



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:09 AM GMT

PDB ID : 3MV2
Title : Crystal Structure of α -COP in Complex with e-COP
Authors : Hoelz, A.; Hsia, K.C.
Deposited on : 2010-05-03
Resolution : 2.90 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>

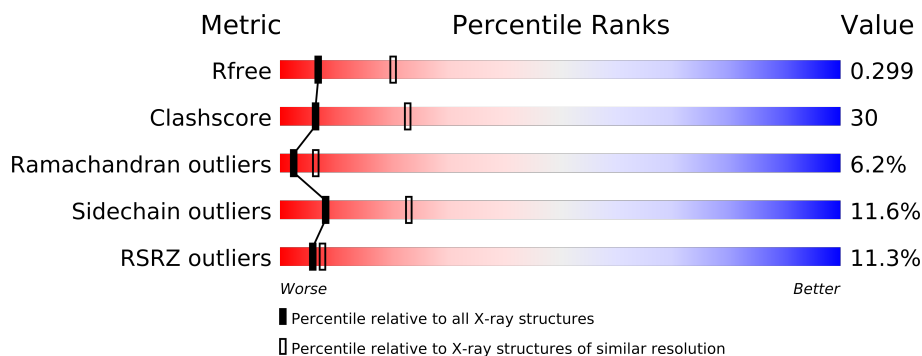
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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	325	
1	C	325	
1	E	325	
2	B	310	
2	D	310	
2	F	310	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14273 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 Coatomer subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2405	1542	403	449	11			
1	C	303	Total	C	N	O	S	0	0	0
			2388	1531	399	447	11			
1	E	303	Total	C	N	O	S	0	0	0
			2388	1531	399	447	11			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP P53622
A	-21	GLY	-	EXPRESSION TAG	UNP P53622
A	-20	SER	-	EXPRESSION TAG	UNP P53622
A	-19	SER	-	EXPRESSION TAG	UNP P53622
A	-18	HIS	-	EXPRESSION TAG	UNP P53622
A	-17	HIS	-	EXPRESSION TAG	UNP P53622
A	-16	HIS	-	EXPRESSION TAG	UNP P53622
A	-15	HIS	-	EXPRESSION TAG	UNP P53622
A	-14	HIS	-	EXPRESSION TAG	UNP P53622
A	-13	HIS	-	EXPRESSION TAG	UNP P53622
A	-12	SER	-	EXPRESSION TAG	UNP P53622
A	-11	SER	-	EXPRESSION TAG	UNP P53622
A	-10	GLY	-	EXPRESSION TAG	UNP P53622
A	-9	LEU	-	EXPRESSION TAG	UNP P53622
A	-8	GLU	-	EXPRESSION TAG	UNP P53622
A	-7	VAL	-	EXPRESSION TAG	UNP P53622
A	-6	LEU	-	EXPRESSION TAG	UNP P53622
A	-5	PHE	-	EXPRESSION TAG	UNP P53622
A	-4	GLN	-	EXPRESSION TAG	UNP P53622
A	-3	GLY	-	EXPRESSION TAG	UNP P53622
A	-2	PRO	-	EXPRESSION TAG	UNP P53622
A	-1	HIS	-	EXPRESSION TAG	UNP P53622
A	0	MET	-	EXPRESSION TAG	UNP P53622

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MET	-	EXPRESSION TAG	UNP P53622
C	-21	GLY	-	EXPRESSION TAG	UNP P53622
C	-20	SER	-	EXPRESSION TAG	UNP P53622
C	-19	SER	-	EXPRESSION TAG	UNP P53622
C	-18	HIS	-	EXPRESSION TAG	UNP P53622
C	-17	HIS	-	EXPRESSION TAG	UNP P53622
C	-16	HIS	-	EXPRESSION TAG	UNP P53622
C	-15	HIS	-	EXPRESSION TAG	UNP P53622
C	-14	HIS	-	EXPRESSION TAG	UNP P53622
C	-13	HIS	-	EXPRESSION TAG	UNP P53622
C	-12	SER	-	EXPRESSION TAG	UNP P53622
C	-11	SER	-	EXPRESSION TAG	UNP P53622
C	-10	GLY	-	EXPRESSION TAG	UNP P53622
C	-9	LEU	-	EXPRESSION TAG	UNP P53622
C	-8	GLU	-	EXPRESSION TAG	UNP P53622
C	-7	VAL	-	EXPRESSION TAG	UNP P53622
C	-6	LEU	-	EXPRESSION TAG	UNP P53622
C	-5	PHE	-	EXPRESSION TAG	UNP P53622
C	-4	GLN	-	EXPRESSION TAG	UNP P53622
C	-3	GLY	-	EXPRESSION TAG	UNP P53622
C	-2	PRO	-	EXPRESSION TAG	UNP P53622
C	-1	HIS	-	EXPRESSION TAG	UNP P53622
C	0	MET	-	EXPRESSION TAG	UNP P53622
E	-22	MET	-	EXPRESSION TAG	UNP P53622
E	-21	GLY	-	EXPRESSION TAG	UNP P53622
E	-20	SER	-	EXPRESSION TAG	UNP P53622
E	-19	SER	-	EXPRESSION TAG	UNP P53622
E	-18	HIS	-	EXPRESSION TAG	UNP P53622
E	-17	HIS	-	EXPRESSION TAG	UNP P53622
E	-16	HIS	-	EXPRESSION TAG	UNP P53622
E	-15	HIS	-	EXPRESSION TAG	UNP P53622
E	-14	HIS	-	EXPRESSION TAG	UNP P53622
E	-13	HIS	-	EXPRESSION TAG	UNP P53622
E	-12	SER	-	EXPRESSION TAG	UNP P53622
E	-11	SER	-	EXPRESSION TAG	UNP P53622
E	-10	GLY	-	EXPRESSION TAG	UNP P53622
E	-9	LEU	-	EXPRESSION TAG	UNP P53622
E	-8	GLU	-	EXPRESSION TAG	UNP P53622
E	-7	VAL	-	EXPRESSION TAG	UNP P53622
E	-6	LEU	-	EXPRESSION TAG	UNP P53622
E	-5	PHE	-	EXPRESSION TAG	UNP P53622
E	-4	GLN	-	EXPRESSION TAG	UNP P53622

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	EXPRESSION TAG	UNP P53622
E	-2	PRO	-	EXPRESSION TAG	UNP P53622
E	-1	HIS	-	EXPRESSION TAG	UNP P53622
E	0	MET	-	EXPRESSION TAG	UNP P53622

- Molecule 2 is a protein called Coatomer subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	293	Total	C	N	O	S	0	0	0
			2364	1508	371	480	5			
2	D	293	Total	C	N	O	S	0	0	0
			2364	1508	371	480	5			
2	F	293	Total	C	N	O	S	0	0	0
			2364	1508	371	480	5			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	EXPRESSION TAG	UNP P40509
B	-12	GLY	-	EXPRESSION TAG	UNP P40509
B	-11	SER	-	EXPRESSION TAG	UNP P40509
B	-10	SER	-	EXPRESSION TAG	UNP P40509
B	-9	HIS	-	EXPRESSION TAG	UNP P40509
B	-8	HIS	-	EXPRESSION TAG	UNP P40509
B	-7	HIS	-	EXPRESSION TAG	UNP P40509
B	-6	HIS	-	EXPRESSION TAG	UNP P40509
B	-5	HIS	-	EXPRESSION TAG	UNP P40509
B	-4	HIS	-	EXPRESSION TAG	UNP P40509
B	-3	SER	-	EXPRESSION TAG	UNP P40509
B	-2	GLN	-	EXPRESSION TAG	UNP P40509
B	-1	ASP	-	EXPRESSION TAG	UNP P40509
B	0	PRO	-	EXPRESSION TAG	UNP P40509
D	-13	MET	-	EXPRESSION TAG	UNP P40509
D	-12	GLY	-	EXPRESSION TAG	UNP P40509
D	-11	SER	-	EXPRESSION TAG	UNP P40509
D	-10	SER	-	EXPRESSION TAG	UNP P40509
D	-9	HIS	-	EXPRESSION TAG	UNP P40509
D	-8	HIS	-	EXPRESSION TAG	UNP P40509
D	-7	HIS	-	EXPRESSION TAG	UNP P40509
D	-6	HIS	-	EXPRESSION TAG	UNP P40509
D	-5	HIS	-	EXPRESSION TAG	UNP P40509
D	-4	HIS	-	EXPRESSION TAG	UNP P40509

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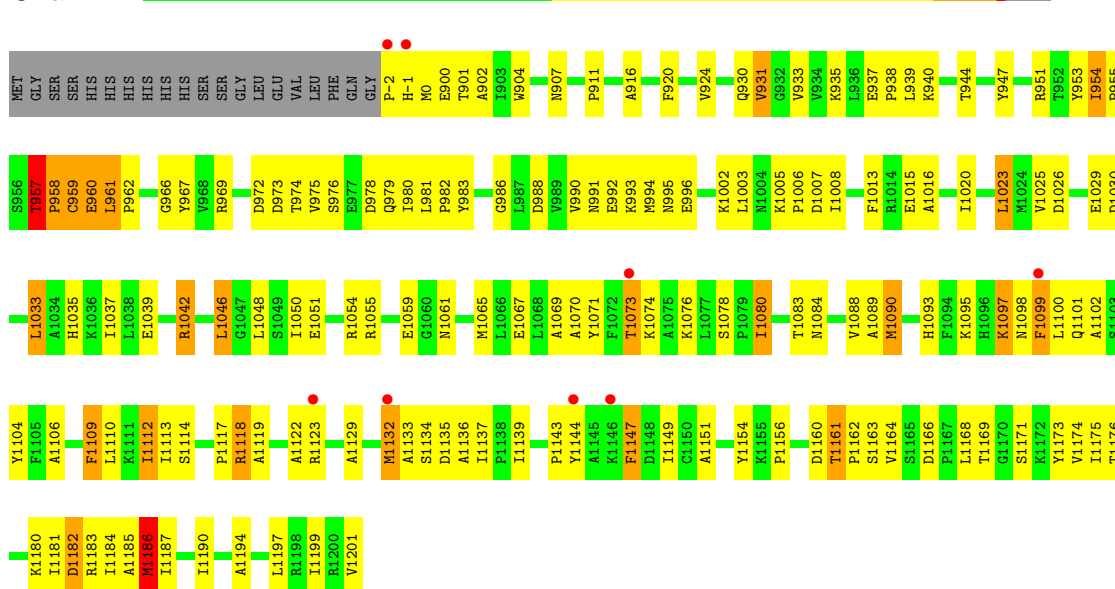
Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	SER	-	EXPRESSION TAG	UNP P40509
D	-2	GLN	-	EXPRESSION TAG	UNP P40509
D	-1	ASP	-	EXPRESSION TAG	UNP P40509
D	0	PRO	-	EXPRESSION TAG	UNP P40509
F	-13	MET	-	EXPRESSION TAG	UNP P40509
F	-12	GLY	-	EXPRESSION TAG	UNP P40509
F	-11	SER	-	EXPRESSION TAG	UNP P40509
F	-10	SER	-	EXPRESSION TAG	UNP P40509
F	-9	HIS	-	EXPRESSION TAG	UNP P40509
F	-8	HIS	-	EXPRESSION TAG	UNP P40509
F	-7	HIS	-	EXPRESSION TAG	UNP P40509
F	-6	HIS	-	EXPRESSION TAG	UNP P40509
F	-5	HIS	-	EXPRESSION TAG	UNP P40509
F	-4	HIS	-	EXPRESSION TAG	UNP P40509
F	-3	SER	-	EXPRESSION TAG	UNP P40509
F	-2	GLN	-	EXPRESSION TAG	UNP P40509
F	-1	ASP	-	EXPRESSION TAG	UNP P40509
F	0	PRO	-	EXPRESSION TAG	UNP P40509

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.

