



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:10 AM GMT

PDB ID : 1R1N
Title : Tri-nuclear oxo-iron clusters in the ferric binding protein from *N. gonorrhoeae*
Authors : Zhu, H.; Alexeev, D.; Hunter, D.J.; Campopiano, D.J.; Sadler, P.J.
Deposited on : 2003-09-24
Resolution : 1.74 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>

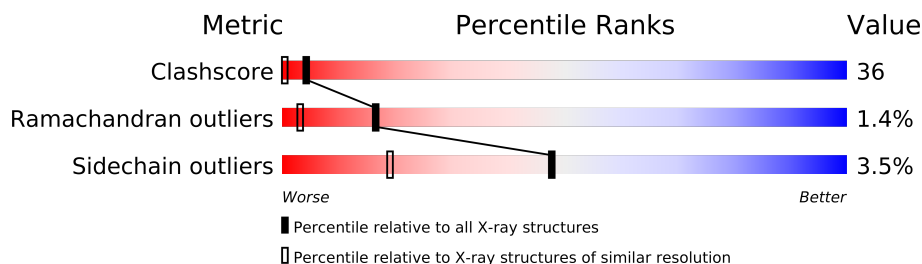
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 1.74 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))
Clashscore	79885	1881 (1.76-1.72)
Ramachandran outliers	78287	1859 (1.76-1.72)
Sidechain outliers	78261	1859 (1.76-1.72)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	309	
1	B	309	
1	C	309	
1	D	309	
1	E	309	
1	F	309	
1	G	309	
1	H	309	
1	I	309	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24350 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.

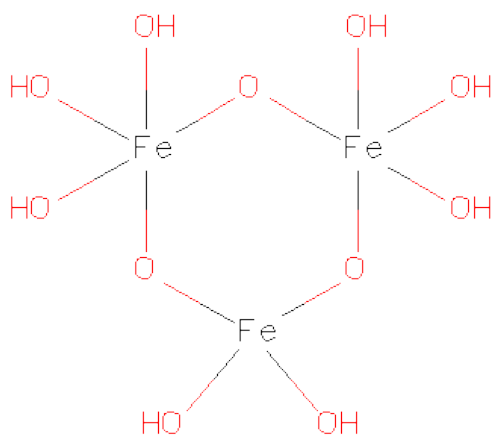
- Molecule 1 is a protein called Ferric-iron Binding Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	B	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	C	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	D	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	E	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	F	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	G	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	H	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	I	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			

There are 9 discrepancies between the modelled and reference sequences:

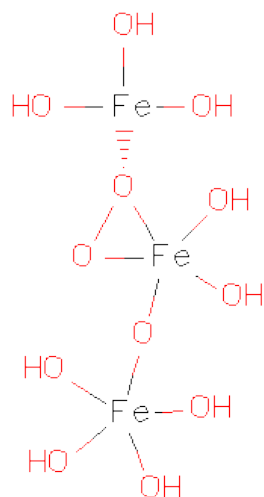
Chain	Residue	Modelled	Actual	Comment	Reference
A	87	VAL	ILE	CONFLICT	UNP P17259
B	87	VAL	ILE	CONFLICT	UNP P17259
C	87	VAL	ILE	CONFLICT	UNP P17259
D	87	VAL	ILE	CONFLICT	UNP P17259
E	87	VAL	ILE	CONFLICT	UNP P17259
F	87	VAL	ILE	CONFLICT	UNP P17259
G	87	VAL	ILE	CONFLICT	UNP P17259
H	87	VAL	ILE	CONFLICT	UNP P17259
I	87	VAL	ILE	CONFLICT	UNP P17259

- Molecule 2 is OXO-IRON CLUSTER 1 (three-letter code: CNB) (formula: $\text{Fe}_3\text{H}_8\text{O}_{11}$).



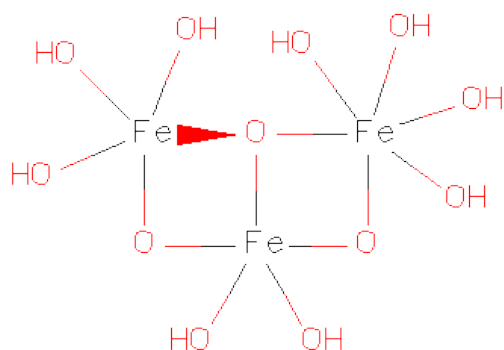
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	O	0	0
			14	3	11		
2	B	1	Total	Fe	O	0	0
			14	3	11		
2	D	1	Total	Fe	O	0	0
			14	3	11		
2	H	1	Total	Fe	O	0	0
			14	3	11		

- Molecule 3 is OXO-IRON CLUSTER 2 (three-letter code: CN1) (formula: $\text{Fe}_3\text{H}_9\text{O}_{12}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	Fe	O	0	0
			15	3	12		
3	E	1	Total	Fe	O	0	0
			15	3	12		
3	G	1	Total	Fe	O	0	0
			15	3	12		
3	I	1	Total	Fe	O	0	0
			15	3	12		

- Molecule 4 is OXO-IRON CLUSTER 3 (three-letter code: CNF) (formula: $\text{Fe}_3\text{H}_9\text{O}_{12}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	Fe	O	0	0
			15	3	12		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	367	Total	O	0	0
			367	367		
5	B	323	Total	O	0	0
			323	323		
5	C	298	Total	O	0	0
			298	298		
5	D	291	Total	O	0	0
			291	291		
5	E	331	Total	O	0	0
			331	331		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	301	Total 301	O 301	0	0
5	G	340	Total 340	O 340	0	0
5	H	295	Total 295	O 295	0	0
5	I	271	Total 271	O 271	0	0

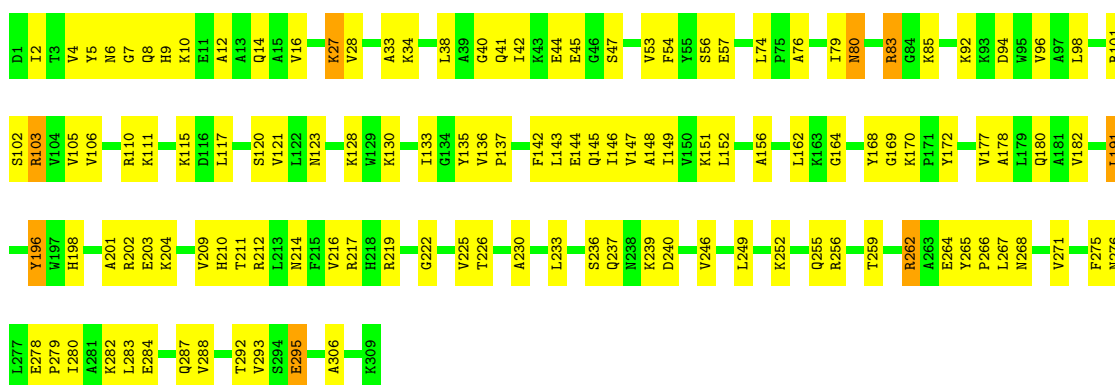
3 Residue-property plots

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.

Note EDS was not executed.

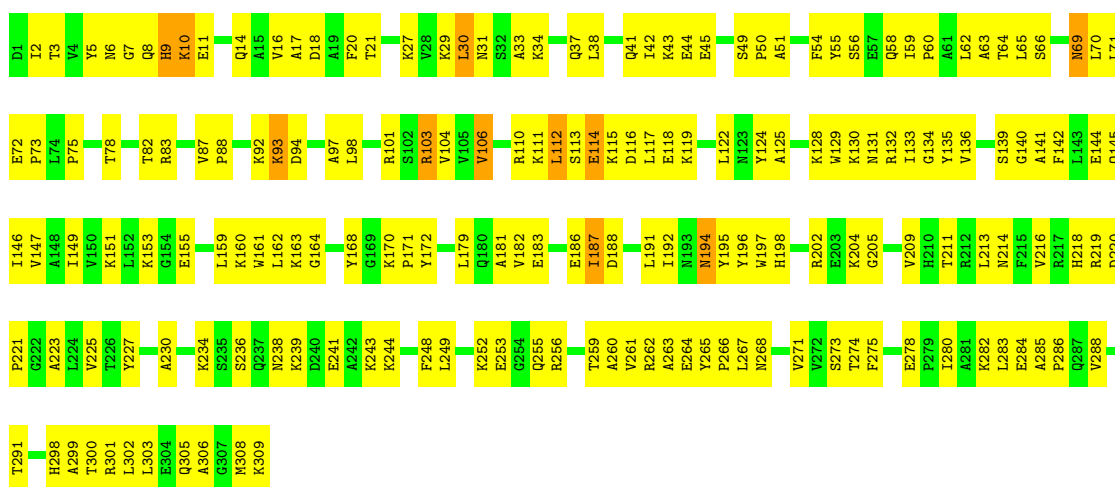
• Molecule 1: Ferric-iron Binding Protein

Chain A:



• Molecule 1: Ferric-iron Binding Protein

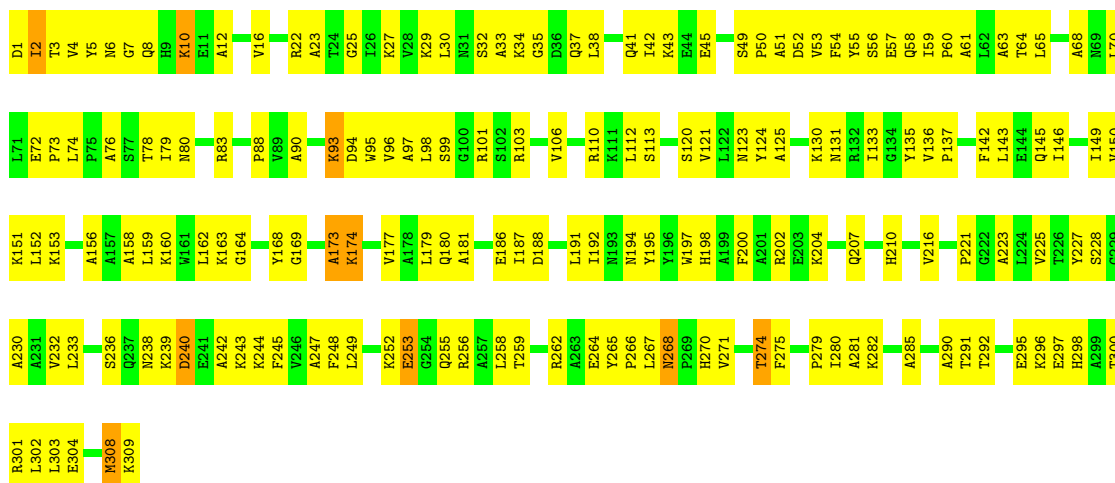
Chain B:



• Molecule 1: Ferric-iron Binding Protein

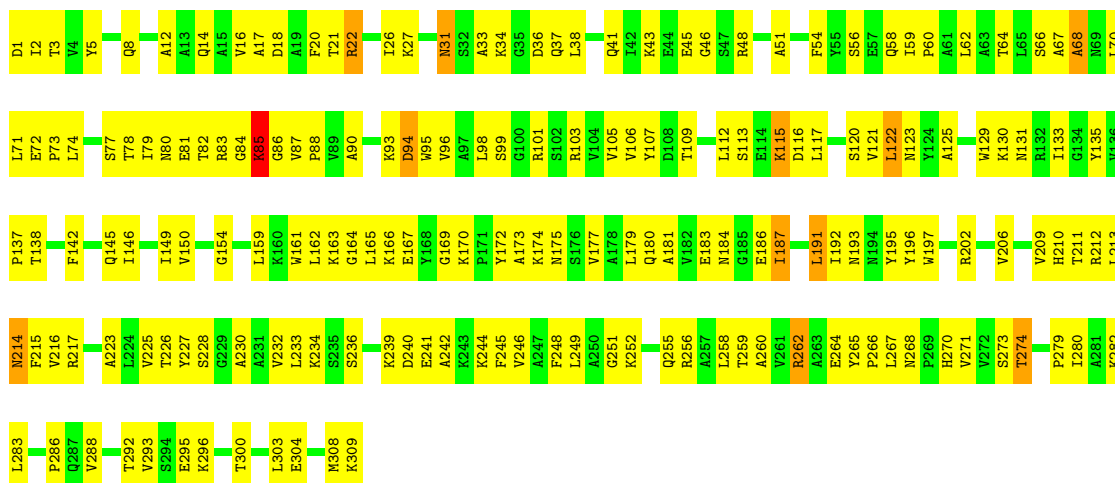
Chain C:





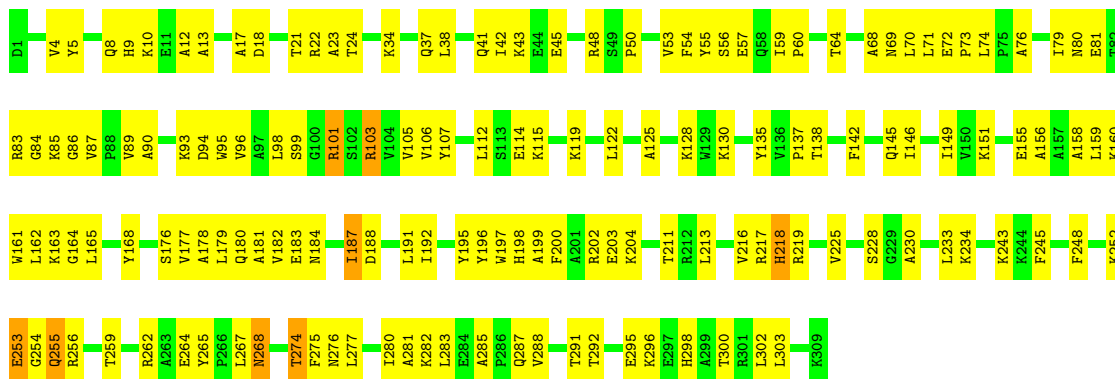
• Molecule 1: Ferric-iron Binding Protein

Chain D:



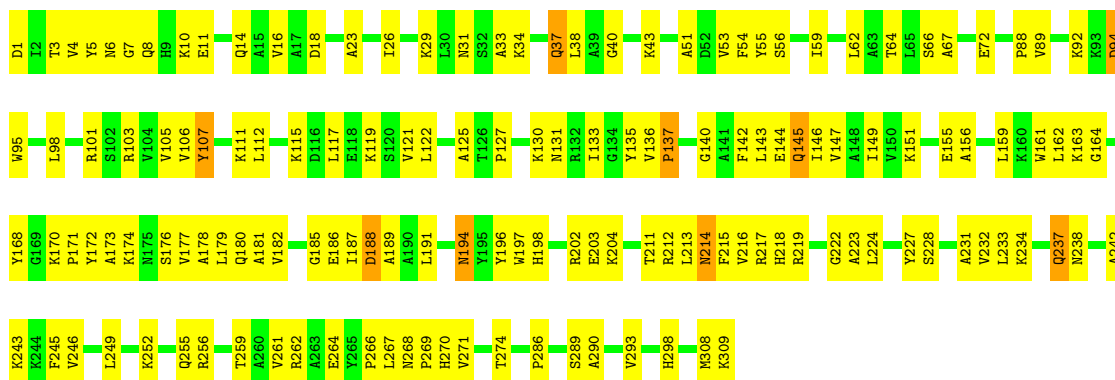
• Molecule 1: Ferric-iron Binding Protein

Chain E:



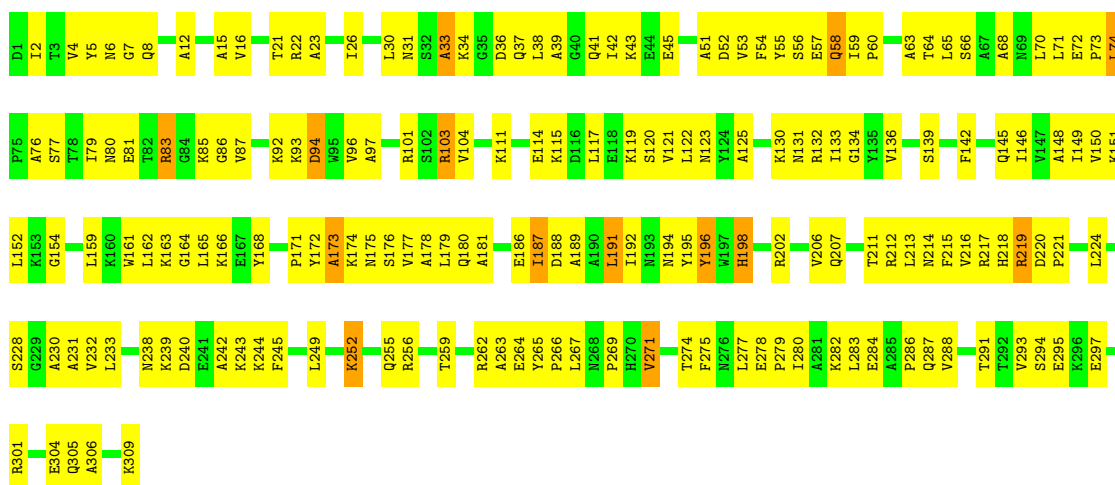
• Molecule 1: Ferric-iron Binding Protein

Chain F:



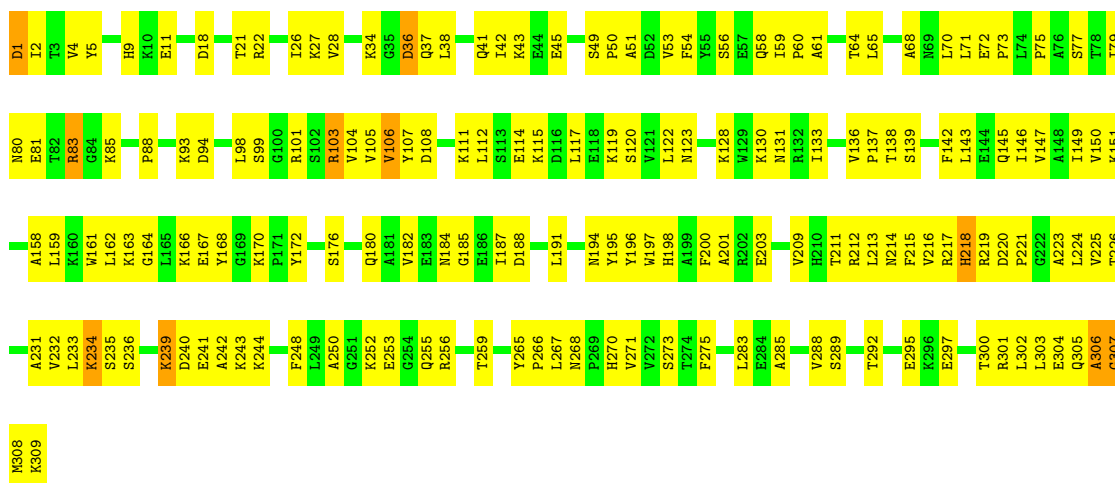
• Molecule 1: Ferric-iron Binding Protein

Chain G:



• Molecule 1: Ferric-iron Binding Protein

Chain H:



• Molecule 1: Ferric-iron Binding Protein

Chain I:

R309	L233	A156		D1
	K234	A157	I79	I2
	S235	A158	N80	T3
	S236	L159	E81	V4
		K160	T82	Y5
	K239	W161	R83	H9
	D240	L162	G84	K10
	E241	K163		E11
	A242	G164	V89	A12
	K243	L165	A90	
		K166		V16
	V246	E167	D94	A17
	A247	V168	W95	A18
	F248	G169		A19
	L249	K170	L98	F20
				T21
	G254	K174	R101	R22
	Q255	N175	S102	A23
	R256	S176	R103	
	A257		V104	
	L258	V182	V105	L30
	T259	E183	V106	N31
	A260			S32
	V261	I187	L112	A33
	R262	D188	S113	K34
	A263		E114	G35
		L191	K115	D36
	P266	I192	D116	Q37
	L267	N193	L117	L38
	N268	N194		
	P269	V196	W121	Q41
	H270	V197	L122	I42
	V271	H198	N123	K43
	V272	H198	Y124	E44
	S273	A199	A125	E45
		F200	T126	
	T280	A201	P127	R48
	A281		K128	
	K282	K204	W129	A51
	L283	G205	K130	D52
	E284	V206	N131	V53
	A285	Q207	R132	F54
	P286	N208	I133	Y55
	Q287	V209		S56
	V288	H210	V136	E57
	S289	T211		Q58
		R212	A141	I59
		L213	F142	P60
	E295			A61
	K296	R217	Q145	
	E297	H218	I146	T64
	H298	D219	V147	L65
	A299	R220	A148	S66
	T300	P221	I149	A67
	R301		V150	A68
	L302	A223	K151	N69
			L152	L70
	Q305	A230	K153	L71
	A306	G307	G154	L72
	V308	V232	E155	D73

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	146.50Å 146.50Å 114.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.74	Depositor
% Data completeness (in resolution range)	99.0 (30.00-1.74)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.167 , 0.300	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24350	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CNF, CNB, CN1

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	0.33	0/2423	0.59	1/3280 (0.0%)
1	B	0.33	0/2423	0.61	0/3280
1	C	0.33	0/2423	0.56	0/3280
1	D	0.32	0/2423	0.58	0/3280
1	E	0.33	0/2423	0.60	0/3280
1	F	0.31	0/2423	0.58	0/3280
1	G	0.32	0/2423	0.58	1/3280 (0.0%)
1	H	0.32	0/2423	0.58	0/3280
1	I	0.34	0/2423	0.54	0/3280
All	All	0.33	0/21807	0.58	2/29520 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	196	TYR	CB-CG-CD1	6.02	124.61	121.00
1	A	196	TYR	CB-CG-CD1	5.42	124.25	121.00

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	2378	0	2424	123	0
1	B	2378	0	2424	195	0
1	C	2378	0	2425	197	0
1	D	2378	0	2424	216	0
1	E	2378	0	2425	149	0
1	F	2378	0	2425	160	0
1	G	2378	0	2425	197	0
1	H	2378	0	2423	177	0
1	I	2378	0	2425	157	0
2	A	14	0	0	2	0
2	B	14	0	0	2	0
2	D	14	0	0	1	0
2	H	14	0	0	0	0
3	C	15	0	0	2	0
3	E	15	0	0	0	0
3	G	15	0	0	7	0
3	I	15	0	0	2	0
4	F	15	0	0	0	0
5	A	367	0	0	37	0
5	B	323	0	0	43	0
5	C	298	0	0	41	0
5	D	291	0	0	34	0
5	E	331	0	0	40	0
5	F	301	0	0	33	0
5	G	340	0	0	34	0
5	H	295	0	0	36	0
5	I	271	0	0	19	0
All	All	24350	0	21820	1567	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 36.

