Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 05:27 PM EDT

PDB ID	:	3KDP
Title	:	Crystal structure of the sodium-potassium pump
Authors	:	Morth, J.P.; Pedersen, B.P.; Nissen, P.
Deposited on	:	2009-10-23
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

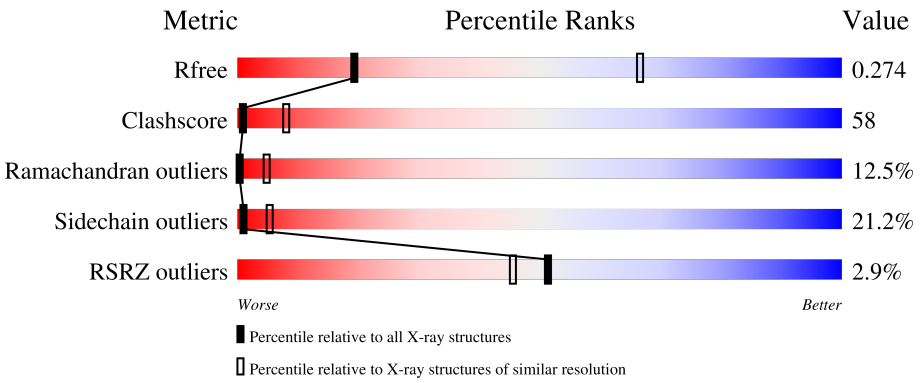
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	998	%, 25%, 52%, 22%, •
1	C	998	24%, 52%, 22%, •
2	B	286	6%, 28%, 50%, 20%, •
2	D	286	13%, 30%, 50%, 18%, •
3	G	27	37%, 59%, 41%

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Mol	Chain	Length	Quality of chain
3	H	27	19% 59% 37%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 20630 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Sodium/potassium-transporting ATPase subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	998	7740	4931	1304	1458	47	0	0	0
1	C	998	7740	4931	1304	1458	47	0	0	0

- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	286	2330	1502	382	433	13	0	0	0
2	D	286	2330	1502	382	433	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	151	SER	PHE	SEE REMARK 999	UNP P05027
D	151	SER	PHE	SEE REMARK 999	UNP P05027

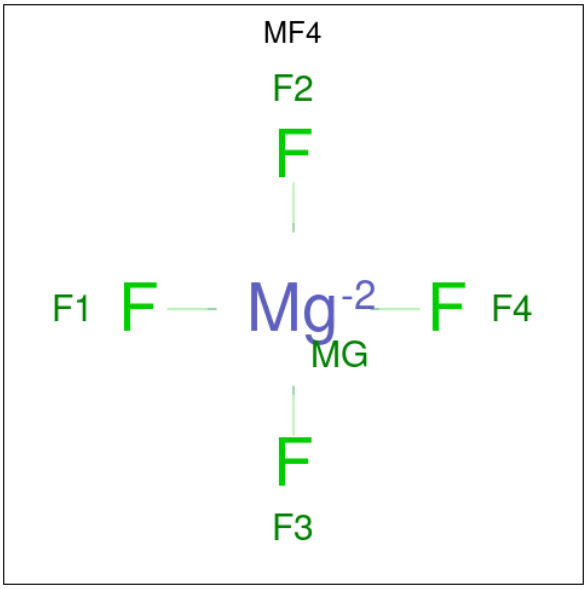
- Molecule 3 is a protein called Na+/K+ ATPase gamma subunit transcript variant a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	G	27	208	140	35	33	0	0	0
3	H	27	208	140	35	33	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	45	LEU	ILE	CONFLICT	UNP Q58K79
H	45	LEU	ILE	CONFLICT	UNP Q58K79

- Molecule 4 is TETRAFLUOROMAGNESATE(2-) (three-letter code: MF4) (formula: F_4Mg).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total F Mg 5 4 1	0	0
4	C	1	Total F Mg 5 4 1	0	0

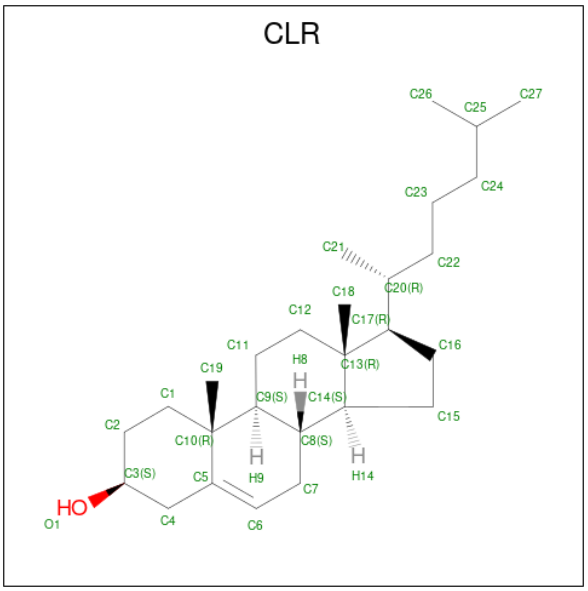
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0

- Molecule 6 is RUBIDIUM ION (three-letter code: RB) (formula: Rb).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total Rb 3 3	0	0
6	C	3	Total Rb 3 3	0	0

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



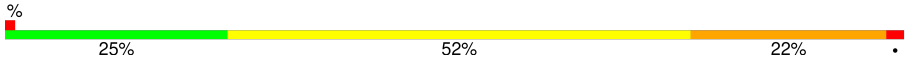
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	B	1	28	27	1	0	0
			Total	C	O		
7	D	1	28	27	1	0	0

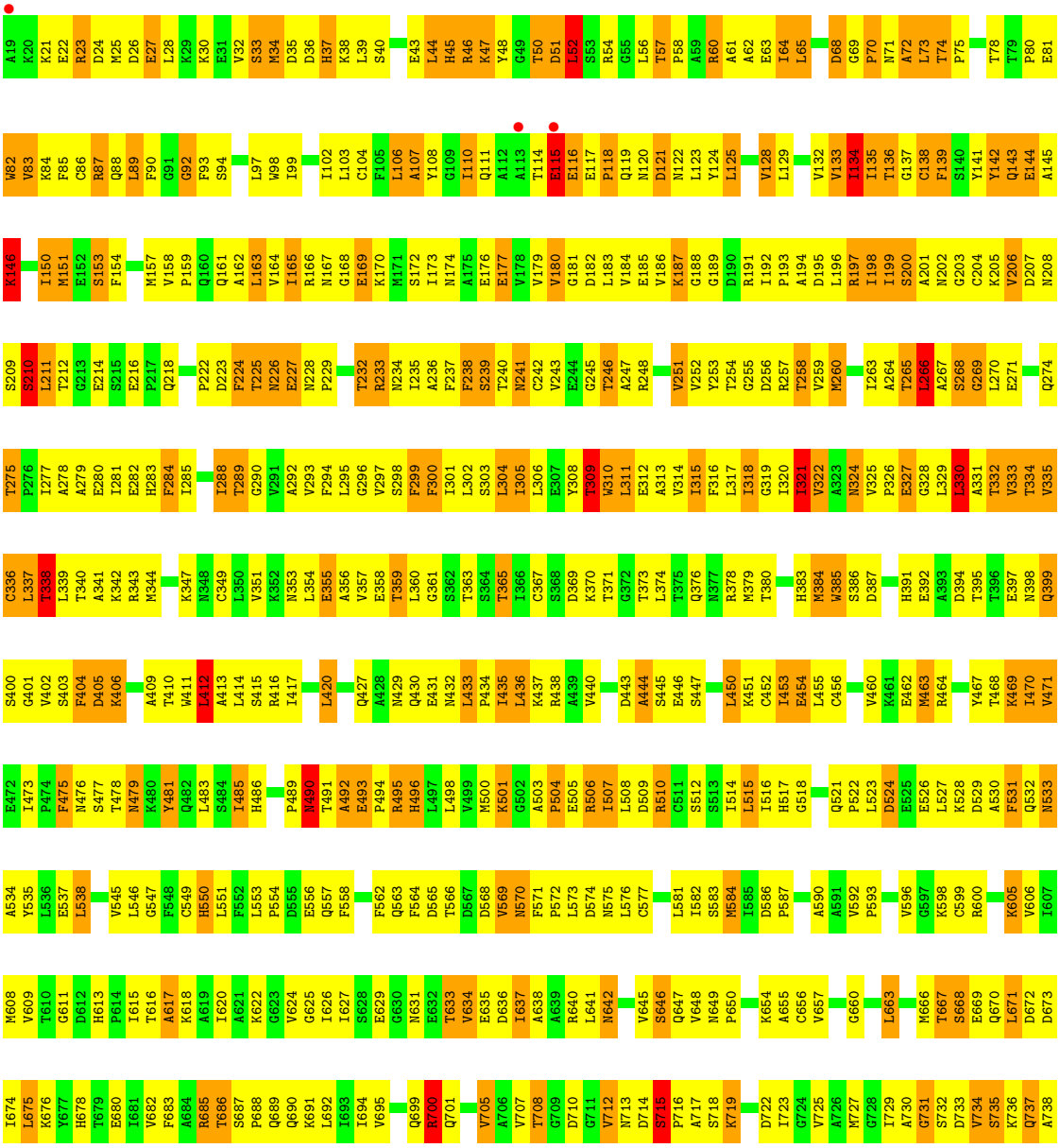
3 Residue-property plots (i)

