Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 06:16 AM GMT

PDB ID : 1C16
Title : CRYSTAL STRUCTURE ANALYSIS OF THE GAMMA/DELTA T CELL LIGAND T22
Authors : Wingren, C.; Crowley, M.P.; Degano, M.; Chien, Y.; Wilson, I.A.
Deposited on : 1999-07-20
Resolution : 3.10 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
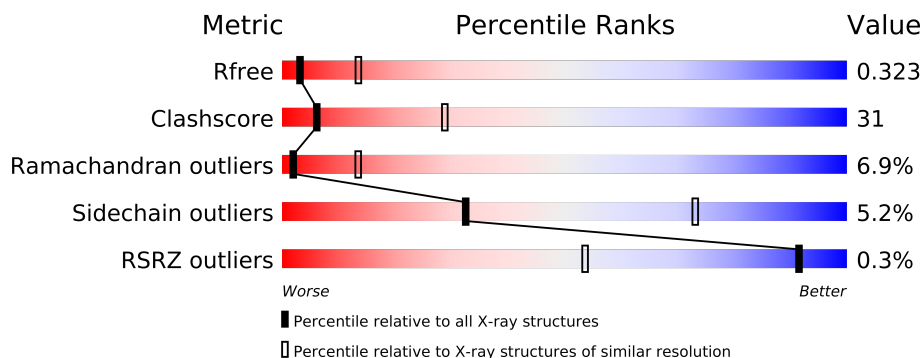A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

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

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

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 3.10 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	Percentile Ranks	Value
Rfree		0.323
Clashscore		31
Ramachandran outliers		6.9%
Sidechain outliers		5.2%
RSRZ outliers		0.3%

Worse — Better

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	260	
1	C	260	
1	E	260	
1	G	260	
2	B	99	
2	D	99	
2	F	99	
2	H	99	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 11652 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MHC-LIKE PROTEIN T22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2098	1325	362	400	11			
1	C	260	Total	C	N	O	S	0	0	0
			2093	1322	360	400	11			
1	E	254	Total	C	N	O	S	0	0	0
			2050	1297	353	389	11			
1	G	260	Total	C	N	O	S	0	0	0
			2095	1322	362	400	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	GLY	GLU	CONFLICT	UNP Q31615
A	276	GLY	PRO	CONFLICT	UNP Q31615
C	275	GLY	GLU	CONFLICT	UNP Q31615
C	276	GLY	PRO	CONFLICT	UNP Q31615
E	275	GLY	GLU	CONFLICT	UNP Q31615
E	276	GLY	PRO	CONFLICT	UNP Q31615
G	275	GLY	GLU	CONFLICT	UNP Q31615
G	276	GLY	PRO	CONFLICT	UNP Q31615

- Molecule 2 is a protein called PROTEIN (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.
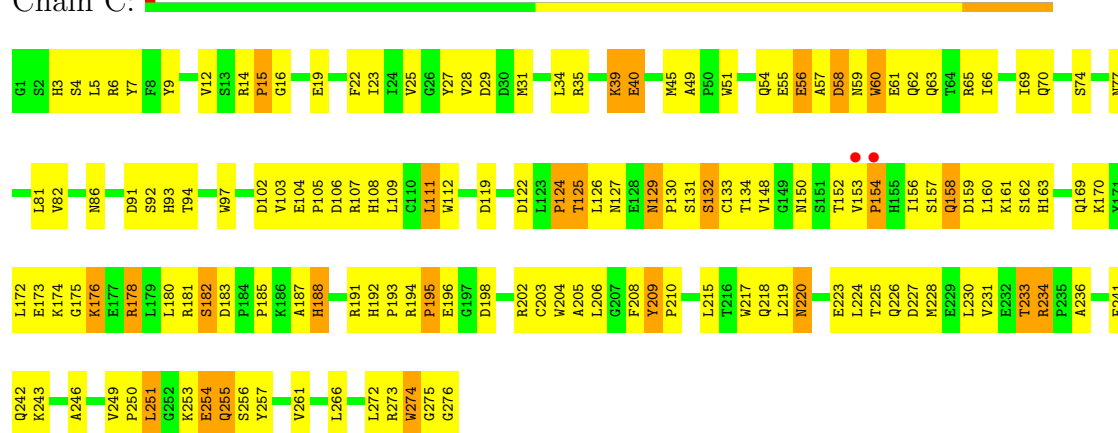
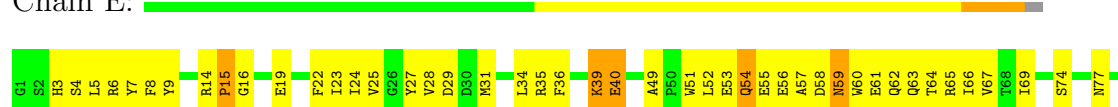• Molecule 1: MHC-LIKE PROTEIN T22

Chain A:
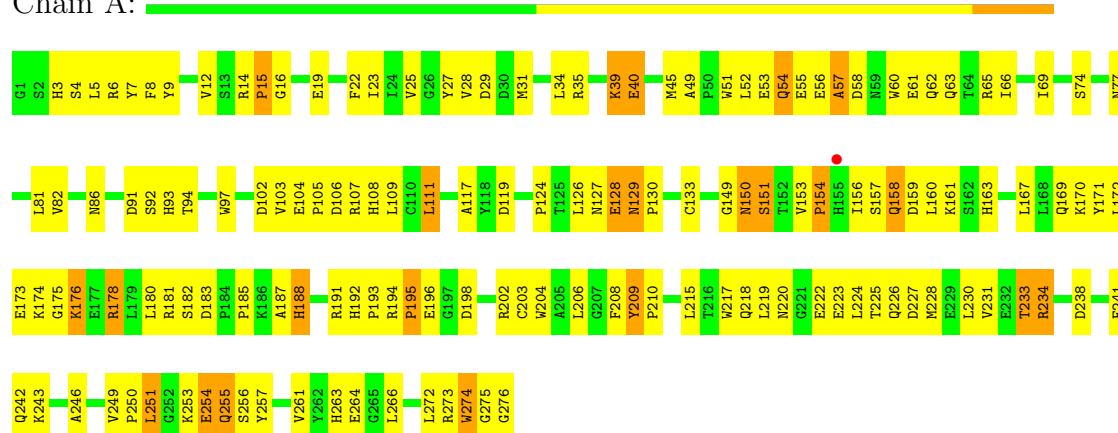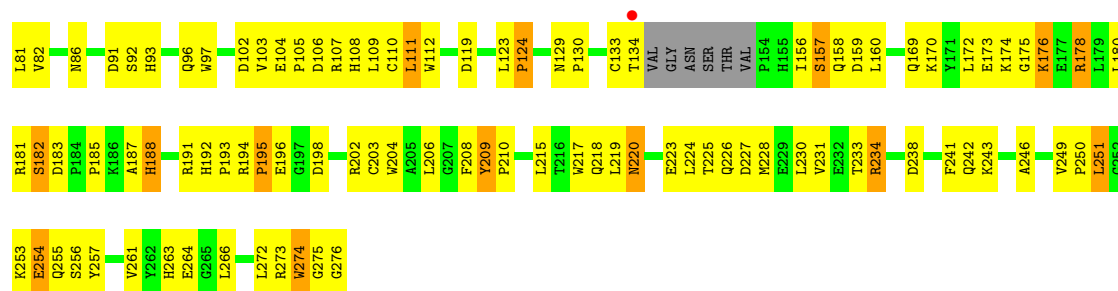

• Molecule 1: MHC-LIKE PROTEIN T22
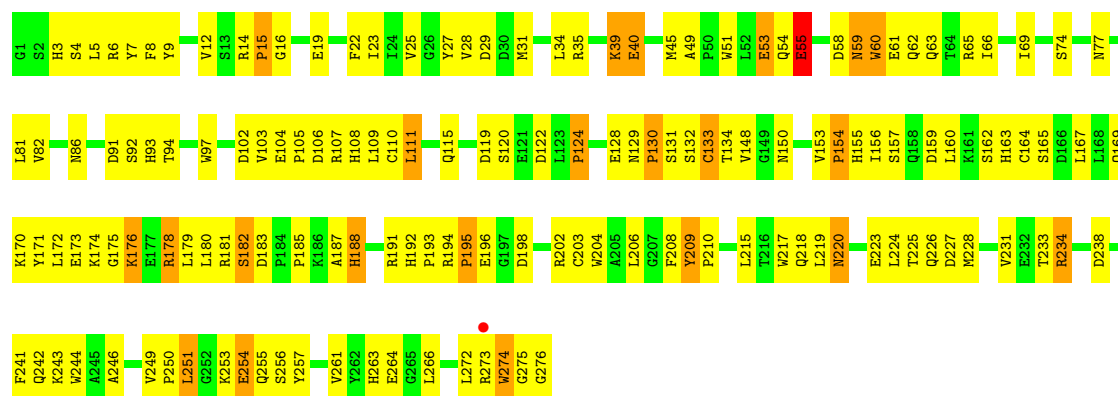
Chain C:

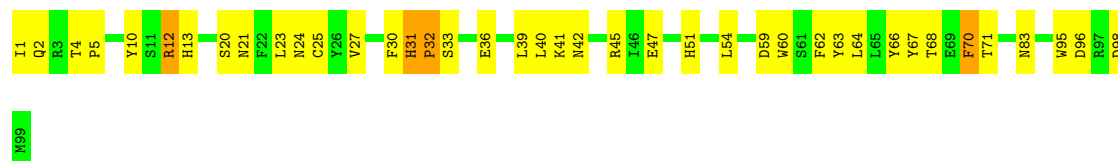• Molecule 1: MHC-LIKE PROTEIN T22

Chain E:

L81 V82 N86 D91 S92 H93 Q96 W97 D102 V103 E104 P105 D106 R107 H108 L109 C110 L111 W112 D119 L123 P124 N129 P130 C133 T134 VAL GLY ASN SER THR VAL P154 H155 I156 S157 Q158 D159 L160 Q169 K170 Y171 L172 E173 K174 G175 K176 E177 R178 L179 L180