All (1567) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:111:LYS:NZ	1:H:188:ASP:OD1	1.59	1.34
1:G:202:ARG:HH22	1:G:274:THR:HG22	1.08	1.09
1:G:80:ASN:HA	1:G:83:ARG:HG2	1.33	1.07
1:F:259:THR:HG21	1:F:266:PRO:HG3	1.31	1.06
1:C:202:ARG:HH22	1:C:274:THR:HG23	1.17	1.06
1:H:252:LYS:HE2	1:H:270:HIS:HB3	1.38	1.05
1:E:202:ARG:HH22	1:E:274:THR:HG23	1.22	1.03
1:D:304:GLU:HG2	1:D:309:LYS:HD3	1.38	1.02
1:C:112:LEU:HD11	1:C:188:ASP:HB3	1.38	1.00

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:182:VAL:HG22	1:F:187:ILE:HD11	1.39	1.00
1:D:260:ALA:HA	1:D:274:THR:HB	1.44	0.99
1:C:93:LYS:HA	1:C:93:LYS:HE3	1.45	0.98
1:G:202:ARG:NH2	1:G:274:THR:HG22	1.79	0.97
1:A:259:THR:HG21	1:A:266:PRO:HG3	1.42	0.97
1:E:181:ALA:HB3	1:E:187:ILE:HD11	1.47	0.96
1:A:146:ILE:HD11	1:A:162:LEU:HD21	1.47	0.95
1:B:125:ALA:HB1	1:B:164:GLY:HA3	1.48	0.95
1:F:187:ILE:CD1	1:F:189:ALA:O	2.17	0.93
1:F:125:ALA:HB1	1:F:164:GLY:HA3	1.49	0.93
1:B:16:VAL:HG21	1:B:249:LEU:HD23	1.51	0.93
1:D:34:LYS:HE3	1:D:36:ASP:HB2	1.49	0.92
1:G:252:LYS:HD2	1:G:252:LYS:H	1.31	0.92
1:F:187:ILE:HD13	1:F:189:ALA:O	1.69	0.92
1:F:3:THR:HG23	1:F:29:LYS:HD2	1.53	0.91
1:H:259:THR:HG23	1:H:273:SER:HA	1.51	0.90
1:E:181:ALA:CB	1:E:187:ILE:HD11	2.03	0.87
1:F:182:VAL:HG22	1:F:187:ILE:CD1	2.04	0.86
1:H:106:VAL:HG22	1:H:211:THR:CG2	2.05	0.86
1:F:34:LYS:CG	1:F:37:GLN:HB2	2.07	0.85
1:E:197:TRP:HE1	1:E:211:THR:HG23	1.41	0.85
1:I:72:GLU:OE1	1:I:73:PRO:HD2	1.78	0.84
1:D:197:TRP:HE1	1:D:211:THR:HG23	1.40	0.84
1:C:74:LEU:HB2	1:C:79:ILE:HD11	1.58	0.84
1:E:149:ILE:HG21	5:E:731:HOH:O	1.78	0.83
1:C:42:ILE:HD13	1:C:233:LEU:HD21	1.60	0.83
1:D:80:ASN:HA	1:D:83:ARG:HG2	1.60	0.83
1:D:308:MET:HG3	5:D:672:HOH:O	1.78	0.82
1:F:259:THR:CG2	1:F:266:PRO:HG3	2.06	0.82
1:D:1:ASP:HB2	5:D:573:HOH:O	1.78	0.82
1:C:35:GLY:HA3	1:C:58:GLN:HE21	1.44	0.82
1:E:34:LYS:HB2	1:E:37:GLN:HE21	1.45	0.82
1:D:99:SER:HB2	1:D:264:GLU:HG3	1.62	0.82
1:D:202:ARG:HH22	1:D:274:THR:HG22	1.43	0.81
1:F:261:VAL:HG12	5:F:551:HOH:O	1.79	0.81
1:G:12:ALA:HB2	1:G:262:ARG:HG3	1.63	0.81
1:F:156:ALA:HB3	5:F:447:HOH:O	1.79	0.80
1:H:234:LYS:HE3	5:H:617:HOH:O	1.81	0.80
1:I:68:ALA:HB2	5:I:483:HOH:O	1.82	0.80
1:F:101:ARG:HD2	1:F:264:GLU:OE2	1.80	0.80
1:F:237:GLN:H	1:F:237:GLN:CD	1.82	0.80
1:G:286:PRO:HG2	5:G:723:HOH:O	1.81	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:72:GLU:HG2	1:E:234:LYS:HA	1.63	0.80
1:A:133:ILE:HD11	1:A:191:LEU:HD13	1.63	0.80
1:E:156:ALA:O	1:E:160:LYS:HG2	1.81	0.80
1:D:262:ARG:HA	1:D:262:ARG:HH11	1.46	0.80
1:A:94:ASP:HA	5:A:574:HOH:O	1.81	0.79
1:D:255:GLN:NE2	1:D:268:ASN:H	1.80	0.79
1:D:175:ASN:HB2	2:D:400:CNB:O2U	1.82	0.79
1:H:130:LYS:HE2	5:H:513:HOH:O	1.80	0.79
3:G:400:CN1:O23	5:G:640:HOH:O	1.99	0.79
1:C:78:THR:HG23	1:C:247:ALA:HA	1.64	0.79
1:C:6:ASN:HB2	1:C:30:LEU:HD22	1.65	0.79
1:H:59:ILE:N	1:H:60:PRO:HD2	1.98	0.79
1:F:5:TYR:CE1	1:F:51:ALA:HB2	2.18	0.79
1:F:259:THR:HG21	1:F:266:PRO:CG	2.09	0.78
1:I:197:TRP:HE1	1:I:211:THR:HG23	1.48	0.78
1:I:182:VAL:HG22	1:I:187:ILE:HG13	1.64	0.78
1:A:130:LYS:HA	1:A:168:TYR:HB3	1.66	0.78
1:C:192:ILE:HD12	5:C:651:HOH:O	1.84	0.78
1:F:34:LYS:HG3	1:F:37:GLN:HB2	1.64	0.77
1:B:131:ASN:O	1:B:187:ILE:HG22	1.83	0.77
1:A:16:VAL:HG11	1:A:249:LEU:HD23	1.66	0.77
1:H:106:VAL:HG22	1:H:211:THR:HG22	1.65	0.77
1:B:134:GLY:HA3	1:B:172:TYR:HE2	1.49	0.77
1:I:152:LEU:HD12	5:I:649:HOH:O	1.83	0.77
1:C:202:ARG:NH2	1:C:274:THR:HG23	1.98	0.77
1:G:163:LYS:HZ2	1:G:306:ALA:HA	1.48	0.77
1:B:248:PHE:CE1	1:B:253:GLU:HB3	2.20	0.76
1:G:80:ASN:HA	1:G:83:ARG:CG	2.12	0.76
1:B:112:LEU:CD1	1:B:116:ASP:HB2	2.16	0.76
1:C:59:ILE:N	1:C:60:PRO:HD2	2.00	0.76
1:C:202:ARG:HH22	1:C:274:THR:CG2	1.97	0.76
1:A:137:PRO:HG3	5:A:634:HOH:O	1.86	0.76
1:G:41:GLN:O	1:G:45:GLU:HG3	1.86	0.75
1:G:6:ASN:HB3	5:G:726:HOH:O	1.85	0.75
1:D:79:ILE:HG12	1:D:96:VAL:HG22	1.68	0.75
1:A:16:VAL:HG11	1:A:249:LEU:CD2	2.17	0.75
1:B:59:ILE:N	1:B:60:PRO:HD2	2.01	0.75
1:F:182:VAL:CG2	1:F:187:ILE:HD11	2.16	0.75
1:H:255:GLN:HE21	1:H:266:PRO:HB3	1.50	0.75
1:I:219:ARG:NH1	1:I:284:GLU:HA	2.01	0.75
1:G:146:ILE:HD13	1:G:162:LEU:HD11	1.67	0.75
1:C:153:LYS:HG2	5:C:585:HOH:O	1.86	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:106:VAL:HG23	1:H:213:LEU:HD23	1.67	0.75
1:F:16:VAL:HG11	1:F:249:LEU:HD23	1.69	0.74
1:A:226:THR:HG23	5:A:447:HOH:O	1.88	0.74
1:G:12:ALA:HB2	1:G:262:ARG:CG	2.16	0.74
1:I:255:GLN:NE2	1:I:268:ASN:HB2	2.01	0.74
1:B:71:LEU:HB2	1:B:94:ASP:HB2	1.69	0.74
1:G:131:ASN:C	1:G:187:ILE:HD11	2.07	0.74
1:C:80:ASN:HA	1:C:83:ARG:HH22	1.51	0.74
1:H:259:THR:CG2	1:H:273:SER:HA	2.18	0.74
1:D:181:ALA:CB	1:D:187:ILE:HD11	2.18	0.73
1:G:174:LYS:HB3	3:G:400:CN1:O3A	1.88	0.73
1:B:43:LYS:HD3	1:B:44:GLU:N	2.03	0.73
1:E:106:VAL:HG22	1:E:211:THR:OG1	1.88	0.73
1:G:175:ASN:HB2	3:G:400:CN1:O3U	1.87	0.73
1:E:202:ARG:HH22	1:E:274:THR:CG2	1.99	0.73
1:H:136:VAL:HG22	5:H:690:HOH:O	1.88	0.73
1:E:83:ARG:HH11	1:E:83:ARG:HG2	1.54	0.73
1:E:202:ARG:NH2	1:E:274:THR:HG23	2.02	0.73
1:H:297:GLU:O	1:H:301:ARG:HG2	1.89	0.73
1:F:293:VAL:HG23	5:F:456:HOH:O	1.87	0.73
1:F:216:VAL:HG23	1:F:223:ALA:HB2	1.71	0.72
1:H:201:ALA:HA	1:H:209:VAL:HG21	1.71	0.72
1:E:99:SER:HA	1:E:267:LEU:HG	1.70	0.72
1:D:244:LYS:HE2	5:D:594:HOH:O	1.88	0.72
1:B:9:HIS:CD2	1:B:10:LYS:H	2.07	0.72
1:C:101:ARG:NH2	1:C:228:SER:HB3	2.05	0.72
1:G:239:LYS:HG2	1:G:243:LYS:HE3	1.72	0.72
1:G:72:GLU:HG2	1:G:239:LYS:HD3	1.70	0.72
1:D:279:PRO:HB2	1:D:282:LYS:HG2	1.72	0.72
1:E:255:GLN:O	1:E:259:THR:HG22	1.90	0.72
1:B:262:ARG:HG3	1:B:264:GLU:HG3	1.71	0.72
1:A:41:GLN:O	1:A:45:GLU:HG3	1.91	0.71
1:B:253:GLU:HB2	5:B:672:HOH:O	1.89	0.71
1:F:145:GLN:O	1:F:149:ILE:HG13	1.91	0.71
1:H:255:GLN:NE2	1:H:266:PRO:HB3	2.06	0.71
1:B:209:VAL:HG12	1:B:211:THR:H	1.56	0.71
1:D:255:GLN:HB2	1:D:271:VAL:HG21	1.72	0.70
1:I:59:ILE:HB	1:I:60:PRO:HD3	1.73	0.70
1:F:145:GLN:HE21	1:F:145:GLN:HA	1.55	0.70
1:D:137:PRO:HB3	1:D:308:MET:HE3	1.72	0.70
1:C:146:ILE:O	1:C:150:VAL:HG23	1.91	0.70
1:E:55:TYR:HE1	1:E:98:LEU:HD12	1.57	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:6:ASN:HB3	1:C:32:SER:HA	1.72	0.70
1:B:149:ILE:HB	5:B:634:HOH:O	1.91	0.70
1:B:41:GLN:O	1:B:45:GLU:HG3	1.92	0.70
1:B:106:VAL:HG22	1:B:211:THR:HG23	1.72	0.70
1:G:83:ARG:HA	1:G:83:ARG:HE	1.57	0.70
1:C:160:LYS:HE3	5:C:600:HOH:O	1.90	0.70
1:E:41:GLN:O	1:E:45:GLU:HG3	1.92	0.69
1:C:97:ALA:HB3	5:C:649:HOH:O	1.92	0.69
1:C:79:ILE:HG12	1:C:96:VAL:HB	1.74	0.69
1:C:195:TYR:CE1	3:C:400:CN1:O1B	2.45	0.69
1:E:112:LEU:HD11	1:E:188:ASP:HB3	1.73	0.69
1:H:252:LYS:CE	1:H:270:HIS:HB3	2.20	0.69
1:E:34:LYS:HB2	1:E:37:GLN:NE2	2.06	0.69
1:F:67:ALA:HB3	5:F:487:HOH:O	1.91	0.69
1:A:130:LYS:HD2	1:A:168:TYR:HA	1.75	0.69
1:D:202:ARG:HH22	1:D:274:THR:CG2	2.05	0.69
1:D:256:ARG:HG2	1:D:271:VAL:HG13	1.74	0.69
1:I:80:ASN:HA	1:I:83:ARG:HH11	1.56	0.69
1:G:219:ARG:O	1:G:286:PRO:HB3	1.93	0.69
1:B:182:VAL:CG2	1:B:187:ILE:HD12	2.21	0.69
1:I:105:VAL:HG22	1:I:191:LEU:HD13	1.75	0.69
1:B:255:GLN:NE2	1:B:268:ASN:H	1.92	0.68
1:C:195:TYR:HE1	3:C:400:CN1:O1B	1.75	0.68
1:H:80:ASN:HA	1:H:83:ARG:HB2	1.74	0.68
1:F:255:GLN:NE2	1:F:268:ASN:H	1.91	0.68
1:B:17:ALA:HA	5:B:618:HOH:O	1.94	0.68
1:D:34:LYS:HB3	1:D:37:GLN:HG2	1.75	0.68
1:G:163:LYS:NZ	1:G:306:ALA:HA	2.08	0.68
1:B:113:SER:HB3	1:B:116:ASP:OD2	1.94	0.68
1:I:104:VAL:HG21	1:I:213:LEU:HD22	1.74	0.68
1:D:163:LYS:HE2	5:D:688:HOH:O	1.91	0.68
1:C:63:ALA:HA	5:C:486:HOH:O	1.93	0.68
1:G:58:GLN:HB2	1:G:60:PRO:HD2	1.76	0.68
1:D:20:PHE:HB2	1:D:248:PHE:CE2	2.27	0.68
1:G:85:LYS:HE3	5:G:682:HOH:O	1.94	0.68
1:B:59:ILE:HD11	1:B:227:TYR:HB2	1.76	0.68
1:F:179:LEU:HD23	1:F:196:TYR:CE2	2.28	0.68
1:I:259:THR:HB	1:I:273:SER:HA	1.75	0.68
1:I:58:GLN:HG2	1:I:60:PRO:HD2	1.75	0.68
1:D:18:ASP:O	1:D:22:ARG:HG3	1.93	0.68
1:G:74:LEU:H	1:G:74:LEU:HD23	1.59	0.68
1:F:7:GLY:HA2	1:F:33:ALA:O	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:5:TYR:HA	1:F:31:ASN:HB3	1.74	0.68
1:D:181:ALA:HB1	1:D:187:ILE:HD11	1.76	0.68
1:C:162:LEU:HD22	1:C:308:MET:HE2	1.75	0.68
1:A:92:LYS:HD3	5:A:671:HOH:O	1.93	0.68
1:C:279:PRO:HB2	1:C:282:LYS:HG2	1.76	0.68
1:E:197:TRP:NE1	1:E:211:THR:HG23	2.07	0.68
1:D:101:ARG:HG3	1:D:264:GLU:OE2	1.94	0.68
1:H:80:ASN:HD21	1:H:83:ARG:HH11	1.42	0.67
1:F:197:TRP:HB3	1:F:213:LEU:HD11	1.75	0.67
1:D:197:TRP:NE1	1:D:211:THR:HG23	2.09	0.67
1:G:130:LYS:HD2	1:G:168:TYR:HA	1.75	0.67
1:I:136:VAL:HG11	1:I:174:LYS:HA	1.75	0.67
1:E:160:LYS:HD3	5:E:568:HOH:O	1.93	0.67
1:B:182:VAL:HG22	1:B:187:ILE:HD12	1.75	0.67
1:B:88:PRO:HB2	5:B:620:HOH:O	1.93	0.67
1:D:71:LEU:HB2	1:D:94:ASP:HB3	1.75	0.67
1:B:112:LEU:HD11	1:B:116:ASP:HB2	1.76	0.67
1:D:279:PRO:HD2	1:D:282:LYS:HG3	1.76	0.67
1:H:163:LYS:NZ	1:H:306:ALA:HA	2.08	0.67
1:A:8:GLN:HG3	1:A:9:HIS:N	2.09	0.67
1:B:255:GLN:HE21	1:B:268:ASN:HB2	1.59	0.67
1:G:252:LYS:CD	1:G:252:LYS:H	2.02	0.67
1:D:70:LEU:HB3	5:D:555:HOH:O	1.93	0.67
1:H:234:LYS:HD2	1:H:235:SER:N	2.10	0.67
1:B:255:GLN:CB	1:B:271:VAL:HG21	2.25	0.67
1:B:30:LEU:CD2	1:B:31:ASN:H	2.06	0.67
1:F:34:LYS:HG2	1:F:37:GLN:HB2	1.75	0.67
1:H:159:LEU:O	1:H:163:LYS:HG2	1.94	0.67
1:H:240:ASP:O	1:H:244:LYS:HD3	1.94	0.67
1:C:152:LEU:HB2	5:C:585:HOH:O	1.95	0.66
1:E:176:SER:O	1:E:180:GLN:HG2	1.94	0.66
1:F:130:LYS:HE3	1:F:131:ASN:ND2	2.10	0.66
1:E:18:ASP:O	1:E:22:ARG:HG3	1.94	0.66
1:H:106:VAL:HG22	1:H:211:THR:HG21	1.76	0.66
1:B:255:GLN:HB3	1:B:271:VAL:HG21	1.78	0.66
1:A:255:GLN:HB2	1:A:271:VAL:HG21	1.78	0.66
1:B:256:ARG:HA	1:B:259:THR:HG22	1.77	0.66
1:C:41:GLN:OE1	5:C:634:HOH:O	2.13	0.66
1:F:130:LYS:HE3	1:F:131:ASN:HD21	1.59	0.66
1:F:133:ILE:HD11	1:F:191:LEU:CD1	2.26	0.66
1:F:1:ASP:HA	1:F:26:ILE:HG23	1.76	0.66
1:H:130:LYS:HE3	1:H:131:ASN:ND2	2.10	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:265:TYR:HB3	1:D:280:ILE:HG12	1.77	0.66
1:E:8:GLN:HB2	5:E:723:HOH:O	1.95	0.66
1:H:65:LEU:HA	5:H:565:HOH:O	1.96	0.66
1:F:180:GLN:HB3	5:F:589:HOH:O	1.96	0.66
1:E:54:PHE:CE2	1:E:56:SER:HB3	2.30	0.66
1:G:255:GLN:HB2	1:G:271:VAL:HG21	1.77	0.66
1:H:159:LEU:HD12	5:H:405:HOH:O	1.95	0.66
1:G:121:VAL:HG13	5:G:503:HOH:O	1.95	0.66
1:A:178:ALA:O	1:A:182:VAL:HG23	1.95	0.66
1:D:255:GLN:HE21	1:D:268:ASN:H	1.44	0.65
1:B:63:ALA:O	1:B:66:SER:HB3	1.95	0.65
1:G:86:GLY:HA2	1:G:287:GLN:HE21	1.60	0.65
1:D:216:VAL:HG23	1:D:223:ALA:HB2	1.79	0.65
1:C:101:ARG:HH22	1:C:228:SER:HB3	1.61	0.65
1:E:23:ALA:HB2	5:E:717:HOH:O	1.96	0.65
1:I:4:VAL:HG22	1:I:53:VAL:HB	1.78	0.65
1:D:300:THR:O	1:D:304:GLU:HG3	1.96	0.65
1:B:18:ASP:HA	1:B:21:THR:HG22	1.77	0.65
1:A:102:SER:HB2	1:A:225:VAL:HG22	1.79	0.65
1:G:233:LEU:HD12	1:G:233:LEU:N	2.11	0.65
1:G:36:ASP:HB3	5:G:433:HOH:O	1.97	0.65
1:B:261:VAL:HG12	5:B:539:HOH:O	1.95	0.65
1:D:296:LYS:HE2	5:D:638:HOH:O	1.97	0.65
1:F:135:TYR:CD2	1:F:137:PRO:HD3	2.31	0.65
1:G:12:ALA:CB	1:G:262:ARG:HG3	2.26	0.65
1:H:143:LEU:O	1:H:147:VAL:HG23	1.96	0.65
1:E:156:ALA:HB3	5:E:439:HOH:O	1.97	0.65
1:H:72:GLU:OE2	1:H:239:LYS:HD3	1.96	0.65
1:B:303:LEU:HD22	5:B:432:HOH:O	1.95	0.65
1:I:112:LEU:HD22	1:I:116:ASP:HB2	1.79	0.65
1:D:113:SER:O	1:D:117:LEU:HD13	1.97	0.65
1:G:39:ALA:HA	1:G:65:LEU:HD11	1.79	0.65
1:G:264:GLU:HG2	5:G:693:HOH:O	1.97	0.65
1:D:270:HIS:HA	5:D:528:HOH:O	1.96	0.64
1:E:162:LEU:HD13	1:E:303:LEU:HD23	1.79	0.64
1:B:202:ARG:HH22	1:B:274:THR:HB	1.62	0.64
1:B:130:LYS:HA	1:B:168:TYR:O	1.97	0.64
1:B:60:PRO:HG3	5:B:713:HOH:O	1.97	0.64
1:C:54:PHE:CZ	1:C:56:SER:HB3	2.32	0.64
1:F:5:TYR:CD1	1:F:51:ALA:HB2	2.32	0.64
1:C:146:ILE:HD11	1:C:303:LEU:HD21	1.79	0.64
1:E:72:GLU:OE1	1:E:73:PRO:HD2	1.98	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:106:VAL:HG23	1:B:213:LEU:HD23	1.79	0.64
1:C:297:GLU:O	1:C:301:ARG:HG2	1.97	0.64
1:C:233:LEU:N	1:C:233:LEU:HD12	2.12	0.64
1:D:16:VAL:HG12	1:D:248:PHE:CE2	2.31	0.64
1:D:78:THR:HG22	1:D:96:VAL:HG21	1.80	0.64
1:G:74:LEU:HD23	1:G:74:LEU:N	2.13	0.64
2:A:400:CNB:O12	5:A:488:HOH:O	2.15	0.64
1:F:187:ILE:HD12	1:F:189:ALA:O	1.97	0.64
1:D:106:VAL:HG21	1:D:179:LEU:CD1	2.28	0.64
1:G:76:ALA:HB1	1:G:80:ASN:HD22	1.62	0.64
1:A:144:GLU:HA	5:A:672:HOH:O	1.98	0.64
1:I:12:ALA:O	1:I:16:VAL:HG23	1.97	0.64
1:C:99:SER:HB2	1:C:264:GLU:HB3	1.79	0.63
1:A:255:GLN:CB	1:A:271:VAL:HG21	2.28	0.63
1:F:172:TYR:OH	1:F:187:ILE:HG21	1.98	0.63
1:A:278:GLU:HG2	5:A:434:HOH:O	1.98	0.63
1:F:259:THR:HG22	5:F:665:HOH:O	1.99	0.63
1:A:8:GLN:HG3	1:A:9:HIS:H	1.64	0.63
1:H:71:LEU:HB3	1:H:94:ASP:HB2	1.79	0.63
1:G:133:ILE:HG13	1:G:134:GLY:H	1.63	0.63
1:H:185:GLY:HA2	5:H:534:HOH:O	1.98	0.63
1:B:29:LYS:HE2	5:B:694:HOH:O	1.97	0.63
1:H:306:ALA:C	1:H:308:MET:H	2.00	0.63
1:C:98:LEU:HD11	1:C:230:ALA:HB2	1.81	0.63
1:B:34:LYS:HE3	1:B:37:GLN:OE1	1.98	0.63
1:G:103:ARG:HG3	1:G:224:LEU:HB3	1.80	0.63
1:H:138:THR:HG22	5:H:455:HOH:O	1.97	0.63
1:G:79:ILE:HG21	5:G:416:HOH:O	1.98	0.63
1:H:120:SER:HB3	1:H:123:ASN:ND2	2.14	0.63
1:B:101:ARG:HA	5:B:697:HOH:O	1.99	0.63
1:F:34:LYS:HG3	1:F:37:GLN:H	1.64	0.62
1:B:11:GLU:HA	5:B:608:HOH:O	1.99	0.62
1:H:18:ASP:O	1:H:22:ARG:HG3	1.98	0.62
1:D:138:THR:HB	5:D:404:HOH:O	1.98	0.62
1:F:105:VAL:HB	5:F:459:HOH:O	1.99	0.62
1:E:135:TYR:CD2	1:E:137:PRO:HD3	2.33	0.62
1:C:106:VAL:HG21	1:C:179:LEU:HD13	1.81	0.62
1:H:301:ARG:HB3	5:H:562:HOH:O	1.99	0.62
1:I:58:GLN:HB2	5:I:543:HOH:O	1.99	0.62
1:G:159:LEU:O	1:G:163:LYS:HG2	1.98	0.62
1:A:177:VAL:HG21	5:I:668:HOH:O	2.00	0.62
1:B:204:LYS:HE2	5:B:711:HOH:O	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:291:THR:HB	5:B:713:HOH:O	1.99	0.62
1:B:106:VAL:HG22	1:B:211:THR:CG2	2.29	0.62
1:I:236:SER:HA	5:I:476:HOH:O	1.98	0.62
1:D:130:LYS:HE3	1:D:131:ASN:HD21	1.63	0.62
1:D:183:GLU:OE1	1:D:211:THR:HG22	2.00	0.62
1:E:158:ALA:HA	5:E:731:HOH:O	1.98	0.62
1:I:58:GLN:CG	1:I:60:PRO:HD2	2.30	0.62
1:D:173:ALA:O	1:D:174:LYS:HD3	1.99	0.62
