



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:05 PM GMT

PDB ID : 2R6C
Title : Crystal Form BH2
Authors : Bailey, S.; Eliason, W.K.; Steitz, T.A.
Deposited on : 2007-09-05
Resolution : 4.00 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>

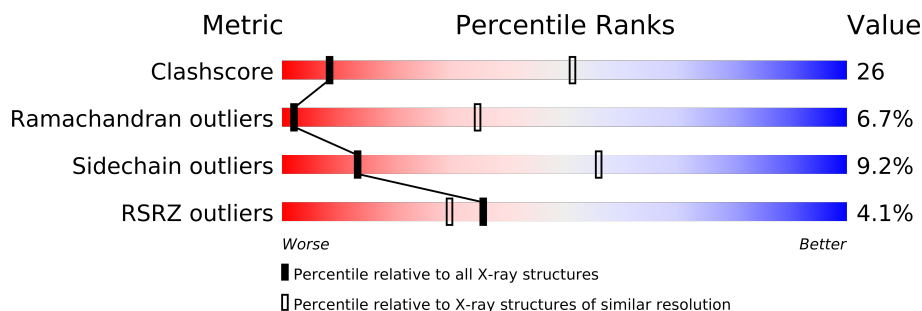
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 4.00 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	1235 (4.50-3.50)
Ramachandran outliers	78287	1170 (4.50-3.50)
Sidechain outliers	78261	1156 (4.50-3.50)
RSRZ outliers	66119	1035 (4.52-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	454	
1	B	454	
1	C	454	
1	D	454	
1	E	454	
1	F	454	
2	G	143	
2	H	143	
2	I	143	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19920 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 Replicative helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2759	1737	473	536	13			
1	B	358	Total	C	N	O	S	0	0	0
			2759	1737	473	536	13			
1	C	358	Total	C	N	O	S	0	0	0
			2759	1737	473	536	13			
1	D	358	Total	C	N	O	S	0	0	0
			2759	1737	473	536	13			
1	E	358	Total	C	N	O	S	0	0	0
			2759	1737	473	536	13			
1	F	358	Total	C	N	O	S	0	0	0
			2759	1737	473	536	13			

- Molecule 2 is a protein called DnaG Primase, Helicase Binding Domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	138	Total	C	N	O	Se	0	0	0
			1122	712	199	205	6			
2	H	138	Total	C	N	O	Se	0	0	0
			1122	712	199	205	6			
2	I	138	Total	C	N	O	Se	0	0	0
			1122	712	199	205	6			

There are 6 discrepancies between the modelled and reference sequences:

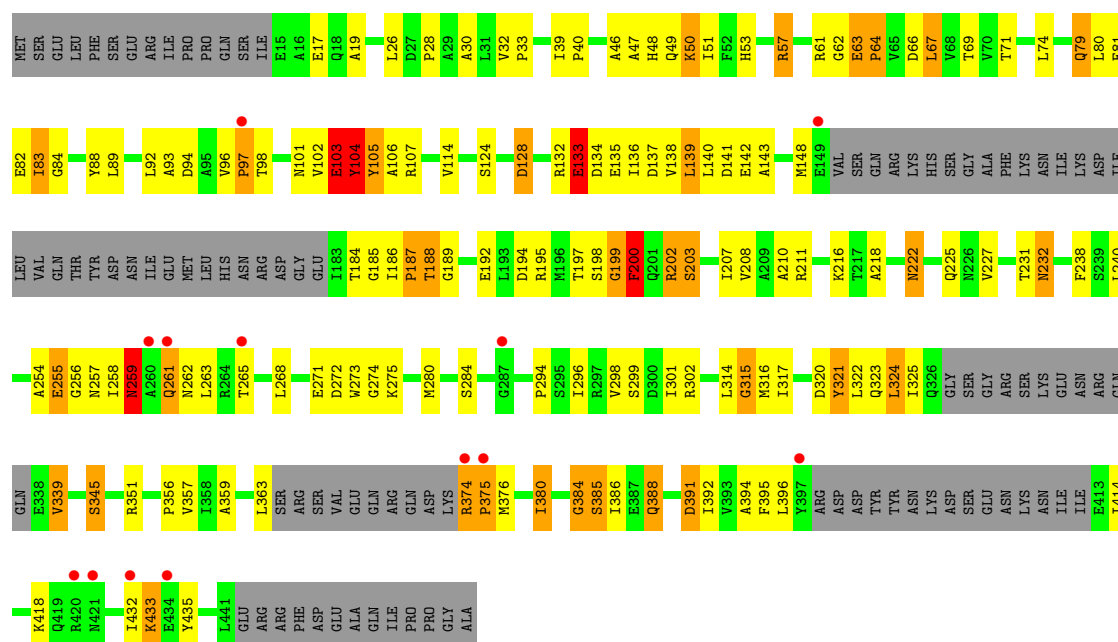
Chain	Residue	Modelled	Actual	Comment	Reference
G	530	GLU	ASP	CONFLICT	UNP Q9X4D0
G	531	LEU	VAL	CONFLICT	UNP Q9X4D0
H	530	GLU	ASP	CONFLICT	UNP Q9X4D0
H	531	LEU	VAL	CONFLICT	UNP Q9X4D0
I	530	GLU	ASP	CONFLICT	UNP Q9X4D0
I	531	LEU	VAL	CONFLICT	UNP Q9X4D0

3 Residue-property plots

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

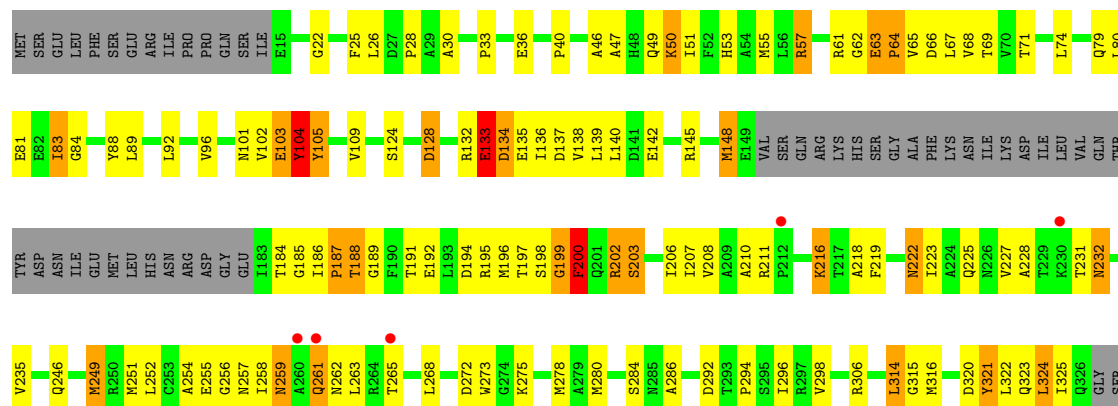
• Molecule 1: Replicative helicase

Chain A:



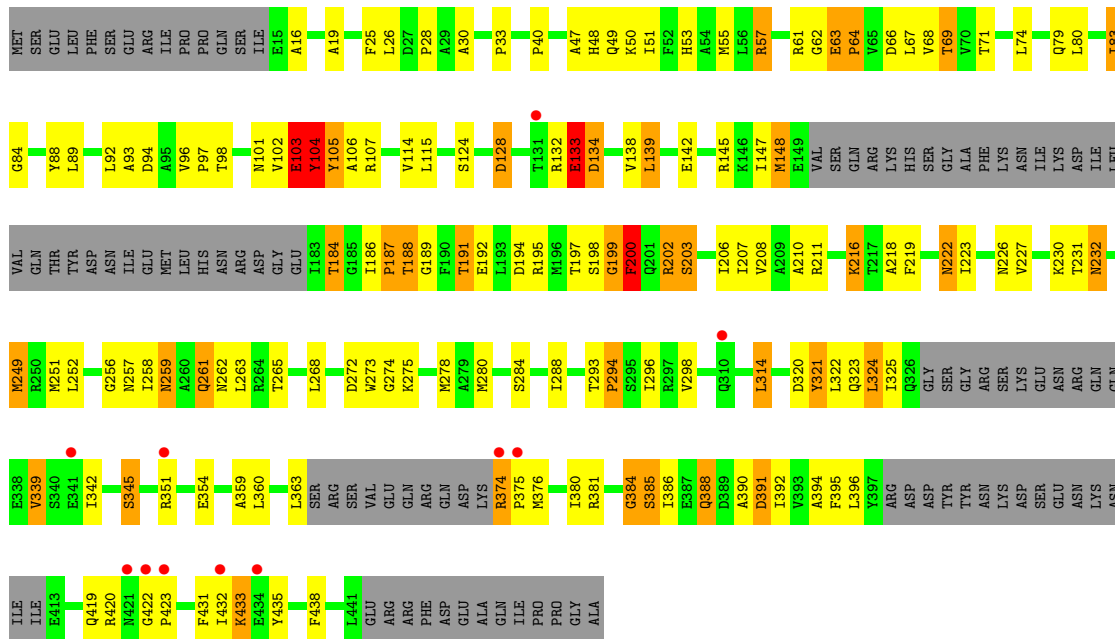
• Molecule 1: Replicative helicase

Chain B:



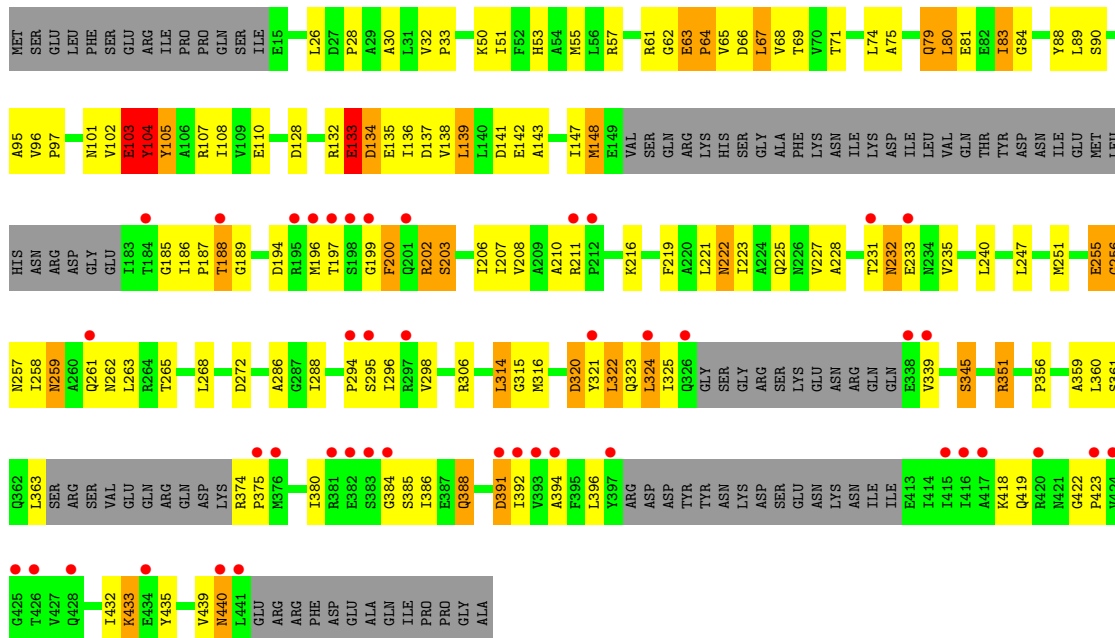
- Molecule 1: Replicative helicase

Chain E:



- Molecule 1: Replicative helicase

Chain F:



- Molecule 2: DnaG Primase, Helicase Binding Domain

Chain G:





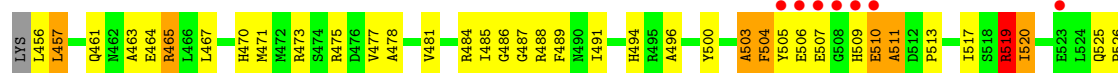
• Molecule 2: DnaG Primase, Helicase Binding Domain

Chain H:



• Molecule 2: DnaG Primase, Helicase Binding Domain

Chain I:



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	228.78Å 228.78Å 192.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.00 19.98 – 4.00	Depositor EDS
% Data completeness (in resolution range)	90.8 (20.00-4.00) 90.8 (19.98-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 4.07Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.320 , 0.344 0.316 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	127.3	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 181.6	EDS
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 44598 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	19920	wwPDB-VP
Average B, all atoms (Å ²)	166.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/2789	0.79	7/3770 (0.2%)
1	B	0.47	0/2789	0.78	4/3770 (0.1%)
1	C	0.51	0/2789	0.81	7/3770 (0.2%)
1	D	0.51	0/2789	0.79	6/3770 (0.2%)
1	E	0.50	0/2789	0.80	8/3770 (0.2%)
1	F	0.47	0/2789	0.76	3/3770 (0.1%)
2	G	0.42	0/1134	0.70	1/1514 (0.1%)
2	H	0.47	0/1134	0.71	1/1514 (0.1%)
2	I	0.42	0/1134	0.69	1/1514 (0.1%)
All	All	0.49	0/20136	0.77	38/27162 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	5
1	B	1	3
1	C	1	5
1	D	2	4
1	E	2	4
1	F	1	2
2	G	0	1
2	H	0	1
2	I	0	1
All	All	8	26

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	519	ARG	N-CA-C	7.51	131.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	519	ARG	N-CA-C	7.41	131.01	111.00
2	G	519	ARG	N-CA-C	7.37	130.89	111.00
1	D	261	GLN	N-CA-C	6.80	129.35	111.00
1	A	261	GLN	N-CA-C	6.45	128.43	111.00
1	E	133	GLU	N-CA-C	6.38	128.21	111.00
1	C	261	GLN	N-CA-C	6.20	127.75	111.00
1	A	133	GLU	N-CA-C	6.18	127.69	111.00
1	B	133	GLU	N-CA-C	6.06	127.37	111.00
1	E	261	GLN	N-CA-C	6.03	127.29	111.00
1	F	133	GLU	N-CA-C	6.00	127.21	111.00
1	B	261	GLN	N-CA-C	5.99	127.17	111.00
1	C	104	TYR	CA-CB-CG	-5.96	102.08	113.40
1	D	133	GLU	N-CA-C	5.93	127.02	111.00
1	A	199	GLY	N-CA-C	-5.93	98.28	113.10
1	C	199	GLY	N-CA-C	-5.93	98.28	113.10
1	C	133	GLU	N-CA-C	5.87	126.83	111.00
1	C	103	GLU	N-CA-C	5.85	126.80	111.00
1	E	199	GLY	N-CA-C	-5.82	98.55	113.10
1	A	321	TYR	N-CA-C	5.79	126.64	111.00
1	F	104	TYR	CA-CB-CG	-5.74	102.49	113.40
1	E	184	THR	N-CA-C	5.72	126.45	111.00
1	A	103	GLU	N-CA-C	5.65	126.26	111.00
1	A	184	THR	N-CA-C	5.63	126.19	111.00
1	E	104	TYR	CA-CB-CG	-5.54	102.87	113.40
1	D	199	GLY	N-CA-C	-5.54	99.26	113.10
1	C	321	TYR	N-CA-C	5.45	125.72	111.00
1	A	104	TYR	CA-CB-CG	-5.38	103.19	113.40
1	E	321	TYR	N-CA-C	5.36	125.48	111.00
1	D	321	TYR	N-CA-C	5.35	125.43	111.00
1	B	199	GLY	N-CA-C	-5.32	99.81	113.10
1	D	104	TYR	CA-CB-CG	-5.32	103.30	113.40
1	E	104	TYR	N-CA-CB	5.31	120.16	110.60
1	D	103	GLU	N-CA-C	5.30	125.30	111.00
1	C	184	THR	N-CA-C	5.21	125.08	111.00
1	F	103	GLU	N-CA-C	5.19	125.01	111.00
1	E	103	GLU	N-CA-C	5.16	124.92	111.00
1	B	321	TYR	N-CA-C	5.04	124.62	111.00

