Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 02:28 AM EDT

PDB ID	:	6A29
Title	:	Crystal structure of PprA A139R mutant
Authors	:	Adachi, M.; Shibazaki, C.; Shimizu, R.; Arai, S.; Satoh, K.; Narumi, I.; Kuroki, R.
Deposited on	:	2018-06-09
Resolution	:	2.40 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:

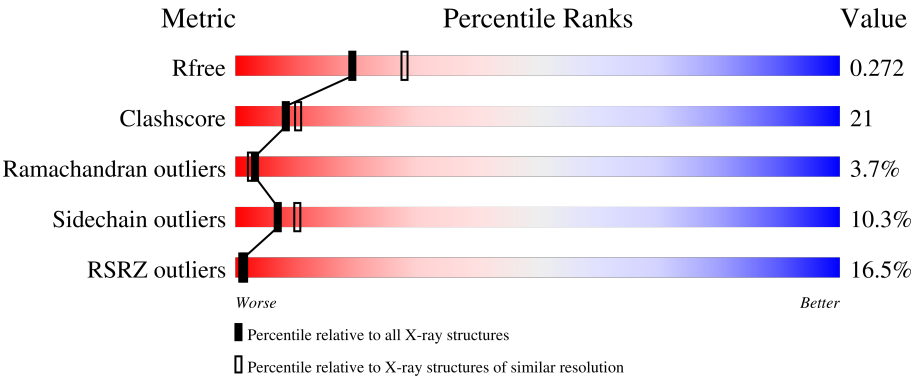
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	284	7% 64% 27% 5%
1	B	284	7% 76% 18%
1	C	284	7% 60% 31% 5%
1	D	284	8% 68% 24% 5%
1	E	284	12% 67% 24% 7%

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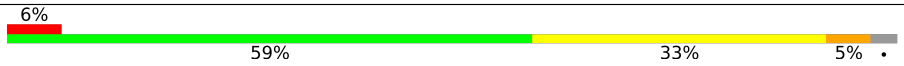
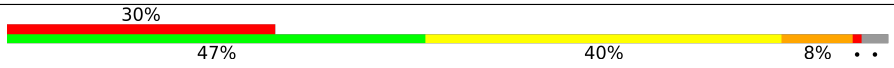
Mol	Chain	Length	Quality of chain
1	F	284	
1	G	284	
1	H	284	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17205 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 DNA repair protein PprA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2083	1290	383	406	4			
1	B	275	Total	C	N	O	S	0	0	0
			2083	1290	383	406	4			
1	C	275	Total	C	N	O	S	0	0	0
			2083	1290	383	406	4			
1	D	275	Total	C	N	O	S	0	0	0
			2083	1290	383	406	4			
1	E	278	Total	C	N	O	S	0	0	0
			2109	1305	388	412	4			
1	F	275	Total	C	N	O	S	0	0	0
			2083	1290	383	406	4			
1	G	275	Total	C	N	O	S	0	0	0
			2083	1290	383	406	4			
1	H	275	Total	C	N	O	S	0	0	0
			2083	1290	383	406	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	ARG	ALA	engineered mutation	UNP O32504
B	139	ARG	ALA	engineered mutation	UNP O32504
C	139	ARG	ALA	engineered mutation	UNP O32504
D	139	ARG	ALA	engineered mutation	UNP O32504
E	139	ARG	ALA	engineered mutation	UNP O32504
F	139	ARG	ALA	engineered mutation	UNP O32504
G	139	ARG	ALA	engineered mutation	UNP O32504
H	139	ARG	ALA	engineered mutation	UNP O32504

- Molecule 2 is water.

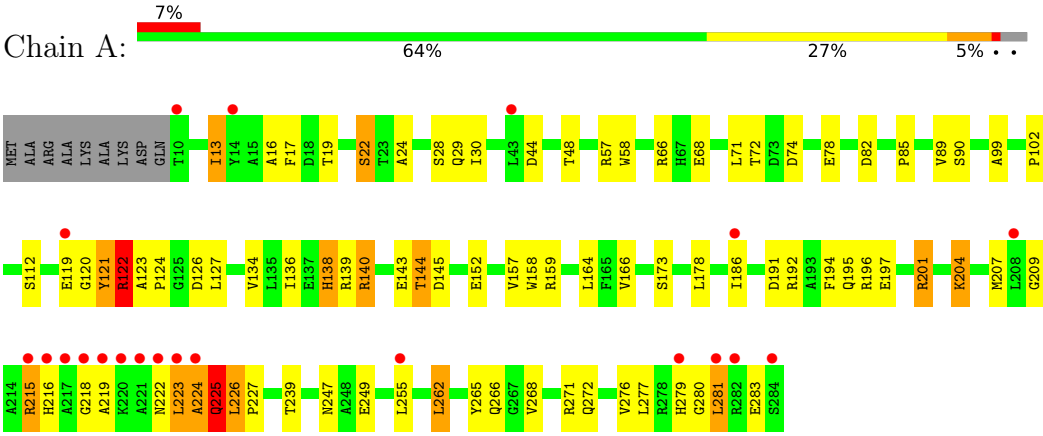
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	33	Total O 33 33	0	0
2	B	154	Total O 154 154	0	0
2	C	67	Total O 67 67	0	0
2	D	75	Total O 75 75	0	0
2	E	113	Total O 113 113	0	0
2	F	15	Total O 15 15	0	0
2	G	32	Total O 32 32	0	0
2	H	26	Total O 26 26	0	0

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.

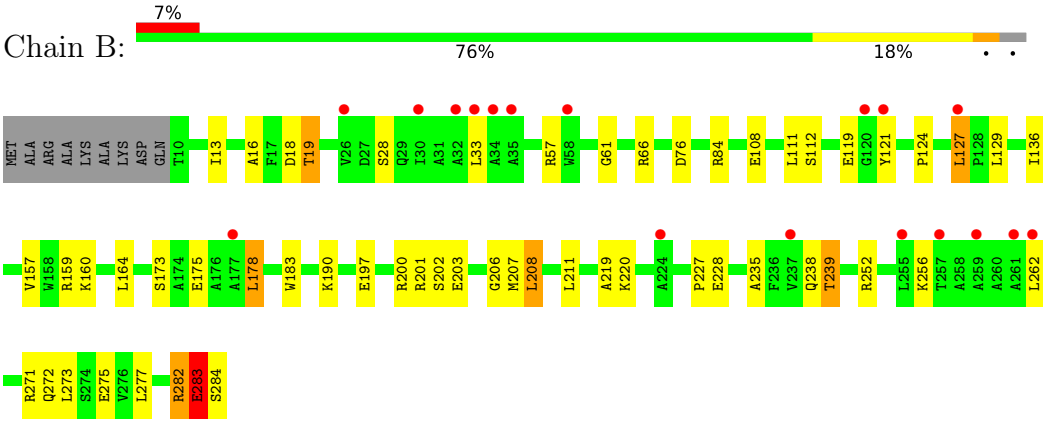
• Molecule 1: DNA repair protein PprA

Chain A:



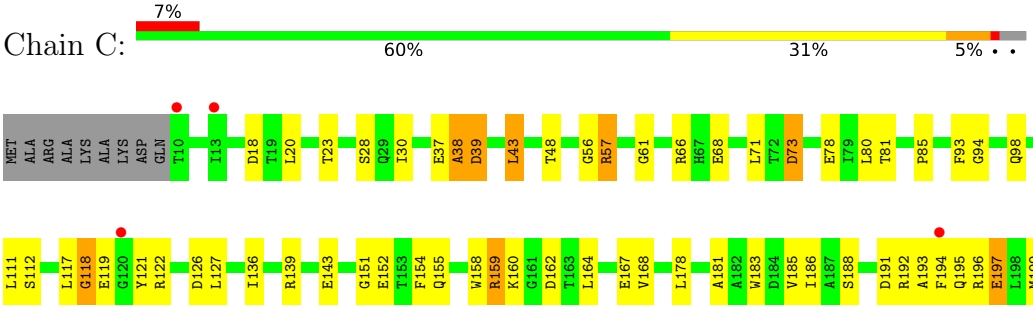
• Molecule 1: DNA repair protein PprA

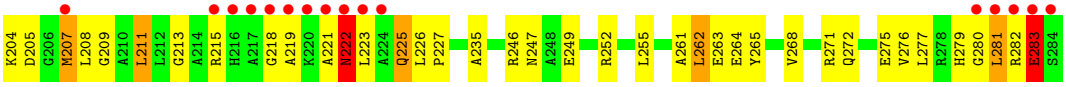
Chain B:



• Molecule 1: DNA repair protein PprA

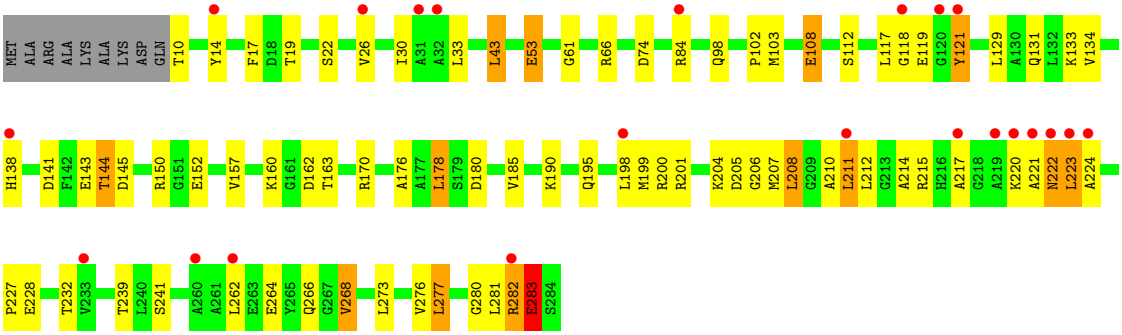
Chain C:





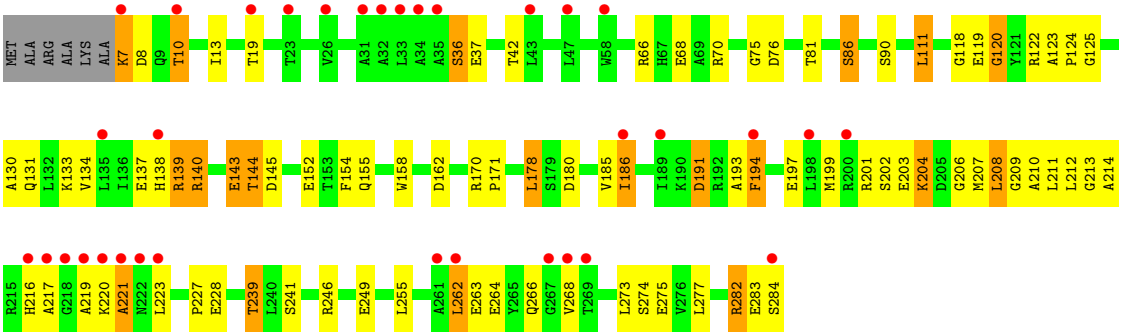
• Molecule 1: DNA repair protein PprA

Chain D:



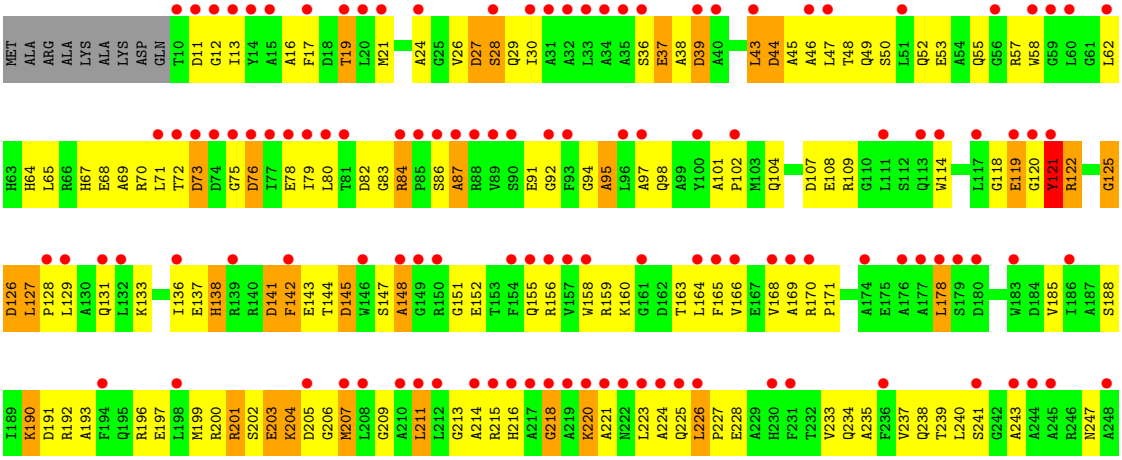
• Molecule 1: DNA repair protein PprA

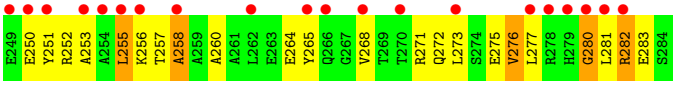
Chain E:



• Molecule 1: DNA repair protein PprA

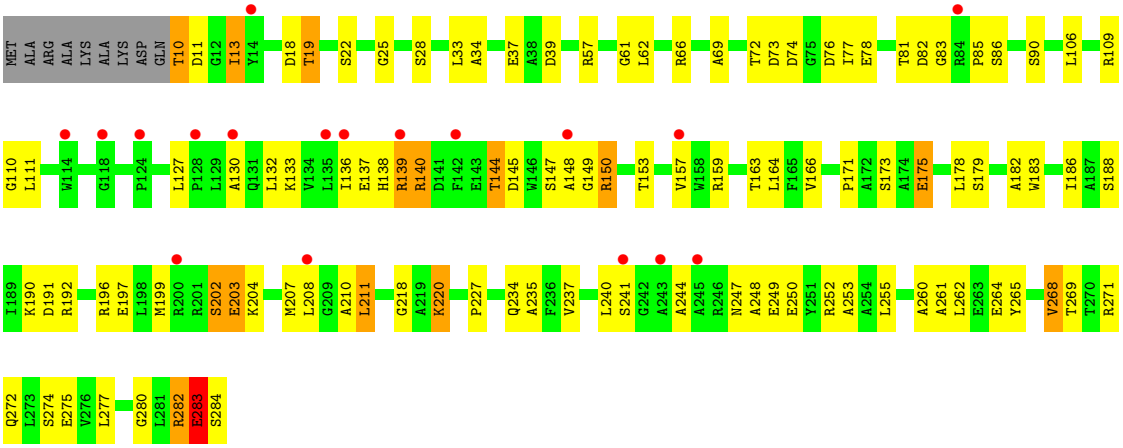
Chain F:





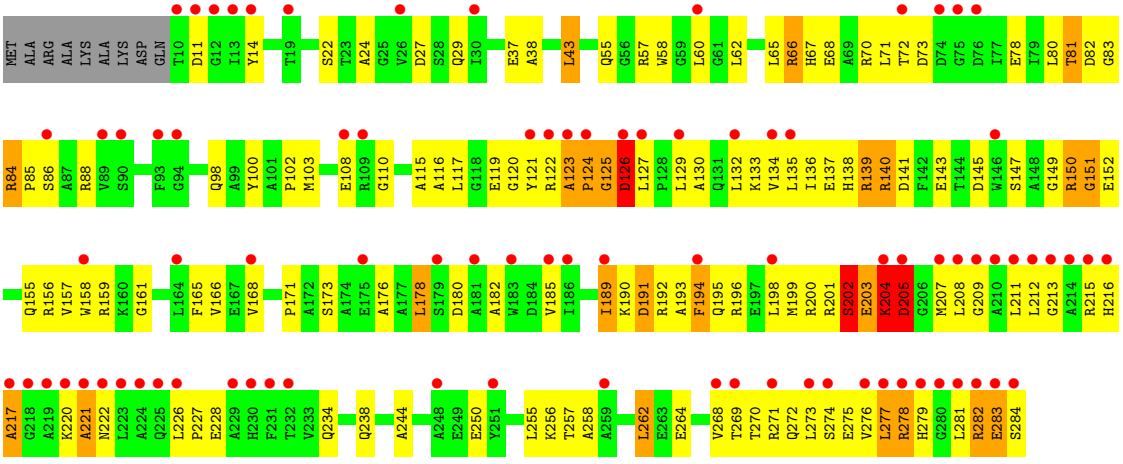
• Molecule 1: DNA repair protein PprA

Chain G:



• Molecule 1: DNA repair protein PprA

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.19Å 272.26Å 104.89Å 90.00° 98.64° 90.00°	Depositor
Resolution (Å)	48.63 – 2.40 48.63 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.63-2.40) 95.3 (48.63-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.212 , 0.271 0.215 , 0.272	Depositor DCC
R_{free} test set	5260 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	48.9	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 63.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17205	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.43	0/2118	0.56	0/2866
1	B	0.65	0/2118	0.72	1/2866 (0.0%)
1	C	0.49	0/2118	0.65	1/2866 (0.0%)
1	D	0.49	0/2118	0.61	0/2866
1	E	0.55	0/2144	0.66	1/2900 (0.0%)
1	F	0.27	0/2118	0.45	0/2866
1	G	0.43	0/2118	0.55	0/2866
1	H	0.34	0/2118	0.50	0/2866
All	All	0.47	0/16970	0.59	3/22962 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	127	LEU	CA-CB-CG	6.47	130.17	115.30
1	E	120	GLY	N-CA-C	-5.68	98.91	113.10
1	C	159	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2083	0	2024	85	1
1	B	2083	0	2024	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2083	0	2024	84	0
1	D	2083	0	2024	67	1
1	E	2109	0	2049	84	0
1	F	2083	0	2024	168	3
1	G	2083	0	2024	73	1
1	H	2083	0	2024	119	1
2	A	33	0	0	2	0
2	B	154	0	0	12	1
2	C	67	0	0	11	0
2	D	75	0	0	14	0
2	E	113	0	0	16	1
2	F	15	0	0	1	0
2	G	32	0	0	1	0
2	H	26	0	0	15	0
All	All	17205	0	16217	691	5

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 21.