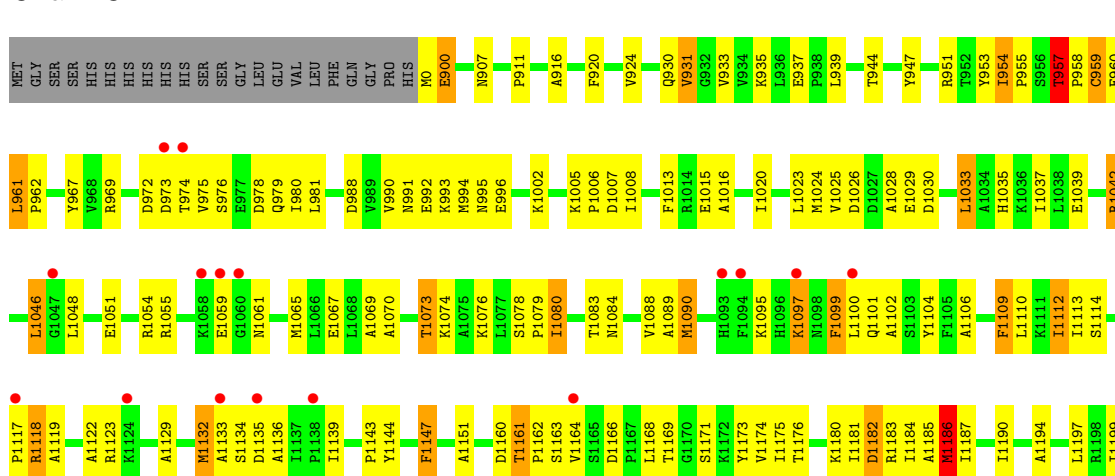
- Molecule 1: Coatomer subunit alpha

Chain A:



- Molecule 1: Coatomer subunit alpha

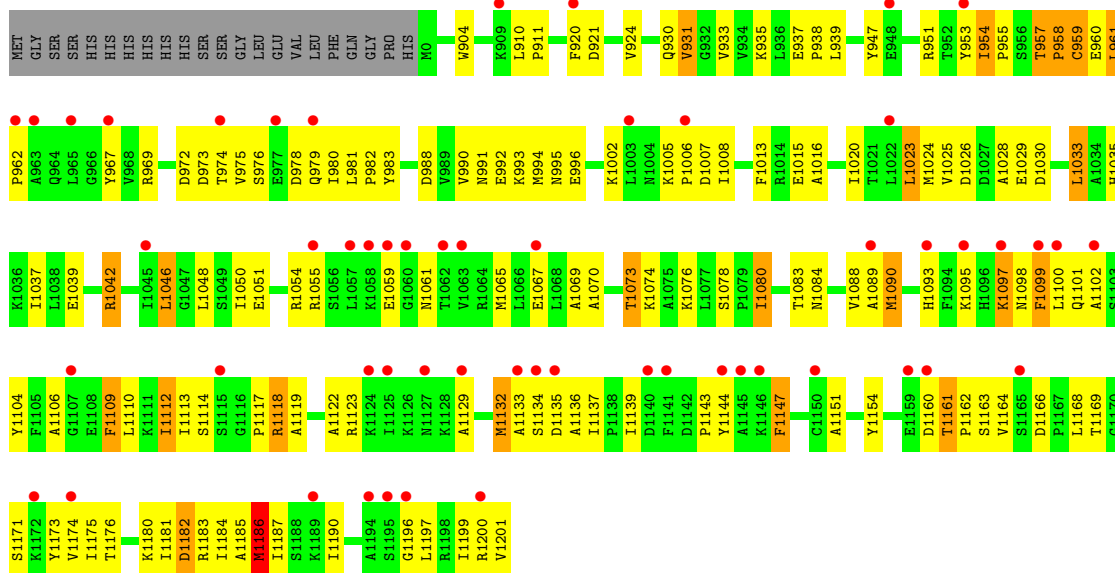
Chain C:



R1200
V1201

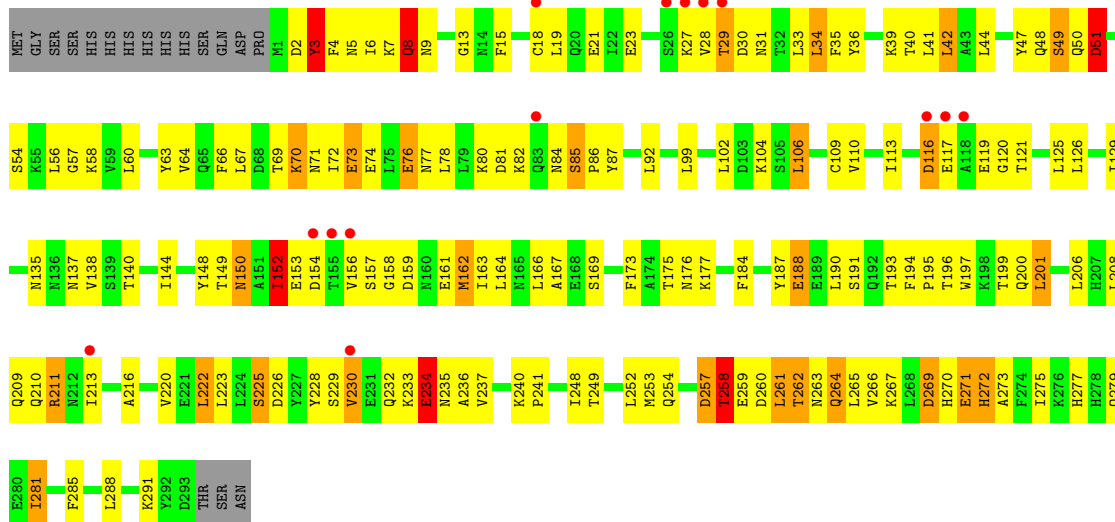
• Molecule 1: Coatomer subunit alpha

Chain E:



• Molecule 2: Coatomer subunit epsilon

Chain B:



• Molecule 2: Coatomer subunit epsilon

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	329.13Å 74.38Å 97.25Å 90.00° 102.27° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.02 – 2.90	Depositor EDS
% Data completeness (in resolution range)	85.4 (20.00-2.90) 85.9 (20.02-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.297 0.247 , 0.299	Depositor DCC
R_{free} test set	1938 reflections (4.43%)	DCC
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 78.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	4 of 47412 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14273	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.52	0/2454	0.74	1/3317 (0.0%)
1	C	0.52	0/2435	0.74	1/3291 (0.0%)
1	E	0.49	0/2435	0.73	1/3291 (0.0%)
2	B	0.53	0/2403	0.79	3/3261 (0.1%)
2	D	0.51	0/2403	0.76	1/3261 (0.0%)
2	F	0.49	0/2403	0.76	1/3261 (0.0%)
All	All	0.51	0/14533	0.75	8/19682 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	116	ASP	CB-CA-C	-5.51	99.39	110.40
2	F	264	GLN	N-CA-C	-5.44	96.31	111.00
2	D	264	GLN	N-CA-C	-5.43	96.34	111.00
2	B	264	GLN	N-CA-C	-5.41	96.40	111.00
1	A	961	LEU	N-CA-C	-5.10	97.23	111.00
1	C	961	LEU	N-CA-C	-5.07	97.31	111.00
1	E	961	LEU	N-CA-C	-5.05	97.37	111.00
2	B	116	ASP	N-CA-C	5.02	124.56	111.00

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	2405	0	2455	161	0
1	C	2388	0	2441	137	0
1	E	2388	0	2441	148	0
2	B	2364	0	2319	140	0
2	D	2364	0	2319	160	0
2	F	2364	0	2319	165	0
All	All	14273	0	14294	863	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 30.