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	104	TYR	CA

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Mol	Chain	Res	Type	Atom
1	B	104	TYR	CA
1	C	104	TYR	CA
1	D	104	TYR	CA
1	D	184	THR	CA
1	E	104	TYR	CA
1	E	184	THR	CA
1	F	104	TYR	CA

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	GLU	Peptide
1	A	187	PRO	Peptide
1	A	259	ASN	Peptide
1	A	320	ASP	Peptide
1	A	374	ARG	Peptide
1	B	187	PRO	Peptide
1	B	320	ASP	Peptide
1	B	374	ARG	Peptide
1	C	103	GLU	Peptide
1	C	187	PRO	Peptide
1	C	259	ASN	Peptide
1	C	320	ASP	Peptide
1	C	374	ARG	Peptide
1	D	103	GLU	Peptide
1	D	187	PRO	Peptide
1	D	320	ASP	Peptide
1	D	374	ARG	Peptide
1	E	103	GLU	Peptide
1	E	187	PRO	Peptide
1	E	320	ASP	Peptide
1	E	374	ARG	Peptide
1	F	103	GLU	Peptide
1	F	320	ASP	Peptide
2	G	519	ARG	Peptide
2	H	519	ARG	Peptide
2	I	519	ARG	Peptide

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	2759	0	2806	160	0
1	B	2759	0	2806	151	0
1	C	2759	0	2805	163	0
1	D	2759	0	2807	187	0
1	E	2759	0	2806	162	0
1	F	2759	0	2807	124	0
2	G	1122	0	1144	62	0
2	H	1122	0	1144	61	0
2	I	1122	0	1144	56	0
All	All	19920	0	20269	1051	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 26.

All (1051) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:255:GLU:O	1:A:257:ASN:N	1.60	1.34
1:C:188:THR:OG1	1:C:194:ASP:OD1	1.52	1.27
1:C:306:ARG:CZ	1:D:32:VAL:HG21	1.64	1.26
1:D:255:GLU:O	1:D:257:ASN:N	1.70	1.23
1:A:132:ARG:O	1:A:133:GLU:HB2	1.40	1.20
1:E:188:THR:OG1	1:E:194:ASP:OD1	1.60	1.16
1:D:188:THR:OG1	1:D:194:ASP:OD1	1.63	1.14
1:B:132:ARG:O	1:B:133:GLU:HB2	1.46	1.14
1:F:255:GLU:O	1:F:257:ASN:N	1.79	1.14
1:C:227:VAL:O	1:C:231:THR:HG22	1.49	1.13
2:H:475:ARG:NH1	2:H:505:TYR:HB2	1.64	1.12
1:B:63:GLU:H	1:B:64:PRO:HA	0.99	1.11
1:E:104:TYR:HE2	1:F:63:GLU:HB2	1.16	1.10
1:D:63:GLU:H	1:D:64:PRO:HA	1.12	1.08
1:C:132:ARG:O	1:C:133:GLU:HB2	1.43	1.08
1:E:132:ARG:O	1:E:133:GLU:HB2	1.47	1.07
1:F:132:ARG:O	1:F:133:GLU:HB2	1.50	1.07
1:F:227:VAL:O	1:F:231:THR:HG22	1.56	1.06
1:C:94:ASP:HB3	2:H:591:LYS:NZ	1.69	1.06
1:E:63:GLU:H	1:E:64:PRO:HA	1.13	1.06
1:D:132:ARG:HD2	1:D:139:LEU:HG	1.35	1.05
1:F:188:THR:OG1	1:F:194:ASP:OD1	1.74	1.05