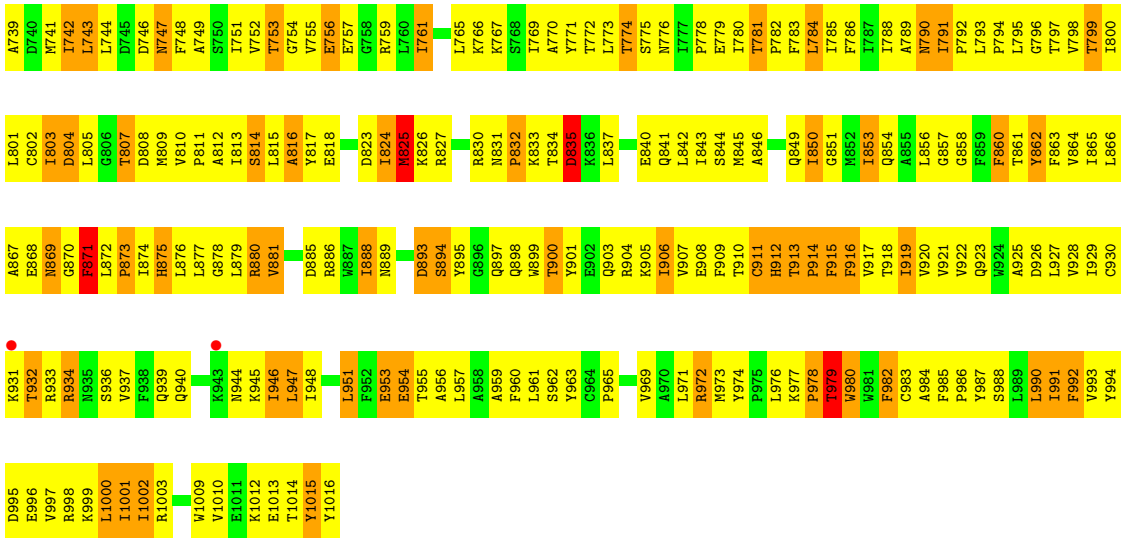
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

Chain A:

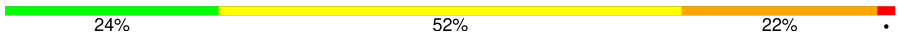


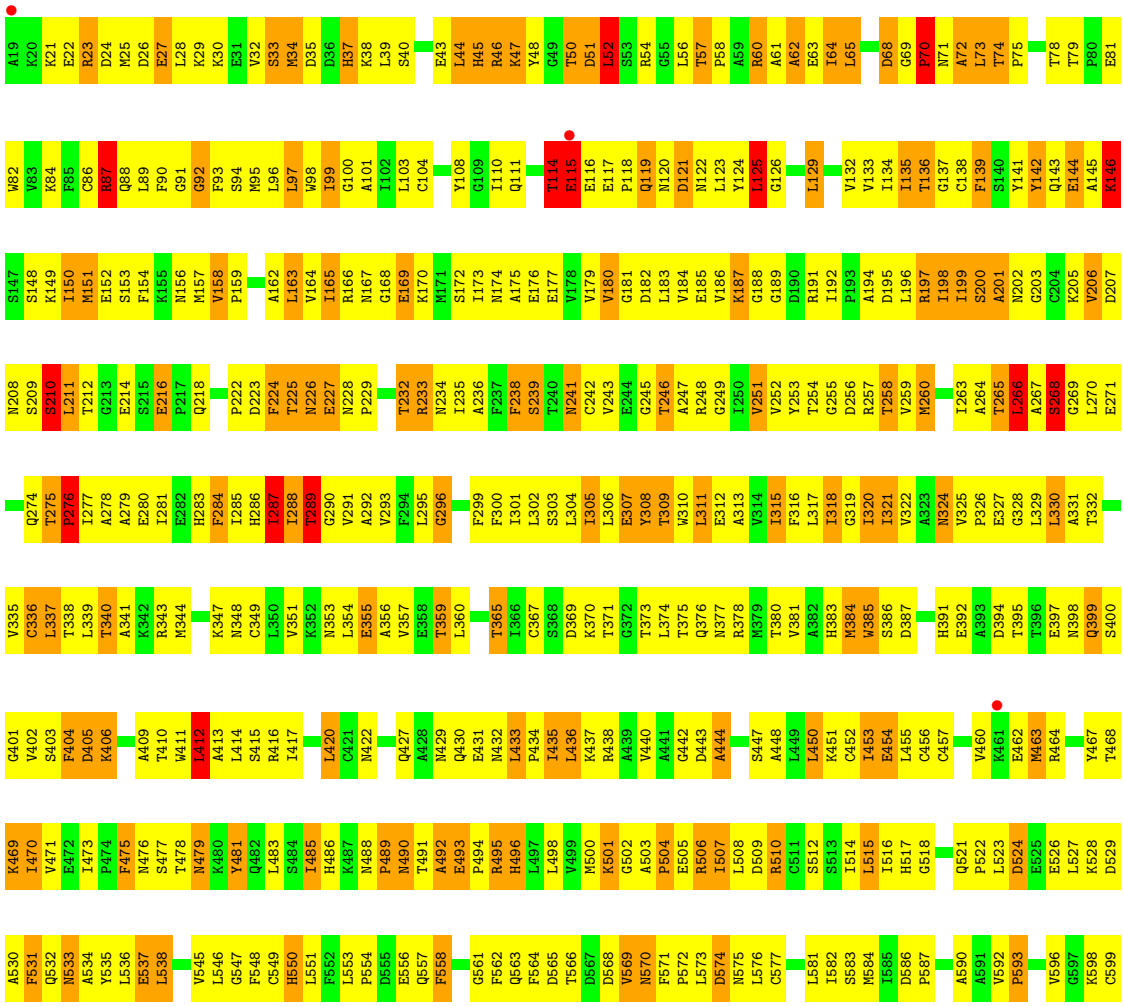


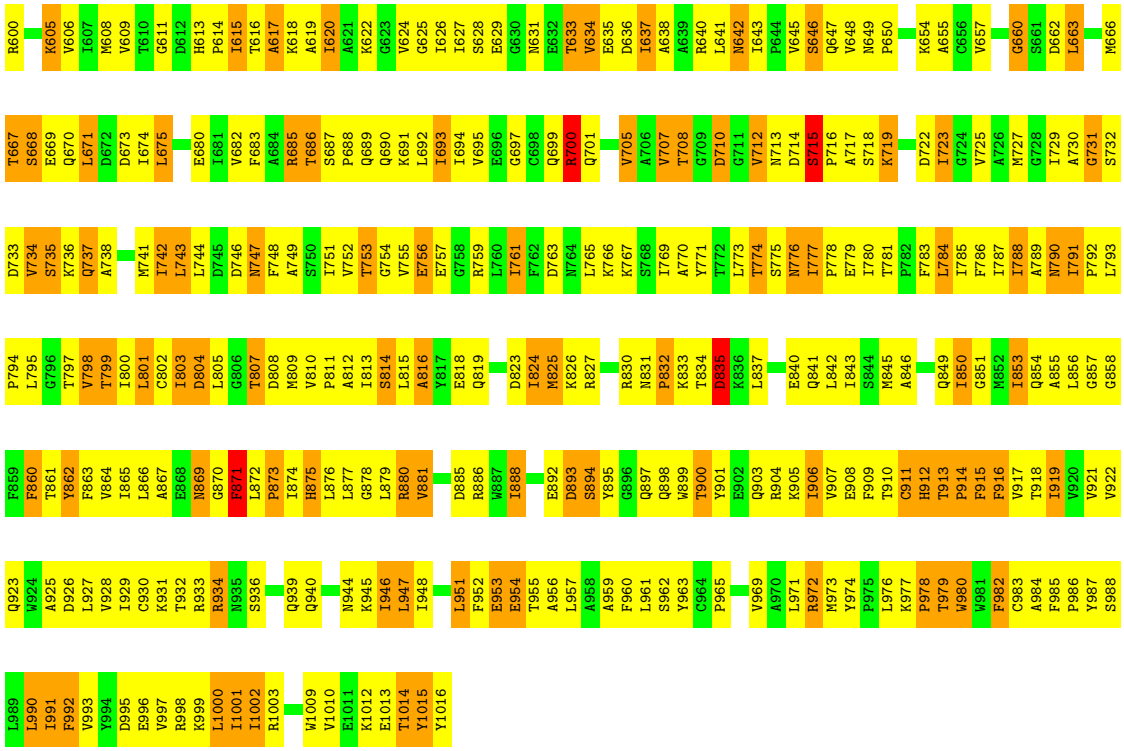


• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

Chain C:

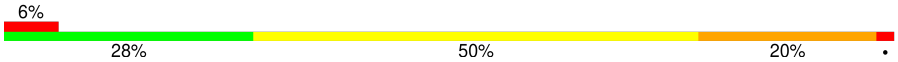


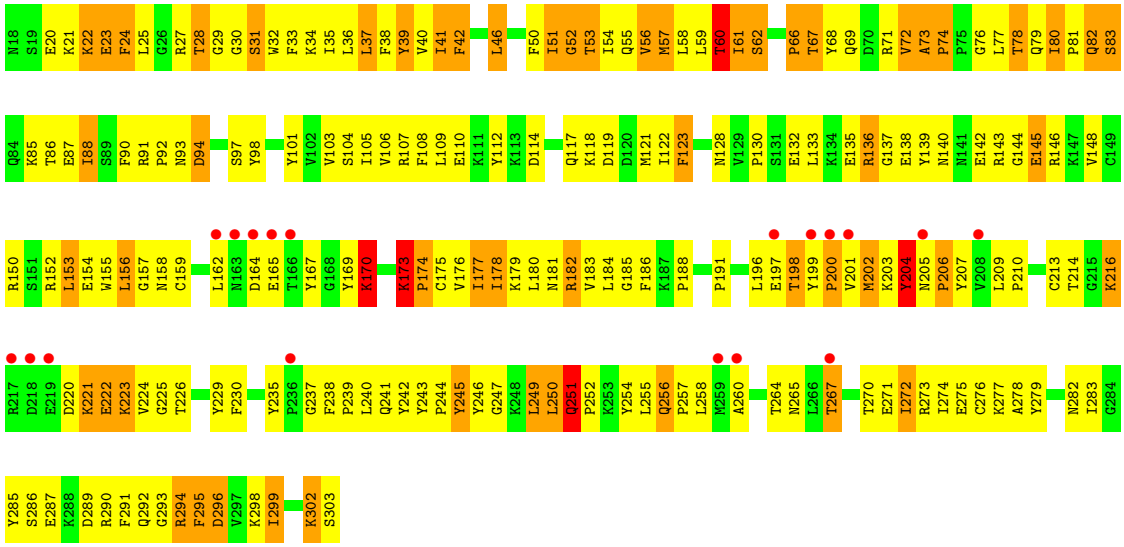




- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

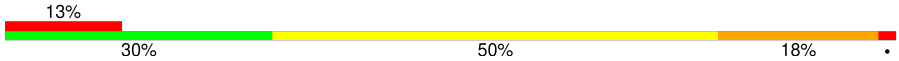
Chain B:

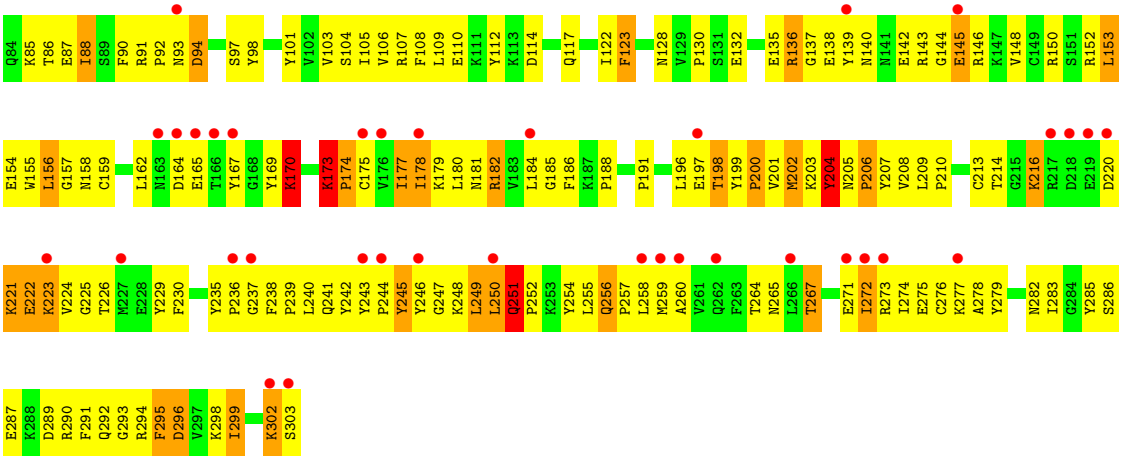




- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

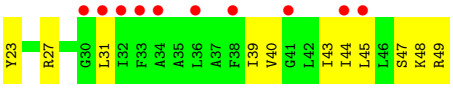
Chain D:





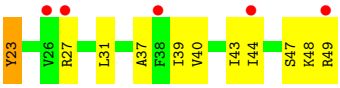
- Molecule 3: Na+/K+ ATPase gamma subunit transcript variant a

Chain G:



- Molecule 3: Na+/K+ ATPase gamma subunit transcript variant a

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.93Å 261.50Å 334.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.86 – 3.50 48.03 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.86-3.50) 99.6 (48.03-3.50)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	0.26	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.242 , 0.286 0.230 , 0.274	Depositor DCC
R_{free} test set	1550 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	89.0	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 82.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	20630	wwPDB-VP
Average B, all atoms (Å^2)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MF4, CLR, MG, RB

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	0.55	2/7890 (0.0%)	0.72	0/10706
1	C	0.55	0/7890	0.72	0/10706
2	B	0.37	0/2389	0.56	0/3221
2	D	0.37	0/2389	0.56	0/3221
3	G	0.24	0/210	0.44	0/282
3	H	0.25	0/210	0.44	0/282
All	All	0.51	2/20978 (0.0%)	0.68	0/28418

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	GLU	CG-CD	5.55	1.60	1.51
1	A	336	CYS	CB-SG	-5.21	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7740	0	7795	930	0
1	C	7740	0	7795	910	0
2	B	2330	0	2304	290	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2330	0	2304	288	0
3	G	208	0	230	6	0
3	H	208	0	230	8	0
4	A	5	0	0	1	0
4	C	5	0	0	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	3	0	0	0	0
6	C	3	0	0	0	0
7	B	28	0	46	2	0
7	D	28	0	46	4	0
All	All	20630	0	20750	2387	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 58.