R181 S182 D183 P184 P185 K186 A187 H188 R191 H192 P193 R194 P195 E196 G197 D198 R202 C203 W204 A205 L206 G207 F208 Y209 P210 L215 T216 Q218 L219 N220 E223 L224 T225 Q226 D227 M228 E229 L230 V231 E232 T233 R234 D238 F241 Q242 K243 A246 V249 P250 L251 G252

K253 E254 Q255 S256 Y257 V261 Y262 H263 E264 G265 L266 L272 R273 W274 G275 G276

● Molecule 1: MHC-LIKE PROTEIN T22

Chain G:

G1 S2 H3 S4 L5 R6 Y7 F8 Y9 V12 S13 R14 P15 G16 E19 F22 I23 I24 V25 G26 Y27 V28 D29 D30 M31 L34 R35 K39 E40 M45 A49 P50 W51 L52 E53 Q54 E55 D58 N59 W60 E61 Q62 Q63 T64 R65 I66 I69 S74 N77

L81 V82 N86 D91 S92 H93 T94 W97 D102 V103 E104 P105 D106 R107 H108 L109 C110 L111 Q115 D119 S120 E121 D122 L123 P124 E128 N129 P130 S131 S132 C133 T134 V148 G149 N150 V153 P154 H155 I156 S157 Q158 D159 L160 K161 S162 H163 C164 S165 D166 L167 L168 Q169

K170 Y171 L172 E173 K174 G175 K176 E177 R178 L179 L180 R181 S182 D183 P184 P185 K186 A187 H188 R191 H192 P193 R194 P195 E196 G197 D198 R202 C203 W204 A205 L206 G207 F208 Y209 P210 L215 T216 W217 Q218 L219 N220 E223 L224 T225 Q226 D227 M228 V231 E232 T233 R234 D238

F241 Q242 K243 W244 A245 A246 V249 P250 L251 G252 K253 E254 Q255 S256 Y257 V261 Y262 H263 E264 G265 L266 L272 R273 W274 G275 G276

● Molecule 2: PROTEIN (BETA-2-MICROGLOBULIN)

Chain B:

I1 Q2 R3 T4 P5 Y10 S11 R12 H13 S20 N21 F22 L23 N24 C25 Y26 V27 F30 H31 P32 S33 E36 L39 L40 K41 N42 R45 I46 E47 H51 L54 D59 W60 S61 F62 Y63 L64 L65 Y66 Y67 T68 E69 F70 T71 N83 W95 D96 R97 D98

M99

● Molecule 2: PROTEIN (BETA-2-MICROGLOBULIN)

Chain D:

I1 Q2 R3 T4 P5 K6 I7 Q8 V9 Y10 S11 R12 H13 S20 N21 F22 L23 N24 C25 F30 H31 P32 S33 E36 L39 L40 K41 N42 R45 I46 E47 H51 L54 S57 K58 D59 W60 S61 F62 Y63 L64 L65 Y66 Y67 T68 E69 F70 T71 N83 W95

D96 R97 D98 M99

● Molecule 2: PROTEIN (BETA-2-MICROGLOBULIN)

Chain F:

I1 Q2 R3 T4 P5 Y10 S11 R12 H13 S20 N21 F22 L23 N24 C25 Y26 V27 F30 H31 P32 S33 E36 L39 L40 R45 I46 E47 H51 L54 S57 K58 D59 W60 S61 F62 Y63 L64 L65 Y66 Y67 T68 E69 F70 T71 N83 W95 D96 R97 D98

M99

• Molecule 2: PROTEIN (BETA-2-MICROGLOBULIN)

Chain H:

I1 Q2 R3 T4 P5 Y10 S11 R12 H13 S20 N21 F22 L23 N24 C25 Y26 V27 F30 H31 P32 S33 E36 L39 L40 K41 N42 R45 I46 E47 H51 L54 S57 K58 D59 W60 S61 F62 Y63 L64 L65 Y66 Y67 T68 E69 F70 T71 N83 W95 D96

R97 D98 M99

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	167.11Å 91.47Å 122.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 49.39 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-3.10) 97.2 (49.39-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.22 (at 3.01Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.284 , 0.334 0.276 , 0.323	Depositor DCC
R_{free} test set	1169 reflections (3.44%)	DCC
Wilson B-factor (Å^2)	49.1	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 17.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Outliers	1 of 37213 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	11652	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.49	0/2158	0.73	0/2942
1	C	0.56	0/2152	0.73	0/2934
1	E	0.52	0/2108	0.75	0/2871
1	G	0.46	0/2155	0.71	0/2938
2	B	0.42	0/852	0.64	0/1152
2	D	0.47	0/852	0.66	0/1152
2	F	0.42	0/852	0.64	0/1152
2	H	0.41	0/852	0.65	0/1152
All	All	0.49	0/11981	0.71	0/16293

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2098	0	1992	138	0
1	C	2093	0	1987	150	0
1	E	2050	0	1944	148	0
1	G	2095	0	1983	159	0
2	B	829	0	794	38	0
2	D	829	0	794	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	829	0	794	34	0
2	H	829	0	794	38	0
All	All	11652	0	11082	697	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

All (697) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:129:ASN:HB3	1:E:130:PRO:HD3	1.36	1.02
1:E:53:GLU:O	1:E:55:GLU:HG3	1.64	0.97
1:C:56:GLU:HG2	1:C:57:ALA:H	1.30	0.96
1:C:129:ASN:HB3	1:C:130:PRO:CD	2.02	0.90
1:C:54:GLN:HE22	1:C:60:TRP:HE1	1.21	0.88
1:G:187:ALA:HB1	1:G:272:LEU:HD11	1.56	0.88
1:C:187:ALA:HB1	1:C:272:LEU:HD11	1.56	0.88
1:G:181:ARG:HD2	1:G:183:ASP:OD2	1.74	0.86
1:A:187:ALA:HB1	1:A:272:LEU:HD11	1.57	0.86
1:E:187:ALA:HB1	1:E:272:LEU:HD11	1.56	0.86
1:C:181:ARG:HD2	1:C:183:ASP:OD2	1.76	0.85
2:F:31:HIS:HB3	2:F:32:PRO:HD3	1.58	0.84
2:D:31:HIS:HB3	2:D:32:PRO:HD3	1.58	0.83
1:A:209:TYR:HB3	1:A:210:PRO:HD3	1.61	0.83
1:C:209:TYR:HB3	1:C:210:PRO:HD3	1.61	0.83
2:B:31:HIS:HB3	2:B:32:PRO:HD3	1.61	0.82
1:A:129:ASN:HB3	1:A:130:PRO:HD3	1.60	0.82
1:A:251:LEU:H	1:A:251:LEU:HD22	1.44	0.82
1:A:181:ARG:HD2	1:A:183:ASP:OD2	1.80	0.82
1:E:251:LEU:HD22	1:E:251:LEU:H	1.44	0.81
1:E:223:GLU:OE2	1:G:108:HIS:CE1	2.34	0.81
1:G:209:TYR:HB3	1:G:210:PRO:HD3	1.62	0.81
1:C:251:LEU:H	1:C:251:LEU:HD22	1.45	0.81
2:H:31:HIS:HB3	2:H:32:PRO:HD3	1.63	0.80
1:G:251:LEU:H	1:G:251:LEU:HD22	1.43	0.80
1:E:65:ARG:O	1:E:69:ILE:HG12	1.81	0.80
1:E:209:TYR:HB3	1:E:210:PRO:HD3	1.63	0.80
2:B:20:SER:HA	2:B:71:THR:HG22	1.64	0.80
1:G:65:ARG:O	1:G:69:ILE:HG12	1.82	0.80
1:A:39:LYS:O	1:A:40:GLU:HG3	1.82	0.80
1:E:129:ASN:HB3	1:E:130:PRO:CD	2.12	0.80
1:A:65:ARG:O	1:A:69:ILE:HG12	1.82	0.80
1:G:110:CYS:HB3	1:G:133:CYS:O	1.82	0.79

