
1:C:3036:PHE:HA	1:C:3040:GLU:OE1	1.83	0.78
1:E:5007:TYR:O	1:E:5098:LEU:HD12	1.84	0.77
1:A:1201:LEU:HD12	1:A:1249:VAL:HG21	1.67	0.77
1:E:5061:GLU:O	1:E:5065:HIS:HB2	1.83	0.77
1:C:3201:LEU:HG	1:C:3249:VAL:HB	1.67	0.77
1:A:1194:ARG:NH1	1:A:1196:GLU:OE2	2.17	0.77
1:C:3201:LEU:HD11	1:C:3254:VAL:CG1	2.14	0.77
1:G:7119:ASP:O	1:G:7120:SER:OG	2.02	0.77
1:C:3050:PRO:HA	1:C:3054:GLN:NE2	2.00	0.76
1:A:1194:ARG:HB2	1:A:1194:ARG:HH11	1.50	0.76
1:C:3160:LEU:HD12	1:C:3163:HIS:ND1	2.01	0.76
1:E:5095:LEU:HD12	1:E:5117:ALA:O	1.85	0.76
2:H:8007:ILE:CD1	2:H:8082:VAL:HG21	2.15	0.76
1:A:1129:ASN:HB3	1:A:1130:PRO:HD3	1.69	0.75
1:E:5183:ASP:HB2	1:E:5209:TYR:HB3	1.67	0.75
1:C:3246:ALA:O	1:C:3247:VAL:HG13	1.86	0.75
1:C:3051:TRP:CD2	1:C:3178:ARG:HD2	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3023:ILE:HD13	1:C:3023:ILE:O	1.85	0.75
2:B:2037:VAL:HG22	2:B:2082:VAL:HG13	1.67	0.75
1:C:3205:ALA:O	1:C:3206:LEU:HD23	1.86	0.75
1:E:5052:LEU:HD22	1:E:5174:LYS:HB2	1.69	0.75
2:B:2002:GLN:HE21	2:B:2086:THR:HG22	1.51	0.75
1:A:1015:PRO:O	1:A:1017:LEU:HG	1.87	0.74
1:C:3110:CYS:HB3	1:C:3133:CYS:O	1.87	0.74
1:E:5186:LYS:HG2	1:E:5206:LEU:O	1.88	0.74
1:E:5079:MET:O	1:E:5082:VAL:HG12	1.88	0.74
2:D:4020:SER:HA	2:D:4071:THR:HG22	1.70	0.73
1:A:1233:THR:HG22	1:A:1243:LYS:HD2	1.69	0.73
1:A:1069:ILE:O	1:A:1073:LEU:HD21	1.87	0.73
1:A:1055:GLU:HA	1:A:1058:ASP:HB2	1.69	0.73
1:C:3007:TYR:O	1:C:3098:LEU:HD12	1.88	0.73
1:E:5051:TRP:CE3	1:E:5178:ARG:HG3	2.23	0.73
1:G:7063:GLN:O	1:G:7067:VAL:HG23	1.87	0.73
1:G:7062:GLN:O	1:G:7066:ILE:HG12	1.87	0.73
2:F:6007:ILE:HD12	2:F:6027:VAL:CG2	2.11	0.73
1:C:3189:VAL:HG13	1:C:3202:ARG:O	1.89	0.73
1:A:1194:ARG:HH12	1:A:1198:ASP:HB2	1.53	0.73
1:C:3192:HIS:HB2	1:C:3200:THR:HB	1.70	0.73
1:E:5065:HIS:O	1:E:5069:ILE:HG12	1.88	0.73
2:H:8016:GLU:O	2:H:8019:LYS:HB2	1.88	0.73
2:D:4023:LEU:HB3	2:D:4068:THR:HG22	1.71	0.73
1:G:7194:ARG:HE	1:G:7196:GLU:HB2	1.52	0.72
1:A:1009:TYR:HE1	1:A:1071:GLY:HA2	1.53	0.72
1:E:5102:ASP:HB2	1:E:5111:LEU:HB2	1.70	0.72
1:E:5201:LEU:HD21	1:E:5254:VAL:HG21	1.70	0.72
1:G:7077:ASN:O	1:G:7081:LEU:HD13	1.90	0.72
1:A:1103:VAL:HG12	1:A:1104:GLU:H	1.54	0.72
1:C:3249:VAL:HG11	1:C:3254:VAL:HA	1.72	0.72
1:A:1274:TRP:O	1:A:1275:GLU:HB2	1.89	0.72
1:A:1017:LEU:HD22	2:H:8070:PHE:HA	1.72	0.72
1:G:7170:LYS:HA	1:G:7170:LYS:CE	2.16	0.72
1:G:7197:GLY:O	1:G:7251:LEU:HD21	1.90	0.72
1:C:3111:LEU:HD13	1:C:3130:PRO:HB3	1.70	0.71
1:C:3104:GLU:HB3	1:C:3109:LEU:HB2	1.71	0.71
1:C:3069:ILE:O	1:C:3073:LEU:HD12	1.90	0.71
1:E:5101:CYS:HA	1:E:5111:LEU:O	1.89	0.71
2:B:2073:THR:HG22	2:B:2075:LYS:H	1.54	0.71
2:D:4003:ARG:HG2	2:D:4029:GLY:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2001:ILE:HD12	2:B:2002:GLN:CG	2.21	0.71
1:G:7172:LEU:O	1:G:7176:LYS:HG2	1.91	0.71
1:E:5163:HIS:HA	1:E:5166:ASP:OD1	1.91	0.71
1:A:1120:SER:HB2	2:B:2031:HIS:NE2	2.06	0.71
1:E:5105:PRO:O	1:E:5106:ASP:OD1	2.09	0.70
1:E:5068:THR:O	1:E:5072:GLN:NE2	2.20	0.70
1:C:3213:ILE:HD11	1:C:3261:VAL:HG13	1.73	0.70
1:C:3062:GLN:O	1:C:3066:ILE:HG12	1.91	0.70
1:G:7101:CYS:HA	1:G:7111:LEU:O	1.90	0.70
1:A:1215:LEU:HD21	1:A:1261:VAL:HG22	1.74	0.70
1:G:7223:GLU:O	1:G:7224:LEU:HG	1.91	0.70
1:G:7109:LEU:HD11	1:G:7111:LEU:HD11	1.72	0.70
1:C:3224:LEU:O	1:C:3228:VAL:HG23	1.92	0.70
2:B:2001:ILE:HD12	2:B:2002:GLN:HG3	1.73	0.70
2:D:4001:ILE:HG23	2:D:4002:GLN:H	1.56	0.70
2:B:2041:LYS:O	2:B:2044:GLU:HG2	1.92	0.70
1:C:3133:CYS:O	1:C:3134:THR:HG23	1.92	0.69
2:H:8073:THR:OG1	2:H:8075:LYS:HD3	1.92	0.69
1:G:7102:ASP:HB2	1:G:7111:LEU:HD13	1.74	0.69
1:E:5217:TRP:O	1:E:5224:LEU:HB2	1.92	0.69
1:C:3073:LEU:HG	1:C:3076:ARG:NH1	2.07	0.69
1:A:1273:ARG:HH11	1:A:1273:ARG:HB2	1.58	0.69
1:G:7201:LEU:HB2	1:G:7247:VAL:HG22	1.75	0.69
1:E:5008:PHE:O	1:E:5024:ILE:HG23	1.92	0.69
2:F:6083:ASN:ND2	2:F:6090:PRO:HG3	2.07	0.69
1:A:1051:TRP:CE3	1:A:1178:ARG:HG3	2.28	0.69
2:F:6099:MET:OXT	2:F:6099:MET:HG3	1.92	0.69
1:A:1193:PRO:N	1:A:1199:VAL:HG13	2.08	0.69
1:G:7176:LYS:HE2	1:G:7180:LEU:HG	1.74	0.68
2:F:6020:SER:HA	2:F:6071:THR:HG22	1.74	0.68
1:G:7249:VAL:CG2	1:G:7254:VAL:HG22	2.22	0.68
1:G:7119:ASP:HB3	2:H:8001:ILE:HD13	1.74	0.68
1:C:3024:ILE:HD12	1:C:3067:VAL:CG1	2.24	0.68
1:A:1111:LEU:HA	1:A:1132:SER:HA	1.76	0.68
1:A:1230:PHE:HD1	1:A:1230:PHE:C	1.97	0.68
1:C:3021:TRP:HB2	1:C:3038:SER:OG	1.93	0.68
1:A:1201:LEU:CD1	1:A:1254:VAL:HG13	2.18	0.68
1:G:7053:GLU:CD	1:G:7174:LYS:HD3	2.14	0.67
1:A:1009:TYR:OH	1:A:1074:SER:HB3	1.95	0.67
1:E:5228:VAL:HG13	1:E:5228:VAL:O	1.94	0.67
1:E:5111:LEU:HD23	1:E:5113:TYR:OH	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3213:ILE:HD13	1:C:3214:THR:C	2.15	0.67
1:A:1034:LEU:HD12	1:A:1045:MET:CE	2.25	0.66
1:C:3069:ILE:HD13	1:C:3072:GLN:OE1	1.96	0.66
1:A:1260:HIS:HA	1:A:1270:LEU:O	1.95	0.66
1:C:3075:GLU:O	1:C:3079:MET:HB2	1.96	0.66
1:G:7185:PRO:HB3	1:G:7208:PHE:HD2	1.60	0.66
2:B:2098:ASP:O	2:B:2099:MET:HG3	1.95	0.66
2:D:4007:ILE:HD12	2:D:4027:VAL:HG12	1.77	0.66
1:A:1188:HIS:HE1	1:A:1206:LEU:HD11	1.61	0.66
2:D:4017:ASN:ND2	2:D:4074:GLU:HG2	2.11	0.66
2:H:8016:GLU:HG2	2:H:8019:LYS:HD2	1.77	0.66
1:A:1110:CYS:HB3	1:A:1133:CYS:N	2.10	0.66
1:A:1060:TRP:CH2	1:A:1170:LYS:HG2	2.30	0.66
2:D:4007:ILE:CD1	2:D:4082:VAL:HG21	2.26	0.66
1:E:5113:TYR:HA	1:E:5129:ASN:O	1.96	0.66
1:A:1254:VAL:O	1:A:1254:VAL:HG12	1.96	0.65
1:A:1059:ASP:H	1:A:1170:LYS:NZ	1.95	0.65
1:C:3185:PRO:HA	1:C:3206:LEU:O	1.97	0.65
2:D:4003:ARG:HB3	2:D:4030:PHE:HA	1.79	0.65
1:C:3189:VAL:HG12	1:C:3274:TRP:HD1	1.59	0.65
1:A:1052:LEU:HB2	1:A:1054:GLN:HE22	1.62	0.65
1:C:3213:ILE:HD13	1:C:3214:THR:N	2.12	0.65
2:F:6073:THR:HG22	2:F:6075:LYS:H	1.61	0.65
1:E:5201:LEU:HD11	1:E:5254:VAL:CG2	2.27	0.65
1:A:1073:LEU:O	1:A:1077:ASN:HB2	1.96	0.65
1:E:5059:ASP:OD1	1:E:5061:GLU:HG3	1.97	0.65
1:A:1263:HIS:H	1:A:1266:LEU:HD12	1.62	0.64
1:A:1052:LEU:HB2	1:A:1054:GLN:NE2	2.12	0.64
1:G:7185:PRO:HB3	1:G:7208:PHE:CD2	2.32	0.64
1:C:3028:VAL:HG11	1:C:3179:LEU:HD13	1.79	0.64
1:G:7215:LEU:HD12	1:G:7261:VAL:HG22	1.78	0.64
1:E:5063:GLN:NE2	1:E:5171:TYR:OH	2.29	0.64
1:A:1230:PHE:C	1:A:1230:PHE:CD1	2.69	0.64
1:A:1013:SER:HA	1:A:1020:PRO:HB3	1.79	0.64
2:B:2046:ILE:HD13	1:G:7017:LEU:HD21	1.77	0.64
1:G:7194:ARG:HH21	1:G:7196:GLU:HB3	1.61	0.64
2:D:4084:HIS:O	2:D:4087:LEU:HB2	1.98	0.64
1:A:1194:ARG:HH21	1:A:1248:VAL:HB	1.63	0.64
1:G:7192:HIS:O	1:G:7200:THR:HG23	1.96	0.64
1:A:1191:ARG:HG3	1:A:1274:TRP:HE1	1.63	0.64
1:A:1049:ALA:O	1:A:1054:GLN:NE2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7069:ILE:HD13	1:G:7072:GLN:NE2	2.13	0.64
1:C:3035:ARG:O	1:C:3043:PRO:HA	1.98	0.64
1:A:1191:ARG:HD3	1:A:1274:TRP:CE2	2.33	0.63
2:H:8081:ARG:HB2	2:H:8092:ILE:CD1	2.28	0.63
2:D:4079:ALA:HB1	2:D:4093:VAL:O	1.97	0.63
1:E:5009:TYR:HB3	1:E:5097:TRP:HB3	1.81	0.63