All (863) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1166:ASP:OD2	1:A:1169:THR:HB	1.59	1.03
1:E:1166:ASP:OD2	1:E:1169:THR:HB	1.59	1.03
1:C:1166:ASP:OD2	1:C:1169:THR:HB	1.59	1.02
2:D:248:ILE:HD11	2:D:263:ASN:HB3	1.43	0.99
2:F:248:ILE:HD11	2:F:263:ASN:HB3	1.43	0.98
2:D:264:GLN:HA	2:D:264:GLN:OE1	1.65	0.97
2:B:248:ILE:HD11	2:B:263:ASN:HB3	1.44	0.97
1:C:1080:ILE:HB	2:F:227:TYR:CD2	2.02	0.95
2:B:264:GLN:HA	2:B:264:GLN:OE1	1.65	0.94
2:F:264:GLN:HA	2:F:264:GLN:OE1	1.65	0.93
2:F:41:LEU:HB3	2:F:47:TYR:HA	1.49	0.91
1:A:957:THR:HG22	1:A:958:PRO:N	1.82	0.90
2:F:34:LEU:HD11	2:F:57:GLY:CA	2.01	0.90
2:F:277:HIS:O	2:F:281:ILE:HG22	1.72	0.90
1:A:-2:PRO:H3	1:A:901:THR:HG21	1.35	0.90
2:D:277:HIS:O	2:D:281:ILE:HG22	1.72	0.88
2:B:277:HIS:O	2:B:281:ILE:HG22	1.73	0.87
1:C:1080:ILE:HB	2:F:227:TYR:CE2	2.10	0.87
2:F:157:SER:O	2:F:161:GLU:HB2	1.76	0.86
1:C:957:THR:HG22	1:C:958:PRO:N	1.90	0.86
1:E:1074:LYS:HE3	1:E:1147:PHE:HE1	1.40	0.86
1:E:1169:THR:HG22	1:E:1171:SER:H	1.42	0.85
1:C:1169:THR:HG22	1:C:1171:SER:H	1.41	0.85
1:A:1008:ILE:HD12	1:A:1008:ILE:H	1.43	0.84
1:E:1008:ILE:H	1:E:1008:ILE:HD12	1.43	0.83
1:A:-2:PRO:N	1:A:901:THR:HG21	1.93	0.83
1:C:1008:ILE:H	1:C:1008:ILE:HD12	1.43	0.83
1:A:1097:LYS:HG3	1:A:1099:PHE:HE1	1.43	0.83
1:A:1169:THR:HG22	1:A:1171:SER:H	1.42	0.83
1:E:1097:LYS:HG3	1:E:1099:PHE:HE1	1.43	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:1074:LYS:HE3	1:E:1147:PHE:CE1	2.15	0.82
2:B:248:ILE:CD1	2:B:263:ASN:HB3	2.10	0.81
2:B:157:SER:O	2:B:161:GLU:HB2	1.80	0.81
2:D:252:LEU:HD21	2:D:259:GLU:HG3	1.62	0.81
1:C:1028:ALA:HB2	1:C:1200:ARG:HH12	1.44	0.81
2:D:216:ALA:O	2:D:220:VAL:HG23	1.81	0.81
2:F:216:ALA:O	2:F:220:VAL:HG23	1.81	0.81
1:E:957:THR:HG22	1:E:958:PRO:N	1.94	0.81
1:A:-2:PRO:CA	1:A:901:THR:HG21	2.10	0.80
2:F:248:ILE:CD1	2:F:263:ASN:HB3	2.10	0.80
1:C:1097:LYS:HG3	1:C:1099:PHE:HE1	1.43	0.80
2:B:252:LEU:HD21	2:B:259:GLU:HG3	1.63	0.80
1:A:1113:ILE:HG23	2:D:150:ASN:ND2	1.97	0.80
2:F:252:LEU:HD21	2:F:259:GLU:HG3	1.62	0.80
2:D:248:ILE:CD1	2:D:263:ASN:HB3	2.10	0.80
1:E:1100:LEU:HD22	1:E:1135:ASP:OD1	1.81	0.80
2:B:216:ALA:O	2:B:220:VAL:HG23	1.81	0.80
1:A:-2:PRO:HA	1:A:901:THR:HG21	1.65	0.79
2:D:60:LEU:O	2:D:64:VAL:HG23	1.83	0.79
1:C:1005:LYS:HB3	1:C:1008:ILE:HD13	1.64	0.78
2:F:60:LEU:O	2:F:64:VAL:HG23	1.83	0.78
1:E:1005:LYS:HB3	1:E:1008:ILE:HD13	1.64	0.78
1:E:931:VAL:HG12	1:E:933:VAL:HG23	1.66	0.78
2:B:60:LEU:O	2:B:64:VAL:HG23	1.84	0.78
1:A:1005:LYS:HB3	1:A:1008:ILE:HD13	1.64	0.78
2:B:50:GLN:O	2:B:51:ASP:HB3	1.83	0.77
1:A:931:VAL:HG12	1:A:933:VAL:HG23	1.66	0.77
1:A:931:VAL:HG13	1:A:1168:LEU:HB2	1.67	0.77
2:F:50:GLN:O	2:F:51:ASP:HB3	1.83	0.77
1:E:920:PHE:O	1:E:924:VAL:HG23	1.85	0.76
2:D:227:TYR:HE1	1:E:1113:ILE:CD1	1.98	0.76
1:C:920:PHE:O	1:C:924:VAL:HG23	1.85	0.76
1:C:1074:LYS:HE3	1:C:1147:PHE:HE1	1.49	0.76
1:A:1118:ARG:HB3	2:D:146:ASP:OD2	1.85	0.76
1:C:931:VAL:HG12	1:C:933:VAL:HG23	1.66	0.76
1:C:1099:PHE:HA	1:C:1102:ALA:HB3	1.69	0.76
1:A:1097:LYS:O	1:A:1136:ALA:HB2	1.86	0.75
2:D:175:THR:HG21	2:D:177:LYS:HD3	1.68	0.75
2:F:41:LEU:CB	2:F:47:TYR:HA	2.16	0.75
1:A:920:PHE:O	1:A:924:VAL:HG23	1.85	0.75
1:C:1074:LYS:HE3	1:C:1147:PHE:CE1	2.20	0.75
2:F:175:THR:HG21	2:F:177:LYS:HD3	1.68	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:175:THR:HG21	2:B:177:LYS:HD3	1.68	0.75
1:A:944:THR:HA	2:B:281:ILE:HD11	1.68	0.75
1:E:954:ILE:HD13	1:E:955:PRO:N	2.02	0.75
2:D:50:GLN:O	2:D:51:ASP:HB3	1.83	0.75
1:C:1028:ALA:HB2	1:C:1200:ARG:NH1	2.01	0.75
1:A:954:ILE:HD13	1:A:955:PRO:N	2.02	0.75
1:A:1097:LYS:HG3	1:A:1099:PHE:CE1	2.21	0.75
2:B:15:PHE:HB3	2:B:40:THR:HG23	1.69	0.74
1:A:1099:PHE:HA	1:A:1102:ALA:HB3	1.69	0.74
1:E:1097:LYS:HG3	1:E:1099:PHE:CE1	2.21	0.74
2:D:15:PHE:HB3	2:D:40:THR:HG23	1.69	0.74
2:F:38:ALA:HB1	2:F:47:TYR:HE1	1.50	0.74
1:C:954:ILE:HD13	1:C:955:PRO:N	2.02	0.74
1:C:1097:LYS:HG3	1:C:1099:PHE:CE1	2.21	0.74
2:F:15:PHE:HB3	2:F:40:THR:HG23	1.69	0.74
2:F:210:GLN:O	2:F:211:ARG:HB2	1.88	0.73
2:D:57:GLY:HA2	2:D:60:LEU:HD12	1.70	0.73
2:F:57:GLY:HA2	2:F:60:LEU:HD12	1.70	0.73
1:A:1118:ARG:HD2	2:D:146:ASP:OD2	1.87	0.73
2:D:112:GLY:O	2:D:115:ASN:HB2	1.89	0.73
2:B:2:ASP:O	2:B:4:PHE:N	2.20	0.73
1:E:1099:PHE:HA	1:E:1102:ALA:HB3	1.69	0.73
2:B:210:GLN:O	2:B:211:ARG:HB2	1.88	0.73
1:A:1132:MET:O	1:A:1134:SER:N	2.22	0.73
2:F:112:GLY:O	2:F:115:ASN:HB2	1.88	0.73
2:B:275:ILE:O	2:B:279:GLN:HG3	1.89	0.73
2:D:210:GLN:O	2:D:211:ARG:HB2	1.88	0.73
2:D:275:ILE:O	2:D:279:GLN:HG3	1.89	0.73
1:A:-2:PRO:HA	1:A:901:THR:CG2	2.19	0.72
1:E:938:PRO:HG2	1:E:1187:ILE:HD11	1.70	0.72
1:C:972:ASP:O	1:C:974:THR:N	2.22	0.72
1:C:1090:MET:HG3	1:C:1106:ALA:HB2	1.72	0.72
1:A:1181:ILE:O	1:A:1181:ILE:HD12	1.90	0.72
1:C:1181:ILE:O	1:C:1181:ILE:HD12	1.90	0.72
1:E:1097:LYS:O	1:E:1136:ALA:HB2	1.90	0.72
1:E:947:TYR:CD2	2:F:281:ILE:HD12	2.25	0.71
1:A:-1:HIS:H	1:A:901:THR:HB	1.55	0.71
2:F:275:ILE:O	2:F:279:GLN:HG3	1.89	0.71
1:E:972:ASP:O	1:E:974:THR:N	2.22	0.71
1:A:972:ASP:O	1:A:974:THR:N	2.22	0.71
1:E:1181:ILE:HD12	1:E:1181:ILE:O	1.90	0.71
1:C:931:VAL:HG13	1:C:1168:LEU:HB2	1.73	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1090:MET:HG3	1:A:1106:ALA:HB2	1.72	0.71
1:E:1067:GLU:HG3	1:E:1139:ILE:HG22	1.71	0.71
2:B:57:GLY:HA2	2:B:60:LEU:HD12	1.70	0.71
1:A:957:THR:CG2	1:A:958:PRO:N	2.54	0.71
1:E:1090:MET:HG3	1:E:1106:ALA:HB2	1.72	0.71
1:E:1113:ILE:CG2	1:E:1119:ALA:HB2	2.21	0.70
1:C:1113:ILE:CG2	1:C:1119:ALA:HB2	2.21	0.70
1:A:1113:ILE:CG2	1:A:1119:ALA:HB2	2.21	0.70
2:F:196:THR:HG22	2:F:197:TRP:H	1.56	0.70
1:A:1074:LYS:HE3	1:A:1147:PHE:HE1	1.57	0.70
2:B:19:LEU:O	2:B:23:GLU:HG2	1.92	0.69
1:C:1113:ILE:HD12	2:F:231:GLU:HB3	1.74	0.69
2:D:19:LEU:O	2:D:23:GLU:HG2	1.92	0.69
2:F:19:LEU:O	2:F:23:GLU:HG2	1.92	0.69
1:A:1070:ALA:O	1:A:1073:THR:HB	1.92	0.69
2:B:106:LEU:O	2:B:110:VAL:HG23	1.92	0.69
1:C:1070:ALA:O	1:C:1073:THR:HB	1.92	0.69
2:F:106:LEU:O	2:F:110:VAL:HG23	1.92	0.69
2:B:196:THR:HG22	2:B:197:TRP:H	1.56	0.69
1:E:1151:ALA:HB3	1:E:1173:TYR:CE2	2.28	0.69
2:D:196:THR:HG22	2:D:197:TRP:H	1.56	0.69
2:D:106:LEU:O	2:D:110:VAL:HG23	1.92	0.69
2:B:196:THR:HG22	2:B:197:TRP:N	2.08	0.69
2:F:28:VAL:HG12	2:F:28:VAL:O	1.93	0.69
1:C:1151:ALA:HB3	1:C:1173:TYR:CE2	2.28	0.69
1:E:1070:ALA:O	1:E:1073:THR:HB	1.92	0.68
1:A:1151:ALA:HB3	1:A:1173:TYR:CE2	2.28	0.68
2:D:28:VAL:HG12	2:D:28:VAL:O	1.93	0.68
1:C:1132:MET:O	1:C:1134:SER:N	2.27	0.68
2:F:196:THR:HG22	2:F:197:TRP:N	2.08	0.68
2:D:196:THR:HG22	2:D:197:TRP:N	2.08	0.68
2:B:28:VAL:HG12	2:B:28:VAL:O	1.93	0.68
1:C:957:THR:HG22	1:C:958:PRO:CD	2.24	0.68
2:F:1:MET:C	2:F:3:TYR:H	1.95	0.68
2:D:222:LEU:O	2:D:225:SER:HB3	1.94	0.68
2:F:222:LEU:O	2:F:225:SER:HB3	1.94	0.68
2:F:44:LEU:HA	2:F:234:GLU:OE1	1.95	0.67
1:A:1099:PHE:HD1	1:A:1134:SER:HB3	1.58	0.67
1:C:944:THR:HA	2:D:281:ILE:HD11	1.75	0.67
1:E:957:THR:HB	2:F:130:GLU:OE2	1.95	0.67
1:E:1099:PHE:HD1	1:E:1134:SER:HB3	1.60	0.67
2:B:222:LEU:O	2:B:225:SER:HB3	1.95	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:41:LEU:HB3	2:F:47:TYR:CA	2.25	0.67
1:A:957:THR:HG22	1:A:958:PRO:CD	2.25	0.67
1:A:1006:PRO:HB3	1:A:1048:LEU:HD22	1.77	0.67
1:E:1008:ILE:N	1:E:1008:ILE:HD12	2.10	0.66
2:B:15:PHE:HB2	2:B:44:LEU:HD21	1.77	0.66
1:C:1197:LEU:HD21	1:C:1199:ILE:HD11	1.76	0.66
1:C:1100:LEU:HD22	1:C:1135:ASP:OD1	1.95	0.66
1:E:1006:PRO:HB3	1:E:1048:LEU:HD22	1.77	0.66
1:C:1008:ILE:HD12	1:C:1008:ILE:N	2.10	0.66
1:A:1100:LEU:HD22	1:A:1135:ASP:OD1	1.94	0.66
1:C:1006:PRO:HB3	1:C:1048:LEU:HD22	1.77	0.66
2:D:227:TYR:CE1	1:E:1113:ILE:CD1	2.78	0.66
1:A:1197:LEU:HD21	1:A:1199:ILE:HD11	1.77	0.66
1:E:1132:MET:O	1:E:1134:SER:N	2.29	0.66
1:E:1100:LEU:HB2	1:E:1134:SER:O	1.95	0.65
2:F:190:LEU:HB3	2:F:199:THR:HG22	1.78	0.65
2:F:15:PHE:HB2	2:F:44:LEU:HD21	1.78	0.65
1:E:1197:LEU:HD21	1:E:1199:ILE:HD11	1.77	0.65
2:D:15:PHE:HB2	2:D:44:LEU:HD21	1.77	0.65
1:C:1109:PHE:HZ	1:C:1118:ARG:HD3	1.62	0.65
2:D:190:LEU:HB3	2:D:199:THR:HG22	1.78	0.64
2:F:257:ASP:O	2:F:259:GLU:N	2.31	0.64
2:D:227:TYR:CE1	1:E:1113:ILE:HD11	2.32	0.64
1:A:1074:LYS:HE3	1:A:1147:PHE:CE1	2.32	0.64
1:A:1008:ILE:N	1:A:1008:ILE:HD12	2.10	0.64
2:B:257:ASP:O	2:B:259:GLU:N	2.31	0.64
2:B:190:LEU:HB3	2:B:199:THR:HG22	1.78	0.64
2:F:8:GLN:O	2:F:8:GLN:HG3	1.98	0.64
2:D:257:ASP:O	2:D:259:GLU:N	2.31	0.64
1:A:1109:PHE:HZ	1:A:1118:ARG:HD3	1.62	0.64
2:F:34:LEU:HD11	2:F:57:GLY:HA3	1.80	0.64
2:F:42:LEU:CD2	2:F:64:VAL:HG13	2.28	0.64
1:A:1169:THR:HG22	1:A:1171:SER:N	2.13	0.63
2:D:227:TYR:HE1	1:E:1113:ILE:HD13	1.61	0.63
1:E:1083:THR:HG21	1:E:1118:ARG:NH1	2.14	0.63
1:A:1083:THR:HG21	1:A:1118:ARG:NH1	2.14	0.63
2:D:269:ASP:OD1	2:D:269:ASP:C	2.37	0.63
1:C:1169:THR:HG22	1:C:1171:SER:N	2.13	0.63
1:C:1104:TYR:CE2	1:C:1143:PRO:HB3	2.33	0.63
1:E:1109:PHE:HZ	1:E:1118:ARG:HD3	1.62	0.62
2:F:269:ASP:C	2:F:269:ASP:OD1	2.37	0.62
2:B:8:GLN:HG3	2:B:8:GLN:O	1.98	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:269:ASP:C	2:B:269:ASP:OD1	2.37	0.62
1:A:957:THR:O	1:A:959:CYS:N	2.32	0.62
1:C:1109:PHE:CD2	1:C:1109:PHE:C	2.73	0.62
1:C:1083:THR:HG21	1:C:1118:ARG:NH1	2.14	0.62
1:C:1042:ARG:HB2	1:C:1184:ILE:HG21	1.80	0.62
1:A:1003:LEU:HD21	2:D:110:VAL:HG21	1.81	0.62
1:C:957:THR:CG2	1:C:958:PRO:N	2.63	0.62
1:A:1109:PHE:CD2	1:A:1109:PHE:C	2.73	0.62
2:D:8:GLN:O	2:D:8:GLN:HG3	1.98	0.62
2:F:261:LEU:O	2:F:261:LEU:HD12	2.00	0.62
2:F:211:ARG:HG2	2:F:211:ARG:HH11	1.65	0.62
1:E:1169:THR:HG22	1:E:1171:SER:N	2.13	0.61
2:D:211:ARG:HH11	2:D:211:ARG:HG2	1.65	0.61
2:B:211:ARG:HG2	2:B:211:ARG:HH11	1.65	0.61
1:C:924:VAL:HG21	2:D:288:LEU:HD13	1.81	0.61
2:F:125:LEU:HD22	2:F:148:TYR:CD2	2.36	0.61
2:D:3:TYR:HB3	2:D:6:ILE:HD13	1.81	0.61
2:D:261:LEU:O	2:D:261:LEU:HD12	2.00	0.61
2:F:3:TYR:HB3	2:F:6:ILE:HD13	1.81	0.61
2:B:3:TYR:HB3	2:B:6:ILE:HD13	1.81	0.61
1:A:1042:ARG:HB2	1:A:1184:ILE:HG21	1.83	0.61
1:E:1109:PHE:C	1:E:1109:PHE:CD2	2.73	0.61
1:A:1113:ILE:HG21	1:A:1119:ALA:HB2	1.83	0.61
1:E:931:VAL:HG13	1:E:1168:LEU:HB2	1.83	0.60
2:D:125:LEU:HD22	2:D:148:TYR:CD2	2.36	0.60
2:B:125:LEU:O	2:B:129:ILE:HD13	2.01	0.60
2:B:85:SER:HB2	2:B:117:GLU:HG3	1.82	0.60
2:B:261:LEU:HD12	2:B:261:LEU:O	2.00	0.60
1:E:1067:GLU:HA	1:E:1139:ILE:HG21	1.83	0.60
1:C:957:THR:O	1:C:959:CYS:N	2.34	0.60
1:E:957:THR:O	1:E:959:CYS:N	2.34	0.60
1:A:1113:ILE:HG23	2:D:150:ASN:HD21	1.66	0.60
2:F:125:LEU:O	2:F:129:ILE:HD13	2.01	0.60
1:C:990:VAL:HG11	1:C:1020:ILE:HD11	1.83	0.60
2:B:262:THR:HG22	2:B:263:ASN:N	2.17	0.60
2:B:125:LEU:HD22	2:B:148:TYR:CD2	2.36	0.60
2:F:262:THR:HG22	2:F:263:ASN:N	2.17	0.60
1:A:1113:ILE:HG22	1:A:1119:ALA:HB2	1.84	0.60
1:E:990:VAL:HG11	1:E:1020:ILE:HD11	1.83	0.60
1:A:990:VAL:HG11	1:A:1020:ILE:HD11	1.83	0.60
1:C:1113:ILE:HG21	1:C:1119:ALA:HB2	1.84	0.59
2:D:125:LEU:O	2:D:129:ILE:HD13	2.01	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1008:ILE:CD1	1:A:1008:ILE:H	2.13	0.59
1:E:1113:ILE:HG22	1:E:1119:ALA:HB2	1.84	0.59
1:A:1067:GLU:HG3	1:A:1139:ILE:HG22	1.84	0.59
1:E:1042:ARG:HB2	1:E:1184:ILE:HG21	1.84	0.59
2:D:262:THR:HG22	2:D:263:ASN:N	2.17	0.59
2:F:34:LEU:HD11	2:F:57:GLY:HA2	1.82	0.59
1:E:1113:ILE:HG21	1:E:1119:ALA:HB2	1.83	0.59
2:F:41:LEU:HD13	2:F:46:GLN:O	2.02	0.59
1:C:933:VAL:HG13	1:C:1187:ILE:HG23	1.85	0.58
2:F:72:ILE:HG13	2:F:99:LEU:CD1	2.33	0.58
1:A:940:LYS:HG3	2:B:285:PHE:CD2	2.39	0.58
2:D:47:TYR:CE2	2:D:64:VAL:HG21	2.39	0.58
2:B:184:PHE:O	2:B:188:GLU:HB2	2.03	0.58
2:D:44:LEU:HD23	2:D:234:GLU:OE1	2.03	0.58
2:B:162:MET:HG2	2:B:163:ILE:N	2.18	0.58
2:D:157:SER:O	2:D:161:GLU:HB2	2.04	0.58
1:C:957:THR:HG22	1:C:958:PRO:HD3	1.85	0.58
2:F:37:LYS:HE2	2:F:50:GLN:OE1	2.03	0.58
2:F:184:PHE:O	2:F:188:GLU:HB2	2.03	0.58
2:F:162:MET:HG2	2:F:163:ILE:N	2.18	0.58
1:E:1008:ILE:H	1:E:1008:ILE:CD1	2.13	0.58
2:D:194:PHE:O	2:D:196:THR:N	2.36	0.58
2:F:47:TYR:CE2	2:F:64:VAL:HG21	2.39	0.58
2:B:194:PHE:O	2:B:196:THR:N	2.36	0.58
1:C:1008:ILE:H	1:C:1008:ILE:CD1	2.13	0.58
1:C:1113:ILE:HG22	1:C:1119:ALA:HB2	1.84	0.58
2:B:47:TYR:CE2	2:B:64:VAL:HG21	2.39	0.57
1:C:1007:ASP:HB2	1:C:1008:ILE:HD12	1.86	0.57
1:C:1025:VAL:CG1	1:C:1030:ASP:HB2	2.35	0.57
2:D:184:PHE:O	2:D:188:GLU:HB2	2.03	0.57
1:E:1007:ASP:HB2	1:E:1008:ILE:HD12	1.86	0.57
2:F:260:ASP:O	2:F:264:GLN:HG2	2.05	0.57
1:E:1025:VAL:CG1	1:E:1030:ASP:HB2	2.35	0.57
1:C:961:LEU:HD13	2:D:94:THR:HG23	1.86	0.57
2:B:261:LEU:O	2:B:264:GLN:HB2	2.04	0.57
2:F:261:LEU:O	2:F:264:GLN:HB2	2.05	0.57
1:C:1099:PHE:HD1	1:C:1134:SER:HB3	1.70	0.57
2:F:194:PHE:O	2:F:196:THR:N	2.36	0.57
2:D:166:LEU:O	2:D:169:SER:HB3	2.05	0.57
1:A:1097:LYS:HG2	1:A:1097:LYS:O	2.05	0.57
1:E:1097:LYS:HG2	1:E:1097:LYS:O	2.05	0.57
2:D:222:LEU:C	2:D:222:LEU:CD2	2.73	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:162:MET:HG2	2:D:163:ILE:N	2.18	0.57
1:A:930:GLN:O	1:A:1194:ALA:HB1	2.05	0.57
1:A:983:TYR:CE2	2:B:253:MET:HG2	2.40	0.57
2:F:222:LEU:HD23	2:F:222:LEU:O	2.05	0.57