All (2387) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:LYS:CB	2:B:22:LYS:HB2	1.69	1.21
1:A:861:THR:HG21	1:A:918:THR:HG21	1.21	1.17
1:C:861:THR:HG21	1:C:918:THR:HG21	1.20	1.16
1:A:226:ASN:HD22	1:A:227:GLU:N	1.45	1.14
2:D:21:LYS:CB	2:D:22:LYS:HB2	1.82	1.10
1:C:747:ASN:ND2	1:C:749:ALA:H	1.49	1.09
1:A:790:ASN:HD22	1:A:880:ARG:HD3	1.18	1.06
1:A:747:ASN:ND2	1:A:749:ALA:H	1.53	1.04
1:C:154:PHE:CD1	1:C:264:ALA:HB2	1.92	1.04
1:C:226:ASN:HD22	1:C:227:GLU:N	1.54	1.04
1:C:440:VAL:HG11	1:C:447:SER:HB2	1.37	1.04
1:C:790:ASN:HD22	1:C:880:ARG:HD3	1.14	1.04
2:D:21:LYS:HB3	2:D:22:LYS:HB2	1.11	1.04
1:C:569:VAL:HG12	1:C:570:ASN:H	1.25	1.00
2:B:21:LYS:HB3	2:B:22:LYS:CB	1.90	1.00
1:C:336:CYS:SG	1:C:816:ALA:HB2	2.03	0.98
1:C:120:ASN:HB3	1:C:124:TYR:CE1	1.98	0.98
1:A:440:VAL:HG11	1:A:447:SER:HB2	1.45	0.98
1:A:340:THR:HG22	1:A:343:ARG:HH21	1.29	0.97
1:A:404:PHE:O	1:A:405:ASP:HB2	1.66	0.96
1:C:73:LEU:H	1:C:73:LEU:HD12	1.28	0.96
1:A:977:LYS:H	1:A:980:TRP:HD1	1.14	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PHE:CD1	1:A:264:ALA:HB2	2.00	0.95
1:A:304:LEU:HD13	1:A:310:TRP:CZ3	2.02	0.94
1:A:73:LEU:HD12	1:A:73:LEU:H	1.30	0.94
2:B:21:LYS:HB3	2:B:22:LYS:HB2	0.94	0.94
1:C:404:PHE:O	1:C:405:ASP:HB2	1.66	0.94
1:A:241:ASN:HD22	1:A:241:ASN:H	1.16	0.94
1:C:795:LEU:HD13	1:C:915:PHE:HB3	1.49	0.93
1:C:747:ASN:HD22	1:C:749:ALA:H	1.08	0.93
1:C:874:ILE:H	1:C:874:ILE:HD12	1.31	0.93
1:A:1001:ILE:HG21	1:A:1010:VAL:HG21	1.49	0.93
1:A:874:ILE:HD12	1:A:874:ILE:H	1.29	0.93
1:C:747:ASN:HD22	1:C:747:ASN:C	1.72	0.93
1:A:304:LEU:HD13	1:A:310:TRP:HZ3	1.34	0.92
1:A:142:TYR:CD2	1:A:142:TYR:O	2.22	0.92
1:A:110:ILE:HG21	1:A:311:LEU:HD22	1.52	0.92
1:C:907:VAL:HG22	2:D:71:ARG:HD3	1.52	0.92
1:A:492:ALA:HA	1:A:493:GLU:HB3	1.52	0.92
1:A:747:ASN:C	1:A:747:ASN:HD22	1.72	0.91
1:C:977:LYS:H	1:C:980:TRP:HD1	1.15	0.91
2:D:60:THR:HG23	2:D:61:ILE:H	1.34	0.91
1:A:747:ASN:HD22	1:A:749:ALA:H	1.13	0.91
1:C:492:ALA:HA	1:C:493:GLU:HB3	1.53	0.90
1:C:241:ASN:HD22	1:C:241:ASN:H	1.17	0.90
2:B:60:THR:HG23	2:B:61:ILE:H	1.34	0.90
2:D:21:LYS:HD2	2:D:22:LYS:HD2	1.53	0.90
2:B:221:LYS:HE3	2:B:223:LYS:HB2	1.51	0.90
1:C:790:ASN:ND2	1:C:880:ARG:HD3	1.87	0.90
2:D:79:GLN:HB3	2:D:295:PHE:HZ	1.35	0.90
1:C:663:LEU:HA	1:C:666:MET:HE2	1.54	0.89
1:A:569:VAL:HG12	1:A:570:ASN:H	1.35	0.89
1:C:977:LYS:HD2	2:D:68:TYR:CE1	2.07	0.89
1:C:654:LYS:HE2	1:C:654:LYS:HA	1.51	0.89
1:C:1001:ILE:HG21	1:C:1010:VAL:HG21	1.55	0.89
1:C:187:LYS:HD2	1:C:188:GLY:H	1.35	0.89
1:A:654:LYS:HA	1:A:654:LYS:HE2	1.54	0.89
2:B:79:GLN:HB3	2:B:295:PHE:HZ	1.36	0.89
1:C:92:GLY:HA3	1:C:285:ILE:HD13	1.52	0.89
1:A:125:LEU:HD21	1:A:797:THR:HG21	1.54	0.89
1:A:795:LEU:HD13	1:A:915:PHE:HB3	1.51	0.88
2:D:221:LYS:HE3	2:D:223:LYS:HB2	1.53	0.88
1:A:85:PHE:O	1:A:88:GLN:HB2	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PHE:CD1	1:A:331:ALA:HB1	2.08	0.88
2:B:245:TYR:HD1	2:B:246:TYR:N	1.71	0.88
1:A:790:ASN:ND2	1:A:880:ARG:HD3	1.89	0.88
1:C:913:THR:HG22	1:C:976:LEU:HD21	1.55	0.88
1:A:340:THR:HG22	1:A:343:ARG:NH2	1.89	0.87
1:C:506:ARG:HH11	1:C:506:ARG:HG3	1.40	0.86
1:C:165:ILE:HG13	1:C:183:LEU:HD23	1.57	0.86
1:A:165:ILE:HG13	1:A:183:LEU:HD23	1.57	0.86
1:C:609:VAL:CG1	1:C:691:LYS:HG2	2.04	0.86
1:A:506:ARG:HH11	1:A:506:ARG:HG3	1.39	0.86
2:D:76:GLY:HA2	2:D:293:GLY:H	1.41	0.86
1:C:98:TRP:CZ2	1:C:133:VAL:HG11	2.11	0.86
1:A:37:HIS:CD2	1:A:232:THR:HG21	2.11	0.85
1:A:492:ALA:N	1:A:493:GLU:HB2	1.91	0.85
1:A:241:ASN:HD22	1:A:241:ASN:N	1.71	0.85
1:C:241:ASN:HD22	1:C:241:ASN:N	1.74	0.85
1:A:50:THR:HB	1:A:56:LEU:HD11	1.56	0.85
1:C:492:ALA:HA	1:C:493:GLU:CB	2.06	0.85
1:C:572:PRO:O	1:C:573:LEU:HD23	1.77	0.85
2:B:76:GLY:HA2	2:B:293:GLY:H	1.41	0.85
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.12	0.84
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.12	0.84
2:D:245:TYR:HD1	2:D:246:TYR:N	1.75	0.84
1:A:871:PHE:HD1	1:A:871:PHE:H	1.24	0.84
2:B:21:LYS:HD2	2:B:22:LYS:HD2	1.57	0.84
1:A:834:THR:HG22	1:A:835:ASP:H	1.43	0.84
1:A:115:GLU:HB3	2:B:85:LYS:HE2	1.59	0.83
1:A:492:ALA:HA	1:A:493:GLU:CB	2.08	0.83
1:A:663:LEU:HA	1:A:666:MET:HE2	1.58	0.83
1:C:510:ARG:HH11	1:C:510:ARG:HB3	1.42	0.83
2:D:31:SER:H	2:D:32:TRP:HB2	1.41	0.83
1:A:47:LYS:HE2	1:A:48:TYR:CZ	2.13	0.83
1:C:73:LEU:HD12	1:C:73:LEU:N	1.93	0.83
1:C:747:ASN:ND2	1:C:749:ALA:N	2.27	0.82
1:A:572:PRO:O	1:A:573:LEU:HD23	1.79	0.82
1:A:97:LEU:HG	1:A:325:VAL:HG11	1.59	0.82
1:A:284:PHE:CD1	1:A:285:ILE:N	2.47	0.82
1:A:73:LEU:HD12	1:A:73:LEU:N	1.94	0.82
2:B:31:SER:H	2:B:32:TRP:HB2	1.42	0.82
1:A:202:ASN:OD1	1:A:203:GLY:N	2.12	0.82
2:B:31:SER:CA	2:B:32:TRP:HB2	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:834:THR:HG22	1:C:835:ASP:H	1.45	0.82
1:A:790:ASN:HD22	1:A:880:ARG:CD	1.92	0.82
1:A:224:PHE:C	1:A:224:PHE:CD2	2.52	0.82
1:A:141:TYR:C	1:A:143:GLN:H	1.82	0.82