1:A:1252:GLY:HA3	1:A:1253:LYS:HE2	1.80	0.63
1:E:5118:TYR:O	1:E:5121:GLU:HG3	1.98	0.63
1:E:5015:PRO:HD3	1:E:5092:SER:HB2	1.81	0.63
1:C:3247:VAL:O	1:C:3248:VAL:HG13	1.99	0.63
1:E:5131:SER:OG	1:E:5132:SER:N	2.30	0.63
2:B:2027:VAL:HG21	2:B:2037:VAL:HG21	1.80	0.63
2:F:6087:LEU:HD13	2:F:6091:LYS:HG2	1.80	0.63
1:G:7249:VAL:HB	1:G:7253:LYS:O	1.98	0.63
2:F:6024:ASN:HB3	2:F:6065:LEU:HD11	1.80	0.63
1:A:1008:PHE:O	1:A:1024:ILE:HG23	1.99	0.63
1:G:7096:GLN:HE21	1:G:7096:GLN:H	1.47	0.63
1:A:1199:VAL:CG2	1:A:1251:LEU:HB2	2.28	0.62
1:A:1191:ARG:NH1	1:A:1199:VAL:HG11	2.14	0.62
1:A:1052:LEU:HD22	1:A:1174:LYS:HB2	1.80	0.62
1:A:1103:VAL:HG21	1:A:1165:SER:HB3	1.80	0.62
1:C:3104:GLU:N	1:C:3109:LEU:HB3	2.07	0.62
1:C:3030:ASP:HB2	1:C:3209:TYR:CE1	2.35	0.62
1:A:1194:ARG:HG3	1:A:1198:ASP:O	2.00	0.62
1:C:3015:PRO:HD3	1:C:3092:SER:HB2	1.81	0.62
1:E:5249:VAL:HG22	1:E:5257:TYR:CZ	2.34	0.62
1:A:1193:PRO:HA	1:A:1199:VAL:HG22	1.82	0.62
1:A:1128:GLU:CG	1:A:1129:ASN:H	2.12	0.62
1:C:3112:TRP:HB3	1:C:3131:SER:HB3	1.82	0.62
2:H:8056:PHE:HA	2:H:8062:PHE:HA	1.82	0.62
1:C:3009:TYR:HB3	1:C:3097:TRP:HB3	1.82	0.61
1:C:3178:ARG:O	1:C:3181:ARG:HB3	2.00	0.61
2:D:4007:ILE:HD12	2:D:4082:VAL:HG21	1.83	0.61
1:C:3260:HIS:HA	1:C:3270:LEU:O	2.00	0.61
1:G:7201:LEU:HD11	1:G:7254:VAL:HG13	1.81	0.61
1:E:5213:ILE:HG13	1:E:5262:ASP:O	2.00	0.61
1:C:3233:THR:HA	1:C:3243:LYS:HB2	1.81	0.61
1:G:7028:VAL:HG23	1:G:7033:VAL:HG21	1.82	0.61
2:H:8007:ILE:HD11	2:H:8082:VAL:HG21	1.82	0.61
1:A:1066:ILE:HD13	1:A:1160:LEU:HB2	1.83	0.61
1:C:3112:TRP:O	1:C:3130:PRO:O	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:GLN:HG2	1:A:1169:GLN:O	2.00	0.61
2:F:6016:GLU:HB3	2:F:6019:LYS:HD3	1.82	0.61
1:G:7068:THR:O	1:G:7072:GLN:HG3	2.00	0.61
1:G:7201:LEU:HB2	1:G:7247:VAL:CG2	2.31	0.61
1:E:5082:VAL:HG23	1:E:5118:TYR:OH	2.01	0.61
1:A:1263:HIS:N	1:A:1266:LEU:HD12	2.16	0.61
1:A:1010:THR:O	1:A:1022:PHE:HA	2.01	0.61
1:G:7189:VAL:HG12	1:G:7274:TRP:HD1	1.64	0.60
1:C:3095:LEU:HG	1:C:3116:LEU:HD21	1.83	0.60
2:H:8075:LYS:HB2	2:H:8075:LYS:NZ	2.16	0.60
2:D:4073:THR:OG1	2:D:4075:LYS:HD3	2.01	0.60
2:F:6037:VAL:HG22	2:F:6082:VAL:HG13	1.83	0.60
1:A:1273:ARG:O	1:A:1274:TRP:HB3	2.02	0.60
1:C:3215:LEU:HD12	1:C:3261:VAL:HG22	1.82	0.60
2:H:8083:ASN:HD21	2:H:8090:PRO:CG	2.08	0.60
2:B:2095:TRP:CH2	2:B:2097:ARG:HG2	2.36	0.60
1:C:3250:PRO:HB2	1:C:3253:LYS:CG	2.31	0.60
2:D:4006:LYS:NZ	2:D:4029:GLY:HA3	2.16	0.60
1:A:1040:GLU:HG3	1:A:1042:THR:H	1.67	0.60
1:C:3112:TRP:CE2	1:C:3161:GLU:HB2	2.37	0.60
1:E:5062:GLN:O	1:E:5066:ILE:HG13	2.01	0.60
1:A:1236:ALA:O	2:B:2012:ARG:HD2	2.01	0.60
1:C:3014:ARG:NH2	1:C:3017:LEU:HD12	2.17	0.60
1:C:3263:HIS:O	1:C:3266:LEU:HB2	2.02	0.60
1:A:1255:GLN:NE2	1:A:1255:GLN:HA	2.17	0.60
1:E:5034:LEU:HD23	1:E:5035:ARG:N	2.17	0.60
1:E:5249:VAL:HG22	1:E:5257:TYR:CE2	2.37	0.59
1:A:1052:LEU:HD23	1:A:1175:GLY:HA3	1.84	0.59
1:A:1252:GLY:CA	1:A:1253:LYS:HE2	2.31	0.59
1:A:1028:VAL:O	1:A:1028:VAL:HG12	2.01	0.59
1:E:5070:GLN:OE1	1:E:5160:LEU:HD13	2.03	0.59
1:A:1105:PRO:O	1:A:1108:HIS:N	2.34	0.59
1:E:5176:LYS:O	1:E:5180:LEU:HB2	2.01	0.59
1:G:7247:VAL:O	1:G:7248:VAL:HG13	2.02	0.59
1:C:3030:ASP:HB2	1:C:3209:TYR:HE1	1.67	0.59
1:C:3168:LEU:HG	1:C:3169:GLN:NE2	2.18	0.59
1:C:3201:LEU:HD12	1:C:3249:VAL:HG21	1.83	0.59
1:G:7170:LYS:O	1:G:7174:LYS:HB2	2.03	0.59
1:G:7103:VAL:HG23	1:G:7168:LEU:HD23	1.83	0.59
1:G:7194:ARG:NE	1:G:7196:GLU:HB2	2.17	0.59
1:A:1170:LYS:CG	1:A:1174:LYS:HE2	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5024:ILE:CD1	1:E:5067:VAL:HG13	2.33	0.59
1:E:5024:ILE:HD12	1:E:5067:VAL:HG13	1.83	0.59
1:A:1103:VAL:HG21	1:A:1165:SER:HA	1.84	0.59
1:C:3034:LEU:HD12	1:C:3043:PRO:HB2	1.83	0.59
1:C:3215:LEU:HD23	1:C:3245:ALA:CB	2.33	0.59
1:A:1066:ILE:O	1:A:1070:GLN:HB3	2.02	0.59
1:G:7024:ILE:HG21	1:G:7067:VAL:HG13	1.84	0.59
1:G:7202:ARG:NH1	2:H:8099:MET:HG3	2.17	0.59
1:C:3228:VAL:N	1:C:3247:VAL:HG12	2.17	0.59
1:G:7075:GLU:O	1:G:7079:MET:HB2	2.02	0.59
1:C:3051:TRP:CG	1:C:3178:ARG:HD2	2.38	0.58
2:H:8019:LYS:O	2:H:8072:PRO:HD2	2.03	0.58
1:A:1126:LEU:N	1:A:1126:LEU:HD13	2.17	0.58
1:E:5258:THR:HA	1:E:5273:ARG:HA	1.84	0.58
2:F:6005:PRO:HB2	2:F:6007:ILE:HD11	1.86	0.58
2:F:6036:GLU:HG2	2:F:6081:ARG:NH2	2.18	0.58
1:E:5224:LEU:O	1:E:5228:VAL:HB	2.03	0.58
2:F:6007:ILE:N	2:F:6007:ILE:HD13	2.18	0.58
1:C:3049:ALA:O	1:C:3052:LEU:HG	2.03	0.58
1:G:7214:THR:HB	1:G:7262:ASP:HB2	1.85	0.58
1:A:1183:ASP:HB2	1:A:1209:TYR:HB3	1.86	0.58
1:A:1049:ALA:HB1	1:A:1051:TRP:NE1	2.19	0.58
1:C:3028:VAL:O	1:C:3029:ASP:HB2	2.04	0.58
2:H:8040:LEU:HD23	2:H:8045:ARG:HA	1.85	0.58
1:A:1005:LEU:O	1:A:1005:LEU:HG	2.03	0.58
2:B:2095:TRP:CZ3	2:B:2097:ARG:HG2	2.38	0.58
2:B:2045:ARG:HG2	2:B:2045:ARG:O	2.04	0.58
1:C:3194:ARG:NH1	1:C:3198:ASP:HB3	2.19	0.58
1:C:3198:ASP:OD1	1:C:3250:PRO:HA	2.04	0.58
1:C:3073:LEU:CD2	1:C:3076:ARG:HH11	2.16	0.58
1:C:3263:HIS:HB3	1:C:3266:LEU:HD12	1.84	0.58
1:C:3120:SER:HB2	2:D:4003:ARG:HH22	1.69	0.58
1:A:1028:VAL:O	1:A:1029:ASP:HB2	2.03	0.58
1:A:1014:ARG:NH2	1:A:1019:GLU:H	2.01	0.57
1:E:5062:GLN:HA	1:E:5062:GLN:NE2	2.19	0.57
1:E:5010:THR:HG1	2:F:6062:PHE:HE2	1.52	0.57
2:F:6027:VAL:HG11	2:F:6035:ILE:CD1	2.34	0.57
1:G:7119:ASP:HB3	2:H:8001:ILE:CD1	2.34	0.57
1:A:1172:LEU:HA	1:A:1179:LEU:HD12	1.87	0.57
2:B:2017:ASN:HA	2:B:2072:PRO:O	2.02	0.57
1:C:3202:ARG:CG	1:C:3246:ALA:HB2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6007:ILE:HG13	2:F:6082:VAL:CG2	2.34	0.57
1:A:1191:ARG:HD2	1:A:1201:LEU:CD2	2.34	0.57
1:A:1049:ALA:HB1	1:A:1051:TRP:CE2	2.40	0.57
1:C:3215:LEU:HD23	1:C:3245:ALA:HB3	1.85	0.57
1:G:7102:ASP:O	1:G:7110:CYS:HA	2.03	0.57
1:E:5104:GLU:HB3	1:E:5109:LEU:HB3	1.85	0.57
1:A:1104:GLU:OE1	1:A:1107:ARG:HB2	2.05	0.57
1:E:5014:ARG:HD3	1:E:5021:TRP:HZ3	1.67	0.57
1:G:7015:PRO:HG2	1:G:7091:ASP:O	2.04	0.57
1:E:5107:ARG:HG2	1:E:5107:ARG:HH11	1.69	0.57
1:A:1185:PRO:HD2	1:A:1266:LEU:CD2	2.28	0.57
2:H:8003:ARG:HB3	2:H:8030:PHE:HA	1.86	0.57
1:G:7104:GLU:HG2	1:G:7104:GLU:O	2.05	0.57
1:C:3172:LEU:HD23	1:C:3179:LEU:HB3	1.86	0.57
1:E:5073:LEU:O	1:E:5077:ASN:HB2	2.04	0.56
2:F:6001:ILE:HD12	2:F:6002:GLN:HG3	1.87	0.56
1:C:3005:LEU:O	1:C:3006:ARG:HD3	2.05	0.56
1:E:5190:THR:CG2	1:E:5192:HIS:CE1	2.88	0.56
1:A:1065:HIS:O	1:A:1069:ILE:HG12	2.05	0.56
1:G:7009:TYR:HE1	1:G:7022:PHE:HB2	1.70	0.56
1:G:7080:THR:OG1	1:G:7081:LEU:HD12	2.05	0.56
1:C:3219:LYS:O	1:C:3220:ASP:HB2	2.04	0.56
1:G:7034:LEU:HG	1:G:7035:ARG:N	2.20	0.56
1:G:7103:VAL:HG12	1:G:7104:GLU:H	1.70	0.56
1:C:3075:GLU:HG3	1:C:3075:GLU:O	2.05	0.56
1:G:7204:TRP:CZ2	2:H:8099:MET:HA	2.40	0.56
1:E:5087:LYS:O	1:E:5088:SER:OG	2.22	0.56
2:H:8051:HIS:HA	2:H:8065:LEU:O	2.06	0.56
2:F:6027:VAL:HG12	2:F:6030:PHE:CD2	2.41	0.56