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:63:GLU:N	1:D:64:PRO:HA	1.71	1.05
1:B:227:VAL:O	1:B:231:THR:HG22	1.56	1.05
1:A:227:VAL:O	1:A:231:THR:HG22	1.52	1.05
1:D:132:ARG:O	1:D:133:GLU:HB2	1.50	1.04
1:A:63:GLU:H	1:A:64:PRO:HA	1.18	1.04
1:F:63:GLU:H	1:F:64:PRO:HA	1.17	1.03
1:A:104:TYR:HE2	1:B:63:GLU:HB2	1.17	1.03
1:C:104:TYR:CE2	1:D:63:GLU:HB2	1.93	1.02
1:B:132:ARG:HD2	1:B:139:LEU:HG	1.41	1.02
1:C:133:GLU:N	1:C:134:ASP:HB2	1.74	1.02
2:H:475:ARG:HH12	2:H:505:TYR:HB2	1.23	1.02
1:B:63:GLU:N	1:B:64:PRO:HA	1.71	1.01
1:D:101:ASN:O	1:D:103:GLU:N	1.93	1.01
1:C:63:GLU:H	1:C:64:PRO:HA	1.23	1.01
1:D:61:ARG:HB2	1:D:62:GLY:HA3	1.43	1.00
1:C:94:ASP:HB3	2:H:591:LYS:HZ3	1.15	1.00
1:B:188:THR:OG1	1:B:194:ASP:OD1	1.80	0.99
1:E:104:TYR:CE2	1:F:63:GLU:HB2	1.96	0.99
1:C:104:TYR:HE2	1:D:63:GLU:HB2	1.23	0.99
1:E:257:ASN:C	1:E:435:TYR:CE2	2.35	0.99
1:B:63:GLU:H	1:B:64:PRO:CA	1.77	0.98
1:A:104:TYR:CE2	1:B:63:GLU:HB2	1.99	0.98
1:A:188:THR:OG1	1:A:194:ASP:OD1	1.83	0.96
1:D:227:VAL:O	1:D:231:THR:HG22	1.62	0.96
1:E:133:GLU:N	1:E:134:ASP:HB2	1.80	0.96
1:C:257:ASN:C	1:C:435:TYR:CE2	2.39	0.96
1:B:133:GLU:N	1:B:134:ASP:HB2	1.80	0.95
1:C:61:ARG:HB2	1:C:62:GLY:HA3	1.45	0.95
1:D:257:ASN:C	1:D:435:TYR:CE2	2.40	0.95
1:B:104:TYR:OH	2:G:537:ALA:HB2	1.67	0.94
1:D:63:GLU:H	1:D:64:PRO:CA	1.82	0.93
1:B:62:GLY:HA2	1:B:63:GLU:HB3	1.50	0.93
1:F:63:GLU:N	1:F:64:PRO:HA	1.82	0.93
1:A:61:ARG:HB2	1:A:62:GLY:HA3	1.49	0.93
1:A:257:ASN:C	1:A:435:TYR:CE2	2.43	0.93
1:E:227:VAL:O	1:E:231:THR:HG22	1.68	0.92
1:B:257:ASN:C	1:B:435:TYR:CE2	2.43	0.92
1:C:231:THR:HG23	1:C:232:ASN:H	1.33	0.92
1:E:63:GLU:N	1:E:64:PRO:HA	1.83	0.92
1:C:132:ARG:HD2	1:C:139:LEU:HG	1.52	0.92
1:E:322:LEU:O	1:E:325:ILE:HG22	1.70	0.92
1:B:101:ASN:O	1:B:103:GLU:N	2.02	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:61:ARG:HB2	1:F:62:GLY:HA3	1.53	0.90
1:B:66:ASP:H	1:B:69:THR:HG22	1.35	0.90
1:C:322:LEU:O	1:C:325:ILE:HG22	1.70	0.90
2:H:475:ARG:HH12	2:H:505:TYR:CB	1.84	0.89
1:F:363:LEU:HD23	1:F:380:ILE:HG23	1.51	0.89
1:A:104:TYR:HH	1:B:69:THR:HG1	1.17	0.89
1:E:61:ARG:HB2	1:E:62:GLY:HA3	1.54	0.89
1:D:322:LEU:O	1:D:325:ILE:HG22	1.73	0.89
1:E:63:GLU:H	1:E:64:PRO:CA	1.86	0.89
1:A:322:LEU:O	1:A:325:ILE:HG22	1.73	0.89
1:F:132:ARG:HD2	1:F:139:LEU:HG	1.54	0.88
1:E:257:ASN:C	1:E:435:TYR:HE2	1.77	0.88
1:E:94:ASP:HB3	2:I:591:LYS:NZ	1.88	0.88
1:F:322:LEU:O	1:F:325:ILE:HG22	1.72	0.88
1:B:322:LEU:O	1:B:325:ILE:HG22	1.72	0.87
1:F:63:GLU:H	1:F:64:PRO:CA	1.87	0.87
2:G:475:ARG:NH1	2:G:505:TYR:HB2	1.89	0.87
1:E:93:ALA:HB1	2:I:588:ILE:HD11	1.56	0.87
1:C:302:ARG:HG2	1:C:306:ARG:HH12	1.40	0.87
1:D:66:ASP:H	1:D:69:THR:CG2	1.88	0.87
1:A:63:GLU:H	1:A:64:PRO:CA	1.88	0.86
1:F:101:ASN:O	1:F:103:GLU:N	2.08	0.86
1:F:67:LEU:O	1:F:71:THR:HG23	1.75	0.86
1:B:363:LEU:HD23	1:B:380:ILE:HG23	1.56	0.86
2:H:484:ARG:HH22	2:H:546:GLU:HG2	1.39	0.86
1:A:101:ASN:O	1:A:103:GLU:N	2.10	0.85
1:E:231:THR:HG23	1:E:232:ASN:H	1.40	0.84
1:F:133:GLU:N	1:F:134:ASP:HB2	1.91	0.84
1:A:63:GLU:N	1:A:64:PRO:HA	1.89	0.84
2:H:475:ARG:HH11	2:H:475:ARG:HG3	1.41	0.84
1:D:133:GLU:N	1:D:134:ASP:HB2	1.93	0.83
2:G:456:LEU:O	2:G:457:LEU:HB2	1.78	0.83
1:C:93:ALA:HB1	2:H:588:ILE:HD11	1.61	0.83
2:I:475:ARG:NH1	2:I:505:TYR:HB2	1.94	0.83
1:E:83:ILE:HG22	1:E:84:GLY:H	1.42	0.83
1:D:231:THR:HG23	1:D:232:ASN:H	1.43	0.83
1:E:101:ASN:O	1:E:103:GLU:N	2.11	0.82
1:D:255:GLU:C	1:D:257:ASN:H	1.81	0.82
1:E:132:ARG:HD2	1:E:139:LEU:HG	1.62	0.82
1:D:66:ASP:H	1:D:69:THR:HG22	1.44	0.81
1:F:66:ASP:H	1:F:69:THR:HG22	1.44	0.81
1:C:63:GLU:N	1:C:64:PRO:HA	1.96	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:LEU:O	1:A:71:THR:HG23	1.81	0.81
1:B:66:ASP:H	1:B:69:THR:CG2	1.93	0.80
1:B:62:GLY:HA2	1:B:63:GLU:CB	2.07	0.80
1:C:187:PRO:O	1:C:189:GLY:N	2.14	0.80
1:A:61:ARG:CB	1:A:62:GLY:HA3	2.12	0.80
1:B:227:VAL:O	1:B:231:THR:CG2	2.31	0.79
1:F:66:ASP:H	1:F:69:THR:CG2	1.95	0.79
1:B:257:ASN:C	1:B:435:TYR:HE2	1.86	0.79
1:B:231:THR:O	1:B:232:ASN:HB2	1.81	0.79
1:E:258:ILE:O	1:E:259:ASN:HB3	1.81	0.79
1:B:135:GLU:O	1:B:137:ASP:N	2.13	0.79
2:G:475:ARG:HG3	2:G:475:ARG:HH11	1.47	0.79
1:A:133:GLU:N	1:A:134:ASP:HB2	1.97	0.79
1:C:63:GLU:H	1:C:64:PRO:CA	1.95	0.79
1:A:197:THR:HB	1:A:199:GLY:O	1.81	0.79
1:A:94:ASP:HB3	2:G:591:LYS:NZ	1.98	0.78
1:A:231:THR:HG23	1:A:232:ASN:H	1.49	0.78
1:C:67:LEU:O	1:C:71:THR:HG23	1.83	0.78
1:C:74:LEU:HD22	1:C:83:ILE:HD11	1.65	0.78
1:F:148:MET:HA	1:F:148:MET:CE	2.13	0.78
1:A:66:ASP:H	1:A:69:THR:HG22	1.48	0.78
1:D:61:ARG:CB	1:D:62:GLY:HA3	2.07	0.77
1:B:61:ARG:HB2	1:B:62:GLY:HA3	1.66	0.77
1:F:62:GLY:HA2	1:F:63:GLU:HB3	1.65	0.77
1:C:51:ILE:HD11	1:C:83:ILE:HG21	1.66	0.77
1:B:132:ARG:O	1:B:133:GLU:CB	2.30	0.77
1:E:74:LEU:HD22	1:E:83:ILE:HD11	1.66	0.77
1:A:363:LEU:HD23	1:A:380:ILE:HG23	1.67	0.76
1:A:62:GLY:HA2	1:A:63:GLU:HB3	1.67	0.76
1:C:315:GLY:O	1:C:356:PRO:HD2	1.85	0.76
1:C:61:ARG:CB	1:C:62:GLY:HA3	2.15	0.76
1:F:71:THR:HG22	1:F:89:LEU:HD12	1.68	0.76
1:E:62:GLY:HA2	1:E:63:GLU:HB3	1.66	0.75
1:A:222:ASN:N	1:A:222:ASN:HD22	1.85	0.75
1:D:363:LEU:HD23	1:D:380:ILE:HG23	1.65	0.75
1:C:306:ARG:NH2	1:D:32:VAL:HG21	2.00	0.75
1:E:257:ASN:O	1:E:435:TYR:HE2	1.69	0.75
1:C:101:ASN:O	1:C:103:GLU:N	2.19	0.75
1:A:93:ALA:HB1	2:G:588:ILE:HD11	1.67	0.75
1:C:104:TYR:HH	1:D:69:THR:HG1	0.97	0.75
1:C:66:ASP:H	1:C:69:THR:HG22	1.50	0.75
1:B:187:PRO:O	1:B:189:GLY:N	2.19	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:30:ALA:O	1:B:33:PRO:HD2	1.87	0.74
1:F:132:ARG:O	1:F:133:GLU:CB	2.35	0.74
1:E:363:LEU:HD23	1:E:380:ILE:HG23	1.70	0.74
2:G:475:ARG:HH12	2:G:505:TYR:CB	2.00	0.73
1:F:135:GLU:O	1:F:137:ASP:N	2.21	0.73
1:D:218:ALA:O	1:D:222:ASN:ND2	2.21	0.73
1:A:218:ALA:O	1:A:222:ASN:ND2	2.21	0.73
1:C:104:TYR:H	1:C:107:ARG:H	1.36	0.73
1:E:104:TYR:HH	1:F:69:THR:HG1	0.83	0.73
1:B:74:LEU:HD22	1:B:83:ILE:HD11	1.71	0.73
1:C:307:ARG:CZ	1:D:36:GLU:OE2	2.36	0.73
1:E:66:ASP:H	1:E:69:THR:HG22	1.53	0.73
1:E:67:LEU:O	1:E:71:THR:HG23	1.88	0.73
1:E:132:ARG:O	1:E:133:GLU:CB	2.31	0.72
1:C:363:LEU:HD23	1:C:380:ILE:HG23	1.71	0.72
1:A:132:ARG:HD2	1:A:139:LEU:HG	1.70	0.72
1:A:104:TYR:H	1:A:107:ARG:H	1.38	0.72
1:C:258:ILE:O	1:C:259:ASN:HB3	1.90	0.72
1:E:388:GLN:H	1:E:388:GLN:HE21	1.36	0.72
1:D:135:GLU:O	1:D:137:ASP:N	2.15	0.72
1:A:132:ARG:O	1:A:133:GLU:CB	2.27	0.72
1:E:94:ASP:HB3	2:I:591:LYS:HZ3	1.54	0.72
1:A:26:LEU:HD22	2:G:592:LYS:HE3	1.72	0.72
1:D:257:ASN:O	1:D:435:TYR:CE2	2.42	0.71
1:F:62:GLY:HA2	1:F:63:GLU:CB	2.19	0.71
1:A:94:ASP:HB3	2:G:591:LYS:HZ3	1.54	0.71
1:F:231:THR:HG23	1:F:232:ASN:H	1.55	0.71
1:D:104:TYR:OH	2:H:537:ALA:HB2	1.90	0.71
1:F:74:LEU:HD22	1:F:83:ILE:HD11	1.73	0.71
1:A:268:LEU:HB3	1:A:272:ASP:HB2	1.73	0.71
1:A:74:LEU:HD22	1:A:83:ILE:HD11	1.72	0.71
1:C:132:ARG:O	1:C:133:GLU:CB	2.30	0.70
1:B:218:ALA:O	1:B:222:ASN:ND2	2.24	0.70
1:D:187:PRO:O	1:D:189:GLY:N	2.24	0.70
1:A:255:GLU:C	1:A:257:ASN:N	2.44	0.70
1:D:62:GLY:HA2	1:D:63:GLU:HB3	1.71	0.70
1:E:197:THR:HB	1:E:199:GLY:O	1.91	0.70
1:A:114:VAL:HG11	1:D:140:LEU:HD11	1.72	0.70
2:H:484:ARG:NH2	2:H:546:GLU:HG2	2.06	0.70
1:C:187:PRO:C	1:C:189:GLY:H	1.95	0.70
1:B:257:ASN:O	1:B:435:TYR:HE2	1.74	0.70
1:B:339:VAL:HG13	1:B:384:GLY:HA3	1.73	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:231:THR:O	1:A:232:ASN:HB2	1.90	0.70
2:H:475:ARG:NH1	2:H:505:TYR:CB	2.47	0.70
1:C:257:ASN:C	1:C:435:TYR:HE2	1.90	0.70
2:G:475:ARG:NH1	2:G:505:TYR:CB	2.54	0.70
1:F:227:VAL:O	1:F:231:THR:CG2	2.39	0.69
1:C:257:ASN:O	1:C:435:TYR:CE2	2.44	0.69
2:I:475:ARG:HG2	2:I:511:ALA:CB	2.22	0.69
1:B:47:ALA:HB1	1:B:83:ILE:HG23	1.74	0.69
1:A:187:PRO:O	1:A:189:GLY:N	2.24	0.69
1:A:192:GLU:HA	1:A:195:ARG:HG3	1.73	0.69
2:G:487:GLY:HA3	2:G:489:PHE:H	1.57	0.69
1:B:258:ILE:O	1:B:259:ASN:HB3	1.92	0.69
1:C:306:ARG:NH1	1:D:32:VAL:HG21	2.08	0.69
1:A:258:ILE:O	1:A:259:ASN:HB3	1.93	0.69
2:H:510:GLU:O	2:H:511:ALA:HB2	1.92	0.68
1:A:62:GLY:CA	1:A:63:GLU:HB3	2.23	0.68
1:B:148:MET:CE	1:B:148:MET:HA	2.24	0.68
1:F:104:TYR:OH	2:I:537:ALA:HB2	1.93	0.68
1:E:227:VAL:O	1:E:231:THR:CG2	2.41	0.68
1:D:51:ILE:HD11	1:D:83:ILE:HG21	1.76	0.68
1:D:388:GLN:HE21	1:D:388:GLN:H	1.40	0.68
1:F:132:ARG:C	1:F:134:ASP:HB2	2.14	0.68
1:C:83:ILE:HG22	1:C:84:GLY:H	1.58	0.68
1:A:210:ALA:HB2	1:A:396:LEU:HB2	1.76	0.68
1:E:218:ALA:O	1:E:222:ASN:ND2	2.27	0.68
1:E:268:LEU:HB3	1:E:272:ASP:HB2	1.76	0.68
1:E:257:ASN:O	1:E:435:TYR:CE2	2.44	0.67
1:E:94:ASP:HB3	2:I:591:LYS:HZ2	1.57	0.67
1:A:257:ASN:C	1:A:435:TYR:HE2	1.94	0.67
1:A:299:SER:HB3	1:B:36:GLU:HB3	1.75	0.67
1:A:432:ILE:O	1:A:433:LYS:HB2	1.94	0.67
2:G:491:ILE:HB	2:G:494:HIS:HD2	1.59	0.67
1:F:233:GLU:HG2	1:F:315:GLY:HA3	1.76	0.67
2:H:491:ILE:HB	2:H:494:HIS:HD2	1.60	0.67
1:E:105:TYR:HE2	1:F:68:VAL:HG12	1.59	0.67
1:A:197:THR:CB	1:A:199:GLY:O	2.41	0.67
1:F:148:MET:HA	1:F:148:MET:HE3	1.75	0.67
2:H:583:ILE:O	2:H:587:MSE:HG3	1.94	0.67
1:E:257:ASN:HA	1:E:435:TYR:CD2	2.29	0.67
1:A:388:GLN:HE21	1:A:388:GLN:H	1.43	0.67
1:E:192:GLU:HA	1:E:195:ARG:HG3	1.77	0.67
1:D:258:ILE:O	1:D:259:ASN:HB3	1.95	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:231:THR:O	1:D:232:ASN:HB2	1.95	0.66
1:C:257:ASN:O	1:C:435:TYR:HE2	1.76	0.66
1:E:231:THR:O	1:E:232:ASN:HB2	1.94	0.66
2:H:487:GLY:HA3	2:H:489:PHE:H	1.61	0.66
1:E:105:TYR:OH	1:F:68:VAL:HB	1.95	0.66
1:C:62:GLY:HA2	1:C:63:GLU:HB3	1.75	0.66
1:B:262:ASN:OD1	1:B:263:LEU:N	2.29	0.66
1:D:62:GLY:HA2	1:D:63:GLU:CB	2.24	0.66
1:E:432:ILE:O	1:E:433:LYS:HB2	1.96	0.66
1:E:83:ILE:HG22	1:E:84:GLY:N	2.10	0.66
1:A:47:ALA:HB1	1:A:83:ILE:HG23	1.76	0.66
1:B:222:ASN:N	1:B:222:ASN:HD22	1.93	0.66
1:D:262:ASN:HB3	1:D:265:THR:HG22	1.78	0.66
1:A:257:ASN:O	1:A:435:TYR:CE2	2.49	0.66
1:C:194:ASP:O	1:C:198:SER:N	2.29	0.66
1:B:231:THR:HG23	1:B:232:ASN:H	1.61	0.66
1:C:222:ASN:HD22	1:C:222:ASN:N	1.93	0.66
1:B:257:ASN:O	1:B:435:TYR:CE2	2.48	0.65
1:B:197:THR:HB	1:B:199:GLY:O	1.95	0.65
1:A:114:VAL:CG1	1:D:140:LEU:HD11	2.26	0.65
1:D:74:LEU:HD22	1:D:83:ILE:HD11	1.78	0.65
2:H:491:ILE:HB	2:H:494:HIS:CD2	2.32	0.65
1:C:388:GLN:H	1:C:388:GLN:HE21	1.44	0.65
1:D:141:ASP:OD2	1:D:297:ARG:HD3	1.95	0.65
2:I:484:ARG:HH22	2:I:546:GLU:HG2	1.60	0.65
1:E:187:PRO:O	1:E:189:GLY:N	2.28	0.65
1:F:374:ARG:HB3	1:F:375:PRO:HA	1.77	0.65
1:C:432:ILE:O	1:C:433:LYS:HB2	1.97	0.65
2:G:475:ARG:HG2	2:G:511:ALA:CB	2.26	0.65
1:C:19:ALA:HA	1:C:96:VAL:HG21	1.79	0.64
1:F:339:VAL:HG13	1:F:384:GLY:HA3	1.79	0.64
1:A:227:VAL:O	1:A:231:THR:CG2	2.38	0.64
1:B:432:ILE:O	1:B:433:LYS:HB2	1.97	0.64
1:D:257:ASN:O	1:D:435:TYR:HE2	1.79	0.64
1:D:71:THR:HG22	1:D:89:LEU:HD12	1.79	0.64
1:A:138:VAL:O	1:A:142:GLU:HG2	1.98	0.64
2:H:510:GLU:O	2:H:511:ALA:CB	2.44	0.64
1:F:262:ASN:HB3	1:F:265:THR:HG22	1.80	0.64
1:F:66:ASP:O	1:F:69:THR:HG22	1.98	0.64
1:A:66:ASP:H	1:A:69:THR:CG2	2.11	0.64
2:I:538:ASP:O	2:I:539:ASP:HB2	1.98	0.64
1:B:388:GLN:HE21	1:B:388:GLN:H	1.46	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:197:THR:HB	1:D:199:GLY:O	1.97	0.63
1:D:30:ALA:O	1:D:33:PRO:HD2	1.99	0.63
2:G:486:GLY:H	2:G:488:ARG:HB2	1.64	0.63
1:F:28:PRO:C	1:F:30:ALA:H	2.01	0.63
1:C:94:ASP:HB3	2:H:591:LYS:HZ2	1.63	0.63
2:I:456:LEU:O	2:I:457:LEU:HB2	1.98	0.63
1:A:97:PRO:HG2	1:A:98:THR:HG22	1.80	0.63
1:F:388:GLN:H	1:F:388:GLN:HE21	1.45	0.63
1:E:273:TRP:C	1:E:275:LYS:H	2.03	0.63
1:D:222:ASN:N	1:D:222:ASN:HD22	1.96	0.63
1:F:63:GLU:N	1:F:64:PRO:CA	2.55	0.62
1:C:431:PHE:CE2	1:C:433:LYS:HG3	2.33	0.62
1:F:262:ASN:OD1	1:F:263:LEU:N	2.31	0.62
1:C:26:LEU:HD22	2:H:592:LYS:HE3	1.81	0.62
1:E:222:ASN:N	1:E:222:ASN:HD22	1.97	0.62
2:G:491:ILE:HB	2:G:494:HIS:CD2	2.34	0.62
1:E:280:MET:O	1:E:284:SER:HB2	1.99	0.62
2:H:562:LYS:HA	2:H:565:GLU:HB3	1.81	0.62
1:C:66:ASP:H	1:C:69:THR:CG2	2.12	0.62
1:A:296:ILE:O	1:A:325:ILE:HG13	1.98	0.62
1:C:197:THR:HB	1:C:199:GLY:O	1.98	0.62
2:H:456:LEU:O	2:H:457:LEU:HB2	2.00	0.62
1:F:228:ALA:HB1	1:F:286:ALA:HB1	1.82	0.62
1:D:432:ILE:O	1:D:433:LYS:HB2	1.99	0.62
2:I:475:ARG:HG2	2:I:511:ALA:HB1	1.80	0.62
1:D:104:TYR:HA	1:D:106:ALA:H	1.65	0.62
1:F:210:ALA:HB2	1:F:396:LEU:HB2	1.81	0.62
1:F:231:THR:O	1:F:232:ASN:HB2	1.99	0.62
1:C:257:ASN:C	1:C:435:TYR:CD2	2.73	0.62
2:G:464:GLU:HG3	2:G:489:PHE:CD1	2.35	0.62
1:C:148:MET:HA	1:C:148:MET:CE	2.30	0.62
1:C:105:TYR:OH	1:D:68:VAL:HB	2.00	0.62
2:G:464:GLU:HG3	2:G:489:PHE:HD1	1.64	0.62
1:C:268:LEU:HB3	1:C:272:ASP:HB2	1.81	0.62
1:A:257:ASN:O	1:A:435:TYR:HE2	1.82	0.61
1:A:104:TYR:HA	1:A:106:ALA:N	2.14	0.61
2:I:560:MSE:O	2:I:562:LYS:N	2.32	0.61
2:I:464:GLU:HG3	2:I:489:PHE:HD1	1.65	0.61
1:B:132:ARG:C	1:B:134:ASP:HB2	2.20	0.61
1:A:208:VAL:HG22	1:A:394:ALA:HB3	1.81	0.61
1:F:258:ILE:O	1:F:259:ASN:CB	2.48	0.61
1:E:61:ARG:CB	1:E:62:GLY:HA3	2.26	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:187:PRO:C	1:D:189:GLY:H	2.04	0.61
1:A:187:PRO:C	1:A:189:GLY:H	2.04	0.61
1:D:208:VAL:HB	1:D:360:LEU:HD23	1.81	0.61
2:G:510:GLU:O	2:G:511:ALA:CB	2.49	0.61
2:I:519:ARG:H	2:I:520:ILE:HB	1.65	0.61
1:C:105:TYR:HE2	1:D:68:VAL:HG12	1.65	0.61
1:B:63:GLU:N	1:B:64:PRO:CA	2.48	0.61
1:D:63:GLU:N	1:D:64:PRO:CA	2.45	0.61
1:C:231:THR:O	1:C:232:ASN:HB2	2.01	0.60
1:E:197:THR:CB	1:E:199:GLY:O	2.49	0.60
1:C:105:TYR:CE2	1:D:68:VAL:HG12	2.36	0.60
1:A:188:THR:HG22	1:A:200:PHE:CE2	2.37	0.60
1:A:93:ALA:HB1	2:G:588:ILE:CD1	2.30	0.60
1:C:431:PHE:HE2	1:C:433:LYS:HG3	1.65	0.60
1:A:53:HIS:CE1	1:A:57:ARG:NH1	2.69	0.60
2:H:475:ARG:NH1	2:H:475:ARG:HG3	2.15	0.60
1:D:391:ASP:OD1	1:D:391:ASP:N	2.33	0.60
1:D:339:VAL:HG13	1:D:384:GLY:HA3	1.82	0.60
1:D:257:ASN:C	1:D:435:TYR:HE2	1.98	0.60
1:D:75:ALA:HB2	1:D:80:LEU:HD12	1.82	0.60
1:D:132:ARG:O	1:D:133:GLU:CB	2.34	0.60
1:A:104:TYR:HA	1:A:106:ALA:H	1.67	0.60
2:I:463:ALA:O	2:I:467:LEU:HB2	2.01	0.60
2:G:562:LYS:HA	2:G:565:GLU:HB3	1.83	0.60
1:E:187:PRO:C	1:E:189:GLY:H	2.05	0.60
1:C:64:PRO:O	1:C:69:THR:HG21	2.01	0.59
2:I:562:LYS:HA	2:I:565:GLU:HB3	1.83	0.59
1:C:28:PRO:C	1:C:30:ALA:H	2.05	0.59
1:D:257:ASN:C	1:D:435:TYR:CD2	2.75	0.59
1:E:93:ALA:HB1	2:I:588:ILE:CD1	2.29	0.59
1:B:392:ILE:HA	1:B:418:LYS:O	2.01	0.59
1:E:257:ASN:C	1:E:435:TYR:CD2	2.75	0.59
1:A:273:TRP:C	1:A:275:LYS:H	2.04	0.59
1:B:374:ARG:HB3	1:B:375:PRO:HA	1.83	0.59
1:E:47:ALA:HB1	1:E:83:ILE:HG23	1.84	0.59
1:A:93:ALA:CB	2:G:588:ILE:HD11	2.31	0.59
1:C:296:ILE:O	1:C:325:ILE:HG13	2.02	0.59
2:G:583:ILE:O	2:G:587:MSE:HG3	2.02	0.59
2:H:486:GLY:H	2:H:488:ARG:HB2	1.67	0.59
1:C:50:LYS:NZ	1:C:82:GLU:OE2	2.35	0.59
1:A:262:ASN:HB3	1:A:265:THR:HG22	1.85	0.59
1:A:83:ILE:HG22	1:A:84:GLY:H	1.68	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:464:GLU:HG3	2:I:489:PHE:CD1	2.38	0.59
1:B:67:LEU:O	1:B:71:THR:HG23	2.02	0.59
2:G:475:ARG:HG2	2:G:511:ALA:HB2	1.84	0.59
2:I:510:GLU:O	2:I:511:ALA:CB	2.49	0.59
2:I:487:GLY:HA3	2:I:489:PHE:H	1.67	0.59
1:D:32:VAL:O	1:D:36:GLU:HG3	2.03	0.59
1:B:133:GLU:HG2	1:E:115:LEU:CD1	2.33	0.59
1:E:93:ALA:CB	2:I:588:ILE:HD11	2.30	0.59
1:A:257:ASN:HA	1:A:435:TYR:CD2	2.38	0.58
1:A:105:TYR:CE2	1:B:68:VAL:HG12	2.38	0.58
1:E:64:PRO:O	1:E:69:THR:HG21	2.02	0.58
1:A:199:GLY:HA3	1:A:200:PHE:O	2.03	0.58
