



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 11:11 AM UTC

PDB ID : 1R3H / pdb_00001r3h
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

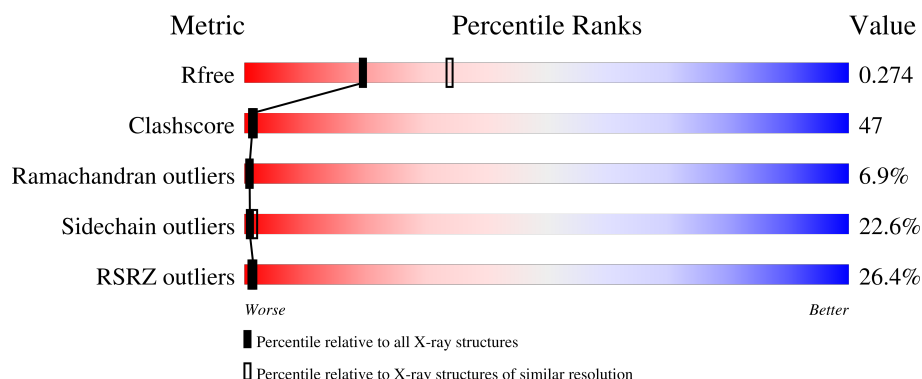
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	260	30% 23% 47% 23% 5%
1	C	260	33% 23% 51% 21% 5%
1	E	260	27% 27% 50% 18% 5%
1	G	260	30% 25% 46% 22% 6%
2	B	99	10% 36% 51% 12%

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Mol	Chain	Length	Quality of chain
2	D	99	21% 45% 48% 6%
2	F	99	12% 43% 45% 10%
2	H	99	13% 30% 51% 19%

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			

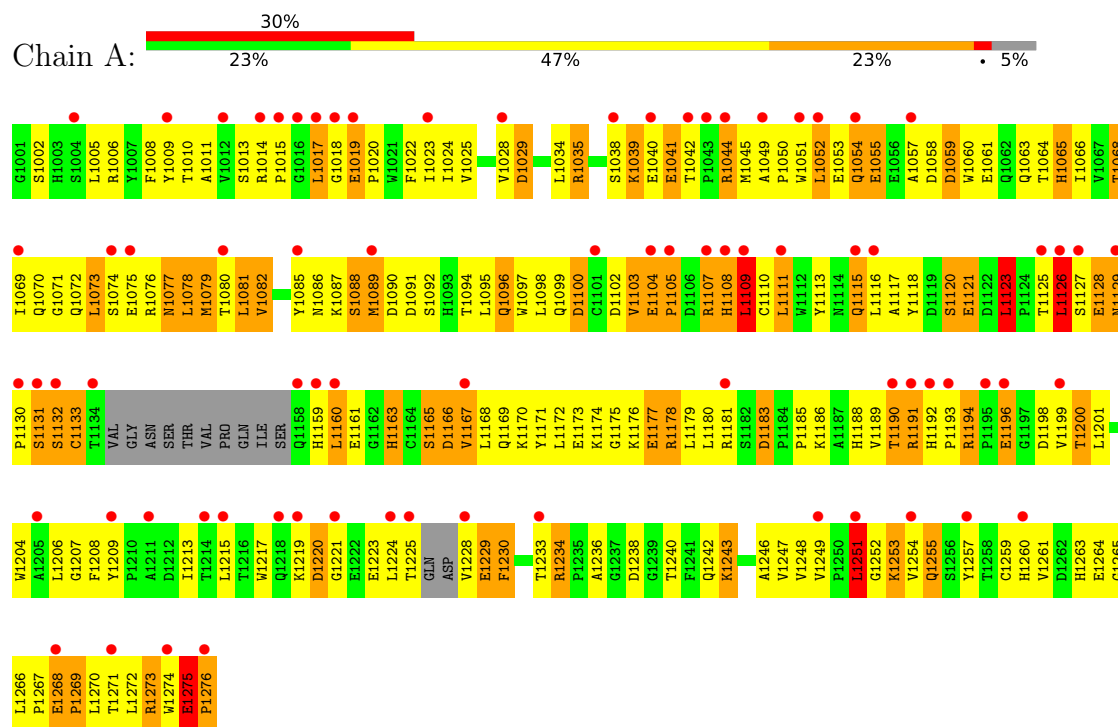
- Molecule 2 is a protein called Beta-2-microglobulin.

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			

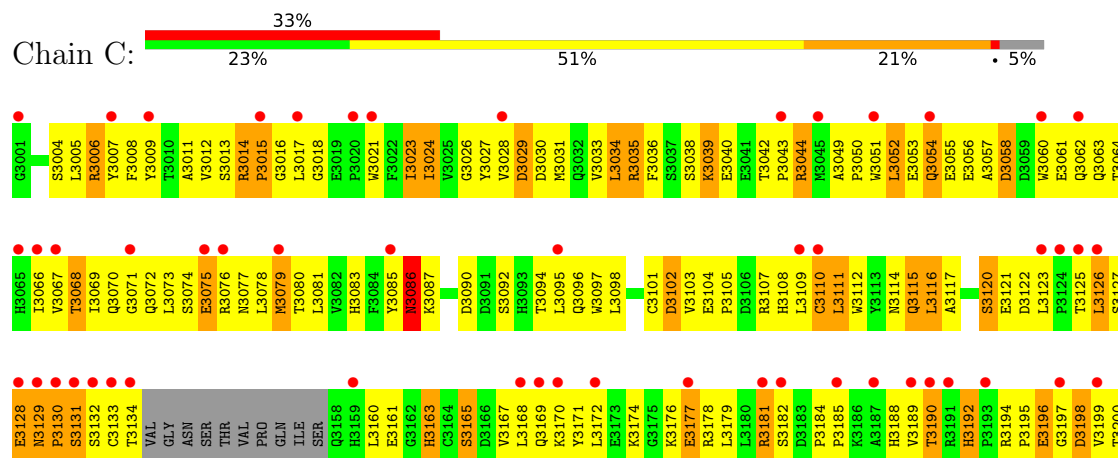
3 Residue-property plots [i](#)

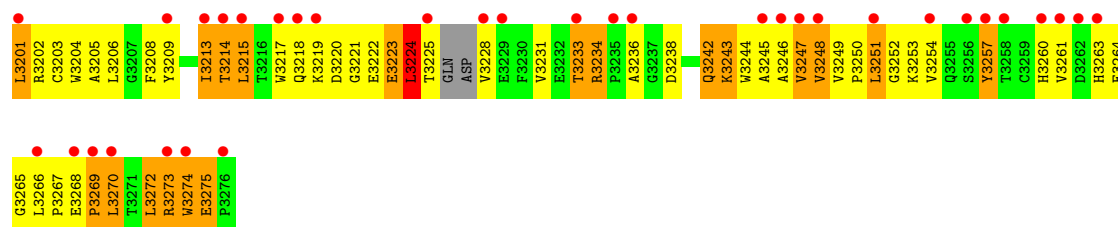
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: MHC H2-TL-T10-129