1:E:5010:THR:HG21	2:F:6054:LEU:CD2	2.36	0.56
1:A:1039:LYS:HE2	1:A:1039:LYS:O	2.06	0.56
1:C:3250:PRO:HB2	1:C:3253:LYS:HG3	1.86	0.56
1:G:7206:LEU:CD2	1:G:7242:GLN:HG2	2.33	0.56
1:A:1125:THR:C	1:A:1126:LEU:HD22	2.26	0.56
2:F:6001:ILE:O	2:F:6001:ILE:HD13	2.05	0.56
2:B:2087:LEU:HD13	2:B:2091:LYS:HG3	1.87	0.56
1:A:1061:GLU:O	1:A:1064:THR:HG22	2.06	0.56
1:C:3234:ARG:HH11	1:C:3242:GLN:HB3	1.70	0.56
1:A:1009:TYR:HD1	1:A:1024:ILE:HD11	1.71	0.56
1:G:7107:ARG:O	1:G:7108:HIS:HB2	2.06	0.56
2:B:2024:ASN:HB3	2:B:2065:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3024:ILE:HD12	1:C:3067:VAL:HG12	1.86	0.55
1:C:3125:THR:O	1:C:3127:SER:N	2.39	0.55
1:C:3172:LEU:O	1:C:3176:LYS:HG2	2.06	0.55
1:G:7039:LYS:HE3	1:G:7040:GLU:N	2.21	0.55
2:H:8027:VAL:HG23	2:H:8064:LEU:HB2	1.88	0.55
1:G:7081:LEU:HD22	1:G:7095:LEU:HD13	1.89	0.55
1:E:5035:ARG:NH2	1:E:5040:GLU:OE1	2.39	0.55
1:A:1242:GLN:O	1:A:1243:LYS:HB2	2.06	0.55
1:E:5258:THR:HB	1:E:5273:ARG:HG2	1.88	0.55
2:B:2056:PHE:HB3	2:B:2062:PHE:CD2	2.41	0.55
1:G:7167:VAL:HG12	1:G:7171:TYR:CE2	2.41	0.55
2:B:2001:ILE:O	2:B:2001:ILE:HD13	2.06	0.55
2:H:8022:PHE:CE2	2:H:8069:GLU:HG3	2.41	0.55
1:C:3014:ARG:HG3	1:C:3021:TRP:HZ3	1.70	0.55
1:C:3236:ALA:O	2:D:4024:ASN:ND2	2.40	0.55
1:C:3249:VAL:HG22	1:C:3257:TYR:CD2	2.41	0.55
2:B:2096:ASP:HB3	2:B:2099:MET:HB2	1.88	0.55
1:G:7202:ARG:HG2	1:G:7204:TRP:NE1	2.21	0.55
1:A:1002:SER:HB2	1:A:1103:VAL:O	2.06	0.55
1:G:7087:LYS:O	1:G:7088:SER:OG	2.17	0.55
1:G:7088:SER:HB3	1:G:7091:ASP:HB2	1.89	0.55
1:E:5199:VAL:CG2	1:E:5251:LEU:HA	2.35	0.55
1:G:7215:LEU:HB3	1:G:7243:LYS:NZ	2.22	0.55
1:C:3101:CYS:HA	1:C:3111:LEU:O	2.06	0.55
1:C:3129:ASN:HB2	1:C:3130:PRO:HD3	1.88	0.55
1:C:3203:CYS:HB2	1:C:3217:TRP:CZ2	2.41	0.55
1:A:1058:ASP:HA	1:A:1170:LYS:HZ1	1.72	0.55
1:C:3040:GLU:OE2	1:C:3044:ARG:NH2	2.39	0.55
1:E:5061:GLU:HA	1:E:5064:THR:CG2	2.34	0.55
2:B:2003:ARG:HD3	2:B:2031:HIS:HB3	1.88	0.55
1:A:1009:TYR:HB3	1:A:1097:TRP:O	2.07	0.55
1:G:7102:ASP:HB2	1:G:7111:LEU:CD1	2.37	0.55
2:F:6005:PRO:HB2	2:F:6007:ILE:CD1	2.36	0.55
2:B:2007:ILE:HD13	2:B:2082:VAL:CG2	2.37	0.55
1:A:1215:LEU:CD2	1:A:1261:VAL:HG22	2.36	0.55
1:E:5169:GLN:O	1:E:5169:GLN:HG2	2.08	0.55
1:A:1201:LEU:HD11	1:A:1254:VAL:CG1	2.24	0.54
1:G:7213:ILE:CG2	1:G:7243:LYS:HE2	2.37	0.54
1:C:3231:VAL:O	1:C:3243:LYS:HG3	2.06	0.54
1:E:5010:THR:HG21	2:F:6054:LEU:HD23	1.90	0.54
1:C:3222:GLU:HG3	1:C:3223:GLU:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1082:VAL:HG22	1:A:1089:MET:HG2	1.89	0.54
1:C:3272:LEU:HD12	1:C:3273:ARG:O	2.06	0.54
1:C:3242:GLN:O	1:C:3243:LYS:HB2	2.07	0.54
1:G:7200:THR:HA	1:G:7248:VAL:HA	1.88	0.54
1:G:7250:PRO:HD2	1:G:7253:LYS:HB2	1.89	0.54
1:G:7185:PRO:HA	1:G:7206:LEU:O	2.07	0.54
1:G:7215:LEU:CD1	1:G:7261:VAL:HG22	2.37	0.54
1:C:3128:GLU:HG2	1:C:3129:ASN:N	2.23	0.54
1:A:1053:GLU:HG3	1:A:1174:LYS:HA	1.89	0.54
1:C:3005:LEU:CD1	1:C:3028:VAL:HG22	2.38	0.54
1:G:7191:ARG:HH12	1:G:7193:PRO:HB3	1.73	0.54
1:E:5034:LEU:CD1	1:E:5063:GLN:NE2	2.71	0.54
1:C:3009:TYR:HB2	1:C:3070:GLN:NE2	2.23	0.54
1:G:7235:PRO:HG2	2:H:8065:LEU:HD13	1.89	0.54
1:G:7219:LYS:O	1:G:7221:GLY:N	2.41	0.54
1:A:1191:ARG:HD3	1:A:1274:TRP:NE1	2.23	0.54
1:C:3200:THR:HG22	1:C:3200:THR:O	2.07	0.54
2:F:6006:LYS:C	2:F:6007:ILE:HD13	2.27	0.54
1:A:1085:TYR:HB3	1:A:1087:LYS:NZ	2.23	0.54
2:F:6024:ASN:HD22	2:F:6067:TYR:HB3	1.72	0.54
1:G:7189:VAL:CG1	1:G:7274:TRP:HD1	2.21	0.54
1:A:1170:LYS:O	1:A:1174:LYS:HG2	2.07	0.54
1:A:1229:GLU:O	1:A:1230:PHE:HB3	2.08	0.54
1:A:1189:VAL:H	1:A:1275:GLU:HG3	1.72	0.53
1:C:3050:PRO:HA	1:C:3054:GLN:HE21	1.72	0.53
2:B:2025:CYS:HB2	2:B:2039:LEU:HD21	1.90	0.53
2:B:2016:GLU:HA	2:B:2016:GLU:OE2	2.09	0.53
1:A:1194:ARG:CB	1:A:1194:ARG:HH11	2.19	0.53
1:E:5254:VAL:O	1:E:5254:VAL:HG22	2.07	0.53
1:A:1111:LEU:HD23	1:A:1113:TYR:OH	2.08	0.53
1:A:1194:ARG:NH2	1:A:1248:VAL:HB	2.23	0.53
1:C:3028:VAL:HG11	1:C:3179:LEU:CD1	2.38	0.53
1:G:7249:VAL:HG12	1:G:7257:TYR:CE2	2.44	0.53
1:G:7109:LEU:O	1:G:7110:CYS:HB2	2.09	0.53
1:E:5249:VAL:HG11	1:E:5254:VAL:HG23	1.90	0.53
1:C:3051:TRP:CE3	1:C:3178:ARG:HD2	2.43	0.53
1:C:3189:VAL:HB	1:C:3274:TRP:HA	1.90	0.53
1:C:3081:LEU:HD22	1:C:3095:LEU:CD1	2.38	0.53
1:C:3128:GLU:HG2	1:C:3129:ASN:H	1.73	0.53
2:B:2087:LEU:HD13	2:B:2091:LYS:CG	2.38	0.53
1:C:3103:VAL:O	1:C:3105:PRO:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:8081:ARG:HA	2:H:8091:LYS:O	2.09	0.53
1:G:7010:THR:O	1:G:7022:PHE:HA	2.08	0.53
1:E:5038:SER:O	1:E:5039:LYS:HB3	2.08	0.53
2:F:6017:ASN:N	2:F:6017:ASN:HD22	2.06	0.53
2:H:8055:SER:HB3	2:H:8063:TYR:CE1	2.44	0.53
1:A:1189:VAL:HG12	1:A:1190:THR:H	1.74	0.53
1:G:7009:TYR:HD2	1:G:7097:TRP:HB3	1.73	0.53
1:G:7028:VAL:O	1:G:7029:ASP:HB2	2.08	0.53
1:A:1126:LEU:H	1:A:1126:LEU:HD13	1.72	0.53
1:C:3104:GLU:HB3	1:C:3109:LEU:CB	2.39	0.53
1:E:5181:ARG:HD2	1:E:5183:ASP:OD2	2.08	0.53
1:A:1213:ILE:HD11	1:A:1261:VAL:HG13	1.91	0.53
1:C:3079:MET:HE1	1:C:3083:HIS:HB2	1.91	0.52
1:G:7191:ARG:HD2	1:G:7274:TRP:CZ2	2.44	0.52
1:G:7123:LEU:HB3	1:G:7124:PRO:HD2	1.90	0.52
1:G:7233:THR:HG22	1:G:7243:LYS:HD3	1.90	0.52
1:C:3023:ILE:HD11	2:D:4054:LEU:O	2.09	0.52
2:H:8056:PHE:HB3	2:H:8062:PHE:CD2	2.44	0.52
1:C:3249:VAL:HG13	1:C:3257:TYR:CE1	2.44	0.52
1:A:1128:GLU:HG2	1:A:1129:ASN:N	2.19	0.52
1:E:5041:GLU:O	1:E:5041:GLU:HG2	2.09	0.52
1:A:1128:GLU:OE2	1:A:1131:SER:N	2.43	0.52
1:C:3125:THR:C	1:C:3126:LEU:HD23	2.29	0.52
1:G:7194:ARG:NH2	1:G:7196:GLU:HB3	2.24	0.52
1:E:5194:ARG:CD	1:E:5196:GLU:OE2	2.55	0.52
1:A:1061:GLU:HA	1:A:1064:THR:HG22	1.90	0.52
1:A:1081:LEU:HD12	1:A:1095:LEU:HD13	1.91	0.52
2:H:8027:VAL:CG2	2:H:8064:LEU:HB2	2.40	0.52
2:H:8009:VAL:HG12	2:H:8023:LEU:HD11	1.92	0.52
2:F:6027:VAL:HG12	2:F:6030:PHE:CE2	2.44	0.52
1:E:5112:TRP:O	1:E:5129:ASN:O	2.27	0.52
1:A:1081:LEU:CD1	1:A:1095:LEU:HD13	2.40	0.52
1:C:3008:PHE:CD2	1:C:3098:LEU:HD13	2.45	0.52
1:C:3096:GLN:HE22	2:D:4031:HIS:CD2	2.27	0.52
1:G:7036:PHE:CD2	1:G:7067:VAL:HG12	2.45	0.52
1:G:7103:VAL:CG2	1:G:7168:LEU:HD23	2.40	0.52
1:G:7095:LEU:HD21	1:G:7116:LEU:HD21	1.92	0.52
1:C:3096:GLN:O	1:C:3116:LEU:HA	2.10	0.52
1:C:3064:THR:O	1:C:3068:THR:OG1	2.28	0.52
1:C:3028:VAL:CG1	1:C:3179:LEU:HD13	2.40	0.52
1:G:7232:GLU:HA	1:G:7232:GLU:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5043:PRO:HG2	1:E:5064:THR:CB	2.40	0.51
2:B:2069:GLU:O	1:G:7017:LEU:HG	2.10	0.51
2:F:6041:LYS:HG2	2:F:6041:LYS:O	2.10	0.51
1:A:1248:VAL:HG23	1:A:1248:VAL:O	2.10	0.51
1:E:5206:LEU:HD23	1:E:5242:GLN:HG2	1.92	0.51
1:C:3104:GLU:HG2	1:C:3107:ARG:HB2	1.91	0.51
1:E:5008:PHE:HB2	1:E:5025:VAL:HB	1.92	0.51
1:G:7006:ARG:HG3	1:G:7098:LEU:HD11	1.93	0.51
1:G:7160:LEU:O	1:G:7160:LEU:HD12	2.09	0.51
2:F:6036:GLU:HG2	2:F:6081:ARG:HH22	1.75	0.51
1:A:1052:LEU:HD23	1:A:1175:GLY:CA	2.41	0.51