1:C:774:THR:HG23	1:C:846:ALA:HA	1.62	0.82
1:C:790:ASN:HD22	1:C:880:ARG:CD	1.91	0.81
1:C:416:ARG:HD2	1:C:467:TYR:CE1	2.14	0.81
1:A:50:THR:HB	1:A:56:LEU:CD1	2.10	0.81
1:C:84:LYS:HD2	1:C:146:LYS:HZ2	1.43	0.81
2:D:31:SER:CA	2:D:32:TRP:HB2	2.10	0.81
1:A:52:LEU:CD2	1:A:199:ILE:HD13	2.10	0.81
2:B:31:SER:N	2:B:32:TRP:HB2	1.96	0.81
1:A:913:THR:HG22	1:A:976:LEU:HD21	1.60	0.81
2:D:31:SER:N	2:D:32:TRP:HB2	1.95	0.81
2:B:153:LEU:H	2:B:153:LEU:HD12	1.46	0.81
2:B:170:LYS:HD2	2:B:170:LYS:N	1.97	0.80
1:C:50:THR:HB	1:C:56:LEU:HD11	1.61	0.80
1:C:416:ARG:O	1:C:420:LEU:HB2	1.80	0.80
1:A:226:ASN:HD22	1:A:227:GLU:H	1.30	0.80
1:C:120:ASN:HB3	1:C:124:TYR:HE1	1.43	0.80
2:B:30:GLY:O	2:B:31:SER:HB3	1.80	0.80
1:C:103:LEU:HD23	1:C:318:ILE:HG13	1.64	0.80
2:D:153:LEU:H	2:D:153:LEU:HD12	1.47	0.80
1:C:354:LEU:O	1:C:357:VAL:HG23	1.81	0.80
1:A:37:HIS:HD2	1:A:232:THR:HG21	1.43	0.80
1:C:492:ALA:N	1:C:493:GLU:HB2	1.97	0.80
1:C:840:GLU:HG2	1:C:841:GLN:H	1.46	0.80
1:A:416:ARG:O	1:A:420:LEU:HB2	1.82	0.79
1:A:609:VAL:CG1	1:A:691:LYS:HG2	2.12	0.79
1:A:341:ALA:HB2	1:A:357:VAL:HG21	1.63	0.79
1:C:196:LEU:HB2	1:C:236:ALA:HB3	1.62	0.79
2:B:21:LYS:HG2	2:B:22:LYS:HG3	1.65	0.79
1:A:747:ASN:ND2	1:A:749:ALA:N	2.31	0.79
1:A:774:THR:HG23	1:A:846:ALA:HA	1.64	0.79
1:A:37:HIS:ND1	1:A:37:HIS:N	2.30	0.79
1:A:510:ARG:HB3	1:A:510:ARG:HH11	1.46	0.79
1:C:37:HIS:CD2	1:C:232:THR:HG21	2.18	0.79
1:A:690:GLN:O	1:A:694:ILE:HG13	1.82	0.79
1:A:196:LEU:HB2	1:A:236:ALA:HB3	1.65	0.78
1:C:151:MET:C	1:C:153:SER:H	1.86	0.78
1:C:690:GLN:O	1:C:694:ILE:HG13	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:VAL:HG12	1:C:570:ASN:N	1.98	0.78
1:A:507:ILE:HG23	1:A:507:ILE:O	1.84	0.78
1:C:98:TRP:CE2	1:C:133:VAL:HG11	2.19	0.78
1:C:202:ASN:OD1	1:C:203:GLY:N	2.15	0.78
1:A:56:LEU:HD13	1:A:182:ASP:HA	1.65	0.78
1:C:166:ARG:C	1:C:168:GLY:H	1.87	0.78
1:A:284:PHE:HD1	1:A:285:ILE:N	1.80	0.78
1:C:110:ILE:HG21	1:C:311:LEU:HB3	1.65	0.78
1:A:727:MET:HB3	1:A:746:ASP:OD1	1.83	0.78
1:A:907:VAL:HG22	2:B:71:ARG:HD3	1.66	0.77
1:C:977:LYS:HD2	2:D:68:TYR:HE1	1.49	0.77
2:D:170:LYS:HD2	2:D:170:LYS:N	1.99	0.77
1:A:34:MET:SD	1:A:34:MET:N	2.58	0.77
1:A:187:LYS:HD2	1:A:188:GLY:H	1.49	0.77
1:A:521:GLN:HB3	1:A:522:PRO:HD2	1.67	0.77
1:C:84:LYS:HD2	1:C:146:LYS:NZ	1.99	0.77
1:C:727:MET:HB3	1:C:746:ASP:OD1	1.84	0.77
1:C:521:GLN:HB3	1:C:522:PRO:HD2	1.66	0.77
2:B:206:PRO:HB2	2:B:207:TYR:CD2	2.20	0.77
1:C:871:PHE:H	1:C:871:PHE:HD1	1.29	0.77
1:A:299:PHE:O	1:A:316:PHE:HE2	1.66	0.77
1:C:224:PHE:C	1:C:224:PHE:CD2	2.58	0.77
2:D:88:ILE:HD11	2:D:299:ILE:HG22	1.67	0.77
1:A:977:LYS:HD2	2:B:68:TYR:CE1	2.20	0.76
2:B:123:PHE:HD2	2:B:123:PHE:N	1.82	0.76
2:D:206:PRO:HB2	2:D:207:TYR:CD2	2.20	0.76
1:A:492:ALA:CA	1:A:493:GLU:CB	2.63	0.76
1:A:840:GLU:HG2	1:A:841:GLN:H	1.49	0.76
1:C:365:THR:HB	1:C:705:VAL:HG13	1.68	0.76
1:C:901:TYR:HA	1:C:904:ARG:NH1	2.00	0.76
2:B:123:PHE:N	2:B:123:PHE:CD2	2.53	0.76
1:A:983:CYS:O	1:A:986:PRO:HD2	1.85	0.76
1:C:37:HIS:ND1	1:C:37:HIS:N	2.31	0.76
2:B:216:LYS:HD2	2:B:221:LYS:HB2	1.68	0.76
2:D:224:VAL:HG13	2:D:267:THR:HG21	1.68	0.76
1:A:911:CYS:O	1:A:914:PRO:HD2	1.85	0.76
2:D:157:GLY:HA3	2:D:230:PHE:CE1	2.21	0.76
1:A:354:LEU:O	1:A:357:VAL:HG23	1.86	0.75
2:B:88:ILE:HG22	2:B:101:TYR:CE1	2.21	0.75
2:D:30:GLY:O	2:D:31:SER:HB3	1.86	0.75
2:B:143:ARG:HH11	2:B:143:ARG:HG3	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:88:ILE:HG22	2:D:101:TYR:CE1	2.22	0.75
1:C:278:ALA:HB2	1:C:355:GLU:OE1	1.85	0.75
1:C:381:VAL:HG21	1:C:452:CYS:HB2	1.68	0.75
2:D:94:ASP:HB2	2:D:97:SER:HB2	1.68	0.75
2:D:294:ARG:HG3	2:D:295:PHE:N	2.00	0.75
2:B:94:ASP:HB2	2:B:97:SER:HB2	1.68	0.75
1:A:142:TYR:HE2	1:A:338:THR:CG2	2.00	0.75
2:D:123:PHE:CD2	2:D:123:PHE:N	2.54	0.75
2:D:123:PHE:N	2:D:123:PHE:HD2	1.82	0.75
1:A:103:LEU:HD21	1:A:317:LEU:HD12	1.68	0.74
1:C:284:PHE:CD1	1:C:284:PHE:C	2.59	0.74
1:C:492:ALA:CA	1:C:493:GLU:CB	2.66	0.74
1:A:416:ARG:HD2	1:A:467:TYR:CE1	2.22	0.74
1:A:860:PHE:HE1	2:B:53:THR:O	1.69	0.74
1:C:92:GLY:HA3	1:C:285:ILE:CD1	2.18	0.74
2:B:239:PRO:HB2	2:B:241:GLN:HG2	1.70	0.74
2:D:216:LYS:HD2	2:D:221:LYS:HB2	1.68	0.74
1:C:37:HIS:HD2	1:C:232:THR:HG21	1.53	0.74
2:D:198:THR:HG23	2:D:203:LYS:HE2	1.69	0.74
2:B:157:GLY:HA3	2:B:230:PHE:CE1	2.22	0.74
1:C:898:GLN:HG3	2:D:182:ARG:HG3	1.70	0.74
1:A:365:THR:HB	1:A:705:VAL:HG13	1.69	0.74
2:B:88:ILE:HD11	2:B:299:ILE:HG22	1.69	0.74
1:A:901:TYR:HA	1:A:904:ARG:NH1	2.02	0.73
1:C:199:ILE:O	1:C:222:PRO:HG3	1.88	0.73
1:C:507:ILE:HG23	1:C:507:ILE:O	1.85	0.73
1:C:911:CYS:O	1:C:914:PRO:HD2	1.87	0.73
2:D:143:ARG:HH11	2:D:143:ARG:HG3	1.53	0.73
1:C:983:CYS:O	1:C:986:PRO:HD2	1.88	0.73
1:A:166:ARG:C	1:A:168:GLY:H	1.90	0.73
1:C:378:ARG:CZ	1:C:436:LEU:HD22	2.18	0.73
1:C:199:ILE:HD12	1:C:200:SER:H	1.54	0.73
1:C:861:THR:HG22	1:C:983:CYS:HB3	1.71	0.73