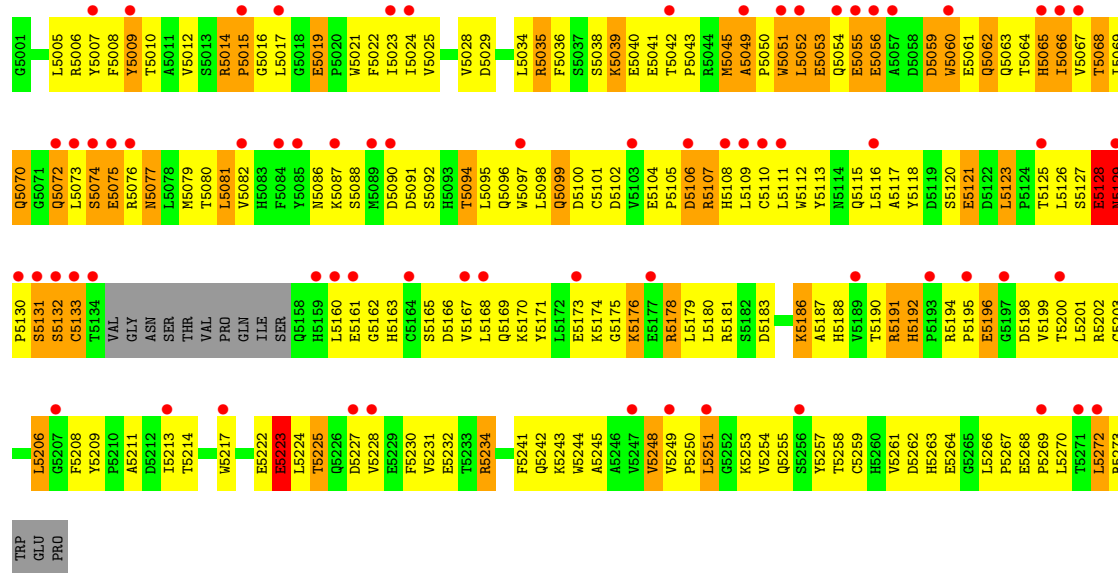


• Molecule 1: MHC H2-TL-T10-129

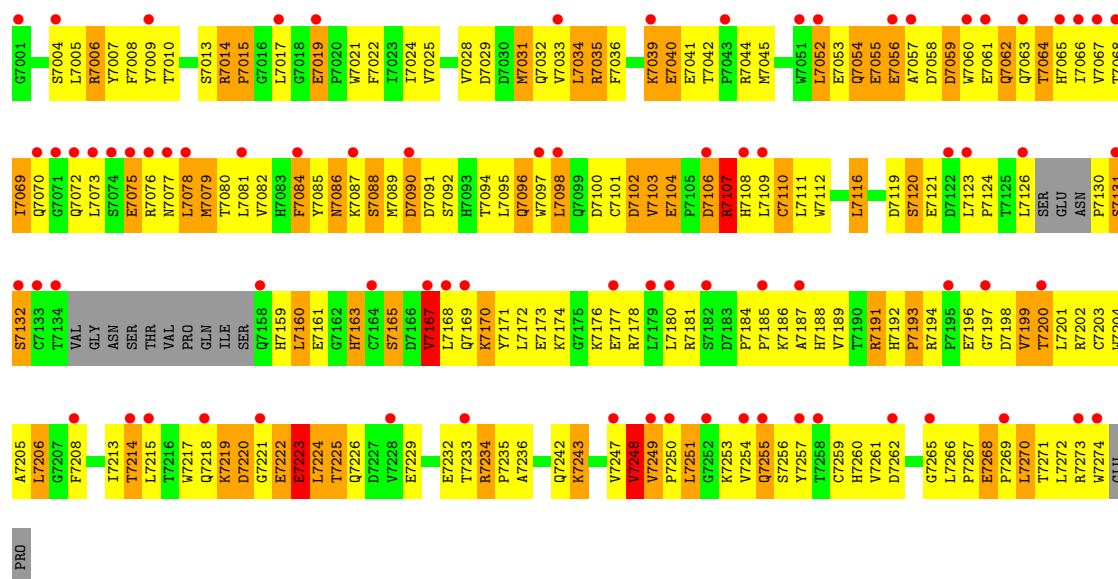




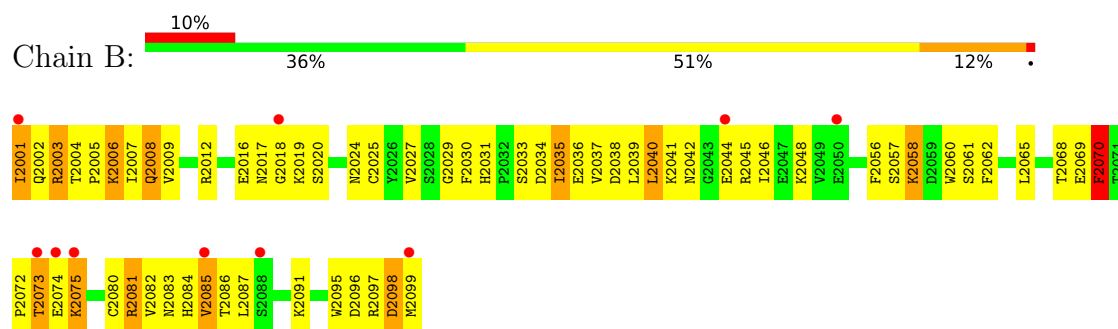
● Molecule 1: MHC H2-TL-T10-129



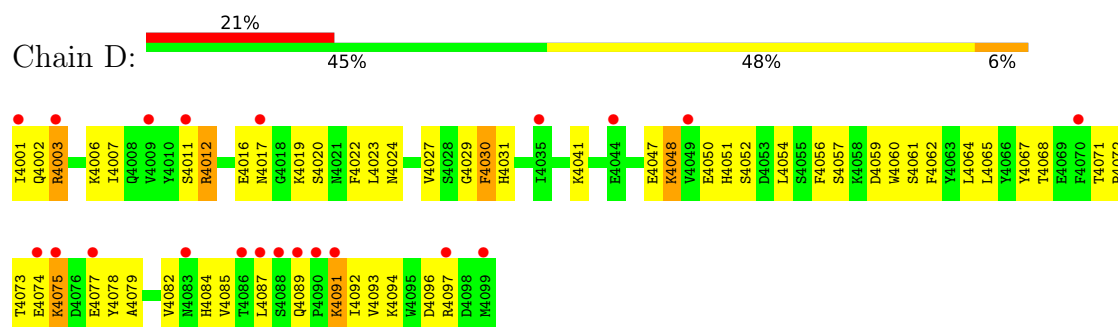
● Molecule 1: MHC H2-TL-T10-129



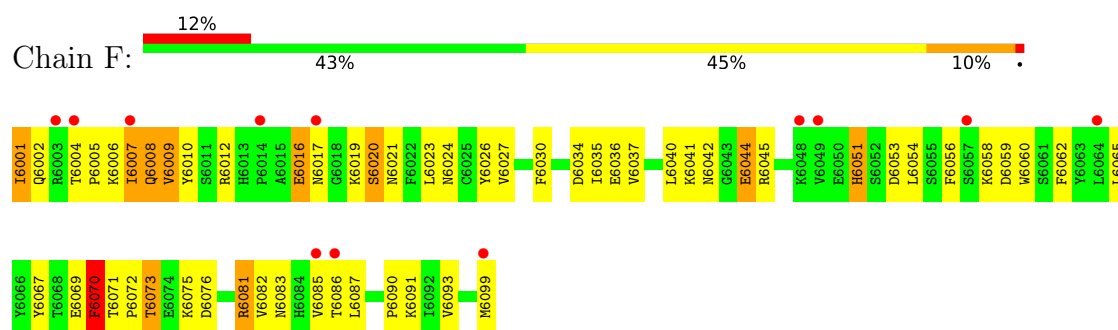
- Molecule 2: Beta-2-microglobulin



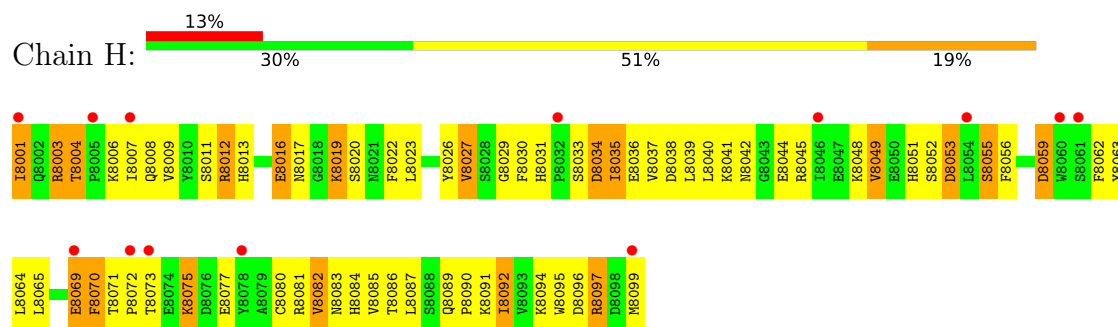
- Molecule 2: Beta-2-microglobulin



- 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 46.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.5 (46.00-2.50) 91.9 (46.00-2.50)	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 , 0.274	Depositor DCC
R_{free} test set	2225 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 71.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.407 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.78	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.43	0/2078	1.00	5/2830 (0.2%)
1	C	0.43	0/2058	1.01	3/2803 (0.1%)
1	E	0.45	1/2062 (0.0%)	1.03	11/2809 (0.4%)
1	G	0.46	1/2043 (0.0%)	1.03	3/2784 (0.1%)
2	B	0.36	0/852	1.00	1/1152 (0.1%)
2	D	0.34	0/852	0.93	1/1152 (0.1%)
2	F	0.36	0/852	1.01	1/1152 (0.1%)
2	H	0.35	0/852	1.00	2/1152 (0.2%)
All	All	0.42	2/11649 (0.0%)	1.01	27/15834 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	7255	GLN	CD-OE1	5.69	1.34	1.23
1	E	5049	ALA	N-CA	5.30	1.51	1.45

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	5070	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	E	5051	TRP	N-CA-C	7.84	120.72	111.71
2	F	6070	PHE	CA-CB-CG	7.03	120.83	113.80
1	E	5123	LEU	O-C-N	6.98	127.60	121.39
1	E	5123	LEU	CA-C-N	6.88	127.26	119.83
1	E	5123	LEU	C-N-CA	6.88	127.26	119.83
1	E	5070	GLN	CG-CD-NE2	6.62	126.34	116.40
2	D	4030	PHE	N-CA-C	6.55	118.48	109.18
1	A	1208	PHE	N-CA-C	6.36	119.47	110.50
1	G	7219	LYS	O-C-N	6.30	130.35	123.10
1	C	3052	LEU	CA-C-N	6.07	133.13	121.54
1	C	3052	LEU	C-N-CA	6.07	133.13	121.54
1	E	5009	TYR	CA-CB-CG	5.87	124.47	113.90
1	E	5050	PRO	O-C-N	-5.65	115.01	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	7120	SER	N-CA-CB	-5.51	107.89	114.17
1	E	5230	PHE	N-CA-C	5.51	116.63	108.86
2	H	8070	PHE	CA-CB-CG	5.42	119.22	113.80
1	E	5208	PHE	N-CA-C	5.31	118.34	110.48
1	C	3086	ASN	CA-CB-CG	5.26	117.86	112.60
1	A	1268	GLU	O-C-N	5.24	125.92	121.84
1	E	5053	GLU	N-CA-C	-5.17	101.44	109.72
1	G	7219	LYS	CA-C-O	-5.11	115.25	121.28
1	A	1123	LEU	CA-C-N	5.10	125.34	119.83
1	A	1123	LEU	C-N-CA	5.10	125.34	119.83
1	A	1275	GLU	N-CA-C	5.08	121.03	109.81
2	H	8031	HIS	N-CA-C	-5.07	98.60	109.81
2	B	2070	PHE	CA-CB-CG	5.04	118.84	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2019	0	1901	248	0
1	C	2001	0	1871	228	0
1	E	2005	0	1891	187	0
1	G	1986	0	1866	182	0
2	B	829	0	791	63	0
2	D	829	0	791	41	0
2	F	829	0	791	56	0
2	H	829	0	791	76	0
All	All	11327	0	10693	1034	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 47.