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:20:SER:HA	2:H:71:THR:HG22	1.65	0.79
1:C:193:PRO:O	1:C:195:PRO:HD3	1.83	0.78
2:D:20:SER:HA	2:D:71:THR:HG22	1.63	0.78
1:E:39:LYS:O	1:E:40:GLU:HG3	1.82	0.78
1:E:9:TYR:OH	1:E:74:SER:HB3	1.84	0.78
1:G:129:ASN:HB3	1:G:130:PRO:HD3	1.64	0.78
1:G:39:LYS:O	1:G:40:GLU:HG3	1.83	0.78
1:A:233:THR:HG22	1:A:243:LYS:HD2	1.66	0.77
1:C:54:GLN:NE2	1:C:60:TRP:HE1	1.82	0.77
2:F:12:ARG:HG2	2:F:13:HIS:CE1	2.19	0.77
1:E:193:PRO:O	1:E:195:PRO:HD3	1.84	0.77
1:A:193:PRO:O	1:A:195:PRO:HD3	1.85	0.77
1:C:39:LYS:O	1:C:40:GLU:HG3	1.86	0.76
2:B:12:ARG:HG2	2:B:13:HIS:CE1	2.20	0.76
2:D:12:ARG:HG2	2:D:13:HIS:CE1	2.20	0.76
1:C:59:ASN:HB2	1:C:61:GLU:HG3	1.68	0.76
2:F:20:SER:HA	2:F:71:THR:HG22	1.64	0.76
1:A:222:GLU:HG3	1:C:150:ASN:OD1	1.86	0.76
1:G:233:THR:HG22	1:G:243:LYS:HD2	1.68	0.75
1:G:193:PRO:O	1:G:195:PRO:HD3	1.86	0.75
1:G:34:LEU:HD23	1:G:35:ARG:N	2.02	0.75
1:A:54:GLN:HA	1:A:54:GLN:NE2	2.01	0.75
2:H:12:ARG:HG2	2:H:13:HIS:CE1	2.21	0.74
1:C:65:ARG:O	1:C:69:ILE:HG12	1.87	0.74
1:G:150:ASN:HB3	1:G:153:VAL:HG22	1.67	0.74
1:A:34:LEU:HD23	1:A:35:ARG:N	2.03	0.74
1:G:9:TYR:OH	1:G:74:SER:HB3	1.87	0.74
1:C:9:TYR:OH	1:C:74:SER:HB3	1.87	0.73
1:C:56:GLU:HG2	1:C:57:ALA:N	2.02	0.73
1:A:9:TYR:OH	1:A:74:SER:HB3	1.88	0.73
2:B:1:ILE:HG23	2:B:2:GLN:HG3	1.71	0.73
2:D:31:HIS:O	2:D:32:PRO:C	2.25	0.73
1:C:129:ASN:HB3	1:C:130:PRO:HD3	1.71	0.73
1:E:34:LEU:HD23	1:E:35:ARG:N	2.04	0.73
1:C:209:TYR:O	1:C:210:PRO:C	2.27	0.72
2:F:31:HIS:O	2:F:32:PRO:C	2.26	0.72
1:E:233:THR:HG22	1:E:243:LYS:HD2	1.71	0.72
1:A:194:ARG:HB3	1:A:198:ASP:O	1.89	0.72
2:D:1:ILE:HG23	2:D:2:GLN:HG3	1.71	0.71
1:C:233:THR:HG22	1:C:243:LYS:HD2	1.71	0.71
1:E:129:ASN:CB	1:E:130:PRO:HD3	2.17	0.71
2:H:1:ILE:HG23	2:H:2:GLN:HG3	1.72	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:1:ILE:HG23	2:F:2:GLN:HG3	1.73	0.71
2:H:31:HIS:O	2:H:32:PRO:C	2.26	0.71
1:C:194:ARG:HB3	1:C:198:ASP:O	1.89	0.71
1:G:194:ARG:HB3	1:G:198:ASP:O	1.91	0.70
1:G:194:ARG:O	1:G:196:GLU:N	2.22	0.70
1:E:209:TYR:O	1:E:210:PRO:C	2.29	0.70
1:A:149:GLY:HA3	1:C:223:GLU:HG3	1.73	0.70
1:E:194:ARG:HB3	1:E:198:ASP:O	1.90	0.70
1:C:109:LEU:HD11	1:C:111:LEU:HD13	1.73	0.70
1:G:109:LEU:HD11	1:G:111:LEU:HD13	1.73	0.69
1:E:194:ARG:O	1:E:196:GLU:N	2.23	0.69
1:C:194:ARG:O	1:C:196:GLU:N	2.23	0.69
2:B:31:HIS:O	2:B:32:PRO:C	2.27	0.68
1:A:129:ASN:CB	1:A:130:PRO:HD3	2.22	0.68
2:B:21:ASN:HB3	2:B:70:PHE:HE1	1.58	0.68
1:C:181:ARG:HG2	1:C:182:SER:N	2.09	0.68
1:A:109:LEU:HD11	1:A:111:LEU:HD13	1.75	0.68
1:E:109:LEU:HD11	1:E:111:LEU:HD13	1.75	0.67
1:E:157:SER:O	1:E:158:GLN:HB3	1.95	0.67
2:F:21:ASN:HB3	2:F:70:PHE:HE1	1.59	0.67
1:G:77:ASN:O	1:G:81:LEU:HD23	1.94	0.67
1:A:194:ARG:O	1:A:196:GLU:N	2.23	0.67
1:C:34:LEU:HD23	1:C:35:ARG:N	2.10	0.67
1:C:157:SER:O	1:C:159:ASP:N	2.27	0.66
1:C:77:ASN:O	1:C:81:LEU:HD23	1.95	0.66
1:G:60:TRP:CE3	1:G:60:TRP:HA	2.29	0.66
1:C:5:LEU:O	1:C:6:ARG:HD3	1.94	0.66
1:A:209:TYR:O	1:A:210:PRO:C	2.33	0.66
2:B:36:GLU:HB3	2:B:83:ASN:HB3	1.78	0.65
1:E:181:ARG:HG2	1:E:182:SER:N	2.12	0.65
1:G:251:LEU:H	1:G:251:LEU:CD2	2.10	0.65
2:H:21:ASN:HB3	2:H:70:PHE:HE1	1.61	0.65
1:G:181:ARG:HG2	1:G:182:SER:N	2.12	0.65
2:B:54:LEU:HD11	2:B:62:PHE:CD2	2.31	0.65
1:G:148:VAL:HG13	1:G:150:ASN:O	1.95	0.65
1:E:251:LEU:H	1:E:251:LEU:CD2	2.10	0.65
1:E:192:HIS:NE2	2:F:98:ASP:HB3	2.12	0.64
1:G:59:ASN:O	1:G:60:TRP:HB2	1.97	0.64
1:E:69:ILE:HB	1:E:158:GLN:HE22	1.62	0.64
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.32	0.64
2:D:31:HIS:HB3	2:D:32:PRO:CD	2.27	0.64
2:F:36:GLU:HB3	2:F:83:ASN:HB3	1.79	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:36:GLU:HB3	2:D:83:ASN:HB3	1.79	0.64
2:F:21:ASN:HB3	2:F:70:PHE:CE1	2.32	0.64
2:H:36:GLU:HB3	2:H:83:ASN:HB3	1.80	0.64
1:A:251:LEU:H	1:A:251:LEU:CD2	2.10	0.64
1:E:181:ARG:HD2	1:E:183:ASP:OD2	1.97	0.64
2:F:31:HIS:HB3	2:F:32:PRO:CD	2.26	0.64
1:E:77:ASN:O	1:E:81:LEU:HD23	1.98	0.64
1:C:251:LEU:H	1:C:251:LEU:CD2	2.11	0.63
1:A:52:LEU:O	1:A:54:GLN:N	2.31	0.63
1:C:59:ASN:O	1:C:60:TRP:HB2	1.97	0.63
2:H:21:ASN:HB3	2:H:70:PHE:CE1	2.33	0.63
1:A:181:ARG:HG2	1:A:182:SER:N	2.13	0.63
1:G:209:TYR:O	1:G:210:PRO:C	2.32	0.63
2:D:21:ASN:HB3	2:D:70:PHE:HE1	1.62	0.63
1:A:5:LEU:O	1:A:6:ARG:HD3	1.98	0.63
1:G:5:LEU:O	1:G:6:ARG:HD3	1.98	0.63
1:G:234:ARG:HD3	2:H:10:TYR:CZ	2.33	0.63
1:C:274:TRP:O	1:C:276:GLY:N	2.32	0.63
1:C:159:ASP:OD2	1:C:161:LYS:HB3	1.98	0.62
1:G:34:LEU:HD23	1:G:34:LEU:C	2.19	0.62
1:C:254:GLU:O	1:C:256:SER:N	2.32	0.62
1:G:194:ARG:HG2	1:G:196:GLU:HB2	1.82	0.62
1:G:192:HIS:NE2	2:H:98:ASP:HB3	2.15	0.62
2:D:21:ASN:HB3	2:D:70:PHE:CE1	2.34	0.62
1:G:148:VAL:HG23	1:G:165:SER:OG	1.99	0.62
1:E:110:CYS:HB3	1:E:133:CYS:O	1.98	0.62
1:A:77:ASN:O	1:A:81:LEU:HD23	2.00	0.62
1:G:194:ARG:HG2	1:G:196:GLU:OE1	2.00	0.62
1:E:274:TRP:O	1:E:276:GLY:N	2.33	0.61
1:E:194:ARG:HG2	1:E:196:GLU:HB2	1.82	0.61
1:G:274:TRP:O	1:G:276:GLY:N	2.33	0.61
1:A:34:LEU:HD23	1:A:34:LEU:C	2.20	0.61
1:A:194:ARG:HG2	1:A:196:GLU:OE1	2.00	0.61
1:G:153:VAL:N	1:G:154:PRO:HD2	2.15	0.61
1:E:194:ARG:HG2	1:E:196:GLU:OE1	2.00	0.61
2:B:31:HIS:HB3	2:B:32:PRO:CD	2.30	0.61
1:G:153:VAL:H	1:G:154:PRO:HD2	1.65	0.61
1:E:54:GLN:O	1:E:55:GLU:HB2	2.00	0.61
1:E:223:GLU:OE1	1:G:108:HIS:CE1	2.54	0.60
1:C:194:ARG:HG2	1:C:196:GLU:OE1	2.01	0.60
1:A:274:TRP:O	1:A:276:GLY:N	2.33	0.60
1:E:5:LEU:O	1:E:6:ARG:HD3	2.02	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:51:HIS:HB3	2:F:66:TYR:CD2	2.36	0.60
1:E:108:HIS:CE1	1:G:223:GLU:OE1	2.55	0.60
1:E:49:ALA:O	1:E:54:GLN:NE2	2.32	0.60
1:G:233:THR:HG22	1:G:243:LYS:NZ	2.17	0.60
1:A:254:GLU:O	1:A:256:SER:N	2.34	0.60
1:E:223:GLU:CD	1:G:108:HIS:NE2	2.55	0.60
1:A:233:THR:HG22	1:A:243:LYS:NZ	2.15	0.60
1:A:194:ARG:HG2	1:A:196:GLU:HB2	1.83	0.60
1:C:156:ILE:HA	1:C:163:HIS:HE1	1.66	0.60
2:H:54:LEU:HD11	2:H:62:PHE:CD2	2.37	0.59
2:H:31:HIS:HB3	2:H:32:PRO:CD	2.32	0.59
1:E:233:THR:HG22	1:E:243:LYS:NZ	2.17	0.59
1:C:194:ARG:HG2	1:C:196:GLU:HB2	1.84	0.59
1:A:191:ARG:HB2	1:A:274:TRP:HE1	1.67	0.59
1:A:159:ASP:OD1	1:A:161:LYS:HB3	2.02	0.59
1:C:233:THR:HG22	1:C:243:LYS:NZ	2.17	0.59
1:G:191:ARG:HB2	1:G:274:TRP:HE1	1.68	0.59
1:A:129:ASN:HB3	1:A:130:PRO:CD	2.33	0.59
1:G:60:TRP:HE3	1:G:60:TRP:HA	1.66	0.58
1:G:234:ARG:HD3	2:H:10:TYR:CE2	2.38	0.58
2:D:51:HIS:HB3	2:D:66:TYR:CD2	2.39	0.58
1:C:126:LEU:HD22	1:C:126:LEU:N	2.18	0.58
1:A:206:LEU:CD2	1:A:242:GLN:HB3	2.33	0.58
1:G:45:MET:CE	1:G:60:TRP:CD1	2.86	0.58
1:C:209:TYR:HB3	1:C:210:PRO:CD	2.33	0.58
1:A:209:TYR:HB3	1:A:210:PRO:CD	2.33	0.58
1:E:223:GLU:CD	1:G:108:HIS:CE1	2.77	0.58
1:E:34:LEU:HD23	1:E:34:LEU:C	2.23	0.58
2:F:23:LEU:HD23	2:F:39:LEU:HD13	1.86	0.58
2:B:51:HIS:HB3	2:B:66:TYR:CD2	2.39	0.58
2:B:23:LEU:HD23	2:B:39:LEU:HD13	1.86	0.57
1:E:254:GLU:O	1:E:256:SER:N	2.37	0.57
2:F:5:PRO:HB3	2:F:30:PHE:HB3	1.86	0.57
2:H:51:HIS:HB3	2:H:66:TYR:CD2	2.39	0.57
1:E:223:GLU:OE2	1:G:108:HIS:HE1	1.86	0.57
1:E:112:TRP:O	1:E:130:PRO:HA	2.05	0.57
1:A:157:SER:O	1:A:159:ASP:N	2.38	0.57
1:A:187:ALA:CB	1:A:272:LEU:HD11	2.34	0.57
1:G:187:ALA:CB	1:G:272:LEU:HD11	2.33	0.56
2:F:54:LEU:HD11	2:F:62:PHE:CD2	2.40	0.56
2:D:59:ASP:O	2:D:60:TRP:HB2	2.04	0.56
1:C:129:ASN:CB	1:C:130:PRO:CD	2.80	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:187:ALA:CB	1:C:272:LEU:HD11	2.33	0.56
1:E:209:TYR:HB3	1:E:210:PRO:CD	2.35	0.56
1:A:233:THR:HG22	1:A:243:LYS:CD	2.35	0.56
1:E:191:ARG:HB2	1:E:274:TRP:HE1	1.70	0.56
1:A:22:PHE:CD1	1:A:22:PHE:C	2.78	0.56
1:G:209:TYR:CB	1:G:210:PRO:HD3	2.36	0.56
1:A:209:TYR:CB	1:A:210:PRO:HD3	2.35	0.56
1:E:158:GLN:OE1	1:E:158:GLN:HA	2.05	0.56
1:G:22:PHE:C	1:G:22:PHE:CD1	2.79	0.56
2:H:5:PRO:HB3	2:H:30:PHE:HB3	1.87	0.56
1:E:22:PHE:C	1:E:22:PHE:CD1	2.79	0.56
1:G:156:ILE:HG12	1:G:157:SER:N	2.21	0.56
1:G:115:GLN:NE2	1:G:129:ASN:HD21	2.03	0.56
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.40	0.56
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.88	0.56
2:D:23:LEU:HD23	2:D:39:LEU:HD13	1.87	0.56
1:C:34:LEU:C	1:C:34:LEU:HD23	2.26	0.56
2:D:54:LEU:HD11	2:D:62:PHE:CD2	2.40	0.55
2:B:59:ASP:O	2:B:60:TRP:HB2	2.05	0.55
1:C:22:PHE:C	1:C:22:PHE:CD1	2.79	0.55
1:C:31:MET:HG2	1:C:209:TYR:OH	2.07	0.55
1:E:219:LEU:HB2	1:E:224:LEU:HD11	1.89	0.55
1:C:191:ARG:HB2	1:C:274:TRP:HE1	1.71	0.55
1:G:254:GLU:O	1:G:256:SER:N	2.39	0.55
1:G:45:MET:HE3	1:G:60:TRP:CD1	2.41	0.55
1:E:223:GLU:OE1	1:G:108:HIS:NE2	2.40	0.54
1:A:15:PRO:HD3	1:A:92:SER:HB2	1.89	0.54
1:E:187:ALA:CB	1:E:272:LEU:HD11	2.33	0.54
1:A:7:TYR:OH	1:A:63:GLN:NE2	2.38	0.54
1:E:234:ARG:HD3	2:F:10:TYR:CZ	2.41	0.54
1:E:156:ILE:HD13	1:E:159:ASP:HB3	1.89	0.54
1:E:209:TYR:CB	1:E:210:PRO:HD3	2.36	0.54
1:A:192:HIS:NE2	2:B:98:ASP:HB3	2.23	0.54
1:C:107:ARG:O	1:C:108:HIS:C	2.46	0.54
1:E:206:LEU:HD22	1:E:242:GLN:HB3	1.90	0.54
1:E:108:HIS:NE2	1:G:223:GLU:CD	2.61	0.54
1:C:55:GLU:O	1:C:56:GLU:HB2	2.08	0.53
1:C:112:TRP:O	1:C:130:PRO:HA	2.08	0.53
1:A:3:HIS:HD2	1:A:29:ASP:OD2	1.90	0.53
1:C:219:LEU:HB2	1:C:224:LEU:HD11	1.90	0.53
1:G:219:LEU:HB2	1:G:224:LEU:HD11	1.88	0.53
1:G:209:TYR:HB3	1:G:210:PRO:CD	2.34	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:5:PRO:CA	2:F:30:PHE:HB3	2.38	0.53
1:E:249:VAL:HG22	1:E:257:TYR:CE2	2.43	0.53
2:H:23:LEU:HD23	2:H:39:LEU:HD13	1.90	0.53
1:C:66:ILE:HD13	1:C:160:LEU:HA	1.90	0.53
1:C:14:ARG:HD3	1:C:19:GLU:O	2.09	0.53
1:G:15:PRO:HD3	1:G:92:SER:HB2	1.89	0.53
1:C:56:GLU:HG2	1:C:58:ASP:H	1.73	0.53
1:A:209:TYR:CG	1:A:210:PRO:N	2.76	0.53
2:F:59:ASP:O	2:F:60:TRP:HB2	2.09	0.53
1:C:187:ALA:HA	1:C:204:TRP:O	2.08	0.53
1:E:206:LEU:CD2	1:E:242:GLN:HB3	2.39	0.53
1:G:206:LEU:CD2	1:G:242:GLN:HB3	2.39	0.53
1:E:169:GLN:O	1:E:173:GLU:HG3	2.09	0.53