1:B:62:LEU:HA	5:B:682:HOH:O	1.99	0.62
1:C:80:ASN:HA	1:C:83:ARG:NH2	2.15	0.62
1:G:21:THR:HA	1:G:26:ILE:O	2.00	0.62
1:H:133:ILE:HD11	1:H:191:LEU:CD1	2.30	0.62
1:I:183:GLU:HG3	1:I:200:PHE:CE1	2.34	0.62
1:B:112:LEU:HD13	1:B:113:SER:N	2.15	0.62
1:F:255:GLN:HG3	1:F:268:ASN:HB2	1.81	0.62
1:C:256:ARG:HA	1:C:259:THR:HG22	1.81	0.62
1:D:202:ARG:HG2	5:D:454:HOH:O	1.99	0.61
1:F:159:LEU:O	1:F:163:LYS:HG2	2.00	0.61
1:B:236:SER:O	1:B:239:LYS:HG3	1.99	0.61
1:F:232:VAL:HG21	1:F:243:LYS:HG2	1.81	0.61
1:C:5:TYR:HB3	1:C:38:LEU:HD13	1.82	0.61
1:B:103:ARG:HH21	1:B:141:ALA:HB3	1.65	0.61
1:B:223:ALA:HB3	1:B:286:PRO:HD3	1.80	0.61
1:D:255:GLN:CB	1:D:271:VAL:HG21	2.30	0.61
1:C:279:PRO:HD2	1:C:282:LYS:HG3	1.81	0.61
1:H:93:LYS:HD3	5:H:430:HOH:O	2.00	0.61
1:H:300:THR:HG23	1:H:309:LYS:NZ	2.15	0.61
1:B:133:ILE:HD11	1:B:191:LEU:HD13	1.80	0.61
1:H:1:ASP:H2	1:H:241:GLU:CD	2.03	0.61
1:I:248:PHE:O	1:I:254:GLY:HA3	2.01	0.61
1:C:202:ARG:HH12	1:C:274:THR:HG21	1.65	0.61
1:A:38:LEU:O	1:A:42:ILE:HG13	1.99	0.61
1:H:54:PHE:CE2	1:H:56:SER:HB2	2.36	0.61
1:F:140:GLY:O	1:F:144:GLU:HG2	1.99	0.61
1:E:115:LYS:HE2	1:E:115:LYS:HA	1.82	0.61
1:H:58:GLN:OE1	1:H:61:ALA:HB2	2.01	0.61
1:B:130:LYS:O	1:B:131:ASN:HB2	2.00	0.61
1:D:12:ALA:HB1	1:D:258:LEU:CD1	2.30	0.61
1:C:110:ARG:HD3	1:C:210:HIS:CG	2.35	0.61
1:F:112:LEU:HA	5:F:483:HOH:O	2.00	0.61
1:D:267:LEU:HD23	1:D:280:ILE:HD12	1.83	0.61
1:H:266:PRO:HG3	5:H:423:HOH:O	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:103:ARG:NH2	5:E:432:HOH:O	2.33	0.61
1:A:233:LEU:N	1:A:233:LEU:HD12	2.16	0.61
1:C:240:ASP:HB3	5:C:432:HOH:O	2.01	0.61
1:I:182:VAL:HG23	1:I:187:ILE:HD11	1.83	0.61
1:H:105:VAL:HB	1:H:214:ASN:HB3	1.82	0.61
1:D:292:THR:O	1:D:296:LYS:HD2	2.01	0.61
1:H:5:TYR:HB3	1:H:38:LEU:HD13	1.83	0.61
1:D:304:GLU:CG	1:D:309:LYS:HD3	2.24	0.60
1:D:106:VAL:HG21	1:D:179:LEU:HD13	1.83	0.60
1:H:59:ILE:N	1:H:60:PRO:CD	2.64	0.60
1:I:268:ASN:HB3	1:I:271:VAL:HG23	1.83	0.60
1:I:82:THR:HG22	1:I:255:GLN:NE2	2.16	0.60
1:D:172:TYR:OH	1:D:187:ILE:HG12	2.01	0.60
1:F:55:TYR:HE1	1:F:98:LEU:HD13	1.67	0.60
1:H:268:ASN:OD1	1:H:270:HIS:HB2	2.01	0.60
1:G:38:LEU:O	1:G:42:ILE:HG13	1.99	0.60
1:A:40:GLY:O	1:A:44:GLU:HG3	2.02	0.60
1:E:85:LYS:HE3	5:E:699:HOH:O	2.01	0.60
1:G:76:ALA:HB1	1:G:80:ASN:ND2	2.17	0.60
1:A:27:LYS:HE2	5:A:631:HOH:O	2.00	0.60
1:D:186:GLU:C	1:D:187:ILE:HG13	2.20	0.60
1:G:72:GLU:CD	1:G:73:PRO:HD2	2.21	0.60
1:C:25:GLY:HA3	1:D:210:HIS:NE2	2.17	0.60
1:D:37:GLN:HB3	5:D:483:HOH:O	2.01	0.60
1:D:106:VAL:HG22	1:D:211:THR:OG1	2.01	0.60
1:A:74:LEU:HG	5:A:574:HOH:O	2.02	0.60
1:G:131:ASN:O	1:G:187:ILE:CD1	2.49	0.60
1:I:195:TYR:HA	1:I:263:ALA:HB3	1.82	0.60
1:D:85:LYS:HB2	1:D:85:LYS:HZ3	1.66	0.60
1:C:12:ALA:O	1:C:16:VAL:HG23	2.00	0.60
1:I:182:VAL:HG22	1:I:187:ILE:CG1	2.30	0.60
1:C:304:GLU:HG2	5:C:663:HOH:O	2.00	0.60
1:C:130:LYS:HA	1:C:168:TYR:HB3	1.83	0.60
1:I:82:THR:HG22	1:I:255:GLN:HE22	1.66	0.60
1:G:133:ILE:HG13	1:G:134:GLY:N	2.16	0.60
1:I:217:ARG:HD3	5:I:652:HOH:O	2.01	0.60
1:H:255:GLN:HB2	1:H:271:VAL:HG21	1.83	0.60
1:C:262:ARG:HG3	1:C:264:GLU:HG2	1.83	0.60
1:D:2:ILE:HG23	1:D:241:GLU:OE2	2.02	0.60
1:D:256:ARG:HA	1:D:259:THR:HG22	1.83	0.60
1:H:101:ARG:HB2	1:H:226:THR:HB	1.83	0.60
1:F:174:LYS:HB2	1:F:177:VAL:HG23	1.84	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:132:ARG:O	1:G:188:ASP:HB2	2.01	0.60
1:F:92:LYS:HB2	1:F:94:ASP:OD1	2.02	0.60
1:A:137:PRO:HA	1:A:142:PHE:CD2	2.37	0.59
1:C:101:ARG:HH22	1:C:228:SER:CB	2.15	0.59
1:E:8:GLN:HG3	1:E:9:HIS:N	2.17	0.59
1:E:218:HIS:HB2	5:E:620:HOH:O	2.02	0.59
1:H:34:LYS:HB2	1:H:37:GLN:HG3	1.83	0.59
1:E:101:ARG:O	1:E:225:VAL:HA	2.02	0.59
1:B:239:LYS:O	1:B:243:LYS:HG3	2.02	0.59
1:H:115:LYS:HG2	5:H:689:HOH:O	2.02	0.59
1:C:79:ILE:HG21	1:C:93:LYS:HE2	1.84	0.59
1:D:166:LYS:HD3	5:D:672:HOH:O	2.01	0.59
1:I:41:GLN:O	1:I:45:GLU:HG3	2.02	0.59
1:D:54:PHE:CZ	1:D:56:SER:HB3	2.37	0.59
1:H:151:LYS:HE2	1:H:295:GLU:OE2	2.01	0.59
1:G:87:VAL:HG13	1:G:267:LEU:HD13	1.84	0.59
1:G:57:GLU:O	1:G:57:GLU:HG2	2.02	0.59
1:H:107:TYR:O	1:H:211:THR:HG23	2.03	0.59
1:G:74:LEU:HD11	1:G:96:VAL:HG23	1.85	0.59
1:D:117:LEU:HD23	1:D:214:ASN:OD1	2.03	0.59
1:C:135:TYR:CD2	1:C:137:PRO:HD3	2.37	0.59
1:C:58:GLN:CD	1:C:61:ALA:HB2	2.22	0.59
1:H:53:VAL:CG2	1:H:242:ALA:HB1	2.32	0.59
1:G:214:ASN:ND2	1:G:215:PHE:N	2.50	0.59
1:I:122:LEU:HD11	1:I:153:LYS:HG3	1.85	0.59
1:H:224:LEU:HD11	5:H:603:HOH:O	2.01	0.59
1:C:204:LYS:HA	1:C:204:LYS:HE2	1.85	0.59
1:C:252:LYS:HE2	1:C:270:HIS:CB	2.33	0.59
1:B:278:GLU:HG2	5:B:466:HOH:O	2.03	0.59
1:C:174:LYS:HE2	1:C:177:VAL:HG23	1.84	0.59
1:E:248:PHE:O	1:E:254:GLY:HA3	2.03	0.59
1:B:106:VAL:HB	1:B:192:ILE:HD11	1.84	0.59
1:A:47:SER:HB2	5:A:527:HOH:O	2.03	0.59
1:A:226:THR:HG21	5:A:647:HOH:O	2.02	0.59
1:I:236:SER:HB3	1:I:239:LYS:HG2	1.84	0.59
1:F:135:TYR:O	1:F:171:PRO:HA	2.03	0.58
1:H:38:LEU:O	1:H:42:ILE:HG13	2.02	0.58
1:F:111:LYS:HG3	5:F:537:HOH:O	2.03	0.58
1:H:60:PRO:O	1:H:64:THR:HG23	2.03	0.58
1:B:82:THR:HB	1:B:267:LEU:HB3	1.84	0.58
1:F:143:LEU:O	1:F:147:VAL:HG23	2.02	0.58
1:E:183:GLU:OE1	1:E:211:THR:HG22	2.02	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:106:VAL:HG21	1:C:179:LEU:CD1	2.32	0.58
1:G:83:ARG:CA	1:G:83:ARG:HE	2.16	0.58
1:G:119:LYS:N	1:G:119:LYS:HD3	2.19	0.58
1:C:121:VAL:HA	1:C:124:TYR:HD2	1.69	0.58
1:H:218:HIS:CE1	1:H:220:ASP:HB2	2.39	0.58
1:A:115:LYS:HB2	5:A:517:HOH:O	2.02	0.58
1:G:139:SER:HB3	1:G:142:PHE:HB2	1.85	0.58
1:G:80:ASN:OD1	1:G:83:ARG:HG3	2.03	0.58
1:E:182:VAL:HG22	1:E:187:ILE:HD12	1.85	0.58
1:A:74:LEU:N	5:A:574:HOH:O	2.29	0.58
1:H:306:ALA:HB2	5:H:405:HOH:O	2.03	0.58
1:A:239:LYS:HD3	5:A:615:HOH:O	2.03	0.58
1:B:225:VAL:HG23	1:B:285:ALA:HB2	1.85	0.58
1:D:31:ASN:HB2	5:D:589:HOH:O	2.04	0.58
1:E:178:ALA:O	1:E:182:VAL:HG23	2.03	0.58
1:C:303:LEU:HD22	5:C:601:HOH:O	2.03	0.58
1:E:69:ASN:HB3	5:E:492:HOH:O	2.03	0.58
1:H:36:ASP:OD2	1:H:36:ASP:N	2.36	0.58
1:G:72:GLU:OE2	1:G:73:PRO:HD2	2.03	0.58
1:I:80:ASN:O	1:I:83:ARG:HB2	2.02	0.58
1:H:80:ASN:HD21	1:H:83:ARG:NH1	2.02	0.58
1:I:22:ARG:O	1:I:23:ALA:HB2	2.04	0.58
1:I:90:ALA:HB2	1:I:95:TRP:CE2	2.39	0.58
1:B:263:ALA:HB3	5:B:585:HOH:O	2.04	0.58
1:E:10:LYS:HG3	5:E:523:HOH:O	2.03	0.58
1:B:259:THR:HB	5:B:706:HOH:O	2.03	0.58
1:B:59:ILE:HD12	5:B:571:HOH:O	2.04	0.57
1:B:198:HIS:HE1	1:B:213:LEU:HD12	1.69	0.57
1:B:197:TRP:HE1	1:B:211:THR:HG22	1.70	0.57
1:H:72:GLU:HG3	1:H:73:PRO:HD2	1.85	0.57
1:F:54:PHE:CE2	1:F:56:SER:HB2	2.40	0.57
1:G:131:ASN:O	1:G:187:ILE:HD12	2.05	0.57
1:H:198:HIS:HD2	1:H:275:PHE:HB3	1.69	0.57
1:B:114:GLU:O	1:B:114:GLU:HG2	2.03	0.57
1:I:204:LYS:O	1:I:208:ASN:HB2	2.03	0.57
1:A:12:ALA:HB2	1:A:262:ARG:HD3	1.86	0.57
1:I:33:ALA:HB3	1:I:38:LEU:HD21	1.85	0.57
1:A:201:ALA:HA	1:A:209:VAL:HG21	1.85	0.57
1:I:79:ILE:HG22	1:I:83:ARG:NH1	2.20	0.57
1:A:256:ARG:HD3	5:A:556:HOH:O	2.05	0.57
1:G:5:TYR:HB3	1:G:38:LEU:HD13	1.85	0.57
1:B:219:ARG:O	1:B:286:PRO:HB3	2.05	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:71:LEU:HB2	1:G:94:ASP:HB3	1.84	0.57
1:E:177:VAL:HG22	5:E:487:HOH:O	2.04	0.57
1:G:259:THR:CG2	1:G:266:PRO:HG3	2.35	0.57
1:B:144:GLU:HB3	5:B:487:HOH:O	2.04	0.57
1:G:4:VAL:HG22	1:G:53:VAL:HB	1.85	0.57
1:F:115:LYS:NZ	1:F:115:LYS:HB3	2.19	0.57
1:G:277:LEU:HD21	5:G:739:HOH:O	2.04	0.57
1:H:159:LEU:HD13	1:H:302:LEU:HD22	1.86	0.57
1:A:202:ARG:HB2	5:A:681:HOH:O	2.04	0.57
1:A:110:ARG:NH1	1:F:23:ALA:HA	2.19	0.57
1:D:33:ALA:HB3	1:D:38:LEU:HG	1.87	0.57
1:G:219:ARG:NH1	1:G:284:GLU:HA	2.19	0.57
1:B:112:LEU:HD13	1:B:116:ASP:HB2	1.85	0.57
1:H:43:LYS:NZ	1:H:68:ALA:HB1	2.19	0.57
1:C:158:ALA:O	1:C:162:LEU:HG	2.05	0.57
1:B:255:GLN:HE21	1:B:268:ASN:H	1.52	0.57
1:G:59:ILE:N	1:G:60:PRO:CD	2.68	0.57
1:B:65:LEU:HD22	1:B:70:LEU:HD12	1.87	0.57
1:E:122:LEU:HA	1:E:161:TRP:CD1	2.40	0.57
1:H:252:LYS:HE3	5:H:434:HOH:O	2.04	0.56
1:E:197:TRP:HB3	1:E:213:LEU:HD11	1.87	0.56
1:G:5:TYR:CD1	1:G:51:ALA:HB2	2.40	0.56
1:C:202:ARG:HH12	1:C:274:THR:CG2	2.18	0.56
1:E:45:GLU:HB3	1:E:48:ARG:O	2.05	0.56
1:H:163:LYS:HZ3	1:H:305:GLN:C	2.08	0.56
1:D:214:ASN:HD22	1:D:215:PHE:N	2.03	0.56
1:F:164:GLY:O	1:F:168:TYR:HB2	2.04	0.56
1:F:34:LYS:HB2	5:F:472:HOH:O	2.05	0.56
1:H:83:ARG:HD3	5:H:620:HOH:O	2.06	0.56
1:B:202:ARG:HH22	1:B:274:THR:CB	2.18	0.56
1:C:29:LYS:HE3	5:C:602:HOH:O	2.04	0.56
1:A:79:ILE:HA	1:A:96:VAL:HG21	1.88	0.56
1:C:248:PHE:CE1	1:C:253:GLU:HB2	2.41	0.56
5:C:431:HOH:O	1:E:253:GLU:HG2	2.04	0.56
1:B:106:VAL:HG23	1:B:213:LEU:CD2	2.36	0.56
1:B:197:TRP:NE1	1:B:211:THR:HG22	2.20	0.56
1:G:93:LYS:HG2	5:G:416:HOH:O	2.05	0.56
1:E:43:LYS:HE3	1:E:64:THR:HG22	1.88	0.56
1:E:86:GLY:HA2	1:E:287:GLN:OE1	2.06	0.56
1:B:308:MET:O	1:B:309:LYS:HB3	2.06	0.56
1:B:204:LYS:HD2	5:B:548:HOH:O	2.05	0.56
1:H:122:LEU:HD21	1:H:149:ILE:HD13	1.86	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:269:PRO:HG3	1:I:48:ARG:HD2	1.86	0.56
1:D:180:GLN:HG3	1:D:184:ASN:HD21	1.70	0.56
1:F:255:GLN:HE22	1:F:267:LEU:H	1.53	0.56
1:C:258:LEU:HD13	5:C:697:HOH:O	2.04	0.56
1:B:16:VAL:HG21	1:B:249:LEU:CD2	2.31	0.56
1:D:135:TYR:CD2	1:D:137:PRO:HD3	2.40	0.56
1:A:130:LYS:CD	1:A:168:TYR:HA	2.36	0.56
1:I:124:TYR:CD1	1:I:133:ILE:HD13	2.41	0.56
1:A:6:ASN:OD1	1:A:8:GLN:HB3	2.05	0.56
1:H:214:ASN:HD22	1:H:215:PHE:H	1.53	0.56
1:C:73:PRO:HA	1:C:94:ASP:HA	1.88	0.56
1:D:67:ALA:HB2	5:D:446:HOH:O	2.04	0.56
1:A:120:SER:HB3	1:A:123:ASN:ND2	2.21	0.56
1:F:16:VAL:HG11	1:F:249:LEU:CD2	2.35	0.56
1:H:214:ASN:HD22	1:H:215:PHE:N	2.04	0.56
1:F:92:LYS:HB2	1:F:94:ASP:CG	2.27	0.56
1:G:151:LYS:HG3	5:G:432:HOH:O	2.05	0.56
1:E:265:TYR:CE2	1:E:283:LEU:HD11	2.41	0.56
1:F:136:VAL:HG13	1:F:172:TYR:O	2.07	0.55
1:H:163:LYS:HZ2	1:H:306:ALA:HA	1.70	0.55
1:C:130:LYS:HD3	1:C:168:TYR:HD2	1.71	0.55
1:C:255:GLN:HE21	1:C:268:ASN:HB3	1.69	0.55
1:G:240:ASP:O	1:G:244:LYS:HG3	2.06	0.55
1:I:256:ARG:HH22	1:I:272:VAL:HG23	1.70	0.55
1:B:5:TYR:CE1	1:B:51:ALA:HB2	2.41	0.55
1:D:106:VAL:HG13	1:D:106:VAL:O	2.06	0.55
1:C:162:LEU:HD22	1:C:308:MET:CE	2.35	0.55
1:D:43:LYS:HE3	1:D:64:THR:HG22	1.88	0.55
1:G:176:SER:O	1:G:180:GLN:HG2	2.05	0.55
1:D:120:SER:HB3	1:D:123:ASN:OD1	2.07	0.55
1:C:133:ILE:N	1:C:187:ILE:HD11	2.20	0.55
1:H:198:HIS:CD2	1:H:275:PHE:HB3	2.41	0.55
1:C:53:VAL:HG23	1:C:242:ALA:HB1	1.88	0.55
1:I:182:VAL:CG2	1:I:187:ILE:HD11	2.36	0.55
1:A:237:GLN:HB3	5:A:698:HOH:O	2.06	0.55
1:B:147:VAL:O	1:B:151:LYS:HG3	2.06	0.55
1:C:27:LYS:HD2	5:C:589:HOH:O	2.07	0.55
1:A:204:LYS:HB3	5:A:747:HOH:O	2.06	0.55
1:B:252:LYS:O	1:B:256:ARG:HG3	2.06	0.55
1:G:161:TRP:CZ2	1:G:165:LEU:HD11	2.40	0.55
1:F:122:LEU:HA	1:F:161:TRP:CD1	2.42	0.55
1:G:148:ALA:O	1:G:152:LEU:HG	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:219:ARG:HD3	1:A:284:GLU:O	2.07	0.55
1:G:206:VAL:HG13	1:G:207:GLN:N	2.21	0.55
1:D:101:ARG:O	1:D:225:VAL:HA	2.07	0.55
1:I:183:GLU:OE2	1:I:211:THR:HG22	2.07	0.55
1:G:58:GLN:HA	5:G:423:HOH:O	2.06	0.55
1:B:300:THR:HA	1:B:303:LEU:HD12	1.87	0.55
1:C:5:TYR:CE1	1:C:51:ALA:HB2	2.42	0.55
1:H:292:THR:OG1	1:H:295:GLU:HG3	2.06	0.55
1:F:64:THR:HG23	5:F:580:HOH:O	2.07	0.55
1:G:293:VAL:HG21	5:G:692:HOH:O	2.07	0.55
1:B:104:VAL:HG21	1:B:213:LEU:HD22	1.88	0.55
1:H:80:ASN:ND2	1:H:83:ARG:HH11	2.05	0.55
1:E:180:GLN:HA	1:E:180:GLN:HE21	1.72	0.55
1:F:176:SER:O	1:F:180:GLN:HG3	2.06	0.55
1:G:54:PHE:CE2	1:G:56:SER:HB2	2.42	0.55
1:G:206:VAL:HG13	1:G:207:GLN:H	1.71	0.55
1:I:259:THR:HG22	1:I:266:PRO:HG3	1.88	0.55
1:G:119:LYS:O	1:G:216:VAL:HG23	2.07	0.55
1:F:117:LEU:HD12	1:F:214:ASN:OD1	2.06	0.55
1:B:59:ILE:N	1:B:60:PRO:CD	2.69	0.55
1:B:30:LEU:HD23	1:B:31:ASN:H	1.72	0.55
1:D:21:THR:HA	1:D:26:ILE:O	2.07	0.55
1:D:202:ARG:HH12	1:D:274:THR:CG2	2.20	0.55
1:H:151:LYS:HE2	1:H:295:GLU:CD	2.27	0.55
1:B:122:LEU:HA	1:B:161:TRP:CD1	2.42	0.55
1:B:194:ASN:CG	1:B:195:TYR:N	2.60	0.54
1:E:291:THR:CG2	1:E:296:LYS:HG3	2.37	0.54
1:I:34:LYS:HB2	1:I:37:GLN:HB2	1.88	0.54
1:C:74:LEU:HB2	1:C:79:ILE:CD1	2.36	0.54
1:E:181:ALA:HB1	1:E:187:ILE:HD11	1.88	0.54
1:C:58:GLN:HB3	5:C:598:HOH:O	2.06	0.54
1:C:59:ILE:N	1:C:60:PRO:CD	2.67	0.54
1:E:160:LYS:HB3	5:E:520:HOH:O	2.07	0.54
1:H:214:ASN:ND2	1:H:215:PHE:N	2.56	0.54
1:A:135:TYR:CD2	1:A:137:PRO:HD3	2.43	0.54
1:G:214:ASN:HD22	1:G:215:PHE:H	1.55	0.54
1:B:142:PHE:O	1:B:146:ILE:HG13	2.08	0.54
1:C:309:LYS:HB3	5:C:663:HOH:O	2.07	0.54
1:A:239:LYS:HE2	5:A:724:HOH:O	2.07	0.54
1:H:41:GLN:O	1:H:45:GLU:HG3	2.08	0.54
1:D:105:VAL:HB	1:D:214:ASN:HB3	1.89	0.54
1:G:12:ALA:O	1:G:16:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:58:GLN:HB3	1:B:60:PRO:HD2	1.88	0.54
1:F:245:PHE:CE2	1:F:249:LEU:HD11	2.43	0.54
1:F:23:ALA:HB1	5:F:607:HOH:O	2.08	0.54
1:E:43:LYS:NZ	1:E:68:ALA:HB2	2.23	0.54
1:I:261:VAL:O	1:I:261:VAL:HG12	2.08	0.54
1:F:95:TRP:HB3	1:F:231:ALA:HB2	1.88	0.54
1:D:202:ARG:NH1	5:D:524:HOH:O	2.37	0.54
1:B:134:GLY:HA3	1:B:172:TYR:CE2	2.37	0.54
1:E:8:GLN:HG3	1:E:9:HIS:H	1.72	0.54
1:E:262:ARG:HB2	5:E:639:HOH:O	2.07	0.54
1:C:90:ALA:HB2	1:C:95:TRP:O	2.07	0.54
1:H:170:LYS:HD2	1:H:172:TYR:OH	2.08	0.54
1:C:244:LYS:HG2	5:C:677:HOH:O	2.07	0.54
1:H:162:LEU:HB2	5:H:405:HOH:O	2.07	0.54
1:E:42:ILE:HG21	1:E:233:LEU:HD11	1.90	0.54
1:D:304:GLU:HB3	5:D:432:HOH:O	2.09	0.54
1:G:224:LEU:C	1:G:224:LEU:HD13	2.28	0.54
1:H:226:THR:HA	5:H:456:HOH:O	2.08	0.54
1:E:79:ILE:HD12	5:E:653:HOH:O	2.08	0.54
1:B:196:TYR:HE2	2:B:400:CNB:O3U	1.91	0.54
1:B:44:GLU:HG3	1:B:45:GLU:N	2.23	0.53
1:H:306:ALA:C	1:H:308:MET:N	2.62	0.53
1:B:114:GLU:OE1	1:B:115:LYS:HE3	2.08	0.53
1:D:41:GLN:O	1:D:45:GLU:HG3	2.08	0.53
1:D:5:TYR:HB2	5:D:690:HOH:O	2.08	0.53
1:C:239:LYS:O	1:C:243:LYS:HG3	2.07	0.53
1:D:260:ALA:HA	1:D:274:THR:CB	2.30	0.53
1:D:66:SER:C	1:D:68:ALA:H	2.11	0.53
1:I:130:LYS:HD3	1:I:168:TYR:HD2	1.72	0.53
1:C:120:SER:HB3	1:C:123:ASN:ND2	2.23	0.53
1:B:131:ASN:HA	1:B:170:LYS:HG3	1.91	0.53