1:D:227:VAL:O	1:D:231:THR:CG2	2.44	0.58
1:E:138:VAL:O	1:E:142:GLU:HG2	2.03	0.58
1:C:93:ALA:CB	2:H:588:ILE:HD11	2.31	0.58
2:G:471:MSE:HB2	2:G:478:ALA:HB2	1.85	0.58
2:H:485:ILE:HG22	2:H:487:GLY:HA2	1.86	0.58
1:E:104:TYR:HB3	1:E:105:TYR:HB2	1.84	0.58
1:B:194:ASP:O	1:B:198:SER:N	2.31	0.58
1:D:249:MET:HA	1:D:252:LEU:HB2	1.86	0.58
1:B:66:ASP:O	1:B:69:THR:HG22	2.04	0.58
1:F:187:PRO:O	1:F:189:GLY:N	2.37	0.58
2:G:465:ARG:HG3	2:G:531:LEU:HD21	1.85	0.58
1:E:26:LEU:HD22	2:I:592:LYS:HE3	1.85	0.58
1:B:104:TYR:HA	1:B:105:TYR:HB2	1.86	0.58
1:F:74:LEU:HD13	1:F:83:ILE:CD1	2.34	0.58
1:C:207:ILE:HD13	1:C:386:ILE:HG21	1.85	0.58
1:C:188:THR:HG22	1:C:200:PHE:CE2	2.39	0.57
1:B:187:PRO:C	1:B:189:GLY:H	2.06	0.57
1:B:273:TRP:C	1:B:275:LYS:H	2.07	0.57
2:G:504:PHE:O	2:G:507:GLU:HB3	2.05	0.57
1:D:67:LEU:O	1:D:71:THR:HG23	2.04	0.57
1:F:61:ARG:CB	1:F:62:GLY:HA3	2.23	0.57
1:B:88:TYR:O	1:B:92:LEU:HG	2.04	0.57
1:A:202:ARG:O	1:A:203:SER:HB2	2.03	0.57
1:C:208:VAL:HG22	1:C:394:ALA:HB3	1.87	0.57
1:A:322:LEU:HB3	1:A:323:GLN:NE2	2.19	0.57
1:C:47:ALA:HB1	1:C:83:ILE:HG23	1.86	0.57
1:E:105:TYR:CE2	1:F:68:VAL:HG12	2.39	0.57
1:B:225:GLN:NE2	1:B:251:MET:HB2	2.19	0.57
1:F:391:ASP:N	1:F:391:ASP:OD1	2.38	0.57
2:I:510:GLU:O	2:I:511:ALA:HB2	2.03	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:268:LEU:HB3	1:F:272:ASP:HB2	1.85	0.57
1:B:207:ILE:HD13	1:B:386:ILE:HG21	1.87	0.57
1:E:257:ASN:CA	1:E:435:TYR:CD2	2.87	0.57
2:G:538:ASP:O	2:G:539:ASP:HB2	2.05	0.57
1:C:104:TYR:HA	1:C:106:ALA:N	2.20	0.57
1:E:148:MET:HA	1:E:148:MET:CE	2.34	0.57
1:E:28:PRO:C	1:E:30:ALA:H	2.07	0.56
1:B:51:ILE:HD11	1:B:83:ILE:HG21	1.86	0.56
1:B:262:ASN:HB3	1:B:265:THR:HG22	1.88	0.56
1:A:374:ARG:HB3	1:A:375:PRO:HA	1.86	0.56
1:D:273:TRP:C	1:D:275:LYS:H	2.08	0.56
1:C:138:VAL:O	1:C:142:GLU:HG2	2.05	0.56
2:I:475:ARG:HH12	2:I:505:TYR:CB	2.19	0.56
1:F:196:MET:O	1:F:419:GLN:NE2	2.34	0.56
1:D:148:MET:CE	1:D:148:MET:HA	2.35	0.56
1:A:135:GLU:O	1:A:137:ASP:N	2.33	0.56
2:H:504:PHE:O	2:H:507:GLU:HB3	2.06	0.56
1:C:132:ARG:C	1:C:134:ASP:HB2	2.25	0.56
2:I:475:ARG:NH1	2:I:505:TYR:CB	2.67	0.56
1:C:71:THR:HG22	1:C:89:LEU:CD1	2.36	0.56
1:B:148:MET:HE2	1:B:148:MET:HA	1.86	0.56
1:B:71:THR:HG22	1:B:89:LEU:HD12	1.88	0.56
1:E:296:ILE:O	1:E:325:ILE:HG13	2.05	0.56
1:D:296:ILE:O	1:D:325:ILE:HG13	2.05	0.56
1:F:258:ILE:O	1:F:259:ASN:HB3	2.06	0.56
1:D:53:HIS:CE1	1:D:57:ARG:HD2	2.40	0.56
1:B:71:THR:HG22	1:B:89:LEU:CD1	2.36	0.56
1:D:381:ARG:HD3	1:D:387:GLU:HB2	1.85	0.56
1:B:257:ASN:C	1:B:435:TYR:CD2	2.79	0.56
1:E:66:ASP:H	1:E:69:THR:CG2	2.16	0.56
1:C:62:GLY:CA	1:C:63:GLU:HB3	2.35	0.56
1:F:83:ILE:HG22	1:F:84:GLY:H	1.71	0.55
1:A:302:ARG:HD2	1:B:36:GLU:OE2	2.05	0.55
1:C:262:ASN:OD1	1:C:263:LEU:N	2.39	0.55
1:E:202:ARG:O	1:E:203:SER:HB2	2.06	0.55
2:H:475:ARG:HG2	2:H:511:ALA:CB	2.35	0.55
1:E:105:TYR:CE2	1:F:68:VAL:CG1	2.90	0.55
1:C:227:VAL:O	1:C:231:THR:CG2	2.39	0.55
1:F:79:GLN:O	1:F:83:ILE:HG13	2.07	0.55
1:A:257:ASN:C	1:A:435:TYR:CD2	2.80	0.55
1:E:194:ASP:O	1:E:198:SER:N	2.29	0.55
1:A:64:PRO:O	1:A:69:THR:HG21	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:53:HIS:CE1	1:A:57:ARG:HH11	2.25	0.55
1:C:262:ASN:HB3	1:C:265:THR:HG22	1.89	0.55
1:F:207:ILE:HD11	1:F:361:SER:HB2	1.89	0.55
1:D:40:PRO:O	1:D:49:GLN:HG3	2.05	0.55
2:G:510:GLU:O	2:G:511:ALA:HB2	2.07	0.55
1:A:67:LEU:CD1	2:G:584:ALA:HB3	2.36	0.55
1:D:262:ASN:OD1	1:D:263:LEU:N	2.38	0.55
2:H:519:ARG:H	2:H:520:ILE:HB	1.71	0.55
1:E:53:HIS:CE1	1:E:57:ARG:HD2	2.42	0.55
1:A:207:ILE:HD13	1:A:386:ILE:HG21	1.89	0.55
2:I:583:ILE:O	2:I:587:MSE:HG3	2.06	0.55
1:D:52:PHE:CD1	1:D:55:MET:HE2	2.42	0.55
1:C:93:ALA:HB1	2:H:588:ILE:CD1	2.35	0.54
1:F:148:MET:HE2	1:F:148:MET:HA	1.89	0.54
2:H:538:ASP:O	2:H:539:ASP:HB2	2.07	0.54
1:E:262:ASN:OD1	1:E:263:LEU:N	2.40	0.54
1:B:257:ASN:HA	1:B:435:TYR:CD2	2.41	0.54
1:C:83:ILE:HG22	1:C:84:GLY:N	2.22	0.54
1:D:200:PHE:CD1	1:D:206:ILE:HD13	2.42	0.54
1:A:315:GLY:O	1:A:356:PRO:HD2	2.07	0.54
1:B:62:GLY:CA	1:B:63:GLU:CB	2.83	0.54
1:D:61:ARG:CB	1:D:62:GLY:CA	2.82	0.54
1:C:210:ALA:HB2	1:C:396:LEU:HB2	1.87	0.54
1:B:210:ALA:HB2	1:B:396:LEU:HB2	1.90	0.54
1:B:197:THR:CB	1:B:199:GLY:O	2.55	0.54
1:A:262:ASN:OD1	1:A:263:LEU:N	2.40	0.54
1:E:262:ASN:HB3	1:E:265:THR:HG22	1.88	0.54
1:E:374:ARG:HB3	1:E:375:PRO:HA	1.89	0.54
1:F:202:ARG:O	1:F:203:SER:HB2	2.08	0.54
1:C:103:GLU:N	1:C:104:TYR:CB	2.71	0.54
1:E:258:ILE:O	1:E:259:ASN:CB	2.54	0.54
2:H:477:VAL:O	2:H:481:VAL:HG23	2.07	0.54
1:E:19:ALA:HA	1:E:96:VAL:HG21	1.90	0.54
1:C:257:ASN:HA	1:C:435:TYR:CD2	2.42	0.54
1:D:315:GLY:O	1:D:356:PRO:HD2	2.08	0.54
1:C:202:ARG:O	1:C:203:SER:HB2	2.07	0.54
1:D:194:ASP:O	1:D:198:SER:N	2.38	0.54
1:A:71:THR:HG22	1:A:89:LEU:HD12	1.90	0.54
2:I:538:ASP:O	2:I:539:ASP:CB	2.56	0.54
1:B:391:ASP:N	1:B:391:ASP:OD1	2.37	0.54
1:D:392:ILE:HA	1:D:418:LYS:O	2.08	0.54
1:D:64:PRO:O	1:D:69:THR:HG21	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:225:GLN:NE2	1:C:251:MET:HB2	2.23	0.54
2:H:471:MSE:HB2	2:H:478:ALA:HB2	1.90	0.53
1:A:222:ASN:HD22	1:A:222:ASN:H	1.56	0.53
1:C:306:ARG:NH2	1:C:352:GLU:OE1	2.41	0.53
1:D:32:VAL:HB	1:D:33:PRO:HD3	1.89	0.53
1:C:231:THR:HG23	1:C:232:ASN:N	2.13	0.53
1:D:132:ARG:C	1:D:134:ASP:HB2	2.28	0.53
1:E:51:ILE:HD11	1:E:83:ILE:HG21	1.89	0.53
1:A:105:TYR:HE2	1:B:68:VAL:HG12	1.71	0.53
1:F:185:GLY:O	1:F:186:ILE:HG13	2.09	0.53
1:D:141:ASP:C	1:D:143:ALA:H	2.12	0.53
2:I:560:MSE:O	2:I:563:VAL:N	2.36	0.53
2:H:475:ARG:HG2	2:H:511:ALA:HB1	1.90	0.53
1:D:231:THR:HG23	1:D:232:ASN:N	2.21	0.53
1:B:246:GLN:HE22	1:E:376:MET:CE	2.21	0.53
1:E:257:ASN:CA	1:E:435:TYR:CE2	2.92	0.53
1:F:322:LEU:HD12	1:F:359:ALA:HB1	1.91	0.53
2:I:475:ARG:HG2	2:I:511:ALA:HB2	1.90	0.53
2:G:560:MSE:O	2:G:562:LYS:N	2.42	0.53
1:E:40:PRO:O	1:E:49:GLN:HG3	2.08	0.53
1:E:62:GLY:CA	1:E:63:GLU:HB3	2.35	0.53
1:C:374:ARG:HB3	1:C:375:PRO:HA	1.91	0.53
1:E:210:ALA:HB2	1:E:396:LEU:HB2	1.91	0.53
1:F:208:VAL:HG22	1:F:394:ALA:HB3	1.90	0.53
1:B:268:LEU:HB3	1:B:272:ASP:HB2	1.91	0.53
1:B:83:ILE:HG22	1:B:84:GLY:H	1.74	0.52
1:E:207:ILE:HA	1:E:359:ALA:O	2.09	0.52
1:D:257:ASN:HA	1:D:435:TYR:CD2	2.45	0.52
1:A:105:TYR:OH	1:B:68:VAL:HB	2.09	0.52
1:F:71:THR:HG22	1:F:89:LEU:CD1	2.38	0.52
1:A:51:ILE:HD11	1:A:83:ILE:HG21	1.90	0.52
1:E:431:PHE:CE2	1:E:433:LYS:HG3	2.44	0.52
2:H:560:MSE:O	2:H:562:LYS:N	2.43	0.52
1:F:221:LEU:HD21	1:F:247:LEU:HD11	1.91	0.52
1:B:53:HIS:CE1	1:B:57:ARG:HD2	2.45	0.52
1:E:200:PHE:CD1	1:E:206:ILE:HD13	2.44	0.52
1:F:62:GLY:CA	1:F:63:GLU:CB	2.87	0.52
1:A:79:GLN:O	1:A:83:ILE:HG13	2.09	0.52
1:F:235:VAL:HG12	1:F:316:MET:HB2	1.91	0.52
1:E:88:TYR:O	1:E:92:LEU:HG	2.09	0.52
1:B:104:TYR:HH	2:G:537:ALA:HB2	1.70	0.52
1:C:84:GLY:HA3	1:C:88:TYR:HB2	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:202:ARG:O	1:A:203:SER:CB	2.58	0.52
1:B:185:GLY:O	1:B:186:ILE:HG13	2.09	0.52
1:A:19:ALA:HA	1:A:96:VAL:HG21	1.92	0.52
1:B:296:ILE:O	1:B:325:ILE:HG13	2.10	0.52
1:F:28:PRO:C	1:F:30:ALA:N	2.62	0.52
1:D:223:ILE:HG22	1:D:316:MET:HE1	1.91	0.52
1:C:97:PRO:HG2	1:C:98:THR:HG22	1.92	0.52
1:D:66:ASP:N	1:D:69:THR:HG22	2.21	0.52
2:I:475:ARG:HG3	2:I:475:ARG:HH11	1.75	0.52
1:D:432:ILE:HD12	1:D:437:LYS:HE3	1.92	0.52
1:E:231:THR:HG23	1:E:232:ASN:N	2.19	0.51
1:E:25:PHE:CZ	1:E:89:LEU:HD22	2.44	0.51
1:A:83:ILE:CG2	1:A:84:GLY:H	2.22	0.51
1:E:101:ASN:C	1:E:103:GLU:H	2.10	0.51
1:A:32:VAL:HB	1:A:33:PRO:HD3	1.91	0.51
1:A:141:ASP:C	1:A:143:ALA:H	2.14	0.51
1:B:105:TYR:O	1:B:109:VAL:HG23	2.09	0.51
1:A:339:VAL:HG13	1:A:384:GLY:HA3	1.92	0.51
1:E:206:ILE:HG23	1:E:392:ILE:HG12	1.92	0.51
1:F:432:ILE:O	1:F:433:LYS:HB2	2.10	0.51
1:A:103:GLU:N	1:A:104:TYR:CB	2.74	0.51
1:A:375:PRO:HG2	1:A:395:PHE:HB3	1.93	0.51
1:D:210:ALA:HB2	1:D:396:LEU:HB2	1.91	0.51
2:H:501:ILE:O	2:H:504:PHE:HB3	2.11	0.51
2:H:507:GLU:O	2:H:507:GLU:HG3	2.10	0.51
1:F:139:LEU:O	1:F:143:ALA:HB2	2.10	0.51
1:C:197:THR:CB	1:C:199:GLY:O	2.58	0.51
1:A:17:GLU:HB3	1:A:48:HIS:HD1	1.74	0.51
2:I:477:VAL:O	2:I:481:VAL:HG23	2.11	0.51
1:C:395:PHE:HB2	1:C:415:ILE:HB	1.93	0.51
1:C:105:TYR:CE2	1:D:68:VAL:CG1	2.94	0.51
1:C:187:PRO:C	1:C:189:GLY:N	2.62	0.51
1:A:268:LEU:HB3	1:A:272:ASP:CB	2.38	0.51
1:A:30:ALA:O	1:A:33:PRO:HD2	2.10	0.51
1:D:280:MET:O	1:D:284:SER:HB2	2.11	0.51
1:A:194:ASP:O	1:A:198:SER:N	2.39	0.51
2:G:475:ARG:HH12	2:G:505:TYR:HB3	1.74	0.51
1:D:197:THR:CB	1:D:199:GLY:O	2.58	0.51
2:G:519:ARG:H	2:G:520:ILE:HB	1.75	0.51
1:C:257:ASN:CA	1:C:435:TYR:CD2	2.94	0.51
2:G:538:ASP:O	2:G:539:ASP:CB	2.59	0.51
1:A:104:TYR:OH	1:B:69:THR:OG1	2.05	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:28:PRO:C	1:B:30:ALA:H	2.13	0.51
1:C:307:ARG:NH2	1:D:36:GLU:OE2	2.43	0.50
2:I:486:GLY:H	2:I:488:ARG:HB2	1.76	0.50
1:C:202:ARG:O	1:C:203:SER:CB	2.59	0.50
1:D:207:ILE:HD13	1:D:386:ILE:HG21	1.93	0.50
1:C:135:GLU:O	1:C:137:ASP:N	2.38	0.50
1:E:25:PHE:HZ	1:E:89:LEU:HD22	1.75	0.50
1:E:202:ARG:O	1:E:203:SER:CB	2.58	0.50
1:E:385:SER:OG	1:E:386:ILE:N	2.44	0.50
1:D:202:ARG:O	1:D:203:SER:CB	2.60	0.50
1:E:391:ASP:HB3	1:E:420:ARG:HD2	1.93	0.50
1:B:133:GLU:CA	1:B:134:ASP:HB2	2.41	0.50
1:A:28:PRO:C	1:A:30:ALA:H	2.14	0.50
1:F:197:THR:HB	1:F:199:GLY:O	2.10	0.50
1:A:258:ILE:O	1:A:259:ASN:CB	2.59	0.50
1:B:340:SER:CB	1:B:385:SER:HB3	2.41	0.50
1:F:75:ALA:HB2	1:F:80:LEU:HD12	1.93	0.50
1:D:66:ASP:O	1:D:69:THR:HG22	2.12	0.50
1:D:101:ASN:C	1:D:103:GLU:N	2.64	0.50
1:D:104:TYR:HA	1:D:106:ALA:N	2.25	0.50
2:H:487:GLY:CA	2:H:489:PHE:H	2.23	0.50
1:C:273:TRP:C	1:C:275:LYS:H	2.14	0.50
1:E:104:TYR:H	1:E:107:ARG:H	1.59	0.50
1:C:71:THR:HG22	1:C:89:LEU:HD12	1.92	0.50
1:C:192:GLU:HA	1:C:195:ARG:HG3	1.92	0.50
1:E:219:PHE:HB2	1:E:438:PHE:CE1	2.47	0.50
1:C:96:VAL:HG13	1:C:97:PRO:HD2	1.94	0.50
1:A:66:ASP:O	1:A:69:THR:HG22	2.12	0.50
1:A:222:ASN:ND2	1:A:222:ASN:N	2.57	0.50
2:H:470:HIS:HE1	2:H:537:ALA:O	1.95	0.50
2:G:485:ILE:HG22	2:G:487:GLY:HA2	1.94	0.50
2:G:467:LEU:O	2:G:471:MSE:HG2	2.11	0.50
1:B:25:PHE:HZ	1:B:89:LEU:HD22	1.77	0.49
1:D:139:LEU:O	1:D:143:ALA:HB2	2.12	0.49
1:B:315:GLY:O	1:B:356:PRO:HD2	2.10	0.49
1:A:257:ASN:CA	1:A:435:TYR:CD2	2.95	0.49
1:B:101:ASN:C	1:B:103:GLU:H	2.06	0.49
1:F:207:ILE:HD13	1:F:386:ILE:HG21	1.93	0.49
1:A:385:SER:OG	1:A:386:ILE:N	2.46	0.49
1:E:103:GLU:N	1:E:104:TYR:CB	2.76	0.49
2:H:464:GLU:HG3	2:H:489:PHE:HD1	1.77	0.49
1:B:208:VAL:HB	1:B:360:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:140:LEU:HD11	1:D:114:VAL:HG11	1.94	0.49
1:F:200:PHE:CD1	1:F:206:ILE:HD13	2.47	0.49
1:B:257:ASN:CA	1:B:435:TYR:CD2	2.96	0.49
1:F:84:GLY:HA3	1:F:88:TYR:HB2	1.95	0.49
1:D:25:PHE:HZ	1:D:89:LEU:HD22	1.77	0.49
1:F:138:VAL:O	1:F:142:GLU:HG2	2.12	0.49
2:I:471:MSE:HB2	2:I:478:ALA:HB2	1.95	0.49
1:D:268:LEU:HB3	1:D:272:ASP:HB2	1.93	0.49
2:G:475:ARG:HH21	2:G:501:ILE:HG22	1.77	0.49
1:D:71:THR:HG22	1:D:89:LEU:CD1	2.42	0.49
1:B:83:ILE:CG2	1:B:84:GLY:H	2.25	0.49
1:B:140:LEU:HD11	1:E:114:VAL:HG11	1.95	0.49
1:F:222:ASN:N	1:F:222:ASN:HD22	2.11	0.49
1:B:25:PHE:CZ	1:B:89:LEU:HD22	2.48	0.49
1:F:53:HIS:CE1	1:F:57:ARG:NH1	2.81	0.49
1:D:142:GLU:HA	1:D:145:ARG:HB3	1.95	0.49
1:B:192:GLU:HA	1:B:195:ARG:HG3	1.94	0.49
1:D:192:GLU:HA	1:D:195:ARG:HG3	1.94	0.49
1:E:71:THR:HG22	1:E:89:LEU:HD13	1.93	0.49
1:D:104:TYR:O	1:D:104:TYR:CD2	2.66	0.49
1:F:392:ILE:HA	1:F:418:LYS:O	2.12	0.49
1:D:228:ALA:HB1	1:D:286:ALA:HB1	1.95	0.49
1:E:97:PRO:HG2	1:E:98:THR:HG22	1.95	0.49
1:D:62:GLY:CA	1:D:63:GLU:CB	2.89	0.49
1:A:63:GLU:N	1:A:64:PRO:CA	2.59	0.49
1:C:259:ASN:OD1	1:C:259:ASN:C	2.51	0.49
1:D:104:TYR:HD1	1:D:105:TYR:CG	2.31	0.49
1:A:238:PHE:CE2	1:A:301:ILE:HG23	2.48	0.49
1:C:53:HIS:CE1	1:C:57:ARG:NH1	2.81	0.49
1:F:255:GLU:C	1:F:257:ASN:H	2.05	0.49
1:C:84:GLY:HA3	1:C:88:TYR:CB	2.43	0.49
2:H:464:GLU:HG3	2:H:489:PHE:CD1	2.47	0.49
1:D:317:ILE:HB	1:D:357:VAL:HG22	1.95	0.49
1:D:262:ASN:HB3	1:D:265:THR:CG2	2.43	0.48
1:A:53:HIS:CE1	1:A:57:ARG:HD2	2.48	0.48
1:E:28:PRO:C	1:E:30:ALA:N	2.67	0.48
1:D:202:ARG:HB3	1:D:354:GLU:C	2.32	0.48
1:B:228:ALA:HB1	1:B:286:ALA:HB1	1.95	0.48
1:E:249:MET:HA	1:E:252:LEU:HB2	1.95	0.48
1:A:83:ILE:HG22	1:A:84:GLY:N	2.29	0.48
2:G:487:GLY:CA	2:G:489:PHE:H	2.24	0.48
1:F:132:ARG:NH1	1:F:135:GLU:OE1	2.46	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:503:ALA:O	2:G:506:GLU:N	2.46	0.48
1:B:133:GLU:N	1:B:134:ASP:CB	2.67	0.48
1:D:141:ASP:OD2	1:D:297:ARG:CD	2.59	0.48
1:E:104:TYR:OH	1:F:69:THR:OG1	1.87	0.48
1:E:259:ASN:OD1	1:E:259:ASN:C	2.51	0.48
1:D:25:PHE:CZ	1:D:89:LEU:HD22	2.49	0.48
1:C:226:ASN:O	1:C:230:LYS:HB2	2.14	0.48
1:A:105:TYR:CE2	1:B:68:VAL:CG1	2.96	0.48
1:B:219:PHE:CZ	1:B:223:ILE:HD11	2.48	0.48
1:F:219:PHE:CZ	1:F:223:ILE:HD11	2.48	0.48
1:B:381:ARG:HD3	1:B:387:GLU:HB2	1.96	0.48
1:E:322:LEU:HB3	1:E:323:GLN:NE2	2.28	0.48
1:B:83:ILE:HG22	1:B:84:GLY:N	2.28	0.48
1:A:46:ALA:O	1:A:50:LYS:HD2	2.14	0.48
1:C:258:ILE:N	1:C:435:TYR:CD2	2.82	0.48
2:G:475:ARG:HG2	2:G:511:ALA:HB1	1.94	0.48
1:D:222:ASN:HD22	1:D:222:ASN:H	1.60	0.48
2:H:541:SER:HB3	2:H:544:GLU:HG3	1.96	0.48
2:H:475:ARG:CG	2:H:475:ARG:NH1	2.77	0.48
1:C:66:ASP:O	1:C:69:THR:HG22	2.14	0.48
1:B:391:ASP:O	1:B:419:GLN:HA	2.14	0.48
2:I:504:PHE:O	2:I:507:GLU:HB3	2.14	0.48
1:D:225:GLN:HE22	1:D:254:ALA:HB3	1.78	0.48
1:D:255:GLU:C	1:D:257:ASN:N	2.45	0.47
2:H:503:ALA:O	2:H:506:GLU:N	2.45	0.47
1:C:104:TYR:HD1	1:C:105:TYR:CG	2.31	0.47
1:D:325:ILE:HG23	1:D:342:ILE:HD13	1.95	0.47
2:G:487:GLY:HA3	2:G:489:PHE:N	2.27	0.47
2:G:464:GLU:CG	2:G:489:PHE:HD1	2.27	0.47
1:B:395:PHE:HB2	1:B:415:ILE:HB	1.95	0.47
2:I:465:ARG:HG3	2:I:531:LEU:HD21	1.95	0.47
1:D:132:ARG:NH1	1:D:135:GLU:OE1	2.48	0.47
1:A:271:GLU:O	1:A:275:LYS:HB2	2.14	0.47
1:E:216:LYS:HA	1:E:396:LEU:HD12	1.96	0.47
1:D:225:GLN:NE2	1:D:251:MET:HB2	2.29	0.47
1:C:280:MET:O	1:C:284:SER:HB2	2.14	0.47
1:C:392:ILE:HA	1:C:418:LYS:O	2.14	0.47
1:E:63:GLU:N	1:E:64:PRO:CA	2.56	0.47
1:B:222:ASN:H	1:B:222:ASN:HD22	1.61	0.47
1:D:235:VAL:HG12	1:D:316:MET:HB2	1.96	0.47
1:D:257:ASN:CA	1:D:435:TYR:CD2	2.98	0.47
2:H:538:ASP:O	2:H:539:ASP:CB	2.61	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:32:VAL:HB	1:F:33:PRO:HD3	1.96	0.47
1:A:392:ILE:HA	1:A:418:LYS:O	2.14	0.47
1:B:66:ASP:N	1:B:69:THR:HG22	2.16	0.47
1:B:104:TYR:HB3	1:B:105:TYR:HB2	1.95	0.47
1:F:83:ILE:CG2	1:F:84:GLY:H	2.26	0.47
1:A:50:LYS:NZ	1:A:82:GLU:OE2	2.48	0.47
1:C:391:ASP:O	1:C:419:GLN:HA	2.15	0.47
1:A:185:GLY:O	1:A:186:ILE:HG13	2.13	0.47
1:D:66:ASP:OD1	1:D:69:THR:HG22	2.15	0.47
1:D:105:TYR:O	1:D:109:VAL:HG23	2.15	0.47
2:I:503:ALA:O	2:I:506:GLU:N	2.46	0.47
1:A:104:TYR:HD1	1:A:105:TYR:CG	2.33	0.47
1:A:231:THR:HG23	1:A:232:ASN:N	2.25	0.47
1:D:323:GLN:HE21	1:D:361:SER:HA	1.79	0.47
1:A:322:LEU:C	1:A:324:LEU:H	2.18	0.47
2:G:507:GLU:O	2:G:507:GLU:HG3	2.15	0.47
2:H:463:ALA:O	2:H:467:LEU:HB2	2.14	0.47
1:C:258:ILE:O	1:C:259:ASN:CB	2.61	0.47
1:C:148:MET:HE3	1:C:148:MET:HA	1.97	0.47
1:F:202:ARG:O	1:F:203:SER:CB	2.63	0.47
1:D:298:VAL:HG11	1:D:345:SER:HB3	1.96	0.47
2:I:513:PRO:O	2:I:517:ILE:HG12	2.15	0.47
1:E:104:TYR:HD1	1:E:105:TYR:CG	2.32	0.47