All (691) 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:H:283:GLU:O	1:H:284:SER:OXT	1.65	1.15
1:H:271:ARG:HA	1:H:274:SER:OG	1.44	1.15
1:E:7:LYS:HB3	2:E:329:HOH:O	0.96	1.13
1:E:203:GLU:HB2	1:F:205:ASP:OD1	1.47	1.13
1:D:150:ARG:HD2	2:D:320:HOH:O	1.47	1.12
1:F:155:GLN:OE1	1:F:255:LEU:HD11	1.50	1.12
1:G:149:GLY:HA3	1:G:153:THR:O	1.51	1.09
1:B:271:ARG:HD3	2:B:301:HOH:O	1.52	1.08
1:B:190:LYS:HD2	1:E:241:SER:OG	1.54	1.07
1:G:163:THR:HG23	1:G:240:LEU:O	1.55	1.05
1:F:71:LEU:HD22	1:F:75:GLY:O	1.55	1.05
1:C:202:SER:O	1:C:203:GLU:HB3	1.48	1.04
1:F:126:ASP:O	1:F:127:LEU:O	1.76	1.03
1:H:200:ARG:NH2	2:H:301:HOH:O	1.90	1.03
1:H:279:HIS:HE1	2:H:310:HOH:O	1.45	1.00
1:D:282:ARG:O	1:D:283:GLU:HB2	1.62	0.99
1:H:279:HIS:CE1	2:H:310:HOH:O	2.14	0.97
1:H:122:ARG:O	1:H:123:ALA:O	1.82	0.97
1:E:202:SER:HB2	1:F:206:GLY:O	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LEU:O	1:C:118:GLY:O	1.83	0.96
1:D:217:ALA:HB1	2:D:315:HOH:O	1.63	0.96
1:H:122:ARG:HG3	2:H:306:HOH:O	1.64	0.95
1:F:272:GLN:O	1:F:276:VAL:HG23	1.66	0.95
1:F:163:THR:HG22	1:F:241:SER:OG	1.65	0.95
1:E:137:GLU:O	1:E:246:ARG:NH2	1.97	0.95
1:F:75:GLY:O	1:F:76:ASP:O	1.85	0.95
1:F:216:HIS:HE1	1:F:224:ALA:O	1.49	0.94
1:H:220:LYS:O	1:H:220:LYS:HD3	1.66	0.94
1:H:264:GLU:O	1:H:268:VAL:HG22	1.68	0.93
1:C:68:GLU:HB2	2:C:325:HOH:O	1.69	0.92
1:E:139:ARG:O	1:E:140:ARG:HB2	1.68	0.92
1:A:191:ASP:OD2	1:A:194:PHE:N	2.01	0.92
1:D:10:THR:HG21	2:D:335:HOH:O	1.70	0.92
1:H:140:ARG:HG3	2:H:316:HOH:O	1.69	0.90
1:G:249:GLU:OE1	1:G:249:GLU:HA	1.72	0.90
1:A:271:ARG:HD2	2:A:329:HOH:O	1.72	0.90
1:H:81:THR:HG23	1:H:86:SER:OG	1.71	0.89
1:F:71:LEU:HD22	1:F:76:ASP:O	1.72	0.88
1:C:139:ARG:O	1:C:246:ARG:NH2	2.07	0.88
1:C:252:ARG:CD	2:C:302:HOH:O	2.22	0.87
1:F:215:ARG:HG2	1:F:280:GLY:O	1.74	0.87
1:B:252:ARG:HD2	2:B:430:HOH:O	1.73	0.86
1:D:281:LEU:O	1:D:282:ARG:HG3	1.75	0.86
1:F:12:GLY:O	1:F:16:ALA:HB2	1.76	0.86
1:E:219:ALA:HB1	2:E:384:HOH:O	1.76	0.85
1:G:25:GLY:HA2	2:G:315:HOH:O	1.77	0.84
1:C:215:ARG:HG2	1:C:279:HIS:O	1.78	0.84
1:F:120:GLY:O	1:F:121:TYR:HB3	1.76	0.84
1:C:202:SER:O	1:C:203:GLU:CB	2.25	0.83
1:G:106:LEU:HD22	1:G:110:GLY:O	1.78	0.83
1:G:76:ASP:OD2	1:G:90:SER:OG	1.96	0.83
1:F:57:ARG:HA	1:F:235:ALA:O	1.78	0.83
1:A:140:ARG:O	1:A:159:ARG:NH1	2.12	0.82
1:H:83:GLY:O	1:H:84:ARG:O	1.97	0.82
1:E:138:HIS:CE1	2:E:373:HOH:O	2.32	0.81
1:F:118:GLY:O	1:F:119:GLU:O	1.97	0.81
1:D:264:GLU:O	1:D:268:VAL:HG12	1.79	0.81
1:F:216:HIS:CE1	1:F:224:ALA:O	2.34	0.80
1:E:138:HIS:O	1:E:139:ARG:O	2.00	0.80
1:H:189:ILE:HG22	1:H:189:ILE:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:ASP:O	1:F:142:PHE:HB3	1.81	0.79
1:F:260:ALA:O	1:F:264:GLU:HG3	1.82	0.79
1:H:180:ASP:OD2	2:H:302:HOH:O	2.01	0.79
1:E:10:THR:HB	2:E:329:HOH:O	1.82	0.78
1:F:72:THR:O	1:F:73:ASP:HB2	1.83	0.78
1:H:140:ARG:CG	2:H:316:HOH:O	2.24	0.78
1:A:120:GLY:O	1:A:122:ARG:N	2.16	0.78
1:F:144:THR:HG22	1:F:145:ASP:O	1.83	0.77
1:F:204:LYS:O	1:F:204:LYS:HG3	1.82	0.77
1:E:220:LYS:HG3	2:E:395:HOH:O	1.84	0.77
1:F:191:ASP:OD2	1:F:193:ALA:HB3	1.85	0.76
1:F:250:GLU:OE1	1:F:250:GLU:HA	1.84	0.76
1:F:257:THR:O	1:F:260:ALA:N	2.18	0.76
1:F:209:GLY:O	1:F:213:GLY:N	2.19	0.75
1:A:212:LEU:O	1:A:215:ARG:HB2	1.87	0.75
1:H:140:ARG:CB	2:H:316:HOH:O	2.34	0.75
1:F:252:ARG:O	1:F:256:LYS:HG2	1.86	0.74
1:A:191:ASP:O	1:A:195:GLN:HG3	1.87	0.74
1:H:211:LEU:O	1:H:215:ARG:HG3	1.86	0.74
1:C:48:THR:HG23	1:C:68:GLU:HA	1.67	0.74
1:F:30:ILE:HG22	1:F:30:ILE:O	1.87	0.74
1:C:252:ARG:NE	2:C:302:HOH:O	2.17	0.74
1:F:237:VAL:HG12	1:F:237:VAL:O	1.87	0.74
1:H:73:ASP:OD1	2:H:303:HOH:O	2.04	0.73
1:G:139:ARG:O	1:G:159:ARG:NH1	2.21	0.73
1:G:202:SER:O	1:G:203:GLU:CB	2.36	0.73
1:F:272:GLN:O	1:F:276:VAL:CG2	2.35	0.73
1:G:66:ARG:HB3	1:G:82:ASP:HA	1.70	0.73
1:H:198:LEU:O	1:H:202:SER:OG	2.06	0.73
1:F:43:LEU:O	1:F:44:ASP:OD1	2.06	0.73
1:D:134:VAL:O	1:D:138:HIS:ND1	2.21	0.73
1:H:140:ARG:HH11	1:H:141:ASP:H	1.37	0.73
1:B:190:LYS:CD	1:E:241:SER:OG	2.36	0.72
1:E:282:ARG:O	1:E:284:SER:N	2.21	0.72
1:H:78:GLU:OE1	1:H:80:LEU:HD11	1.88	0.72
1:H:129:LEU:HB3	1:H:133:LYS:HE3	1.70	0.72
1:F:133:LYS:NZ	1:F:137:GLU:OE2	2.23	0.72
1:A:216:HIS:ND1	1:A:222:ASN:OD1	2.22	0.72
1:A:215:ARG:HE	1:A:279:HIS:HB3	1.54	0.72
1:A:215:ARG:HH22	1:A:222:ASN:HA	1.55	0.71
1:A:224:ALA:O	1:A:226:LEU:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:ARG:O	1:G:159:ARG:NH1	2.24	0.71
1:F:239:THR:O	1:F:240:LEU:HD23	1.89	0.71
1:H:120:GLY:O	2:H:304:HOH:O	2.08	0.71
1:C:282:ARG:O	1:C:283:GLU:HB3	1.90	0.71
1:E:139:ARG:O	1:E:140:ARG:CB	2.38	0.71
1:D:228:GLU:OE2	2:D:301:HOH:O	2.09	0.71
1:C:196:ARG:HE	1:D:176:ALA:HB1	1.54	0.71
1:B:200:ARG:O	1:B:203:GLU:HB2	1.90	0.71
1:G:191:ASP:HB2	1:G:284:SER:OG	1.91	0.71
1:E:207:MET:O	1:E:210:ALA:HB3	1.91	0.71
1:A:207:MET:HG3	1:B:202:SER:OG	1.90	0.70
1:H:98:GLN:O	1:H:102:PRO:CD	2.40	0.70
1:E:203:GLU:O	1:E:204:LYS:HB2	1.89	0.70
1:H:273:LEU:O	1:H:277:LEU:HD12	1.91	0.70
1:F:27:ASP:O	1:F:29:GLN:N	2.25	0.70
1:C:191:ASP:O	1:C:195:GLN:HG3	1.92	0.70
1:F:168:VAL:O	1:F:235:ALA:CB	2.40	0.70
1:F:19:THR:HG22	1:F:227:PRO:HG3	1.73	0.69
1:F:178:LEU:HD11	1:F:226:LEU:HD13	1.73	0.69
1:G:202:SER:O	1:G:203:GLU:HG3	1.92	0.69
1:B:271:ARG:NH2	2:B:303:HOH:O	2.24	0.69
1:A:225:GLN:O	1:A:226:LEU:C	2.30	0.69
1:E:37:GLU:HA	1:E:37:GLU:OE1	1.93	0.69
1:F:83:GLY:O	1:F:84:ARG:O	2.10	0.69
1:C:139:ARG:CB	2:C:357:HOH:O	2.40	0.69
1:E:220:LYS:O	1:E:221:ALA:HB2	1.93	0.69
1:F:168:VAL:O	1:F:235:ALA:HB1	1.93	0.69
1:A:209:GLY:O	1:A:213:GLY:N	2.15	0.69
1:D:232:THR:OG1	2:D:303:HOH:O	2.10	0.69
1:D:103:MET:O	2:D:302:HOH:O	2.09	0.69
1:E:81:THR:HG23	1:E:86:SER:OG	1.93	0.69
1:F:218:GLY:O	1:F:282:ARG:NH2	2.26	0.69
1:F:91:GLU:HG2	1:F:91:GLU:O	1.91	0.68
1:H:138:HIS:O	1:H:139:ARG:O	2.11	0.68
1:A:30:ILE:HG22	1:A:30:ILE:O	1.92	0.68
1:B:19:THR:HG23	1:B:227:PRO:HG3	1.75	0.68
1:F:121:TYR:O	1:F:122:ARG:O	2.11	0.68
1:G:76:ASP:OD1	1:G:77:ILE:N	2.23	0.68
1:F:13:ILE:HG21	1:F:76:ASP:OD1	1.93	0.68
1:F:188:SER:O	1:F:190:LYS:HG2	1.94	0.68
1:F:84:ARG:HG2	2:F:307:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:ARG:NH1	1:E:68:GLU:OE1	2.27	0.68
1:F:13:ILE:CG2	1:F:76:ASP:OD1	2.42	0.68
1:A:66:ARG:NH1	1:A:68:GLU:OE2	2.26	0.67
1:F:268:VAL:HG12	1:F:271:ARG:HH21	1.60	0.67
1:F:52:GLN:NE2	1:F:67:HIS:O	2.26	0.67
1:H:204:LYS:O	1:H:205:ASP:CB	2.42	0.67
1:H:122:ARG:HG2	1:H:145:ASP:OD1	1.95	0.67
1:C:126:ASP:OD1	1:C:126:ASP:N	2.26	0.67
1:C:159:ARG:CD	2:C:326:HOH:O	2.42	0.67
1:F:192:ARG:O	1:F:196:ARG:HG3	1.94	0.67
1:A:276:VAL:O	1:A:279:HIS:HB2	1.93	0.67
1:G:13:ILE:HD11	1:G:90:SER:HB3	1.77	0.67
1:H:124:PRO:O	1:H:125:GLY:O	2.13	0.67
1:H:220:LYS:O	1:H:221:ALA:CB	2.42	0.67
1:A:19:THR:O	1:A:22:SER:HB2	1.95	0.67
1:C:56:GLY:O	2:C:301:HOH:O	2.11	0.67
1:A:134:VAL:O	1:A:138:HIS:O	2.13	0.67
1:F:94:GLY:O	1:F:97:ALA:HB3	1.95	0.67
1:G:220:LYS:O	1:G:220:LYS:HD3	1.95	0.67
1:F:215:ARG:CG	1:F:280:GLY:O	2.42	0.66
1:C:38:ALA:O	1:C:39:ASP:O	2.13	0.66
1:F:48:THR:O	1:F:48:THR:HG22	1.93	0.66
1:B:160:LYS:CE	2:B:307:HOH:O	2.43	0.66
1:D:150:ARG:NH2	2:D:304:HOH:O	2.28	0.66
1:F:151:GLY:O	1:F:170:ARG:NH2	2.28	0.66
1:G:202:SER:O	1:G:203:GLU:HB2	1.96	0.66
1:A:218:GLY:HA3	1:A:280:GLY:O	1.95	0.66
1:C:215:ARG:HH22	1:C:223:LEU:HD12	1.60	0.66
1:H:70:ARG:HH21	1:H:72:THR:HG22	1.61	0.65
1:E:76:ASP:OD2	1:E:90:SER:OG	2.11	0.65
1:F:144:THR:CG2	1:F:145:ASP:O	2.44	0.65
1:H:270:THR:O	1:H:274:SER:OG	2.13	0.65
1:B:160:LYS:HE2	2:B:307:HOH:O	1.94	0.65
1:A:99:ALA:O	1:A:102:PRO:HD2	1.97	0.65
1:E:138:HIS:HE1	2:E:373:HOH:O	1.74	0.65
1:D:10:THR:CG2	2:D:335:HOH:O	2.34	0.65
1:H:168:VAL:HG12	1:H:262:LEU:HD12	1.79	0.65
1:A:192:ARG:O	1:A:196:ARG:HG3	1.96	0.64
1:C:197:GLU:OE2	1:C:201:ARG:HD2	1.97	0.64
1:E:203:GLU:HG3	1:F:204:LYS:H	1.62	0.64
1:F:163:THR:HG22	1:F:241:SER:HG	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:66:ARG:NH2	1:H:68:GLU:OE2	2.30	0.64
1:A:207:MET:HG2	1:B:207:MET:HG2	1.80	0.64
1:F:44:ASP:HA	1:F:47:LEU:HB2	1.77	0.64
1:F:197:GLU:O	1:F:201:ARG:HG3	1.96	0.64
1:B:283:GLU:O	1:B:284:SER:CB	2.45	0.64
1:F:69:ALA:HA	1:F:78:GLU:O	1.97	0.64
1:C:94:GLY:O	1:C:98:GLN:HG3	1.96	0.64
1:C:280:GLY:O	1:C:281:LEU:O	2.16	0.64
1:F:26:VAL:HG12	1:F:28:SER:H	1.62	0.64
1:F:55:GLN:OE1	1:F:62:LEU:HD12	1.97	0.64
1:G:132:LEU:O	1:G:136:ILE:HG12	1.97	0.64
1:H:132:LEU:O	1:H:136:ILE:HG12	1.97	0.64
1:F:272:GLN:HA	1:F:275:GLU:HG2	1.80	0.64
1:D:205:ASP:OD1	1:D:206:GLY:N	2.31	0.64
1:E:19:THR:HG22	1:E:227:PRO:HG3	1.80	0.64
1:F:240:LEU:HD11	1:F:250:GLU:O	1.98	0.64
1:H:200:ARG:O	1:H:202:SER:O	2.16	0.64
1:G:202:SER:O	1:G:203:GLU:CG	2.47	0.63
1:H:204:LYS:O	1:H:205:ASP:HB2	1.98	0.63
1:F:137:GLU:O	1:F:138:HIS:HB2	1.97	0.63
1:B:16:ALA:O	1:B:19:THR:HG22	1.97	0.63
1:C:23:THR:HG21	1:C:227:PRO:HB2	1.81	0.63
1:A:78:GLU:OE2	1:A:85:PRO:HB3	1.99	0.63
1:C:117:LEU:O	1:C:118:GLY:C	2.37	0.63
1:B:136:ILE:O	1:B:159:ARG:NH2	2.32	0.63
1:E:197:GLU:O	1:E:201:ARG:HG3	1.99	0.63
1:C:207:MET:SD	1:D:207:MET:HG2	2.39	0.62
1:B:144:THR:HG21	2:B:416:HOH:O	1.98	0.62
1:E:203:GLU:O	1:E:204:LYS:CB	2.47	0.62
1:A:215:ARG:O	1:A:219:ALA:HB3	1.99	0.62
1:C:219:ALA:HB2	1:C:280:GLY:HA2	1.80	0.62
1:H:78:GLU:HG3	1:H:88:ARG:HG2	1.82	0.62
1:B:207:MET:C	1:B:208:LEU:O	2.34	0.62
1:H:122:ARG:N	2:H:306:HOH:O	2.32	0.62
1:C:207:MET:HA	1:D:207:MET:HE3	1.82	0.61
1:F:204:LYS:O	1:F:204:LYS:CG	2.47	0.61
1:F:126:ASP:OD1	1:F:126:ASP:N	2.33	0.61
1:H:201:ARG:O	1:H:205:ASP:HB2	2.00	0.61
1:G:220:LYS:O	1:G:220:LYS:CG	2.48	0.61
1:H:83:GLY:O	1:H:84:ARG:C	2.39	0.61
1:C:196:ARG:NH2	1:D:180:ASP:OD2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:PRO:HG2	1:F:228:GLU:OE1	2.01	0.61
1:B:275:GLU:OE2	2:B:302:HOH:O	2.15	0.61
1:H:98:GLN:O	1:H:102:PRO:HD3	1.98	0.61
1:H:157:VAL:HG23	1:H:165:PHE:O	2.00	0.61
1:H:220:LYS:O	1:H:221:ALA:HB2	2.01	0.61
1:C:28:SER:HB2	1:C:30:ILE:HG12	1.81	0.61
1:D:201:ARG:HH22	1:D:214:ALA:HB2	1.66	0.60
1:E:202:SER:CB	1:F:206:GLY:O	2.46	0.60
1:C:276:VAL:O	1:C:279:HIS:HB3	2.00	0.60
1:F:71:LEU:CD2	1:F:76:ASP:O	2.47	0.60
1:H:283:GLU:O	1:H:284:SER:C	2.38	0.60
1:C:159:ARG:HD2	2:C:326:HOH:O	2.01	0.60
1:G:163:THR:CG2	1:G:240:LEU:O	2.43	0.60