1:C:249:VAL:HG22	1:C:257:TYR:CE2	2.44	0.53
1:C:209:TYR:CB	1:C:210:PRO:HD3	2.34	0.53
2:D:5:PRO:HB3	2:D:30:PHE:HB3	1.89	0.53
1:E:108:HIS:NE2	1:G:223:GLU:OE2	2.42	0.53
1:A:249:VAL:HG22	1:A:257:TYR:CE2	2.43	0.53
1:E:251:LEU:N	1:E:251:LEU:HD22	2.21	0.53
1:A:206:LEU:HD22	1:A:242:GLN:HB3	1.89	0.53
1:C:3:HIS:HD2	1:C:29:ASP:OD2	1.92	0.53
1:C:169:GLN:O	1:C:173:GLU:HG3	2.09	0.52
1:G:107:ARG:O	1:G:108:HIS:C	2.47	0.52
1:G:233:THR:HG22	1:G:243:LYS:CD	2.37	0.52
1:E:187:ALA:HA	1:E:204:TRP:O	2.09	0.52
1:C:273:ARG:NH1	1:C:273:ARG:HG2	2.25	0.52
2:H:59:ASP:O	2:H:60:TRP:HB2	2.10	0.52
1:G:194:ARG:CG	1:G:196:GLU:OE1	2.57	0.52
2:B:5:PRO:CA	2:B:30:PHE:HB3	2.39	0.52
1:A:127:ASN:O	1:A:128:GLU:HB3	2.10	0.52
2:H:5:PRO:CA	2:H:30:PHE:HB3	2.39	0.52
2:B:95:TRP:CD1	2:B:96:ASP:N	2.77	0.52
1:A:222:GLU:CG	1:C:150:ASN:OD1	2.56	0.52
1:A:194:ARG:CG	1:A:196:GLU:OE1	2.58	0.52
1:E:108:HIS:NE2	1:G:223:GLU:OE1	2.42	0.52
1:E:66:ILE:HD13	1:E:160:LEU:HA	1.91	0.52
1:A:107:ARG:O	1:A:108:HIS:C	2.47	0.52
1:E:9:TYR:HH	1:E:74:SER:HB3	1.72	0.52
1:E:194:ARG:CG	1:E:196:GLU:OE1	2.57	0.52
1:G:206:LEU:HD22	1:G:242:GLN:HB3	1.90	0.52
1:E:107:ARG:O	1:E:108:HIS:C	2.47	0.52
1:G:249:VAL:HG22	1:G:257:TYR:CE2	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:28:VAL:O	1:G:29:ASP:HB2	2.10	0.52
1:A:219:LEU:HB2	1:A:224:LEU:HD11	1.90	0.51
1:G:3:HIS:HD2	1:G:29:ASP:OD2	1.92	0.51
1:C:56:GLU:CG	1:C:57:ALA:H	2.11	0.51
1:A:251:LEU:N	1:A:251:LEU:HD22	2.20	0.51
1:A:127:ASN:O	1:A:128:GLU:CB	2.57	0.51
1:A:14:ARG:HD3	1:A:19:GLU:O	2.09	0.51
1:C:15:PRO:HD3	1:C:92:SER:HB2	1.92	0.51
2:H:95:TRP:CD1	2:H:96:ASP:N	2.78	0.51
1:C:178:ARG:HH11	1:C:178:ARG:CG	2.24	0.51
1:G:129:ASN:HB3	1:G:130:PRO:CD	2.37	0.51
1:E:233:THR:HG22	1:E:243:LYS:CD	2.39	0.51
1:A:62:GLN:OE1	1:A:157:SER:HB2	2.10	0.51
1:A:14:ARG:NH1	1:A:19:GLU:O	2.40	0.51
1:E:14:ARG:NH1	1:E:19:GLU:O	2.43	0.51
1:E:202:ARG:HG2	1:E:204:TRP:NE1	2.26	0.51
1:E:209:TYR:CG	1:E:210:PRO:N	2.78	0.51
1:G:93:HIS:HD2	1:G:119:ASP:OD2	1.94	0.51
1:E:15:PRO:HD3	1:E:92:SER:HB2	1.91	0.51
1:A:187:ALA:HA	1:A:204:TRP:O	2.11	0.51
1:C:194:ARG:CG	1:C:196:GLU:OE1	2.59	0.51
1:A:66:ILE:HD13	1:A:160:LEU:HA	1.92	0.51
2:D:5:PRO:CA	2:D:30:PHE:HB3	2.41	0.51
1:E:55:GLU:O	1:E:57:ALA:N	2.43	0.51
1:C:59:ASN:HB2	1:C:61:GLU:CG	2.38	0.51
1:G:273:ARG:NH1	1:G:273:ARG:HG2	2.26	0.51
1:E:14:ARG:HD3	1:E:19:GLU:O	2.09	0.51
1:E:55:GLU:C	1:E:57:ALA:N	2.62	0.51
1:G:178:ARG:CG	1:G:178:ARG:HH11	2.24	0.51
1:A:108:HIS:HE2	1:C:223:GLU:CD	2.13	0.51
2:F:95:TRP:CD1	2:F:96:ASP:N	2.78	0.51
1:C:192:HIS:NE2	2:D:98:ASP:HB3	2.26	0.50
1:A:169:GLN:O	1:A:173:GLU:HG3	2.11	0.50
1:G:14:ARG:HD3	1:G:19:GLU:O	2.11	0.50
1:C:234:ARG:HD3	2:D:10:TYR:CZ	2.46	0.50
1:E:7:TYR:OH	1:E:63:GLN:NE2	2.42	0.50
1:E:52:LEU:O	1:E:54:GLN:HG3	2.11	0.50
1:A:31:MET:HG2	1:A:209:TYR:OH	2.11	0.50
1:A:129:ASN:CB	1:A:130:PRO:CD	2.88	0.50
1:C:14:ARG:NH1	1:C:19:GLU:O	2.42	0.50
1:G:66:ILE:HD13	1:G:160:LEU:HA	1.93	0.50
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:208:PHE:CE1	1:A:241:PHE:HB2	2.46	0.50
1:G:209:TYR:CG	1:G:210:PRO:N	2.75	0.50
1:E:273:ARG:NH1	1:E:273:ARG:HG2	2.26	0.50
1:C:250:PRO:HB2	1:C:253:LYS:HG3	1.94	0.50
1:E:82:VAL:O	1:E:86:ASN:N	2.45	0.50
1:G:251:LEU:N	1:G:251:LEU:HD22	2.20	0.50
1:G:238:ASP:HB3	2:H:12:ARG:HD2	1.94	0.50
1:A:223:GLU:OE2	1:C:108:HIS:CE1	2.65	0.50
1:E:93:HIS:HD2	1:E:119:ASP:OD2	1.94	0.50
1:G:202:ARG:HG2	1:G:204:TRP:NE1	2.26	0.50
1:C:233:THR:HG22	1:C:243:LYS:CD	2.39	0.50
1:C:59:ASN:C	1:C:61:GLU:H	2.15	0.50
1:E:238:ASP:HB3	2:F:12:ARG:HD2	1.94	0.50
1:A:54:GLN:HA	1:A:54:GLN:HE21	1.76	0.50
1:C:122:ASP:O	1:C:124:PRO:HD3	2.12	0.50
1:C:181:ARG:CG	1:C:182:SER:N	2.74	0.49
1:C:209:TYR:CG	1:C:210:PRO:N	2.76	0.49
2:H:24:ASN:HD22	2:H:67:TYR:HB3	1.77	0.49
2:F:39:LEU:CD1	2:F:68:THR:HG22	2.42	0.49
1:A:28:VAL:O	1:A:29:ASP:HB2	2.12	0.49
2:D:95:TRP:CD1	2:D:96:ASP:N	2.80	0.49
1:A:82:VAL:O	1:A:86:ASN:N	2.45	0.49
1:E:215:LEU:CD2	1:E:261:VAL:HG22	2.42	0.49
1:E:9:TYR:HB3	1:E:97:TRP:HB3	1.94	0.49
1:C:153:VAL:O	1:C:154:PRO:O	2.30	0.49
1:G:273:ARG:HG2	1:G:273:ARG:HH11	1.78	0.49
1:C:273:ARG:HG2	1:C:273:ARG:HH11	1.76	0.49
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.47	0.49
1:A:215:LEU:CD2	1:A:261:VAL:HG22	2.41	0.49
1:G:169:GLN:O	1:G:173:GLU:HG3	2.12	0.49
1:C:7:TYR:OH	1:C:63:GLN:NE2	2.42	0.49
1:C:209:TYR:CB	1:C:210:PRO:CD	2.90	0.49
1:E:3:HIS:HD2	1:E:29:ASP:OD2	1.95	0.49
1:G:9:TYR:HB3	1:G:97:TRP:HB3	1.94	0.49
1:E:234:ARG:HD3	2:F:10:TYR:CE2	2.48	0.49
1:A:223:GLU:OE1	1:C:108:HIS:NE2	2.46	0.49
1:G:250:PRO:HB2	1:G:253:LYS:HG3	1.93	0.49
1:G:187:ALA:HA	1:G:204:TRP:O	2.12	0.49
1:G:208:PHE:CE1	1:G:241:PHE:HB2	2.47	0.49
1:E:53:GLU:O	1:E:55:GLU:N	2.45	0.49
1:A:157:SER:O	1:A:158:GLN:C	2.51	0.49
2:B:39:LEU:CD1	2:B:68:THR:HG22	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:150:ASN:O	1:A:151:SER:HB2	2.13	0.49
2:F:24:ASN:HD22	2:F:67:TYR:HB3	1.78	0.49
1:A:181:ARG:CG	1:A:182:SER:N	2.76	0.49
1:C:65:ARG:NH1	1:C:157:SER:HB2	2.28	0.49
1:G:14:ARG:NH1	1:G:19:GLU:O	2.42	0.49
1:G:82:VAL:O	1:G:86:ASN:N	2.46	0.49
2:B:70:PHE:CD1	2:B:70:PHE:C	2.86	0.49
2:B:24:ASN:HD22	2:B:67:TYR:HB3	1.78	0.49
1:C:61:GLU:O	1:C:62:GLN:C	2.51	0.48
1:G:181:ARG:CG	1:G:182:SER:N	2.76	0.48
1:G:150:ASN:HB3	1:G:153:VAL:CG2	2.40	0.48
2:F:54:LEU:HA	2:F:64:LEU:CD2	2.44	0.48
1:C:93:HIS:HD2	1:C:119:ASP:OD2	1.95	0.48
1:C:206:LEU:CD2	1:C:242:GLN:HB3	2.43	0.48
1:G:153:VAL:O	1:G:155:HIS:CE1	2.67	0.48
1:A:273:ARG:NH1	1:A:273:ARG:HG2	2.27	0.48
1:A:129:ASN:CG	1:A:130:PRO:HD3	2.34	0.48
1:A:238:ASP:HB3	2:B:12:ARG:HD2	1.95	0.48
1:C:274:TRP:HE3	1:C:274:TRP:O	1.97	0.48
1:C:150:ASN:HB3	1:C:153:VAL:HG21	1.96	0.48
1:E:178:ARG:CG	1:E:178:ARG:HH11	2.26	0.48
1:E:28:VAL:O	1:E:29:ASP:HB2	2.13	0.48
1:A:45:MET:HE3	1:A:60:TRP:CD1	2.48	0.48
1:E:53:GLU:O	1:E:54:GLN:C	2.51	0.48
1:A:209:TYR:CB	1:A:210:PRO:CD	2.91	0.48
1:G:109:LEU:CD1	1:G:111:LEU:HD13	2.43	0.48
1:E:181:ARG:CG	1:E:182:SER:N	2.77	0.48
1:A:250:PRO:HB2	1:A:253:LYS:HG3	1.95	0.48
1:C:82:VAL:O	1:C:86:ASN:N	2.46	0.48
1:C:202:ARG:HG2	1:C:204:TRP:NE1	2.29	0.48
2:D:54:LEU:HA	2:D:64:LEU:CD2	2.44	0.48
1:G:215:LEU:CD2	1:G:261:VAL:HG22	2.44	0.48
2:H:31:HIS:O	2:H:33:SER:N	2.47	0.48
1:C:206:LEU:HD22	1:C:242:GLN:HB3	1.95	0.48
1:E:273:ARG:HH11	1:E:273:ARG:HG2	1.78	0.48
2:H:54:LEU:HA	2:H:64:LEU:CD2	2.44	0.48
1:C:208:PHE:CE1	1:C:241:PHE:HB2	2.49	0.48
2:D:31:HIS:O	2:D:33:SER:N	2.47	0.48
2:H:40:LEU:HD23	2:H:45:ARG:HA	1.96	0.48
1:E:208:PHE:CE1	1:E:241:PHE:HB2	2.48	0.48
1:C:125:THR:HB	1:C:127:ASN:OD1	2.14	0.48
2:F:31:HIS:O	2:F:33:SER:N	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:223:GLU:OE2	1:G:108:HIS:NE2	2.47	0.47
1:E:215:LEU:HD22	1:E:261:VAL:HG22	1.96	0.47
1:C:170:LYS:O	1:C:174:LYS:HG2	2.14	0.47
1:G:274:TRP:HE3	1:G:274:TRP:O	1.97	0.47
1:C:156:ILE:HD12	1:C:156:ILE:C	2.35	0.47
1:E:54:GLN:O	1:E:55:GLU:CB	2.61	0.47
1:A:202:ARG:HG2	1:A:204:TRP:NE1	2.29	0.47
2:B:54:LEU:HA	2:B:64:LEU:CD2	2.43	0.47
2:D:39:LEU:CD1	2:D:68:THR:HG22	2.43	0.47
1:G:219:LEU:HB3	1:G:224:LEU:HD21	1.96	0.47
1:A:219:LEU:HB3	1:A:224:LEU:HD21	1.96	0.47
1:A:209:TYR:CD1	1:A:209:TYR:C	2.86	0.47
1:E:9:TYR:OH	1:E:74:SER:CB	2.58	0.47
2:D:70:PHE:CD1	2:D:70:PHE:C	2.87	0.47
1:C:126:LEU:CD2	1:C:126:LEU:N	2.77	0.47
2:F:40:LEU:HD23	2:F:45:ARG:HA	1.96	0.47
2:F:70:PHE:CD1	2:F:70:PHE:C	2.87	0.47
1:E:219:LEU:HB3	1:E:224:LEU:HD21	1.96	0.47
1:E:55:GLU:C	1:E:57:ALA:H	2.18	0.47
1:G:31:MET:HG2	1:G:209:TYR:OH	2.14	0.47
1:G:9:TYR:OH	1:G:74:SER:CB	2.61	0.47
1:A:9:TYR:HB3	1:A:97:TRP:HB3	1.95	0.47
1:A:273:ARG:HH11	1:A:273:ARG:HG2	1.79	0.47
1:E:203:CYS:HB2	1:E:217:TRP:CZ2	2.50	0.47
1:C:215:LEU:CD2	1:C:261:VAL:HG22	2.44	0.47
1:C:178:ARG:NH1	1:C:178:ARG:HG2	2.30	0.47
1:E:209:TYR:CB	1:E:210:PRO:CD	2.92	0.47
2:H:39:LEU:CD1	2:H:68:THR:HG22	2.45	0.47
1:E:61:GLU:O	1:E:62:GLN:C	2.53	0.47
1:G:122:ASP:O	1:G:124:PRO:HD3	2.14	0.47
1:C:131:SER:O	1:C:132:SER:HB3	2.15	0.47
1:A:103:VAL:HG12	1:A:104:GLU:N	2.30	0.47
1:C:129:ASN:HB3	1:C:130:PRO:HD2	1.90	0.47
1:C:9:TYR:HB3	1:C:97:TRP:HB3	1.96	0.47
1:A:61:GLU:O	1:A:62:GLN:C	2.52	0.47
1:E:169:GLN:HA	1:E:169:GLN:OE1	2.15	0.47
1:E:157:SER:OG	1:E:157:SER:O	2.21	0.46
1:A:52:LEU:C	1:A:54:GLN:H	2.17	0.46
2:H:70:PHE:CD1	2:H:70:PHE:C	2.87	0.46
2:F:5:PRO:HA	2:F:30:PHE:HB3	1.98	0.46
1:G:274:TRP:O	1:G:274:TRP:CE3	2.68	0.46
1:G:54:GLN:O	1:G:55:GLU:C	2.54	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:24:ASN:HD22	2:D:67:TYR:HB3	1.81	0.46
1:E:250:PRO:HB2	1:E:253:LYS:HG3	1.96	0.46
1:A:178:ARG:HH12	1:A:181:ARG:CZ	2.29	0.46
1:A:191:ARG:C	1:A:192:HIS:HD1	2.19	0.46
2:D:40:LEU:HD23	2:D:45:ARG:HA	1.98	0.46
2:B:31:HIS:O	2:B:33:SER:N	2.49	0.46
1:E:274:TRP:HE3	1:E:274:TRP:O	1.97	0.46
1:A:178:ARG:HH11	1:A:178:ARG:CG	2.29	0.46
2:H:24:ASN:ND2	2:H:67:TYR:HB3	2.31	0.46
1:A:25:VAL:HG11	1:A:27:TYR:HE1	1.80	0.46
1:G:187:ALA:O	1:G:188:HIS:HB3	2.15	0.46
1:C:274:TRP:O	1:C:274:TRP:CE3	2.69	0.46
2:H:5:PRO:CB	2:H:30:PHE:HB3	2.46	0.46
1:E:103:VAL:HG12	1:E:104:GLU:N	2.31	0.46
1:G:159:ASP:OD2	1:G:162:SER:OG	2.27	0.46
2:B:5:PRO:HA	2:B:30:PHE:HB3	1.98	0.46
1:G:173:GLU:O	1:G:176:LYS:HE3	2.16	0.46
2:F:24:ASN:ND2	2:F:67:TYR:HB3	2.31	0.46
1:G:170:LYS:O	1:G:174:LYS:HG2	2.16	0.46
1:E:6:ARG:NH2	1:E:102:ASP:OD1	2.47	0.46
1:G:209:TYR:CB	1:G:210:PRO:CD	2.91	0.46
1:E:274:TRP:O	1:E:274:TRP:CE3	2.69	0.46
1:A:273:ARG:O	1:A:274:TRP:C	2.54	0.46
1:G:61:GLU:O	1:G:62:GLN:C	2.53	0.45
1:C:273:ARG:O	1:C:274:TRP:C	2.54	0.45
2:F:5:PRO:CB	2:F:30:PHE:HB3	2.45	0.45
1:C:25:VAL:HG11	1:C:27:TYR:HE1	1.81	0.45
2:B:40:LEU:HD23	2:B:45:ARG:HA	1.98	0.45
1:C:103:VAL:HG12	1:C:104:GLU:N	2.31	0.45
1:A:170:LYS:O	1:A:174:LYS:HG2	2.16	0.45
1:E:228:MET:HG3	1:E:246:ALA:O	2.15	0.45