1:B:223:ILE:O	1:B:227:VAL:HG23	2.15	0.47
1:E:83:ILE:CG2	1:E:84:GLY:H	2.09	0.47
1:D:207:ILE:CD1	1:D:386:ILE:HG21	2.45	0.47
1:C:216:LYS:HB2	1:C:360:LEU:HD22	1.97	0.47
1:E:208:VAL:HG22	1:E:394:ALA:HB3	1.96	0.47
1:A:391:ASP:N	1:A:391:ASP:OD1	2.43	0.47
1:F:251:MET:CE	1:F:288:ILE:HD13	2.45	0.47
1:B:196:MET:O	1:B:419:GLN:NE2	2.40	0.46
1:F:208:VAL:HA	1:F:394:ALA:O	2.15	0.46
1:D:374:ARG:HB3	1:D:375:PRO:HA	1.96	0.46
2:G:475:ARG:NH1	2:G:475:ARG:HG3	2.20	0.46
1:B:258:ILE:O	1:B:259:ASN:CB	2.62	0.46
1:C:28:PRO:C	1:C:30:ALA:N	2.68	0.46
1:C:86:VAL:HG22	2:H:572:GLU:HG3	1.98	0.46
1:C:104:TYR:N	1:C:107:ARG:H	2.09	0.46
1:D:202:ARG:O	1:D:203:SER:HB2	2.15	0.46
1:A:132:ARG:NH1	1:A:135:GLU:OE1	2.48	0.46
1:E:132:ARG:C	1:E:134:ASP:HB2	2.36	0.46
1:E:62:GLY:HA2	1:E:63:GLU:CB	2.33	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:315:GLY:O	1:F:356:PRO:HD2	2.16	0.46
1:B:235:VAL:HG12	1:B:316:MET:HB2	1.98	0.46
1:C:104:TYR:HA	1:C:106:ALA:H	1.79	0.46
1:F:188:THR:HG22	1:F:200:PHE:CE2	2.51	0.46
1:C:25:PHE:CZ	1:C:89:LEU:HD22	2.51	0.46
1:E:339:VAL:HG13	1:E:384:GLY:HA3	1.98	0.46
2:G:550:ARG:CB	2:G:550:ARG:HH11	2.28	0.46
1:F:187:PRO:C	1:F:189:GLY:H	2.18	0.46
2:H:467:LEU:HA	2:H:467:LEU:HD12	1.85	0.46
1:F:240:LEU:HD22	1:F:295:SER:HA	1.97	0.46
1:A:280:MET:O	1:A:284:SER:HB2	2.15	0.46
1:E:191:THR:O	1:E:194:ASP:HB2	2.16	0.45
2:H:471:MSE:O	2:H:475:ARG:HD2	2.16	0.45
1:F:64:PRO:HB2	1:F:65:VAL:H	1.64	0.45
1:C:101:ASN:HB2	1:C:105:TYR:CD1	2.51	0.45
1:D:128:ASP:HB3	1:D:139:LEU:HD21	1.96	0.45
1:C:62:GLY:CA	1:C:63:GLU:CB	2.93	0.45
1:B:222:ASN:ND2	1:B:222:ASN:N	2.63	0.45
2:I:519:ARG:O	2:I:519:ARG:HD3	2.16	0.45
1:D:200:PHE:CD1	1:D:200:PHE:N	2.83	0.45
2:I:541:SER:HB3	2:I:544:GLU:HG3	1.98	0.45
1:A:88:TYR:O	1:A:92:LEU:HG	2.16	0.45
2:I:491:ILE:HB	2:I:494:HIS:CD2	2.51	0.45
1:D:28:PRO:C	1:D:30:ALA:H	2.19	0.45
1:B:104:TYR:HD1	1:B:105:TYR:CG	2.34	0.45
1:D:322:LEU:HB3	1:D:323:GLN:NE2	2.31	0.45
1:B:148:MET:HE3	1:B:148:MET:HA	1.97	0.45
2:I:487:GLY:HA2	2:I:488:ARG:HB2	1.97	0.45
2:G:565:GLU:O	2:G:569:THR:HG22	2.15	0.45
1:C:351:ARG:HH11	1:C:351:ARG:HB2	1.80	0.45
1:A:61:ARG:CB	1:A:62:GLY:CA	2.90	0.45
1:E:202:ARG:HB3	1:E:354:GLU:C	2.36	0.45
2:G:519:ARG:O	2:G:519:ARG:HD3	2.17	0.45
1:C:258:ILE:N	1:C:435:TYR:CE2	2.85	0.45
1:E:84:GLY:HA3	1:E:88:TYR:CB	2.46	0.45
1:D:185:GLY:O	1:D:186:ILE:HG13	2.17	0.45
1:E:187:PRO:C	1:E:189:GLY:N	2.69	0.45
1:D:246:GLN:HG2	1:D:246:GLN:O	2.17	0.45
1:B:249:MET:HA	1:B:252:LEU:HB2	1.98	0.45
1:F:298:VAL:HG11	1:F:345:SER:HB3	1.98	0.45
1:B:280:MET:O	1:B:284:SER:HB2	2.17	0.45
1:A:67:LEU:HD12	2:G:584:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:148:MET:HE3	1:D:148:MET:HA	1.98	0.45
1:C:219:PHE:CZ	1:C:223:ILE:HD11	2.51	0.45
1:E:251:MET:HE3	1:E:288:ILE:HD13	1.99	0.45
1:A:104:TYR:CD2	1:A:104:TYR:O	2.69	0.45
1:B:200:PHE:CD1	1:B:206:ILE:HD13	2.52	0.45
2:G:475:ARG:CG	2:G:475:ARG:HH11	2.23	0.45
1:E:48:HIS:NE2	1:E:88:TYR:OH	2.37	0.45
1:F:51:ILE:HD11	1:F:83:ILE:HG21	1.99	0.45
1:F:233:GLU:CG	1:F:315:GLY:HA3	2.43	0.45
2:H:487:GLY:HA3	2:H:489:PHE:N	2.27	0.45
1:E:273:TRP:O	1:E:275:LYS:N	2.47	0.45
1:E:208:VAL:HB	1:E:360:LEU:HD23	1.99	0.45
2:I:470:HIS:HE1	2:I:537:ALA:O	2.00	0.45
1:C:222:ASN:ND2	1:C:222:ASN:N	2.62	0.45
1:C:148:MET:HA	1:C:148:MET:HE2	1.99	0.45
1:C:135:GLU:C	1:C:137:ASP:H	2.19	0.45
1:C:101:ASN:C	1:C:103:GLU:H	2.17	0.45
1:D:74:LEU:HD13	1:D:83:ILE:CD1	2.47	0.45
1:C:385:SER:OG	1:C:386:ILE:N	2.49	0.45
1:E:251:MET:CE	1:E:288:ILE:HD13	2.47	0.45
1:B:439:VAL:HG12	1:B:440:ASN:N	2.32	0.45
1:B:202:ARG:O	1:B:203:SER:CB	2.64	0.45
1:E:298:VAL:HG11	1:E:345:SER:HB3	1.99	0.45
1:F:439:VAL:HG12	1:F:440:ASN:H	1.82	0.45
1:D:259:ASN:OD1	1:D:259:ASN:C	2.56	0.45
1:A:200:PHE:N	1:A:200:PHE:CD1	2.85	0.45
1:F:296:ILE:O	1:F:325:ILE:HG13	2.17	0.45
1:C:200:PHE:CD1	1:C:206:ILE:HD13	2.52	0.44
1:C:133:GLU:CA	1:C:134:ASP:HB2	2.46	0.44
1:C:322:LEU:C	1:C:324:LEU:H	2.21	0.44
1:C:322:LEU:HB3	1:C:323:GLN:NE2	2.31	0.44
1:A:187:PRO:C	1:A:189:GLY:N	2.69	0.44
2:I:473:ARG:HD2	2:I:536:ILE:HD11	1.99	0.44
1:C:231:THR:CG2	1:C:232:ASN:H	2.15	0.44
1:C:316:MET:HG2	1:C:356:PRO:HG2	1.99	0.44
1:B:259:ASN:C	1:B:259:ASN:OD1	2.55	0.44
1:B:202:ARG:HB3	1:B:354:GLU:C	2.37	0.44
1:B:28:PRO:C	1:B:30:ALA:N	2.68	0.44
1:F:104:TYR:H	1:F:107:ARG:HB2	1.82	0.44
1:E:142:GLU:HA	1:E:145:ARG:HB3	1.99	0.44
1:E:219:PHE:CZ	1:E:223:ILE:HD11	2.52	0.44
1:A:298:VAL:HG11	1:A:345:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:196:MET:O	1:D:419:GLN:NE2	2.43	0.44
1:A:257:ASN:CA	1:A:435:TYR:CE2	3.00	0.44
1:E:104:TYR:HA	1:E:106:ALA:N	2.33	0.44
1:D:104:TYR:H	1:D:107:ARG:H	1.65	0.44
1:F:197:THR:CB	1:F:199:GLY:O	2.65	0.44
1:C:104:TYR:HB3	1:C:105:TYR:HB2	2.00	0.44
1:F:83:ILE:HG22	1:F:84:GLY:N	2.32	0.44
1:A:273:TRP:C	1:A:275:LYS:N	2.70	0.44
2:I:503:ALA:O	2:I:504:PHE:C	2.56	0.44
1:C:391:ASP:OD1	1:C:391:ASP:N	2.46	0.44
2:H:496:ALA:O	2:H:500:TYR:HD2	2.00	0.44
1:A:104:TYR:OH	1:B:63:GLU:HG3	2.17	0.44
1:E:16:ALA:HA	1:F:68:VAL:HG11	2.00	0.44
1:D:133:GLU:N	1:D:134:ASP:CB	2.74	0.44
1:C:88:TYR:O	1:C:92:LEU:HG	2.18	0.44
2:G:582:ARG:HB3	2:G:582:ARG:HE	1.56	0.44
1:C:83:ILE:CG2	1:C:84:GLY:H	2.17	0.44
1:C:48:HIS:NE2	1:C:88:TYR:OH	2.42	0.44
1:A:207:ILE:HA	1:A:359:ALA:O	2.17	0.44
2:H:503:ALA:O	2:H:504:PHE:C	2.56	0.44
1:E:98:THR:HG23	1:E:101:ASN:HD21	1.83	0.44
1:E:133:GLU:CA	1:E:134:ASP:HB2	2.48	0.44
1:E:66:ASP:O	1:E:69:THR:HG22	2.18	0.44
1:D:322:LEU:C	1:D:324:LEU:H	2.21	0.44
1:C:207:ILE:HA	1:C:359:ALA:O	2.17	0.44
1:A:132:ARG:C	1:A:134:ASP:HB2	2.38	0.44
2:H:509:HIS:O	2:H:510:GLU:C	2.57	0.44
1:F:141:ASP:C	1:F:143:ALA:H	2.21	0.44
1:E:322:LEU:O	1:E:324:LEU:N	2.51	0.44
1:E:84:GLY:HA3	1:E:88:TYR:HB3	2.00	0.44
1:C:40:PRO:O	1:C:49:GLN:HG3	2.17	0.44
1:E:200:PHE:CD1	1:E:200:PHE:N	2.85	0.43
1:E:322:LEU:C	1:E:324:LEU:H	2.20	0.43
1:A:396:LEU:CD2	1:A:414:ILE:HG12	2.48	0.43
1:B:225:GLN:HE22	1:B:254:ALA:HB3	1.82	0.43
1:D:28:PRO:C	1:D:30:ALA:N	2.71	0.43
1:C:104:TYR:OH	1:D:63:GLU:HG3	2.18	0.43
1:D:67:LEU:HD23	1:D:67:LEU:HA	1.83	0.43
2:I:565:GLU:O	2:I:569:THR:HG22	2.18	0.43
1:C:340:SER:HB3	1:C:385:SER:HB3	2.00	0.43
1:E:422:GLY:HA3	1:E:423:PRO:HD3	1.82	0.43
1:A:101:ASN:HB2	1:A:105:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:226:ASN:O	1:E:230:LYS:HB2	2.19	0.43
1:F:351:ARG:HH11	1:F:351:ARG:HB2	1.82	0.43
1:F:422:GLY:HA3	1:F:423:PRO:HD3	1.83	0.43
1:A:104:TYR:N	1:A:107:ARG:H	2.12	0.43
1:B:61:ARG:HB2	1:B:62:GLY:CA	2.44	0.43
1:E:62:GLY:CA	1:E:63:GLU:CB	2.95	0.43
1:D:47:ALA:HB1	1:D:83:ILE:HG23	2.00	0.43
2:G:465:ARG:CG	2:G:531:LEU:HD21	2.46	0.43
1:B:216:LYS:HA	1:B:396:LEU:HD12	2.00	0.43
1:B:53:HIS:CE1	1:B:57:ARG:NH1	2.86	0.43
1:C:381:ARG:HD3	1:C:387:GLU:HB2	2.00	0.43
1:E:101:ASN:HB2	1:E:105:TYR:CD1	2.54	0.43
1:C:61:ARG:CB	1:C:62:GLY:CA	2.93	0.43
1:C:323:GLN:HE21	1:C:361:SER:HA	1.83	0.43
1:F:323:GLN:HE21	1:F:361:SER:HA	1.83	0.43
1:D:84:GLY:HA3	1:D:88:TYR:CB	2.49	0.43
1:D:273:TRP:C	1:D:275:LYS:N	2.72	0.43
1:B:202:ARG:O	1:B:203:SER:HB2	2.19	0.43
1:B:138:VAL:O	1:B:142:GLU:HG2	2.19	0.43
1:A:124:SER:O	1:A:128:ASP:HB2	2.19	0.43
1:A:101:ASN:HB3	1:A:104:TYR:CD1	2.53	0.43
1:D:124:SER:O	1:D:128:ASP:HB2	2.18	0.43
2:G:501:ILE:O	2:G:504:PHE:HB3	2.18	0.43
1:D:102:VAL:O	1:D:104:TYR:HA	2.19	0.43
1:A:316:MET:HG2	1:A:356:PRO:HG2	2.01	0.43
1:B:22:GLY:HA3	1:B:96:VAL:HG21	2.00	0.43
1:D:133:GLU:CA	1:D:134:ASP:HB2	2.48	0.43
1:A:67:LEU:HD21	1:A:89:LEU:HB3	2.00	0.43
1:E:273:TRP:C	1:E:275:LYS:N	2.69	0.43
1:A:28:PRO:C	1:A:30:ALA:N	2.72	0.43
1:D:255:GLU:HB3	1:D:256:GLY:H	1.61	0.43
1:B:322:LEU:C	1:B:324:LEU:H	2.22	0.43
1:D:79:GLN:O	1:D:83:ILE:HG13	2.18	0.43
1:E:148:MET:HA	1:E:148:MET:HE2	2.00	0.43
1:A:374:ARG:HG2	1:A:376:MET:HE3	2.01	0.43
2:G:484:ARG:HH22	2:G:546:GLU:HG2	1.84	0.43
1:B:187:PRO:C	1:B:189:GLY:N	2.69	0.43
2:I:461:GLN:HG3	2:I:491:ILE:HD11	2.00	0.43
1:D:439:VAL:HG12	1:D:440:ASN:H	1.84	0.43
1:B:61:ARG:CB	1:B:62:GLY:HA3	2.34	0.42
1:E:101:ASN:HB3	1:E:104:TYR:CD1	2.53	0.42
1:A:376:MET:CE	1:D:246:GLN:HE22	2.32	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:258:ILE:N	1:D:435:TYR:CD2	2.87	0.42
1:E:104:TYR:CD2	1:E:104:TYR:C	2.90	0.42
2:H:546:GLU:O	2:H:550:ARG:HB2	2.19	0.42
1:A:210:ALA:CB	1:A:396:LEU:HB2	2.48	0.42
1:C:340:SER:CB	1:C:385:SER:HB3	2.49	0.42
1:E:391:ASP:O	1:E:419:GLN:HA	2.19	0.42
1:B:40:PRO:O	1:B:49:GLN:HG3	2.19	0.42
1:C:101:ASN:HB2	1:C:102:VAL:H	1.69	0.42
1:F:101:ASN:C	1:F:103:GLU:N	2.72	0.42
2:H:565:GLU:O	2:H:569:THR:HG22	2.19	0.42
1:D:207:ILE:HG23	1:D:393:VAL:HG13	2.00	0.42
1:B:298:VAL:HG11	1:B:345:SER:HB3	2.00	0.42
1:C:306:ARG:NH2	1:D:32:VAL:CG2	2.79	0.42
1:A:101:ASN:C	1:A:103:GLU:N	2.73	0.42
1:C:98:THR:HG23	1:C:101:ASN:HD21	1.85	0.42
2:G:487:GLY:HA2	2:G:488:ARG:HB2	2.01	0.42
1:B:207:ILE:HG23	1:B:393:VAL:HG13	2.01	0.42
1:A:140:LEU:HD11	1:D:114:VAL:CG1	2.50	0.42
1:F:251:MET:HE3	1:F:288:ILE:HD13	2.02	0.42
1:A:40:PRO:O	1:A:49:GLN:HG3	2.19	0.42
1:F:96:VAL:HA	1:F:97:PRO:HD3	1.92	0.42
1:E:104:TYR:O	1:E:104:TYR:CD2	2.72	0.42
1:A:322:LEU:O	1:A:324:LEU:N	2.52	0.42
1:D:186:ILE:HA	1:D:187:PRO:HD3	1.92	0.42
2:G:486:GLY:N	2:G:488:ARG:HB2	2.33	0.42
1:C:339:VAL:HG13	1:C:384:GLY:HA3	2.00	0.42
2:G:487:GLY:HA3	2:G:489:PHE:HD2	1.85	0.42
1:D:83:ILE:CG2	1:D:84:GLY:H	2.30	0.42
1:E:268:LEU:HB3	1:E:272:ASP:CB	2.46	0.42
1:D:395:PHE:HB2	1:D:415:ILE:HB	2.01	0.42
1:F:84:GLY:HA3	1:F:88:TYR:CB	2.49	0.42
1:D:48:HIS:HE2	1:D:88:TYR:HH	1.68	0.42
1:D:84:GLY:HA3	1:D:88:TYR:HB2	2.02	0.42
2:H:486:GLY:N	2:H:488:ARG:HB2	2.33	0.42
1:E:26:LEU:HA	1:E:26:LEU:HD23	1.76	0.42
1:C:249:MET:HA	1:C:252:LEU:HB2	2.01	0.42
1:D:41:GLU:N	1:D:41:GLU:OE1	2.51	0.42
2:H:516:LEU:HD23	2:H:516:LEU:HA	1.93	0.42
2:H:468:LEU:HD23	2:H:497:LEU:HD13	2.01	0.42
1:E:105:TYR:CZ	1:F:68:VAL:HB	2.55	0.42
1:C:25:PHE:HZ	1:C:89:LEU:HD22	1.84	0.42
1:A:225:GLN:HE22	1:A:254:ALA:HB3	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:391:ASP:HB3	1:C:420:ARG:NH1	2.34	0.42
1:C:314:LEU:HD13	1:C:355:VAL:HG21	2.02	0.42
2:H:582:ARG:HE	2:H:582:ARG:HB3	1.45	0.42
1:B:351:ARG:HH11	1:B:351:ARG:HB2	1.85	0.42
1:A:62:GLY:CA	1:A:63:GLU:CB	2.89	0.42
1:C:66:ASP:C	1:C:66:ASP:OD1	2.58	0.42
1:F:105:TYR:H	1:F:108:ILE:HD12	1.85	0.42
2:I:487:GLY:HA3	2:I:489:PHE:N	2.33	0.42
2:G:467:LEU:HA	2:G:467:LEU:HD12	1.91	0.42
1:B:142:GLU:HA	1:B:145:ARG:HB3	2.01	0.42
1:C:124:SER:O	1:C:128:ASP:HB2	2.19	0.42
1:F:320:ASP:HA	1:F:360:LEU:HD12	2.01	0.42
1:C:91:GLU:O	1:C:95:ALA:HB2	2.20	0.42
1:D:238:PHE:O	1:D:320:ASP:N	2.46	0.42
1:B:292:ASP:OD1	1:B:292:ASP:N	2.50	0.42
1:F:61:ARG:HB2	1:F:62:GLY:CA	2.39	0.41
1:B:84:GLY:HA3	1:B:88:TYR:CB	2.50	0.41
2:H:457:LEU:HA	2:H:458:PRO:HD3	1.83	0.41
1:B:375:PRO:HG2	1:B:395:PHE:HB3	2.01	0.41
1:D:22:GLY:HA3	1:D:96:VAL:HG21	2.02	0.41
2:G:505:TYR:O	2:G:508:GLY:N	2.52	0.41
1:F:74:LEU:HD13	1:F:83:ILE:HD11	2.02	0.41
1:D:187:PRO:C	1:D:189:GLY:N	2.69	0.41
1:F:104:TYR:HD1	1:F:105:TYR:CG	2.37	0.41
1:E:222:ASN:H	1:E:222:ASN:HD22	1.67	0.41
1:E:30:ALA:O	1:E:33:PRO:HD2	2.20	0.41
1:D:375:PRO:HG2	1:D:395:PHE:HB3	2.02	0.41
1:E:293:THR:HA	1:E:294:PRO:HD2	1.76	0.41
1:D:115:LEU:HA	1:D:115:LEU:HD23	1.93	0.41
1:D:256:GLY:O	1:D:257:ASN:C	2.57	0.41
2:I:509:HIS:O	2:I:510:GLU:C	2.58	0.41
2:I:564:LYS:HE3	2:I:587:MSE:HG2	2.01	0.41
1:A:141:ASP:C	1:A:143:ALA:N	2.73	0.41
1:D:216:LYS:HA	1:D:396:LEU:HD12	2.01	0.41
2:I:525:GLN:N	2:I:526:PRO:HD2	2.34	0.41
2:G:500:TYR:CZ	2:G:521:PRO:HD3	2.55	0.41
1:F:257:ASN:C	1:F:435:TYR:CE2	2.93	0.41
1:C:344:ARG:HH11	1:D:61:ARG:CG	2.33	0.41
1:D:141:ASP:C	1:D:143:ALA:N	2.74	0.41
1:D:104:TYR:CD1	1:D:105:TYR:N	2.88	0.41
1:A:259:ASN:C	1:A:259:ASN:OD1	2.58	0.41
2:G:557:LYS:O	2:G:560:MSE:HB3	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:64:PRO:HB2	1:B:65:VAL:H	1.63	0.41
1:B:200:PHE:CD1	1:B:200:PHE:N	2.87	0.41
2:G:503:ALA:O	2:G:504:PHE:C	2.57	0.41
2:I:496:ALA:O	2:I:500:TYR:HD2	2.03	0.41
1:B:66:ASP:O	1:B:67:LEU:C	2.59	0.41
1:B:64:PRO:O	1:B:69:THR:HG21	2.20	0.41
1:E:186:ILE:HA	1:E:187:PRO:HD3	1.89	0.41
1:D:271:GLU:O	1:D:275:LYS:HB2	2.21	0.41
1:E:375:PRO:HG2	1:E:395:PHE:HB3	2.03	0.41
1:D:96:VAL:HA	1:D:97:PRO:HD3	1.90	0.41
1:E:104:TYR:HA	1:E:106:ALA:H	1.85	0.41
2:I:554:ASN:HB2	2:I:557:LYS:HD2	2.02	0.41
1:C:80:LEU:HD23	1:C:80:LEU:HA	1.93	0.41
1:E:103:GLU:N	1:E:104:TYR:HB2	2.36	0.41
1:E:216:LYS:HA	1:E:396:LEU:CD1	2.51	0.41
1:F:225:GLN:NE2	1:F:251:MET:HB2	2.36	0.41
1:B:422:GLY:HA3	1:B:423:PRO:HD3	1.84	0.41
1:D:257:ASN:CA	1:D:435:TYR:CE2	3.04	0.41
1:A:103:GLU:N	1:A:104:TYR:HB2	2.36	0.41
1:A:188:THR:CG2	1:A:200:PHE:CE2	3.04	0.41
1:D:322:LEU:C	1:D:324:LEU:N	2.73	0.41
2:G:475:ARG:CG	2:G:475:ARG:NH1	2.83	0.41
1:E:222:ASN:N	1:E:222:ASN:ND2	2.66	0.41
1:B:208:VAL:HG22	1:B:394:ALA:HB3	2.02	0.41
1:D:351:ARG:HB2	1:D:351:ARG:HH11	1.86	0.41
1:A:317:ILE:HB	1:A:357:VAL:HG22	2.02	0.41
1:B:323:GLN:HE21	1:B:361:SER:HA	1.85	0.41
1:F:255:GLU:CG	1:F:256:GLY:H	2.33	0.41
1:E:104:TYR:OH	1:F:63:GLU:HG3	2.21	0.41
1:C:94:ASP:CB	2:H:591:LYS:NZ	2.61	0.41
1:D:135:GLU:C	1:D:137:ASP:N	2.74	0.41
1:B:188:THR:HG22	1:B:200:PHE:CE2	2.56	0.41
1:E:325:ILE:HG23	1:E:342:ILE:HD13	2.03	0.41
2:I:484:ARG:NH2	2:I:546:GLU:HG2	2.32	0.41
1:F:95:ALA:HA	2:I:457:LEU:O	2.20	0.41
1:A:273:TRP:O	1:A:275:LYS:N	2.53	0.41
1:B:340:SER:HB3	1:B:385:SER:HB3	2.03	0.41
1:E:124:SER:O	1:E:128:ASP:HB2	2.20	0.41
1:E:188:THR:HG22	1:E:200:PHE:CE2	2.57	0.40
1:F:432:ILE:HG22	1:F:435:TYR:H	1.85	0.40
1:E:258:ILE:N	1:E:435:TYR:CE2	2.85	0.40
1:E:322:LEU:C	1:E:324:LEU:N	2.74	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:464:GLU:CG	2:I:489:PHE:HD1	2.33	0.40
1:B:273:TRP:C	1:B:275:LYS:N	2.72	0.40
1:E:391:ASP:HB3	1:E:420:ARG:NH1	2.36	0.40
1:B:124:SER:O	1:B:128:ASP:HB2	2.21	0.40
1:C:16:ALA:HA	1:D:68:VAL:HG11	2.03	0.40
1:F:322:LEU:C	1:F:324:LEU:H	2.24	0.40
1:F:104:TYR:CD1	1:F:104:TYR:C	2.91	0.40
2:I:485:ILE:HG22	2:I:487:GLY:HA2	2.04	0.40
1:A:39:ILE:HB	1:A:40:PRO:HD2	2.03	0.40
1:A:396:LEU:HD23	1:A:414:ILE:HG12	2.03	0.40
1:D:422:GLY:HA3	1:D:423:PRO:HD3	1.80	0.40
1:B:67:LEU:HA	1:B:67:LEU:HD23	1.94	0.40
1:C:67:LEU:HA	1:C:67:LEU:HD23	1.88	0.40
1:D:222:ASN:N	1:D:222:ASN:ND2	2.66	0.40
1:D:439:VAL:HG12	1:D:440:ASN:N	2.36	0.40
2:H:475:ARG:NH1	2:H:504:PHE:HD2	2.20	0.40
1:D:104:TYR:C	1:D:104:TYR:CD1	2.81	0.40
1:D:381:ARG:HD2	1:D:381:ARG:HA	1.91	0.40
1:E:207:ILE:HG22	1:E:390:ALA:HB1	2.04	0.40
1:D:202:ARG:HB3	1:D:354:GLU:O	2.21	0.40
1:B:46:ALA:HB1	1:B:50:LYS:HE3	2.03	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	348/454 (77%)	284 (82%)	41 (12%)	23 (7%)	2	35
1	B	348/454 (77%)	285 (82%)	40 (12%)	23 (7%)	2	35
1	C	348/454 (77%)	283 (81%)	40 (12%)	25 (7%)	2	32
1	D	348/454 (77%)	285 (82%)	42 (12%)	21 (6%)	2	38
1	E	348/454 (77%)	283 (81%)	42 (12%)	23 (7%)	2	35
1	F	348/454 (77%)	289 (83%)	38 (11%)	21 (6%)	2	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	136/143 (95%)	113 (83%)	13 (10%)	10 (7%)	2	31
2	H	136/143 (95%)	109 (80%)	17 (12%)	10 (7%)	2	31
2	I	136/143 (95%)	111 (82%)	14 (10%)	11 (8%)	1	27
All	All	2496/3153 (79%)	2042 (82%)	287 (12%)	167 (7%)	2	34