All (1034) 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:A:1034:LEU:HD12	1:A:1045:MET:HE1	1.55	0.88
1:E:5261:VAL:HB	1:E:5270:LEU:HB3	1.53	0.88
1:C:3265:GLY:O	1:C:3267:PRO:HD3	1.73	0.88
1:G:7206:LEU:HD22	1:G:7242:GLN:HG2	1.53	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:A:1095:LEU:HD21	1:A:1116:LEU:HD23	1.60	0.84
1:E:5225:THR:O	1:E:5228:VAL:HG12	1.76	0.84
1:A:1103:VAL:HG11	1:A:1165:SER:HB3	1.60	0.84
1:E:5051:TRP:CD1	1:E:5051:TRP:H	1.94	0.83
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1228:VAL:O	1:A:1228:VAL:HG13	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:1128:GLU:HG2	1:A:1129:ASN:H	1.48	0.79
1:A:1263:HIS:CD2	1:A:1265:GLY:H	2.01	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:C:3050:PRO:HA	1:C:3054:GLN:NE2	2.00	0.76
1:A:1194:ARG:HH11	1:A:1194:ARG:HB2	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:G:7119:ASP:O	1:G:7120:SER:OG	2.02	0.75
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:3023:ILE:HD13	1:C:3023:ILE:O	1.85	0.75
1:C:3051:TRP:CD2	1:C:3178:ARG:HD2	2.21	0.75
1:C:3246:ALA:O	1:C:3247:VAL:HG13	1.86	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
1:A:1233:THR:HG22	1:A:1243:LYS:HD2	1.69	0.73
2:D:4020:SER:HA	2:D:4071:THR:HG22	1.70	0.73
1:A:1069:ILE:O	1:A:1073:LEU:HD21	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1194:ARG:HH12	1:A:1198:ASP:HB2	1.53	0.73
1:C:3189:VAL:HG13	1:C:3202:ARG:O	1.89	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:A:1009:TYR:HE1	1:A:1071:GLY:HA2	1.53	0.72
1:G:7194:ARG:HE	1:G:7196:GLU:HB2	1.52	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:G:7053:GLU:CD	1:G:7174:LYS:HD3	2.14	0.72
1:A:1103:VAL:HG12	1:A:1104:GLU:H	1.54	0.72
1:C:3213:ILE:HD13	1:C:3214:THR:C	2.15	0.72
1:A:1017:LEU:HD22	2:H:8070:PHE:HA	1.72	0.72
1:A:1274:TRP:O	1:A:1275:GLU:HB2	1.89	0.72
1:C:3249:VAL:HG11	1:C:3254:VAL: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:A:1230:PHE:HD1	1:A:1230:PHE:C	1.97	0.71
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
2:B:2073:THR:HG22	2:B:2075:LYS:H	1.54	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:D:4003:ARG:HG2	2:D:4029:GLY:O	1.89	0.71
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:A:1120:SER:HB2	2:B:2031:HIS:NE2	2.06	0.71
1:E:5163:HIS:HA	1:E:5166:ASP:OD1	1.91	0.71
1:E:5105:PRO:O	1:E:5106:ASP:OD1	2.09	0.70
1:C:3062:GLN:O	1:C:3066:ILE:HG12	1.91	0.70
1:C:3213:ILE:HD11	1:C:3261:VAL:HG13	1.73	0.70
1:E:5068:THR:O	1:E:5072:GLN:NE2	2.20	0.70
1:G:7101:CYS:HA	1:G:7111:LEU:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:2041:LYS:O	2:B:2044:GLU:HG2	1.92	0.70
2:D:4001:ILE:HG23	2:D:4002:GLN:H	1.56	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:C:3073:LEU:HG	1:C:3076:ARG:NH1	2.07	0.69
1:E:5217:TRP:O	1:E:5224:LEU:HB2	1.92	0.69
1:A:1273:ARG:HH11	1:A:1273:ARG:HB2	1.58	0.69
1:E:5008:PHE:O	1:E:5024:ILE:HG23	1.92	0.69
1:G:7201:LEU:HB2	1:G:7247:VAL:HG22	1.75	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:7119:ASP:HB3	2:H:8001:ILE:HD13	1.74	0.68
1:G:7249:VAL:CG2	1:G:7254:VAL:HG22	2.22	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: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:A:1009:TYR:OH	1:A:1074:SER:HB3	1.95	0.67
1:A:1230:PHE:C	1:A:1230:PHE:CD1	2.69	0.67
1:E:5111:LEU:HD23	1:E:5113:TYR:OH	1.95	0.67
1:A:1260:HIS:HA	1:A:1270:LEU:O	1.95	0.66
1:C:3069:ILE:HD13	1:C:3072:GLN:OE1	1.96	0.66
1:A:1034:LEU:HD12	1:A:1045:MET:CE	2.25	0.66
1:C:3075:GLU:O	1:C:3079:MET:HB2	1.96	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:E:5228:VAL:O	1:E:5228:VAL:HG13	1.94	0.66
1:G:7185:PRO:HB3	1:G:7208:PHE:HD2	1.60	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
1:A:1060:TRP:CH2	1:A:1170:LYS:HG2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1110:CYS:HB3	1:A:1133:CYS:N	2.10	0.66
2:D:4007:ILE:CD1	2:D:4082:VAL:HG21	2.26	0.66
2:H:8016:GLU:HG2	2:H:8019:LYS:HD2	1.77	0.66
1:E:5113:TYR:HA	1:E:5129:ASN:O	1.96	0.66
1:A:1254:VAL:HG12	1:A:1254:VAL:O	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:A:1052:LEU:HB2	1:A:1054:GLN:HE22	1.62	0.65
1:C:3189:VAL:HG12	1:C:3274:TRP:HD1	1.59	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:A:1073:LEU:O	1:A:1077:ASN:HB2	1.96	0.65
1:E:5201:LEU:HD11	1:E:5254:VAL:CG2	2.27	0.65
1:E:5059:ASP:OD1	1:E:5061:GLU:HG3	1.97	0.65
1:A:1052:LEU:HB2	1:A:1054:GLN:NE2	2.12	0.64
1:A:1263:HIS:H	1:A:1266:LEU:HD12	1.62	0.64
1:C:3028:VAL:HG11	1:C:3179:LEU:HD13	1.79	0.64
1:G:7185:PRO:HB3	1:G:7208:PHE:CD2	2.32	0.64
1:G:7215:LEU:HD12	1:G:7261:VAL:HG22	1.78	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:E:5063:GLN:NE2	1:E:5171:TYR:OH	2.29	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:1049:ALA:O	1:A:1054:GLN:NE2	2.30	0.64
1:A:1191:ARG:HG3	1:A:1274:TRP:HE1	1.63	0.64
1:C:3035:ARG:O	1:C:3043:PRO:HA	1.98	0.64
1:G:7069:ILE:HD13	1:G:7072:GLN:NE2	2.13	0.64
1:A:1191:ARG:HD3	1:A:1274:TRP:CE2	2.33	0.63
2:D:4079:ALA:HB1	2:D:4093:VAL:O	1.97	0.63
2:H:8081:ARG:HB2	2:H:8092:ILE:CD1	2.28	0.63
1:A:1252:GLY:HA3	1:A:1253:LYS:HE2	1.80	0.63
1:E:5009:TYR:HB3	1:E:5097:TRP:HB3	1.81	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
2:B:2027:VAL:HG21	2:B:2037:VAL:HG21	1.80	0.63
1:E:5131:SER:OG	1:E:5132:SER:N	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6087:LEU:HD13	2:F:6091:LYS:HG2	1.80	0.63
2:F:6024:ASN:HB3	2:F:6065:LEU:HD11	1.80	0.63
1:G:7249:VAL:HB	1:G:7253:LYS:O	1.98	0.63
1:A:1008:PHE:O	1:A:1024:ILE:HG23	1.99	0.63
1:G:7096:GLN:H	1:G:7096:GLN:HE21	1.47	0.63
1:A:1199:VAL:CG2	1:A:1251:LEU:HB2	2.28	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:A:1191:ARG:NH1	1:A:1199:VAL:HG11	2.14	0.62
1:C:3030:ASP:HB2	1:C:3209:TYR:CE1	2.35	0.62
1:C:3104:GLU:N	1:C:3109:LEU:HB3	2.07	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:1128:GLU:CG	1:A:1129:ASN:H	2.12	0.62
1:A:1193:PRO:HA	1:A:1199:VAL:HG22	1.82	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
1:C:3260:HIS:HA	1:C:3270:LEU:O	2.00	0.61
2:D:4007:ILE:HD12	2:D:4082:VAL:HG21	1.83	0.61
1:C:3233:THR:HA	1:C:3243:LYS:HB2	1.81	0.61
1:E:5213:ILE:HG13	1:E:5262:ASP:O	2.00	0.61
1:G:7028:VAL:HG23	1:G:7033:VAL:HG21	1.82	0.61
1:G:7201:LEU:HD11	1:G:7254:VAL:HG13	1.81	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
2:H:8007:ILE:HD11	2:H:8082:VAL:HG21	1.82	0.61
1:A:1169:GLN:O	1:A:1169:GLN:HG2	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:E:5010:THR:HG1	2:F:6062:PHE:HE2	1.49	0.61
1:E:5082:VAL:HG23	1:E:5118:TYR:OH	2.01	0.61
1:G:7201:LEU:HB2	1:G:7247:VAL:CG2	2.31	0.61
1:A:1010:THR:O	1:A:1022:PHE:HA	2.01	0.61
1:A:1263:HIS:N	1:A:1266:LEU:HD12	2.16	0.61
1:A:1125:THR:C	1:A:1126:LEU:HD22	2.26	0.60
1:C:3095:LEU:HG	1:C:3116:LEU:HD21	1.83	0.60
2:D:4073:THR:OG1	2:D:4075:LYS:HD3	2.01	0.60
1:G:7189:VAL:HG12	1:G:7274:TRP:HD1	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:8075:LYS:HB2	2:H:8075:LYS:NZ	2.16	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:B:2095:TRP:CH2	2:B:2097:ARG:HG2	2.36	0.60
2:H:8083:ASN:HD21	2:H:8090:PRO:CG	2.08	0.60
1:A:1040:GLU:HG3	1:A:1042:THR:H	1.67	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:C:3031:MET:HE2	1:C:3178:ARG:HB3	1.82	0.60
1:C:3112:TRP:CE2	1:C:3161:GLU:HB2	2.37	0.60
1:A:1236:ALA:O	2:B:2012:ARG:HD2	2.01	0.60
1:E:5062:GLN:O	1:E:5066:ILE:HG13	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:HA	1:A:1255:GLN:NE2	2.17	0.60
1:E:5034:LEU:HD23	1:E:5035:ARG:N	2.17	0.60
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:E:5249:VAL:HG22	1:E:5257:TYR:CE2	2.37	0.59
1:A:1028:VAL:HG12	1:A:1028:VAL:O	2.01	0.59
1:A:1105:PRO:O	1:A:1108:HIS:N	2.34	0.59
1:E:5070:GLN:OE1	1:E:5160:LEU:HD13	2.03	0.59
1:E:5176:LYS:O	1:E:5180:LEU:HB2	2.01	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:G:7247:VAL:O	1:G:7248:VAL:HG13	2.02	0.59
1:C:3201:LEU:HD12	1:C:3249:VAL:HG21	1.83	0.59
1:G:7103:VAL:HG23	1:G:7168:LEU:HD23	1.83	0.59
1:G:7170:LYS:O	1:G:7174:LYS:HB2	2.03	0.59
1:A:1103:VAL:HG21	1:A:1165:SER:HA	1.84	0.59
1:A:1170:LYS:CG	1:A:1174:LYS:HE2	2.30	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:E:5024:ILE:HD12	1:E:5067:VAL:HG13	1.83	0.59
1:E:5024:ILE:CD1	1:E:5067:VAL:HG13	2.33	0.59
1:G:7194:ARG:NE	1:G:7196:GLU:HB2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1126:LEU:HD13	1:A:1126:LEU:N	2.17	0.58
1:E:5258:THR:HA	1:E:5273:ARG:HA	1.84	0.58
2:F:6006:LYS:C	2:F:6007:ILE:HD13	2.27	0.58
2:H:8019:LYS:O	2:H:8072:PRO:HD2	2.03	0.58
1:E:5224:LEU:O	1:E:5228:VAL:HB	2.03	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:C:3049:ALA:O	1:C:3052:LEU:HG	2.03	0.58
2:F:6007:ILE:HD13	2:F:6007:ILE:N	2.18	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:HG	1:A:1005:LEU:O	2.03	0.58
2:B:2045:ARG:HG2	2:B:2045:ARG:O	2.04	0.58
2:B:2095:TRP:CZ3	2:B:2097:ARG:HG2	2.38	0.58
1:A:1028:VAL:O	1:A:1029:ASP:HB2	2.03	0.58
1:C:3073:LEU:CD2	1:C:3076:ARG:HH11	2.16	0.58
1:C:3120:SER:HB2	2:D:4003:ARG:HH22	1.69	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:3263:HIS:HB3	1:C:3266:LEU:HD12	1.84	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
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:A:1049:ALA:HB1	1:A:1051:TRP:CE2	2.40	0.57
1:A:1191:ARG:HD2	1:A:1201:LEU:CD2	2.34	0.57
1:C:3202:ARG:CG	1:C:3246:ALA:HB2	2.34	0.57
1:C:3215:LEU:HD23	1:C:3245:ALA:HB3	1.85	0.57
1:E:5104:GLU:HB3	1:E:5109:LEU:HB3	1.85	0.57
2:F:6007:ILE:HG13	2:F:6082:VAL:CG2	2.34	0.57
1:G:7102:ASP:O	1:G:7110:CYS:HA	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:3125:THR:C	1:C:3126:LEU:HD23	2.29	0.57
2:H:8003:ARG:HB3	2:H:8030:PHE:HA	1.86	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:3075:GLU:O	1:C:3075:GLU:HG3	2.05	0.56
1:E:5087:LYS:O	1:E:5088:SER:OG	2.22	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:G:7104:GLU:O	1:G:7104:GLU:HG2	2.05	0.56
1:G:7204:TRP:CZ2	2:H:8099:MET:HA	2.40	0.56
2:H:8051:HIS:HA	2:H:8065:LEU:O	2.06	0.56
1:A:1039:LYS:HE2	1:A:1039:LYS:O	2.06	0.56
1:C:3219:LYS:O	1:C:3220:ASP:HB2	2.04	0.56
1:E:5010:THR:HG21	2:F:6054:LEU:CD2	2.36	0.56
2:F:6027:VAL:HG12	2:F:6030:PHE:CD2	2.41	0.56
1:C:3250:PRO:HB2	1:C:3253:LYS:HG3	1.86	0.56
2:F:6001:ILE:HD13	2:F:6001:ILE:O	2.05	0.56
1:G:7064:THR:O	1:G:7068:THR:OG1	2.19	0.56
1:G:7206:LEU:CD2	1:G:7242:GLN:HG2	2.33	0.56
1:A:1252:GLY:C	1:A:1253:LYS:HE2	2.30	0.56
2:B:2087:LEU:HD13	2:B:2091:LYS:HG3	1.87	0.56
1:A:1009:TYR:HD1	1:A:1024:ILE:HD11	1.71	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
2:B:2024:ASN:HB3	2:B:2065:LEU:HD11	1.87	0.56
1:G:7107:ARG:O	1:G:7108:HIS:HB2	2.06	0.56
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:E:5202:ARG:NH2	2:F:6099:MET:HE1	2.20	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:A:1242:GLN:O	1:A:1243:LYS:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2056:PHE:HB3	2:B:2062:PHE:CD2	2.41	0.55
1:E:5035:ARG:NH2	1:E:5040:GLU:OE1	2.39	0.55
1:E:5258:THR:HB	1:E:5273:ARG:HG2	1.88	0.55
1:G:7081:LEU:HD22	1:G:7095:LEU:HD13	1.89	0.55
2:B:2001:ILE:HD13	2:B:2001:ILE:O	2.06	0.55
1:G:7167:VAL:HG12	1:G:7171:TYR:CE2	2.41	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
2:B:2096:ASP:HB3	2:B:2099:MET:HB2	1.88	0.55
1:C:3249:VAL:HG22	1:C:3257:TYR:CD2	2.41	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: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: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: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:A:1009:TYR:HB3	1:A:1097:TRP:O	2.07	0.55
2:B:2003:ARG:HD3	2:B:2031:HIS:HB3	1.88	0.55
1:E:5061:GLU:HA	1:E:5064:THR:CG2	2.34	0.55
1:G:7102:ASP:HB2	1:G:7111:LEU:CD1	2.37	0.55
1:A:1215:LEU:CD2	1:A:1261:VAL:HG22	2.36	0.55
2:B:2007:ILE:HD13	2:B:2082:VAL:CG2	2.37	0.55
1:E:5169:GLN:O	1:E:5169:GLN:HG2	2.08	0.55
2:F:6005:PRO:HB2	2:F:6007:ILE:CD1	2.36	0.55
1:A:1082:VAL:HG22	1:A:1089:MET:HG2	1.89	0.54
1:A:1201:LEU:HD11	1:A:1254:VAL:CG1	2.24	0.54
1:C:3222:GLU:HG3	1:C:3223:GLU:N	2.22	0.54
1:C:3231:VAL:O	1:C:3243:LYS:HG3	2.06	0.54
1:C:3272:LEU:HD12	1:C:3273:ARG:O	2.06	0.54
1:E:5010:THR:HG21	2:F:6054:LEU:HD23	1.90	0.54
1:G:7213:ILE:CG2	1:G:7243:LYS:HE2	2.37	0.54
1:C:3079:MET:HE3	1:C:3079:MET:O	2.07	0.54
1:C:3242:GLN:O	1:C:3243:LYS:HB2	2.07	0.54
1:G:7185:PRO:HA	1:G:7206:LEU:O	2.07	0.54
1:G:7200:THR:HA	1:G:7248:VAL:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7250:PRO:HD2	1:G:7253:LYS:HB2	1.89	0.54
1:C:3128:GLU:HG2	1:C:3129:ASN:N	2.23	0.54
1:G:7215:LEU:CD1	1:G:7261:VAL:HG22	2.37	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:C:3009:TYR:HB2	1:C:3070:GLN:NE2	2.23	0.54
1:E:5034:LEU:CD1	1:E:5063:GLN:NE2	2.71	0.54
1:G:7191:ARG:HH12	1:G:7193:PRO:HB3	1.73	0.54
1:G:7219:LYS:O	1:G:7221:GLY:N	2.41	0.54
1:G:7235:PRO:HG2	2:H:8065:LEU:HD13	1.89	0.54