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.51	0.45
1:G:115:GLN:HE21	1:G:129:ASN:HD21	1.64	0.45
1:C:28:VAL:O	1:C:29:ASP:HB2	2.16	0.45
1:A:172:LEU:HD22	1:A:180:LEU:HD21	1.97	0.45
1:A:56:GLU:O	1:A:57:ALA:HB2	2.17	0.45
1:E:223:GLU:OE2	1:G:134:THR:HB	2.15	0.45
1:G:209:TYR:CD1	1:G:209:TYR:C	2.86	0.45
1:E:31:MET:HG2	1:E:209:TYR:OH	2.16	0.45
1:G:233:THR:HG22	1:G:243:LYS:HZ2	1.80	0.45
1:A:109:LEU:CD1	1:A:111:LEU:HD13	2.45	0.45
1:A:60:TRP:HZ3	1:A:167:LEU:HD23	1.82	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:185:PRO:HD2	1:E:266:LEU:HD21	1.99	0.45
1:C:251:LEU:N	1:C:251:LEU:HD22	2.22	0.45
1:E:158:GLN:O	1:E:158:GLN:HG3	2.16	0.45
1:C:159:ASP:HB3	1:C:162:SER:OG	2.16	0.45
1:G:131:SER:OG	1:G:132:SER:N	2.49	0.45
1:A:233:THR:HG22	1:A:243:LYS:HZ2	1.82	0.45
1:E:273:ARG:O	1:E:274:TRP:C	2.55	0.45
2:B:5:PRO:CB	2:B:30:PHE:HB3	2.47	0.45
1:C:234:ARG:HD3	2:D:10:TYR:CE2	2.52	0.45
1:C:236:ALA:O	2:D:12:ARG:HD3	2.17	0.45
1:C:109:LEU:CD1	1:C:111:LEU:HD13	2.44	0.45
1:A:274:TRP:O	1:A:274:TRP:HE3	1.99	0.45
1:A:234:ARG:H	1:A:234:ARG:HG3	1.67	0.45
1:G:25:VAL:HG11	1:G:27:TYR:HE1	1.82	0.45
1:G:172:LEU:HD22	1:G:180:LEU:HD21	1.98	0.45
1:A:228:MET:HG3	1:A:246:ALA:O	2.17	0.45
1:E:191:ARG:C	1:E:192:HIS:HD1	2.21	0.45
1:E:209:TYR:CD1	1:E:209:TYR:C	2.88	0.44
1:C:169:GLN:OE1	1:C:169:GLN:HA	2.16	0.44
1:C:175:GLY:O	1:C:176:LYS:C	2.55	0.44
1:C:236:ALA:O	2:D:12:ARG:CD	2.64	0.44
1:G:59:ASN:C	1:G:61:GLU:H	2.20	0.44
2:H:5:PRO:HA	2:H:30:PHE:HB3	1.99	0.44
1:C:185:PRO:HD2	1:C:266:LEU:HD21	2.00	0.44
1:E:220:ASN:HD22	1:E:220:ASN:HA	1.54	0.44
2:F:27:VAL:HG12	2:F:30:PHE:CD2	2.52	0.44
1:C:219:LEU:HB3	1:C:224:LEU:HD21	1.99	0.44
1:C:228:MET:HG3	1:C:246:ALA:O	2.17	0.44
1:E:24:ILE:HD12	1:E:67:VAL:HG13	1.99	0.44
1:C:172:LEU:HD22	1:C:180:LEU:HD21	1.99	0.44
1:E:170:LYS:O	1:E:174:LYS:HG2	2.18	0.44
1:C:187:ALA:O	1:C:188:HIS:HB3	2.16	0.44
1:C:173:GLU:O	1:C:176:LYS:HE3	2.17	0.44
1:C:178:ARG:HH12	1:C:181:ARG:CZ	2.31	0.44
1:E:109:LEU:CD1	1:E:111:LEU:HD13	2.47	0.44
1:A:274:TRP:CE3	1:A:274:TRP:O	2.71	0.44
1:G:191:ARG:C	1:G:192:HIS:HD1	2.21	0.44
1:G:273:ARG:O	1:G:274:TRP:C	2.55	0.44
1:C:4:SER:HB3	1:C:102:ASP:OD1	2.18	0.44
1:G:22:PHE:HD1	1:G:23:ILE:N	2.15	0.44
1:E:234:ARG:HG3	1:E:234:ARG:H	1.65	0.44
1:A:175:GLY:O	1:A:176:LYS:C	2.56	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:45:MET:O	1:G:49:ALA:C	2.56	0.44
1:G:234:ARG:H	1:G:234:ARG:HG3	1.65	0.44
1:A:215:LEU:HD22	1:A:261:VAL:HG22	1.99	0.44
1:G:53:GLU:HB2	1:G:174:LYS:HD2	2.00	0.44
1:G:120:SER:HB2	2:H:31:HIS:NE2	2.32	0.44
1:A:185:PRO:HD2	1:A:266:LEU:HD21	1.99	0.44
2:D:41:LYS:O	2:D:42:ASN:HB2	2.18	0.43
2:B:54:LEU:HA	2:B:64:LEU:HD21	2.00	0.43
2:F:27:VAL:O	2:F:63:TYR:HA	2.19	0.43
1:E:24:ILE:N	1:E:36:PHE:O	2.50	0.43
1:C:45:MET:O	1:C:49:ALA:C	2.56	0.43
1:A:55:GLU:HA	1:A:58:ASP:HB2	2.00	0.43
1:G:234:ARG:NH1	2:H:10:TYR:CG	2.87	0.43
1:G:169:GLN:OE1	1:G:169:GLN:HA	2.18	0.43
2:B:24:ASN:ND2	2:B:67:TYR:HB3	2.32	0.43
1:G:228:MET:HG3	1:G:246:ALA:O	2.18	0.43
1:G:115:GLN:HG2	1:G:129:ASN:OD1	2.18	0.43
1:C:205:ALA:O	1:C:206:LEU:HD23	2.19	0.43
1:G:175:GLY:O	1:G:176:LYS:C	2.56	0.43
1:E:53:GLU:O	1:E:55:GLU:CG	2.49	0.43
1:A:22:PHE:HD1	1:A:23:ILE:N	2.16	0.43
1:G:7:TYR:OH	1:G:63:GLN:NE2	2.43	0.43
1:C:56:GLU:CD	1:C:58:ASP:HB3	2.39	0.43
1:C:175:GLY:O	1:C:178:ARG:N	2.51	0.43
1:C:209:TYR:CD1	1:C:209:TYR:C	2.88	0.43
1:G:238:ASP:HB3	2:H:12:ARG:CD	2.48	0.43
1:G:215:LEU:HD22	1:G:261:VAL:HG22	1.99	0.43
1:G:12:VAL:HG22	1:G:94:THR:HG22	2.01	0.43
2:B:41:LYS:O	2:B:42:ASN:HB2	2.19	0.43
1:C:230:LEU:HA	1:C:230:LEU:HD23	1.83	0.43
1:E:25:VAL:HG11	1:E:27:TYR:HE1	1.84	0.43
1:C:6:ARG:NH2	1:C:102:ASP:OD1	2.50	0.43
1:C:191:ARG:C	1:C:192:HIS:HD1	2.20	0.43
1:E:60:TRP:O	1:E:64:THR:HG23	2.18	0.43
1:E:123:LEU:O	1:E:124:PRO:C	2.57	0.43
1:G:203:CYS:HB2	1:G:217:TRP:CZ2	2.52	0.43
1:E:172:LEU:HD22	1:E:180:LEU:HD21	2.01	0.43
1:E:156:ILE:HD13	1:E:159:ASP:CB	2.48	0.43
2:D:5:PRO:HA	2:D:30:PHE:HB3	2.00	0.43
1:G:220:ASN:HD22	1:G:220:ASN:HA	1.55	0.43
1:E:219:LEU:HD13	1:E:257:TYR:CE1	2.54	0.43
1:G:167:LEU:O	1:G:171:TYR:HD2	2.02	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:134:THR:HG21	1:C:150:ASN:HD22	1.84	0.43
2:B:27:VAL:HG12	2:B:30:PHE:CD2	2.54	0.43
1:C:203:CYS:HB2	1:C:217:TRP:CZ2	2.53	0.43
1:G:178:ARG:HG2	1:G:178:ARG:NH1	2.33	0.42
2:D:31:HIS:CB	2:D:32:PRO:CD	2.96	0.42
2:H:54:LEU:HA	2:H:64:LEU:HD21	2.01	0.42
1:A:219:LEU:HD13	1:A:257:TYR:CE1	2.54	0.42
1:G:4:SER:HB3	1:G:102:ASP:OD1	2.19	0.42
1:G:178:ARG:HH12	1:G:181:ARG:CZ	2.32	0.42
1:E:187:ALA:O	1:E:188:HIS:HB3	2.18	0.42
1:A:105:PRO:C	1:A:107:ARG:H	2.22	0.42
1:A:60:TRP:HA	1:A:60:TRP:CE3	2.53	0.42
1:C:225:THR:C	1:C:227:ASP:H	2.23	0.42
1:G:103:VAL:HG12	1:G:104:GLU:N	2.33	0.42
1:C:125:THR:HG22	1:C:127:ASN:HD21	1.85	0.42
1:A:230:LEU:HA	1:A:230:LEU:HD23	1.87	0.42
1:C:233:THR:HG22	1:C:243:LYS:HZ2	1.84	0.42
1:C:181:ARG:NH2	1:C:209:TYR:CE1	2.87	0.42
2:D:24:ASN:ND2	2:D:67:TYR:HB3	2.34	0.42
1:G:12:VAL:HG13	1:G:94:THR:HG22	2.01	0.42
1:E:172:LEU:HA	1:E:172:LEU:HD23	1.91	0.42
1:G:185:PRO:HD2	1:G:266:LEU:HD21	2.00	0.42
1:E:178:ARG:HG2	1:E:178:ARG:NH1	2.34	0.42
2:H:27:VAL:HG12	2:H:30:PHE:CD2	2.55	0.42
1:G:93:HIS:CD2	1:G:119:ASP:OD2	2.73	0.42
1:A:154:PRO:HB2	1:A:156:ILE:HG22	2.02	0.42
1:E:22:PHE:HD1	1:E:23:ILE:N	2.18	0.42
2:H:25:CYS:HB2	2:H:39:LEU:HD21	2.02	0.42
1:A:187:ALA:O	1:A:188:HIS:HB3	2.19	0.42
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.55	0.42
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.48	0.42
2:F:54:LEU:HA	2:F:64:LEU:HD21	2.00	0.42
1:E:96:GLN:NE2	2:F:31:HIS:NE2	2.67	0.42
1:E:178:ARG:CG	1:E:178:ARG:NH1	2.83	0.42
1:A:4:SER:HB3	1:A:102:ASP:OD1	2.20	0.42
2:B:27:VAL:O	2:B:63:TYR:HA	2.20	0.42
1:G:219:LEU:HD13	1:G:257:TYR:CE1	2.54	0.42
1:A:169:GLN:OE1	1:A:169:GLN:HA	2.20	0.42
1:A:173:GLU:O	1:A:176:LYS:HE3	2.18	0.42
1:C:178:ARG:NH1	1:C:178:ARG:CG	2.81	0.41
2:D:5:PRO:CB	2:D:30:PHE:HB3	2.49	0.41
1:E:58:ASP:O	1:E:59:ASN:C	2.57	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:45:MET:HE1	1:G:60:TRP:CD1	2.55	0.41
1:A:14:ARG:CD	1:A:19:GLU:O	2.68	0.41
1:A:25:VAL:CG1	1:A:27:TYR:CE1	3.03	0.41
1:G:225:THR:C	1:G:227:ASP:H	2.23	0.41
2:D:7:ILE:HG22	2:D:8:GLN:N	2.35	0.41
1:C:58:ASP:OD1	1:C:58:ASP:O	2.38	0.41
1:E:178:ARG:HH12	1:E:181:ARG:CZ	2.33	0.41
1:C:255:GLN:NE2	1:C:274:TRP:HB3	2.36	0.41
2:D:54:LEU:HA	2:D:64:LEU:HD21	2.01	0.41
1:C:25:VAL:CG1	1:C:27:TYR:CE1	3.04	0.41
1:E:8:PHE:N	1:E:8:PHE:CD1	2.88	0.41
1:A:238:ASP:HB3	2:B:12:ARG:CD	2.51	0.41
1:G:59:ASN:CG	1:G:60:TRP:N	2.74	0.41
2:F:25:CYS:HB2	2:F:39:LEU:HD21	2.03	0.41
1:G:179:LEU:HD23	1:G:179:LEU:HA	1.91	0.41
1:C:181:ARG:HG2	1:C:182:SER:H	1.82	0.41
1:E:225:THR:C	1:E:227:ASP:H	2.23	0.41
2:H:41:LYS:O	2:H:42:ASN:HB2	2.20	0.41
1:E:52:LEU:C	1:E:54:GLN:N	2.74	0.41
1:C:215:LEU:HD22	1:C:261:VAL:HG22	2.02	0.41
1:G:163:HIS:O	1:G:164:CYS:C	2.57	0.41
1:C:220:ASN:HD22	1:C:220:ASN:HA	1.54	0.41
1:A:8:PHE:CD1	1:A:8:PHE:N	2.89	0.41
1:A:12:VAL:HG22	1:A:94:THR:HG22	2.03	0.41
1:G:105:PRO:C	1:G:107:ARG:H	2.23	0.41
1:C:69:ILE:O	1:C:70:GLN:C	2.59	0.41
1:C:9:TYR:OH	1:C:74:SER:CB	2.61	0.41
1:A:167:LEU:O	1:A:171:TYR:HD2	2.03	0.41
1:G:172:LEU:HD23	1:G:172:LEU:HA	1.88	0.41
1:E:230:LEU:HD23	1:E:230:LEU:HA	1.88	0.41
1:E:175:GLY:O	1:E:176:LYS:C	2.58	0.41
1:E:69:ILE:HB	1:E:158:GLN:NE2	2.33	0.41
1:A:52:LEU:C	1:A:54:GLN:N	2.74	0.41
1:E:105:PRO:C	1:E:107:ARG:H	2.24	0.41
1:E:108:HIS:CE1	1:E:134:THR:HG22	2.56	0.41
2:B:25:CYS:HB2	2:B:39:LEU:HD21	2.03	0.41
1:C:14:ARG:CD	1:C:19:GLU:O	2.68	0.41
1:G:8:PHE:CD1	1:G:8:PHE:N	2.89	0.41
1:A:238:ASP:HB3	2:B:12:ARG:NE	2.36	0.41
1:A:255:GLN:NE2	1:A:274:TRP:HB3	2.35	0.41
1:G:22:PHE:CD1	1:G:23:ILE:N	2.89	0.41
1:G:157:SER:C	1:G:159:ASP:H	2.24	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:14:ARG:CD	1:G:19:GLU:O	2.69	0.41
1:A:45:MET:O	1:A:49:ALA:C	2.58	0.41
1:G:263:HIS:CG	1:G:264:GLU:N	2.89	0.41
1:C:12:VAL:HG13	1:C:94:THR:HG22	2.02	0.41
1:C:59:ASN:OD1	1:C:59:ASN:N	2.53	0.41
1:A:178:ARG:NH1	1:A:181:ARG:CZ	2.84	0.41
1:E:4:SER:HB3	1:E:102:ASP:OD1	2.21	0.41
1:G:156:ILE:HG12	1:G:157:SER:H	1.86	0.41
1:C:219:LEU:HD13	1:C:257:TYR:CE1	2.56	0.41
1:C:234:ARG:H	1:C:234:ARG:HG3	1.62	0.41
1:A:25:VAL:CG1	1:A:27:TYR:HE1	2.34	0.41
1:E:263:HIS:CG	1:E:264:GLU:N	2.89	0.41
1:C:22:PHE:HD1	1:C:23:ILE:N	2.19	0.40
1:G:192:HIS:HA	1:G:193:PRO:HD2	1.96	0.40
1:G:274:TRP:C	1:G:274:TRP:CE3	2.95	0.40
2:B:54:LEU:HD11	2:B:62:PHE:HD2	1.79	0.40
1:G:6:ARG:HA	1:G:6:ARG:HD3	1.83	0.40
1:C:105:PRO:C	1:C:107:ARG:H	2.24	0.40
2:H:27:VAL:O	2:H:63:TYR:HA	2.21	0.40
2:D:25:CYS:HB2	2:D:39:LEU:HD21	2.04	0.40
1:E:14:ARG:CD	1:E:19:GLU:O	2.69	0.40
1:G:25:VAL:CG1	1:G:27:TYR:CE1	3.04	0.40
1:G:39:LYS:HA	1:G:39:LYS:NZ	2.37	0.40
1:G:243:LYS:HG2	1:G:244:TRP:N	2.36	0.40
1:G:153:VAL:N	1:G:154:PRO:CD	2.82	0.40
1:E:181:ARG:HG2	1:E:182:SER:H	1.85	0.40
1:A:191:ARG:HB2	1:A:274:TRP:NE1	2.35	0.40
1:A:153:VAL:HG13	1:A:163:HIS:NE2	2.37	0.40
1:A:225:THR:C	1:A:227:ASP:H	2.24	0.40
1:C:242:GLN:NE2	2:D:12:ARG:O	2.53	0.40
1:G:238:ASP:HB3	2:H:12:ARG:NE	2.35	0.40
1:E:6:ARG:HD3	1:E:6:ARG:HA	1.82	0.40
1:E:156:ILE:HG23	1:E:159:ASP:H	1.87	0.40
1:A:263:HIS:CG	1:A:264:GLU:N	2.90	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	258/260 (99%)	204 (79%)	32 (12%)	22 (8%)	1	9
1	C	258/260 (99%)	204 (79%)	31 (12%)	23 (9%)	1	8
1	E	250/260 (96%)	200 (80%)	30 (12%)	20 (8%)	1	10
1	G	258/260 (99%)	202 (78%)	35 (14%)	21 (8%)	1	10
2	B	97/99 (98%)	87 (90%)	7 (7%)	3 (3%)	7	36
2	D	97/99 (98%)	87 (90%)	7 (7%)	3 (3%)	7	36
2	F	97/99 (98%)	86 (89%)	8 (8%)	3 (3%)	7	36
2	H	97/99 (98%)	89 (92%)	5 (5%)	3 (3%)	7	36
All	All	1412/1436 (98%)	1159 (82%)	155 (11%)	98 (7%)	2	13