1:E:170:ARG:NH2	1:E:263:GLU:OE1	2.33	0.60
1:C:122:ARG:O	1:C:122:ARG:HG3	2.01	0.60
1:D:221:ALA:O	1:D:222:ASN:CB	2.49	0.60
1:G:159:ARG:HB2	1:G:164:LEU:HD12	1.83	0.60
1:H:140:ARG:HB3	2:H:316:HOH:O	2.00	0.60
1:D:117:LEU:O	1:D:119:GLU:N	2.26	0.60
1:E:220:LYS:O	1:E:221:ALA:CB	2.49	0.60
1:H:110:GLY:O	1:H:171:PRO:HB3	2.01	0.60
1:H:151:GLY:O	1:H:152:GLU:HB2	2.01	0.59
1:F:126:ASP:O	1:F:127:LEU:C	2.41	0.59
1:F:141:ASP:O	1:F:142:PHE:CB	2.51	0.59
1:D:26:VAL:HG22	1:D:53:GLU:HG2	1.85	0.59
1:F:125:GLY:O	1:F:127:LEU:N	2.35	0.59
1:F:143:GLU:HG3	1:F:158:TRP:HB3	1.83	0.59
1:H:281:LEU:O	1:H:283:GLU:N	2.35	0.59
1:A:140:ARG:H	1:A:140:ARG:HD2	1.68	0.59
1:B:283:GLU:O	1:B:284:SER:HB2	2.03	0.59
1:C:271:ARG:NH2	2:C:303:HOH:O	2.29	0.59
1:F:216:HIS:O	1:F:221:ALA:O	2.21	0.59
1:F:92:GLY:O	1:F:95:ALA:HB3	2.03	0.59
1:H:204:LYS:O	1:H:205:ASP:OD1	2.21	0.59
1:G:173:SER:HB2	1:G:175:GLU:HG2	1.85	0.59
1:G:197:GLU:OE1	1:G:282:ARG:NH1	2.36	0.59
1:H:137:GLU:HG2	2:H:309:HOH:O	2.02	0.59
1:C:209:GLY:O	1:C:213:GLY:N	2.36	0.58
1:E:130:ALA:O	1:E:133:LYS:HG2	2.03	0.58
1:H:98:GLN:O	1:H:102:PRO:HD2	2.03	0.58
1:D:280:GLY:O	1:D:281:LEU:HD23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:MET:O	1:G:210:ALA:HB3	2.03	0.58
1:A:262:LEU:O	1:A:266:GLN:HG3	2.03	0.58
1:D:10:THR:HG22	1:D:10:THR:O	2.04	0.58
1:D:19:THR:HG22	1:D:227:PRO:HG3	1.86	0.58
1:F:86:SER:O	1:F:87:ALA:HB2	2.04	0.58
1:H:122:ARG:CG	1:H:145:ASP:OD1	2.52	0.58
1:H:276:VAL:HG12	1:H:276:VAL:O	2.03	0.58
1:E:144:THR:HG23	1:E:145:ASP:O	2.03	0.57
1:H:173:SER:OG	1:H:176:ALA:HB2	2.04	0.57
1:E:209:GLY:O	1:E:213:GLY:N	2.36	0.57
1:F:192:ARG:O	1:F:196:ARG:CG	2.52	0.57
1:D:152:GLU:HG3	2:D:360:HOH:O	2.04	0.57
1:G:220:LYS:O	1:G:220:LYS:CD	2.53	0.57
1:F:46:ALA:HA	1:F:49:GLN:HG3	1.85	0.57
1:D:268:VAL:HG11	1:G:268:VAL:HG11	1.86	0.57
1:B:197:GLU:OE2	1:B:201:ARG:NH1	2.38	0.57
1:A:66:ARG:N	1:A:82:ASP:OD1	2.36	0.57
1:A:71:LEU:HD12	1:A:71:LEU:H	1.69	0.57
1:F:21:MET:HB3	1:F:26:VAL:HB	1.86	0.57
1:H:27:ASP:OD1	1:H:29:GLN:HG2	2.04	0.57
1:H:209:GLY:O	1:H:213:GLY:N	2.38	0.57
1:C:43:LEU:HD23	1:C:71:LEU:HD11	1.87	0.57
1:H:244:ALA:HB1	1:H:250:GLU:OE1	2.04	0.57
1:G:136:ILE:O	1:G:159:ARG:NH2	2.37	0.57
1:F:47:LEU:O	1:F:69:ALA:HB3	2.05	0.56
1:E:70:ARG:HD2	2:E:362:HOH:O	2.05	0.56
1:F:43:LEU:O	1:F:44:ASP:CG	2.43	0.56
1:E:191:ASP:OD2	1:E:193:ALA:HB3	2.06	0.56
1:F:17:PHE:O	1:F:21:MET:HG2	2.06	0.56
1:G:260:ALA:O	1:G:264:GLU:HG3	2.06	0.56
1:A:28:SER:O	1:A:29:GLN:HG2	2.04	0.56
1:D:163:THR:HG23	1:D:239:THR:OG1	2.06	0.56
1:A:224:ALA:O	1:A:225:GLN:C	2.42	0.56
1:A:72:THR:OG1	1:A:74:ASP:OD1	2.22	0.56
1:E:144:THR:CG2	1:E:145:ASP:O	2.53	0.56
1:H:123:ALA:O	1:H:125:GLY:N	2.39	0.56
1:C:107:ASP:OD1	1:C:109:ARG:N	2.39	0.56
1:B:124:PRO:HD2	1:B:127:LEU:HD21	1.89	0.55
1:C:215:ARG:CG	1:C:279:HIS:O	2.52	0.55
1:E:7:LYS:HD3	1:E:8:ASP:H	1.69	0.55
1:G:175:GLU:CD	1:G:175:GLU:H	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:211:LEU:O	1:H:281:LEU:HD21	2.06	0.55
1:C:37:GLU:OE2	1:C:37:GLU:HA	2.05	0.55
1:C:191:ASP:OD1	1:C:193:ALA:N	2.38	0.55
1:F:257:THR:O	1:F:258:ALA:C	2.45	0.55
1:H:55:GLN:NE2	1:H:60:LEU:HD12	2.22	0.55
1:A:108:GLU:CD	1:A:108:GLU:H	2.10	0.55
1:A:121:TYR:O	1:A:122:ARG:CG	2.55	0.55
1:G:272:GLN:O	1:G:275:GLU:HG2	2.06	0.55
1:D:74:ASP:OD1	1:D:74:ASP:N	2.39	0.55
1:E:214:ALA:O	1:E:217:ALA:HB2	2.07	0.55
1:A:272:GLN:O	1:A:276:VAL:HG23	2.07	0.55
1:C:265:TYR:HA	1:C:268:VAL:HG22	1.89	0.55
1:H:173:SER:OG	1:H:176:ALA:CB	2.55	0.55
1:C:57:ARG:HA	1:C:235:ALA:O	2.06	0.54
1:F:27:ASP:O	1:F:29:GLN:HG2	2.06	0.54
1:F:101:ALA:HB3	1:F:102:PRO:HD3	1.89	0.54
1:E:208:LEU:HD22	1:E:212:LEU:HG	1.89	0.54
1:F:36:SER:O	1:F:37:GLU:HB2	2.07	0.54
1:F:70:ARG:O	1:F:71:LEU:HD23	2.07	0.54
1:B:178:LEU:HD13	1:B:208:LEU:HD11	1.89	0.54
1:F:164:LEU:HD21	1:F:251:TYR:HD2	1.71	0.54
1:F:104:GLN:HA	1:F:114:TRP:HE1	1.72	0.54
1:B:119:GLU:HG3	1:B:119:GLU:O	2.07	0.54
1:D:33:LEU:HD23	1:D:43:LEU:HD13	1.89	0.54
1:F:214:ALA:HA	1:F:218:GLY:HA3	1.89	0.54
1:H:182:ALA:O	1:H:185:VAL:HB	2.07	0.54
1:E:170:ARG:HH12	1:E:263:GLU:CD	2.10	0.54
1:F:272:GLN:O	1:F:276:VAL:CB	2.55	0.54
1:G:218:GLY:HA3	1:G:280:GLY:O	2.08	0.54
1:A:265:TYR:HA	1:A:268:VAL:HG22	1.89	0.54
1:E:170:ARG:NH1	1:E:263:GLU:OE1	2.41	0.54
1:A:225:GLN:OE1	1:A:225:GLN:HA	2.08	0.54
1:G:139:ARG:O	1:G:140:ARG:O	2.26	0.54
1:A:191:ASP:OD2	1:A:194:PHE:CB	2.56	0.54
1:D:178:LEU:HD23	1:D:273:LEU:HD21	1.90	0.54
1:H:192:ARG:O	1:H:196:ARG:HG2	2.06	0.54
1:C:203:GLU:N	1:C:205:ASP:O	2.41	0.54
1:E:239:THR:HB	2:E:371:HOH:O	2.07	0.54
1:F:148:ALA:O	1:F:155:GLN:HG2	2.08	0.53
1:H:58:TRP:O	1:H:234:GLN:HB2	2.08	0.53
1:F:48:THR:O	1:F:48:THR:CG2	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:ALA:HA	1:G:133:LYS:HD2	1.89	0.53
1:B:173:SER:OG	1:B:175:GLU:HG2	2.08	0.53
1:D:61:GLY:HA3	1:D:112:SER:HB2	1.89	0.53
1:A:122:ARG:HG3	1:A:122:ARG:O	2.08	0.53
1:A:276:VAL:O	1:A:279:HIS:CB	2.57	0.53
1:E:68:GLU:CD	2:E:302:HOH:O	2.46	0.53
1:F:281:LEU:HD23	1:F:282:ARG:HD2	1.90	0.53
1:C:263:GLU:O	1:C:264:GLU:C	2.45	0.53
1:E:119:GLU:O	1:E:122:ARG:HB3	2.08	0.53
1:F:17:PHE:HE1	1:F:79:ILE:HD11	1.73	0.53
1:C:268:VAL:O	1:C:272:GLN:HG3	2.07	0.53
1:D:190:LYS:HG3	1:G:241:SER:HB2	1.89	0.53
1:D:220:LYS:HD2	1:G:39:ASP:HB3	1.90	0.53
1:G:171:PRO:HA	1:G:234:GLN:OE1	2.08	0.53
1:G:247:ASN:OD1	1:G:249:GLU:HB2	2.09	0.53
1:A:157:VAL:HG23	1:A:166:VAL:HG22	1.90	0.53
1:F:12:GLY:O	1:F:16:ALA:CB	2.53	0.52
1:B:160:LYS:NZ	2:B:307:HOH:O	2.41	0.52
1:C:136:ILE:O	1:C:159:ARG:NH2	2.40	0.52
1:F:78:GLU:O	1:F:80:LEU:HD12	2.08	0.52
1:H:244:ALA:CB	1:H:250:GLU:OE1	2.57	0.52
1:F:166:VAL:HB	1:F:238:GLN:HB3	1.90	0.52
1:G:192:ARG:O	1:G:196:ARG:HG3	2.10	0.52
1:D:144:THR:HG23	1:D:145:ASP:O	2.09	0.52
1:F:152:GLU:O	1:F:152:GLU:HG2	2.09	0.52
1:H:122:ARG:O	1:H:123:ALA:C	2.48	0.52
1:C:122:ARG:O	1:C:122:ARG:CG	2.58	0.52
1:D:282:ARG:O	1:D:283:GLU:CB	2.45	0.52
1:D:212:LEU:O	1:D:215:ARG:HB2	2.09	0.52
1:G:57:ARG:HA	1:G:235:ALA:O	2.08	0.52
1:G:61:GLY:O	1:G:62:LEU:HD23	2.10	0.52
1:B:282:ARG:HG2	2:B:363:HOH:O	2.10	0.52
1:E:7:LYS:HD3	1:E:8:ASP:N	2.25	0.52
1:G:109:ARG:O	1:G:171:PRO:HG2	2.09	0.52
1:F:136:ILE:HG23	1:F:159:ARG:NH2	2.24	0.51
1:F:200:ARG:O	1:F:202:SER:O	2.28	0.51
1:H:199:MET:O	1:H:202:SER:OG	2.27	0.51
1:A:123:ALA:N	1:A:143:GLU:O	2.35	0.51
1:A:124:PRO:HB2	1:A:126:ASP:OD1	2.11	0.51
1:F:202:SER:O	1:F:203:GLU:HB3	2.11	0.51
1:H:275:GLU:HA	1:H:278:ARG:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:LYS:O	1:E:120:GLY:HA3	2.09	0.51
1:C:215:ARG:NE	1:C:276:VAL:O	2.43	0.51
1:G:19:THR:HG23	1:G:227:PRO:HG3	1.92	0.51
1:B:190:LYS:HD2	1:E:241:SER:HG	1.70	0.51
1:C:282:ARG:O	1:C:283:GLU:CB	2.58	0.51
1:E:219:ALA:CB	2:E:384:HOH:O	2.46	0.51
1:F:215:ARG:O	1:F:216:HIS:C	2.48	0.51
1:C:143:GLU:HB2	1:C:158:TRP:HB3	1.93	0.51
1:E:216:HIS:CE1	1:E:223:LEU:HD22	2.46	0.51
1:F:62:LEU:HD22	1:F:65:LEU:HD12	1.93	0.51
1:H:122:ARG:C	1:H:123:ALA:O	2.50	0.51
1:B:61:GLY:HA3	1:B:112:SER:HB2	1.92	0.51
1:C:159:ARG:HD3	2:C:326:HOH:O	2.09	0.51
1:E:178:LEU:HD13	1:E:208:LEU:HD11	1.93	0.51
1:D:223:LEU:HD23	1:D:224:ALA:O	2.10	0.50
1:E:139:ARG:H	1:E:246:ARG:NH2	2.09	0.50
1:H:24:ALA:HB1	1:H:57:ARG:HB2	1.93	0.50
1:A:194:PHE:CZ	1:A:281:LEU:HB3	2.47	0.50
1:C:192:ARG:HB3	1:C:196:ARG:NH1	2.26	0.50
1:H:273:LEU:O	1:H:273:LEU:HG	2.10	0.50
1:E:131:GLN:O	1:E:134:VAL:HB	2.11	0.50
1:G:147:SER:O	1:G:148:ALA:C	2.49	0.50
1:B:228:GLU:HG2	1:B:273:LEU:HD22	1.94	0.50
1:F:276:VAL:O	1:F:276:VAL:CG1	2.59	0.50
1:G:265:TYR:O	1:G:269:THR:OG1	2.23	0.50
1:B:159:ARG:HB2	1:B:164:LEU:HD12	1.92	0.50
1:F:64:HIS:CE1	1:F:65:LEU:HG	2.46	0.50
1:F:243:ALA:O	1:F:247:ASN:HB2	2.12	0.50
1:G:204:LYS:O	1:H:203:GLU:OE1	2.30	0.50
1:B:268:VAL:O	1:B:272:GLN:HG3	2.12	0.50
1:H:149:GLY:O	1:H:150:ARG:C	2.50	0.50
1:H:269:THR:HA	1:H:272:GLN:HB2	1.94	0.50
1:E:122:ARG:NH2	2:E:306:HOH:O	2.44	0.49
1:F:83:GLY:O	1:F:84:ARG:C	2.51	0.49
1:H:282:ARG:O	1:H:282:ARG:HG3	2.11	0.49
1:A:207:MET:HG2	1:B:207:MET:CG	2.41	0.49
1:D:53:GLU:OE1	1:G:275:GLU:OE1	2.30	0.49
1:H:276:VAL:O	1:H:276:VAL:CG1	2.59	0.49
1:F:240:LEU:CD1	1:F:250:GLU:O	2.60	0.49
1:G:182:ALA:HB1	1:G:211:LEU:HD12	1.94	0.49
1:A:191:ASP:OD2	1:A:194:PHE:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:ILE:HD13	1:E:76:ASP:HA	1.94	0.49
1:A:24:ALA:O	1:A:57:ARG:HD2	2.13	0.49
1:C:38:ALA:O	1:C:39:ASP:C	2.49	0.49
1:F:215:ARG:CB	1:F:280:GLY:O	2.60	0.49
1:A:283:GLU:HG3	1:A:283:GLU:O	2.13	0.49
1:G:144:THR:HG23	1:G:145:ASP:O	2.12	0.49
1:H:220:LYS:O	1:H:220:LYS:CD	2.50	0.49
1:B:144:THR:HG22	1:B:157:VAL:H	1.78	0.49
1:C:66:ARG:O	1:C:81:THR:HA	2.12	0.49
1:H:123:ALA:HB1	1:H:124:PRO:HD2	1.94	0.49
1:C:155:GLN:HA	1:C:167:GLU:O	2.13	0.48
1:E:143:GLU:HB2	1:E:158:TRP:HB3	1.95	0.48
1:H:125:GLY:O	1:H:126:ASP:C	2.51	0.48
1:H:178:LEU:HD23	1:H:273:LEU:HD21	1.94	0.48
1:A:30:ILE:O	1:A:30:ILE:CG2	2.60	0.48
1:D:144:THR:HG21	2:D:347:HOH:O	2.11	0.48
1:G:220:LYS:O	1:G:220:LYS:HG2	2.12	0.48
1:F:98:GLN:O	1:F:102:PRO:HD3	2.14	0.48
1:G:34:ALA:O	1:G:37:GLU:N	2.40	0.48
1:E:119:GLU:N	1:E:120:GLY:HA3	2.28	0.48
1:F:147:SER:O	1:F:148:ALA:O	2.31	0.48
1:G:69:ALA:HA	1:G:78:GLU:O	2.14	0.48
1:A:225:GLN:NE2	2:A:303:HOH:O	2.46	0.48
1:G:81:THR:O	1:G:82:ASP:HB2	2.14	0.48
1:A:136:ILE:O	1:A:159:ARG:NH2	2.46	0.48
1:G:138:HIS:O	1:G:139:ARG:C	2.51	0.48
1:G:72:THR:OG1	1:G:74:ASP:OD1	2.16	0.48
1:G:144:THR:HG22	1:G:157:VAL:H	1.78	0.48
1:H:238:GLN:HB2	1:H:258:ALA:HB2	1.95	0.48
1:A:13:ILE:HD11	1:A:90:SER:HB3	1.96	0.48
1:A:247:ASN:OD1	1:A:249:GLU:N	2.47	0.48
1:E:203:GLU:CG	1:F:204:LYS:H	2.26	0.48
1:F:125:GLY:C	1:F:126:ASP:OD1	2.53	0.48
1:C:181:ALA:O	1:C:185:VAL:HG23	2.14	0.47
1:D:121:TYR:HD1	1:D:121:TYR:H	1.62	0.47
1:D:170:ARG:HB3	1:D:266:GLN:HE22	1.79	0.47
1:E:197:GLU:OE2	1:E:201:ARG:HD2	2.14	0.47
1:F:282:ARG:O	1:F:283:GLU:HB3	2.13	0.47
1:G:183:TRP:CE2	1:H:195:GLN:HG2	2.49	0.47
1:D:221:ALA:O	1:D:222:ASN:HB2	2.13	0.47
1:G:166:VAL:O	1:G:237:VAL:HA	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ILE:HG23	1:B:183:TRP:CH2	2.49	0.47
1:C:37:GLU:O	1:C:38:ALA:HB2	2.14	0.47
1:D:204:LYS:NZ	2:D:311:HOH:O	2.44	0.47
1:F:202:SER:O	1:F:203:GLU:CB	2.62	0.47