2:F:6083:ASN:HD22	2:F:6090:PRO:HG3	1.75	0.51
2:B:2056:PHE:HB3	2:B:2062:PHE:CE2	2.45	0.51
1:C:3251:LEU:HD22	1:C:3252:GLY:N	2.25	0.51
1:A:1059:ASP:HA	1:A:1061:GLU:OE1	2.10	0.51
1:E:5034:LEU:HD12	1:E:5045:MET:SD	2.50	0.51
1:C:3120:SER:HG	2:D:4001:ILE:N	2.09	0.51
1:A:1252:GLY:C	1:A:1253:LYS:HE2	2.30	0.51
2:F:6041:LYS:O	2:F:6042:ASN:HB2	2.09	0.51
1:E:5234:ARG:NH1	1:E:5242:GLN:OE1	2.44	0.51
2:D:4019:LYS:O	2:D:4071:THR:HB	2.09	0.51
1:E:5263:HIS:HB3	1:E:5266:LEU:HD12	1.93	0.51
1:C:3058:ASP:OD2	1:C:3174:LYS:NZ	2.39	0.51
1:A:1076:ARG:HG2	1:A:1076:ARG:HH11	1.75	0.51
1:G:7131:SER:O	1:G:7132:SER:O	2.29	0.51
1:G:7191:ARG:HH11	1:G:7193:PRO:HD3	1.76	0.51
1:G:7068:THR:HG22	1:G:7072:GLN:OE1	2.11	0.51
1:C:3077:ASN:O	1:C:3081:LEU:HD13	2.10	0.51
1:C:3218:GLN:OE1	1:C:3221:GLY:HA2	2.11	0.51
1:A:1163:HIS:HA	1:A:1166:ASP:OD1	2.11	0.51
2:B:2018:GLY:O	2:B:2019:LYS:HE3	2.11	0.51
1:G:7163:HIS:CD2	1:G:7163:HIS:N	2.77	0.51
1:A:1077:ASN:O	1:A:1081:LEU:HB2	2.11	0.51
1:A:1002:SER:HB3	1:A:1104:GLU:HB2	1.93	0.51
1:A:1103:VAL:HG21	1:A:1165:SER:CA	2.41	0.51
1:C:3131:SER:OG	1:C:3132:SER:N	2.41	0.51
2:H:8006:LYS:CE	2:H:8029:GLY:HA3	2.37	0.51
2:F:6001:ILE:CD1	2:F:6002:GLN:HG3	2.41	0.51
2:H:8009:VAL:CG1	2:H:8023:LEU:HD11	2.40	0.51
1:A:1194:ARG:HH22	1:A:1198:ASP:HB3	1.76	0.50
1:C:3168:LEU:CD2	1:C:3169:GLN:HE22	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5227:ASP:OD1	1:E:5248:VAL:HG23	2.10	0.50
1:G:7199:VAL:HG23	1:G:7251:LEU:CD1	2.41	0.50
1:A:1006:ARG:HG3	1:A:1006:ARG:HH11	1.76	0.50
1:G:7086:ASN:O	1:G:7086:ASN:OD1	2.29	0.50
1:G:7032:GLN:NE2	2:H:8053:ASP:OD2	2.44	0.50
2:B:2009:VAL:HG22	2:B:2080:CYS:HB2	1.93	0.50
1:E:5162:GLY:O	1:E:5166:ASP:OD1	2.30	0.50
2:H:8004:THR:O	2:H:8029:GLY:O	2.29	0.50
1:C:3199:VAL:O	1:C:3248:VAL:HA	2.12	0.50
1:A:1273:ARG:NH1	1:A:1273:ARG:HB2	2.24	0.50
1:A:1014:ARG:NH2	1:A:1018:GLY:HA3	2.16	0.50
1:A:1009:TYR:CD1	1:A:1024:ILE:HD11	2.46	0.50
2:B:2096:ASP:OD1	2:B:2098:ASP:OD2	2.29	0.50
2:F:6051:HIS:HA	2:F:6065:LEU:O	2.12	0.50
2:D:4041:LYS:HG3	2:D:4078:TYR:CE1	2.45	0.50
1:A:1161:GLU:O	1:A:1161:GLU:HG2	2.11	0.50
1:E:5170:LYS:O	1:E:5173:GLU:HB2	2.12	0.50
1:A:1177:GLU:O	1:A:1181:ARG:HB2	2.11	0.50
1:E:5249:VAL:HG13	1:E:5250:PRO:HD2	1.94	0.50
1:A:1160:LEU:HD12	1:A:1160:LEU:O	2.11	0.50
1:G:7168:LEU:O	1:G:7172:LEU:HG	2.12	0.50
1:A:1253:LYS:HE2	1:A:1253:LYS:N	2.27	0.50
1:G:7187:ALA:HA	1:G:7204:TRP:O	2.11	0.50
1:G:7106:ASP:O	1:G:7107:ARG:HG2	2.11	0.50
1:E:5195:PRO:O	1:E:5196:GLU:HG3	2.11	0.50
1:C:3190:THR:HA	1:C:3274:TRP:HE1	1.75	0.50
1:A:1247:VAL:HG23	1:A:1249:VAL:HG23	1.94	0.50
1:A:1005:LEU:CD2	1:A:1167:VAL:HG12	2.41	0.50
1:E:5090:ASP:O	1:E:5091:ASP:OD2	2.30	0.50
1:G:7069:ILE:HD13	1:G:7072:GLN:HE22	1.77	0.50
1:E:5181:ARG:NH1	1:E:5183:ASP:OD2	2.44	0.50
1:G:7176:LYS:CE	1:G:7180:LEU:HG	2.41	0.50
1:C:3006:ARG:NH1	1:C:3102:ASP:OD1	2.44	0.50
2:D:4041:LYS:HG3	2:D:4078:TYR:CZ	2.47	0.50
2:D:4077:GLU:OE2	2:D:4078:TYR:N	2.45	0.50
1:A:1087:LYS:O	1:A:1088:SER:O	2.30	0.49
1:A:1064:THR:O	1:A:1068:THR:OG1	2.29	0.49
2:H:8080:CYS:O	2:H:8092:ILE:HA	2.12	0.49
1:G:7077:ASN:ND2	1:G:7097:TRP:HZ3	2.10	0.49
2:B:2001:ILE:HD12	2:B:2002:GLN:HG2	1.93	0.49
1:G:7199:VAL:HG23	1:G:7251:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3251:LEU:HD22	1:C:3252:GLY:H	1.77	0.49
1:A:1221:GLY:O	1:A:1223:GLU:OE2	2.30	0.49
1:A:1189:VAL:H	1:A:1275:GLU:CG	2.25	0.49
1:A:1085:TYR:HB3	1:A:1087:LYS:CE	2.42	0.49
1:E:5170:LYS:HZ2	1:E:5174:LYS:HE3	1.76	0.49
1:A:1172:LEU:HD23	1:A:1179:LEU:HD13	1.93	0.49
1:G:7025:VAL:HG21	2:H:8053:ASP:HB2	1.93	0.49
1:A:1103:VAL:CG1	1:A:1165:SER:HB3	2.37	0.49
1:E:5095:LEU:HA	1:E:5117:ALA:O	2.13	0.49
1:G:7111:LEU:HD23	1:G:7130:PRO:HG2	1.93	0.49
1:G:7223:GLU:OE1	1:G:7225:THR:OG1	2.25	0.49
1:C:3083:HIS:O	1:C:3086:ASN:HB3	2.11	0.49
1:E:5130:PRO:O	1:E:5131:SER:O	2.30	0.49
1:G:7009:TYR:CD2	1:G:7097:TRP:HB3	2.47	0.49
1:A:1207:GLY:O	1:A:1240:THR:HG22	2.13	0.49
1:G:7208:PHE:CE2	1:G:7213:ILE:HD12	2.48	0.49
1:E:5202:ARG:HA	1:E:5245:ALA:O	2.12	0.49
2:H:8017:ASN:HA	2:H:8072:PRO:O	2.13	0.49
1:A:1017:LEU:HD23	2:H:8071:THR:HG23	1.93	0.49
1:E:5194:ARG:NH1	1:E:5196:GLU:OE2	2.45	0.49
1:C:3050:PRO:HA	1:C:3054:GLN:HE22	1.75	0.49
1:E:5126:LEU:HD22	1:E:5126:LEU:N	2.28	0.49
1:G:7013:SER:O	1:G:7092:SER:OG	2.28	0.49
1:E:5112:TRP:HB2	1:E:5133:CYS:SG	2.52	0.49
2:H:8003:ARG:O	2:H:8086:THR:HG21	2.13	0.49
1:A:1072:GLN:HG3	1:A:1072:GLN:O	2.13	0.49
1:G:7095:LEU:HD11	1:G:7116:LEU:HD23	1.95	0.49
1:C:3024:ILE:HD12	1:C:3067:VAL:HG13	1.93	0.49
1:C:3034:LEU:HG	1:C:3035:ARG:N	2.28	0.49
1:E:5034:LEU:HD13	1:E:5063:GLN:NE2	2.28	0.49
1:G:7222:GLU:O	1:G:7223:GLU:O	2.30	0.49
1:G:7096:GLN:N	1:G:7096:GLN:HE21	2.11	0.49
1:E:5077:ASN:O	1:E:5081:LEU:HB2	2.13	0.49
1:C:3014:ARG:NH2	1:C:3018:GLY:HA3	2.10	0.49
2:D:4077:GLU:OE2	2:D:4078:TYR:O	2.31	0.49
2:H:8041:LYS:O	2:H:8042:ASN:HB2	2.13	0.49
1:E:5213:ILE:HD11	1:E:5261:VAL:HG13	1.95	0.48
1:C:3112:TRP:HB3	1:C:3131:SER:CB	2.43	0.48
1:C:3055:GLU:O	1:C:3057:ALA:N	2.38	0.48
1:C:3228:VAL:O	1:C:3228:VAL:HG12	2.13	0.48
1:A:1217:TRP:CZ3	1:A:1257:TYR:HB3	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5007:TYR:OH	1:E:5063:GLN:OE1	2.31	0.48
1:C:3215:LEU:HD12	1:C:3261:VAL:CG2	2.43	0.48
1:A:1204:TRP:CZ2	2:B:2099:MET:HA	2.48	0.48
1:E:5104:GLU:CB	1:E:5109:LEU:HD22	2.43	0.48
1:C:3056:GLU:O	1:C:3057:ALA:HB3	2.13	0.48
1:G:7203:CYS:HB2	1:G:7217:TRP:CZ2	2.48	0.48
1:E:5200:THR:O	1:E:5201:LEU:HD23	2.12	0.48
1:G:7200:THR:O	1:G:7201:LEU:HD23	2.13	0.48
1:E:5194:ARG:HE	1:E:5248:VAL:HG11	1.77	0.48
1:E:5170:LYS:NZ	1:E:5174:LYS:HE3	2.28	0.48
1:E:5075:GLU:O	1:E:5079:MET:HB2	2.12	0.48
1:A:1261:VAL:HB	1:A:1270:LEU:HB2	1.95	0.48
2:H:8033:SER:O	2:H:8035:ILE:N	2.46	0.48
1:C:3177:GLU:OE2	1:C:3177:GLU:N	2.46	0.48
2:H:8016:GLU:HG2	2:H:8019:LYS:CD	2.42	0.48
1:C:3261:VAL:O	1:C:3266:LEU:HD13	2.13	0.48
1:C:3128:GLU:CG	1:C:3129:ASN:H	2.26	0.48
1:A:1172:LEU:HD22	1:A:1180:LEU:CD1	2.43	0.48
1:E:5201:LEU:HD11	1:E:5254:VAL:HG23	1.93	0.48
1:C:3181:ARG:HG2	1:C:3181:ARG:O	2.13	0.48
1:G:7208:PHE:CD2	1:G:7213:ILE:HD12	2.49	0.48
1:E:5035:ARG:HG3	2:F:6053:ASP:CG	2.34	0.48
1:E:5217:TRP:CZ3	1:E:5257:TYR:HB3	2.49	0.48
1:G:7188:HIS:HA	1:G:7272:LEU:HD11	1.96	0.48
1:G:7194:ARG:NH1	1:G:7198:ASP:OD2	2.47	0.48
1:G:7189:VAL:HG12	1:G:7274:TRP:CD1	2.47	0.48
1:C:3036:PHE:HB2	1:C:3043:PRO:HB3	1.96	0.48
1:C:3050:PRO:C	1:C:3052:LEU:H	2.16	0.48
1:A:1060:TRP:HZ2	1:A:1174:LYS:HG3	1.79	0.48
1:C:3185:PRO:HD3	1:C:3263:HIS:CD2	2.48	0.48
1:G:7199:VAL:O	1:G:7199:VAL:HG12	2.13	0.48
1:C:3111:LEU:HB3	1:C:3130:PRO:HB3	1.95	0.48
1:G:7006:ARG:HB3	1:G:7008:PHE:CE1	2.49	0.48
1:G:7268:GLU:HG2	1:G:7269:PRO:HD2	1.96	0.48
2:D:4006:LYS:HZ3	2:D:4029:GLY:HA3	1.77	0.48
1:A:1034:LEU:HD12	1:A:1045:MET:HE1	1.94	0.48