1:A:645:VAL:O	1:A:648:VAL:HG23	1.89	0.73
2:B:294:ARG:HG3	2:B:295:PHE:N	2.02	0.73
2:D:23:GLU:C	2:D:25:LEU:H	1.92	0.73
1:A:378:ARG:CZ	1:A:436:LEU:HD22	2.19	0.72
1:C:284:PHE:C	1:C:284:PHE:HD1	1.92	0.72
1:C:645:VAL:O	1:C:648:VAL:HG23	1.89	0.72
1:A:743:LEU:N	1:A:743:LEU:HD23	2.04	0.72
1:A:874:ILE:H	1:A:874:ILE:CD1	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:ARG:HG3	1:A:881:VAL:N	2.04	0.72
2:D:21:LYS:HG2	2:D:22:LYS:HG3	1.71	0.72
2:B:198:THR:HG23	2:B:203:LYS:HE2	1.68	0.72
2:D:60:THR:HG23	2:D:61:ILE:N	2.05	0.72
1:A:93:PHE:CE2	1:A:326:PRO:HD2	2.25	0.72
1:A:238:PHE:HD1	1:A:239:SER:N	1.87	0.72
2:D:239:PRO:HB2	2:D:241:GLN:HG2	1.70	0.72
2:D:170:LYS:HD3	2:D:175:CYS:HB2	1.70	0.72
1:A:370:LYS:HB2	1:A:608:MET:HE3	1.72	0.72
1:A:922:VAL:HA	1:A:988:SER:OG	1.89	0.72
2:B:156:LEU:HD13	2:B:159:CYS:CB	2.20	0.72
2:D:58:LEU:C	2:D:60:THR:HB	2.10	0.72
1:C:907:VAL:CG2	2:D:71:ARG:HD3	2.18	0.72
1:C:922:VAL:HA	1:C:988:SER:OG	1.90	0.72
2:B:136:ARG:HB3	2:B:146:ARG:HD3	1.72	0.71
2:B:224:VAL:HG13	2:B:267:THR:HG21	1.70	0.71
1:C:139:PHE:HE1	1:C:335:VAL:HG23	1.55	0.71
1:A:999:LYS:O	1:A:1003:ARG:HG3	1.91	0.71
2:B:23:GLU:C	2:B:25:LEU:H	1.90	0.71
1:C:435:ILE:HD13	1:C:438:ARG:NH2	2.05	0.71
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.71	0.71
1:C:645:VAL:C	1:C:647:GLN:H	1.94	0.71
2:D:156:LEU:HD13	2:D:159:CYS:HB3	1.72	0.71
1:C:47:LYS:HE2	1:C:48:TYR:CZ	2.26	0.71
1:C:460:VAL:CG1	1:C:464:ARG:HD3	2.21	0.71
1:A:48:TYR:HB2	1:A:50:THR:HG22	1.73	0.71
1:A:645:VAL:C	1:A:647:GLN:H	1.91	0.71
1:C:34:MET:N	1:C:34:MET:SD	2.63	0.71
1:A:732:SER:O	1:A:733:ASP:C	2.29	0.71
1:C:732:SER:O	1:C:733:ASP:C	2.28	0.71
2:D:73:ALA:HB1	2:D:74:PRO:CD	2.21	0.71
2:B:60:THR:HG23	2:B:61:ILE:N	2.05	0.71
2:B:59:LEU:N	2:B:60:THR:HA	2.06	0.71
2:B:73:ALA:HB1	2:B:74:PRO:CD	2.21	0.71
2:B:265:ASN:ND2	2:B:267:THR:HG22	2.05	0.71
1:A:327:GLU:HB3	1:A:805:LEU:HD11	1.73	0.70
2:B:156:LEU:HD13	2:B:159:CYS:HB3	1.72	0.70
1:C:50:THR:HB	1:C:56:LEU:CD1	2.20	0.70
1:C:94:SER:O	1:C:98:TRP:HB2	1.91	0.70
1:C:910:THR:O	1:C:914:PRO:HD3	1.91	0.70
1:A:460:VAL:HG12	1:A:464:ARG:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:TYR:HB2	1:C:50:THR:HG22	1.71	0.70
1:C:166:ARG:O	1:C:167:ASN:HB2	1.91	0.70
2:D:59:LEU:N	2:D:60:THR:HA	2.05	0.70
3:H:47:SER:O	3:H:48:LYS:HB2	1.92	0.70
1:A:275:THR:OG1	1:A:277:ILE:HG22	1.90	0.70
1:C:640:ARG:O	1:C:641:LEU:HD12	1.90	0.70
2:D:31:SER:HA	2:D:32:TRP:HB2	1.74	0.70
1:A:166:ARG:O	1:A:167:ASN:HB2	1.89	0.70
1:A:310:TRP:CE3	1:A:310:TRP:HA	2.25	0.70
1:C:277:ILE:O	1:C:280:GLU:N	2.24	0.70
1:C:303:SER:O	1:C:308:TYR:HD2	1.74	0.70
1:A:142:TYR:CE2	1:A:338:THR:HG21	2.27	0.70
2:B:170:LYS:HD3	2:B:175:CYS:HB2	1.74	0.70
1:C:840:GLU:HG2	1:C:841:GLN:N	2.06	0.70
1:A:288:ILE:HG22	1:A:289:THR:N	2.07	0.70
1:A:913:THR:HG21	1:A:974:TYR:O	1.91	0.70
2:B:188:PRO:CD	2:B:243:TYR:HD1	2.05	0.70
1:C:110:ILE:HG22	1:C:111:GLN:HG3	1.71	0.70
2:D:21:LYS:CD	2:D:22:LYS:HD2	2.22	0.70
1:A:549:CYS:HB2	1:A:577:CYS:O	1.92	0.70
1:C:145:ALA:C	1:C:146:LYS:HG3	2.10	0.70
1:A:182:ASP:O	1:A:251:VAL:HG22	1.92	0.70
1:A:187:LYS:O	1:A:242:CYS:SG	2.50	0.69
1:A:569:VAL:HG12	1:A:570:ASN:N	2.05	0.69
2:B:58:LEU:C	2:B:60:THR:HB	2.12	0.69
2:D:265:ASN:ND2	2:D:267:THR:HG22	2.06	0.69
2:B:22:LYS:N	2:B:25:LEU:HD12	2.07	0.69
2:D:31:SER:HA	2:D:33:PHE:H	1.58	0.69
1:A:897:GLN:HA	2:B:182:ARG:O	1.92	0.69
2:B:265:ASN:HD22	2:B:267:THR:HG22	1.56	0.69
1:C:308:TYR:OH	1:C:787:ILE:HD13	1.91	0.69
1:C:936:SER:HA	1:C:996:GLU:OE2	1.93	0.69
1:A:122:ASN:HD21	1:A:315:ILE:HD11	1.57	0.69
1:A:301:ILE:HD12	1:A:302:LEU:N	2.07	0.69
1:A:910:THR:O	1:A:914:PRO:HD3	1.92	0.69
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.75	0.69
1:C:898:GLN:OE1	2:D:182:ARG:HD3	1.92	0.69
2:D:156:LEU:HD13	2:D:159:CYS:CB	2.21	0.69
2:B:21:LYS:CD	2:B:22:LYS:HD2	2.22	0.69
1:C:56:LEU:HD13	1:C:182:ASP:HA	1.74	0.69
1:C:999:LYS:O	1:C:1003:ARG:HG3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ASN:ND2	1:A:227:GLU:N	2.31	0.69
1:A:267:ALA:O	1:A:269:GLY:N	2.24	0.69
1:A:460:VAL:CG1	1:A:464:ARG:HD3	2.22	0.69
2:B:216:LYS:CD	2:B:221:LYS:HB2	2.23	0.69
1:C:151:MET:C	1:C:153:SER:N	2.46	0.69
1:C:151:MET:O	1:C:153:SER:N	2.26	0.69
1:C:202:ASN:OD1	1:C:202:ASN:C	2.32	0.69
2:B:20:GLU:CD	2:B:28:THR:OG1	2.32	0.69
2:B:31:SER:HA	2:B:33:PHE:H	1.57	0.69
1:C:406:LYS:O	1:C:406:LYS:HD3	1.93	0.69
1:A:52:LEU:HD21	1:A:199:ILE:HD13	1.73	0.69
1:A:853:ILE:HD13	2:B:46:LEU:HD21	1.75	0.69
3:G:40:VAL:O	3:G:44:ILE:HG13	1.93	0.68
1:C:874:ILE:H	1:C:874:ILE:CD1	2.04	0.68
1:A:791:ILE:HG23	1:A:862:TYR:OH	1.94	0.68
3:G:47:SER:O	3:G:48:LYS:HB2	1.94	0.68
1:C:238:PHE:HD1	1:C:239:SER:N	1.90	0.68
1:A:687:SER:HB2	1:A:690:GLN:H	1.58	0.68
1:A:1001:ILE:HG21	1:A:1010:VAL:CG2	2.22	0.68
1:C:710:ASP:O	1:C:731:GLY:HA2	1.93	0.68
2:B:21:LYS:CB	2:B:22:LYS:CB	2.62	0.68
1:C:321:ILE:HG22	1:C:322:VAL:N	2.08	0.68