1:E:938:PRO:HG2	1:E:1187:ILE:CD1	2.35	0.57
2:D:109:CYS:O	2:D:113:ILE:HG13	2.05	0.57
1:A:924:VAL:HG21	2:B:288:LEU:HD13	1.87	0.56
2:D:197:TRP:O	2:D:201:LEU:HB2	2.05	0.56
2:D:222:LEU:O	2:D:222:LEU:HD23	2.04	0.56
1:C:1067:GLU:HG3	1:C:1139:ILE:HG22	1.87	0.56
1:C:1097:LYS:HG2	1:C:1097:LYS:O	2.05	0.56
2:F:197:TRP:O	2:F:201:LEU:HB2	2.05	0.56
2:F:122:THR:HG21	2:F:160:ASN:HB3	1.87	0.56
2:B:166:LEU:O	2:B:169:SER:HB3	2.05	0.56
1:A:1025:VAL:CG1	1:A:1030:ASP:HB2	2.35	0.56
2:D:261:LEU:O	2:D:264:GLN:HB2	2.04	0.56
1:A:1007:ASP:HB2	1:A:1008:ILE:HD12	1.86	0.56
2:F:222:LEU:CD2	2:F:222:LEU:C	2.74	0.56
2:D:260:ASP:O	2:D:264:GLN:HG2	2.05	0.56
2:F:166:LEU:O	2:F:169:SER:HB3	2.05	0.56
2:F:109:CYS:O	2:F:113:ILE:HG13	2.05	0.56
2:B:260:ASP:O	2:B:264:GLN:HG2	2.05	0.56
2:B:222:LEU:HD23	2:B:222:LEU:O	2.05	0.56
1:C:1025:VAL:O	1:C:1201:VAL:HG23	2.06	0.56
2:D:227:TYR:HE1	1:E:1113:ILE:HD11	1.66	0.56
2:B:109:CYS:O	2:B:113:ILE:HG13	2.06	0.56
1:A:1117:PRO:CB	2:D:177:LYS:NZ	2.69	0.56
2:B:222:LEU:CD2	2:B:222:LEU:C	2.74	0.56
1:C:1042:ARG:NH1	1:C:1169:THR:O	2.39	0.55
1:A:1113:ILE:HD12	2:D:150:ASN:ND2	2.21	0.55
1:A:1117:PRO:CB	2:D:177:LYS:HZ1	2.19	0.55
2:B:197:TRP:O	2:B:201:LEU:HB2	2.05	0.55
2:D:118:ALA:O	2:D:121:THR:HB	2.06	0.55
1:E:994:MET:HE3	1:E:1016:ALA:HB3	1.88	0.55
1:C:994:MET:HE3	1:C:1016:ALA:HB3	1.89	0.55
2:B:28:VAL:O	2:B:30:ASP:N	2.40	0.55
1:C:1079:PRO:HG3	2:F:195:PRO:HG3	1.89	0.55
2:F:28:VAL:O	2:F:30:ASP:N	2.40	0.55
1:C:1117:PRO:HG2	1:C:1118:ARG:H	1.72	0.54
2:D:28:VAL:O	2:D:30:ASP:N	2.40	0.54
1:E:1117:PRO:HG2	1:E:1118:ARG:H	1.72	0.54
1:E:954:ILE:HD13	1:E:955:PRO:CD	2.37	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1100:LEU:HB2	1:A:1134:SER:O	2.07	0.54
1:A:1117:PRO:HG2	1:A:1118:ARG:H	1.72	0.54
2:F:230:VAL:O	2:F:233:LYS:HG3	2.08	0.54
2:F:173:PHE:CD1	2:F:209:GLN:NE2	2.76	0.54
1:A:954:ILE:HD13	1:A:955:PRO:CD	2.37	0.54
2:D:230:VAL:O	2:D:233:LYS:HG3	2.08	0.54
1:A:940:LYS:HB2	2:B:285:PHE:CE2	2.43	0.54
2:D:122:THR:HG22	2:D:163:ILE:HG21	1.90	0.54
1:E:930:GLN:HB3	1:E:1196:GLY:O	2.09	0.54
2:B:230:VAL:O	2:B:233:LYS:HG3	2.08	0.54
1:C:954:ILE:HD13	1:C:955:PRO:CD	2.37	0.53
1:E:1093:HIS:NE2	1:E:1139:ILE:CD1	2.72	0.53
2:B:187:TYR:CD1	2:B:206:LEU:HD21	2.43	0.53
2:D:248:ILE:HG12	2:D:262:THR:CG2	2.38	0.53
1:E:1104:TYR:CE2	1:E:1143:PRO:HB3	2.43	0.53
2:F:187:TYR:CD1	2:F:206:LEU:HD21	2.44	0.53
2:B:270:HIS:CD2	2:B:272:HIS:HB3	2.43	0.53
2:B:86:PRO:CD	2:B:117:GLU:HB2	2.38	0.53
2:D:270:HIS:CD2	2:D:272:HIS:HB3	2.44	0.53
2:F:42:LEU:HD21	2:F:64:VAL:HG13	1.90	0.53
1:A:1093:HIS:NE2	1:A:1139:ILE:CD1	2.71	0.53
2:F:270:HIS:CD2	2:F:272:HIS:HB3	2.44	0.53
1:A:1098:ASN:ND2	1:A:1137:ILE:O	2.37	0.53
2:F:248:ILE:HG12	2:F:262:THR:CG2	2.38	0.53
1:E:931:VAL:HG23	1:E:1197:LEU:HA	1.90	0.52
2:D:50:GLN:O	2:D:51:ASP:CB	2.56	0.52
2:D:102:LEU:HB3	2:D:135:ASN:HB2	1.91	0.52
2:B:248:ILE:HG12	2:B:262:THR:CG2	2.39	0.52
2:D:4:PHE:C	2:D:4:PHE:CD2	2.82	0.52
2:B:50:GLN:O	2:B:51:ASP:CB	2.55	0.52
1:A:974:THR:HG22	1:A:974:THR:O	2.10	0.52
2:F:85:SER:HB2	2:F:117:GLU:OE1	2.10	0.52
2:D:187:TYR:CD1	2:D:206:LEU:HD21	2.44	0.52
1:A:957:THR:HG22	1:A:958:PRO:HD3	1.91	0.52
1:C:1025:VAL:HG11	1:C:1030:ASP:HB2	1.91	0.52
2:B:4:PHE:CD2	2:B:4:PHE:C	2.82	0.52
1:A:994:MET:HE3	1:A:1016:ALA:HB3	1.91	0.52
1:A:900:GLU:OE2	1:A:969:ARG:HD3	2.10	0.52
1:C:954:ILE:C	1:C:954:ILE:HD13	2.30	0.52
2:F:38:ALA:HB1	2:F:47:TYR:CE1	2.39	0.52
1:A:1113:ILE:HG23	2:D:150:ASN:CG	2.30	0.52
1:E:1197:LEU:HG	1:E:1199:ILE:HG13	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:974:THR:HG22	1:C:974:THR:O	2.10	0.52
1:E:910:LEU:HD11	1:E:1024:MET:HG3	1.92	0.52
1:E:954:ILE:C	1:E:954:ILE:HD13	2.30	0.52
2:F:4:PHE:C	2:F:4:PHE:CD2	2.83	0.52
1:E:1025:VAL:HG11	1:E:1030:ASP:HB2	1.91	0.52
2:F:15:PHE:HB2	2:F:44:LEU:CD2	2.40	0.52
1:C:1083:THR:HG23	1:C:1109:PHE:CE1	2.45	0.52
1:A:1025:VAL:HG11	1:A:1030:ASP:HB2	1.91	0.52
1:C:1197:LEU:HG	1:C:1199:ILE:HG13	1.92	0.51
1:A:938:PRO:HG2	1:A:1187:ILE:HD11	1.92	0.51
2:F:37:LYS:HD3	2:F:50:GLN:OE1	2.10	0.51
2:F:50:GLN:O	2:F:51:ASP:CB	2.55	0.51
2:B:15:PHE:HB2	2:B:44:LEU:CD2	2.40	0.51
1:E:993:LYS:HG2	1:E:1015:GLU:HG2	1.93	0.51
2:B:72:ILE:HG22	2:B:76:GLU:HB2	1.92	0.51
2:B:173:PHE:CD1	2:B:209:GLN:NE2	2.76	0.51
2:D:258:THR:O	2:D:259:GLU:C	2.49	0.51
1:A:933:VAL:HG13	1:A:1187:ILE:HG23	1.93	0.51
1:E:1083:THR:HG23	1:E:1109:PHE:CE1	2.45	0.51
2:F:66:PHE:CE1	2:F:72:ILE:HG12	2.45	0.51
2:D:267:LYS:O	2:D:269:ASP:N	2.40	0.51
2:D:248:ILE:HG12	2:D:262:THR:HG22	1.92	0.51
2:F:72:ILE:HG22	2:F:76:GLU:HB2	1.92	0.51
1:A:980:ILE:C	1:A:981:LEU:HG	2.31	0.51
2:B:149:THR:HG22	2:B:150:ASN:N	2.25	0.51
2:D:173:PHE:CD1	2:D:209:GLN:NE2	2.76	0.51
1:C:1002:LYS:NZ	1:C:1080:ILE:HD11	2.26	0.51
1:E:1143:PRO:HG2	1:E:1144:TYR:CD1	2.45	0.51
1:C:1143:PRO:HG2	1:C:1144:TYR:CD1	2.45	0.51
2:D:149:THR:HG22	2:D:150:ASN:N	2.26	0.51
1:E:920:PHE:CD2	2:F:285:PHE:HD1	2.29	0.51
1:A:1083:THR:HG23	1:A:1109:PHE:CE1	2.45	0.51
1:A:1002:LYS:NZ	1:A:1080:ILE:HD11	2.26	0.51
2:F:248:ILE:HG12	2:F:262:THR:HG22	1.93	0.51
1:C:1025:VAL:O	1:C:1200:ARG:HA	2.11	0.51
1:E:1002:LYS:NZ	1:E:1080:ILE:HD11	2.26	0.51
1:C:980:ILE:C	1:C:981:LEU:HG	2.31	0.51
1:E:974:THR:O	1:E:974:THR:HG22	2.10	0.51
1:C:993:LYS:HG2	1:C:1015:GLU:HG2	1.93	0.51
2:D:15:PHE:HA	2:D:18:CYS:HB3	1.93	0.51
2:F:6:ILE:H	2:F:6:ILE:HD12	1.76	0.51
1:A:1197:LEU:HG	1:A:1199:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:72:ILE:HG22	2:F:72:ILE:O	2.10	0.51
2:D:72:ILE:O	2:D:72:ILE:HG22	2.11	0.51
1:C:916:ALA:O	1:C:951:ARG:NH2	2.44	0.51
1:A:1143:PRO:HG2	1:A:1144:TYR:CD1	2.45	0.50
2:D:6:ILE:HD12	2:D:6:ILE:H	1.76	0.50
2:B:42:LEU:HD21	2:B:64:VAL:HG13	1.92	0.50
1:A:954:ILE:HD13	1:A:954:ILE:C	2.30	0.50
2:D:235:ASN:O	2:D:235:ASN:ND2	2.44	0.50
1:E:1093:HIS:NE2	1:E:1139:ILE:HD11	2.27	0.50
1:A:1005:LYS:NZ	2:D:107:GLU:OE2	2.44	0.50
1:C:1100:LEU:HB2	1:C:1134:SER:O	2.12	0.50
1:C:1109:PHE:HD2	1:C:1109:PHE:C	2.15	0.50
2:B:72:ILE:HG22	2:B:72:ILE:O	2.11	0.50
1:E:980:ILE:C	1:E:981:LEU:HG	2.31	0.50
2:D:291:LYS:HG2	2:D:292:TYR:CE2	2.47	0.50
1:E:957:THR:CG2	1:E:958:PRO:N	2.66	0.50
1:E:1025:VAL:HB	1:E:1199:ILE:HG22	1.93	0.50
1:E:1028:ALA:HB2	1:E:1200:ARG:NH1	2.27	0.50
1:A:931:VAL:HG11	1:A:1168:LEU:HD13	1.94	0.50
2:F:15:PHE:HA	2:F:18:CYS:HB3	1.93	0.50
2:F:15:PHE:O	2:F:44:LEU:HD11	2.11	0.50
1:A:993:LYS:HG2	1:A:1015:GLU:HG2	1.93	0.50
2:B:248:ILE:HD11	2:B:263:ASN:CB	2.30	0.50
1:A:1104:TYR:CE2	1:A:1143:PRO:HB3	2.47	0.50
2:B:235:ASN:O	2:B:235:ASN:ND2	2.44	0.50
2:D:72:ILE:HG22	2:D:76:GLU:HB2	1.92	0.50
2:D:29:THR:HG22	2:D:29:THR:O	2.12	0.50
2:F:235:ASN:ND2	2:F:235:ASN:O	2.44	0.50
2:F:149:THR:HG22	2:F:150:ASN:N	2.26	0.50
2:B:258:THR:O	2:B:259:GLU:C	2.49	0.50
2:F:37:LYS:CE	2:F:50:GLN:OE1	2.59	0.50
2:B:15:PHE:HA	2:B:18:CYS:HB3	1.94	0.50
2:D:15:PHE:HB2	2:D:44:LEU:CD2	2.40	0.50
2:B:191:SER:HA	2:B:199:THR:HB	1.94	0.50
1:A:900:GLU:HG2	1:A:967:TYR:CG	2.46	0.50
2:B:15:PHE:O	2:B:44:LEU:HD11	2.12	0.49
2:B:6:ILE:HD12	2:B:6:ILE:H	1.77	0.49
1:C:961:LEU:HG	1:C:962:PRO:HD2	1.94	0.49
2:B:173:PHE:CE1	2:B:209:GLN:NE2	2.80	0.49
2:F:29:THR:O	2:F:29:THR:HG22	2.12	0.49
2:B:267:LYS:O	2:B:269:ASP:N	2.40	0.49
2:F:72:ILE:CG1	2:F:99:LEU:CD1	2.90	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:173:PHE:CE1	2:D:209:GLN:NE2	2.80	0.49
1:A:1069:ALA:O	1:A:1089:ALA:HB2	2.12	0.49
1:C:1069:ALA:O	1:C:1089:ALA:HB2	2.12	0.49
2:B:69:THR:O	2:B:70:LYS:C	2.50	0.49
1:C:1097:LYS:O	1:C:1136:ALA:HB2	2.12	0.49
2:F:258:THR:O	2:F:259:GLU:C	2.49	0.49
2:B:248:ILE:HG12	2:B:262:THR:HG22	1.93	0.49
1:C:930:GLN:O	1:C:1194:ALA:HB1	2.12	0.49
2:D:248:ILE:HD11	2:D:263:ASN:CB	2.30	0.49
2:F:38:ALA:CB	2:F:47:TYR:HE1	2.21	0.49
2:F:1:MET:C	2:F:3:TYR:N	2.64	0.49
2:F:72:ILE:HD11	2:F:99:LEU:HD12	1.93	0.49
1:E:1069:ALA:O	1:E:1089:ALA:HB2	2.12	0.49
2:D:15:PHE:O	2:D:44:LEU:HD11	2.12	0.49
1:E:904:TRP:CH2	1:E:982:PRO:HB3	2.47	0.49
2:D:73:GLU:OE1	2:D:73:GLU:HA	2.13	0.49
2:F:191:SER:HA	2:F:199:THR:HB	1.95	0.49
2:D:13:GLY:HA3	2:D:196:THR:HG21	1.95	0.49
1:A:1067:GLU:HA	1:A:1139:ILE:HG21	1.95	0.49
2:B:29:THR:O	2:B:29:THR:HG22	2.12	0.49
1:A:1185:ALA:O	1:A:1187:ILE:N	2.46	0.48
1:C:1185:ALA:O	1:C:1187:ILE:N	2.46	0.48
1:E:1185:ALA:O	1:E:1187:ILE:N	2.46	0.48
1:A:1123:ARG:HG2	1:A:1123:ARG:HH11	1.78	0.48
2:F:104:LYS:HG2	2:F:104:LYS:O	2.13	0.48
1:A:-1:HIS:O	1:A:0:MET:C	2.52	0.48
2:F:173:PHE:CE1	2:F:209:GLN:NE2	2.80	0.48
1:A:994:MET:HE1	1:A:1013:PHE:HD2	1.78	0.48
1:E:961:LEU:HG	1:E:962:PRO:HD2	1.95	0.48
1:E:931:VAL:HG11	1:E:1168:LEU:HD13	1.95	0.48
2:D:104:LYS:HG2	2:D:104:LYS:O	2.13	0.48
1:C:1109:PHE:CZ	1:C:1118:ARG:HD3	2.46	0.48
1:A:1035:HIS:O	1:A:1039:GLU:HG2	2.14	0.48
1:C:1123:ARG:HH11	1:C:1123:ARG:HG2	1.78	0.48
2:B:102:LEU:HB3	2:B:135:ASN:HB2	1.95	0.48
2:D:191:SER:HA	2:D:199:THR:HB	1.95	0.48
1:E:1123:ARG:HH11	1:E:1123:ARG:HG2	1.78	0.48
2:D:2:ASP:O	2:D:159:ASP:OD2	2.31	0.48
1:A:1080:ILE:HG13	2:D:147:ASN:OD1	2.14	0.48
1:C:1035:HIS:O	1:C:1039:GLU:HG2	2.14	0.48
1:E:1098:ASN:ND2	1:E:1137:ILE:H	2.12	0.48
1:E:1042:ARG:CB	1:E:1184:ILE:HG21	2.43	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:66:PHE:CD2	2:F:67:LEU:HD12	2.49	0.48
1:A:916:ALA:O	1:A:951:ARG:NH2	2.47	0.48
1:C:920:PHE:CZ	2:D:281:ILE:HG13	2.49	0.48
2:D:227:TYR:CE1	1:E:1113:ILE:HD13	2.45	0.48
1:E:1109:PHE:C	1:E:1109:PHE:HD2	2.15	0.48
1:E:1035:HIS:O	1:E:1039:GLU:HG2	2.14	0.48
2:D:240:LYS:N	2:D:241:PRO:HD2	2.29	0.48
1:C:1029:GLU:HB3	2:F:185:TYR:OH	2.14	0.48
2:B:270:HIS:ND1	2:B:271:GLU:N	2.60	0.48
1:E:976:SER:C	1:E:978:ASP:N	2.67	0.48
1:A:969:ARG:HD2	1:A:980:ILE:HG23	1.95	0.47
2:F:66:PHE:HD2	2:F:67:LEU:HD12	1.79	0.47
2:F:72:ILE:HD11	2:F:99:LEU:CD1	2.44	0.47
2:F:73:GLU:OE1	2:F:73:GLU:HA	2.13	0.47
2:B:2:ASP:C	2:B:4:PHE:H	2.15	0.47
2:D:230:VAL:C	2:D:232:GLN:H	2.18	0.47
2:D:66:PHE:HD2	2:D:67:LEU:HD12	1.79	0.47
1:A:961:LEU:HG	1:A:962:PRO:HD2	1.95	0.47
2:D:1:MET:C	2:D:3:TYR:H	2.16	0.47
1:C:1029:GLU:HG3	2:F:185:TYR:OH	2.14	0.47
1:E:1051:GLU:O	1:E:1055:ARG:HG3	2.15	0.47
2:B:74:GLU:HA	2:B:77:ASN:HB2	1.96	0.47
2:B:34:LEU:HD11	2:B:57:GLY:CA	2.45	0.47
1:E:955:PRO:HD3	2:F:242:THR:HG21	1.96	0.47
1:C:1160:ASP:O	1:C:1161:THR:C	2.53	0.47
2:B:5:ASN:O	2:B:6:ILE:C	2.53	0.47
1:E:969:ARG:HD2	1:E:980:ILE:HG23	1.95	0.47
1:A:1160:ASP:O	1:A:1161:THR:C	2.53	0.47
1:C:976:SER:C	1:C:978:ASP:N	2.67	0.47
1:E:983:TYR:CE2	2:F:253:MET:HG2	2.49	0.47
2:B:222:LEU:HD22	2:B:228:TYR:CD1	2.50	0.47
2:B:73:GLU:HA	2:B:73:GLU:OE1	2.13	0.47
2:D:66:PHE:CD2	2:D:67:LEU:HD12	2.49	0.47
2:B:104:LYS:O	2:B:104:LYS:HG2	2.13	0.47
2:B:66:PHE:CD2	2:B:67:LEU:HD12	2.49	0.47
1:A:1113:ILE:HG22	1:A:1119:ALA:CB	2.45	0.47
1:A:1109:PHE:HD2	1:A:1109:PHE:C	2.15	0.47
1:A:1118:ARG:NH2	2:D:143:THR:OG1	2.47	0.47
2:F:5:ASN:O	2:F:6:ILE:C	2.53	0.47
2:D:6:ILE:CD1	2:D:6:ILE:H	2.28	0.47
2:B:117:GLU:OE1	2:B:117:GLU:HA	2.15	0.47
1:C:969:ARG:HD2	1:C:980:ILE:HG23	1.95	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:7:LYS:HE2	2:F:36:TYR:OH	2.15	0.47
2:B:80:LYS:C	2:B:82:LYS:H	2.18	0.47
2:D:48:GLN:O	2:D:50:GLN:NE2	2.48	0.47
1:E:1090:MET:HE3	1:E:1106:ALA:HA	1.97	0.47
2:D:227:TYR:CE2	1:E:1080:ILE:HB	2.50	0.47
1:E:1113:ILE:HG22	1:E:1119:ALA:CB	2.45	0.47
2:B:240:LYS:N	2:B:241:PRO:HD2	2.29	0.47
1:C:1051:GLU:O	1:C:1055:ARG:HG3	2.15	0.47
2:D:7:LYS:HE2	2:D:36:TYR:OH	2.15	0.47
1:A:1101:GLN:O	1:A:1104:TYR:N	2.48	0.46
1:C:1101:GLN:O	1:C:1104:TYR:N	2.48	0.46
1:A:1025:VAL:O	1:A:1201:VAL:HG23	2.14	0.46
2:F:230:VAL:C	2:F:232:GLN:H	2.18	0.46
2:B:66:PHE:HD2	2:B:67:LEU:HD12	1.79	0.46
1:A:1051:GLU:O	1:A:1055:ARG:HG3	2.15	0.46
2:F:159:ASP:O	2:F:162:MET:HE1	2.14	0.46
1:C:900:GLU:OE2	1:C:969:ARG:HD3	2.15	0.46
1:A:1174:VAL:HG23	1:A:1176:THR:HB	1.98	0.46
2:D:80:LYS:C	2:D:82:LYS:H	2.18	0.46
2:F:240:LYS:N	2:F:241:PRO:HD2	2.29	0.46
1:A:1109:PHE:CZ	1:A:1118:ARG:HD3	2.47	0.46
2:D:5:ASN:O	2:D:6:ILE:C	2.53	0.46
2:F:122:THR:HG22	2:F:163:ILE:HG21	1.97	0.46
2:D:206:LEU:HD22	2:D:206:LEU:N	2.31	0.46
1:E:1160:ASP:O	1:E:1161:THR:C	2.53	0.46
1:E:1101:GLN:O	1:E:1104:TYR:N	2.48	0.46
1:E:1025:VAL:O	1:E:1200:ARG:HA	2.15	0.46
2:B:42:LEU:CD2	2:B:64:VAL:HG13	2.46	0.46
2:B:6:ILE:CD1	2:B:6:ILE:H	2.28	0.46
2:F:6:ILE:H	2:F:6:ILE:CD1	2.28	0.46
2:D:74:GLU:HA	2:D:77:ASN:HB2	1.96	0.46
1:A:976:SER:C	1:A:978:ASP:N	2.67	0.46
2:F:222:LEU:HD22	2:F:228:TYR:CD1	2.50	0.46
2:B:206:LEU:HD22	2:B:206:LEU:N	2.31	0.46
1:A:947:TYR:CE1	1:A:951:ARG:NH2	2.84	0.46
2:F:74:GLU:HA	2:F:77:ASN:HB2	1.96	0.46
2:F:80:LYS:C	2:F:82:LYS:H	2.18	0.46
2:B:13:GLY:HA3	2:B:196:THR:HG21	1.97	0.46
2:B:230:VAL:C	2:B:232:GLN:H	2.18	0.46
1:C:1174:VAL:HG23	1:C:1176:THR:HB	1.98	0.46
2:D:62:LEU:HD23	2:D:62:LEU:HA	1.73	0.46
1:A:1042:ARG:NH1	1:A:1169:THR:O	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:11:TYR:CE1	2:F:163:ILE:HD11	2.51	0.46
1:A:904:TRP:CZ3	1:A:982:PRO:HB3	2.51	0.46
2:D:222:LEU:HD22	2:D:228:TYR:CD1	2.51	0.46