1:H:191:ASP:OD1	1:H:191:ASP:O	2.32	0.47
1:E:37:GLU:OE1	1:E:37:GLU:CA	2.58	0.47
1:D:66:ARG:NH2	2:D:312:HOH:O	2.47	0.47
1:E:111:LEU:HD21	1:E:154:PHE:CD2	2.50	0.47
1:H:122:ARG:NE	1:H:145:ASP:OD1	2.47	0.47
1:A:126:ASP:O	1:A:127:LEU:C	2.53	0.47
1:A:194:PHE:O	1:A:197:GLU:HB3	2.14	0.47
1:C:158:TRP:O	1:C:164:LEU:HD12	2.15	0.47
1:D:84:ARG:NH2	2:D:313:HOH:O	2.48	0.47
1:D:201:ARG:NH2	1:D:214:ALA:HB2	2.28	0.47
1:E:111:LEU:HD13	1:E:171:PRO:HG3	1.96	0.47
1:E:180:ASP:OD1	1:F:196:ARG:NE	2.46	0.47
1:F:107:ASP:OD2	1:F:109:ARG:NH2	2.48	0.47
1:G:78:GLU:OE2	1:G:85:PRO:HB3	2.15	0.47
1:A:216:HIS:CG	1:A:222:ASN:OD1	2.68	0.47
1:G:248:ALA:O	1:G:252:ARG:HG2	2.15	0.47
1:H:117:LEU:C	1:H:119:GLU:H	2.18	0.47
1:A:212:LEU:O	1:A:215:ARG:CB	2.61	0.47
1:C:222:ASN:CG	1:C:222:ASN:O	2.52	0.47
1:F:185:VAL:HB	1:F:211:LEU:HD11	1.96	0.47
1:H:212:LEU:O	1:H:216:HIS:N	2.31	0.47
1:A:78:GLU:OE2	1:A:85:PRO:HG3	2.15	0.46
1:G:133:LYS:O	1:G:137:GLU:HG3	2.15	0.46
1:D:141:ASP:OD2	1:D:160:LYS:HA	2.15	0.46
1:F:38:ALA:O	1:F:39:ASP:O	2.34	0.46
1:H:136:ILE:O	1:H:159:ARG:NH2	2.45	0.46
1:D:207:MET:O	1:D:210:ALA:HB3	2.15	0.46
1:F:30:ILE:HG21	1:F:47:LEU:HD21	1.97	0.46
1:F:243:ALA:O	1:F:247:ASN:CB	2.64	0.46
1:C:252:ARG:HB3	1:C:252:ARG:NH1	2.31	0.46
1:D:133:LYS:HD2	2:D:368:HOH:O	2.15	0.46
1:G:244:ALA:HA	1:G:250:GLU:HG3	1.97	0.46
1:A:19:THR:HG22	1:A:227:PRO:HG3	1.97	0.46
1:E:186:ILE:HD13	1:E:211:LEU:HD12	1.97	0.46
1:F:58:TRP:O	1:F:234:GLN:NE2	2.44	0.46
1:F:199:MET:O	1:F:202:SER:HB2	2.14	0.46
1:D:117:LEU:HD12	1:D:143:GLU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:207:MET:HE1	1:F:211:LEU:HD12	1.98	0.46
1:H:129:LEU:H	1:H:129:LEU:HD12	1.81	0.46
1:A:138:HIS:HA	1:A:139:ARG:HA	1.66	0.46
1:C:183:TRP:CZ3	1:D:195:GLN:O	2.69	0.46
1:G:19:THR:CG2	1:G:227:PRO:HG3	2.46	0.46
1:A:218:GLY:CA	1:A:280:GLY:O	2.63	0.45
1:F:91:GLU:O	1:F:91:GLU:CG	2.62	0.45
1:E:219:ALA:CA	2:E:384:HOH:O	2.63	0.45
1:F:252:ARG:O	1:F:256:LYS:CG	2.60	0.45
1:H:62:LEU:HD22	1:H:65:LEU:HD12	1.98	0.45
1:H:65:LEU:O	1:H:67:HIS:CD2	2.69	0.45
1:F:206:GLY:HA3	1:F:207:MET:HA	1.83	0.45
1:H:121:TYR:CA	2:H:306:HOH:O	2.64	0.45
1:B:219:ALA:HA	1:E:42:THR:OG1	2.17	0.45
1:F:121:TYR:O	1:F:122:ARG:C	2.55	0.45
1:F:128:PRO:HD2	1:F:131:GLN:HB2	1.98	0.45
1:F:265:TYR:HA	1:F:268:VAL:HG22	1.98	0.45
1:A:16:ALA:O	1:A:17:PHE:C	2.54	0.45
1:A:201:ARG:HA	1:A:201:ARG:HD2	1.75	0.45
1:G:199:MET:SD	1:H:208:LEU:HB2	2.56	0.45
1:H:115:ALA:HB1	1:H:143:GLU:OE1	2.17	0.45
1:H:270:THR:O	1:H:270:THR:HG22	2.16	0.45
1:A:106:LEU:HD23	1:A:112:SER:HA	1.98	0.44
1:D:134:VAL:O	1:D:138:HIS:CE1	2.70	0.44
1:H:116:ALA:H	1:H:143:GLU:CD	2.20	0.44
1:H:204:LYS:O	1:H:205:ASP:CG	2.55	0.44
1:D:220:LYS:O	1:D:220:LYS:HG2	2.17	0.44
1:F:253:ALA:O	1:F:256:LYS:HB2	2.16	0.44
1:A:143:GLU:HG3	1:A:158:TRP:HB3	1.99	0.44
1:B:18:ASP:HA	1:B:28:SER:OG	2.17	0.44
1:B:197:GLU:OE1	1:B:282:ARG:NH1	2.46	0.44
1:C:61:GLY:HA3	1:C:112:SER:HB2	1.99	0.44
1:E:185:VAL:CG2	1:E:274:SER:O	2.65	0.44
1:F:276:VAL:O	1:F:276:VAL:HG13	2.16	0.44
1:G:10:THR:HA	1:G:13:ILE:HD12	1.99	0.44
1:F:24:ALA:HB3	1:F:26:VAL:HG23	1.98	0.44
1:G:188:SER:O	1:G:190:LYS:HG2	2.18	0.44
1:A:44:ASP:OD1	1:A:71:LEU:HD12	2.18	0.44
1:A:213:GLY:C	1:A:215:ARG:H	2.21	0.44
1:E:130:ALA:O	1:E:133:LYS:CG	2.66	0.44
1:F:75:GLY:C	1:F:76:ASP:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:166:VAL:HG11	1:H:255:LEU:HA	2.00	0.44
1:C:247:ASN:OD1	1:C:249:GLU:N	2.51	0.44
1:F:75:GLY:O	1:F:76:ASP:C	2.51	0.44
1:F:156:ARG:HG3	1:F:158:TRP:HZ3	1.81	0.44
1:H:14:TYR:HE1	1:H:71:LEU:HD21	1.81	0.44
1:H:129:LEU:O	1:H:133:LYS:HG3	2.17	0.44
1:C:78:GLU:OE2	1:C:85:PRO:HB3	2.17	0.44
1:C:199:MET:CE	1:D:208:LEU:HB2	2.47	0.44
1:D:14:TYR:N	1:D:14:TYR:CD1	2.86	0.44
1:B:264:GLU:O	1:B:268:VAL:HG13	2.18	0.43
1:H:43:LEU:HD12	1:H:43:LEU:HA	1.89	0.43
1:H:121:TYR:HA	2:H:306:HOH:O	2.17	0.43
1:D:185:VAL:HG21	1:D:277:LEU:HB3	2.00	0.43
1:A:121:TYR:O	1:A:122:ARG:HG3	2.18	0.43
1:F:45:ALA:O	1:F:49:GLN:HG2	2.18	0.43
1:F:80:LEU:HB3	1:F:84:ARG:O	2.18	0.43
1:G:138:HIS:O	1:G:138:HIS:ND1	2.49	0.43
1:A:216:HIS:CE1	1:A:222:ASN:OD1	2.71	0.43
1:B:256:LYS:CE	2:B:333:HOH:O	2.65	0.43
1:E:7:LYS:HZ2	1:E:8:ASP:H	1.67	0.43
1:C:38:ALA:C	1:C:39:ASP:O	2.56	0.43
1:F:24:ALA:HA	1:F:233:VAL:HG22	2.01	0.43
1:E:7:LYS:NZ	1:E:7:LYS:HA	2.34	0.43
1:E:206:GLY:CA	1:F:202:SER:HB3	2.48	0.43
1:G:261:ALA:O	1:G:262:LEU:C	2.57	0.43
1:G:283:GLU:HB3	1:G:284:SER:H	1.56	0.43
1:H:100:TYR:O	1:H:103:MET:HG3	2.18	0.43
1:B:121:TYR:HA	2:B:319:HOH:O	2.19	0.43
1:F:30:ILE:O	1:F:30:ILE:CG2	2.59	0.43
1:F:48:THR:HG23	1:F:68:GLU:HA	2.00	0.43
1:F:281:LEU:HD23	1:F:283:GLU:H	1.83	0.43
1:A:225:GLN:O	1:A:226:LEU:O	2.37	0.43
1:E:264:GLU:O	1:E:268:VAL:HG13	2.19	0.43
1:A:48:THR:HG23	1:A:68:GLU:HA	2.01	0.43
1:D:162:ASP:O	1:D:241:SER:HA	2.19	0.43
1:F:119:GLU:O	1:F:120:GLY:C	2.55	0.43
1:A:204:LYS:H	1:A:204:LYS:HG3	1.76	0.43
1:F:169:ALA:O	1:F:171:PRO:HD3	2.18	0.43
1:E:228:GLU:HG2	1:E:273:LEU:HD22	2.01	0.42
1:F:28:SER:HB2	1:F:30:ILE:HG12	2.01	0.42
1:G:186:ILE:HG13	1:G:211:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:216:HIS:O	1:H:217:ALA:HB2	2.18	0.42
1:C:191:ASP:OD1	1:C:191:ASP:C	2.58	0.42
1:E:216:HIS:HD2	2:E:316:HOH:O	2.02	0.42
1:F:86:SER:O	1:F:87:ALA:CB	2.67	0.42
1:F:209:GLY:O	1:F:213:GLY:CA	2.66	0.42
1:G:18:ASP:OD1	1:G:28:SER:OG	2.29	0.42
1:H:158:TRP:NE1	1:H:165:PHE:CD1	2.88	0.42
1:B:238:GLN:NE2	1:B:239:THR:H	2.17	0.42
1:E:118:GLY:C	1:E:120:GLY:HA3	2.40	0.42
1:F:272:GLN:O	1:F:276:VAL:HB	2.19	0.42
1:C:226:LEU:HA	1:C:227:PRO:HD2	1.85	0.42
1:C:252:ARG:NH1	2:C:304:HOH:O	2.30	0.42
1:D:144:THR:HG22	1:D:157:VAL:H	1.84	0.42
1:F:204:LYS:N	1:F:205:ASP:HA	2.33	0.42
1:C:194:PHE:HD1	1:C:282:ARG:HH21	1.67	0.42
1:C:196:ARG:NH1	1:D:180:ASP:OD1	2.52	0.42
1:C:226:LEU:HA	1:C:226:LEU:HD23	1.76	0.42
1:D:264:GLU:HG2	1:G:264:GLU:HA	2.02	0.42
1:A:17:PHE:CD2	1:A:30:ILE:HG13	2.54	0.42
1:A:78:GLU:OE2	1:A:85:PRO:CG	2.67	0.42
1:A:159:ARG:HG3	1:A:164:LEU:HB2	2.00	0.42
1:C:73:ASP:OD2	1:C:73:ASP:N	2.23	0.42
1:F:228:GLU:HG2	1:F:273:LEU:HD22	2.01	0.42
1:H:122:ARG:CD	1:H:145:ASP:OD1	2.67	0.42
1:A:249:GLU:OE2	1:D:103:MET:HG2	2.20	0.42
1:D:198:LEU:HD22	1:D:211:LEU:HD13	2.01	0.42
1:H:132:LEU:O	1:H:135:LEU:HB3	2.20	0.42
1:H:140:ARG:O	1:H:159:ARG:HD2	2.20	0.42
1:A:215:ARG:HB3	1:A:215:ARG:NH1	2.34	0.42
1:A:223:LEU:O	1:A:224:ALA:O	2.38	0.42
1:B:57:ARG:HA	1:B:235:ALA:O	2.20	0.42
1:C:20:LEU:HB2	1:C:93:PHE:CE1	2.55	0.42
1:C:154:PHE:O	1:C:168:VAL:HA	2.19	0.42
1:D:17:PHE:CD2	1:D:30:ILE:HG13	2.55	0.42
1:F:121:TYR:C	1:F:122:ARG:O	2.58	0.42
1:A:24:ALA:HB2	1:A:58:TRP:NE1	2.35	0.42
1:E:208:LEU:HB2	2:E:354:HOH:O	2.20	0.42
1:E:262:LEU:HD22	1:E:266:GLN:HG3	2.02	0.42
1:C:261:ALA:O	1:C:262:LEU:C	2.55	0.42
1:F:215:ARG:HB2	1:F:216:HIS:H	1.71	0.42
1:C:18:ASP:OD1	1:C:30:ILE:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:37:GLU:O	1:H:38:ALA:C	2.57	0.41
1:H:140:ARG:HD3	1:H:141:ASP:N	2.34	0.41
1:H:271:ARG:CA	1:H:274:SER:OG	2.38	0.41
1:A:215:ARG:HD2	1:A:276:VAL:O	2.20	0.41
1:C:151:GLY:O	1:C:152:GLU:HB2	2.20	0.41
1:E:246:ARG:HE	1:E:246:ARG:HB3	1.59	0.41
1:A:13:ILE:HG23	1:A:89:VAL:HG11	2.02	0.41
1:A:78:GLU:OE2	1:A:85:PRO:CB	2.67	0.41
1:A:207:MET:CG	1:B:207:MET:HG2	2.50	0.41
1:B:13:ILE:HD13	1:B:76:ASP:HA	2.02	0.41
1:F:43:LEU:O	1:F:44:ASP:CB	2.68	0.41
1:B:256:LYS:HE2	2:B:333:HOH:O	2.21	0.41
1:C:225:GLN:HA	2:C:306:HOH:O	2.19	0.41
1:D:220:LYS:O	1:D:221:ALA:HB3	2.20	0.41
1:A:144:THR:CG2	1:A:145:ASP:O	2.68	0.41
1:E:13:ILE:HD12	1:E:75:GLY:O	2.20	0.41
1:D:98:GLN:O	1:D:102:PRO:HD3	2.20	0.41
1:F:226:LEU:HD22	1:F:228:GLU:HB2	2.01	0.41
1:F:197:GLU:OE1	1:F:201:ARG:NH1	2.54	0.41
1:F:207:MET:HE2	1:F:207:MET:HB3	1.98	0.41
1:H:80:LEU:HG	1:H:85:PRO:HA	2.03	0.41
1:H:227:PRO:HG2	1:H:228:GLU:OE1	2.20	0.41
1:B:206:GLY:O	1:B:208:LEU:O	2.39	0.41
1:C:207:MET:HB2	1:D:199:MET:HE3	2.03	0.41
1:E:162:ASP:O	1:E:241:SER:HA	2.21	0.41
1:F:120:GLY:O	1:F:121:TYR:CB	2.55	0.41
1:F:121:TYR:O	1:F:121:TYR:CD2	2.73	0.41
1:F:136:ILE:HG23	1:F:159:ARG:HH22	1.85	0.41
1:F:152:GLU:O	1:F:152:GLU:CG	2.69	0.41
1:G:149:GLY:CA	1:G:153:THR:O	2.44	0.41
1:H:155:GLN:O	1:H:156:ARG:HB3	2.21	0.41
1:H:244:ALA:HA	1:H:250:GLU:OE1	2.21	0.41
1:A:207:MET:SD	1:B:207:MET:HG2	2.61	0.41
1:B:283:GLU:HB3	1:B:284:SER:H	1.36	0.41
1:C:107:ASP:OD1	1:C:107:ASP:C	2.60	0.41
1:F:158:TRP:HE1	1:F:165:PHE:HD2	1.68	0.41
1:D:108:GLU:CD	1:D:108:GLU:H	2.24	0.40
1:E:123:ALA:HB1	1:E:124:PRO:HD2	2.02	0.40
1:H:130:ALA:O	1:H:134:VAL:HG23	2.21	0.40
1:H:226:LEU:HD22	1:H:228:GLU:OE1	2.21	0.40
1:C:117:LEU:CD2	1:C:160:LYS:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:SER:O	1:E:37:GLU:HB2	2.21	0.40
1:F:50:SER:HA	1:F:53:GLU:OE1	2.21	0.40
1:F:282:ARG:O	1:F:283:GLU:CB	2.68	0.40
1:E:194:PHE:HD1	1:E:194:PHE:HA	1.80	0.40
1:E:201:ARG:NH2	2:E:316:HOH:O	2.53	0.40
1:E:220:LYS:HA	2:E:395:HOH:O	2.21	0.40
1:F:44:ASP:OD2	1:F:69:ALA:O	2.40	0.40
1:H:126:ASP:CG	1:H:147:SER:HB3	2.41	0.40
1:H:194:PHE:CE2	1:H:281:LEU:HB3	2.57	0.40
1:C:215:ARG:NE	1:C:279:HIS:O	2.55	0.40
1:C:211:LEU:HD23	1:C:281:LEU:HD21	2.04	0.40
1:C:271:ARG:O	1:C:275:GLU:HG2	2.21	0.40
1:E:206:GLY:HA2	1:F:202:SER:HB3	2.03	0.40
1:F:50:SER:O	1:F:53:GLU:HG2	2.22	0.40
1:F:129:LEU:H	1:F:129:LEU:HD12	1.86	0.40
1:G:250:GLU:O	1:G:253:ALA:N	2.55	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:TYR:OH	1:F:118:GLY:O[2_445]	1.95	0.25
1:F:11:ASP:OD2	1:H:222:ASN:ND2[2_556]	1.96	0.24
2:B:420:HOH:O	2:E:339:HOH:O[1_655]	2.14	0.06
1:G:73:ASP:OD1	1:G:150:ARG:NH2[1_655]	2.15	0.05
1:D:131:GLN:NE2	1:F:137:GLU:OE1[2_445]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	273/284 (96%)	243 (89%)	25 (9%)	5 (2%)	8 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	273/284 (96%)	267 (98%)	5 (2%)	1 (0%)	34 48
1	C	273/284 (96%)	236 (86%)	29 (11%)	8 (3%)	4 4
1	D	273/284 (96%)	256 (94%)	13 (5%)	4 (2%)	10 14
1	E	276/284 (97%)	256 (93%)	13 (5%)	7 (2%)	5 6
1	F	273/284 (96%)	207 (76%)	38 (14%)	28 (10%)	0 0
1	G	273/284 (96%)	247 (90%)	21 (8%)	5 (2%)	8 10
1	H	273/284 (96%)	220 (81%)	31 (11%)	22 (8%)	1 0
All	All	2187/2272 (96%)	1932 (88%)	175 (8%)	80 (4%)	3 2