All (167) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	A	188	THR
1	A	200	PHE
1	A	203	SER
1	A	232	ASN
1	A	256	GLY
1	A	259	ASN
1	A	385	SER
1	B	63	GLU
1	B	102	VAL
1	B	104	TYR
1	B	188	THR
1	B	200	PHE
1	B	203	SER
1	B	232	ASN
1	B	256	GLY
1	B	259	ASN
1	B	385	SER
1	C	63	GLU
1	C	104	TYR
1	C	188	THR
1	C	200	PHE
1	C	203	SER
1	C	232	ASN
1	C	256	GLY
1	C	259	ASN
1	C	385	SER
1	D	102	VAL
1	D	136	ILE
1	D	188	THR
1	D	200	PHE
1	D	203	SER
1	D	232	ASN

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Mol	Chain	Res	Type
1	D	256	GLY
1	D	385	SER
1	E	63	GLU
1	E	104	TYR
1	E	188	THR
1	E	200	PHE
1	E	203	SER
1	E	232	ASN
1	E	256	GLY
1	E	259	ASN
1	E	385	SER
1	F	63	GLU
1	F	102	VAL
1	F	104	TYR
1	F	188	THR
1	F	203	SER
1	F	232	ASN
1	F	256	GLY
1	F	259	ASN
1	F	385	SER
2	G	504	PHE
2	G	510	GLU
2	G	511	ALA
2	G	534	LEU
2	G	535	LEU
2	G	539	ASP
2	H	504	PHE
2	H	510	GLU
2	H	511	ALA
2	H	535	LEU
2	H	539	ASP
2	I	504	PHE
2	I	510	GLU
2	I	511	ALA
2	I	534	LEU
2	I	539	ASP
1	A	83	ILE
1	A	102	VAL
1	A	104	TYR
1	A	133	GLU
1	A	433	LYS
1	B	83	ILE