2:H:8030:PHE:CE1	2:H:8035:ILE:HD12	2.49	0.48
1:C:3218:GLN:HG2	1:C:3222:GLU:N	2.29	0.48
1:A:1193:PRO:CA	1:A:1199:VAL:HG13	2.43	0.48
1:A:1088:SER:O	1:A:1090:ASP:OD1	2.32	0.48
1:C:3127:SER:O	1:C:3128:GLU:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3199:VAL:HG22	1:C:3249:VAL:O	2.13	0.48
1:C:3178:ARG:C	1:C:3181:ARG:HB3	2.35	0.48
1:G:7185:PRO:HG3	1:G:7208:PHE:HB3	1.96	0.48
1:E:5052:LEU:HD23	1:E:5175:GLY:N	2.28	0.48
1:A:1191:ARG:HG3	1:A:1274:TRP:NE1	2.28	0.47
1:A:1017:LEU:HD22	2:H:8070:PHE:CA	2.43	0.47
1:A:1103:VAL:O	1:A:1104:GLU:HB2	2.13	0.47
1:C:3043:PRO:HD2	1:C:3064:THR:HB	1.96	0.47
1:C:3026:GLY:O	1:C:3033:VAL:HG22	2.14	0.47
1:A:1110:CYS:O	1:A:1111:LEU:HD12	2.13	0.47
1:E:5036:PHE:CE2	1:E:5068:THR:HG23	2.48	0.47
1:A:1095:LEU:HD12	1:A:1117:ALA:O	2.13	0.47
1:E:5097:TRP:NE1	1:E:5099:GLN:NE2	2.62	0.47
1:A:1079:MET:O	1:A:1082:VAL:HG13	2.14	0.47
2:B:2001:ILE:HG23	2:B:2002:GLN:HG3	1.97	0.47
1:A:1228:VAL:CG1	1:A:1228:VAL:O	2.53	0.47
1:C:3073:LEU:HB3	1:C:3077:ASN:ND2	2.30	0.47
1:E:5249:VAL:HG21	1:E:5254:VAL:HG23	1.96	0.47
1:E:5227:ASP:O	1:E:5227:ASP:OD2	2.32	0.47
1:C:3268:GLU:HG3	1:C:3269:PRO:HD2	1.96	0.47
1:E:5107:ARG:HG2	1:E:5107:ARG:NH1	2.29	0.47
2:H:8027:VAL:O	2:H:8063:TYR:HA	2.14	0.47
1:E:5054:GLN:O	1:E:5056:GLU:N	2.46	0.47
1:A:1014:ARG:NH1	2:H:8048:LYS:HD3	2.29	0.47
1:G:7079:MET:O	1:G:7082:VAL:HB	2.15	0.47
1:G:7055:GLU:HG3	1:G:7056:GLU:N	2.29	0.47
2:D:4048:LYS:O	2:D:4048:LYS:HG3	2.14	0.47
2:H:8007:ILE:O	2:H:8008:GLN:HG3	2.15	0.47
1:E:5095:LEU:HD12	1:E:5117:ALA:C	2.35	0.47
1:E:5170:LYS:HZ2	1:E:5174:LYS:CE	2.27	0.47
1:C:3111:LEU:HD22	1:C:3130:PRO:HB2	1.96	0.47
1:G:7014:ARG:HG2	1:G:7021:TRP:HZ3	1.78	0.47
1:A:1194:ARG:NH1	1:A:1198:ASP:O	2.48	0.47
1:A:1070:GLN:O	1:A:1073:LEU:HG	2.15	0.47
1:A:1009:TYR:O	1:A:1096:GLN:HA	2.14	0.47
2:B:2069:GLU:HG2	2:B:2070:PHE:N	2.30	0.47
2:F:6023:LEU:HD13	2:F:6070:PHE:CE2	2.50	0.47
1:G:7249:VAL:HG12	1:G:7257:TYR:CZ	2.50	0.47
1:G:7015:PRO:HB2	1:G:7090:ASP:HA	1.97	0.47
1:A:1189:VAL:O	1:A:1275:GLU:OE1	2.32	0.46
1:A:1273:ARG:CB	1:A:1273:ARG:NH1	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3218:GLN:HG2	1:C:3222:GLU:C	2.35	0.46
1:E:5223:GLU:OE2	1:E:5223:GLU:N	2.49	0.46
1:G:7088:SER:CB	1:G:7091:ASP:HB2	2.46	0.46
1:A:1274:TRP:O	1:A:1275:GLU:CB	2.62	0.46
1:A:1050:PRO:O	1:A:1054:GLN:NE2	2.48	0.46
1:A:1006:ARG:HH21	1:A:1102:ASP:CG	2.17	0.46
1:A:1085:TYR:OH	1:A:1123:LEU:HD21	2.15	0.46
1:A:1103:VAL:HG21	1:A:1165:SER:CB	2.43	0.46
1:C:3052:LEU:O	1:C:3053:GLU:HG3	2.15	0.46
1:E:5014:ARG:NH2	1:E:5019:GLU:O	2.48	0.46
1:A:1191:ARG:HH22	1:A:1199:VAL:HG21	1.80	0.46
1:A:1254:VAL:O	1:A:1254:VAL:CG1	2.62	0.46
1:C:3178:ARG:HA	1:C:3181:ARG:HB3	1.98	0.46
1:C:3095:LEU:CG	1:C:3116:LEU:HD21	2.45	0.46
1:E:5060:TRP:CE3	1:E:5060:TRP:HA	2.51	0.46
1:E:5052:LEU:HA	1:E:5174:LYS:O	2.15	0.46
1:C:3111:LEU:HD22	1:C:3130:PRO:CB	2.46	0.46
1:E:5109:LEU:HG	1:E:5110:CYS:N	2.30	0.46
1:A:1194:ARG:NE	1:A:1200:THR:HG22	2.31	0.46
1:G:7192:HIS:O	1:G:7194:ARG:N	2.48	0.46
2:H:8016:GLU:HG3	2:H:8016:GLU:O	2.14	0.46
1:C:3182:SER:OG	1:C:3265:GLY:CA	2.63	0.46
1:C:3182:SER:OG	1:C:3265:GLY:HA2	2.15	0.46
1:A:1005:LEU:HD22	1:A:1167:VAL:HG12	1.96	0.46
1:E:5012:VAL:HG22	1:E:5094:THR:HB	1.98	0.46
1:A:1108:HIS:O	1:A:1109:LEU:CD1	2.58	0.46
1:C:3112:TRP:CE3	1:C:3161:GLU:HA	2.50	0.46
1:A:1271:THR:HG22	1:A:1271:THR:O	2.15	0.46
1:A:1104:GLU:HA	1:A:1105:PRO:HD3	1.80	0.46
1:C:3063:GLN:NE2	1:C:3171:TYR:OH	2.49	0.46
2:B:2046:ILE:HG21	1:G:7017:LEU:CD2	2.45	0.46
2:B:2081:ARG:HE	2:B:2081:ARG:HB3	1.55	0.46
1:E:5014:ARG:O	1:E:5016:GLY:N	2.49	0.46
1:E:5211:ALA:HB2	1:E:5241:PHE:CE1	2.51	0.46
1:E:5005:LEU:HB2	1:E:5168:LEU:HD13	1.97	0.46
1:C:3224:LEU:O	1:C:3225:THR:O	2.34	0.46
2:F:6035:ILE:HG12	2:F:6036:GLU:N	2.31	0.46
1:E:5223:GLU:O	1:E:5224:LEU:HD23	2.16	0.46
1:C:3007:TYR:OH	1:C:3063:GLN:NE2	2.49	0.46
1:C:3160:LEU:HD12	1:C:3163:HIS:CE1	2.51	0.46
2:H:8095:TRP:CZ3	2:H:8097:ARG:HD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7273:ARG:O	1:G:7273:ARG:HG2	2.16	0.46
1:A:1201:LEU:HD12	1:A:1249:VAL:CG2	2.43	0.46
1:G:7073:LEU:O	1:G:7077:ASN:ND2	2.49	0.46
1:E:5231:VAL:CG2	1:E:5244:TRP:H	2.29	0.46
2:D:4071:THR:HA	2:D:4072:PRO:HD2	1.83	0.46
1:E:5019:GLU:H	1:E:5019:GLU:HG3	1.54	0.46
2:F:6040:LEU:HA	2:F:6044:GLU:O	2.16	0.46
1:A:1107:ARG:O	1:A:1107:ARG:HD3	2.16	0.45
1:C:3060:TRP:O	1:C:3064:THR:HG23	2.15	0.45
1:E:5082:VAL:O	1:E:5086:ASN:N	2.49	0.45
1:C:3005:LEU:HD12	1:C:3028:VAL:HG22	1.97	0.45
1:C:3218:GLN:HG2	1:C:3222:GLU:H	1.81	0.45
1:A:1014:ARG:HH12	2:H:8048:LYS:HZ2	1.63	0.45
1:A:1108:HIS:O	1:A:1109:LEU:CB	2.64	0.45
1:G:7080:THR:OG1	1:G:7081:LEU:N	2.50	0.45
1:G:7172:LEU:N	1:G:7172:LEU:HD23	2.31	0.45
1:G:7172:LEU:O	1:G:7176:LYS:N	2.49	0.45
1:A:1040:GLU:HG3	1:A:1041:GLU:N	2.31	0.45
2:B:2040:LEU:HD11	2:B:2081:ARG:HB2	1.99	0.45
1:E:5010:THR:O	1:E:5022:PHE:HA	2.15	0.45
1:G:7061:GLU:O	1:G:7065:HIS:ND1	2.48	0.45
2:F:6009:VAL:HG23	2:F:6093:VAL:HG12	1.98	0.45
1:E:5163:HIS:O	1:E:5167:VAL:HG23	2.16	0.45
2:B:2003:ARG:HH12	2:B:2061:SER:CA	2.29	0.45
1:G:7069:ILE:HG22	1:G:7070:GLN:N	2.31	0.45
1:C:3215:LEU:HB3	1:C:3243:LYS:HZ3	1.82	0.45
1:G:7007:TYR:OH	1:G:7063:GLN:NE2	2.49	0.45
2:F:6017:ASN:HA	2:F:6072:PRO:O	2.16	0.45
1:A:1191:ARG:HD2	1:A:1201:LEU:HD21	1.99	0.45
1:A:1090:ASP:OD1	1:A:1091:ASP:N	2.49	0.45
1:E:5174:LYS:HA	1:E:5174:LYS:HD3	1.78	0.45
1:A:1238:ASP:OD1	1:A:1238:ASP:N	2.50	0.45
1:A:1194:ARG:NH2	1:A:1198:ASP:HB3	2.31	0.45
1:G:7271:THR:HG22	1:G:7272:LEU:N	2.31	0.45
1:C:3234:ARG:NH1	1:C:3242:GLN:OE1	2.50	0.45
1:E:5234:ARG:HB3	2:F:6026:TYR:CD2	2.52	0.45
1:E:5192:HIS:CD2	1:E:5192:HIS:N	2.82	0.45
1:G:7165:SER:O	1:G:7169:GLN:NE2	2.45	0.45
1:E:5268:GLU:CD	1:E:5269:PRO:HD2	2.36	0.45
2:D:4091:LYS:HA	2:D:4091:LYS:HD2	1.50	0.45
2:D:4096:ASP:OD2	2:D:4097:ARG:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3014:ARG:O	1:C:3016:GLY:N	2.50	0.45
1:E:5067:VAL:HA	1:E:5070:GLN:HB2	1.98	0.45
1:G:7028:VAL:HG23	1:G:7033:VAL:CG2	2.46	0.45
2:F:6059:ASP:O	2:F:6060:TRP:HB2	2.17	0.45
1:A:1191:ARG:HD2	1:A:1201:LEU:HD23	1.99	0.45
1:A:1249:VAL:HG22	1:A:1257:TYR:CE2	2.51	0.45
1:E:5199:VAL:HG12	1:E:5200:THR:N	2.32	0.45
1:E:5201:LEU:HD11	1:E:5249:VAL:HG21	1.99	0.45
1:G:7215:LEU:HB3	1:G:7243:LYS:HZ1	1.82	0.45
1:A:1103:VAL:HG12	1:A:1104:GLU:N	2.29	0.45
1:G:7073:LEU:HB3	1:G:7077:ASN:ND2	2.31	0.45
1:G:7095:LEU:HD11	1:G:7116:LEU:CD2	2.46	0.45
1:C:3115:GLN:O	1:C:3116:LEU:HB2	2.16	0.45
1:C:3034:LEU:HD12	1:C:3043:PRO:CB	2.47	0.45
1:C:3004:SER:HB2	1:C:3006:ARG:NH1	2.32	0.45
2:F:6021:ASN:N	2:F:6070:PHE:O	2.50	0.45
1:C:3246:ALA:O	1:C:3247:VAL:CG1	2.63	0.45
1:C:3014:ARG:NH2	1:C:3017:LEU:O	2.50	0.45
2:D:4023:LEU:O	2:D:4067:TYR:HA	2.17	0.45