2:D:126:LEU:HD12	2:D:167:ALA:HB2	1.98	0.46
2:B:7:LYS:HE2	2:B:36:TYR:OH	2.15	0.46
2:F:270:HIS:ND1	2:F:271:GLU:N	2.60	0.46
2:F:102:LEU:HB3	2:F:135:ASN:HB2	1.99	0.46
1:E:1028:ALA:HB2	1:E:1200:ARG:HH12	1.80	0.45
2:F:48:GLN:O	2:F:50:GLN:NE2	2.48	0.45
2:B:234:GLU:HB3	2:B:235:ASN:H	1.67	0.45
1:A:1093:HIS:NE2	1:A:1139:ILE:HD11	2.31	0.45
2:F:7:LYS:O	2:F:9:ASN:N	2.49	0.45
1:E:1180:LYS:O	1:E:1190:ILE:HG13	2.16	0.45
2:B:48:GLN:O	2:B:50:GLN:NE2	2.48	0.45
1:C:1113:ILE:HG22	1:C:1119:ALA:CB	2.45	0.45
2:F:267:LYS:O	2:F:269:ASP:N	2.40	0.45
1:C:1180:LYS:O	1:C:1190:ILE:HG13	2.16	0.45
2:F:69:THR:O	2:F:70:LYS:C	2.55	0.45
1:C:1084:ASN:O	1:C:1088:VAL:HG23	2.17	0.45
2:F:248:ILE:CG1	2:F:262:THR:CG2	2.95	0.45
1:E:920:PHE:HD2	2:F:285:PHE:HD1	1.64	0.45
2:F:3:TYR:CD2	2:F:33:LEU:HD21	2.52	0.45
1:C:0:MET:O	1:C:900:GLU:C	2.54	0.45
1:C:907:ASN:CG	1:C:978:ASP:O	2.54	0.45
1:A:972:ASP:OD1	1:A:972:ASP:N	2.50	0.45
1:C:1118:ARG:NH1	2:F:231:GLU:OE2	2.50	0.45
2:D:3:TYR:CD2	2:D:33:LEU:HD21	2.52	0.45
2:B:86:PRO:HD2	2:B:117:GLU:HB2	1.98	0.45
1:A:907:ASN:CG	1:A:978:ASP:O	2.55	0.45
2:B:7:LYS:O	2:B:9:ASN:N	2.49	0.45
1:A:1084:ASN:O	1:A:1088:VAL:HG23	2.17	0.45
1:A:920:PHE:CZ	2:B:281:ILE:HG13	2.52	0.45
1:A:1180:LYS:O	1:A:1190:ILE:HG13	2.16	0.45
2:B:35:PHE:O	2:B:39:LYS:HB2	2.17	0.45
1:C:1028:ALA:CB	1:C:1200:ARG:NH1	2.76	0.45
2:D:47:TYR:CZ	2:D:64:VAL:HG21	2.52	0.45
2:F:112:GLY:HA2	2:F:115:ASN:HB2	1.99	0.45
1:E:1067:GLU:HG3	1:E:1139:ILE:CG2	2.42	0.45
2:D:222:LEU:CD2	2:D:222:LEU:O	2.65	0.45
2:F:63:TYR:O	2:F:66:PHE:HB3	2.17	0.45
2:F:166:LEU:HA	2:F:166:LEU:HD12	1.68	0.45
1:A:951:ARG:NH1	1:A:967:TYR:HE2	2.15	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:1174:VAL:HG23	1:E:1176:THR:HB	1.97	0.45
2:B:41:LEU:HB3	2:B:47:TYR:HA	1.98	0.45
1:C:1078:SER:OG	1:C:1080:ILE:HG23	2.17	0.45
1:C:1101:GLN:O	1:C:1102:ALA:C	2.55	0.45
1:E:910:LEU:HD23	1:E:1201:VAL:HA	1.99	0.45
2:D:270:HIS:ND1	2:D:271:GLU:N	2.60	0.45
2:B:222:LEU:CD2	2:B:222:LEU:O	2.65	0.45
1:E:1109:PHE:CZ	1:E:1118:ARG:HD3	2.46	0.45
2:B:3:TYR:CD2	2:B:33:LEU:HD21	2.52	0.45
2:B:63:TYR:O	2:B:66:PHE:HB3	2.17	0.45
2:D:35:PHE:O	2:D:39:LYS:HB2	2.17	0.45
1:E:1084:ASN:O	1:E:1088:VAL:HG23	2.16	0.45
1:A:1042:ARG:CB	1:A:1184:ILE:HG21	2.47	0.44
1:E:947:TYR:CG	2:F:281:ILE:HD12	2.52	0.44
1:E:1135:ASP:O	1:E:1136:ALA:C	2.56	0.44
2:D:159:ASP:O	2:D:162:MET:HE1	2.16	0.44
1:C:994:MET:HE1	1:C:1013:PHE:HD2	1.82	0.44
1:A:995:ASN:O	1:A:996:GLU:C	2.56	0.44
2:F:54:SER:O	2:F:58:LYS:HB2	2.17	0.44
1:C:995:ASN:O	1:C:996:GLU:C	2.56	0.44
2:F:47:TYR:CZ	2:F:64:VAL:HG21	2.53	0.44
1:A:-1:HIS:N	1:A:901:THR:HB	2.28	0.44
2:D:41:LEU:HB3	2:D:47:TYR:HA	1.99	0.44
1:C:972:ASP:N	1:C:972:ASP:OD1	2.50	0.44
1:E:972:ASP:N	1:E:972:ASP:OD1	2.50	0.44
2:F:206:LEU:HD22	2:F:206:LEU:N	2.31	0.44
2:D:7:LYS:O	2:D:9:ASN:N	2.50	0.44
2:F:35:PHE:O	2:F:39:LYS:HB2	2.17	0.44
2:D:54:SER:O	2:D:58:LYS:HB2	2.18	0.44
2:B:248:ILE:CG1	2:B:262:THR:CG2	2.95	0.44
2:F:48:GLN:O	2:F:49:SER:C	2.55	0.44
1:E:1078:SER:OG	1:E:1080:ILE:HG23	2.18	0.44
1:A:1117:PRO:HB3	2:D:177:LYS:HZ1	1.81	0.44
1:C:1090:MET:HE3	1:C:1106:ALA:HA	1.99	0.44
2:F:6:ILE:HD12	2:F:21:GLU:HB3	2.00	0.44
2:D:248:ILE:CG1	2:D:262:THR:CG2	2.95	0.44
1:A:1147:PHE:CD1	1:A:1147:PHE:N	2.83	0.44
1:E:951:ARG:NH1	1:E:967:TYR:HE2	2.15	0.44
2:F:222:LEU:O	2:F:222:LEU:CD2	2.66	0.44
1:C:1025:VAL:HB	1:C:1199:ILE:HG22	1.99	0.44
2:D:122:THR:HG22	2:D:163:ILE:CG2	2.47	0.44
1:A:1078:SER:OG	1:A:1080:ILE:HG23	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:126:LEU:HD12	2:B:167:ALA:HB2	2.00	0.44
1:A:1008:ILE:N	1:A:1008:ILE:CD1	2.78	0.44
1:E:1101:GLN:O	1:E:1102:ALA:C	2.55	0.44
2:B:47:TYR:CZ	2:B:64:VAL:HG21	2.53	0.44
2:D:63:TYR:O	2:D:66:PHE:HB3	2.17	0.44
2:B:54:SER:O	2:B:58:LYS:HB2	2.17	0.44
2:B:48:GLN:O	2:B:49:SER:C	2.56	0.44
1:A:966:GLY:HA3	2:B:173:PHE:CE2	2.53	0.44
2:D:181:THR:HB	2:D:182:SER:H	1.52	0.44
2:F:6:ILE:HD12	2:F:6:ILE:N	2.33	0.44
2:D:265:LEU:O	2:D:269:ASP:HB3	2.18	0.44
1:A:1123:ARG:HG2	1:A:1123:ARG:NH1	2.33	0.44
1:C:1046:LEU:HD22	1:C:1046:LEU:O	2.18	0.44
1:E:1147:PHE:CD1	1:E:1147:PHE:N	2.83	0.43
1:C:1135:ASP:O	1:C:1136:ALA:C	2.56	0.43
1:E:994:MET:HE1	1:E:1013:PHE:HD2	1.84	0.43
1:E:1098:ASN:ND2	1:E:1137:ILE:O	2.44	0.43
2:F:31:ASN:OD1	2:F:56:LEU:HD23	2.18	0.43
2:F:152:ILE:HD13	2:F:156:VAL:HG21	2.00	0.43
2:D:261:LEU:HD12	2:D:261:LEU:C	2.39	0.43
2:D:196:THR:CG2	2:D:197:TRP:N	2.78	0.43
2:B:6:ILE:HD12	2:B:21:GLU:HB3	2.00	0.43
2:B:152:ILE:CG2	2:B:156:VAL:HB	2.49	0.43
1:A:1101:GLN:O	1:A:1102:ALA:C	2.55	0.43
2:F:265:LEU:O	2:F:269:ASP:HB3	2.18	0.43
2:D:6:ILE:HD12	2:D:6:ILE:N	2.33	0.43
2:D:166:LEU:HD12	2:D:166:LEU:HA	1.68	0.43
1:E:1123:ARG:NH1	1:E:1123:ARG:HG2	2.33	0.43
2:B:140:THR:O	2:B:144:ILE:HG12	2.18	0.43
2:F:140:THR:O	2:F:144:ILE:HG12	2.18	0.43
1:A:986:GLY:HA2	1:A:1023:LEU:HD21	1.99	0.43
1:E:910:LEU:CD2	1:E:1201:VAL:HA	2.48	0.43
2:D:48:GLN:O	2:D:49:SER:C	2.56	0.43
2:F:28:VAL:O	2:F:28:VAL:CG1	2.64	0.43
2:D:6:ILE:HD12	2:D:21:GLU:HB3	2.00	0.43
2:B:6:ILE:HD12	2:B:6:ILE:N	2.33	0.43
2:B:72:ILE:O	2:B:73:GLU:C	2.56	0.43
1:E:991:ASN:O	1:E:992:GLU:C	2.57	0.43
1:A:1050:ILE:HG12	1:A:1154:TYR:CD2	2.53	0.43
1:A:-2:PRO:CA	1:A:901:THR:CG2	2.84	0.43
2:D:193:THR:HG22	2:D:194:PHE:CE1	2.54	0.43
1:E:1054:ARG:NH2	1:E:1088:VAL:CG1	2.82	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:152:ILE:HD13	2:B:156:VAL:HG21	2.00	0.43
1:E:935:LYS:HE2	1:E:937:GLU:OE1	2.19	0.43
1:E:1183:ARG:N	1:E:1183:ARG:HD3	2.34	0.43
1:C:1183:ARG:HD3	1:C:1183:ARG:N	2.34	0.43
1:A:1029:GLU:N	1:A:1029:GLU:CD	2.72	0.43
2:F:261:LEU:C	2:F:261:LEU:HD12	2.39	0.43
1:A:1099:PHE:HB3	1:A:1129:ALA:HB1	2.00	0.43
1:C:1123:ARG:HG2	1:C:1123:ARG:NH1	2.33	0.43
1:E:1046:LEU:O	1:E:1046:LEU:HD22	2.18	0.43
1:C:1099:PHE:HB3	1:C:1129:ALA:HB1	2.00	0.43
1:E:904:TRP:CZ3	1:E:982:PRO:HB3	2.54	0.43
1:A:939:LEU:HD12	1:A:939:LEU:HA	1.87	0.43
1:A:1135:ASP:O	1:A:1136:ALA:C	2.56	0.43
2:D:42:LEU:HD21	2:D:64:VAL:HG13	2.01	0.43
2:F:193:THR:HG22	2:F:194:PHE:CE1	2.53	0.43
2:F:196:THR:H	2:F:199:THR:HG1	1.67	0.43
2:F:72:ILE:O	2:F:73:GLU:C	2.56	0.43
1:C:991:ASN:O	1:C:992:GLU:C	2.57	0.43
1:A:1046:LEU:O	1:A:1046:LEU:HD22	2.18	0.43
2:B:193:THR:HG22	2:B:194:PHE:CE1	2.53	0.43
2:F:222:LEU:HD23	2:F:222:LEU:C	2.40	0.43
2:B:166:LEU:HA	2:B:166:LEU:HD12	1.68	0.43
1:C:951:ARG:NH1	1:C:967:TYR:HE2	2.16	0.43
1:C:947:TYR:CE1	1:C:951:ARG:NH2	2.87	0.43
1:C:1029:GLU:CG	2:F:185:TYR:OH	2.67	0.43
2:D:126:LEU:CD1	2:D:167:ALA:HB2	2.49	0.43
2:D:54:SER:C	2:D:56:LEU:H	2.23	0.43
2:F:152:ILE:CG2	2:F:156:VAL:HB	2.49	0.43
2:B:31:ASN:HB2	2:B:119:GLU:OE2	2.19	0.43
2:B:44:LEU:HA	2:B:234:GLU:OE1	2.19	0.43
2:D:72:ILE:O	2:D:73:GLU:C	2.56	0.43
1:C:1054:ARG:NH2	1:C:1088:VAL:CG1	2.81	0.43
1:A:1054:ARG:NH2	1:A:1088:VAL:CG1	2.82	0.43
2:D:140:THR:O	2:D:144:ILE:HG12	2.19	0.43
2:B:87:TYR:CE2	2:B:120:GLY:HA2	2.54	0.43
2:B:261:LEU:HD12	2:B:261:LEU:C	2.39	0.42
2:D:152:ILE:CG2	2:D:156:VAL:HB	2.48	0.42
1:A:1112:ILE:HG22	1:A:1112:ILE:O	2.19	0.42
2:F:248:ILE:HD11	2:F:263:ASN:CB	2.30	0.42
1:E:1029:GLU:CD	1:E:1029:GLU:N	2.72	0.42
2:B:196:THR:H	2:B:199:THR:HG1	1.67	0.42
2:D:152:ILE:HD13	2:D:156:VAL:HG21	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:1033:LEU:CD2	1:E:1037:ILE:HG13	2.50	0.42
2:D:208:LEU:HA	2:D:208:LEU:HD23	1.82	0.42
1:E:1008:ILE:N	1:E:1008:ILE:CD1	2.78	0.42
1:C:1147:PHE:N	1:C:1147:PHE:CD1	2.83	0.42
1:C:931:VAL:HG11	1:C:1168:LEU:HD13	2.02	0.42
2:F:175:THR:HG22	2:F:177:LYS:HB3	2.02	0.42
2:B:222:LEU:HD23	2:B:222:LEU:C	2.39	0.42
2:D:291:LYS:O	2:D:292:TYR:CD2	2.73	0.42
1:A:1033:LEU:CD2	1:A:1037:ILE:HG13	2.50	0.42
1:E:1099:PHE:HB3	1:E:1129:ALA:HB1	2.00	0.42
2:F:122:THR:HG22	2:F:163:ILE:CG2	2.50	0.42
1:A:1163:SER:N	1:A:1175:ILE:HD11	2.35	0.42
1:C:935:LYS:HE2	1:C:937:GLU:OE1	2.19	0.42
2:B:265:LEU:O	2:B:269:ASP:HB3	2.18	0.42
1:E:1182:ASP:OD2	1:E:1184:ILE:HB	2.20	0.42
2:F:54:SER:C	2:F:56:LEU:H	2.23	0.42
1:E:1033:LEU:O	1:E:1033:LEU:HD23	2.20	0.42
1:C:975:VAL:HG12	1:C:979:GLN:HB3	2.02	0.42
1:C:1166:ASP:OD2	1:C:1169:THR:CB	2.49	0.42
1:C:933:VAL:HG22	1:C:1187:ILE:CG2	2.49	0.42
2:D:222:LEU:C	2:D:222:LEU:HD23	2.39	0.42
2:B:159:ASP:O	2:B:162:MET:HE1	2.20	0.42
1:C:1033:LEU:HD23	1:C:1033:LEU:O	2.20	0.42
1:A:1183:ARG:N	1:A:1183:ARG:HD3	2.34	0.42
1:C:1042:ARG:CB	1:C:1184:ILE:HG21	2.47	0.42
1:E:1074:LYS:HG3	1:E:1147:PHE:CE1	2.54	0.42
2:D:175:THR:HG22	2:D:177:LYS:HB3	2.02	0.42
2:F:2:ASP:C	2:F:3:TYR:CD1	2.93	0.42
1:A:1033:LEU:HD23	1:A:1033:LEU:O	2.20	0.42
1:A:991:ASN:O	1:A:992:GLU:C	2.57	0.42
1:C:1182:ASP:OD2	1:C:1184:ILE:HB	2.20	0.42
2:F:37:LYS:CD	2:F:50:GLN:OE1	2.68	0.42
1:A:960:GLU:OE1	2:B:63:TYR:OH	2.35	0.42
1:A:935:LYS:HE2	1:A:937:GLU:OE1	2.19	0.42
1:A:953:TYR:CD1	1:A:953:TYR:N	2.88	0.42
2:B:208:LEU:HA	2:B:208:LEU:HD23	1.82	0.42
1:E:995:ASN:O	1:E:996:GLU:C	2.56	0.42
1:A:1166:ASP:OD2	1:A:1169:THR:CB	2.49	0.42
2:D:234:GLU:HB3	2:D:235:ASN:H	1.67	0.42
2:D:44:LEU:O	2:D:45:GLY:C	2.58	0.42
1:A:1162:PRO:C	1:A:1175:ILE:HD11	2.41	0.42
1:C:1112:ILE:HG22	1:C:1112:ILE:O	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1182:ASP:OD2	1:A:1184:ILE:HB	2.20	0.41
1:E:1185:ALA:O	1:E:1186:MET:C	2.58	0.41
1:A:1110:LEU:HD21	1:A:1122:ALA:HB3	2.02	0.41
1:C:1185:ALA:O	1:C:1186:MET:C	2.58	0.41
1:E:994:MET:HE3	1:E:1016:ALA:CB	2.50	0.41
1:A:-2:PRO:HA	1:A:901:THR:HG22	1.99	0.41
1:E:975:VAL:HG12	1:E:979:GLN:HB3	2.02	0.41
1:E:1162:PRO:C	1:E:1175:ILE:HD11	2.41	0.41
1:E:957:THR:HG22	1:E:958:PRO:CD	2.49	0.41
1:A:1185:ALA:O	1:A:1186:MET:C	2.58	0.41
1:A:1090:MET:HE3	1:A:1106:ALA:HA	2.03	0.41
1:C:981:LEU:HD13	1:C:1024:MET:HE1	2.02	0.41
2:B:56:LEU:C	2:B:58:LYS:N	2.73	0.41
1:E:1163:SER:N	1:E:1175:ILE:HD11	2.35	0.41
1:A:1071:TYR:CZ	1:A:1156:PRO:HD3	2.55	0.41
1:E:1110:LEU:HD21	1:E:1122:ALA:HB3	2.02	0.41
1:C:1110:LEU:HD21	1:C:1122:ALA:HB3	2.02	0.41
1:E:1186:MET:SD	1:E:1186:MET:N	2.94	0.41
1:C:953:TYR:CD1	1:C:953:TYR:N	2.88	0.41
1:E:1112:ILE:HG22	1:E:1112:ILE:O	2.20	0.41
2:F:34:LEU:HD11	2:F:57:GLY:N	2.33	0.41
2:B:197:TRP:NE1	2:B:236:ALA:HB2	2.35	0.41
2:D:197:TRP:NE1	2:D:236:ALA:HB2	2.36	0.41
1:C:994:MET:HE3	1:C:1016:ALA:CB	2.51	0.41
1:E:953:TYR:CD1	1:E:953:TYR:N	2.88	0.41
1:C:939:LEU:HD22	1:C:1187:ILE:HD12	2.02	0.41
2:B:196:THR:O	2:B:200:GLN:HB2	2.21	0.41
2:B:71:ASN:OD1	2:B:73:GLU:HB2	2.21	0.41
1:E:980:ILE:O	1:E:980:ILE:HG22	2.19	0.41
2:F:56:LEU:C	2:F:58:LYS:N	2.74	0.41
1:A:920:PHE:N	1:A:920:PHE:CD1	2.89	0.41
1:C:1090:MET:CE	1:C:1106:ALA:HA	2.51	0.41
2:D:223:LEU:HD23	2:D:223:LEU:HA	1.83	0.41
2:B:257:ASP:C	2:B:259:GLU:N	2.75	0.41
1:E:920:PHE:N	1:E:920:PHE:CD1	2.89	0.41
2:B:210:GLN:O	2:B:211:ARG:CB	2.63	0.41
2:D:210:GLN:O	2:D:211:ARG:CB	2.63	0.41
1:E:1090:MET:CE	1:E:1106:ALA:HA	2.51	0.41
2:F:196:THR:O	2:F:200:GLN:HB2	2.20	0.41
2:F:28:VAL:C	2:F:30:ASP:N	2.74	0.41
2:D:71:ASN:OD1	2:D:73:GLU:HB2	2.20	0.41
2:D:291:LYS:HG2	2:D:292:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:939:LEU:HD12	1:E:939:LEU:HA	1.88	0.41
2:B:54:SER:C	2:B:56:LEU:H	2.22	0.41
2:B:223:LEU:HD23	2:B:223:LEU:HA	1.83	0.41
2:F:222:LEU:HD21	2:F:228:TYR:CE1	2.57	0.40
2:B:222:LEU:HD21	2:B:228:TYR:CE1	2.56	0.40
2:F:71:ASN:OD1	2:F:73:GLU:HB2	2.21	0.40
1:A:980:ILE:O	1:A:980:ILE:HG22	2.19	0.40
1:A:975:VAL:HG12	1:A:979:GLN:HB3	2.02	0.40
1:C:920:PHE:N	1:C:920:PHE:CD1	2.89	0.40
2:D:196:THR:O	2:D:200:GLN:HB2	2.20	0.40
2:B:206:LEU:HD22	2:B:206:LEU:H	1.86	0.40
1:E:921:ASP:N	2:F:288:LEU:HD11	2.36	0.40
2:D:69:THR:O	2:D:70:LYS:C	2.59	0.40
1:C:1163:SER:N	1:C:1175:ILE:HD11	2.35	0.40
1:C:1162:PRO:C	1:C:1175:ILE:HD11	2.41	0.40
1:A:901:THR:HG22	1:A:902:ALA:N	2.37	0.40
2:B:175:THR:HG22	2:B:177:LYS:HB3	2.02	0.40
1:C:1029:GLU:N	1:C:1029:GLU:CD	2.72	0.40
2:D:56:LEU:C	2:D:58:LYS:N	2.74	0.40
1:C:1033:LEU:CD2	1:C:1037:ILE:HG13	2.50	0.40
2:F:126:LEU:HD12	2:F:167:ALA:HB2	2.03	0.40
1:E:1025:VAL:O	1:E:1201:VAL:HG23	2.21	0.40
1:A:1186:MET:SD	1:A:1186:MET:N	2.94	0.40
1:C:933:VAL:HG22	1:C:1187:ILE:HG22	2.02	0.40
1:A:1090:MET:CE	1:A:1106:ALA:HA	2.51	0.40
2:D:222:LEU:HD21	2:D:228:TYR:CE1	2.56	0.40
1:E:1020:ILE:O	1:E:1023:LEU:HB2	2.22	0.40
2:D:157:SER:O	2:D:158:GLY:C	2.60	0.40
2:D:206:LEU:HD22	2:D:206:LEU:H	1.86	0.40
1:E:1050:ILE:HG12	1:E:1154:TYR:CD2	2.56	0.40
1:E:957:THR:O	1:E:958:PRO:C	2.58	0.40
2:F:197:TRP:NE1	2:F:236:ALA:HB2	2.36	0.40
2:D:197:TRP:NE1	2:D:236:ALA:CB	2.85	0.40
1:A:1071:TYR:HB3	1:A:1149:ILE:HG12	2.02	0.40
2:F:208:LEU:HD23	2:F:208:LEU:HA	1.82	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	303/325 (93%)	256 (84%)	32 (11%)	15 (5%)	3	11
1	C	301/325 (93%)	255 (85%)	31 (10%)	15 (5%)	3	11
1	E	301/325 (93%)	255 (85%)	31 (10%)	15 (5%)	3	11
2	B	291/310 (94%)	227 (78%)	41 (14%)	23 (8%)	1	3
2	D	291/310 (94%)	226 (78%)	44 (15%)	21 (7%)	2	4
2	F	291/310 (94%)	228 (78%)	42 (14%)	21 (7%)	2	4
All	All	1778/1905 (93%)	1447 (81%)	221 (12%)	110 (6%)	2	6