1:B:30:LEU:HD22	1:B:31:ASN:H	1.71	0.53
1:G:269:PRO:HD3	5:G:478:HOH:O	2.07	0.53
1:I:147:VAL:HG12	1:I:151:LYS:HE3	1.91	0.53
1:B:14:GLN:HE21	1:B:14:GLN:HA	1.74	0.53
1:F:130:LYS:HB2	5:F:561:HOH:O	2.09	0.53
1:D:21:THR:HG21	5:D:444:HOH:O	2.09	0.53
1:E:57:GLU:O	1:E:101:ARG:NH1	2.38	0.53
1:D:31:ASN:HA	5:D:654:HOH:O	2.07	0.53
1:C:245:PHE:O	1:C:249:LEU:HG	2.09	0.53
1:C:43:LYS:HE3	1:C:65:LEU:HD23	1.90	0.53
1:A:198:HIS:CD2	1:A:275:PHE:HB3	2.43	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:83:ARG:NH1	1:E:83:ARG:HG2	2.23	0.53
1:B:183:GLU:OE1	1:B:209:VAL:HG13	2.08	0.53
1:F:179:LEU:C	1:F:181:ALA:H	2.12	0.53
1:E:8:GLN:HG3	1:E:12:ALA:HB3	1.91	0.53
1:G:259:THR:HG21	1:G:266:PRO:HG3	1.91	0.53
1:D:173:ALA:HB1	1:D:174:LYS:HE2	1.91	0.53
1:F:214:ASN:HD22	1:F:215:PHE:N	2.06	0.53
1:C:245:PHE:CE2	1:C:249:LEU:HD11	2.43	0.53
1:I:297:GLU:O	1:I:301:ARG:HG2	2.09	0.53
1:B:56:SER:OG	1:B:58:GLN:O	2.25	0.53
1:F:155:GLU:OE2	1:F:298:HIS:HE1	1.92	0.53
1:D:202:ARG:NH2	1:D:274:THR:O	2.42	0.53
1:A:146:ILE:HD12	1:A:162:LEU:HD11	1.91	0.53
1:G:5:TYR:CE1	1:G:51:ALA:HB2	2.43	0.53
1:G:111:LYS:HD2	5:G:466:HOH:O	2.09	0.53
1:C:159:LEU:HD11	1:C:163:LYS:HE3	1.90	0.53
1:D:242:ALA:O	1:D:246:VAL:HG23	2.09	0.53
5:F:640:HOH:O	1:G:252:LYS:HE2	2.08	0.53
1:H:305:GLN:C	1:H:307:GLY:H	2.11	0.53
1:B:21:THR:HG23	5:B:421:HOH:O	2.08	0.53
1:F:159:LEU:O	1:F:159:LEU:HD13	2.08	0.53
1:F:92:LYS:HB2	1:F:94:ASP:OD2	2.09	0.53
1:I:5:TYR:CE1	1:I:51:ALA:HB2	2.44	0.53
1:D:223:ALA:HB3	1:D:286:PRO:HD3	1.90	0.53
1:I:106:VAL:HG22	1:I:211:THR:OG1	2.09	0.53
1:G:265:TYR:CE2	1:G:283:LEU:HD11	2.44	0.53
1:H:300:THR:O	1:H:304:GLU:HG3	2.09	0.53
1:H:216:VAL:HG23	1:H:223:ALA:HB2	1.90	0.53
1:I:66:SER:C	1:I:68:ALA:H	2.13	0.52
1:C:106:VAL:O	1:C:106:VAL:HG13	2.08	0.52
1:B:255:GLN:HE21	1:B:268:ASN:CB	2.20	0.52
1:E:54:PHE:CZ	1:E:56:SER:HB3	2.45	0.52
1:H:233:LEU:HD12	1:H:233:LEU:N	2.24	0.52
1:A:54:PHE:CE2	1:A:56:SER:HB3	2.43	0.52
1:H:5:TYR:CE1	1:H:51:ALA:HB2	2.45	0.52
1:B:216:VAL:HG12	1:B:218:HIS:CE1	2.44	0.52
1:D:256:ARG:HD3	5:D:434:HOH:O	2.10	0.52
1:D:87:VAL:HG22	1:D:267:LEU:HD22	1.91	0.52
1:C:197:TRP:O	1:C:200:PHE:N	2.41	0.52
1:C:5:TYR:CD2	1:C:38:LEU:HD22	2.43	0.52
1:H:250:ALA:HB2	5:H:627:HOH:O	2.10	0.52
1:H:98:LEU:O	1:H:267:LEU:HG	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:106:VAL:HB	1:D:192:ILE:HD11	1.90	0.52
1:F:237:GLN:HG2	5:F:605:HOH:O	2.08	0.52
1:G:72:GLU:CG	1:G:239:LYS:HD3	2.38	0.52
1:A:240:ASP:HB3	5:A:687:HOH:O	2.09	0.52
1:B:198:HIS:HD2	1:B:275:PHE:HB3	1.74	0.52
1:B:266:PRO:HG3	5:B:706:HOH:O	2.10	0.52
1:C:53:VAL:CG2	1:C:242:ALA:HB1	2.40	0.52
1:I:42:ILE:HD12	1:I:65:LEU:HD11	1.91	0.52
1:H:120:SER:HB3	1:H:123:ASN:HD21	1.74	0.52
1:F:14:GLN:HG3	1:F:18:ASP:OD2	2.10	0.52
1:D:90:ALA:HB3	1:D:93:LYS:HA	1.92	0.52
1:B:2:ILE:HG22	1:B:238:ASN:HB2	1.92	0.52
1:G:15:ALA:HB1	5:G:452:HOH:O	2.08	0.52
1:H:107:TYR:OH	1:H:114:GLU:HG2	2.10	0.52
1:I:208:ASN:N	1:I:208:ASN:ND2	2.56	0.52
1:H:68:ALA:HB3	5:H:565:HOH:O	2.09	0.52
1:E:74:LEU:CD1	1:E:96:VAL:HG13	2.40	0.52
1:E:159:LEU:HB2	1:E:302:LEU:HD22	1.91	0.52
1:G:294:SER:O	1:G:297:GLU:HB3	2.09	0.52
1:C:22:ARG:HD3	5:C:466:HOH:O	2.09	0.52
1:D:105:VAL:HG23	5:D:570:HOH:O	2.09	0.52
1:D:130:LYS:HE3	1:D:131:ASN:ND2	2.24	0.52
1:D:5:TYR:CD1	1:D:51:ALA:HB2	2.45	0.52
1:B:75:PRO:HG2	1:B:78:THR:OG1	2.10	0.52
1:E:281:ALA:HB3	5:E:661:HOH:O	2.09	0.52
1:G:59:ILE:HD11	5:G:511:HOH:O	2.09	0.52
1:H:300:THR:HG23	1:H:309:LYS:HZ1	1.75	0.52
1:D:167:GLU:HG3	1:D:167:GLU:O	2.10	0.52
1:A:105:VAL:HG22	1:A:191:LEU:HD12	1.91	0.51
1:B:59:ILE:H	1:B:60:PRO:HD2	1.75	0.51
1:B:198:HIS:CE1	1:B:213:LEU:HD12	2.45	0.51
1:F:255:GLN:HE22	1:F:267:LEU:N	2.09	0.51
1:G:132:ARG:HB3	1:G:132:ARG:HH11	1.75	0.51
1:C:29:LYS:HD3	1:C:29:LYS:C	2.30	0.51
1:A:198:HIS:HD2	1:A:275:PHE:HB3	1.75	0.51
1:H:81:GLU:HB3	1:H:250:ALA:HB1	1.91	0.51
1:H:288:VAL:HG12	1:H:289:SER:N	2.24	0.51
1:F:131:ASN:CB	1:F:170:LYS:HE3	2.40	0.51
1:H:36:ASP:HB3	5:H:473:HOH:O	2.10	0.51
1:F:4:VAL:HG22	1:F:53:VAL:HB	1.92	0.51
1:E:122:LEU:HB3	5:E:431:HOH:O	2.10	0.51
1:I:84:GLY:HA3	5:I:560:HOH:O	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:VAL:HG11	1:A:249:LEU:HD21	1.92	0.51
1:F:112:LEU:HD23	5:F:483:HOH:O	2.09	0.51
1:I:201:ALA:HA	1:I:209:VAL:HG21	1.91	0.51
1:A:287:GLN:NE2	1:A:287:GLN:HA	2.26	0.51
1:C:149:ILE:HB	5:C:653:HOH:O	2.11	0.51
1:F:255:GLN:HB2	1:F:271:VAL:HG21	1.91	0.51
1:G:164:GLY:O	1:G:168:TYR:HB2	2.09	0.51
1:A:143:LEU:O	1:A:147:VAL:HG23	2.10	0.51
1:H:233:LEU:HD23	5:H:610:HOH:O	2.10	0.51
1:A:145:GLN:O	1:A:149:ILE:HG13	2.11	0.51
1:C:121:VAL:HA	1:C:124:TYR:CD2	2.46	0.51
1:E:300:THR:HA	5:E:650:HOH:O	2.11	0.51
1:I:89:VAL:HG22	5:I:522:HOH:O	2.09	0.51
1:I:58:GLN:OE1	1:I:60:PRO:HB2	2.10	0.51
1:A:252:LYS:NZ	1:A:252:LYS:HB3	2.25	0.51
1:B:162:LEU:O	1:B:306:ALA:HB1	2.11	0.51
1:B:112:LEU:HD13	1:B:113:SER:H	1.75	0.51
1:I:194:ASN:CG	1:I:195:TYR:N	2.64	0.51
1:I:122:LEU:HA	1:I:161:TRP:CD1	2.46	0.51
1:C:255:GLN:HE21	1:C:268:ASN:CB	2.22	0.51
1:H:145:GLN:O	1:H:149:ILE:HG13	2.11	0.51
1:E:89:VAL:HG22	5:E:605:HOH:O	2.09	0.51
1:I:208:ASN:N	1:I:208:ASN:HD22	2.08	0.51
1:E:38:LEU:O	1:E:42:ILE:HG13	2.11	0.51
1:G:34:LYS:HB2	1:G:37:GLN:HG3	1.93	0.51
1:D:259:THR:HG23	5:D:407:HOH:O	2.10	0.51
1:G:52:ASP:HB3	1:G:242:ALA:HB2	1.92	0.51
1:D:293:VAL:HA	1:D:296:LYS:HD3	1.91	0.51
1:G:42:ILE:HD12	1:G:65:LEU:HD11	1.93	0.51
1:B:218:HIS:N	1:B:284:GLU:OE2	2.41	0.51
1:C:198:HIS:HB3	1:C:275:PHE:CD2	2.45	0.50
1:D:282:LYS:HA	1:D:282:LYS:HE2	1.91	0.50
1:H:43:LYS:HD2	1:H:70:LEU:HD11	1.94	0.50
1:H:122:LEU:CD2	1:H:149:ILE:HD13	2.42	0.50
1:I:256:ARG:NH2	1:I:272:VAL:HG23	2.25	0.50
1:F:72:GLU:OE1	1:F:234:LYS:HA	2.11	0.50
1:H:136:VAL:HG13	5:H:690:HOH:O	2.11	0.50
1:I:147:VAL:HB	5:I:630:HOH:O	2.10	0.50
1:G:179:LEU:HD13	1:G:192:ILE:CD1	2.41	0.50
1:A:216:VAL:HG13	5:A:413:HOH:O	2.11	0.50
1:E:119:LYS:HD2	5:E:473:HOH:O	2.10	0.50
1:B:98:LEU:HD13	1:B:249:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:166:LYS:HG2	1:G:306:ALA:O	2.11	0.50
1:I:80:ASN:HB3	5:I:635:HOH:O	2.11	0.50
1:I:136:VAL:CG1	1:I:174:LYS:HA	2.40	0.50
1:E:142:PHE:O	1:E:146:ILE:HG13	2.11	0.50
1:C:309:LYS:OXT	1:C:309:LYS:HD3	2.11	0.50
1:D:252:LYS:O	1:D:256:ARG:HG3	2.11	0.50
1:D:255:GLN:HG3	1:D:268:ASN:CB	2.42	0.50
1:G:111:LYS:HD3	1:G:188:ASP:OD1	2.11	0.50
1:A:236:SER:HB3	1:A:239:LYS:HG3	1.93	0.50
1:C:55:TYR:CE1	1:C:249:LEU:HD13	2.46	0.50
1:B:72:GLU:HG2	1:B:234:LYS:HA	1.94	0.50
1:F:182:VAL:HG12	1:F:211:THR:HG22	1.94	0.50
1:D:135:TYR:CE2	1:D:308:MET:HE3	2.46	0.50
1:C:262:ARG:HG2	1:C:262:ARG:HH11	1.77	0.50
1:D:17:ALA:O	1:D:20:PHE:HB3	2.11	0.50
1:G:120:SER:HA	1:G:216:VAL:HG21	1.92	0.50
1:H:218:HIS:HB3	5:H:495:HOH:O	2.11	0.50
1:I:282:LYS:O	1:I:284:GLU:HG3	2.12	0.50
1:G:239:LYS:CG	1:G:243:LYS:HE3	2.40	0.50
1:C:252:LYS:HE2	1:C:270:HIS:HB2	1.92	0.50
1:G:22:ARG:HB3	5:G:516:HOH:O	2.11	0.50
1:F:289:SER:HB2	5:F:415:HOH:O	2.12	0.50
1:D:170:LYS:HG2	5:D:689:HOH:O	2.12	0.50
1:E:155:GLU:OE2	1:E:298:HIS:CE1	2.64	0.50
1:H:111:LYS:CE	1:H:188:ASP:OD1	2.54	0.50
1:B:131:ASN:O	1:B:187:ILE:CG2	2.58	0.50
1:G:131:ASN:C	1:G:187:ILE:CD1	2.79	0.50
1:H:71:LEU:HG	1:H:231:ALA:HB1	1.91	0.50
1:D:54:PHE:O	1:D:230:ALA:HA	2.11	0.50
1:C:236:SER:HA	5:C:503:HOH:O	2.12	0.50
1:B:155:GLU:OE2	1:B:298:HIS:HE1	1.95	0.50
1:E:81:GLU:OE1	1:E:81:GLU:HA	2.11	0.50
1:C:239:LYS:HD3	5:C:676:HOH:O	2.10	0.50
1:E:195:TYR:CE1	1:E:196:TYR:CE1	3.00	0.50
1:E:128:LYS:HE2	5:E:601:HOH:O	2.10	0.50
1:G:83:ARG:HA	1:G:83:ARG:NE	2.25	0.50
1:E:259:THR:HG23	5:E:414:HOH:O	2.10	0.50
1:C:106:VAL:HB	1:C:192:ILE:HD11	1.94	0.50
1:H:72:GLU:HB3	1:H:232:VAL:HG13	1.93	0.50
1:F:232:VAL:HG21	1:F:243:LYS:CG	2.41	0.50
1:B:73:PRO:HA	1:B:93:LYS:O	2.12	0.50
1:B:244:LYS:HE3	5:B:716:HOH:O	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:224:LEU:HD12	5:F:431:HOH:O	2.12	0.50
1:I:71:LEU:HB2	1:I:94:ASP:OD2	2.11	0.49
1:B:268:ASN:HB3	1:B:271:VAL:HG23	1.92	0.49
1:H:99:SER:HA	1:H:267:LEU:HG	1.94	0.49
1:F:289:SER:HB3	5:F:516:HOH:O	2.12	0.49
1:A:106:VAL:CG2	1:A:211:THR:HB	2.41	0.49
1:G:278:GLU:HG2	5:G:404:HOH:O	2.12	0.49
1:F:217:ARG:HD3	5:F:509:HOH:O	2.13	0.49
1:B:300:THR:O	1:B:303:LEU:HB2	2.11	0.49
1:A:83:ARG:HD3	5:A:661:HOH:O	2.12	0.49
1:F:178:ALA:O	1:F:182:VAL:HG23	2.11	0.49
1:G:195:TYR:HA	1:G:263:ALA:HB3	1.94	0.49
1:G:122:LEU:HD23	5:G:503:HOH:O	2.12	0.49
1:B:65:LEU:HD12	5:B:682:HOH:O	2.11	0.49
1:A:196:TYR:CE2	2:A:400:CNB:O3U	2.66	0.49
1:F:143:LEU:HB2	5:F:534:HOH:O	2.11	0.49
1:B:265:TYR:HB2	1:B:280:ILE:HD13	1.94	0.49
1:B:27:LYS:HE3	5:B:710:HOH:O	2.12	0.49
1:I:16:VAL:HG11	1:I:249:LEU:CD2	2.42	0.49
1:A:236:SER:O	1:A:239:LYS:HE3	2.12	0.49
1:I:131:ASN:OD1	1:I:170:LYS:HE3	2.12	0.49
1:D:265:TYR:HB3	1:D:280:ILE:CG1	2.40	0.49
1:I:106:VAL:O	1:I:106:VAL:HG13	2.13	0.49
1:C:4:VAL:HG22	1:C:53:VAL:HB	1.93	0.49
1:C:52:ASP:HA	1:C:236:SER:HB2	1.94	0.49
1:E:4:VAL:HG22	1:E:53:VAL:HB	1.94	0.49
1:D:77:SER:O	1:D:81:GLU:HG2	2.13	0.49
1:F:107:TYR:N	1:F:107:TYR:CD1	2.79	0.49
1:A:259:THR:HG22	5:A:538:HOH:O	2.12	0.49
1:F:29:LYS:HE3	5:F:529:HOH:O	2.12	0.49
1:F:66:SER:OG	1:F:92:LYS:HD2	2.11	0.49
1:D:58:GLN:HB2	1:D:60:PRO:HD2	1.95	0.49
1:C:216:VAL:HG23	1:C:223:ALA:HB2	1.95	0.49
1:G:171:PRO:HD3	5:G:666:HOH:O	2.12	0.49
1:B:282:LYS:HA	1:B:282:LYS:HE2	1.94	0.49
1:G:233:LEU:CD1	1:G:233:LEU:N	2.75	0.49
1:A:239:LYS:NZ	1:A:239:LYS:HB2	2.28	0.49
1:C:133:ILE:O	1:C:133:ILE:HG23	2.13	0.49
1:B:97:ALA:HB2	5:B:620:HOH:O	2.13	0.49
1:H:53:VAL:HG13	1:H:231:ALA:O	2.13	0.49
1:I:141:ALA:HB1	1:I:193:ASN:HD21	1.77	0.49
1:E:107:TYR:OH	1:E:114:GLU:HG2	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:232:VAL:HG13	1:I:242:ALA:CB	2.42	0.49
1:A:101:ARG:HG2	5:A:675:HOH:O	2.13	0.49
1:A:147:VAL:HG13	1:A:295:GLU:HG2	1.95	0.49
1:G:214:ASN:ND2	1:G:215:PHE:H	2.09	0.49
1:I:61:ALA:O	1:I:64:THR:HG22	2.13	0.49
1:E:202:ARG:HH12	1:E:274:THR:CG2	2.25	0.49
1:I:73:PRO:HA	1:I:94:ASP:HA	1.94	0.49
1:C:59:ILE:CD1	1:C:227:TYR:HB2	2.43	0.49
1:G:196:TYR:CE1	3:G:400:CN1:O3U	2.66	0.49
1:C:8:GLN:NE2	1:C:101:ARG:HH21	2.11	0.49
1:G:33:ALA:HB3	1:G:38:LEU:CD2	2.42	0.49
1:E:303:LEU:HD12	5:E:650:HOH:O	2.12	0.49
1:B:34:LYS:HE3	1:B:37:GLN:CD	2.33	0.49
1:F:6:ASN:O	1:F:38:LEU:HD11	2.12	0.49
1:I:164:GLY:O	1:I:168:TYR:HD1	1.95	0.49
1:F:146:ILE:HD13	1:F:162:LEU:HD11	1.94	0.49
1:B:136:VAL:CG1	1:B:139:SER:HB2	2.42	0.49
1:B:181:ALA:HA	1:B:186:GLU:OE2	2.12	0.49
1:G:239:LYS:O	1:G:243:LYS:HG3	2.13	0.48
1:D:18:ASP:C	1:D:20:PHE:H	2.15	0.48
1:C:174:LYS:H	1:C:174:LYS:HD3	1.77	0.48
1:B:5:TYR:CZ	1:B:51:ALA:HB2	2.48	0.48
1:A:259:THR:CG2	1:A:266:PRO:HG3	2.29	0.48
1:G:16:VAL:HG12	1:G:16:VAL:O	2.13	0.48
1:I:259:THR:HG21	1:I:271:VAL:CG1	2.43	0.48
1:B:9:HIS:CD2	1:B:10:LYS:N	2.80	0.48
1:D:12:ALA:O	1:D:16:VAL:HG23	2.13	0.48
1:B:18:ASP:HA	1:B:21:THR:CG2	2.42	0.48
1:D:33:ALA:HB3	1:D:38:LEU:CG	2.42	0.48
1:F:182:VAL:HB	1:F:211:THR:HG21	1.95	0.48
1:C:179:LEU:O	1:C:179:LEU:HD12	2.14	0.48
1:C:101:ARG:CZ	1:C:228:SER:HB3	2.43	0.48
1:C:125:ALA:HB1	1:C:164:GLY:HA3	1.95	0.48
1:F:145:GLN:NE2	1:F:145:GLN:HA	2.26	0.48
1:E:8:GLN:CG	1:E:9:HIS:H	2.27	0.48
1:I:101:ARG:HB3	1:I:195:TYR:CE2	2.49	0.48
1:E:288:VAL:HB	5:E:621:HOH:O	2.12	0.48
1:D:161:TRP:CE2	1:D:165:LEU:HD11	2.49	0.48
1:D:234:LYS:C	1:D:236:SER:H	2.16	0.48
1:F:151:LYS:NZ	1:F:290:ALA:O	2.47	0.48
1:B:131:ASN:OD1	1:B:170:LYS:HD2	2.13	0.48
1:B:182:VAL:HG23	1:B:187:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:256:ARG:HG2	1:G:271:VAL:HG13	1.96	0.48
1:A:180:GLN:HG3	5:A:464:HOH:O	2.13	0.48
1:H:119:LYS:NZ	5:H:515:HOH:O	2.47	0.48
1:C:57:GLU:N	1:C:57:GLU:OE2	2.41	0.48
1:B:101:ARG:NH1	5:B:557:HOH:O	2.47	0.48
1:C:5:TYR:CD1	1:C:51:ALA:HB2	2.48	0.48
1:H:79:ILE:CD1	1:H:93:LYS:HD2	2.43	0.48
1:H:5:TYR:CD1	1:H:51:ALA:HB2	2.49	0.48
1:D:195:TYR:CZ	1:D:196:TYR:CE1	3.01	0.48
1:I:146:ILE:HG12	1:I:162:LEU:HD21	1.96	0.48
1:E:59:ILE:N	1:E:60:PRO:CD	2.76	0.48
1:D:216:VAL:CG2	1:D:223:ALA:HB2	2.42	0.48
1:B:54:PHE:O	1:B:230:ALA:HA	2.13	0.48
1:I:259:THR:CG2	1:I:266:PRO:HG3	2.43	0.48
1:C:8:GLN:HG3	5:C:664:HOH:O	2.13	0.48
1:F:262:ARG:HG3	5:F:701:HOH:O	2.12	0.48
1:D:265:TYR:HA	1:D:266:PRO:HD3	1.73	0.48
1:F:112:LEU:CD1	1:F:188:ASP:HB3	2.43	0.48
1:D:85:LYS:HG2	5:D:489:HOH:O	2.14	0.48
1:I:217:ARG:HA	1:I:223:ALA:HB2	1.95	0.48
1:H:9:HIS:NE2	1:H:11:GLU:HB3	2.29	0.48
1:I:255:GLN:O	1:I:259:THR:HG23	2.14	0.48
1:I:105:VAL:HG22	1:I:191:LEU:CD1	2.42	0.48
1:D:130:LYS:HB2	5:D:628:HOH:O	2.14	0.48
1:C:236:SER:O	1:C:239:LYS:HG3	2.14	0.48
1:F:252:LYS:O	1:F:256:ARG:HG3	2.14	0.48
1:H:2:ILE:HG13	1:H:28:VAL:HG13	1.96	0.48
1:I:221:PRO:HB3	5:I:649:HOH:O	2.14	0.48
1:I:174:LYS:HB2	3:I:400:CN1:O3U	2.14	0.48
1:G:111:LYS:HD3	1:G:188:ASP:CG	2.34	0.48
1:E:151:LYS:HE2	1:E:295:GLU:OE2	2.14	0.48
1:F:173:ALA:HA	5:F:540:HOH:O	2.14	0.48
1:D:72:GLU:OE2	1:D:73:PRO:HD2	2.13	0.48
1:D:107:TYR:HB2	1:D:112:LEU:HD12	1.96	0.48
1:G:198:HIS:HB3	1:G:275:PHE:CD2	2.48	0.48
1:D:145:GLN:O	1:D:149:ILE:HG13	2.14	0.48
1:B:255:GLN:HB2	1:B:271:VAL:HG21	1.96	0.47
1:F:179:LEU:C	1:F:181:ALA:N	2.68	0.47
1:D:214:ASN:HD22	1:D:215:PHE:H	1.62	0.47
1:H:133:ILE:HD11	1:H:191:LEU:HD13	1.96	0.47
1:G:294:SER:HA	5:G:615:HOH:O	2.13	0.47
1:G:2:ILE:HG22	1:G:238:ASN:HB2	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:262:ARG:C	1:D:264:GLU:H	2.16	0.47
1:I:204:LYS:O	1:I:205:GLY:O	2.31	0.47
1:F:98:LEU:O	1:F:267:LEU:HG	2.13	0.47
1:I:198:HIS:HB2	1:I:263:ALA:CB	2.45	0.47
1:F:38:LEU:HB2	1:F:54:PHE:CE1	2.49	0.47
1:B:114:GLU:CD	1:B:115:LYS:HE3	2.34	0.47
1:H:9:HIS:CD2	1:H:11:GLU:HB3	2.49	0.47
1:C:267:LEU:HD23	1:C:280:ILE:HD13	1.96	0.47
1:E:199:ALA:O	1:E:203:GLU:HB2	2.14	0.47
1:A:4:VAL:HG22	1:A:53:VAL:HB	1.96	0.47
1:C:10:LYS:NZ	1:C:32:SER:HB2	2.29	0.47
1:H:306:ALA:O	1:H:308:MET:N	2.46	0.47