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	57	ALA
1	A	129	ASN
1	A	151	SER
1	A	209	TYR
1	A	254	GLU
1	A	255	GLN
1	A	275	GLY
2	B	31	HIS
2	B	47	GLU
1	C	129	ASN
1	C	154	PRO
1	C	158	GLN
1	C	209	TYR
1	C	254	GLU
1	C	255	GLN
1	C	275	GLY
2	D	31	HIS
2	D	47	GLU

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Mol	Chain	Res	Type
1	E	54	GLN
1	E	209	TYR
1	E	254	GLU
1	E	255	GLN
1	E	275	GLY
2	F	31	HIS
2	F	47	GLU
1	G	209	TYR
1	G	254	GLU
1	G	255	GLN
1	G	275	GLY
2	H	31	HIS
2	H	47	GLU
1	A	51	TRP
1	A	128	GLU
1	A	158	GLN
1	C	56	GLU
1	E	51	TRP
1	E	56	GLU
1	E	59	ASN
1	G	51	TRP
1	G	53	GLU
1	A	274	TRP
1	C	51	TRP
1	C	58	ASP
1	C	182	SER
1	C	274	TRP
1	E	16	GLY
1	E	274	TRP
1	G	128	GLU
1	G	274	TRP
1	A	16	GLY
1	A	40	GLU
1	A	106	ASP
1	A	188	HIS
2	B	32	PRO
1	C	106	ASP
1	C	124	PRO
1	C	188	HIS
1	C	226	GLN
2	D	32	PRO
1	E	106	ASP