1:A:1191:ARG:HD3	1:A:1274:TRP:NE1	2.23	0.54
1:C:3200:THR:O	1:C:3200:THR:HG22	2.07	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: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:G:7189:VAL:CG1	1:G:7274:TRP:HD1	2.21	0.54
1:A:1189:VAL:H	1:A:1275:GLU:HG3	1.72	0.53
2:B:2016:GLU:HA	2:B:2016:GLU:OE2	2.09	0.53
2:B:2025:CYS:HB2	2:B:2039:LEU:HD21	1.90	0.53
1:C:3050:PRO:HA	1:C:3054:GLN:HE21	1.72	0.53
1:A:1111:LEU:HD23	1:A:1113:TYR:OH	2.08	0.53
1:A:1194:ARG:HH11	1:A:1194:ARG:CB	2.19	0.53
1:E:5254:VAL:O	1:E:5254:VAL:HG22	2.07	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:C:3051:TRP:CE3	1:C:3178:ARG:HD2	2.43	0.53
1:E:5249:VAL:HG11	1:E:5254:VAL:HG23	1.90	0.53
2:B:2087:LEU:HD13	2:B:2091:LYS:CG	2.38	0.53
1:C:3081:LEU:HD22	1:C:3095:LEU:CD1	2.38	0.53
1:C:3103:VAL:O	1:C:3105:PRO:HD3	2.09	0.53
1:C:3128:GLU:HG2	1:C:3129:ASN:H	1.73	0.53
1:C:3189:VAL:HB	1:C:3274:TRP:HA	1.90	0.53
1:E:5035:ARG:HG3	2:F:6053:ASP:CG	2.34	0.53
2:F:6017:ASN:HD22	2:F:6017:ASN:N	2.06	0.53
1:G:7010:THR:O	1:G:7022:PHE:HA	2.08	0.53
2:H:8081:ARG:HA	2:H:8091:LYS:O	2.09	0.53
1:A:1014:ARG:HH12	2:H:8048:LYS:HZ2	1.55	0.53
1:G:7109:LEU:O	1:G:7110:CYS:HB2	2.09	0.53
2:H:8055:SER:HB3	2:H:8063:TYR:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1126:LEU:HD13	1:A:1126:LEU:H	1.72	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:1213:ILE:HD11	1:A:1261:VAL:HG13	1.91	0.53
1:C:3050:PRO:C	1:C:3052:LEU:H	2.16	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:C:3178:ARG:C	1:C:3181:ARG:HB3	2.35	0.52
1:G:7123:LEU:HB3	1:G:7124:PRO:HD2	1.90	0.52
1:G:7191:ARG:HD2	1:G:7274:TRP:CZ2	2.44	0.52
1:C:3023:ILE:HD11	2:D:4054:LEU:O	2.09	0.52
1:G:7233:THR:HG22	1:G:7243:LYS:HD3	1.90	0.52
2:H:8056:PHE:HB3	2:H:8062:PHE:CD2	2.44	0.52
1:A:1128:GLU:HG2	1:A:1129:ASN:N	2.19	0.52
1:C:3249:VAL:HG13	1:C:3257:TYR:CE1	2.44	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:E:5038:SER:O	1:E:5039:LYS:HB3	2.08	0.52
1:E:5194:ARG:CD	1:E:5196:GLU:OE2	2.55	0.52
1:G:7194:ARG:NH2	1:G:7196:GLU:HB3	2.24	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:8009:VAL:HG12	2:H:8023:LEU:HD11	1.92	0.52
2:H:8027:VAL:CG2	2:H:8064:LEU:HB2	2.40	0.52
1:E:5112:TRP:O	1:E:5129:ASN:O	2.27	0.52
2:F:6027:VAL:HG12	2:F:6030:PHE:CE2	2.44	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:E:5095:LEU:HD12	1:E:5117:ALA:C	2.35	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:C:3028:VAL:CG1	1:C:3179:LEU:HD13	2.40	0.52
1:C:3064:THR:O	1:C:3068:THR:OG1	2.28	0.52
1:C:3096:GLN:O	1:C:3116:LEU:HA	2.10	0.52
1:G:7095:LEU:HD21	1:G:7116:LEU:HD21	1.92	0.52
1:G:7232:GLU:HA	1:G:7232:GLU:OE1	2.09	0.52
2:B:2069:GLU:O	1:G:7017:LEU:HG	2.10	0.51
1:E:5043:PRO:HG2	1:E:5064:THR:CB	2.40	0.51
1:E:5097:TRP:NE1	1:E:5099:GLN:HE21	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6041:LYS:O	2:F:6041:LYS:HG2	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:C:3218:GLN:HG2	1:C:3222:GLU:C	2.35	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:HD12	1:G:7160:LEU:O	2.09	0.51
1:A:1052:LEU:HD23	1:A:1175:GLY:CA	2.41	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
2:F:6036:GLU:HG2	2:F:6081:ARG:HH22	1.75	0.51
2:F:6083:ASN:HD22	2:F:6090:PRO:HG3	1.75	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:A:1006:ARG:HH21	1:A:1102:ASP:CG	2.17	0.51
2:F:6041:LYS:O	2:F:6042:ASN:HB2	2.09	0.51
1:A:1076:ARG:HH11	1:A:1076:ARG:HG2	1.75	0.51
1:C:3058:ASP:OD2	1:C:3174:LYS:NZ	2.39	0.51
2:D:4019:LYS:O	2:D:4071:THR:HB	2.09	0.51
1:E:5234:ARG:NH1	1:E:5242:GLN:OE1	2.44	0.51
1:E:5263:HIS:HB3	1:E:5266:LEU:HD12	1.93	0.51
1:G:7131:SER:O	1:G:7132:SER:O	2.29	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: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:G:7068:THR:HG22	1:G:7072:GLN:OE1	2.11	0.51
1:G:7163:HIS:N	1:G:7163:HIS:CD2	2.77	0.51
1:G:7191:ARG:HH11	1:G:7193:PRO:HD3	1.76	0.51
1:A:1002:SER:HB3	1:A:1104:GLU:HB2	1.93	0.51
1:A:1014:ARG:NH1	2:H:8048:LYS:HZ2	2.09	0.51
1:A:1077:ASN:O	1:A:1081:LEU:HB2	2.11	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:F:6001:ILE:CD1	2:F:6002:GLN:HG3	2.41	0.51
2:H:8006:LYS:CE	2:H:8029:GLY:HA3	2.37	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
1:A:1006:ARG:HG3	1:A:1006:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2009:VAL:HG22	2:B:2080:CYS:HB2	1.93	0.50
1:E:5227:ASP:OD1	1:E:5248:VAL:HG23	2.10	0.50
1:G:7032:GLN:NE2	2:H:8053:ASP:OD2	2.44	0.50
1:G:7086:ASN:OD1	1:G:7086:ASN:O	2.29	0.50
1:G:7199:VAL:HG23	1:G:7251:LEU:CD1	2.41	0.50
1:E:5082:VAL:HG23	1:E:5118:TYR:HH	1.74	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:A:1009:TYR:CD1	1:A:1024:ILE:HD11	2.46	0.50
1:A:1014:ARG:NH2	1:A:1018:GLY:HA3	2.16	0.50
1:A:1161:GLU:O	1:A:1161:GLU:HG2	2.11	0.50
1:A:1273:ARG:HB2	1:A:1273:ARG:NH1	2.24	0.50
2:B:2096:ASP:OD1	2:B:2098:ASP:OD2	2.29	0.50
1:C:3199:VAL:O	1:C:3248:VAL:HA	2.12	0.50
2:D:4041:LYS:HG3	2:D:4078:TYR:CE1	2.45	0.50
2:F:6051:HIS:HA	2:F:6065:LEU:O	2.12	0.50
1:A:1177:GLU:O	1:A:1181:ARG:HB2	2.11	0.50
1:E:5170:LYS:O	1:E:5173:GLU:HB2	2.12	0.50
1:A:1160:LEU:HD12	1:A:1160:LEU:O	2.11	0.50
1:A:1253:LYS:HE2	1:A:1253:LYS:N	2.27	0.50
1:E:5249:VAL:HG13	1:E:5250:PRO:HD2	1.94	0.50
1:G:7106:ASP:O	1:G:7107:ARG:HG2	2.11	0.50
1:G:7168:LEU:O	1:G:7172:LEU:HG	2.12	0.50
1:G:7187:ALA:HA	1:G:7204:TRP:O	2.11	0.50
1:E:5195:PRO:O	1:E:5196:GLU:HG3	2.11	0.50
1:A:1005:LEU:CD2	1:A:1167:VAL:HG12	2.41	0.50
1:A:1247:VAL:HG23	1:A:1249:VAL:HG23	1.94	0.50
1:C:3190:THR:HA	1:C:3274:TRP:HE1	1.75	0.50
1:E:5090:ASP:O	1:E:5091:ASP:OD2	2.30	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:E:5181:ARG:NH1	1:E:5183:ASP:OD2	2.44	0.50
1:E:5268:GLU:CD	1:E:5269:PRO:HD2	2.36	0.50
1:G:7069:ILE:HD13	1:G:7072:GLN:HE22	1.77	0.50
1:G:7176:LYS:CE	1:G:7180:LEU:HG	2.41	0.50
1:A:1064:THR:O	1:A:1068:THR:OG1	2.29	0.49
1:A:1087:LYS:O	1:A:1088:SER:O	2.30	0.49
1:A:1221:GLY:O	1:A:1223:GLU:OE2	2.30	0.49
2:B:2001:ILE:HD12	2:B:2002:GLN:HG2	1.93	0.49
1:C:3251:LEU:HD22	1:C:3252:GLY:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7077:ASN:ND2	1:G:7097:TRP:HZ3	2.10	0.49
1:G:7199:VAL:HG23	1:G:7251:LEU:HD12	1.93	0.49
2:H:8080:CYS:O	2:H:8092:ILE:HA	2.12	0.49
1:A:1085:TYR:HB3	1:A:1087:LYS:CE	2.42	0.49
1:A:1172:LEU:HD23	1:A:1179:LEU:HD13	1.93	0.49
1:A:1189:VAL:H	1:A:1275:GLU:CG	2.25	0.49
1:E:5170:LYS:HZ2	1:E:5174:LYS:HE3	1.76	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:C:3083:HIS:O	1:C:3086:ASN:HB3	2.11	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:A:1207:GLY:O	1:A:1240:THR:HG22	2.13	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:E:5202:ARG:HA	1:E:5245:ALA:O	2.12	0.49
1:G:7208:PHE:CE2	1:G:7213:ILE:HD12	2.48	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: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:E:5194:ARG:NH1	1:E:5196:GLU:OE2	2.45	0.49
1:G:7013:SER:O	1:G:7092:SER:OG	2.28	0.49
1:A:1268:GLU:CD	1:A:1269:PRO:HD2	2.38	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:O	1:A:1072:GLN:HG3	2.13	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:E:5077:ASN:O	1:E:5081:LEU:HB2	2.13	0.49
1:G:7095:LEU:HD11	1:G:7116:LEU:HD23	1.95	0.49
1:G:7096:GLN:HE21	1:G:7096:GLN:N	2.11	0.49
1:G:7222:GLU:O	1:G:7223:GLU:O	2.30	0.49
1:A:1061:GLU:C	1:A:1064:THR:HG22	2.38	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:F:6001:ILE:HD13	2:F:6001:ILE:C	2.38	0.49
1:C:3055:GLU:O	1:C:3057:ALA:N	2.38	0.48
1:C:3112:TRP:HB3	1:C:3131:SER:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5213:ILE:HD11	1:E:5261:VAL:HG13	1.95	0.48
1:A:1204:TRP:CZ2	2:B:2099:MET:HA	2.48	0.48
1:A:1217:TRP:CZ3	1:A:1257:TYR:HB3	2.47	0.48
1:C:3056:GLU:O	1:C:3057:ALA:HB3	2.13	0.48
1:C:3215:LEU:HD12	1:C:3261:VAL:CG2	2.43	0.48
1:C:3228:VAL:HG12	1:C:3228:VAL:O	2.13	0.48
1:E:5007:TYR:OH	1:E:5063:GLN:OE1	2.31	0.48
1:E:5104:GLU:CB	1:E:5109:LEU:HD22	2.43	0.48
1:G:7203:CYS:HB2	1:G:7217:TRP:CZ2	2.48	0.48
2:H:8041:LYS:O	2:H:8042:ASN:HB2	2.13	0.48
1:A:1261:VAL:HB	1:A:1270:LEU:HB2	1.95	0.48
1:C:3177:GLU:N	1:C:3177:GLU:OE2	2.46	0.48
1:E:5075:GLU:O	1:E:5079:MET:HB2	2.12	0.48
1:E:5170:LYS:NZ	1:E:5174:LYS:HE3	2.28	0.48
1:E:5194:ARG:HE	1:E:5248:VAL:HG11	1.77	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
2:H:8033:SER:O	2:H:8035:ILE:N	2.46	0.48
1:A:1172:LEU:HD22	1:A:1180:LEU:CD1	2.43	0.48
1:C:3128:GLU:CG	1:C:3129:ASN:H	2.26	0.48
1:C:3261:VAL:O	1:C:3266:LEU:HD13	2.13	0.48
2:H:8016:GLU:HG2	2:H:8019:LYS:CD	2.42	0.48
1:C:3181:ARG:O	1:C:3181:ARG:HG2	2.13	0.48
1:E:5201:LEU:HD11	1:E:5254:VAL:HG23	1.93	0.48
1:G:7208:PHE:CD2	1:G:7213:ILE:HD12	2.49	0.48
1:C:3036:PHE:HB2	1:C:3043:PRO:HB3	1.96	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:7189:VAL:HG12	1:G:7274:TRP:CD1	2.47	0.48
1:G:7194:ARG:NH1	1:G:7198:ASP:OD2	2.47	0.48
1:A:1060:TRP:HZ2	1:A:1174:LYS:HG3	1.79	0.48
1:C:3111:LEU:HB3	1:C:3130:PRO:HB3	1.95	0.48
1:C:3185:PRO:HD3	1:C:3263:HIS:CD2	2.48	0.48
1:G:7006:ARG:HB3	1:G:7008:PHE:CE1	2.49	0.48
1:G:7199:VAL:HG12	1:G:7199:VAL:O	2.13	0.48
1:G:7268:GLU:HG2	1:G:7269:PRO:HD2	1.96	0.48
1:C:3218:GLN:HG2	1:C:3222:GLU:N	2.29	0.48
2:D:4006:LYS:HZ3	2:D:4029:GLY:HA3	1.77	0.48
2:H:8030:PHE:CE1	2:H:8035:ILE:HD12	2.49	0.48
1:A:1088:SER:O	1:A:1090:ASP:OD1	2.32	0.48
1:A:1193:PRO:CA	1:A:1199:VAL:HG13	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3127:SER:O	1:C:3128:GLU:HB3	2.13	0.48
1:C:3031:MET:HE1	1:C:3178:ARG:HD3	1.95	0.48
1:C:3199:VAL:HG22	1:C:3249:VAL:O	2.13	0.48
1:E:5052:LEU:HD23	1:E:5175:GLY:N	2.28	0.48
1:G:7185:PRO:HG3	1:G:7208:PHE:HB3	1.96	0.48
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:A:1191:ARG:HG3	1:A:1274:TRP:NE1	2.28	0.47
1:C:3026:GLY:O	1:C:3033:VAL:HG22	2.14	0.47
1:C:3043:PRO:HD2	1:C:3064:THR:HB	1.96	0.47
1:A:1079:MET:O	1:A:1082:VAL:HG13	2.14	0.47
1:A:1095:LEU:HD12	1:A:1117:ALA:O	2.13	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:E:5097:TRP:NE1	1:E:5099:GLN:NE2	2.62	0.47
1:G:7119:ASP:C	1:G:7120:SER:HG	2.09	0.47
1:A:1128:GLU:CD	1:A:1130:PRO:HD2	2.40	0.47
2:B:2001:ILE:HG23	2:B:2002:GLN:HG3	1.97	0.47
1:A:1228:VAL:O	1:A:1228:VAL:CG1	2.53	0.47
1:C:3073:LEU:HB3	1:C:3077:ASN:ND2	2.30	0.47
1:C:3268:GLU:HG3	1:C:3269:PRO:HD2	1.96	0.47
1:E:5054:GLN:O	1:E:5056:GLU:N	2.46	0.47
1:E:5107:ARG:HG2	1:E:5107:ARG:NH1	2.29	0.47
1:E:5227:ASP:O	1:E:5227:ASP:OD2	2.32	0.47
1:E:5249:VAL:HG21	1:E:5254:VAL:HG23	1.96	0.47
2:H:8027:VAL:O	2:H:8063:TYR:HA	2.14	0.47
1:A:1014:ARG:NH1	2:H:8048:LYS:HD3	2.29	0.47
1:C:3122:ASP:CG	2:D:4060:TRP:HE1	2.23	0.47
2:D:4048:LYS:O	2:D:4048:LYS:HG3	2.14	0.47
1:G:7055:GLU:HG3	1:G:7056:GLU:N	2.29	0.47
1:G:7079:MET:O	1:G:7082:VAL:HB	2.15	0.47
1:C:3111:LEU:HD22	1:C:3130:PRO:HB2	1.96	0.47
1:C:3120:SER:HG	2:D:4001:ILE:N	2.12	0.47
1:E:5170:LYS:HZ2	1:E:5174:LYS:CE	2.27	0.47
1:G:7014:ARG:HG2	1:G:7021:TRP:HZ3	1.78	0.47
2:H:8007:ILE:O	2:H:8008:GLN:HG3	2.15	0.47
1:A:1070:GLN:O	1:A:1073:LEU:HG	2.15	0.47
1:A:1194:ARG:NH1	1:A:1198:ASP:O	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1072:GLN:C	1:A:1073:LEU:HD23	2.39	0.47
1:G:7015:PRO:HB2	1:G:7090:ASP:HA	1.97	0.47
1:G:7249:VAL:HG12	1:G:7257:TYR:CZ	2.50	0.47
1:A:1189:VAL:O	1:A:1275:GLU:OE1	2.32	0.46
1:A:1273:ARG:NH1	1:A:1273:ARG:CB	2.78	0.46
1:E:5223:GLU:N	1:E:5223:GLU:OE2	2.49	0.46
1:G:7088:SER:CB	1:G:7091:ASP:HB2	2.46	0.46
1:A:1050:PRO:O	1:A:1054:GLN:NE2	2.48	0.46
1:A:1274:TRP:O	1:A:1275:GLU:CB	2.62	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:A:1274:TRP:C	1:A:1276:PRO:HD3	2.41	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:3095:LEU:CG	1:C:3116:LEU:HD21	2.45	0.46
1:C:3111:LEU:HD22	1:C:3130:PRO:CB	2.46	0.46
1:C:3178:ARG:HA	1:C:3181:ARG:HB3	1.98	0.46
1:E:5052:LEU:HA	1:E:5174:LYS:O	2.15	0.46
1:E:5060:TRP:HA	1:E:5060:TRP:CE3	2.51	0.46
1:E:5109:LEU:HG	1:E:5110:CYS:N	2.30	0.46
1:A:1005:LEU:HD22	1:A:1167:VAL:HG12	1.96	0.46
1:A:1194:ARG:NE	1:A:1200:THR:HG22	2.31	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:E:5012:VAL:HG22	1:E:5094:THR:HB	1.98	0.46
1:G:7192:HIS:O	1:G:7194:ARG:N	2.48	0.46
2:H:8016:GLU:O	2:H:8016:GLU:HG3	2.14	0.46
1:A:1108:HIS:O	1:A:1109:LEU:CD1	2.58	0.46
1:A:1271:THR:O	1:A:1271:THR:HG22	2.15	0.46
1:C:3112:TRP:CE3	1:C:3161:GLU:HA	2.50	0.46
2:H:8096:ASP:CG	2:H:8099:MET:HB3	2.40	0.46
1:A:1104:GLU:HA	1:A:1105:PRO:HD3	1.80	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:C:3063:GLN:NE2	1:C:3171:TYR:OH	2.49	0.46
1:E:5005:LEU:HB2	1:E:5168:LEU:HD13	1.97	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:C:3007:TYR:OH	1:C:3063:GLN:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3160:LEU:HD12	1:C:3163:HIS:CE1	2.51	0.46
1:C:3224:LEU:O	1:C:3225:THR:O	2.34	0.46
1:E:5223:GLU:O	1:E:5224:LEU:HD23	2.16	0.46
2:F:6035:ILE:HG12	2:F:6036:GLU:N	2.31	0.46
1:G:7273:ARG:HG2	1:G:7273:ARG:O	2.16	0.46