1:B:252:LYS:HG2	1:B:256:ARG:HD2	1.96	0.47
1:A:148:ALA:O	1:A:152:LEU:HG	2.15	0.47
1:D:309:LYS:HG2	1:D:309:LYS:OXT	2.14	0.47
1:I:71:LEU:HD12	1:I:94:ASP:OD2	2.13	0.47
1:H:80:ASN:HA	1:H:83:ARG:CB	2.44	0.47
1:G:218:HIS:C	1:G:220:ASP:H	2.16	0.47
1:H:234:LYS:C	1:H:234:LYS:HD2	2.33	0.47
1:I:79:ILE:HG22	1:I:83:ARG:HH12	1.80	0.47
1:D:166:LYS:O	1:D:166:LYS:HD2	2.14	0.47
1:I:183:GLU:HG3	1:I:200:PHE:HE1	1.75	0.47
1:F:137:PRO:HA	1:F:142:PHE:CD2	2.49	0.47
1:E:79:ILE:HG12	1:E:96:VAL:HG12	1.96	0.47
1:G:12:ALA:HB2	1:G:262:ARG:HG2	1.93	0.47
1:D:251:GLY:O	1:D:255:GLN:HG2	2.15	0.47
1:A:246:VAL:HA	1:A:249:LEU:HD12	1.96	0.47
1:E:180:GLN:NE2	5:E:402:HOH:O	2.47	0.47
1:H:304:GLU:HG2	1:H:309:LYS:HE3	1.96	0.47
1:F:112:LEU:HD12	1:F:188:ASP:HB3	1.96	0.47
1:I:159:LEU:HD13	1:I:302:LEU:HD22	1.97	0.47
1:C:143:LEU:HD21	1:C:296:LYS:HG3	1.96	0.47
1:G:117:LEU:N	1:G:117:LEU:HD22	2.30	0.47
1:D:84:GLY:C	1:D:86:GLY:H	2.18	0.47
1:C:58:GLN:OE1	1:C:60:PRO:HG2	2.15	0.47
1:D:252:LYS:HG2	1:D:270:HIS:HB2	1.96	0.47
1:I:219:ARG:O	1:I:286:PRO:HB3	2.15	0.47
1:I:54:PHE:CE2	1:I:56:SER:HB2	2.50	0.47
1:C:300:THR:O	1:C:304:GLU:HG3	2.15	0.47
1:D:59:ILE:O	1:D:62:LEU:HB2	2.15	0.47
1:E:159:LEU:O	1:E:163:LYS:HG3	2.15	0.47
1:B:220:ASP:OD1	1:B:221:PRO:HD2	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:106:VAL:HG22	1:F:211:THR:HB	1.96	0.47
1:D:202:ARG:NH2	1:D:274:THR:HG22	2.20	0.47
1:C:298:HIS:HD2	5:C:633:HOH:O	1.97	0.47
1:E:48:ARG:HG2	5:E:713:HOH:O	2.15	0.47
1:H:43:LYS:CD	1:H:70:LEU:HD11	2.45	0.47
1:H:143:LEU:HD12	1:H:146:ILE:HD12	1.96	0.47
1:I:16:VAL:HG11	1:I:249:LEU:HD23	1.96	0.47
1:B:133:ILE:HD11	1:B:191:LEU:CD1	2.45	0.47
1:I:195:TYR:HA	1:I:263:ALA:CB	2.44	0.47
1:G:120:SER:HB3	1:G:123:ASN:ND2	2.30	0.47
1:B:69:ASN:HB3	1:B:234:LYS:NZ	2.30	0.47
1:E:24:THR:HG22	5:E:686:HOH:O	2.14	0.47
1:I:220:ASP:OD1	1:I:221:PRO:HD2	2.15	0.47
1:C:221:PRO:HG3	5:C:585:HOH:O	2.14	0.47
1:H:146:ILE:O	1:H:150:VAL:HG23	2.15	0.47
1:E:179:LEU:HD13	1:E:192:ILE:HD13	1.97	0.47
1:D:99:SER:HB2	1:D:264:GLU:CG	2.40	0.46
1:I:133:ILE:HD11	1:I:191:LEU:CD2	2.45	0.46
1:F:1:ASP:HA	1:F:26:ILE:CG2	2.45	0.46
1:E:135:TYR:CE2	1:E:137:PRO:HD3	2.51	0.46
1:E:262:ARG:HD3	1:E:264:GLU:CG	2.45	0.46
1:A:110:ARG:HH11	1:F:23:ALA:HA	1.80	0.46
1:B:151:LYS:HD2	1:B:288:VAL:CG1	2.45	0.46
1:I:142:PHE:O	1:I:146:ILE:HG13	2.15	0.46
1:F:218:HIS:HB2	5:F:469:HOH:O	2.15	0.46
1:E:255:GLN:HB3	1:E:255:GLN:HE21	1.60	0.46
1:E:202:ARG:HH12	1:E:274:THR:HG21	1.80	0.46
1:E:72:GLU:CG	1:E:234:LYS:HA	2.41	0.46
1:C:78:THR:O	1:C:78:THR:HG22	2.15	0.46
1:H:220:ASP:OD1	1:H:221:PRO:HD2	2.16	0.46
1:C:181:ALA:HA	1:C:186:GLU:OE2	2.14	0.46
1:E:8:GLN:CG	1:E:9:HIS:N	2.78	0.46
1:C:98:LEU:HD11	1:C:230:ALA:CB	2.45	0.46
1:I:33:ALA:HB3	1:I:38:LEU:CD2	2.46	0.46
1:I:43:LYS:HG2	1:I:70:LEU:CD1	2.45	0.46
1:H:85:LYS:NZ	5:H:582:HOH:O	2.47	0.46
1:G:291:THR:HA	1:G:295:GLU:OE1	2.15	0.46
1:G:173:ALA:HB3	1:G:177:VAL:HG21	1.98	0.46
1:I:191:LEU:N	1:I:191:LEU:HD22	2.31	0.46
1:C:130:LYS:HD2	1:C:168:TYR:HA	1.97	0.46
1:H:265:TYR:CE2	1:H:283:LEU:HD11	2.51	0.46
1:G:304:GLU:HB3	1:G:309:LYS:HB3	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:156:ALA:HB3	5:C:433:HOH:O	2.16	0.46
1:F:204:LYS:HD2	5:F:688:HOH:O	2.14	0.46
1:A:133:ILE:HD11	1:A:191:LEU:CD1	2.40	0.46
1:E:54:PHE:O	1:E:230:ALA:HA	2.16	0.46
1:C:255:GLN:CB	1:C:271:VAL:HG21	2.45	0.46
1:I:232:VAL:HG21	1:I:243:LYS:HA	1.97	0.46
1:A:136:VAL:HG22	1:A:172:TYR:O	2.15	0.46
1:E:93:LYS:HE2	5:E:623:HOH:O	2.15	0.46
1:G:173:ALA:O	1:G:174:LYS:HD3	2.15	0.46
1:C:101:ARG:HH11	1:C:101:ARG:HG3	1.80	0.46
1:B:110:ARG:NH2	1:B:183:GLU:O	2.45	0.46
1:B:129:TRP:O	1:B:133:ILE:HG22	2.16	0.46
1:A:203:GLU:HG2	5:A:604:HOH:O	2.15	0.46
1:B:145:GLN:O	1:B:149:ILE:HG13	2.16	0.46
1:I:83:ARG:HG3	1:I:83:ARG:HH11	1.81	0.46
1:B:14:GLN:HG3	5:B:608:HOH:O	2.15	0.46
1:D:245:PHE:CZ	1:D:249:LEU:HD21	2.51	0.46
1:G:267:LEU:CD2	1:G:280:ILE:HD13	2.45	0.46
1:H:103:ARG:HG3	1:H:224:LEU:HB3	1.98	0.46
1:B:115:LYS:C	1:B:117:LEU:H	2.19	0.46
1:E:159:LEU:HD22	5:E:469:HOH:O	2.15	0.46
1:A:4:VAL:HG23	1:A:28:VAL:HG13	1.98	0.46
1:C:281:ALA:HB1	5:C:560:HOH:O	2.15	0.46
1:A:76:ALA:O	1:A:80:ASN:HB2	2.16	0.46
1:D:217:ARG:HA	1:D:283:LEU:O	2.16	0.46
1:D:255:GLN:HG3	1:D:268:ASN:HB3	1.98	0.46
1:G:195:TYR:CE1	1:G:196:TYR:CE1	3.03	0.46
1:F:233:LEU:HD12	1:F:233:LEU:N	2.30	0.46
1:B:194:ASN:HB2	5:B:519:HOH:O	2.15	0.46
1:G:74:LEU:HD11	1:G:96:VAL:CG2	2.46	0.46
1:E:5:TYR:OH	1:E:50:PRO:HD2	2.16	0.46
1:F:3:THR:CG2	1:F:29:LYS:HD2	2.36	0.46
1:A:164:GLY:O	1:A:168:TYR:HD1	1.99	0.46
1:I:112:LEU:HD11	1:I:129:TRP:CZ3	2.51	0.46
1:I:153:LYS:HB3	5:I:636:HOH:O	2.15	0.46
1:D:206:VAL:HG22	1:D:212:ARG:HH12	1.80	0.46
1:C:265:TYR:HB3	1:C:280:ILE:HB	1.98	0.46
1:A:267:LEU:CD2	1:A:280:ILE:HD13	2.46	0.46
1:C:72:GLU:HB3	1:C:232:VAL:HB	1.97	0.46
1:G:63:ALA:O	1:G:66:SER:HB3	2.16	0.46
1:C:292:THR:HG23	1:C:295:GLU:OE1	2.16	0.46
1:B:182:VAL:HG23	1:B:187:ILE:CD1	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:133:ILE:HD11	1:I:191:LEU:HD22	1.98	0.46
1:D:159:LEU:HD11	1:D:163:LYS:HE3	1.98	0.46
1:D:245:PHE:O	1:D:248:PHE:HB3	2.15	0.46
1:D:26:ILE:HD13	1:D:241:GLU:HB2	1.98	0.46
1:D:59:ILE:N	1:D:60:PRO:CD	2.79	0.46
1:G:211:THR:O	1:G:212:ARG:HG2	2.16	0.46
1:I:113:SER:HB2	5:I:448:HOH:O	2.15	0.46
1:E:138:THR:HG23	5:E:484:HOH:O	2.16	0.46
1:C:136:VAL:HG13	1:C:173:ALA:O	2.15	0.46
1:D:216:VAL:HG23	1:D:217:ARG:N	2.31	0.45
1:G:173:ALA:C	1:G:174:LYS:HD3	2.36	0.45
1:D:282:LYS:CA	1:D:282:LYS:HE2	2.46	0.45
1:H:83:ARG:HD2	5:H:564:HOH:O	2.16	0.45
1:A:147:VAL:O	1:A:151:LYS:HG3	2.17	0.45
1:D:167:GLU:OE2	1:G:115:LYS:HD3	2.15	0.45
1:C:290:ALA:HA	5:C:561:HOH:O	2.16	0.45
1:F:125:ALA:HB1	1:F:164:GLY:CA	2.33	0.45
1:G:232:VAL:HG11	1:G:239:LYS:HG3	1.99	0.45
1:D:115:LYS:HD2	1:D:116:ASP:N	2.31	0.45
1:A:147:VAL:HB	5:A:672:HOH:O	2.16	0.45
1:G:245:PHE:O	1:G:249:LEU:HG	2.16	0.45
1:H:236:SER:HA	5:H:680:HOH:O	2.16	0.45
1:E:84:GLY:O	1:E:87:VAL:HB	2.15	0.45
1:B:38:LEU:O	1:B:42:ILE:HG13	2.15	0.45
1:E:71:LEU:O	1:E:234:LYS:HE3	2.15	0.45
1:D:267:LEU:HD23	1:D:280:ILE:CD1	2.47	0.45
1:C:262:ARG:NH1	1:C:262:ARG:HG2	2.31	0.45
1:C:41:GLN:O	1:C:45:GLU:HG3	2.17	0.45
1:E:161:TRP:CZ2	1:E:165:LEU:HD11	2.51	0.45
1:D:109:THR:HA	1:D:112:LEU:O	2.16	0.45
1:F:219:ARG:O	1:F:286:PRO:HB3	2.17	0.45
1:G:181:ALA:O	1:G:186:GLU:HB2	2.17	0.45
1:F:203:GLU:HB2	5:F:481:HOH:O	2.16	0.45
1:D:1:ASP:CG	1:D:27:LYS:HB2	2.37	0.45
1:E:160:LYS:CB	5:E:520:HOH:O	2.65	0.45
1:C:8:GLN:OE1	1:C:262:ARG:NH1	2.50	0.45
1:D:129:TRP:HB3	1:D:133:ILE:HG22	1.99	0.45
1:A:103:ARG:NH2	5:A:420:HOH:O	2.48	0.45
1:C:180:GLN:HA	1:C:180:GLN:NE2	2.31	0.45
1:I:200:PHE:CZ	1:I:204:LYS:HD2	2.51	0.45
1:H:43:LYS:HZ2	1:H:68:ALA:HB1	1.81	0.45
1:G:221:PRO:HB2	5:G:681:HOH:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:275:PHE:O	1:E:277:LEU:N	2.40	0.45
1:G:172:TYR:HB2	1:G:178:ALA:HB2	1.98	0.45
1:E:252:LYS:O	1:E:256:ARG:N	2.39	0.45
1:I:241:GLU:CD	1:I:241:GLU:H	2.19	0.45
1:C:150:VAL:HG11	1:C:298:HIS:CD2	2.52	0.45
1:H:4:VAL:HG22	1:H:53:VAL:HB	1.98	0.45
1:D:180:GLN:HG3	1:D:184:ASN:ND2	2.32	0.45
1:I:301:ARG:O	1:I:305:GLN:HB2	2.17	0.45
1:B:238:ASN:HB3	1:B:241:GLU:HG3	1.99	0.45
1:E:219:ARG:NH1	1:E:285:ALA:O	2.48	0.45
1:B:118:GLU:HG2	1:B:124:TYR:CE1	2.52	0.45
1:C:60:PRO:O	1:C:63:ALA:HB3	2.16	0.45
1:D:255:GLN:HE22	1:D:267:LEU:H	1.64	0.45
1:H:136:VAL:CG1	1:H:139:SER:HB2	2.46	0.45
1:C:150:VAL:HG22	1:C:158:ALA:CB	2.47	0.45
1:B:29:LYS:NZ	5:B:666:HOH:O	2.49	0.45
1:B:204:LYS:HB2	5:B:548:HOH:O	2.17	0.45
1:H:79:ILE:HD12	1:H:93:LYS:HD2	1.99	0.45
1:H:149:ILE:HD12	1:H:161:TRP:CE3	2.52	0.45
1:A:110:ARG:HH11	1:F:23:ALA:C	2.20	0.45
1:B:196:TYR:CE2	2:B:400:CNB:O3U	2.69	0.45
1:A:54:PHE:CZ	1:A:56:SER:HB3	2.52	0.45
1:D:161:TRP:CZ2	1:D:165:LEU:HD11	2.52	0.45
1:F:202:ARG:NH2	1:F:274:THR:O	2.50	0.45
1:B:16:VAL:HG11	1:B:249:LEU:HD21	1.99	0.45
1:H:107:TYR:C	1:H:211:THR:HG23	2.37	0.45
1:B:112:LEU:HD11	1:B:116:ASP:C	2.38	0.45
1:D:74:LEU:HD21	1:D:232:VAL:CG2	2.47	0.45
1:B:62:LEU:O	1:B:66:SER:HB2	2.17	0.45
1:G:115:LYS:HG3	5:G:639:HOH:O	2.16	0.45
1:B:69:ASN:HD21	1:B:92:LYS:NZ	2.14	0.45
1:H:180:GLN:NE2	5:H:692:HOH:O	2.49	0.45
1:I:219:ARG:HD2	5:I:569:HOH:O	2.17	0.45
1:B:41:GLN:O	1:B:44:GLU:HG2	2.17	0.45
1:C:101:ARG:HG3	1:C:101:ARG:NH1	2.32	0.45
1:G:92:LYS:HB2	1:G:94:ASP:OD1	2.16	0.45
1:D:109:THR:CG2	1:D:212:ARG:HG2	2.47	0.45
1:H:75:PRO:HG3	5:H:683:HOH:O	2.16	0.45
1:A:162:LEU:HB3	1:A:306:ALA:CB	2.46	0.44
1:D:181:ALA:C	1:D:187:ILE:HD11	2.37	0.44
1:H:53:VAL:HG23	1:H:242:ALA:HB1	1.97	0.44
1:B:159:LEU:HD11	1:B:163:LYS:HE3	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:142:PHE:CZ	1:D:308:MET:HE1	2.52	0.44
1:D:27:LYS:HD3	5:D:608:HOH:O	2.17	0.44
1:C:101:ARG:HA	5:C:692:HOH:O	2.17	0.44
1:D:5:TYR:CE1	1:D:51:ALA:HB2	2.53	0.44
1:B:238:ASN:HB3	1:B:241:GLU:CG	2.47	0.44
1:E:292:THR:OG1	1:E:295:GLU:HG3	2.17	0.44
1:I:150:VAL:HG11	1:I:298:HIS:CE1	2.52	0.44
1:G:7:GLY:N	1:G:55:TYR:O	2.46	0.44
1:D:150:VAL:HA	1:D:154:GLY:O	2.18	0.44
1:E:268:ASN:HD22	1:E:268:ASN:C	2.20	0.44
1:B:119:LYS:HA	5:B:700:HOH:O	2.18	0.44
1:C:6:ASN:HB2	1:C:30:LEU:CD2	2.42	0.44
1:I:36:ASP:CG	1:I:58:GLN:HE22	2.21	0.44
1:I:175:ASN:ND2	3:I:400:CN1:O3U	2.50	0.44
1:D:33:ALA:HB3	1:D:38:LEU:CD2	2.48	0.44
1:H:21:THR:OG1	1:H:27:LYS:HA	2.16	0.44
1:B:135:TYR:O	1:B:171:PRO:HA	2.18	0.44
1:E:228:SER:HB3	5:E:680:HOH:O	2.16	0.44
1:F:309:LYS:HG2	1:F:309:LYS:OXT	2.18	0.44
1:B:14:GLN:NE2	1:B:14:GLN:HA	2.32	0.44
1:D:85:LYS:HB2	1:D:85:LYS:NZ	2.32	0.44
1:D:85:LYS:HZ2	1:D:85:LYS:HA	1.82	0.44
1:A:252:LYS:HE3	5:H:438:HOH:O	2.16	0.44
1:D:33:ALA:HB3	1:D:38:LEU:HD21	1.99	0.44
1:D:62:LEU:HD22	1:D:95:TRP:HB3	2.00	0.44
1:B:69:ASN:CG	1:B:92:LYS:HZ3	2.20	0.44
1:A:10:LYS:O	1:A:14:GLN:HB2	2.18	0.44
1:H:139:SER:HB3	1:H:142:PHE:HB2	1.99	0.44
1:G:52:ASP:O	1:G:232:VAL:HA	2.17	0.44
1:F:133:ILE:HD11	1:F:191:LEU:HD13	1.99	0.44
1:F:40:GLY:O	1:F:43:LYS:HB2	2.17	0.44
1:E:296:LYS:HD2	5:E:683:HOH:O	2.16	0.44
1:I:164:GLY:O	1:I:168:TYR:CD1	2.69	0.44
1:I:151:LYS:HE2	1:I:295:GLU:OE1	2.18	0.44
1:C:22:ARG:HB2	5:C:688:HOH:O	2.17	0.44
1:D:162:LEU:HD22	1:D:308:MET:SD	2.58	0.44
1:I:268:ASN:C	1:I:270:HIS:H	2.21	0.44
1:D:71:LEU:HD12	1:D:94:ASP:HB2	1.99	0.44
1:H:1:ASP:H1	1:H:26:ILE:HG23	1.82	0.44
1:G:214:ASN:HD22	1:G:215:PHE:N	2.14	0.44
1:C:64:THR:HG23	5:C:488:HOH:O	2.17	0.44
1:A:217:ARG:HA	1:A:283:LEU:O	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:83:ARG:HG2	1:B:83:ARG:HH11	1.82	0.44
1:E:256:ARG:HD2	5:E:490:HOH:O	2.17	0.44
1:D:3:THR:HG21	5:D:473:HOH:O	2.16	0.44
1:H:49:SER:HA	1:H:50:PRO:HD3	1.83	0.44
1:B:7:GLY:C	1:B:8:GLN:O	2.48	0.44
1:D:78:THR:CG2	1:D:96:VAL:HG21	2.46	0.44
1:H:158:ALA:O	1:H:162:LEU:HG	2.17	0.44
1:D:292:THR:O	1:D:295:GLU:HB2	2.18	0.44
1:G:38:LEU:HB2	1:G:54:PHE:CE1	2.53	0.44
1:G:54:PHE:O	1:G:230:ALA:HA	2.18	0.44
1:A:292:THR:OG1	1:A:295:GLU:HB2	2.18	0.44
1:C:151:LYS:HE2	1:C:295:GLU:OE2	2.17	0.44
1:E:198:HIS:HB3	1:E:275:PHE:CD2	2.52	0.44
1:E:21:THR:HG21	5:E:488:HOH:O	2.17	0.44
1:C:142:PHE:O	1:C:145:GLN:HB3	2.18	0.44
1:I:80:ASN:CA	1:I:83:ARG:HH11	2.29	0.44
1:G:224:LEU:HG	5:G:659:HOH:O	2.18	0.44
1:B:2:ILE:HG22	1:B:238:ASN:CB	2.48	0.44
1:D:125:ALA:HB1	1:D:164:GLY:HA3	1.99	0.44
1:G:263:ALA:HB1	5:G:739:HOH:O	2.18	0.43
1:F:51:ALA:O	1:F:233:LEU:HD22	2.18	0.43
1:E:43:LYS:HG2	1:E:70:LEU:CD1	2.48	0.43
1:F:43:LYS:HE3	1:F:64:THR:HG22	2.00	0.43
1:I:43:LYS:HD2	5:I:593:HOH:O	2.18	0.43
1:D:82:THR:HG22	1:D:267:LEU:HB2	2.00	0.43
1:C:162:LEU:HD12	1:C:302:LEU:HB3	2.00	0.43
1:C:123:ASN:ND2	5:C:631:HOH:O	2.50	0.43
1:C:43:LYS:NZ	1:C:64:THR:HB	2.33	0.43
1:I:9:HIS:CE1	1:I:11:GLU:HB2	2.53	0.43
1:C:58:GLN:O	1:C:58:GLN:HG3	2.17	0.43
1:E:112:LEU:CD1	1:E:188:ASP:HB3	2.47	0.43
1:F:119:LYS:NZ	5:F:662:HOH:O	2.50	0.43
1:F:242:ALA:O	1:F:246:VAL:HG23	2.17	0.43
1:H:211:THR:HG22	1:H:212:ARG:N	2.33	0.43
1:D:146:ILE:HD13	1:D:162:LEU:HD11	2.00	0.43
1:C:59:ILE:HD11	1:C:227:TYR:HB2	2.00	0.43
1:D:87:VAL:HA	1:D:88:PRO:HD3	1.87	0.43
3:G:400:CN1:O2B	5:G:735:HOH:O	2.21	0.43
1:C:221:PRO:CG	5:C:585:HOH:O	2.67	0.43
1:E:83:ARG:NE	5:E:556:HOH:O	2.51	0.43
1:E:115:LYS:CA	1:E:115:LYS:HE2	2.48	0.43
1:E:101:ARG:HG3	1:E:264:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:57:GLU:HA	1:G:228:SER:HB2	1.99	0.43
1:B:216:VAL:HG23	5:B:576:HOH:O	2.18	0.43
1:E:151:LYS:HD2	1:E:288:VAL:HG13	2.01	0.43
1:A:111:LYS:HE2	5:A:512:HOH:O	2.18	0.43
1:H:59:ILE:H	1:H:60:PRO:HD2	1.82	0.43
1:B:54:PHE:CE2	1:B:56:SER:HB3	2.53	0.43
1:H:201:ALA:HA	1:H:209:VAL:CG2	2.46	0.43
1:G:52:ASP:O	1:G:232:VAL:HG13	2.19	0.43
1:E:55:TYR:HE1	1:E:98:LEU:CD1	2.28	0.43
1:G:265:TYR:HA	1:G:266:PRO:HD3	1.91	0.43
1:D:214:ASN:ND2	1:D:215:PHE:N	2.65	0.43
1:C:113:SER:HB3	5:C:484:HOH:O	2.19	0.43
1:H:164:GLY:O	1:H:168:TYR:HB2	2.18	0.43
1:A:7:GLY:HA2	1:A:33:ALA:O	2.19	0.43
1:E:80:ASN:HA	1:E:83:ARG:HB2	1.99	0.43
1:C:41:GLN:NE2	5:C:459:HOH:O	2.52	0.43
1:H:216:VAL:O	1:H:217:ARG:HB2	2.19	0.43
1:A:111:LYS:HB3	5:A:512:HOH:O	2.18	0.43
1:D:48:ARG:HD2	1:D:48:ARG:HA	1.75	0.43
1:I:145:GLN:O	1:I:149:ILE:HG13	2.18	0.43
1:D:226:THR:HG22	5:D:659:HOH:O	2.17	0.43
1:H:195:TYR:CE1	1:H:196:TYR:CZ	3.07	0.43
1:G:114:GLU:OE2	1:G:114:GLU:HA	2.18	0.43
1:C:274:THR:HG22	1:C:275:PHE:CD1	2.54	0.43
1:I:259:THR:HG21	1:I:271:VAL:HG11	2.01	0.43
1:E:146:ILE:HD13	1:E:162:LEU:HD11	2.01	0.43
1:G:53:VAL:HA	1:G:231:ALA:O	2.18	0.43
1:E:280:ILE:HG13	1:E:283:LEU:HD12	2.00	0.43
1:G:293:VAL:HG11	5:G:692:HOH:O	2.19	0.43
1:I:34:LYS:HD2	1:I:37:GLN:HG3	2.00	0.43
1:E:119:LYS:HB2	5:E:503:HOH:O	2.18	0.43
1:I:206:VAL:HB	5:I:616:HOH:O	2.19	0.43
1:A:156:ALA:HB3	5:A:419:HOH:O	2.17	0.43
1:H:104:VAL:HG11	1:H:194:ASN:HB3	1.99	0.43
1:F:131:ASN:HA	1:F:170:LYS:HE3	2.01	0.43
1:D:113:SER:HB3	1:D:115:LYS:HE3	2.00	0.43