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Mol	Chain	Res	Type
1	B	133	GLU
1	B	136	ILE
1	B	433	LYS
1	C	83	ILE
1	C	102	VAL
1	C	133	GLU
1	C	384	GLY
1	D	63	GLU
1	D	83	ILE
1	D	133	GLU
1	D	184	THR
1	D	259	ASN
1	D	433	LYS
1	E	83	ILE
1	E	102	VAL
1	E	133	GLU
1	E	433	LYS
1	F	83	ILE
1	F	133	GLU
1	F	136	ILE
2	G	503	ALA
2	H	503	ALA
2	H	534	LEU
2	I	561	LEU
1	A	294	PRO
1	B	184	THR
1	C	134	ASP
1	D	104	TYR
1	D	105	TYR
1	D	294	PRO
1	D	321	TYR
1	E	184	THR
1	E	294	PRO
1	F	294	PRO
1	F	440	ASN
2	I	503	ALA
2	I	535	LEU
1	A	105	TYR
1	A	384	GLY
1	B	64	PRO
1	B	105	TYR
1	B	294	PRO

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Mol	Chain	Res	Type
1	B	384	GLY
1	C	240	LEU
1	C	294	PRO
1	C	321	TYR
1	C	433	LYS
1	D	384	GLY
1	E	105	TYR
1	E	134	ASP
1	E	384	GLY
1	F	64	PRO
1	F	105	TYR
1	F	200	PHE
1	F	321	TYR
2	G	457	LEU
2	G	561	LEU
2	H	561	LEU
1	A	136	ILE
1	A	240	LEU
1	B	134	ASP
1	B	314	LEU
1	C	105	TYR
1	C	184	THR
1	C	314	LEU
1	C	375	PRO
1	E	191	THR
1	E	314	LEU
1	F	134	ASP
1	F	314	LEU
1	F	433	LYS
2	H	457	LEU
2	I	457	LEU
2	I	560	MSE
1	B	321	TYR
1	D	375	PRO
1	E	274	GLY
1	A	274	GLY
1	A	315	GLY
1	B	375	PRO
2	G	520	ILE
2	H	520	ILE
1	A	97	PRO
1	C	68	VAL