1:G:7102:ASP:N	1:G:7102:ASP:OD1	2.50	0.45
2:D:4027:VAL:HG22	2:D:4064:LEU:O	2.17	0.45
2:B:2058:LYS:HE2	2:B:2058:LYS:HB3	1.44	0.45
1:A:1115:GLN:HE21	1:A:1115:GLN:HB2	1.53	0.45
1:C:3077:ASN:O	1:C:3081:LEU:HB2	2.16	0.44
2:F:6008:GLN:NE2	2:F:6026:TYR:O	2.50	0.44
1:A:1234:ARG:NH1	1:A:1242:GLN:OE1	2.50	0.44
2:H:8035:ILE:HG13	2:H:8084:HIS:HD2	1.81	0.44
1:E:5190:THR:HB	1:E:5192:HIS:CE1	2.53	0.44
1:C:3055:GLU:O	1:C:3055:GLU:OE2	2.35	0.44
2:D:4012:ARG:HD3	2:D:4022:PHE:HB2	1.99	0.44
1:A:1017:LEU:HD21	2:H:8071:THR:OG1	2.17	0.44
2:F:6056:PHE:HA	2:F:6062:PHE:HA	2.00	0.44
1:G:7169:GLN:O	1:G:7173:GLU:HG3	2.16	0.44
1:E:5199:VAL:HG22	1:E:5251:LEU:HD23	1.98	0.44
1:A:1109:LEU:HD12	1:A:1109:LEU:HA	1.79	0.44
1:C:3102:ASP:OD1	1:C:3102:ASP:N	2.49	0.44
1:G:7014:ARG:HD2	1:G:7019:GLU:O	2.17	0.44
1:G:7045:MET:HB3	1:G:7052:LEU:HD12	1.99	0.44
2:H:8059:ASP:N	2:H:8059:ASP:OD1	2.45	0.44
1:E:5052:LEU:HD22	1:E:5174:LYS:CB	2.42	0.44
2:F:6023:LEU:O	2:F:6067:TYR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3221:GLY:O	1:C:3222:GLU:HB2	2.17	0.44
1:A:1268:GLU:CD	1:A:1269:PRO:HD2	2.38	0.44
1:A:1035:ARG:HH12	1:A:1044:ARG:NH1	2.15	0.44
1:C:3194:ARG:HH11	1:C:3198:ASP:HB3	1.82	0.44
1:C:3112:TRP:CZ3	1:C:3161:GLU:HA	2.52	0.44
2:H:8096:ASP:HB3	2:H:8099:MET:HB3	1.99	0.44
2:B:2085:VAL:HG12	2:H:8044:GLU:HG2	1.99	0.44
1:C:3011:ALA:HA	1:C:3021:TRP:O	2.17	0.44
1:A:1061:GLU:C	1:A:1064:THR:HG22	2.38	0.44
1:A:1078:LEU:O	1:A:1081:LEU:N	2.49	0.44
1:A:1128:GLU:OE2	1:A:1131:SER:HB3	2.18	0.44
1:C:3263:HIS:CB	1:C:3266:LEU:HD12	2.47	0.44
1:C:3111:LEU:CB	1:C:3130:PRO:HB3	2.48	0.44
2:F:6001:ILE:HD13	2:F:6001:ILE:C	2.38	0.44
1:A:1076:ARG:HG2	1:A:1076:ARG:NH1	2.33	0.44
2:B:2038:ASP:OD2	2:H:8036:GLU:OE2	2.35	0.44
2:B:2007:ILE:CD1	2:B:2082:VAL:HG21	2.48	0.44
2:F:6073:THR:HG22	2:F:6076:ASP:H	1.82	0.44
1:E:5096:GLN:NE2	2:F:6056:PHE:CG	2.86	0.44
1:A:1039:LYS:CE	1:A:1039:LYS:O	2.66	0.44
1:C:3188:HIS:O	1:C:3204:TRP:HB2	2.17	0.44
2:B:2006:LYS:HD2	2:B:2029:GLY:HA3	2.00	0.44
1:E:5188:HIS:HE1	1:E:5206:LEU:HD11	1.83	0.44
1:C:3071:GLY:O	1:C:3074:SER:HB3	2.17	0.44
1:E:5249:VAL:HG12	1:E:5250:PRO:O	2.18	0.44
1:G:7005:LEU:HD13	1:G:7028:VAL:HG22	1.99	0.44
2:H:8053:ASP:N	2:H:8053:ASP:OD1	2.50	0.44
2:H:8038:ASP:OD1	2:H:8045:ARG:NH1	2.51	0.43
1:C:3103:VAL:HG21	1:C:3165:SER:HA	1.99	0.43
1:C:3103:VAL:HG11	1:C:3165:SER:HB2	1.99	0.43
1:C:3196:GLU:O	1:C:3198:ASP:N	2.50	0.43
1:E:5194:ARG:HA	1:E:5195:PRO:HD3	1.85	0.43
1:E:5066:ILE:O	1:E:5070:GLN:CG	2.58	0.43
1:A:1079:MET:HB3	1:A:1079:MET:HE3	1.87	0.43
1:A:1273:ARG:O	1:A:1276:PRO:HD2	2.18	0.43
1:A:1061:GLU:CA	1:A:1064:THR:HG22	2.48	0.43
2:H:8007:ILE:HD12	2:H:8082:VAL:HG21	1.97	0.43
2:B:2019:LYS:HA	2:B:2019:LYS:HD3	1.88	0.43
1:G:7054:GLN:OE1	1:G:7055:GLU:N	2.33	0.43
1:G:7064:THR:O	1:G:7068:THR:OG1	2.19	0.43
1:C:3035:ARG:HG3	1:C:3036:PHE:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1215:LEU:HD23	1:A:1215:LEU:HA	1.90	0.43
1:E:5258:THR:CG2	1:E:5273:ARG:HG2	2.48	0.43
1:G:7040:GLU:O	1:G:7041:GLU:OE2	2.36	0.43
1:A:1191:ARG:CG	1:A:1274:TRP:NE1	2.81	0.43
1:G:7111:LEU:HB3	1:G:7130:PRO:HB3	2.00	0.43
2:D:4051:HIS:HA	2:D:4065:LEU:O	2.19	0.43
1:C:3073:LEU:CD2	1:C:3076:ARG:NH1	2.81	0.43
2:F:6051:HIS:ND1	2:F:6051:HIS:N	2.67	0.43
1:E:5023:ILE:O	1:E:5023:ILE:HG23	2.19	0.43
1:A:1006:ARG:HG3	1:A:1006:ARG:NH1	2.34	0.43
1:A:1191:ARG:HH22	1:A:1251:LEU:HD12	1.84	0.43
1:A:1015:PRO:HG3	1:A:1091:ASP:O	2.19	0.43
1:E:5118:TYR:HB2	1:E:5123:LEU:HD11	2.01	0.43
1:G:7266:LEU:HA	1:G:7267:PRO:HD3	1.87	0.43
1:A:1199:VAL:HG21	1:A:1251:LEU:HD12	2.00	0.43
1:G:7184:PRO:HA	1:G:7185:PRO:HD3	1.76	0.43
1:A:1035:ARG:CZ	1:A:1044:ARG:HD2	2.48	0.43
2:B:2005:PRO:HB3	2:B:2030:PHE:HB3	2.01	0.43
1:C:3095:LEU:CD1	1:C:3116:LEU:HD21	2.48	0.43
1:E:5203:CYS:O	1:E:5244:TRP:HA	2.18	0.43
1:A:1011:ALA:CB	1:A:1074:SER:HB2	2.49	0.43
2:F:6005:PRO:HB2	2:F:6027:VAL:HG13	1.99	0.43
1:A:1189:VAL:HG12	1:A:1190:THR:N	2.32	0.43
1:A:1128:GLU:CD	1:A:1130:PRO:HD2	2.40	0.43
1:E:5074:SER:OG	1:E:5075:GLU:N	2.50	0.43
1:A:1009:TYR:HB3	1:A:1097:TRP:HB3	2.01	0.43
1:A:1215:LEU:HD23	1:A:1260:HIS:O	2.19	0.43
1:C:3238:ASP:OD1	1:C:3238:ASP:N	2.50	0.43
1:G:7112:TRP:CE2	1:G:7161:GLU:HB2	2.54	0.43
1:G:7234:ARG:HB3	2:H:8026:TYR:CE2	2.54	0.43
1:C:3073:LEU:CG	1:C:3076:ARG:NH1	2.80	0.42
1:C:3009:TYR:OH	1:C:3074:SER:HB3	2.19	0.42
1:A:1180:LEU:N	1:A:1180:LEU:HD12	2.34	0.42
2:H:8052:SER:O	2:H:8064:LEU:HD22	2.18	0.42
1:E:5028:VAL:O	1:E:5029:ASP:HB2	2.19	0.42
2:F:6007:ILE:CD1	2:F:6007:ILE:N	2.82	0.42
1:A:1199:VAL:HG12	1:A:1200:THR:N	2.33	0.42
1:E:5199:VAL:CG2	1:E:5251:LEU:HD23	2.48	0.42
1:G:7192:HIS:HA	1:G:7193:PRO:HD2	1.86	0.42
1:A:1172:LEU:HD22	1:A:1180:LEU:HD11	2.01	0.42
1:E:5014:ARG:HB2	1:E:5017:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1229:GLU:N	1:A:1246:ALA:O	2.43	0.42
1:E:5228:VAL:O	1:E:5228:VAL:CG1	2.63	0.42
1:G:7243:LYS:HB3	1:G:7243:LYS:HE3	1.51	0.42
2:H:8082:VAL:N	2:H:8091:LYS:O	2.50	0.42
1:G:7053:GLU:OE2	1:G:7174:LYS:HA	2.19	0.42
2:B:2007:ILE:HD13	2:B:2082:VAL:HG21	2.00	0.42
1:C:3208:PHE:HB2	1:C:3263:HIS:NE2	2.35	0.42
1:E:5234:ARG:HD3	2:F:6010:TYR:CE2	2.54	0.42
1:A:1011:ALA:HB1	1:A:1074:SER:HB2	2.00	0.42
1:E:5096:GLN:HB3	2:F:6056:PHE:CE2	2.54	0.42
2:B:2005:PRO:CA	2:B:2030:PHE:HB3	2.50	0.42
1:A:1073:LEU:N	1:A:1073:LEU:HD23	2.35	0.42
1:E:5111:LEU:HB3	1:E:5113:TYR:CE1	2.54	0.42
2:B:2045:ARG:O	2:H:8034:ASP:OD2	2.37	0.42
1:C:3217:TRP:O	1:C:3218:GLN:HG3	2.18	0.42
1:E:5266:LEU:HA	1:E:5267:PRO:HD3	1.85	0.42
1:G:7055:GLU:O	1:G:7056:GLU:HB2	2.19	0.42
1:G:7236:ALA:O	2:H:8012:ARG:HD2	2.19	0.42
1:G:7031:MET:CE	1:G:7178:ARG:HB3	2.50	0.42
1:A:1072:GLN:C	1:A:1073:LEU:HD23	2.39	0.42
1:E:5052:LEU:HD23	1:E:5175:GLY:CA	2.49	0.42
1:G:7035:ARG:HG3	1:G:7036:PHE:N	2.34	0.42
1:G:7109:LEU:HG	1:G:7110:CYS:N	2.34	0.42
1:E:5009:TYR:CB	1:E:5097:TRP:HB3	2.47	0.42
2:H:8039:LEU:O	2:H:8045:ARG:HA	2.18	0.42
1:E:5010:THR:HB	1:E:5023:ILE:CG2	2.49	0.42
1:C:3228:VAL:HA	1:C:3247:VAL:CG1	2.50	0.42
1:C:3184:PRO:HA	1:C:3185:PRO:HD3	1.82	0.42
1:E:5052:LEU:HD23	1:E:5175:GLY:HA3	2.02	0.42
2:B:2058:LYS:HG2	2:B:2058:LYS:H	1.41	0.42
2:H:8071:THR:HA	2:H:8072:PRO:HD2	1.94	0.42
1:A:1014:ARG:NH1	2:H:8048:LYS:NZ	2.68	0.42
1:E:5175:GLY:O	1:E:5179:LEU:HG	2.20	0.42
2:D:4075:LYS:H	2:D:4075:LYS:HD3	1.84	0.42
2:H:8096:ASP:CG	2:H:8099:MET:HB3	2.40	0.42
2:H:8030:PHE:CD1	2:H:8035:ILE:HD12	2.55	0.42
2:D:4091:LYS:HD2	2:D:4092:ILE:N	2.35	0.42
1:C:3234:ARG:N	1:C:3242:GLN:O	2.53	0.42
1:A:1249:VAL:HG12	1:A:1254:VAL:HG22	1.96	0.41
1:C:3014:ARG:HG2	1:C:3014:ARG:HH11	1.85	0.41
1:E:5036:PHE:HE2	1:E:5068:THR:HG23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7081:LEU:O	1:G:7085:TYR:HD2	2.03	0.41
1:A:1219:LYS:O	1:A:1220:ASP:HB2	2.20	0.41