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	TYR
1	A	224	ALA
1	A	225	GLN
1	C	39	ASP
1	C	118	GLY
1	C	281	LEU
1	D	222	ASN
1	D	283	GLU
1	E	139	ARG
1	E	140	ARG
1	E	204	LYS
1	E	221	ALA
1	E	283	GLU
1	F	28	SER
1	F	39	ASP
1	F	44	ASP
1	F	73	ASP
1	F	76	ASP
1	F	84	ARG
1	F	119	GLU
1	F	121	TYR
1	F	122	ARG
1	F	126	ASP
1	F	127	LEU
1	F	142	PHE
1	F	148	ALA
1	G	140	ARG
1	G	203	GLU

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Mol	Chain	Res	Type
1	H	84	ARG
1	H	123	ALA
1	H	124	PRO
1	H	125	GLY
1	H	139	ARG
1	H	191	ASP
1	H	217	ALA
1	H	221	ALA
1	H	282	ARG
1	C	38	ALA
1	E	125	GLY
1	F	87	ALA
1	F	125	GLY
1	F	141	ASP
1	F	223	LEU
1	G	283	GLU
1	H	126	ASP
1	H	151	GLY
1	H	161	GLY
1	H	203	GLU
1	H	205	ASP
1	B	283	GLU
1	C	221	ALA
1	C	222	ASN
1	D	118	GLY
1	F	138	HIS
1	F	218	GLY
1	F	220	LYS
1	F	258	ALA
1	F	280	GLY
1	H	11	ASP
1	H	204	LYS
1	A	226	LEU
1	C	218	GLY
1	C	283	GLU
1	D	282	ARG
1	F	37	GLU
1	F	108	GLU
1	G	83	GLY
1	H	127	LEU
1	H	189	ILE
1	H	193	ALA