2:H:8095:TRP:CZ3	2:H:8097:ARG:HD2	2.51	0.46
1:A:1201:LEU:HD12	1:A:1249:VAL:CG2	2.43	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
1:E:5231:VAL:CG2	1:E:5244:TRP:H	2.29	0.46
2:F:6040:LEU:HA	2:F:6044:GLU:O	2.16	0.46
1:G:7073:LEU:O	1:G:7077:ASN:ND2	2.49	0.46
1:A:1107:ARG:HD3	1:A:1107:ARG:O	2.16	0.45
1:C:3005:LEU:HD12	1:C:3028:VAL:HG22	1.97	0.45
1:C:3060:TRP:O	1:C:3064:THR:HG23	2.15	0.45
1:C:3218:GLN:HG2	1:C:3222:GLU:H	1.81	0.45
1:E:5082:VAL:O	1:E:5086:ASN: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
2:F:6009:VAL:HG23	2:F:6093:VAL:HG12	1.98	0.45
1:G:7061:GLU:O	1:G:7065:HIS:ND1	2.48	0.45
1:G:7080:THR:OG1	1:G:7081:LEU:N	2.50	0.45
1:G:7172:LEU:O	1:G:7176:LYS:N	2.49	0.45
1:G:7172:LEU:N	1:G:7172:LEU:HD23	2.31	0.45
2:B:2003:ARG:HH12	2:B:2061:SER:CA	2.29	0.45
1:E:5163:HIS:O	1:E:5167:VAL:HG23	2.16	0.45
2:F:6017:ASN:HA	2:F:6072:PRO:O	2.16	0.45
1:G:7007:TYR:OH	1:G:7063:GLN:NE2	2.49	0.45
1:G:7069:ILE:HG22	1:G:7070:GLN:N	2.31	0.45
1:A:1090:ASP:OD1	1:A:1091:ASP:N	2.49	0.45
1:A:1191:ARG:HD2	1:A:1201:LEU:HD21	1.99	0.45
1:A:1238:ASP:OD1	1:A:1238:ASP:N	2.50	0.45
1:E:5174:LYS:HA	1:E:5174:LYS:HD3	1.78	0.45
1:A:1194:ARG:NH2	1:A:1198:ASP:HB3	2.31	0.45
1:C:3234:ARG:NH1	1:C:3242:GLN:OE1	2.50	0.45
2:D:4091:LYS:HD2	2:D:4091:LYS:HA	1.50	0.45
2:D:4096:ASP:OD2	2:D:4097:ARG:N	2.50	0.45
1:E:5192:HIS:CD2	1:E:5192:HIS:N	2.82	0.45
1:E:5234:ARG:HB3	2:F:6026:TYR:CD2	2.52	0.45
1:G:7165:SER:O	1:G:7169:GLN:NE2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7271:THR:HG22	1:G:7272:LEU:N	2.31	0.45
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:E:5125:THR:C	1:E:5126:LEU:HD22	2.42	0.45
2:F:6059:ASP:O	2:F:6060:TRP:HB2	2.17	0.45
1:G:7028:VAL:HG23	1:G:7033:VAL:CG2	2.46	0.45
1:A:1103:VAL:HG12	1:A:1104:GLU:N	2.29	0.45
1:A:1108:HIS:O	1:A:1109:LEU:CB	2.64	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:C:3004:SER:HB2	1:C:3006:ARG:NH1	2.32	0.45
1:C:3034:LEU:HD12	1:C:3043:PRO:CB	2.47	0.45
1:C:3115:GLN:O	1:C:3116:LEU:HB2	2.16	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: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:G:7215:LEU:HB3	1:G:7243:LYS:HZ1	1.82	0.45
2:F:6021:ASN:N	2:F:6070:PHE:O	2.50	0.45
1:A:1115:GLN:HE21	1:A:1115:GLN:HB2	1.53	0.45
2:B:2058:LYS:HE2	2:B:2058:LYS:HB3	1.44	0.45
1:C:3014:ARG:NH2	1:C:3017:LEU:O	2.50	0.45
1:C:3055:GLU:C	1:C:3057:ALA:N	2.75	0.45
1:C:3246:ALA:O	1:C:3247:VAL:CG1	2.63	0.45
2:D:4023:LEU:O	2:D:4067:TYR:HA	2.17	0.45
2:D:4027:VAL:HG22	2:D:4064:LEU:O	2.17	0.45
1:G:7102:ASP:N	1:G:7102:ASP:OD1	2.50	0.45
1:A:1234:ARG:NH1	1:A:1242:GLN:OE1	2.50	0.44
2:B:2007:ILE:C	2:B:2008:GLN:HG3	2.42	0.44
1:C:3055:GLU:O	1:C:3055:GLU:OE2	2.35	0.44
1:C:3077:ASN:O	1:C:3081:LEU:HB2	2.16	0.44
2:D:4012:ARG:HD3	2:D:4022:PHE:HB2	1.99	0.44
1:E:5190:THR:HB	1:E:5192:HIS:CE1	2.53	0.44
2:F:6008:GLN:NE2	2:F:6026:TYR:O	2.50	0.44
2:H:8035:ILE:HG13	2:H:8084:HIS:HD2	1.81	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:A:1109:LEU:HD12	1:A:1109:LEU:HA	1.79	0.44
1:C:3050:PRO:C	1:C:3052:LEU:N	2.76	0.44
1:C:3102:ASP:OD1	1:C:3102:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5199:VAL:HG22	1:E:5251:LEU:HD23	1.98	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:OD1	2:H:8059:ASP:N	2.45	0.44
1:A:1035:ARG:HH12	1:A:1044:ARG:NH1	2.15	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
1:A:1013:SER:O	1:A:1092:SER:OG	2.28	0.44
2:B:2001:ILE:HD13	2:B:2001:ILE:C	2.43	0.44
2:B:2085:VAL:HG12	2:H:8044:GLU:HG2	1.99	0.44
1:C:3112:TRP:CZ3	1:C:3161:GLU:HA	2.52	0.44
1:C:3194:ARG:HH11	1:C:3198:ASP:HB3	1.82	0.44
2:H:8096:ASP:HB3	2:H:8099:MET:HB3	1.99	0.44
1:A:1076:ARG:HG2	1:A:1076:ARG:NH1	2.33	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
2:B:2038:ASP:OD2	2:H:8036:GLU:OE2	2.35	0.44
1:C:3011:ALA:HA	1:C:3021:TRP:O	2.17	0.44
1:C:3111:LEU:CB	1:C:3130:PRO:HB3	2.48	0.44
1:C:3263:HIS:CB	1:C:3266:LEU:HD12	2.47	0.44
1:E:5115:GLN:C	1:E:5116:LEU:HD12	2.42	0.44
1:A:1039:LYS:O	1:A:1039:LYS:CE	2.66	0.44
2:B:2006:LYS:HD2	2:B:2029:GLY:HA3	2.00	0.44
2:B:2007:ILE:CD1	2:B:2082:VAL:HG21	2.48	0.44
1:C:3188:HIS:O	1:C:3204:TRP:HB2	2.17	0.44
1:E:5096:GLN:NE2	2:F:6056:PHE:CG	2.86	0.44
2:F:6073:THR:HG22	2:F:6076:ASP:H	1.82	0.44
1:C:3071:GLY:O	1:C:3074:SER:HB3	2.17	0.44
1:E:5188:HIS:HE1	1:E:5206:LEU:HD11	1.83	0.44
1:E:5105:PRO:O	1:E:5106:ASP:CG	2.60	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:OD1	2:H:8053:ASP:N	2.50	0.44
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:E:5225:THR:C	1:E:5228:VAL:HG12	2.43	0.43
2:H:8038:ASP:OD1	2:H:8045:ARG:NH1	2.51	0.43
1:C:3196:GLU:O	1:C:3198:ASP:N	2.50	0.43
1:E:5066:ILE:O	1:E:5070:GLN:CG	2.58	0.43
1:E:5194:ARG:HA	1:E:5195:PRO:HD3	1.85	0.43
1:A:1061:GLU:CA	1:A:1064:THR:HG22	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1273:ARG:O	1:A:1276:PRO:HD2	2.18	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
2:H:8007:ILE:HD12	2:H:8082:VAL:HG21	1.97	0.43
1:A:1215:LEU:HD23	1:A:1215:LEU:HA	1.90	0.43
1:C:3035:ARG:HG3	1:C:3036:PHE:N	2.32	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
2:D:4051:HIS:HA	2:D:4065:LEU:O	2.19	0.43
1:G:7111:LEU:HB3	1:G:7130:PRO:HB3	2.00	0.43
1:A:1006:ARG:HG3	1:A:1006:ARG:NH1	2.34	0.43
1:A:1192:HIS:C	1:A:1199:VAL:HG13	2.42	0.43
1:C:3073:LEU:CD2	1:C:3076:ARG:NH1	2.81	0.43
1:C:3221:GLY:O	1:C:3222:GLU:HB2	2.17	0.43
1:E:5023:ILE:HG23	1:E:5023:ILE:O	2.19	0.43
2:F:6051:HIS:ND1	2:F:6051:HIS:N	2.67	0.43
1:A:1015:PRO:HG3	1:A:1091:ASP:O	2.19	0.43
1:A:1191:ARG:HH22	1:A:1251:LEU:HD12	1.84	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:1035:ARG:CZ	1:A:1044:ARG:HD2	2.48	0.43
1:A:1199:VAL:HG21	1:A:1251:LEU:HD12	2.00	0.43
2:B:2005:PRO:HB3	2:B:2030:PHE:HB3	2.01	0.43
1:G:7184:PRO:HA	1:G:7185:PRO:HD3	1.76	0.43
1:A:1011:ALA:CB	1:A:1074:SER:HB2	2.49	0.43
1:C:3055:GLU:C	1:C:3057:ALA:H	2.24	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:1009:TYR:HB3	1:A:1097:TRP:HB3	2.01	0.43
1:A:1189:VAL:HG12	1:A:1190:THR:N	2.32	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:E:5074:SER:OG	1:E:5075:GLU:N	2.50	0.43
2:F:6005:PRO:HB2	2:F:6027:VAL:HG13	1.99	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:A:1180:LEU:N	1:A:1180:LEU:HD12	2.34	0.42
1:C:3009:TYR:OH	1:C:3074:SER:HB3	2.19	0.42
1:C:3073:LEU:CG	1:C:3076:ARG:NH1	2.80	0.42
1:E:5028:VAL:O	1:E:5029:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:8052:SER:O	2:H:8064:LEU:HD22	2.18	0.42
1:A:1172:LEU:HD22	1:A:1180:LEU:HD11	2.01	0.42
1:A:1199:VAL:HG12	1:A:1200:THR:N	2.33	0.42
1:E:5014:ARG:HB2	1:E:5017:LEU:HB2	2.01	0.42
1:E:5199:VAL:CG2	1:E:5251:LEU:HD23	2.48	0.42
2:F:6007:ILE:N	2:F:6007:ILE:CD1	2.82	0.42
1:G:7192:HIS:HA	1:G:7193:PRO:HD2	1.86	0.42
1:A:1229:GLU:N	1:A:1246:ALA:O	2.43	0.42
1:C:3026:GLY:C	1:C:3033:VAL:HG22	2.44	0.42
1:E:5228:VAL:O	1:E:5228:VAL:CG1	2.63	0.42
1:G:7185:PRO:C	1:G:7186:LYS:HD3	2.45	0.42
1:A:1011:ALA:HB1	1:A:1074:SER:HB2	2.00	0.42
2:B:2005:PRO:CA	2:B:2030:PHE:HB3	2.50	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:5096:GLN:HB3	2:F:6056:PHE:CE2	2.54	0.42
1:E:5234:ARG:HD3	2:F:6010:TYR:CE2	2.54	0.42
1:G:7053:GLU:OE2	1:G:7174:LYS:HA	2.19	0.42
1:G:7243:LYS:HE3	1:G:7243:LYS:HB3	1.51	0.42
2:H:8082:VAL:N	2:H:8091:LYS:O	2.50	0.42
1:A:1073:LEU:HD23	1:A:1073:LEU:N	2.35	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:5111:LEU:HB3	1:E:5113:TYR:CE1	2.54	0.42
1:E:5266:LEU:HA	1:E:5267:PRO:HD3	1.85	0.42
1:G:7031:MET:CE	1:G:7178:ARG:HB3	2.50	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:E:5006:ARG:HH21	1:E:5102:ASP:CG	2.27	0.42
1:E:5009:TYR:CB	1:E:5097:TRP:HB3	2.47	0.42
1:E:5010:THR:HB	1:E:5023:ILE:CG2	2.49	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:7053:GLU:CD	1:G:7174:LYS:HZ3	2.27	0.42
1:G:7109:LEU:HG	1:G:7110:CYS:N	2.34	0.42
2:H:8039:LEU:O	2:H:8045:ARG:HA	2.18	0.42
2:B:2058:LYS:H	2:B:2058:LYS:HG2	1.41	0.42
1:C:3184:PRO:HA	1:C:3185:PRO:HD3	1.82	0.42
1:C:3228:VAL:HA	1:C:3247:VAL:CG1	2.50	0.42
1:E:5052:LEU:HD23	1:E:5175:GLY:HA3	2.02	0.42
1:A:1014:ARG:NH1	2:H:8048:LYS:NZ	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3110:CYS:C	1:C:3111:LEU:HD23	2.45	0.42
2:D:4075:LYS:HD3	2:D:4075:LYS:H	1.84	0.42
2:D:4091:LYS:HD2	2:D:4092:ILE:N	2.35	0.42
1:E:5175:GLY:O	1:E:5179:LEU:HG	2.20	0.42
2:H:8030:PHE:CD1	2:H:8035:ILE:HD12	2.55	0.42
2:H:8071:THR:HA	2:H:8072:PRO:HD2	1.94	0.42
1:C:3234:ARG:N	1:C:3242:GLN:O	2.53	0.42
1:A:1219:LYS:O	1:A:1220:ASP:HB2	2.20	0.41
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
1:G:7081:LEU:O	1:G:7085:TYR:HD2	2.03	0.41
1:C:3111:LEU:CD1	1:C:3130:PRO:HB3	2.44	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:3031:MET:CE	1:C:3178:ARG:HD3	2.50	0.41
1:G:7005:LEU:CD1	1:G:7028:VAL:HG22	2.50	0.41
1:G:7087:LYS:C	1:G:7088:SER:HG	2.20	0.41
1:G:7103:VAL:HG12	1:G:7104:GLU:N	2.33	0.41
1:A:1069:ILE:O	1:A:1073:LEU:CD2	2.64	0.41
1:A:1266:LEU:HA	1:A:1267:PRO:HD3	1.85	0.41
2:B:2036:GLU:OE1	2:H:8038:ASP:OD2	2.38	0.41
1:C:3231:VAL:HG13	1:C:3244:TRP:CZ2	2.56	0.41
1:C:3249:VAL:HG13	1:C:3250:PRO:HD2	2.02	0.41
1:E:5060:TRP:CZ3	1:E:5170:LYS:HD3	2.55	0.41
2:H:8097:ARG:HE	2:H:8097:ARG:HB3	1.80	0.41
1:A:1111:LEU:HD23	1:A:1113:TYR:CZ	2.55	0.41
1:C:3014:ARG:CZ	1:C:3017:LEU:HD12	2.49	0.41
1:E:5194:ARG:O	1:E:5196:GLU:N	2.50	0.41
1:G:7025:VAL:CG2	2:H:8053:ASP:HB2	2.51	0.41
2:B:2041:LYS:O	2:B:2042:ASN:HB2	2.20	0.41
1:C:3117:ALA:HB2	2:D:4060:TRP:CE2	2.55	0.41
1:E:5062:GLN:OE1	1:E:5163:HIS:CD2	2.74	0.41
1:E:5077:ASN:HD22	1:E:5077:ASN:HA	1.57	0.41
1:E:5104:GLU:HB3	1:E:5109:LEU:CB	2.51	0.41
2:F:6069:GLU:HG2	2:F:6070:PHE:N	2.36	0.41
1:C:3014:ARG:HH21	1:C:3018:GLY:CA	2.12	0.41
1:C:3122:ASP:O	1:C:3123:LEU:HD23	2.20	0.41
2:D:4003:ARG:HH11	2:D:4061:SER:HB3	1.86	0.41
2:D:4059:ASP:O	2:D:4060:TRP:HB2	2.20	0.41
1:E:5097:TRP:CE2	1:E:5099:GLN:NE2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:8048:LYS:O	2:H:8049:VAL:HG23	2.21	0.41
1:A:1079:MET:HA	1:A:1082:VAL:CG1	2.51	0.41
2:B:2003:ARG:HH12	2:B:2061:SER:HA	1.85	0.41
1:C:3167:VAL:O	1:C:3167:VAL:HG12	2.19	0.41
2:D:4050:GLU:HB2	2:D:4067:TYR:CZ	2.55	0.41
2:D:4056:PHE:HA	2:D:4062:PHE:HA	2.03	0.41
1:E:5066:ILE:O	1:E:5066:ILE:HG22	2.21	0.41
1:E:5255:GLN:HE21	1:E:5255:GLN:HB3	1.61	0.41
1:G:7215:LEU:HD11	1:G:7259:CYS:SG	2.61	0.41
1:G:7225:THR:O	1:G:7225:THR:HG22	2.20	0.41
1:A:1128:GLU:OE2	1:A:1131:SER:CB	2.69	0.41
2:B:2095:TRP:CZ2	2:B:2097:ARG:HA	2.55	0.41
1:C:3027:TYR:HA	1:C:3031:MET:O	2.21	0.41
1:C:3198:ASP:OD2	1:C:3248:VAL:HB	2.21	0.41
1:C:3222:GLU:O	1:C:3223:GLU:O	2.39	0.41
1:E:5104:GLU:HB3	1:E:5109:LEU:HD22	2.03	0.41
1:E:5128:GLU:CG	1:E:5131:SER:HB2	2.50	0.41
2:F:6016:GLU:HB3	2:F:6019:LYS:CD	2.47	0.41
1:G:7205:ALA:O	1:G:7206:LEU:HD23	2.21	0.41
1:A:1060:TRP:HA	1:A:1063:GLN:HG3	2.02	0.41
1:A:1117:ALA:HB2	2:B:2060:TRP:CE2	2.56	0.41
2:B:2035:ILE:CD1	2:B:2083:ASN:O	2.59	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: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
1:G:7167:VAL:O	1:G:7170:LYS:N	2.50	0.41
1:A:1035:ARG:HH12	1:A:1044:ARG:CZ	2.34	0.40
1:E:5187:ALA:HB3	1:E:5272:LEU:HD21	2.03	0.40
1:E:5191:ARG:HH11	1:E:5191:ARG:HG2	1.85	0.40
1:E:5231:VAL:HG23	1:E:5243:LYS:HG3	2.02	0.40
1:A:1100:ASP:O	1:A:1113:TYR:HD1	2.04	0.40
1:A:1102:ASP:OD2	1:A:1113:TYR:OH	2.38	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:A:1059:ASP:N	1:A:1170:LYS:NZ	2.67	0.40
1:A:1191:ARG:C	1:A:1192:HIS:HD1	2.30	0.40
1:C:3085:TYR:C	1:C:3086:ASN:HD22	2.28	0.40
1:C:3233:THR:HA	1:C:3242:GLN:O	2.20	0.40
1:C:3274:TRP:O	1:C:3275:GLU:O	2.40	0.40
1:E:5053:GLU:OE1	1:E:5053:GLU:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5060:TRP:CH2	1:E:5170:LYS:HE3	2.56	0.40
1:E:5200:THR:HG22	1:E:5201:LEU:N	2.36	0.40
2:B:2033:SER:O	2:B:2035:ILE:N	2.54	0.40
1:G:7189:VAL:HG23	1:G:7272:LEU:CD1	2.37	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
1:G:7184:PRO:HB3	1:G:7265:GLY:C	2.46	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%)	0	0
1	C	242/260 (93%)	180 (74%)	40 (16%)	22 (9%)	0	0
1	E	243/260 (94%)	192 (79%)	39 (16%)	12 (5%)	1	2
1	G	239/260 (92%)	178 (74%)	34 (14%)	27 (11%)	0	0
2	B	97/99 (98%)	89 (92%)	5 (5%)	3 (3%)	3	5
2	D	97/99 (98%)	85 (88%)	11 (11%)	1 (1%)	12	24
2	F	97/99 (98%)	86 (89%)	9 (9%)	2 (2%)	5	9
2	H	97/99 (98%)	84 (87%)	11 (11%)	2 (2%)	5	9
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	158 (71%)	65 (29%)	0	0
1	C	219/235 (93%)	172 (78%)	47 (22%)	1	2
1	E	222/235 (94%)	173 (78%)	49 (22%)	1	2
1	G	218/235 (93%)	162 (74%)	56 (26%)	0	1
2	B	94/94 (100%)	77 (82%)	17 (18%)	2	3
2	D	94/94 (100%)	82 (87%)	12 (13%)	4	9
2	F	94/94 (100%)	78 (83%)	16 (17%)	2	4
2	H	94/94 (100%)	72 (77%)	22 (23%)	1	1
All	All	1258/1316 (96%)	974 (77%)	284 (23%)	1	1