1:A:1274:TRP:C	1:A:1276:PRO:HD3	2.41	0.41
1:E:5049:ALA:HB3	1:E:5052:LEU:HD12	2.02	0.41
1:E:5242:GLN:O	1:E:5243:LYS:HB2	2.20	0.41
1:C:3111:LEU:CD1	1:C:3130:PRO:HB3	2.44	0.41
1:C:3031:MET:CE	1:C:3178:ARG:HD3	2.50	0.41
1:G:7103:VAL:HG12	1:G:7104:GLU:N	2.33	0.41
1:G:7005:LEU:CD1	1:G:7028:VAL:HG22	2.50	0.41
1:C:3249:VAL:HG13	1:C:3250:PRO:HD2	2.02	0.41
1:A:1266:LEU:HA	1:A:1267:PRO:HD3	1.85	0.41
1:A:1069:ILE:O	1:A:1073:LEU:CD2	2.64	0.41
1:C:3231:VAL:HG13	1:C:3244:TRP:CZ2	2.56	0.41
1:E:5060:TRP:CZ3	1:E:5170:LYS:HD3	2.55	0.41
2:B:2036:GLU:OE1	2:H:8038:ASP:OD2	2.38	0.41
2:H:8097:ARG:HE	2:H:8097:ARG:HB3	1.80	0.41
1:C:3014:ARG:CZ	1:C:3017:LEU:HD12	2.49	0.41
1:A:1111:LEU:HD23	1:A:1113:TYR:CZ	2.55	0.41
1:E:5194:ARG:O	1:E:5196:GLU:N	2.50	0.41
1:E:5064:THR:O	1:E:5068:THR:OG1	2.36	0.41
1:G:7025:VAL:CG2	2:H:8053:ASP:HB2	2.51	0.41
1:E:5062:GLN:OE1	1:E:5163:HIS:CD2	2.74	0.41
1:E:5118:TYR:O	1:E:5119:ASP:HB2	2.20	0.41
2:B:2041:LYS:O	2:B:2042:ASN:HB2	2.20	0.41
2:F:6069:GLU:HG2	2:F:6070:PHE:N	2.36	0.41
1:E:5104:GLU:HB3	1:E:5109:LEU:CB	2.51	0.41
1:E:5077:ASN:HA	1:E:5077:ASN:HD22	1.57	0.41
1:C:3117:ALA:HB2	2:D:4060:TRP:CE2	2.55	0.41
1:C:3014:ARG:HH21	1:C:3018:GLY:CA	2.12	0.41
1:A:1014:ARG:NH1	2:H:8048:LYS:HZ2	2.18	0.41
2:H:8048:LYS:O	2:H:8049:VAL:HG23	2.21	0.41
2:D:4003:ARG:HH11	2:D:4061:SER:HB3	1.86	0.41
1:E:5097:TRP:CE2	1:E:5099:GLN:NE2	2.89	0.41
1:C:3122:ASP:O	1:C:3123:LEU:HD23	2.20	0.41
2:D:4059:ASP:O	2:D:4060:TRP:HB2	2.20	0.41
1:G:7215:LEU:HD11	1:G:7259:CYS:SG	2.61	0.41
1:E:5066:ILE:O	1:E:5066:ILE:HG22	2.21	0.41
2:B:2003:ARG:HH12	2:B:2061:SER:HA	1.85	0.41
2:D:4050:GLU:HB2	2:D:4067:TYR:CZ	2.55	0.41
1:G:7225:THR:O	1:G:7225:THR:HG22	2.20	0.41
1:A:1079:MET:HA	1:A:1082:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3122:ASP:CG	2:D:4060:TRP:HE1	2.23	0.41
2:D:4056:PHE:HA	2:D:4062:PHE:HA	2.03	0.41
1:C:3167:VAL:O	1:C:3167:VAL:HG12	2.19	0.41
1:E:5255:GLN:HB3	1:E:5255:GLN:HE21	1.61	0.41
1:C:3198:ASP:OD2	1:C:3248:VAL:HB	2.21	0.41
1:C:3027:TYR:HA	1:C:3031:MET:O	2.21	0.41
1:G:7205:ALA:O	1:G:7206:LEU:HD23	2.21	0.41
1:E:5128:GLU:CG	1:E:5131:SER:HB2	2.50	0.41
1:A:1128:GLU:OE2	1:A:1131:SER:CB	2.69	0.41
2:F:6016:GLU:HB3	2:F:6019:LYS:CD	2.47	0.41
2:B:2095:TRP:CZ2	2:B:2097:ARG:HA	2.55	0.41
1:E:5104:GLU:HB3	1:E:5109:LEU:HD22	2.03	0.41
1:C:3222:GLU:O	1:C:3223:GLU:O	2.39	0.41
2:B:2035:ILE:CD1	2:B:2083:ASN:O	2.59	0.41
1:A:1060:TRP:HA	1:A:1063:GLN:HG3	2.02	0.41
1:G:7167:VAL:O	1:G:7170:LYS:N	2.50	0.41
1:A:1117:ALA:HB2	2:B:2060:TRP:CE2	2.56	0.41
1:C:3042:THR:HA	1:C:3043:PRO:HD3	1.90	0.41
1:C:3269:PRO:O	1:C:3270:LEU:HD13	2.21	0.41
2:B:2036:GLU:HG2	2:B:2081:ARG:HH22	1.86	0.41
1:C:3012:VAL:HG12	1:C:3013:SER:N	2.36	0.41
1:E:5231:VAL:HG23	1:E:5243:LYS:HG3	2.02	0.40
1:A:1035:ARG:HH12	1:A:1044:ARG:CZ	2.34	0.40
1:E:5191:ARG:HH11	1:E:5191:ARG:HG2	1.85	0.40
1:E:5187:ALA:HB3	1:E:5272:LEU:HD21	2.03	0.40
1:A:1100:ASP:O	1:A:1113:TYR:HD1	2.04	0.40
1:C:3096:GLN:NE2	2:D:4031:HIS:CD2	2.90	0.40
1:G:7260:HIS:CD2	1:G:7260:HIS:N	2.90	0.40
1:C:3274:TRP:O	1:C:3275:GLU:O	2.40	0.40
1:E:5200:THR:HG22	1:E:5201:LEU:N	2.36	0.40
1:A:1059:ASP:N	1:A:1170:LYS:NZ	2.67	0.40
1:C:3233:THR:HA	1:C:3242:GLN:O	2.20	0.40
1:E:5060:TRP:CH2	1:E:5170:LYS:HE3	2.56	0.40
1:E:5053:GLU:OE1	1:E:5053:GLU:HA	2.21	0.40
1:G:7189:VAL:HG23	1:G:7272:LEU:CD1	2.37	0.40
2:B:2033:SER:O	2:B:2035:ILE:N	2.54	0.40
1:E:5125:THR:C	1:E:5126:LEU:HD22	2.42	0.40
1:G:7260:HIS:HA	1:G:7270:LEU:O	2.22	0.40
1:A:1201:LEU:HD21	1:A:1254:VAL:HG11	2.02	0.40
2:H:8086:THR:O	2:H:8087:LEU:HD23	2.22	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	242/260 (93%)	181 (75%)	37 (15%)	24 (10%)	1	0
1	C	242/260 (93%)	180 (74%)	40 (16%)	22 (9%)	1	1
1	E	243/260 (94%)	192 (79%)	39 (16%)	12 (5%)	3	3
1	G	239/260 (92%)	178 (74%)	34 (14%)	27 (11%)	0	0
2	B	97/99 (98%)	89 (92%)	5 (5%)	3 (3%)	5	7
2	D	97/99 (98%)	85 (88%)	11 (11%)	1 (1%)	19	34
2	F	97/99 (98%)	86 (89%)	9 (9%)	2 (2%)	9	14
2	H	97/99 (98%)	84 (87%)	11 (11%)	2 (2%)	9	14
All	All	1354/1436 (94%)	1075 (79%)	186 (14%)	93 (7%)	1	1

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1052	LEU
1	A	1054	GLN
1	A	1057	ALA
1	A	1088	SER
1	A	1100	ASP
1	A	1109	LEU
1	A	1132	SER
1	A	1275	GLU
1	C	3015	PRO
1	C	3114	ASN
1	C	3126	LEU
1	C	3130	PRO
1	C	3197	GLY
1	C	3223	GLU
1	C	3247	VAL
1	E	5052	LEU
1	E	5100	ASP

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Mol	Chain	Res	Type
1	E	5131	SER
1	E	5223	GLU
1	G	7132	SER
1	G	7220	ASP
1	G	7223	GLU
1	G	7225	THR
1	A	1023	ILE
1	A	1029	ASP
1	A	1059	ASP
1	A	1108	HIS
1	A	1128	GLU
1	A	1131	SER
1	A	1251	LEU
2	B	2034	ASP
2	B	2057	SER
1	C	3029	ASP
1	C	3108	HIS
1	C	3248	VAL
2	F	6034	ASP
1	G	7056	GLU
1	G	7057	ALA
1	G	7058	ASP
1	G	7059	ASP
1	G	7086	ASN
1	G	7088	SER
1	G	7110	CYS
1	G	7131	SER
1	G	7226	GLN
1	G	7248	VAL
2	H	8034	ASP
1	A	1104	GLU
1	A	1126	LEU
1	A	1127	SER
1	A	1129	ASN
1	A	1243	LYS
1	A	1269	PRO
1	C	3116	LEU
1	C	3128	GLU
1	C	3224	LEU
1	C	3275	GLU
1	E	5015	PRO
1	E	5074	SER

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Mol	Chain	Res	Type
1	G	7015	PRO
1	G	7084	PHE
1	G	7107	ARG
1	G	7193	PRO
1	G	7224	LEU
1	A	1105	PRO
1	A	1120	SER
2	B	2068	THR
1	C	3039	LYS
1	C	3110	CYS
1	C	3198	ASP
1	C	3243	LYS
1	C	3269	PRO
2	D	4047	GLU
1	E	5055	GLU
1	E	5056	GLU
1	E	5128	GLU
1	E	5129	ASN
1	E	5196	GLU
1	G	7040	GLU
1	G	7104	GLU
1	A	1055	GLU
1	C	3054	GLN
1	C	3129	ASN
1	G	7052	LEU
1	G	7054	GLN
1	G	7055	GLU
1	G	7100	ASP
2	H	8097	ARG
1	E	5106	ASP
2	F	6020	SER
1	C	3195	PRO
1	G	7167	VAL
1	G	7199	VAL

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	223/235 (95%)	167 (75%)	56 (25%)	1	1
1	C	219/235 (93%)	174 (80%)	45 (20%)	1	2
1	E	222/235 (94%)	175 (79%)	47 (21%)	1	2
1	G	218/235 (93%)	163 (75%)	55 (25%)	1	1
2	B	94/94 (100%)	79 (84%)	15 (16%)	3	5
2	D	94/94 (100%)	78 (83%)	16 (17%)	2	4
2	F	94/94 (100%)	78 (83%)	16 (17%)	2	4
2	H	94/94 (100%)	74 (79%)	20 (21%)	1	2
All	All	1258/1316 (96%)	988 (78%)	270 (22%)	1	2

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1019	GLU
1	A	1035	ARG
1	A	1038	SER
1	A	1039	LYS
1	A	1044	ARG
1	A	1065	HIS
1	A	1068	THR
1	A	1073	LEU
1	A	1075	GLU
1	A	1077	ASN
1	A	1078	LEU
1	A	1080	THR
1	A	1081	LEU
1	A	1082	VAL
1	A	1086	ASN
1	A	1094	THR
1	A	1098	LEU
1	A	1099	GLN
1	A	1107	ARG
1	A	1109	LEU
1	A	1111	LEU
1	A	1115	GLN
1	A	1121	GLU
1	A	1126	LEU
1	A	1133	CYS
1	A	1159	HIS
1	A	1160	LEU

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Mol	Chain	Res	Type
1	A	1163	HIS
1	A	1165	SER
1	A	1166	ASP
1	A	1167	VAL
1	A	1171	TYR
1	A	1173	GLU
1	A	1176	LYS
1	A	1177	GLU
1	A	1178	ARG
1	A	1183	ASP
1	A	1186	LYS
1	A	1191	ARG
1	A	1194	ARG
1	A	1196	GLU
1	A	1198	ASP
1	A	1200	THR
1	A	1220	ASP
1	A	1224	LEU
1	A	1225	THR
1	A	1229	GLU
1	A	1230	PHE