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Mol	Chain	Res	Type
1	E	182	SER
1	E	188	HIS
1	E	226	GLN
2	F	32	PRO
1	G	16	GLY
1	G	40	GLU
1	G	55	GLU
1	G	106	ASP
1	G	176	LYS
1	G	182	SER
1	G	188	HIS
1	G	226	GLN
2	H	32	PRO
1	A	15	PRO
1	A	124	PRO
1	A	176	LYS
1	A	226	GLN
1	C	15	PRO
1	C	16	GLY
1	E	15	PRO
1	E	40	GLU
1	E	157	SER
1	G	15	PRO
1	G	59	ASN
1	C	40	GLU
1	C	132	SER
1	C	176	LYS
1	E	176	LYS
1	C	148	VAL
1	E	124	PRO
1	G	154	PRO
1	A	154	PRO
1	A	195	PRO
1	C	195	PRO
1	E	195	PRO
1	G	130	PRO
1	G	195	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/233 (99%)	217 (94%)	14 (6%)	26	67
1	C	230/233 (99%)	215 (94%)	15 (6%)	24	65
1	E	224/233 (96%)	215 (96%)	9 (4%)	42	82
1	G	230/233 (99%)	216 (94%)	14 (6%)	26	67
2	B	94/94 (100%)	91 (97%)	3 (3%)	51	87
2	D	94/94 (100%)	90 (96%)	4 (4%)	40	80
2	F	94/94 (100%)	90 (96%)	4 (4%)	40	80
2	H	94/94 (100%)	90 (96%)	4 (4%)	40	80
All	All	1291/1308 (99%)	1224 (95%)	67 (5%)	32	73