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Mol	Chain	Res	Type
1	C	136	ILE
1	E	68	VAL
2	I	520	ILE
1	A	375	PRO
1	A	64	PRO
1	C	64	PRO
1	E	64	PRO
1	D	64	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/386 (77%)	269 (91%)	28 (9%)	13	55
1	B	297/386 (77%)	269 (91%)	28 (9%)	13	55
1	C	297/386 (77%)	269 (91%)	28 (9%)	13	55
1	D	297/386 (77%)	267 (90%)	30 (10%)	11	51
1	E	297/386 (77%)	268 (90%)	29 (10%)	12	52
1	F	297/386 (77%)	269 (91%)	28 (9%)	13	55
2	G	117/116 (101%)	108 (92%)	9 (8%)	18	65
2	H	117/116 (101%)	107 (92%)	10 (8%)	15	61
2	I	117/116 (101%)	111 (95%)	6 (5%)	33	79
All	All	2133/2664 (80%)	1937 (91%)	196 (9%)	13	56

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	57	ARG
1	A	67	LEU
1	A	79	GLN
1	A	80	LEU
1	A	81	GLU
1	A	103	GLU

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Mol	Chain	Res	Type
1	A	104	TYR
1	A	128	ASP
1	A	133	GLU
1	A	139	LEU
1	A	148	MET
1	A	200	PHE
1	A	202	ARG
1	A	211	ARG
1	A	216	LYS
1	A	222	ASN
1	A	255	GLU
1	A	261	GLN
1	A	314	LEU
1	A	321	TYR
1	A	324	LEU
1	A	339	VAL
1	A	345	SER
1	A	351	ARG
1	A	380	ILE
1	A	388	GLN
1	A	391	ASP
1	B	26	LEU
1	B	50	LYS
1	B	55	MET
1	B	57	ARG
1	B	79	GLN
1	B	80	LEU
1	B	81	GLU
1	B	103	GLU
1	B	104	TYR
1	B	128	ASP
1	B	148	MET
1	B	191	THR
1	B	200	PHE
1	B	202	ARG
1	B	211	ARG
1	B	216	LYS
1	B	222	ASN
1	B	249	MET
1	B	255	GLU
1	B	261	GLN
1	B	278	MET

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Mol	Chain	Res	Type
1	B	306	ARG
1	B	314	LEU
1	B	324	LEU
1	B	339	VAL
1	B	351	ARG
1	B	388	GLN
1	B	391	ASP
1	C	50	LYS
1	C	57	ARG
1	C	67	LEU
1	C	79	GLN
1	C	80	LEU
1	C	102	VAL
1	C	104	TYR
1	C	128	ASP
1	C	133	GLU
1	C	139	LEU
1	C	147	ILE
1	C	148	MET
1	C	200	PHE
1	C	202	ARG
1	C	211	ARG
1	C	222	ASN
1	C	249	MET
1	C	261	GLN
1	C	278	MET
1	C	314	LEU
1	C	324	LEU
1	C	339	VAL
1	C	345	SER
1	C	351	ARG
1	C	355	VAL
1	C	381	ARG
1	C	388	GLN
1	C	391	ASP
1	D	26	LEU
1	D	50	LYS
1	D	55	MET
1	D	57	ARG
1	D	67	LEU
1	D	79	GLN
1	D	80	LEU

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Mol	Chain	Res	Type
1	D	81	GLU
1	D	103	GLU
1	D	104	TYR
1	D	136	ILE
1	D	139	LEU
1	D	140	LEU
1	D	148	MET
1	D	200	PHE
1	D	202	ARG
1	D	211	ARG
1	D	216	LYS
1	D	222	ASN
1	D	249	MET
1	D	261	GLN
1	D	269	THR
1	D	306	ARG
1	D	314	LEU
1	D	324	LEU
1	D	339	VAL
1	D	351	ARG
1	D	380	ILE
1	D	388	GLN
1	D	391	ASP
1	E	50	LYS
1	E	55	MET
1	E	57	ARG
1	E	69	THR
1	E	79	GLN
1	E	80	LEU
1	E	103	GLU
1	E	104	TYR
1	E	128	ASP
1	E	139	LEU
1	E	147	ILE
1	E	148	MET
1	E	200	PHE
1	E	202	ARG
1	E	211	ARG
1	E	216	LYS
1	E	222	ASN
1	E	249	MET
1	E	261	GLN

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Mol	Chain	Res	Type
1	E	278	MET
1	E	314	LEU
1	E	321	TYR
1	E	324	LEU
1	E	339	VAL
1	E	345	SER
1	E	351	ARG
1	E	381	ARG
1	E	388	GLN
1	E	391	ASP
1	F	26	LEU
1	F	50	LYS
1	F	55	MET
1	F	67	LEU
1	F	79	GLN
1	F	80	LEU
1	F	81	GLU
1	F	90	SER
1	F	104	TYR
1	F	110	GLU
1	F	128	ASP
1	F	139	LEU
1	F	147	ILE
1	F	148	MET
1	F	202	ARG
1	F	211	ARG
1	F	216	LYS
1	F	222	ASN
1	F	255	GLU
1	F	261	GLN
1	F	306	ARG
1	F	314	LEU
1	F	322	LEU
1	F	324	LEU
1	F	345	SER
1	F	351	ARG
1	F	388	GLN
1	F	391	ASP
2	G	465	ARG
2	G	519	ARG
2	G	536	ILE
2	G	538	ASP

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Mol	Chain	Res	Type
2	G	540	VAL
2	G	543	GLN
2	G	550	ARG
2	G	569	THR
2	G	593	MSE
2	H	465	ARG
2	H	497	LEU
2	H	519	ARG
2	H	536	ILE
2	H	538	ASP
2	H	540	VAL
2	H	550	ARG
2	H	561	LEU
2	H	582	ARG
2	H	593	MSE
2	I	465	ARG
2	I	519	ARG
2	I	536	ILE
2	I	538	ASP
2	I	540	VAL
2	I	593	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	222	ASN
1	A	225	GLN
1	A	323	GLN
1	A	388	GLN
1	B	53	HIS
1	B	201	GLN
1	B	222	ASN
1	B	225	GLN
1	B	245	GLN
1	B	246	GLN
1	B	323	GLN
1	B	388	GLN
1	B	421	ASN
1	C	53	HIS
1	C	201	GLN
1	C	222	ASN

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Mol	Chain	Res	Type
1	C	225	GLN
1	C	234	ASN
1	C	245	GLN
1	C	246	GLN
1	C	323	GLN
1	C	388	GLN
1	C	421	ASN
1	D	53	HIS
1	D	201	GLN
1	D	222	ASN
1	D	225	GLN
1	D	246	GLN
1	D	323	GLN
1	D	388	GLN
1	E	53	HIS
1	E	201	GLN
1	E	222	ASN
1	E	225	GLN
1	E	323	GLN
1	E	388	GLN
1	E	421	ASN
1	F	53	HIS
1	F	201	GLN
1	F	225	GLN
1	F	226	ASN
1	F	246	GLN
1	F	323	GLN
1	F	388	GLN
2	G	470	HIS
2	G	494	HIS
2	H	470	HIS
2	H	494	HIS
2	H	509	HIS
2	H	554	ASN
2	I	470	HIS
2	I	494	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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	358/454 (78%)	0.16	13 (3%) 41 33	156, 167, 168, 170	0
1	B	358/454 (78%)	0.25	7 (1%) 62 48	163, 167, 168, 175	0
1	C	358/454 (78%)	0.11	9 (2%) 54 43	157, 167, 168, 170	0
1	D	358/454 (78%)	0.16	9 (2%) 54 43	163, 167, 168, 182	0
1	E	358/454 (78%)	0.16	11 (3%) 47 37	163, 167, 168, 170	0
1	F	358/454 (78%)	0.66	44 (12%) 5 7	162, 167, 168, 187	0
2	G	138/143 (96%)	0.12	3 (2%) 59 46	163, 167, 168, 171	0
2	H	138/143 (96%)	0.13	3 (2%) 59 46	162, 167, 168, 171	0
2	I	138/143 (96%)	0.25	7 (5%) 27 24	163, 167, 168, 171	0
All	All	2562/3153 (81%)	0.24	106 (4%) 35 29	156, 167, 168, 187	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	382	GLU	5.5
1	B	260	ALA	5.2
1	F	394	ALA	5.1
1	F	199	GLY	4.7
1	F	197	THR	4.6
2	I	510	GLU	4.6
1	F	384	GLY	4.5
2	H	510	GLU	4.4
1	D	261	GLN	4.3
1	F	441	LEU	4.3
1	F	326	GLN	4.3
1	D	413	GLU	4.2
1	C	441	LEU	4.0
1	A	261	GLN	3.9
1	F	324	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	231	THR	3.8
1	B	261	GLN	3.8
1	F	383	SER	3.7
2	I	506	GLU	3.7
1	F	417	ALA	3.6
1	A	421	ASN	3.5
1	A	434	GLU	3.4
1	A	287	GLY	3.4
1	F	198	SER	3.4
1	F	261	GLN	3.4
2	I	507	GLU	3.4
1	F	428	GLN	3.3
1	F	423	PRO	3.3
1	F	416	ILE	3.3
1	F	426	THR	3.3
1	F	391	ASP	3.3
1	F	196	MET	3.2
1	F	233	GLU	3.2
1	F	392	ILE	3.2
1	A	374	ARG	3.1
1	F	195	ARG	3.1
1	D	374	ARG	3.1
1	A	265	THR	3.0
1	F	397	TYR	3.0
1	F	420	ARG	3.0
1	E	310	GLN	3.0
1	B	382	GLU	2.9
1	F	424	VAL	2.9
1	F	201	GLN	2.9
1	E	421	ASN	2.9
2	I	509	HIS	2.9
1	B	230	LYS	2.9
1	D	231	THR	2.9
1	C	421	ASN	2.8
1	F	297	ARG	2.8
2	G	510	GLU	2.8
1	E	434	GLU	2.8
1	A	260	ALA	2.8
1	F	321	TYR	2.7
1	A	432	ILE	2.7
1	F	338	GLU	2.7
1	C	260	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	375	PRO	2.6
1	A	397	TYR	2.6
1	F	440	ASN	2.6
1	D	420	ARG	2.6
1	F	425	GLY	2.6
1	E	432	ILE	2.5
1	A	149	GLU	2.5
1	F	415	ILE	2.5
1	F	393	VAL	2.4
2	G	509	HIS	2.4
1	D	230	LYS	2.4
1	F	381	ARG	2.4
2	I	508	GLY	2.4
2	G	523	GLU	2.4
1	E	375	PRO	2.4
2	I	505	TYR	2.4
1	D	382	GLU	2.4
2	I	523	GLU	2.3
1	C	273	TRP	2.3
1	F	376	MET	2.3
1	E	374	ARG	2.3
1	F	184	THR	2.3
1	C	97	PRO	2.3
1	F	294	PRO	2.3
1	E	422	GLY	2.3
1	B	265	THR	2.3
1	B	397	TYR	2.2
1	F	375	PRO	2.2
1	E	351	ARG	2.2
1	A	97	PRO	2.2
1	A	420	ARG	2.2
1	D	423	PRO	2.2
1	F	295	SER	2.2
2	H	519	ARG	2.2
1	F	339	VAL	2.2
2	H	523	GLU	2.1
1	E	423	PRO	2.1
1	F	211	ARG	2.1
1	F	212	PRO	2.1
1	E	341	GLU	2.1
1	F	188	THR	2.1
1	E	131	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	212	PRO	2.1
1	F	434	GLU	2.1
1	C	149	GLU	2.0
1	C	382	GLU	2.0
1	D	428	GLN	2.0
1	C	434	GLU	2.0
1	C	261	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.