1	A	1234	ARG
1	A	1251	LEU
1	A	1253	LYS
1	A	1255	GLN
1	A	1259	CYS
1	A	1264	GLU
1	A	1272	LEU
1	A	1273	ARG
2	B	2001	ILE
2	B	2003	ARG
2	B	2004	THR
2	B	2006	LYS
2	B	2012	ARG
2	B	2020	SER
2	B	2035	ILE
2	B	2045	ARG
2	B	2048	LYS
2	B	2058	LYS
2	B	2070	PHE
2	B	2075	LYS
2	B	2081	ARG

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Mol	Chain	Res	Type
2	B	2085	VAL
2	B	2098	ASP
1	C	3006	ARG
1	C	3014	ARG
1	C	3023	ILE
1	C	3024	ILE
1	C	3034	LEU
1	C	3035	ARG
1	C	3039	LYS
1	C	3044	ARG
1	C	3058	ASP
1	C	3061	GLU
1	C	3068	THR
1	C	3075	GLU
1	C	3078	LEU
1	C	3079	MET
1	C	3083	HIS
1	C	3086	ASN
1	C	3087	LYS
1	C	3090	ASP
1	C	3094	THR
1	C	3102	ASP
1	C	3111	LEU
1	C	3120	SER
1	C	3121	GLU
1	C	3131	SER
1	C	3163	HIS
1	C	3165	SER
1	C	3169	GLN
1	C	3170	LYS
1	C	3171	TYR
1	C	3177	GLU
1	C	3181	ARG
1	C	3190	THR
1	C	3192	HIS
1	C	3196	GLU
1	C	3201	LEU
1	C	3213	ILE
1	C	3224	LEU
1	C	3233	THR
1	C	3234	ARG
1	C	3242	GLN

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Mol	Chain	Res	Type
1	C	3257	TYR
1	C	3264	GLU
1	C	3272	LEU
1	C	3273	ARG
1	C	3274	TRP
2	D	4003	ARG
2	D	4011	SER
2	D	4012	ARG
2	D	4016	GLU
2	D	4020	SER
2	D	4045	ARG
2	D	4048	LYS
2	D	4052	SER
2	D	4057	SER
2	D	4069	GLU
2	D	4070	PHE
2	D	4075	LYS
2	D	4081	ARG
2	D	4085	VAL
2	D	4091	LYS
2	D	4097	ARG
1	E	5014	ARG
1	E	5019	GLU
1	E	5035	ARG
1	E	5039	LYS
1	E	5042	THR
1	E	5045	MET
1	E	5051	TRP
1	E	5055	GLU
1	E	5059	ASP
1	E	5060	TRP
1	E	5062	GLN
1	E	5065	HIS
1	E	5066	ILE
1	E	5068	THR
1	E	5072	GLN
1	E	5076	ARG
1	E	5077	ASN
1	E	5080	THR
1	E	5081	LEU
1	E	5094	THR
1	E	5099	GLN

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Mol	Chain	Res	Type
1	E	5107	ARG
1	E	5108	HIS
1	E	5109	LEU
1	E	5120	SER
1	E	5129	ASN
1	E	5132	SER
1	E	5133	CYS
1	E	5161	GLU
1	E	5165	SER
1	E	5176	LYS
1	E	5178	ARG
1	E	5186	LYS
1	E	5191	ARG
1	E	5192	HIS
1	E	5194	ARG
1	E	5214	THR
1	E	5222	GLU
1	E	5223	GLU
1	E	5225	THR
1	E	5232	GLU
1	E	5234	ARG
1	E	5248	VAL
1	E	5253	LYS
1	E	5255	GLN
1	E	5259	CYS
1	E	5264	GLU
2	F	6001	ILE
2	F	6004	THR
2	F	6007	ILE
2	F	6008	GLN
2	F	6012	ARG
2	F	6016	GLU
2	F	6044	GLU
2	F	6045	ARG
2	F	6051	HIS
2	F	6058	LYS
2	F	6070	PHE
2	F	6073	THR
2	F	6081	ARG
2	F	6085	VAL
2	F	6086	THR
2	F	6091	LYS

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Mol	Chain	Res	Type
1	G	7004	SER
1	G	7006	ARG
1	G	7014	ARG
1	G	7019	GLU
1	G	7031	MET
1	G	7034	LEU
1	G	7035	ARG
1	G	7039	LYS
1	G	7042	THR
1	G	7044	ARG
1	G	7059	ASP
1	G	7062	GLN
1	G	7064	THR
1	G	7075	GLU
1	G	7078	LEU
1	G	7079	MET
1	G	7084	PHE
1	G	7087	LYS
1	G	7090	ASP
1	G	7094	THR
1	G	7096	GLN
1	G	7098	LEU
1	G	7102	ASP
1	G	7106	ASP
1	G	7107	ARG
1	G	7116	LEU
1	G	7121	GLU
1	G	7122	ASP
1	G	7126	LEU
1	G	7159	HIS
1	G	7160	LEU
1	G	7163	HIS
1	G	7165	SER
1	G	7167	VAL
1	G	7170	LYS
1	G	7177	GLU
1	G	7181	ARG
1	G	7191	ARG
1	G	7200	THR
1	G	7206	LEU
1	G	7212	ASP
1	G	7214	THR

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Mol	Chain	Res	Type
1	G	7218	GLN
1	G	7220	ASP
1	G	7222	GLU
1	G	7223	GLU
1	G	7229	GLU
1	G	7234	ARG
1	G	7243	LYS
1	G	7248	VAL
1	G	7251	LEU
1	G	7255	GLN
1	G	7256	SER
1	G	7268	GLU
1	G	7270	LEU
2	H	8001	ILE
2	H	8003	ARG
2	H	8004	THR
2	H	8011	SER
2	H	8012	ARG
2	H	8013	HIS
2	H	8016	GLU
2	H	8019	LYS
2	H	8020	SER
2	H	8027	VAL
2	H	8035	ILE
2	H	8053	ASP
2	H	8055	SER
2	H	8059	ASP
2	H	8070	PHE
2	H	8075	LYS
2	H	8077	GLU
2	H	8088	SER
2	H	8089	GLN
2	H	8099	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1003	HIS
1	A	1054	GLN
1	A	1115	GLN
1	A	1158	GLN
1	A	1169	GLN

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Mol	Chain	Res	Type
1	A	1188	HIS
1	A	1255	GLN
1	A	1260	HIS
1	A	1263	HIS
2	B	2002	GLN
2	B	2024	ASN
1	C	3032	GLN
1	C	3054	GLN
1	C	3063	GLN
1	C	3070	GLN
1	C	3086	ASN
1	C	3169	GLN
1	C	3263	HIS
1	E	5062	GLN
1	E	5077	ASN
1	E	5163	HIS
1	E	5169	GLN
1	E	5188	HIS
1	E	5192	HIS
1	E	5218	GLN
1	E	5255	GLN
1	E	5260	HIS
2	F	6008	GLN
2	F	6013	HIS
2	F	6024	ASN
1	G	7003	HIS
1	G	7063	GLN
1	G	7072	GLN
1	G	7086	ASN
1	G	7096	GLN
2	H	8042	ASN
2	H	8051	HIS
2	H	8083	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	248/260 (95%)	0.82	26 (10%) 8 8	11, 26, 37, 42	0
1	C	248/260 (95%)	1.09	40 (16%) 3 2	9, 29, 40, 42	0
1	E	247/260 (95%)	0.69	24 (9%) 10 10	9, 24, 38, 46	0
1	G	245/260 (94%)	0.67	17 (6%) 20 22	9, 24, 37, 43	0
2	B	99/99 (100%)	0.25	1 (1%) 84 86	9, 15, 25, 31	0
2	D	99/99 (100%)	0.45	3 (3%) 54 59	9, 17, 30, 35	0
2	F	99/99 (100%)	0.24	0 100 100	9, 16, 24, 27	0
2	H	99/99 (100%)	0.28	0 100 100	9, 15, 28, 36	0
All	All	1384/1436 (96%)	0.67	111 (8%) 15 16	9, 23, 37, 46	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1134	THR	6.4
1	C	3134	THR	6.2
1	A	1130	PRO	5.2
1	C	3062	GLN	5.0
1	A	1089	MET	4.8
1	G	7254	VAL	4.4
1	C	3247	VAL	4.2
1	C	3267	PRO	4.2
1	G	7257	TYR	4.2
1	A	1251	LEU	4.1
1	C	3067	VAL	3.9
1	C	3248	VAL	3.8
1	E	5227	ASP	3.7
1	G	7195	PRO	3.6
1	C	3187	ALA	3.5
1	G	7067	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	3073	LEU	3.4
1	E	5089	MET	3.4
1	G	7066	ILE	3.4
1	E	5087	LYS	3.3
1	E	5133	CYS	3.2
1	E	5074	SER	3.2
1	G	7247	VAL	3.2
1	C	3126	LEU	3.1
1	A	1017	LEU	3.1
1	C	3086	ASN	3.1
1	G	7057	ALA	3.0
1	E	5069	ILE	3.0
1	E	5193	PRO	3.0
1	E	5057	ALA	3.0
1	G	7274	TRP	2.9
1	C	3179	LEU	2.9
1	E	5056	GLU	2.9
1	A	1272	LEU	2.9
1	E	5075	GLU	2.8
1	G	7133	CYS	2.8
1	C	3079	MET	2.8
1	A	1088	SER	2.8
1	A	1158	GLN	2.8
1	A	1179	LEU	2.7
1	A	1249	VAL	2.7
1	A	1181	ARG	2.7
1	A	1254	VAL	2.7
1	A	1009	TYR	2.7
1	G	7250	PRO	2.7
1	G	7059	ASP	2.7
1	C	3265	GLY	2.7
1	C	3263	HIS	2.6
1	C	3182	SER	2.6
1	C	3225	THR	2.5
1	E	5249	VAL	2.5
1	C	3269	PRO	2.5
1	E	5105	PRO	2.5
1	E	5073	LEU	2.5
1	C	3254	VAL	2.5
2	D	4001	ILE	2.5
1	G	7065	HIS	2.5
1	C	3009	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	5085	TYR	2.5
1	E	5230	PHE	2.4
1	G	7228	VAL	2.4
1	C	3200	THR	2.4
1	C	3255	GLN	2.3
1	C	3177	GLU	2.3
1	E	5038	SER	2.3
1	E	5228	VAL	2.3
1	G	7200	THR	2.3
1	A	1260	HIS	2.3
1	C	3257	TYR	2.3
1	E	5160	LEU	2.3
1	C	3249	VAL	2.3
1	G	7199	VAL	2.3
1	E	5023	ILE	2.3
1	A	1074	SER	2.3
1	C	3214	THR	2.3
1	A	1199	VAL	2.3
1	A	1219	LYS	2.3
1	E	5200	THR	2.3
1	C	3228	VAL	2.3
1	C	3003	HIS	2.2
1	A	1224	LEU	2.2
1	E	5195	PRO	2.2
2	D	4088	SER	2.2
1	C	3197	GLY	2.2
1	C	3261	VAL	2.2
1	E	5009	TYR	2.2
1	C	3268	GLU	2.2
1	G	7078	LEU	2.2
1	A	1127	SER	2.1
1	G	7256	SER	2.1
2	B	2001	ILE	2.1
1	C	3107	ARG	2.1
1	A	1075	GLU	2.1
1	C	3039	LYS	2.1
1	A	1193	PRO	2.1
1	C	3215	LEU	2.1
1	C	3065	HIS	2.1
1	A	1159	HIS	2.1
1	C	3127	SER	2.1
1	C	3133	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	5116	LEU	2.1
1	C	3125	THR	2.1
1	E	5134	THR	2.1
2	D	4086	THR	2.1
1	A	1107	ARG	2.1
1	C	3066	ILE	2.1
1	C	3258	THR	2.0
1	C	3199	VAL	2.0
1	A	1059	ASP	2.0
1	A	1225	THR	2.0
1	A	1274	TRP	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.