All (110) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	957	THR
1	A	973	ASP
1	A	1114	SER
1	A	1133	ALA
1	A	1186	MET
2	B	29	THR
2	B	51	ASP
2	B	73	GLU
2	B	234	GLU
2	B	258	THR
1	C	973	ASP
1	C	1114	SER
1	C	1133	ALA
1	C	1186	MET
2	D	29	THR
2	D	51	ASP
2	D	73	GLU
2	D	234	GLU
2	D	258	THR
1	E	973	ASP
1	E	1114	SER

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Mol	Chain	Res	Type
1	E	1133	ALA
1	E	1186	MET
2	F	29	THR
2	F	51	ASP
2	F	73	GLU
2	F	234	GLU
2	F	258	THR
1	A	1076	LYS
1	A	1097	LYS
2	B	3	TYR
2	B	8	GLN
2	B	154	ASP
2	B	195	PRO
2	B	273	ALA
1	C	957	THR
1	C	1076	LYS
1	C	1097	LYS
2	D	8	GLN
2	D	154	ASP
2	D	195	PRO
2	D	273	ALA
1	E	1076	LYS
1	E	1097	LYS
2	F	8	GLN
2	F	70	LYS
2	F	154	ASP
2	F	195	PRO
2	F	273	ALA
1	A	959	CYS
1	A	1095	LYS
1	A	1099	PHE
1	A	1132	MET
2	B	27	LYS
2	B	78	LEU
2	B	116	ASP
2	B	150	ASN
2	B	226	ASP
1	C	959	CYS
1	C	1095	LYS
1	C	1099	PHE
1	C	1132	MET
2	D	27	LYS