1:E:303:LEU:HB2	5:E:650:HOH:O	2.19	0.43
1:A:252:LYS:HE2	1:A:256:ARG:CZ	2.49	0.43
1:B:140:GLY:O	1:B:144:GLU:HG2	2.19	0.43
1:D:60:PRO:HG2	5:D:437:HOH:O	2.17	0.43
1:C:292:THR:OG1	1:C:295:GLU:HG3	2.18	0.43
1:H:256:ARG:HD2	5:H:445:HOH:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:59:ILE:O	1:F:62:LEU:HB2	2.18	0.43
1:I:258:LEU:HD11	5:I:595:HOH:O	2.18	0.43
1:H:200:PHE:O	1:H:203:GLU:HB3	2.19	0.43
1:B:49:SER:HA	1:B:50:PRO:HD3	1.84	0.43
1:H:167:GLU:HG3	1:H:167:GLU:O	2.19	0.43
1:G:175:ASN:CB	3:G:400:CN1:O3U	2.64	0.43
1:C:244:LYS:O	1:C:247:ALA:HB3	2.19	0.43
1:G:72:GLU:HG2	1:G:239:LYS:CD	2.45	0.43
1:B:14:GLN:HA	1:B:17:ALA:HB3	2.00	0.43
1:F:197:TRP:CZ2	1:F:212:ARG:HD3	2.54	0.43
1:D:66:SER:C	1:D:68:ALA:N	2.72	0.43
1:G:133:ILE:HD12	1:G:189:ALA:HB3	1.99	0.43
1:A:204:LYS:HD2	5:A:642:HOH:O	2.18	0.43
1:A:240:ASP:HA	5:A:606:HOH:O	2.17	0.43
1:D:212:ARG:O	1:D:213:LEU:HD23	2.19	0.43
1:B:132:ARG:HD2	5:B:639:HOH:O	2.18	0.43
1:E:105:VAL:HG22	1:E:191:LEU:CD1	2.49	0.43
1:D:197:TRP:HE1	1:D:211:THR:CG2	2.22	0.43
1:C:233:LEU:N	1:C:233:LEU:CD1	2.80	0.43
1:D:255:GLN:HE21	1:D:268:ASN:CB	2.31	0.43
1:B:172:TYR:HA	5:B:474:HOH:O	2.19	0.43
1:F:38:LEU:HB2	1:F:54:PHE:HE1	1.83	0.43
1:C:3:THR:HA	5:C:666:HOH:O	2.19	0.43
1:A:80:ASN:HA	1:A:80:ASN:HD22	1.65	0.43
1:H:166:LYS:HG2	5:H:439:HOH:O	2.18	0.43
1:B:179:LEU:HG	5:B:674:HOH:O	2.17	0.43
1:A:128:LYS:HG2	1:A:128:LYS:O	2.18	0.43
1:I:57:GLU:N	1:I:57:GLU:OE2	2.44	0.43
1:H:106:VAL:CG1	1:H:106:VAL:O	2.66	0.42
1:G:132:ARG:HB3	1:G:132:ARG:NH1	2.33	0.42
1:C:174:LYS:N	1:C:174:LYS:HD3	2.34	0.42
1:I:141:ALA:CB	1:I:193:ASN:HD21	2.31	0.42
1:A:152:LEU:HD21	1:A:288:VAL:HG22	2.01	0.42
1:G:43:LYS:HD2	1:G:64:THR:CG2	2.49	0.42
1:B:299:ALA:HA	1:B:302:LEU:HD12	2.00	0.42
1:F:227:TYR:CD1	1:F:227:TYR:N	2.88	0.42
1:F:11:GLU:HB3	1:F:261:VAL:HG11	2.01	0.42
1:F:216:VAL:HG13	5:F:539:HOH:O	2.18	0.42
1:I:58:GLN:HG2	1:I:60:PRO:CD	2.47	0.42
1:C:146:ILE:HG12	1:C:162:LEU:HD21	2.00	0.42
1:D:122:LEU:HA	1:D:161:TRP:CD1	2.54	0.42
1:I:288:VAL:HG12	1:I:289:SER:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:248:PHE:CE1	1:H:253:GLU:HB3	2.54	0.42
1:I:156:ALA:HB3	5:I:482:HOH:O	2.18	0.42
1:B:6:ASN:OD1	1:B:55:TYR:HD2	2.02	0.42
1:C:179:LEU:HD21	1:C:197:TRP:HD1	1.84	0.42
1:G:122:LEU:HG	5:G:681:HOH:O	2.19	0.42
1:G:122:LEU:HA	1:G:161:TRP:CD1	2.54	0.42
1:D:51:ALA:HB3	1:D:233:LEU:HD22	2.01	0.42
1:C:7:GLY:N	1:C:55:TYR:O	2.42	0.42
1:A:106:VAL:HA	1:A:212:ARG:O	2.20	0.42
1:A:2:ILE:CG1	1:A:28:VAL:HG22	2.48	0.42
1:B:128:LYS:O	1:B:132:ARG:HD3	2.20	0.42
1:A:98:LEU:HD11	1:A:230:ALA:CB	2.48	0.42
1:C:207:GLN:NE2	5:C:644:HOH:O	2.37	0.42
1:I:2:ILE:HA	1:I:52:ASP:OD1	2.19	0.42
1:E:259:THR:O	1:E:274:THR:HB	2.20	0.42
1:D:98:LEU:O	1:D:99:SER:HB3	2.19	0.42
1:C:76:ALA:O	1:C:80:ASN:ND2	2.53	0.42
1:B:17:ALA:O	1:B:20:PHE:HB3	2.19	0.42
1:B:3:THR:HG23	1:B:29:LYS:HG3	2.01	0.42
1:E:135:TYR:HE2	1:E:137:PRO:HB3	1.84	0.42
1:H:117:LEU:HD13	1:H:214:ASN:HB2	2.00	0.42
1:G:139:SER:HB3	1:G:142:PHE:CB	2.48	0.42
1:D:48:ARG:NH2	5:D:582:HOH:O	2.50	0.42
1:D:280:ILE:O	1:D:283:LEU:HB2	2.19	0.42
1:F:216:VAL:HG23	1:F:217:ARG:N	2.34	0.42
1:G:239:LYS:HA	1:G:242:ALA:HB3	2.01	0.42
1:G:79:ILE:HG12	1:G:96:VAL:CG2	2.49	0.42
1:G:57:GLU:OE2	1:G:57:GLU:N	2.48	0.42
1:G:136:VAL:HB	1:G:139:SER:HB2	2.02	0.42
1:F:256:ARG:NH2	5:F:583:HOH:O	2.52	0.42
1:F:238:ASN:O	1:F:242:ALA:HB2	2.19	0.42
1:E:217:ARG:HD3	1:E:282:LYS:O	2.19	0.42
1:F:89:VAL:HG11	5:F:611:HOH:O	2.20	0.42
1:G:68:ALA:O	1:G:70:LEU:HG	2.19	0.42
1:C:1:ASP:HB3	5:C:580:HOH:O	2.18	0.42
1:C:59:ILE:CD1	1:C:88:PRO:HG2	2.50	0.42
1:H:130:LYS:HE3	1:H:131:ASN:HD21	1.82	0.42
1:B:9:HIS:HD2	1:B:10:LYS:H	1.62	0.42
1:C:142:PHE:HE2	1:C:308:MET:HE1	1.85	0.42
1:F:127:PRO:HA	5:F:561:HOH:O	2.18	0.42
1:G:133:ILE:HD11	1:G:191:LEU:CD1	2.50	0.42
1:G:26:ILE:HG22	5:G:694:HOH:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2:ILE:H	1:C:2:ILE:HD13	1.85	0.42
1:I:64:THR:HG23	1:I:65:LEU:N	2.34	0.42
1:G:150:VAL:HA	1:G:154:GLY:O	2.19	0.42
1:I:98:LEU:O	1:I:267:LEU:HG	2.19	0.42
1:G:80:ASN:HB2	5:G:579:HOH:O	2.20	0.42
1:H:106:VAL:HA	1:H:212:ARG:O	2.19	0.42
1:D:83:ARG:HA	1:D:83:ARG:HD3	1.88	0.42
1:D:191:LEU:H	1:D:191:LEU:HD22	1.84	0.42
1:D:259:THR:OG1	1:D:273:SER:HA	2.19	0.42
1:C:240:ASP:O	1:C:244:LYS:HG3	2.20	0.42
1:E:55:TYR:CE1	1:E:98:LEU:HD12	2.45	0.42
1:C:236:SER:HA	5:C:498:HOH:O	2.19	0.42
1:D:90:ALA:HB2	1:D:95:TRP:CE2	2.55	0.42
1:A:101:ARG:HB3	1:A:264:GLU:HG2	2.00	0.42
1:A:57:GLU:HB2	1:A:101:ARG:NH2	2.34	0.42
1:I:150:VAL:HG22	1:I:158:ALA:CB	2.50	0.42
1:H:195:TYR:CZ	1:H:196:TYR:CE1	3.08	0.42
1:G:145:GLN:O	1:G:149:ILE:HG13	2.20	0.42
1:H:182:VAL:HG22	1:H:187:ILE:HG23	2.02	0.42
1:B:111:LYS:HD3	1:B:188:ASP:OD1	2.20	0.42
1:A:121:VAL:HB	1:A:222:GLY:HA3	2.02	0.42
1:G:146:ILE:HD11	1:G:162:LEU:HD21	2.02	0.42
1:E:76:ALA:O	1:E:80:ASN:ND2	2.53	0.42
1:G:265:TYR:HB2	1:G:280:ILE:HD12	2.01	0.42
1:I:198:HIS:HB2	1:I:263:ALA:HB2	2.01	0.42
1:I:195:TYR:HB3	1:I:263:ALA:O	2.20	0.42
1:B:7:GLY:HA2	1:B:33:ALA:O	2.20	0.42
1:H:88:PRO:HG3	5:H:526:HOH:O	2.19	0.42
1:B:153:LYS:HE2	5:B:687:HOH:O	2.20	0.42
1:G:279:PRO:HB2	1:G:282:LYS:HG2	2.02	0.42
1:I:31:ASN:ND2	5:I:515:HOH:O	2.47	0.42
1:C:34:LYS:HB2	1:C:37:GLN:OE1	2.20	0.42
1:A:265:TYR:HA	1:A:266:PRO:HD3	1.84	0.42
1:I:121:VAL:HA	1:I:124:TYR:HD2	1.85	0.42
1:E:180:GLN:HA	1:E:180:GLN:NE2	2.34	0.42
1:H:149:ILE:HG12	1:H:221:PRO:HB3	2.02	0.42
1:G:92:LYS:HB2	1:G:94:ASP:CG	2.40	0.42
1:G:218:HIS:C	1:G:220:ASP:N	2.73	0.42
1:A:265:TYR:HD1	1:A:265:TYR:H	1.66	0.42
1:F:8:GLN:NE2	1:F:55:TYR:CE1	2.88	0.42
1:G:38:LEU:HD12	1:G:54:PHE:HE1	1.85	0.42
1:C:252:LYS:HA	1:C:255:GLN:HB2	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:184:ASN:ND2	5:H:460:HOH:O	2.53	0.42
1:H:128:LYS:HG2	1:H:128:LYS:O	2.20	0.42
1:D:191:LEU:N	1:D:191:LEU:HD22	2.34	0.41
1:F:101:ARG:NH1	1:F:228:SER:OG	2.53	0.41
1:I:219:ARG:HD3	1:I:284:GLU:O	2.19	0.41
1:G:163:LYS:HZ3	1:G:305:GLN:C	2.23	0.41
1:D:74:LEU:CD1	1:D:96:VAL:HG23	2.50	0.41
1:C:162:LEU:HB3	1:C:308:MET:HE2	2.01	0.41
1:A:255:GLN:HG3	1:A:268:ASN:CB	2.49	0.41
1:H:303:LEU:HB3	1:H:309:LYS:HE2	2.01	0.41
1:D:193:ASN:HB3	1:D:195:TYR:CE2	2.55	0.41
1:E:13:ALA:O	1:E:17:ALA:HB2	2.20	0.41
1:D:183:GLU:OE1	1:D:209:VAL:HG13	2.20	0.41
1:B:10:LYS:HE2	5:B:704:HOH:O	2.19	0.41
1:G:72:GLU:CD	1:G:239:LYS:HD3	2.40	0.41
1:B:64:THR:C	1:B:66:SER:N	2.72	0.41
1:I:18:ASP:HB3	1:I:22:ARG:NH1	2.35	0.41
1:C:2:ILE:HB	1:C:52:ASP:CB	2.50	0.41
1:C:245:PHE:CZ	1:C:249:LEU:HD11	2.54	0.41
1:H:98:LEU:HD23	5:H:627:HOH:O	2.20	0.41
1:D:8:GLN:NE2	1:D:228:SER:HB3	2.35	0.41
1:C:225:VAL:CG2	1:C:285:ALA:HB2	2.50	0.41
1:D:239:LYS:NZ	5:D:533:HOH:O	2.51	0.41
1:C:49:SER:HA	1:C:50:PRO:HD3	1.82	0.41
1:G:301:ARG:O	1:G:305:GLN:HG3	2.20	0.41
1:F:53:VAL:HG12	1:F:54:PHE:N	2.35	0.41
1:G:117:LEU:CD2	1:G:117:LEU:H	2.34	0.41
1:H:219:ARG:NH1	1:H:285:ALA:O	2.49	0.41
1:I:71:LEU:HD23	1:I:233:LEU:CD2	2.50	0.41
1:D:146:ILE:HD11	1:D:303:LEU:HD21	2.03	0.41
1:C:279:PRO:HB2	1:C:282:LYS:CG	2.48	0.41
1:G:255:GLN:HE21	1:G:266:PRO:HB3	1.86	0.41
1:E:200:PHE:O	1:E:203:GLU:HB3	2.20	0.41
1:I:69:ASN:O	1:I:234:LYS:HD2	2.21	0.41
1:I:132:ARG:O	1:I:188:ASP:HB2	2.21	0.41
1:F:185:GLY:O	1:F:187:ILE:N	2.53	0.41
1:D:166:LYS:HB2	5:D:672:HOH:O	2.19	0.41
1:D:135:TYR:HB3	1:D:191:LEU:HD23	2.02	0.41
1:D:256:ARG:NH1	5:D:434:HOH:O	2.53	0.41
1:B:31:ASN:HA	5:B:663:HOH:O	2.20	0.41
1:F:131:ASN:HB3	1:F:170:LYS:HE3	2.02	0.41
1:B:260:ALA:HB3	5:B:523:HOH:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:256:ARG:HB3	1:C:256:ARG:HH11	1.85	0.41
1:H:300:THR:HG23	1:H:309:LYS:HZ2	1.84	0.41
1:F:214:ASN:HD22	1:F:215:PHE:H	1.67	0.41
1:B:265:TYR:CE2	1:B:283:LEU:HD11	2.55	0.41
1:I:232:VAL:HG13	1:I:242:ALA:HB3	2.01	0.41
1:G:198:HIS:CE1	1:G:213:LEU:HD12	2.56	0.41
1:H:75:PRO:C	1:H:77:SER:N	2.74	0.41
1:I:17:ALA:O	1:I:20:PHE:HB3	2.21	0.41
1:E:90:ALA:HB2	1:E:95:TRP:CE2	2.56	0.41
1:D:274:THR:CG2	1:D:274:THR:O	2.69	0.41
1:D:286:PRO:O	1:D:288:VAL:HG23	2.20	0.41
1:G:125:ALA:HB1	1:G:164:GLY:HA3	2.02	0.41
1:D:85:LYS:CB	1:D:85:LYS:NZ	2.84	0.41
1:G:119:LYS:N	1:G:119:LYS:CD	2.82	0.41
1:I:65:LEU:HD22	1:I:70:LEU:HD13	2.02	0.41
1:B:160:LYS:HE3	5:B:631:HOH:O	2.20	0.41
1:A:293:VAL:HG23	5:A:504:HOH:O	2.19	0.41
1:A:266:PRO:HD2	5:A:751:HOH:O	2.20	0.41
1:D:18:ASP:C	1:D:20:PHE:N	2.74	0.41
1:H:72:GLU:HA	1:H:73:PRO:HD3	1.97	0.41
1:C:130:LYS:O	1:C:131:ASN:HB2	2.19	0.41
1:C:255:GLN:HB3	1:C:271:VAL:HG21	2.03	0.41
1:B:5:TYR:CD1	1:B:51:ALA:HB2	2.55	0.41
1:G:15:ALA:HB2	5:G:517:HOH:O	2.20	0.41
1:G:179:LEU:HD13	1:G:192:ILE:HD13	2.02	0.41
1:B:72:GLU:HB3	5:B:698:HOH:O	2.21	0.41
1:G:23:ALA:N	5:G:516:HOH:O	2.51	0.41
1:H:225:VAL:HG23	1:H:285:ALA:HB2	2.01	0.41
1:F:172:TYR:OH	1:F:187:ILE:CG2	2.65	0.41
1:F:10:LYS:HZ2	1:G:252:LYS:HE2	1.85	0.41
1:C:262:ARG:CG	1:C:264:GLU:HG2	2.50	0.41
1:F:98:LEU:C	1:F:267:LEU:HG	2.41	0.41
1:D:68:ALA:O	1:D:70:LEU:HG	2.21	0.41
1:G:5:TYR:CD2	1:G:38:LEU:HD22	2.56	0.41
1:A:5:TYR:CD2	1:A:38:LEU:HD22	2.56	0.41
1:E:245:PHE:O	1:E:248:PHE:HB3	2.21	0.41
1:D:233:LEU:N	1:D:233:LEU:HD12	2.36	0.41
1:C:3:THR:O	1:C:52:ASP:HB2	2.21	0.41
1:I:125:ALA:HB1	1:I:164:GLY:HA3	2.02	0.41
1:A:212:ARG:HA	1:A:212:ARG:HD3	1.93	0.41
1:G:117:LEU:HD22	1:G:117:LEU:H	1.86	0.41
1:G:104:VAL:CG1	1:G:194:ASN:HB3	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:125:ALA:HB1	1:E:164:GLY:HA3	2.03	0.41
1:E:243:LYS:NZ	5:E:638:HOH:O	2.54	0.41
1:E:130:LYS:HD3	1:E:168:TYR:HD2	1.85	0.41
1:A:34:LYS:HE2	1:A:34:LYS:HB3	1.89	0.41
1:H:104:VAL:HG21	1:H:213:LEU:HD22	2.02	0.41
1:E:145:GLN:O	1:E:149:ILE:HG13	2.21	0.41
1:D:256:ARG:CG	1:D:271:VAL:HG13	2.45	0.41
1:G:196:TYR:CE2	3:G:400:CN1:O3B	2.73	0.41
1:I:152:LEU:HD11	1:I:286:PRO:HB2	2.03	0.41
1:D:240:ASP:O	1:D:244:LYS:HB2	2.21	0.41
1:C:57:GLU:HB2	1:C:101:ARG:HH21	1.86	0.41
1:B:195:TYR:CD1	1:B:262:ARG:NH2	2.89	0.41
1:C:146:ILE:HA	5:C:653:HOH:O	2.21	0.41
1:C:150:VAL:HG22	1:C:158:ALA:HB2	2.02	0.41
1:B:259:THR:OG1	1:B:273:SER:HA	2.21	0.41
1:I:53:VAL:HG12	1:I:54:PHE:N	2.36	0.41
1:B:133:ILE:HG23	1:B:133:ILE:O	2.21	0.41
1:F:94:ASP:OD1	1:F:94:ASP:N	2.53	0.41
1:C:27:LYS:HB2	5:C:589:HOH:O	2.21	0.41
1:F:121:VAL:HB	1:F:222:GLY:HA3	2.03	0.41
1:I:123:ASN:C	1:I:125:ALA:H	2.23	0.41
1:D:90:ALA:HB1	5:D:498:HOH:O	2.19	0.41
1:I:300:THR:C	1:I:302:LEU:N	2.73	0.41
1:C:291:THR:HG22	1:C:292:THR:N	2.36	0.41
1:F:194:ASN:HD22	1:F:198:HIS:CE1	2.39	0.41
1:D:121:VAL:HB	5:D:453:HOH:O	2.21	0.41
1:F:308:MET:HG2	5:F:550:HOH:O	2.21	0.41
1:H:108:ASP:O	1:H:112:LEU:N	2.54	0.41
1:I:103:ARG:HB2	1:I:222:GLY:O	2.21	0.41
1:A:117:LEU:HD13	1:A:214:ASN:ND2	2.36	0.41
1:C:238:ASN:ND2	5:C:636:HOH:O	2.53	0.41
1:H:58:GLN:HB2	1:H:60:PRO:HD2	2.03	0.41
1:I:255:GLN:HB2	1:I:271:VAL:HG21	2.02	0.41
1:D:181:ALA:C	1:D:187:ILE:CD1	2.90	0.41
1:D:14:GLN:HA	1:D:17:ALA:HB3	2.03	0.41
1:B:261:VAL:HG13	5:B:523:HOH:O	2.21	0.41
1:D:174:LYS:HB2	1:D:177:VAL:HG23	2.01	0.41
1:A:233:LEU:N	1:A:233:LEU:CD1	2.82	0.41
1:B:82:THR:O	1:B:87:VAL:HG11	2.21	0.41
1:E:159:LEU:HD21	5:E:548:HOH:O	2.20	0.41
1:A:83:ARG:HH11	1:A:83:ARG:CG	2.34	0.41
1:H:197:TRP:O	1:H:200:PHE:N	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:77:SER:O	1:G:81:GLU:HG3	2.21	0.41
1:A:170:LYS:HE3	1:A:170:LYS:HB2	1.87	0.41
1:D:142:PHE:CE2	1:D:308:MET:HE2	2.56	0.40
1:E:45:GLU:O	1:E:48:ARG:HB2	2.21	0.40
1:F:255:GLN:CB	1:F:271:VAL:HG21	2.51	0.40
1:I:4:VAL:HB	1:I:30:LEU:HD23	2.02	0.40
1:C:68:ALA:O	1:C:70:LEU:HG	2.21	0.40
1:I:230:ALA:HB3	1:I:246:VAL:HG13	2.03	0.40
1:I:166:LYS:HE2	1:I:307:GLY:O	2.22	0.40
1:D:179:LEU:HD11	1:D:197:TRP:HD1	1.86	0.40
1:F:101:ARG:HG3	1:F:264:GLU:HG2	2.03	0.40
1:C:264:GLU:O	1:C:266:PRO:HD3	2.21	0.40
1:B:262:ARG:HA	1:B:262:ARG:HD2	1.79	0.40
1:F:179:LEU:HD23	1:F:196:TYR:CD2	2.55	0.40
1:H:239:LYS:O	1:H:243:LYS:HG3	2.21	0.40
1:I:117:LEU:HD23	1:I:129:TRP:HH2	1.86	0.40
1:H:18:ASP:HB3	1:H:22:ARG:HH11	1.86	0.40
1:H:34:LYS:HE2	5:H:557:HOH:O	2.21	0.40
1:E:43:LYS:HG2	1:E:70:LEU:HD11	2.02	0.40
1:C:94:ASP:N	1:C:94:ASP:OD1	2.52	0.40
1:F:121:VAL:HG22	1:F:161:TRP:HZ2	1.86	0.40
1:G:202:ARG:NH2	1:G:274:THR:O	2.54	0.40
1:C:58:GLN:HG3	1:C:61:ALA:CB	2.52	0.40
1:F:145:GLN:HE21	1:F:145:GLN:CA	2.28	0.40
1:C:33:ALA:HB3	1:C:38:LEU:HD21	2.03	0.40
1:D:2:ILE:CG2	1:D:241:GLU:HG3	2.51	0.40
1:G:92:LYS:HB2	1:G:94:ASP:OD2	2.21	0.40
1:F:214:ASN:ND2	1:F:215:PHE:N	2.70	0.40
1:H:217:ARG:NH1	1:H:283:LEU:HA	2.36	0.40
1:A:279:PRO:HD2	1:A:282:LYS:HD2	2.04	0.40
1:G:83:ARG:HH22	1:G:97:ALA:H	1.69	0.40
1:D:16:VAL:HG11	1:D:249:LEU:CD2	2.52	0.40
1:E:180:GLN:O	1:E:184:ASN:ND2	2.55	0.40
1:A:79:ILE:HA	1:A:96:VAL:CG2	2.50	0.40
1:C:133:ILE:HG13	1:C:191:LEU:CD2	2.52	0.40
1:B:301:ARG:O	1:B:305:GLN:HG3	2.21	0.40
1:A:85:LYS:HA	5:A:421:HOH:O	2.21	0.40
1:F:111:LYS:HE3	1:F:185:GLY:HA2	2.02	0.40
1:I:182:VAL:CG2	1:I:187:ILE:CG1	2.99	0.40
1:G:30:LEU:HB3	5:G:726:HOH:O	2.22	0.40
1:F:268:ASN:ND2	1:F:270:HIS:H	2.20	0.40
1:B:308:MET:HB3	5:B:432:HOH:O	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:252:LYS:HD2	1:A:256:ARG:NH2	2.36	0.40
1:D:109:THR:HG23	1:D:212:ARG:HG2	2.04	0.40
1:E:203:GLU:OE2	1:E:204:LYS:HE2	2.22	0.40
1:A:210:HIS:HD2	5:A:733:HOH:O	2.04	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	307/309 (99%)	289 (94%)	16 (5%)	2 (1%)	30	11
1	B	307/309 (99%)	271 (88%)	31 (10%)	5 (2%)	14	2
1	C	307/309 (99%)	282 (92%)	20 (6%)	5 (2%)	14	2
1	D	307/309 (99%)	268 (87%)	35 (11%)	4 (1%)	18	3
1	E	307/309 (99%)	288 (94%)	18 (6%)	1 (0%)	50	28
1	F	307/309 (99%)	279 (91%)	26 (8%)	2 (1%)	30	11
1	G	307/309 (99%)	271 (88%)	28 (9%)	8 (3%)	8	0
1	H	307/309 (99%)	278 (91%)	23 (8%)	6 (2%)	11	1
1	I	307/309 (99%)	272 (89%)	28 (9%)	7 (2%)	10	1
All	All	2763/2781 (99%)	2498 (90%)	225 (8%)	40 (1%)	16	3