All (284) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1017	LEU
1	A	1019	GLU
1	A	1025	VAL
1	A	1035	ARG
1	A	1038	SER
1	A	1039	LYS
1	A	1041	GLU
1	A	1044	ARG

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Mol	Chain	Res	Type
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	1079	MET
1	A	1080	THR
1	A	1081	LEU
1	A	1082	VAL
1	A	1086	ASN
1	A	1089	MET
1	A	1094	THR
1	A	1096	GLN
1	A	1098	LEU
1	A	1099	GLN
1	A	1103	VAL
1	A	1107	ARG
1	A	1109	LEU
1	A	1111	LEU
1	A	1115	GLN
1	A	1121	GLU
1	A	1123	LEU
1	A	1126	LEU
1	A	1133	CYS
1	A	1159	HIS
1	A	1160	LEU
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	1190	THR
1	A	1191	ARG
1	A	1194	ARG
1	A	1196	GLU

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Mol	Chain	Res	Type
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
1	A	1276	PRO
2	B	2001	ILE
2	B	2003	ARG
2	B	2004	THR
2	B	2006	LYS
2	B	2008	GLN
2	B	2020	SER
2	B	2035	ILE
2	B	2040	LEU
2	B	2048	LYS
2	B	2058	LYS
2	B	2070	PHE
2	B	2073	THR
2	B	2074	GLU
2	B	2075	LYS
2	B	2081	ARG
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