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Mol	Chain	Res	Type
2	D	78	LEU
2	D	150	ASN
2	D	158	GLY
2	D	226	ASP
2	D	291	LYS
1	E	957	THR
1	E	959	CYS
1	E	1095	LYS
1	E	1099	PHE
1	E	1132	MET
2	F	27	LYS
2	F	78	LEU
2	F	150	ASN
2	F	226	ASP
2	F	291	LYS
2	B	49	SER
2	B	70	LYS
2	B	269	ASP
2	B	291	LYS
2	D	3	TYR
2	D	49	SER
2	D	152	ILE
2	D	269	ASP
2	F	49	SER
2	F	269	ASP
1	A	958	PRO
2	B	81	ASP
2	B	152	ILE
1	C	900	GLU
2	D	81	ASP
2	F	81	ASP
2	F	152	ILE
1	A	911	PRO
1	C	911	PRO
1	E	911	PRO
2	B	158	GLY
1	A	1161	THR
2	B	230	VAL
1	C	1161	THR
2	D	230	VAL
1	E	1161	THR
2	F	230	VAL

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Mol	Chain	Res	Type
1	A	1112	ILE
1	C	1112	ILE
1	E	1112	ILE
2	F	158	GLY
1	E	958	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	259/276 (94%)	237 (92%)	22 (8%)	15	42
1	C	257/276 (93%)	235 (91%)	22 (9%)	15	41
1	E	257/276 (93%)	236 (92%)	21 (8%)	17	44
2	B	263/279 (94%)	225 (86%)	38 (14%)	5	13
2	D	263/279 (94%)	224 (85%)	39 (15%)	4	13
2	F	263/279 (94%)	224 (85%)	39 (15%)	4	13
All	All	1562/1665 (94%)	1381 (88%)	181 (12%)	8	23