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	10	LYS
1	C	308	MET
1	F	186	GLU
1	H	239	LYS
1	I	23	ALA
1	C	23	ALA
1	D	46	GLY

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Mol	Chain	Res	Type
1	D	68	ALA
1	I	205	GLY
1	B	10	LYS
1	C	173	ALA
1	D	85	LYS
1	E	276	ASN
1	G	8	GLN
1	H	218	HIS
1	H	306	ALA
1	A	276	ASN
1	B	93	LYS
1	B	114	GLU
1	C	169	GLY
1	G	33	ALA
1	G	173	ALA
1	G	198	HIS
1	H	83	ARG
1	B	69	ASN
1	G	58	GLN
1	G	217	ARG
1	G	219	ARG
1	A	169	GLY
1	B	205	GLY
1	I	67	ALA
1	H	307	GLY
1	I	154	GLY
1	G	271	VAL
1	I	127	PRO
1	I	269	PRO
1	F	137	PRO
1	D	169	GLY
1	H	137	PRO
1	I	280	ILE

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	245/245 (100%)	238 (97%)	7 (3%)	55	27
1	B	245/245 (100%)	237 (97%)	8 (3%)	50	22
1	C	245/245 (100%)	236 (96%)	9 (4%)	45	18
1	D	245/245 (100%)	232 (95%)	13 (5%)	32	8
1	E	245/245 (100%)	235 (96%)	10 (4%)	41	15
1	F	245/245 (100%)	235 (96%)	10 (4%)	41	15
1	G	245/245 (100%)	235 (96%)	10 (4%)	41	15
1	H	245/245 (100%)	239 (98%)	6 (2%)	61	35
1	I	245/245 (100%)	240 (98%)	5 (2%)	68	44
All	All	2205/2205 (100%)	2127 (96%)	78 (4%)	48	19