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Mol	Chain	Res	Type
1	C	3068	THR
1	C	3075	GLU
1	C	3078	LEU
1	C	3079	MET
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	3115	GLN
1	C	3120	SER
1	C	3121	GLU
1	C	3131	SER
1	C	3163	HIS
1	C	3165	SER
1	C	3170	LYS
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	3214	THR
1	C	3215	LEU
1	C	3224	LEU
1	C	3233	THR
1	C	3234	ARG
1	C	3242	GLN
1	C	3251	LEU
1	C	3257	TYR
1	C	3264	GLU
1	C	3270	LEU
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	4048	LYS

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Mol	Chain	Res	Type
2	D	4052	SER
2	D	4057	SER
2	D	4075	LYS
2	D	4085	VAL
2	D	4089	GLN
2	D	4091	LYS
2	D	4094	LYS
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	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	5075	GLU
1	E	5076	ARG
1	E	5077	ASN
1	E	5080	THR
1	E	5081	LEU
1	E	5094	THR
1	E	5099	GLN
1	E	5107	ARG
1	E	5108	HIS
1	E	5120	SER
1	E	5121	GLU
1	E	5128	GLU
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

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Mol	Chain	Res	Type
1	E	5192	HIS
1	E	5206	LEU
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	5251	LEU
1	E	5253	LYS
1	E	5259	CYS
1	E	5264	GLU
1	E	5272	LEU
2	F	6001	ILE
2	F	6004	THR
2	F	6007	ILE
2	F	6008	GLN
2	F	6009	VAL
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
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

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Mol	Chain	Res	Type
1	G	7064	THR
1	G	7069	ILE
1	G	7075	GLU
1	G	7078	LEU
1	G	7079	MET
1	G	7084	PHE
1	G	7089	MET
1	G	7090	ASP
1	G	7094	THR
1	G	7096	GLN
1	G	7098	LEU
1	G	7102	ASP
1	G	7103	VAL
1	G	7106	ASP
1	G	7107	ARG
1	G	7116	LEU
1	G	7121	GLU
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	7214	THR
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	7249	VAL
1	G	7251	LEU
1	G	7255	GLN
1	G	7256	SER

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Mol	Chain	Res	Type
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	8027	VAL
2	H	8035	ILE
2	H	8049	VAL
2	H	8053	ASP
2	H	8055	SER
2	H	8059	ASP
2	H	8069	GLU
2	H	8075	LYS
2	H	8077	GLU
2	H	8082	VAL
2	H	8085	VAL
2	H	8089	GLN
2	H	8092	ILE
2	H	8094	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1003	HIS
1	A	1054	GLN
1	A	1062	GLN
1	A	1086	ASN
1	A	1115	GLN
1	A	1158	GLN
1	A	1163	HIS
1	A	1169	GLN
1	A	1188	HIS
1	A	1218	GLN
1	A	1255	GLN
1	A	1260	HIS
1	A	1263	HIS
2	B	2002	GLN

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Mol	Chain	Res	Type
2	B	2024	ASN
2	B	2031	HIS
1	C	3054	GLN
1	C	3063	GLN
1	C	3070	GLN
1	C	3077	ASN
1	C	3086	ASN
1	C	3169	GLN
1	C	3260	HIS
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	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	248/260 (95%)	1.72	77 (31%) 1 1	11, 26, 37, 42	0
1	C	248/260 (95%)	1.86	86 (34%) 1 1	9, 29, 40, 42	0
1	E	247/260 (95%)	1.59	69 (27%) 1 1	9, 24, 38, 46	0
1	G	245/260 (94%)	1.65	78 (31%) 1 1	9, 24, 37, 43	0
2	B	99/99 (100%)	1.08	10 (10%) 12 10	9, 15, 25, 31	0
2	D	99/99 (100%)	1.33	21 (21%) 2 2	8, 17, 30, 35	0
2	F	99/99 (100%)	1.12	12 (12%) 8 7	9, 16, 24, 27	0
2	H	99/99 (100%)	1.10	13 (13%) 7 6	9, 15, 28, 36	0
All	All	1384/1436 (96%)	1.55	366 (26%) 1 1	8, 23, 37, 46	0