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Mol	Chain	Res	Type
1	H	283	GLU
1	F	43	LEU
1	F	82	ASP
1	F	95	ALA
1	F	203	GLU
1	G	139	ARG
1	H	202	SER
1	A	122	ARG
1	E	191	ASP
1	H	150	ARG

5.3.2 Protein sidechains (i)

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	199/206 (97%)	178 (89%)	21 (11%)	6 9
1	B	199/206 (97%)	180 (90%)	19 (10%)	8 12
1	C	199/206 (97%)	175 (88%)	24 (12%)	5 6
1	D	199/206 (97%)	182 (92%)	17 (8%)	10 16
1	E	202/206 (98%)	181 (90%)	21 (10%)	7 10
1	F	199/206 (97%)	181 (91%)	18 (9%)	9 14
1	G	199/206 (97%)	174 (87%)	25 (13%)	4 5
1	H	199/206 (97%)	179 (90%)	20 (10%)	7 11
All	All	1595/1648 (97%)	1430 (90%)	165 (10%)	7 10

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	22	SER
1	A	119	GLU
1	A	122	ARG
1	A	138	HIS

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Mol	Chain	Res	Type
1	A	140	ARG
1	A	144	THR
1	A	152	GLU
1	A	173	SER
1	A	178	LEU
1	A	201	ARG
1	A	204	LYS
1	A	211	LEU
1	A	215	ARG
1	A	223	LEU
1	A	225	GLN
1	A	239	THR
1	A	255	LEU
1	A	262	LEU
1	A	277	LEU
1	A	281	LEU
1	B	19	THR
1	B	33	LEU
1	B	66	ARG
1	B	84	ARG
1	B	108	GLU
1	B	111	LEU
1	B	129	LEU
1	B	138	HIS
1	B	144	THR
1	B	178	LEU
1	B	208	LEU
1	B	211	LEU
1	B	220	LYS
1	B	239	THR
1	B	262	LEU
1	B	268	VAL
1	B	277	LEU
1	B	282	ARG
1	B	283	GLU
1	C	43	LEU
1	C	57	ARG
1	C	73	ASP
1	C	80	LEU
1	C	108	GLU
1	C	111	LEU
1	C	119	GLU

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Mol	Chain	Res	Type
1	C	121	TYR
1	C	127	LEU
1	C	162	ASP
1	C	178	LEU
1	C	186	ILE
1	C	188	SER
1	C	197	GLU
1	C	202	SER
1	C	207	MET
1	C	208	LEU
1	C	211	LEU
1	C	222	ASN
1	C	225	GLN
1	C	255	LEU
1	C	262	LEU
1	C	277	LEU
1	C	283	GLU
1	D	22	SER
1	D	43	LEU
1	D	53	GLU
1	D	108	GLU
1	D	121	TYR
1	D	129	LEU
1	D	144	THR
1	D	178	LEU
1	D	200	ARG
1	D	208	LEU
1	D	211	LEU
1	D	223	LEU
1	D	262	LEU
1	D	268	VAL
1	D	276	VAL
1	D	277	LEU
1	D	283	GLU
1	E	7	LYS
1	E	10	THR
1	E	36	SER
1	E	86	SER
1	E	111	LEU
1	E	143	GLU
1	E	144	THR
1	E	152	GLU

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Mol	Chain	Res	Type
1	E	155	GLN
1	E	178	LEU
1	E	186	ILE
1	E	194	PHE
1	E	199	MET
1	E	208	LEU
1	E	239	THR
1	E	249	GLU
1	E	255	LEU
1	E	262	LEU
1	E	275	GLU
1	E	277	LEU
1	E	282	ARG
1	F	19	THR
1	F	27	ASP
1	F	121	TYR
1	F	145	ASP
1	F	160	LYS
1	F	178	LEU
1	F	190	LYS
1	F	201	ARG
1	F	204	LYS
1	F	207	MET
1	F	211	LEU
1	F	220	LYS
1	F	225	GLN
1	F	226	LEU
1	F	255	LEU
1	F	276	VAL
1	F	277	LEU
1	F	282	ARG
1	G	10	THR
1	G	11	ASP
1	G	13	ILE
1	G	19	THR
1	G	22	SER
1	G	33	LEU
1	G	86	SER
1	G	111	LEU
1	G	127	LEU
1	G	144	THR
1	G	150	ARG

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Mol	Chain	Res	Type
1	G	175	GLU
1	G	178	LEU
1	G	179	SER
1	G	202	SER
1	G	208	LEU
1	G	211	LEU
1	G	220	LYS
1	G	255	LEU
1	G	268	VAL
1	G	271	ARG
1	G	274	SER
1	G	277	LEU
1	G	282	ARG
1	G	283	GLU
1	H	22	SER
1	H	43	LEU
1	H	66	ARG
1	H	81	THR
1	H	82	ASP
1	H	108	GLU
1	H	126	ASP
1	H	140	ARG
1	H	178	LEU
1	H	190	LYS
1	H	194	PHE
1	H	202	SER
1	H	204	LYS
1	H	205	ASP
1	H	207	MET
1	H	256	LYS
1	H	257	THR
1	H	262	LEU
1	H	277	LEU
1	H	278	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	B	238	GLN
1	D	49	GLN
1	D	216	HIS

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Mol	Chain	Res	Type
1	E	216	HIS
1	F	67	HIS
1	F	104	GLN
1	F	216	HIS
1	F	238	GLN
1	H	29	GLN
1	H	55	GLN
1	H	104	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	275/284 (96%)	0.75	21 (7%) 13 12	47, 61, 91, 112	0
1	B	275/284 (96%)	0.98	20 (7%) 15 13	27, 36, 59, 79	0
1	C	275/284 (96%)	0.78	21 (7%) 13 12	38, 55, 96, 130	0
1	D	275/284 (96%)	0.87	22 (8%) 12 11	34, 48, 89, 123	0
1	E	278/284 (97%)	1.04	34 (12%) 4 3	28, 45, 86, 104	0
1	F	275/284 (96%)	2.59	141 (51%) 0 0	67, 112, 140, 160	0
1	G	275/284 (96%)	0.75	18 (6%) 18 17	42, 63, 83, 97	0
1	H	275/284 (96%)	1.88	86 (31%) 0 0	63, 83, 132, 157	0
All	All	2203/2272 (96%)	1.20	363 (16%) 1 1	27, 60, 120, 160	0