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	80	ASN
1	A	83	ARG
1	A	103	ARG
1	A	191	LEU
1	A	262	ARG
1	A	295	GLU
1	B	9	HIS
1	B	30	LEU
1	B	103	ARG
1	B	106	VAL
1	B	112	LEU
1	B	187	ILE
1	B	194	ASN
1	B	214	ASN
1	C	2	ILE
1	C	93	LYS
1	C	103	ARG
1	C	174	LYS
1	C	194	ASN
1	C	240	ASP
1	C	253	GLU
1	C	268	ASN
1	C	274	THR
1	D	22	ARG
1	D	31	ASN

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Mol	Chain	Res	Type
1	D	85	LYS
1	D	94	ASP
1	D	103	ARG
1	D	115	LYS
1	D	122	LEU
1	D	187	ILE
1	D	191	LEU
1	D	214	ASN
1	D	227	TYR
1	D	262	ARG
1	D	274	THR
1	E	94	ASP
1	E	101	ARG
1	E	103	ARG
1	E	187	ILE
1	E	216	VAL
1	E	218	HIS
1	E	253	GLU
1	E	255	GLN
1	E	268	ASN
1	E	274	THR
1	F	37	GLN
1	F	88	PRO
1	F	94	ASP
1	F	103	ARG
1	F	107	TYR
1	F	145	GLN
1	F	188	ASP
1	F	194	ASN
1	F	214	ASN
1	F	237	GLN
1	G	31	ASN
1	G	74	LEU
1	G	83	ARG
1	G	94	ASP
1	G	101	ARG
1	G	103	ARG
1	G	187	ILE
1	G	191	LEU
1	G	252	LYS
1	G	288	VAL
1	H	1	ASP

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Mol	Chain	Res	Type
1	H	36	ASP
1	H	103	ARG
1	H	106	VAL
1	H	176	SER
1	H	234	LYS
1	I	55	TYR
1	I	114	GLU
1	I	176	SER
1	I	208	ASN
1	I	287	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	31	ASN
1	A	41	GLN
1	A	80	ASN
1	A	123	ASN
1	A	131	ASN
1	A	180	GLN
1	A	198	HIS
1	A	276	ASN
1	A	287	GLN
1	A	298	HIS
1	A	305	GLN
1	B	8	GLN
1	B	9	HIS
1	B	14	GLN
1	B	31	ASN
1	B	58	GLN
1	B	198	HIS
1	B	208	ASN
1	B	238	ASN
1	B	255	GLN
1	B	270	HIS
1	B	298	HIS
1	C	31	ASN
1	C	41	GLN
1	C	123	ASN
1	C	131	ASN
1	C	180	GLN

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Mol	Chain	Res	Type
1	C	207	GLN
1	C	238	ASN
1	C	255	GLN
1	C	268	ASN
1	D	8	GLN
1	D	69	ASN
1	D	80	ASN
1	D	131	ASN
1	D	180	GLN
1	D	184	ASN
1	D	208	ASN
1	D	214	ASN
1	D	255	GLN
1	D	268	ASN
1	D	298	HIS
1	E	37	GLN
1	E	41	GLN
1	E	123	ASN
1	E	180	GLN
1	E	255	GLN
1	E	268	ASN
1	E	298	HIS
1	F	31	ASN
1	F	194	ASN
1	F	255	GLN
1	F	268	ASN
1	F	298	HIS
1	G	31	ASN
1	G	41	GLN
1	G	58	GLN
1	G	69	ASN
1	G	123	ASN
1	G	210	HIS
1	G	214	ASN
1	G	218	HIS
1	G	238	ASN
1	G	255	GLN
1	G	276	ASN
1	G	287	GLN
1	G	305	GLN
1	H	8	GLN
1	H	14	GLN

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Mol	Chain	Res	Type
1	H	80	ASN
1	H	123	ASN
1	H	131	ASN
1	H	184	ASN
1	H	207	GLN
1	H	208	ASN
1	H	214	ASN
1	H	255	GLN
1	H	287	GLN
1	H	298	HIS
1	I	8	GLN
1	I	58	GLN
1	I	69	ASN
1	I	123	ASN
1	I	175	ASN
1	I	193	ASN
1	I	208	ASN
1	I	210	HIS
1	I	276	ASN
1	I	298	HIS

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 ⓘ

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CNB	A	400	1	12,14,14	7.15	12 (100%)	0,29,29	0.00	-
2	CNB	B	400	1	12,14,14	7.14	12 (100%)	0,29,29	0.00	-
3	CN1	C	400	1	8,15,15	10.02	8 (100%)	0,31,31	0.00	-
2	CNB	D	400	1	12,14,14	7.17	12 (100%)	0,29,29	0.00	-
3	CN1	E	400	1	8,15,15	10.04	8 (100%)	0,31,31	0.00	-
4	CNF	F	400	1	13,16,16	6.43	4 (30%)	0,40,40	0.00	-
3	CN1	G	400	1	8,15,15	10.03	8 (100%)	0,31,31	0.00	-
2	CNB	H	400	1	12,14,14	7.12	12 (100%)	0,29,29	0.00	-
3	CN1	I	400	1	8,15,15	10.09	8 (100%)	0,31,31	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CNB	A	400	1	-	0/0/22/22	1/1/1/1
2	CNB	B	400	1	-	0/0/22/22	1/1/1/1
3	CN1	C	400	1	-	0/0/25/25	0/0/1/1
2	CNB	D	400	1	-	0/0/22/22	1/1/1/1
3	CN1	E	400	1	-	0/0/25/25	0/0/1/1
4	CNF	F	400	1	-	0/0/43/43	0/0/2/2
3	CN1	G	400	1	-	0/0/25/25	0/0/1/1
2	CNB	H	400	1	-	0/0/22/22	1/1/1/1
3	CN1	I	400	1	-	0/0/25/25	0/0/1/1

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	400	CNF	O1B-FE1	15.98	2.26	1.92
3	I	400	CN1	O13-FE3	13.80	2.10	1.79
3	I	400	CN1	O13-FE1	13.79	2.10	1.79
3	G	400	CN1	O13-FE1	13.78	2.10	1.79
3	G	400	CN1	O13-FE3	13.77	2.10	1.79
3	E	400	CN1	O13-FE3	13.76	2.10	1.79
3	C	400	CN1	O13-FE3	13.68	2.10	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	400	CN1	O13-FE1	13.67	2.10	1.79
3	C	400	CN1	O13-FE1	13.66	2.10	1.79
4	F	400	CNF	O2B-FE2	11.03	2.15	1.92
4	F	400	CNF	O1U-FE1	9.65	2.13	1.92
2	D	400	CNB	O3B-FE3	8.74	2.11	1.92
2	D	400	CNB	O2U-FE2	8.63	2.10	1.92
2	A	400	CNB	O2U-FE2	8.62	2.10	1.92
2	D	400	CNB	O2A-FE2	8.58	2.10	1.92
2	D	400	CNB	O3U-FE3	8.57	2.10	1.92
3	I	400	CN1	O1U-FE1	8.54	2.10	1.92
3	E	400	CN1	O1A-FE1	8.54	2.10	1.92
3	I	400	CN1	O3B-FE3	8.54	2.10	1.92
3	G	400	CN1	O1U-FE1	8.53	2.10	1.92
3	C	400	CN1	O3B-FE3	8.53	2.10	1.92
2	H	400	CNB	O3U-FE3	8.52	2.10	1.92
3	E	400	CN1	O3A-FE3	8.52	2.10	1.92
3	E	400	CN1	O1U-FE1	8.51	2.10	1.92
3	C	400	CN1	O1U-FE1	8.50	2.10	1.92
2	A	400	CNB	O3U-FE3	8.50	2.10	1.92
2	H	400	CNB	O2A-FE2	8.50	2.10	1.92
2	B	400	CNB	O3B-FE3	8.49	2.10	1.92
3	I	400	CN1	O1B-FE1	8.49	2.10	1.92
3	I	400	CN1	O3A-FE3	8.48	2.10	1.92
2	A	400	CNB	O2A-FE2	8.48	2.10	1.92
2	H	400	CNB	O2B-FE2	8.48	2.10	1.92
2	H	400	CNB	O2U-FE2	8.48	2.10	1.92
3	I	400	CN1	O12-FE1	8.48	2.10	1.92
3	I	400	CN1	O1A-FE1	8.47	2.10	1.92
2	B	400	CNB	O2A-FE2	8.47	2.10	1.92
2	B	400	CNB	O2B-FE2	8.47	2.10	1.92
2	B	400	CNB	O2U-FE2	8.47	2.10	1.92
3	C	400	CN1	O3A-FE3	8.46	2.10	1.92
3	G	400	CN1	O3B-FE3	8.46	2.10	1.92
2	A	400	CNB	O3A-FE3	8.45	2.10	1.92
3	G	400	CN1	O1B-FE1	8.45	2.10	1.92
3	G	400	CN1	O3A-FE3	8.44	2.10	1.92
3	C	400	CN1	O1A-FE1	8.44	2.10	1.92
2	A	400	CNB	O2B-FE2	8.44	2.10	1.92
3	E	400	CN1	O1B-FE1	8.43	2.10	1.92
3	E	400	CN1	O3B-FE3	8.43	2.10	1.92
3	C	400	CN1	O12-FE1	8.42	2.10	1.92
3	C	400	CN1	O1B-FE1	8.41	2.10	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	400	CN1	O12-FE1	8.40	2.10	1.92
2	A	400	CNB	O3B-FE3	8.39	2.10	1.92
2	B	400	CNB	O3U-FE3	8.39	2.10	1.92
2	B	400	CNB	O3A-FE3	8.39	2.10	1.92
2	H	400	CNB	O3A-FE3	8.34	2.10	1.92
3	G	400	CN1	O1A-FE1	8.34	2.10	1.92
2	H	400	CNB	O3B-FE3	8.32	2.10	1.92
3	G	400	CN1	O12-FE1	8.30	2.10	1.92
2	D	400	CNB	O3A-FE3	8.23	2.10	1.92
2	B	400	CNB	O12-FE1	8.22	2.11	1.84
2	D	400	CNB	O2B-FE2	8.17	2.09	1.92
2	D	400	CNB	O12-FE1	8.16	2.10	1.84
2	A	400	CNB	O13-FE1	8.09	2.10	1.84
2	D	400	CNB	O13-FE1	8.06	2.10	1.84
2	H	400	CNB	O12-FE1	8.05	2.10	1.84
2	B	400	CNB	O13-FE1	8.02	2.10	1.84
2	H	400	CNB	O13-FE1	8.01	2.10	1.84
2	A	400	CNB	O12-FE1	8.00	2.10	1.84
4	F	400	CNF	O1A-FE1	-7.60	1.76	1.92
2	D	400	CNB	O23-FE2	3.67	2.10	1.90
2	D	400	CNB	O23-FE3	3.67	2.10	1.90
2	A	400	CNB	O12-FE2	3.64	2.10	1.90
2	H	400	CNB	O12-FE2	3.63	2.10	1.90
2	A	400	CNB	O23-FE2	3.60	2.10	1.90
2	B	400	CNB	O23-FE2	3.60	2.10	1.90
2	B	400	CNB	O23-FE3	3.59	2.10	1.90
2	B	400	CNB	O13-FE3	3.59	2.10	1.90
2	A	400	CNB	O23-FE3	3.59	2.10	1.90
2	D	400	CNB	O13-FE3	3.58	2.10	1.90
2	H	400	CNB	O23-FE3	3.58	2.10	1.90
2	H	400	CNB	O23-FE2	3.57	2.10	1.90
2	A	400	CNB	O13-FE3	3.57	2.10	1.90
2	B	400	CNB	O12-FE2	3.57	2.10	1.90
2	D	400	CNB	O12-FE2	3.55	2.10	1.90
2	H	400	CNB	O13-FE3	3.54	2.10	1.90

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	400	CNB	FE1-FE2-FE3-O12-O13-O23
2	B	400	CNB	FE1-FE2-FE3-O12-O13-O23
2	D	400	CNB	FE1-FE2-FE3-O12-O13-O23
2	A	400	CNB	FE1-FE2-FE3-O12-O13-O23

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.