All (366) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1134	THR	8.3
1	G	7254	VAL	6.7
1	A	1130	PRO	6.7
1	E	5087	LYS	6.0
1	C	3248	VAL	5.9
1	G	7076	ARG	5.4
1	G	7065	HIS	5.4
2	H	8001	ILE	5.0
1	A	1089	MET	4.9
1	A	1075	GLU	4.7
1	E	5074	SER	4.5
1	C	3187	ALA	4.4
1	C	3270	LEU	4.4
1	C	3134	THR	4.4
1	E	5193	PRO	4.3
1	A	1074	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	5073	LEU	4.2
1	A	1009	TYR	4.2
1	G	7066	ILE	4.1
2	D	4099	MET	4.1
1	E	5227	ASP	4.0
1	G	7180	LEU	4.0
1	G	7133	CYS	4.0
1	E	5052	LEU	4.0
1	A	1209	TYR	4.0
1	C	3133	CYS	4.0
1	A	1225	THR	4.0
2	B	2088	SER	3.9
2	D	4077	GLU	3.9
1	C	3051	TRP	3.9
1	C	3130	PRO	3.9
1	C	3017	LEU	3.9
1	C	3266	LEU	3.8
1	A	1016	GLY	3.8
1	C	3197	GLY	3.8
1	G	7074	SER	3.8
1	C	3190	THR	3.8
1	G	7249	VAL	3.8
1	G	7131	SER	3.7
1	A	1004	SER	3.7
1	G	7056	GLU	3.7
1	A	1017	LEU	3.7
1	C	3217	TRP	3.7
1	E	5116	LEU	3.7
1	C	3054	GLN	3.7
1	A	1167	VAL	3.6
1	C	3257	TYR	3.6
1	C	3219	LYS	3.6
1	C	3269	PRO	3.6
2	H	8072	PRO	3.6
1	C	3262	ASP	3.6
1	G	7067	VAL	3.5
1	C	3126	LEU	3.5
1	G	7009	TYR	3.5
1	G	7017	LEU	3.5
1	G	7109	LEU	3.5
1	A	1116	LEU	3.5
1	C	3246	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	3067	VAL	3.4
1	G	7247	VAL	3.4
1	G	7252	GLY	3.4
2	D	4001	ILE	3.4
1	A	1107	ARG	3.4
1	A	1127	SER	3.4
1	A	1274	TRP	3.4
1	C	3254	VAL	3.4
1	A	1181	ARG	3.4
1	C	3062	GLN	3.3
1	A	1224	LEU	3.3
1	C	3182	SER	3.3
1	A	1085	TYR	3.3
1	E	5129	ASN	3.3
1	A	1214	THR	3.3
1	C	3214	THR	3.3
1	C	3079	MET	3.3
1	A	1129	ASN	3.3
1	E	5133	CYS	3.3
1	C	3168	LEU	3.3
1	C	3261	VAL	3.3
1	A	1257	TYR	3.2
1	E	5015	PRO	3.2
1	C	3268	GLU	3.2
1	E	5082	VAL	3.2
1	C	3201	LEU	3.2
1	E	5085	TYR	3.2
1	G	7197	GLY	3.2
1	C	3233	THR	3.2
1	A	1193	PRO	3.2
1	C	3209	TYR	3.2
1	C	3071	GLY	3.2
1	C	3218	GLN	3.1
1	C	3131	SER	3.1
1	A	1019	GLU	3.1
1	A	1215	LEU	3.1
1	A	1254	VAL	3.1
1	G	7057	ALA	3.1
1	C	3228	VAL	3.1
1	G	7167	VAL	3.1
1	A	1276	PRO	3.1
1	A	1052	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	7106	ASP	3.1
1	G	7182	SER	3.1
1	C	3247	VAL	3.1
1	A	1023	ILE	3.1
2	F	6086	THR	3.1
1	C	3213	ILE	3.1
1	G	7072	GLN	3.0
1	A	1057	ALA	3.0
1	C	3009	TYR	3.0
1	G	7257	TYR	3.0
2	H	8061	SER	3.0
1	E	5072	GLN	3.0
1	E	5168	LEU	3.0
1	C	3110	CYS	3.0
1	A	1125	THR	3.0
1	G	7187	ALA	3.0
1	E	5055	GLU	3.0
1	A	1159	HIS	3.0
1	G	7262	ASP	3.0
1	A	1051	TRP	2.9
1	E	5060	TRP	2.9
1	A	1199	VAL	2.9
1	E	5134	THR	2.9
1	G	7068	THR	2.9
1	C	3236	ALA	2.9
1	A	1105	PRO	2.9
1	G	7087	LYS	2.9
1	E	5090	ASP	2.9
1	E	5075	GLU	2.9
1	G	7052	LEU	2.9
2	B	2099	MET	2.9
1	E	5076	ARG	2.9
1	G	7273	ARG	2.9
2	F	6049	VAL	2.9
1	C	3276	PRO	2.9
1	A	1109	LEU	2.9
1	G	7126	LEU	2.9
1	G	7071	GLY	2.9
1	E	5132	SER	2.8
1	E	5195	PRO	2.8
1	C	3225	THR	2.8
1	C	3258	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	5109	LEU	2.8
1	G	7051	TRP	2.8
2	H	8007	ILE	2.8
1	C	3015	PRO	2.8
1	E	5228	VAL	2.8
1	G	7078	LEU	2.8
1	E	5065	HIS	2.8
1	E	5007	TYR	2.8
1	E	5249	VAL	2.8
1	G	7250	PRO	2.8
1	C	3109	LEU	2.8
1	C	3123	LEU	2.8
1	E	5111	LEU	2.8
2	H	8060	TRP	2.7
1	A	1249	VAL	2.7
1	C	3189	VAL	2.7
1	E	5057	ALA	2.7
1	A	1108	HIS	2.7
2	B	2001	ILE	2.7
2	H	8099	MET	2.7
1	E	5177	GLU	2.7
1	A	1018	GLY	2.7
1	A	1218	GLN	2.7
1	E	5054	GLN	2.7
1	C	3065	HIS	2.7
2	H	8046	ILE	2.7
1	G	7077	ASN	2.7
1	E	5067	VAL	2.7
1	A	1049	ALA	2.7
1	G	7061	GLU	2.7
1	G	7221	GLY	2.6
1	C	3193	PRO	2.6
1	G	7164	CYS	2.6
2	D	4091	LYS	2.6
1	C	3215	LEU	2.6
1	E	5247	VAL	2.6
1	E	5131	SER	2.6
1	G	7177	GLU	2.6
1	A	1211	ALA	2.6
1	A	1221	GLY	2.6
1	A	1160	LEU	2.6
1	C	3251	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	7215	LEU	2.6
1	C	3075	GLU	2.6
1	C	3128	GLU	2.6
1	C	3256	SER	2.6
1	G	7255	GLN	2.6
1	C	3085	TYR	2.6
1	E	5159	HIS	2.6
1	A	1219	LYS	2.6
1	G	7081	LEU	2.6
2	D	4074	GLU	2.6
1	A	1038	SER	2.6
1	A	1260	HIS	2.6
1	E	5217	TRP	2.6
2	F	6014	PRO	2.6
1	E	5272	LEU	2.6
2	H	8069	GLU	2.6
1	C	3199	VAL	2.6
2	D	4017	ASN	2.6
1	A	1131	SER	2.6
1	A	1132	SER	2.6
1	E	5125	THR	2.6
1	A	1195	PRO	2.5
1	G	7269	PRO	2.5
1	C	3129	ASN	2.5
1	C	3076	ARG	2.5
1	E	5009	TYR	2.5
1	E	5130	PRO	2.5
1	E	5213	ILE	2.5
1	A	1268	GLU	2.5
1	E	5108	HIS	2.5
1	G	7228	VAL	2.5
1	C	3185	PRO	2.5
1	G	7073	LEU	2.5
1	C	3169	GLN	2.5
1	A	1014	ARG	2.5
1	A	1080	THR	2.5
2	D	4011	SER	2.5
1	G	7075	GLU	2.5
1	G	7158	GLN	2.5
1	G	7169	GLN	2.5
2	D	4003	ARG	2.5
2	D	4097	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	3095	LEU	2.4
1	C	3172	LEU	2.4
1	C	3274	TRP	2.4
1	C	3132	SER	2.4
1	C	3001	GLY	2.4
1	A	1126	LEU	2.4
2	F	6064	LEU	2.4
2	F	6003	ARG	2.4
2	D	4086	THR	2.4
2	D	4088	SER	2.4
1	G	7090	ASP	2.4
1	G	7179	LEU	2.4
1	A	1042	THR	2.4
2	B	2073	THR	2.4
1	C	3260	HIS	2.4
1	E	5251	LEU	2.4
2	F	6099	MET	2.4
1	A	1205	ALA	2.4
1	G	7039	LYS	2.4
1	G	7233	THR	2.3
1	G	7274	TRP	2.4
1	C	3066	ILE	2.3
1	C	3229	GLU	2.3
1	G	7195	PRO	2.3
1	G	7097	TRP	2.3
1	A	1069	ILE	2.3
1	G	7098	LEU	2.3
2	F	6048	LYS	2.3
1	C	3177	GLU	2.3
1	E	5173	GLU	2.3
1	G	7214	THR	2.3
1	C	3191	ARG	2.3
1	E	5051	TRP	2.3
1	G	7060	TRP	2.3
1	G	7070	GLN	2.3
1	G	7108	HIS	2.3
2	D	4089	GLN	2.3
1	A	1251	LEU	2.3
1	E	5106	ASP	2.3
1	G	7208	PHE	2.3
1	G	7019	GLU	2.3
1	C	3235	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	7043	PRO	2.3
2	H	8005	PRO	2.3
1	E	5271	THR	2.3
1	E	5207	GLY	2.3
1	G	7063	GLN	2.3
1	G	7123	LEU	2.3
2	F	6007	ILE	2.3
1	A	1104	GLU	2.3
1	A	1012	VAL	2.3
1	A	1028	VAL	2.3
1	E	5024	ILE	2.2
2	B	2075	LYS	2.2
1	A	1044	ARG	2.2
1	A	1228	VAL	2.2
1	G	7185	PRO	2.2
1	A	1054	GLN	2.2
1	A	1111	LEU	2.2
1	E	5089	MET	2.2
2	H	8054	LEU	2.2
1	E	5066	ILE	2.2
2	B	2074	GLU	2.2
2	D	4083	ASN	2.2
1	A	1192	HIS	2.2
1	A	1101	CYS	2.2
1	G	7258	THR	2.2
2	H	8073	THR	2.2
2	D	4087	LEU	2.2
1	C	3181	ARG	2.2
1	G	7084	PHE	2.2
2	D	4070	PHE	2.2
1	C	3028	VAL	2.2
1	E	5103	VAL	2.2
1	C	3125	THR	2.2
1	E	5200	THR	2.2
1	G	7134	THR	2.2
1	E	5023	ILE	2.2
1	G	7132	SER	2.2
1	E	5056	GLU	2.2
1	E	5161	GLU	2.2
1	G	7122	ASP	2.2
1	C	3021	TRP	2.2
1	A	1158	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	7218	GLN	2.1
1	G	7200	THR	2.1
1	G	7265	GLY	2.1
1	A	1191	ARG	2.1
1	E	5256	SER	2.1
1	G	7004	SER	2.1
1	C	3020	PRO	2.1
1	C	3170	LYS	2.1
2	H	8032	PRO	2.1
1	E	5084	PHE	2.1
1	G	7033	VAL	2.1
1	C	3245	ALA	2.1
1	E	5049	ALA	2.1
1	E	5042	THR	2.1
1	E	5197	GLY	2.1
1	G	7001	GLY	2.1
2	D	4035	ILE	2.1
1	A	1040	GLU	2.1
2	F	6057	SER	2.1
1	A	1015	PRO	2.1
1	C	3159	HIS	2.1
1	E	5167	VAL	2.1
1	E	5189	VAL	2.1
1	C	3060	TRP	2.1
2	F	6004	THR	2.1
1	A	1196	GLU	2.1
1	E	5110	CYS	2.1
1	A	1043	PRO	2.1
1	C	3263	HIS	2.1
2	B	2085	VAL	2.1
1	E	5160	LEU	2.1
2	F	6017	ASN	2.1
1	C	3273	ARG	2.1
2	B	2018	GLY	2.1
1	A	1190	THR	2.1
1	A	1271	THR	2.1
2	B	2044	GLU	2.1
2	B	2050	GLU	2.1
1	C	3007	TYR	2.1
1	E	5164	CYS	2.1
2	D	4090	PRO	2.1
2	D	4049	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	6085	VAL	2.0
1	E	5017	LEU	2.0
1	G	7168	LEU	2.0
1	A	1233	THR	2.0
1	E	5097	TRP	2.0
2	D	4075	LYS	2.0
1	C	3043	PRO	2.0
2	H	8078	TYR	2.0
1	A	1115	GLN	2.0
2	D	4009	VAL	2.0
2	D	4044	GLU	2.0
1	C	3045	MET	2.0
1	C	3124	PRO	2.0
1	E	5269	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.