All (363) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	223	LEU	16.8
1	H	221	ALA	13.4
1	H	224	ALA	12.0
1	F	120	GLY	10.5
1	F	280	GLY	10.5
1	H	281	LEU	10.2
1	H	223	LEU	10.1
1	A	281	LEU	9.7
1	H	218	GLY	9.5
1	H	219	ALA	9.4
1	F	221	ALA	9.0
1	H	280	GLY	8.9
1	A	223	LEU	8.9
1	A	224	ALA	8.8
1	F	281	LEU	8.5
1	F	217	ALA	8.3

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Mol	Chain	Res	Type	RSRZ
1	C	221	ALA	8.2
1	F	10	THR	8.1
1	C	282	ARG	8.0
1	H	121	TYR	8.0
1	H	208	LEU	7.9
1	F	129	LEU	7.7
1	E	217	ALA	7.6
1	F	12	GLY	7.6
1	C	215	ARG	7.3
1	F	77	ILE	7.2
1	F	19	THR	7.0
1	H	216	HIS	7.0
1	H	212	LEU	7.0
1	A	284	SER	6.9
1	F	93	PHE	6.8
1	F	226	LEU	6.7
1	F	208	LEU	6.7
1	F	223	LEU	6.6
1	F	279	HIS	6.6
1	D	223	LEU	6.6
1	C	217	ALA	6.5
1	H	211	LEU	6.5
1	H	222	ASN	6.5
1	F	60	LEU	6.3
1	H	226	LEU	6.2
1	F	231	PHE	6.1
1	D	221	ALA	6.1
1	H	124	PRO	6.0
1	F	218	GLY	5.9
1	F	236	PHE	5.9
1	F	32	ALA	5.9
1	H	277	LEU	5.9
1	F	142	PHE	5.8
1	C	224	ALA	5.8
1	H	185	VAL	5.8
1	F	157	VAL	5.7
1	H	268	VAL	5.7
1	H	194	PHE	5.6
1	C	216	HIS	5.6
1	F	30	ILE	5.5
1	F	47	LEU	5.5
1	H	217	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	F	13	ILE	5.4
1	F	17	PHE	5.4
1	H	215	ARG	5.3
1	H	284	SER	5.3
1	F	87	ALA	5.2
1	F	11	ASP	5.2
1	F	24	ALA	5.2
1	F	224	ALA	5.1
1	F	220	LYS	5.0
1	H	76	ASP	5.0
1	F	241	SER	4.9
1	D	121	TYR	4.9
1	F	164	LEU	4.9
1	E	218	GLY	4.8
1	F	86	SER	4.8
1	F	88	ARG	4.8
1	A	217	ALA	4.8
1	F	211	LEU	4.8
1	A	221	ALA	4.8
1	F	215	ARG	4.7
1	A	10	THR	4.7
1	D	219	ALA	4.7
1	F	169	ALA	4.7
1	H	276	VAL	4.7
1	C	222	ASN	4.7
1	F	150	ARG	4.7
1	F	31	ALA	4.6
1	F	174	ALA	4.6
1	H	60	LEU	4.6
1	C	220	LYS	4.5
1	F	73	ASP	4.5
1	H	279	HIS	4.4
1	F	212	LEU	4.4
1	F	72	THR	4.4
1	H	220	LYS	4.4
1	F	78	GLU	4.4
1	H	181	ALA	4.3
1	F	46	ALA	4.3
1	E	220	LYS	4.3
1	F	117	LEU	4.2
1	H	168	VAL	4.2
1	F	33	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	H	213	GLY	4.2
1	F	273	LEU	4.1
1	H	251	TYR	4.1
1	F	92	GLY	4.1
1	F	219	ALA	4.1
1	F	36	SER	4.1
1	H	10	THR	4.1
1	F	43	LEU	4.1
1	F	222	ASN	4.0
1	F	245	ALA	4.0
1	F	121	TYR	4.0
1	A	220	LYS	4.0
1	H	11	ASP	4.0
1	F	56	GLY	4.0
1	F	154	PHE	4.0
1	F	128	PRO	3.9
1	F	136	ILE	3.9
1	A	216	HIS	3.9
1	F	71	LEU	3.9
1	F	178	LEU	3.9
1	F	35	ALA	3.8
1	F	244	ALA	3.8
1	F	114	TRP	3.8
1	F	14	TYR	3.8
1	D	222	ASN	3.8
1	D	220	LYS	3.8
1	F	111	LEU	3.8
1	F	81	THR	3.7
1	C	281	LEU	3.7
1	B	121	TYR	3.7
1	F	277	LEU	3.7
1	F	15	ALA	3.7
1	H	232	THR	3.7
1	G	135	LEU	3.7
1	E	284	SER	3.6
1	D	120	GLY	3.6
1	F	183	TRP	3.6
1	F	230	HIS	3.6
1	F	85	PRO	3.6
1	F	186	ILE	3.6
1	A	119	GLU	3.6
1	H	19	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	284	SER	3.6
1	G	139	ARG	3.6
1	F	90	SER	3.5
1	F	251	TYR	3.5
1	C	10	THR	3.5
1	G	245	ALA	3.5
1	H	282	ARG	3.5
1	H	13	ILE	3.5
1	H	179	SER	3.5
1	H	271	ARG	3.5
1	B	138	HIS	3.5
1	H	207	MET	3.5
1	F	34	ALA	3.4
1	F	177	ALA	3.4
1	H	230	HIS	3.4
1	F	248	ALA	3.4
1	H	127	LEU	3.4
1	H	278	ARG	3.4
1	H	30	ILE	3.4
1	F	20	LEU	3.4
1	H	122	ARG	3.4
1	E	221	ALA	3.3
1	F	80	LEU	3.3
1	F	194	PHE	3.3
1	F	216	HIS	3.3
1	C	219	ALA	3.3
1	F	253	ALA	3.3
1	F	132	LEU	3.3
1	F	205	ASP	3.3
1	C	207	MET	3.3
1	H	75	GLY	3.3
1	E	222	ASN	3.3
1	F	168	VAL	3.3
1	A	218	GLY	3.2
1	F	179	SER	3.2
1	H	134	VAL	3.2
1	E	223	LEU	3.2
1	C	218	GLY	3.2
1	D	211	LEU	3.2
1	F	282	ARG	3.2
1	E	198	LEU	3.2
1	A	215	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	262	LEU	3.1
1	E	219	ALA	3.1
1	F	214	ALA	3.1
1	F	59	GLY	3.1
1	E	7	LYS	3.1
1	F	75	GLY	3.1
1	F	156	ARG	3.1
1	H	225	GLN	3.0
1	B	268	VAL	3.0
1	F	207	MET	3.0
1	F	39	ASP	3.0
1	F	74	ASP	3.0
1	F	21	MET	3.0
1	H	129	LEU	3.0
1	F	139	ARG	3.0
1	G	208	LEU	3.0
1	F	119	GLU	3.0
1	F	131	GLN	3.0
1	D	84	ARG	3.0
1	F	278	ARG	3.0
1	F	58	TRP	2.9
1	H	89	VAL	2.9
1	F	165	PHE	2.9
1	F	255	LEU	2.9
1	E	34	ALA	2.9
1	H	248	ALA	2.9
1	H	93	PHE	2.9
1	H	274	SER	2.9
1	F	149	GLY	2.9
1	B	224	ALA	2.9
1	F	76	ASP	2.9
1	E	10	THR	2.8
1	D	282	ARG	2.8
1	E	194	PHE	2.8
1	F	79	ILE	2.8
1	F	96	LEU	2.8
1	F	89	VAL	2.8
1	F	28	SER	2.8
1	F	170	ARG	2.8
1	F	262	LEU	2.8
1	H	229	ALA	2.7
1	D	32	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	43	LEU	2.7
1	D	138	HIS	2.7
1	G	136	ILE	2.7
1	F	100	TYR	2.7
1	F	148	ALA	2.7
1	G	157	VAL	2.7
1	F	198	LEU	2.7
1	H	94	GLY	2.7
1	F	243	ALA	2.7
1	F	146	TRP	2.7
1	H	12	GLY	2.7
1	H	189	ILE	2.7
1	B	34	ALA	2.7
1	E	138	HIS	2.7
1	C	280	GLY	2.7
1	C	203	GLU	2.7
1	H	198	LEU	2.7
1	H	72	THR	2.6
1	G	241	SER	2.6
1	A	219	ALA	2.6
1	F	256	LYS	2.6
1	H	86	SER	2.6
1	H	205	ASP	2.6
1	H	283	GLU	2.6
1	D	224	ALA	2.6
1	H	269	THR	2.6
1	H	109	ARG	2.6
1	B	33	LEU	2.6
1	F	166	VAL	2.6
1	F	266	GLN	2.6
1	F	258	ALA	2.6
1	H	164	LEU	2.5
1	D	118	GLY	2.5
1	B	32	ALA	2.5
1	F	62	LEU	2.5
1	F	249	GLU	2.5
1	F	176	ALA	2.5
1	A	279	HIS	2.5
1	F	51	LEU	2.5
1	F	158	TRP	2.5
1	F	225	GLN	2.5
1	D	262	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	90	SER	2.5
1	B	261	ALA	2.5
1	H	123	ALA	2.5
1	A	14	TYR	2.5
1	E	135	LEU	2.5
1	E	189	ILE	2.4
1	H	273	LEU	2.4
1	E	261	ALA	2.4
1	F	210	ALA	2.4
1	B	120	GLY	2.4
1	E	216	HIS	2.4
1	H	14	TYR	2.4
1	C	283	GLU	2.4
1	G	84	ARG	2.4
1	E	268	VAL	2.4
1	G	200	ARG	2.4
1	A	208	LEU	2.4
1	H	126	ASP	2.4
1	E	186	ILE	2.4
1	H	186	ILE	2.4
1	H	210	ALA	2.4
1	G	142	PHE	2.4
1	B	259	ALA	2.3
1	F	102	PRO	2.3
1	G	124	PRO	2.3
1	H	135	LEU	2.3
1	H	146	TRP	2.3
1	D	14	TYR	2.3
1	G	114	TRP	2.3
1	H	26	VAL	2.3
1	F	180	ASP	2.3
1	H	175	GLU	2.3
1	E	33	LEU	2.3
1	E	262	LEU	2.3
1	G	148	ALA	2.3
1	H	74	ASP	2.3
1	G	128	PRO	2.3
1	E	32	ALA	2.3
1	E	23	THR	2.2
1	F	270	THR	2.2
1	E	26	VAL	2.2
1	F	268	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	43	LEU	2.2
1	C	194	PHE	2.2
1	H	158	TRP	2.2
1	A	186	ILE	2.2
1	E	35	ALA	2.2
1	H	132	LEU	2.2
1	F	155	GLN	2.2
1	H	231	PHE	2.2
1	B	26	VAL	2.2
1	F	113	GLN	2.2
1	B	30	ILE	2.2
1	F	84	ARG	2.2
1	D	260	ALA	2.2
1	H	259	ALA	2.2
1	H	209	GLY	2.2
1	F	265	TYR	2.1
1	B	35	ALA	2.1
1	B	177	ALA	2.1
1	B	257	THR	2.1
1	F	250	GLU	2.1
1	H	183	TRP	2.1
1	E	267	GLY	2.1
1	C	13	ILE	2.1
1	A	222	ASN	2.1
1	A	255	LEU	2.1
1	E	47	LEU	2.1
1	D	198	LEU	2.1
1	D	31	ALA	2.1
1	E	19	THR	2.1
1	F	161	GLY	2.1
1	E	200	ARG	2.1
1	E	269	THR	2.1
1	H	108	GLU	2.1
1	G	243	ALA	2.1
1	H	214	ALA	2.1
1	G	118	GLY	2.1
1	G	14	TYR	2.1
1	D	217	ALA	2.0
1	E	31	ALA	2.0
1	F	254	ALA	2.0
1	G	130	ALA	2.0
1	B	58	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	26	VAL	2.0
1	B	127	LEU	2.0
1	B	255	LEU	2.0
1	F	40	ALA	2.0
1	F	97	ALA	2.0
1	A	282	ARG	2.0
1	B	237	VAL	2.0
1	D	233	VAL	2.0
1	H	204	LYS	2.0
1	E	58	TRP	2.0
1	C	120	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.