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	931	VAL
1	A	954	ILE
1	A	957	THR
1	A	960	GLU
1	A	988	ASP
1	A	1023	LEU
1	A	1026	ASP
1	A	1033	LEU
1	A	1042	ARG
1	A	1046	LEU
1	A	1059	GLU
1	A	1061	ASN
1	A	1065	MET
1	A	1073	THR

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Mol	Chain	Res	Type
1	A	1080	ILE
1	A	1090	MET
1	A	1109	PHE
1	A	1118	ARG
1	A	1147	PHE
1	A	1164	VAL
1	A	1182	ASP
1	A	1186	MET
2	B	3	TYR
2	B	8	GLN
2	B	34	LEU
2	B	42	LEU
2	B	51	ASP
2	B	76	GLU
2	B	84	ASN
2	B	85	SER
2	B	92	LEU
2	B	99	LEU
2	B	106	LEU
2	B	121	THR
2	B	137	ASN
2	B	138	VAL
2	B	152	ILE
2	B	153	GLU
2	B	162	MET
2	B	164	LEU
2	B	176	ASN
2	B	188	GLU
2	B	201	LEU
2	B	211	ARG
2	B	213	ILE
2	B	222	LEU
2	B	225	SER
2	B	229	SER
2	B	234	GLU
2	B	237	VAL
2	B	249	THR
2	B	254	GLN
2	B	257	ASP
2	B	258	THR
2	B	261	LEU
2	B	262	THR

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Mol	Chain	Res	Type
2	B	266	VAL
2	B	271	GLU
2	B	272	HIS
2	B	281	ILE
1	C	931	VAL
1	C	954	ILE
1	C	957	THR
1	C	960	GLU
1	C	988	ASP
1	C	1023	LEU
1	C	1026	ASP
1	C	1033	LEU
1	C	1042	ARG
1	C	1046	LEU
1	C	1059	GLU
1	C	1061	ASN
1	C	1065	MET
1	C	1073	THR
1	C	1080	ILE
1	C	1090	MET
1	C	1109	PHE
1	C	1118	ARG
1	C	1147	PHE
1	C	1164	VAL
1	C	1182	ASP
1	C	1186	MET
2	D	2	ASP
2	D	3	TYR
2	D	8	GLN
2	D	34	LEU
2	D	42	LEU
2	D	51	ASP
2	D	76	GLU
2	D	84	ASN
2	D	85	SER
2	D	92	LEU
2	D	99	LEU
2	D	106	LEU
2	D	121	THR
2	D	137	ASN
2	D	138	VAL
2	D	152	ILE

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Mol	Chain	Res	Type
2	D	153	GLU
2	D	162	MET
2	D	164	LEU
2	D	176	ASN
2	D	188	GLU
2	D	201	LEU
2	D	211	ARG
2	D	213	ILE
2	D	222	LEU
2	D	225	SER
2	D	229	SER
2	D	234	GLU
2	D	237	VAL
2	D	249	THR
2	D	254	GLN
2	D	257	ASP
2	D	258	THR
2	D	261	LEU
2	D	262	THR
2	D	266	VAL
2	D	271	GLU
2	D	272	HIS
2	D	281	ILE
1	E	931	VAL
1	E	954	ILE
1	E	960	GLU
1	E	988	ASP
1	E	1023	LEU
1	E	1026	ASP
1	E	1033	LEU
1	E	1042	ARG
1	E	1046	LEU
1	E	1059	GLU
1	E	1061	ASN
1	E	1065	MET
1	E	1073	THR
1	E	1080	ILE
1	E	1090	MET
1	E	1109	PHE
1	E	1118	ARG
1	E	1147	PHE
1	E	1164	VAL

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Mol	Chain	Res	Type
1	E	1182	ASP
1	E	1186	MET
2	F	2	ASP
2	F	3	TYR
2	F	8	GLN
2	F	34	LEU
2	F	42	LEU
2	F	51	ASP
2	F	76	GLU
2	F	84	ASN
2	F	85	SER
2	F	92	LEU
2	F	99	LEU
2	F	106	LEU
2	F	121	THR
2	F	137	ASN
2	F	138	VAL
2	F	152	ILE
2	F	153	GLU
2	F	162	MET
2	F	164	LEU
2	F	176	ASN
2	F	188	GLU
2	F	201	LEU
2	F	211	ARG
2	F	213	ILE
2	F	222	LEU
2	F	225	SER
2	F	229	SER
2	F	234	GLU
2	F	237	VAL
2	F	249	THR
2	F	254	GLN
2	F	257	ASP
2	F	258	THR
2	F	261	LEU
2	F	262	THR
2	F	266	VAL
2	F	271	GLU
2	F	272	HIS
2	F	281	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	907	ASN
1	A	930	GLN
1	A	1087	GLN
2	B	235	ASN
1	C	907	ASN
1	C	930	GLN
1	C	1087	GLN
2	D	150	ASN
2	D	176	ASN
2	D	235	ASN
1	E	930	GLN
1	E	1087	GLN
1	E	1098	ASN
2	F	160	ASN
2	F	176	ASN
2	F	235	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	305/325 (93%)	-0.12	8 (2%) 53 63	55, 89, 144, 199	0
1	C	303/325 (93%)	0.14	16 (5%) 25 31	57, 97, 167, 201	0
1	E	303/325 (93%)	0.95	55 (18%) 2 3	98, 157, 196, 201	0
2	B	293/310 (94%)	0.08	14 (4%) 29 36	59, 99, 166, 201	0
2	D	293/310 (94%)	0.21	17 (5%) 22 26	64, 104, 172, 201	0
2	F	293/310 (94%)	1.68	92 (31%) 1 1	106, 179, 201, 201	0
All	All	1790/1905 (93%)	0.49	202 (11%) 6 7	55, 119, 197, 201	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	29	THR	9.9
2	F	160	ASN	9.5
2	F	153	GLU	9.3
2	F	70	LYS	8.9
2	F	51	ASP	8.7
2	F	50	GLN	8.0
2	D	155	THR	7.9
1	C	1135	ASP	7.2
2	F	257	ASP	7.1
1	C	1133	ALA	6.9
2	D	258	THR	6.7
2	F	83	GLN	6.5
2	F	116	ASP	6.4
2	F	47	TYR	6.3
2	F	178	GLU	6.3
2	F	58	LYS	6.2
1	E	1057	LEU	6.1
2	B	29	THR	6.1
2	F	20	GLN	6.1

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Mol	Chain	Res	Type	RSRZ
2	F	180	ALA	6.1
2	F	151	ALA	5.9
1	E	979	GLN	5.7
2	F	118	ALA	5.7
1	C	1060	GLY	5.7
2	F	48	GLN	5.7
1	E	1165	SER	5.6
1	A	1144	TYR	5.5
2	F	15	PHE	5.4
2	F	27	LYS	5.4
2	F	30	ASP	5.2
2	F	31	ASN	5.2
1	E	1135	ASP	5.2
2	F	28	VAL	5.1
2	D	1	MET	5.1
2	B	154	ASP	5.0
2	F	1	MET	5.0
2	B	156	VAL	5.0
1	E	1144	TYR	4.9
2	F	147	ASN	4.7
1	E	977	GLU	4.7
1	E	1093	HIS	4.6
1	C	1117	PRO	4.6
1	E	1058	LYS	4.5
2	D	81	ASP	4.5
2	F	143	THR	4.5
2	F	84	ASN	4.4
1	E	1055	ARG	4.3
2	F	26	SER	4.3
2	F	152	ILE	4.3
2	B	117	GLU	4.2
2	F	233	LYS	4.2
1	A	1099	PHE	4.1
2	F	177	LYS	4.1
2	F	3	TYR	4.1
1	E	1089	ALA	4.1
2	F	179	THR	4.1
2	F	281	ILE	4.0
2	B	155	THR	4.0
2	B	116	ASP	4.0
2	F	99	LEU	3.9
2	F	2	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
2	F	155	THR	3.9
1	E	1174	VAL	3.9
2	F	121	THR	3.8
2	F	24	LYS	3.8
1	E	1196	GLY	3.8
1	C	1138	PRO	3.8
2	F	107	GLU	3.7
2	F	44	LEU	3.7
1	E	1060	GLY	3.7
2	F	112	GLY	3.7
2	F	161	GLU	3.7
1	E	974	THR	3.7
1	C	973	ASP	3.7
2	F	52	PRO	3.6
2	F	258	THR	3.6
1	E	1115	SER	3.6
2	F	25	PHE	3.5
1	E	1124	LYS	3.5
1	E	1097	LYS	3.5
2	F	91	LEU	3.5
1	C	1059	GLU	3.5
2	F	46	GLN	3.5
2	F	104	LYS	3.5
2	F	135	ASN	3.5
1	A	-2	PRO	3.5
2	D	26	SER	3.4
2	F	18	CYS	3.3
1	E	962	PRO	3.3
2	F	10	TYR	3.3
2	B	18	CYS	3.2
2	F	16	VAL	3.2
1	C	1058	LYS	3.2
1	E	967	TYR	3.2
1	C	1094	PHE	3.2
1	E	909	LYS	3.1
2	D	27	LYS	3.1
1	E	1100	LEU	3.1
1	E	1146	LYS	3.1
1	E	1003	LEU	3.1
1	E	963	ALA	3.1
2	F	194	PHE	3.1
2	F	11	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	1022	LEU	3.1
2	F	89	LEU	3.1
2	F	159	ASP	3.0
2	F	148	TYR	3.0
1	E	965	LEU	3.0
2	F	117	GLU	3.0
1	E	1141	PHE	3.0
1	E	1062	THR	3.0
2	F	293	ASP	2.9
1	E	1067	GLU	2.9
2	B	27	LYS	2.9
2	F	120	GLY	2.9
2	B	118	ALA	2.9
2	F	53	THR	2.9
2	F	129	ILE	2.9
1	E	1059	GLU	2.8
2	D	116	ASP	2.8
2	D	156	VAL	2.8
2	F	249	THR	2.8
1	E	1129	ALA	2.8
2	D	2	ASP	2.8
2	F	85	SER	2.7
1	E	1172	LYS	2.7
2	F	185	TYR	2.7
1	E	1107	GLY	2.7
2	F	287	GLU	2.7
2	F	146	ASP	2.6
2	F	243	PHE	2.6
1	A	-1	HIS	2.6
2	F	88	GLU	2.6
2	F	12	THR	2.5
2	D	70	LYS	2.5
2	B	28	VAL	2.5
1	E	1150	CYS	2.5
2	F	267	LYS	2.5
2	F	211	ARG	2.5
1	A	1146	LYS	2.5
2	D	55	LYS	2.5
2	F	19	LEU	2.5
1	C	1097	LYS	2.5
2	F	268	LEU	2.5
2	F	64	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	290	ARG	2.5
2	D	80	LYS	2.5
1	E	1102	ALA	2.4
2	F	101	ASP	2.4
1	E	920	PHE	2.4
2	F	136	ASN	2.4
1	E	1140	ASP	2.4
1	E	1134	SER	2.4
1	A	1132	MET	2.4
1	E	1133	ALA	2.4
1	C	1124	LYS	2.4
2	F	87	TYR	2.4
1	E	1160	ASP	2.4
2	B	213	ILE	2.4
1	E	1194	ALA	2.4
2	D	257	ASP	2.4
2	D	93	ALA	2.3
1	E	1006	PRO	2.3
1	A	1073	THR	2.3
2	B	230	VAL	2.3
1	E	1127	ASN	2.3
2	D	117	GLU	2.2
2	F	140	THR	2.2
1	E	1063	VAL	2.2
2	F	111	GLU	2.2
2	B	83	GLN	2.2
2	F	244	LEU	2.2
1	E	1145	ALA	2.2
2	D	28	VAL	2.2
1	E	1189	LYS	2.2
1	E	1045	ILE	2.2
2	F	145	PHE	2.2
2	F	77	ASN	2.2
2	D	29	THR	2.1
1	C	1164	VAL	2.1
1	C	1047	GLY	2.1
1	E	1125	ILE	2.1
2	F	246	ASN	2.1
2	F	189	GLU	2.1
1	E	1195	SER	2.1
2	F	245	ALA	2.1
1	E	1159	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	80	LYS	2.1
1	E	1095	LYS	2.1
2	B	26	SER	2.1
2	F	154	ASP	2.1
2	F	119	GLU	2.1
1	C	974	THR	2.1
1	E	948	GLU	2.0
1	C	1100	LEU	2.0
1	E	953	TYR	2.0
1	C	1093	HIS	2.0
2	F	125	LEU	2.0
1	A	1123	ARG	2.0
1	E	1200	ARG	2.0
2	F	8	GLN	2.0
1	E	1099	PHE	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.