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	54	GLN
1	A	91	ASP
1	A	111	LEU
1	A	126	LEU
1	A	133	CYS
1	A	150	ASN
1	A	178	ARG
1	A	218	GLN
1	A	220	ASN
1	A	231	VAL
1	A	233	THR
1	A	234	ARG
1	A	251	LEU
2	B	4	THR
2	B	12	ARG
2	B	70	PHE
1	C	39	LYS
1	C	60	TRP
1	C	91	ASP
1	C	111	LEU
1	C	125	THR
1	C	133	CYS
1	C	152	THR

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Mol	Chain	Res	Type
1	C	158	GLN
1	C	178	ARG
1	C	218	GLN
1	C	220	ASN
1	C	231	VAL
1	C	233	THR
1	C	234	ARG
1	C	251	LEU
2	D	4	THR
2	D	12	ARG
2	D	57	SER
2	D	70	PHE
1	E	39	LYS
1	E	91	ASP
1	E	111	LEU
1	E	178	ARG
1	E	218	GLN
1	E	220	ASN
1	E	231	VAL
1	E	234	ARG
1	E	251	LEU
2	F	4	THR
2	F	12	ARG
2	F	57	SER
2	F	70	PHE
1	G	39	LYS
1	G	55	GLU
1	G	58	ASP
1	G	60	TRP
1	G	91	ASP
1	G	111	LEU
1	G	124	PRO
1	G	133	CYS
1	G	178	ARG
1	G	218	GLN
1	G	220	ASN
1	G	231	VAL
1	G	234	ARG
1	G	251	LEU
2	H	4	THR
2	H	12	ARG
2	H	57	SER

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Mol	Chain	Res	Type
2	H	70	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	54	GLN
1	A	63	GLN
1	A	72	GLN
1	A	86	ASN
1	A	93	HIS
1	A	96	GLN
1	A	220	ASN
1	A	255	GLN
1	A	260	HIS
2	B	24	ASN
1	C	3	HIS
1	C	54	GLN
1	C	63	GLN
1	C	72	GLN
1	C	86	ASN
1	C	93	HIS
1	C	96	GLN
1	C	163	HIS
1	C	220	ASN
1	C	255	GLN
1	C	260	HIS
2	D	24	ASN
1	E	3	HIS
1	E	63	GLN
1	E	70	GLN
1	E	72	GLN
1	E	86	ASN
1	E	93	HIS
1	E	96	GLN
1	E	220	ASN
1	E	255	GLN
1	E	260	HIS
2	F	24	ASN
1	G	3	HIS
1	G	63	GLN
1	G	72	GLN

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Mol	Chain	Res	Type
1	G	86	ASN
1	G	93	HIS
1	G	96	GLN
1	G	115	GLN
1	G	220	ASN
1	G	255	GLN
1	G	260	HIS
2	H	24	ASN

5.3.3　RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5　Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6　Ligand geometry ⓘ

There are no ligands in this entry.

5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	260/260 (100%)	-0.06	1 (0%) 90	45	5, 46, 97, 100	0
1	C	260/260 (100%)	-0.07	2 (0%) 83	28	3, 29, 93, 100	0
1	E	254/260 (97%)	-0.02	1 (0%) 90	45	6, 48, 97, 100	0
1	G	260/260 (100%)	0.10	1 (0%) 90	45	15, 58, 99, 100	0
2	B	99/99 (100%)	0.01	0 100	100	12, 54, 88, 98	0
2	D	99/99 (100%)	-0.21	0 100	100	5, 33, 75, 82	0
2	F	99/99 (100%)	0.10	0 100	100	14, 58, 92, 97	0
2	H	99/99 (100%)	-0.07	0 100	100	15, 56, 89, 95	0
All	All	1430/1436 (99%)	-0.02	5 (0%) 91	53	3, 47, 96, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	134	THR	3.7
1	G	273	ARG	3.5
1	A	155	HIS	2.9
1	C	154	PRO	2.8
1	C	153	VAL	2.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.