1:C:778:PRO:CG	1:C:919:ILE:HD11	2.23	0.68
1:A:38:LYS:HG2	1:A:224:PHE:HE1	1.59	0.68
1:A:92:GLY:HA3	1:A:285:ILE:HD13	1.76	0.68
1:A:304:LEU:HD22	1:A:310:TRP:CZ3	2.28	0.68
1:A:435:ILE:HD13	1:A:438:ARG:NH2	2.08	0.68
1:A:840:GLU:HG2	1:A:841:GLN:N	2.06	0.68
1:C:311:LEU:HD23	1:C:311:LEU:H	1.57	0.68
2:D:22:LYS:N	2:D:25:LEU:HD12	2.08	0.68
2:D:216:LYS:CD	2:D:221:LYS:HB2	2.23	0.68
1:A:824:ILE:O	1:A:827:ARG:HG2	1.94	0.68
1:C:187:LYS:CD	1:C:188:GLY:H	2.06	0.68
1:C:226:ASN:HD22	1:C:227:GLU:H	1.40	0.68
1:C:370:LYS:HB2	1:C:608:MET:HE3	1.76	0.68
1:C:545:VAL:HG22	1:C:583:SER:HB3	1.75	0.68
1:C:743:LEU:HD23	1:C:743:LEU:N	2.09	0.68
1:C:880:ARG:HG3	1:C:881:VAL:N	2.07	0.68
2:D:136:ARG:HB3	2:D:146:ARG:HD3	1.74	0.68
2:D:185:GLY:HA2	2:D:244:PRO:HB3	1.75	0.68
1:A:778:PRO:CG	1:A:919:ILE:HD11	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:PHE:CE1	1:C:335:VAL:HG23	2.28	0.68
2:B:185:GLY:HA2	2:B:244:PRO:HB3	1.76	0.67
1:C:549:CYS:HB2	1:C:577:CYS:O	1.93	0.67
1:C:791:ILE:HG23	1:C:862:TYR:OH	1.94	0.67
1:C:874:ILE:C	1:C:876:LEU:H	1.96	0.67
2:D:199:TYR:CD1	2:D:200:PRO:HD2	2.30	0.67
1:C:767:LYS:HB3	1:C:930:CYS:O	1.95	0.67
2:D:20:GLU:CD	2:D:28:THR:OG1	2.33	0.67
1:A:169:GLU:HG2	1:C:170:LYS:HD2	1.75	0.67
1:C:129:LEU:HD11	1:C:322:VAL:CG2	2.24	0.67
1:C:288:ILE:HD11	1:C:773:LEU:HD11	1.77	0.67
1:C:531:PHE:C	1:C:531:PHE:CD1	2.66	0.67
2:B:199:TYR:CD1	2:B:200:PRO:HD2	2.30	0.67
1:A:44:LEU:O	1:A:46:ARG:N	2.27	0.67
1:A:640:ARG:O	1:A:641:LEU:HD12	1.94	0.67
1:A:736:LYS:C	1:A:738:ALA:H	1.97	0.67
1:C:913:THR:CG2	1:C:976:LEU:HD21	2.23	0.67
1:C:929:ILE:HB	1:C:995:ASP:OD2	1.95	0.67
2:D:143:ARG:HG3	2:D:143:ARG:NH1	2.10	0.67
3:H:40:VAL:O	3:H:44:ILE:HG13	1.95	0.67
1:A:861:THR:HG22	1:A:983:CYS:HB3	1.77	0.67
2:B:31:SER:HA	2:B:32:TRP:HB2	1.75	0.67
2:D:177:ILE:HA	2:D:260:ALA:HA	1.76	0.67
2:D:188:PRO:CD	2:D:243:TYR:HD1	2.07	0.67
1:C:736:LYS:C	1:C:738:ALA:H	1.99	0.67
1:C:913:THR:HG21	1:C:974:TYR:O	1.93	0.67
1:C:995:ASP:OD1	1:C:998:ARG:NH1	2.28	0.67
2:D:39:TYR:HE2	7:D:3001:CLR:H182	1.60	0.67
2:D:40:VAL:HG23	2:D:41:ILE:N	2.10	0.67
1:A:329:LEU:HD21	1:A:769:ILE:HG12	1.76	0.67
1:C:493:GLU:H	1:C:494:PRO:CD	2.08	0.66
1:A:277:ILE:HD13	1:A:358:GLU:HG3	1.77	0.66
1:A:414:LEU:HD12	1:A:414:LEU:O	1.95	0.66
1:C:414:LEU:HD12	1:C:414:LEU:O	1.94	0.66
2:D:273:ARG:HG3	2:D:298:LYS:HG2	1.77	0.66
1:A:871:PHE:N	1:A:871:PHE:CD1	2.63	0.66
1:A:310:TRP:HA	1:A:310:TRP:HE3	1.60	0.66
1:C:747:ASN:HD21	1:C:749:ALA:CB	2.07	0.66
1:A:138:CYS:O	1:A:141:TYR:HB3	1.95	0.66
1:A:506:ARG:HG3	1:A:506:ARG:NH1	2.11	0.66
2:B:177:ILE:HA	2:B:260:ALA:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:687:SER:HB2	1:C:690:GLN:H	1.61	0.66
2:D:73:ALA:CB	2:D:74:PRO:HD2	2.26	0.66
2:D:148:VAL:HG11	2:D:254:TYR:HA	1.78	0.66
1:A:110:ILE:CG2	1:A:311:LEU:HD22	2.24	0.66
1:A:255:GLY:O	1:A:258:THR:HG23	1.96	0.66
1:A:874:ILE:C	1:A:876:LEU:H	1.98	0.66
1:C:795:LEU:HD13	1:C:915:PHE:CB	2.26	0.66
1:C:329:LEU:HD21	1:C:769:ILE:HG12	1.77	0.66
1:C:267:ALA:O	1:C:269:GLY:N	2.25	0.66
1:C:460:VAL:HG12	1:C:464:ARG:HD3	1.75	0.65
1:C:747:ASN:HD22	1:C:749:ALA:N	1.89	0.65
1:C:857:GLY:CA	1:C:987:TYR:CD1	2.78	0.65
2:D:91:ARG:HG2	2:D:302:LYS:O	1.96	0.65
1:A:207:ASP:HB3	1:A:241:ASN:ND2	2.11	0.65
1:A:611:GLY:HA2	1:A:686:THR:H	1.61	0.65
2:B:91:ARG:HG2	2:B:302:LYS:O	1.96	0.65
1:C:150:ILE:CG2	1:C:268:SER:HB2	2.26	0.65
1:A:309:THR:HG22	1:A:310:TRP:H	1.61	0.65
2:B:225:GLY:HA2	2:B:265:ASN:HB3	1.79	0.65
1:C:277:ILE:HG23	1:C:278:ALA:N	2.09	0.65
1:C:44:LEU:O	1:C:46:ARG:N	2.29	0.65
1:A:141:TYR:C	1:A:143:GLN:N	2.50	0.65
2:B:143:ARG:HG3	2:B:143:ARG:NH1	2.09	0.65
2:B:148:VAL:HG11	2:B:254:TYR:HA	1.77	0.65
1:C:386:SER:HB2	1:C:391:HIS:NE2	2.12	0.65
2:D:265:ASN:HD22	2:D:267:THR:HG22	1.60	0.65
1:C:934:ARG:O	1:C:1003:ARG:HD3	1.96	0.65
1:A:373:THR:HG21	1:A:708:THR:HB	1.79	0.65
1:A:936:SER:HA	1:A:996:GLU:OE2	1.96	0.65
2:B:273:ARG:HG3	2:B:298:LYS:HG2	1.79	0.65
1:C:562:PHE:HE2	1:C:570:ASN:HD21	1.45	0.65
1:C:747:ASN:ND2	1:C:747:ASN:C	2.46	0.65
1:A:338:THR:HA	1:A:354:LEU:HD11	1.79	0.65
1:C:462:GLU:O	1:C:464:ARG:N	2.30	0.65
1:C:824:ILE:O	1:C:827:ARG:HG2	1.96	0.65
1:A:463:MET:O	1:A:463:MET:HG2	1.97	0.65
1:A:767:LYS:HB3	1:A:930:CYS:O	1.96	0.65
2:B:73:ALA:CB	2:B:74:PRO:HD2	2.26	0.65
1:C:300:PHE:HA	1:C:303:SER:HB3	1.78	0.65
2:D:112:TYR:HE2	2:D:255:LEU:HB3	1.62	0.65
1:A:708:THR:HG21	1:A:748:PHE:CE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:TRP:O	1:C:413:ALA:N	2.30	0.64
2:D:140:ASN:HB3	2:D:142:GLU:HG3	1.79	0.64
1:A:406:LYS:O	1:A:406:LYS:HD3	1.98	0.64
1:A:462:GLU:O	1:A:464:ARG:N	2.30	0.64
1:A:40:SER:H	1:A:43:GLU:HB2	1.63	0.64
1:A:300:PHE:HA	1:A:303:SER:CB	2.27	0.64
1:A:470:ILE:HG12	1:A:485:ILE:O	1.97	0.64
1:A:494:PRO:O	1:A:495:ARG:O	2.15	0.64
1:C:125:LEU:HD12	1:C:798:VAL:HG23	1.80	0.64
1:C:287:ILE:HG22	1:C:288:ILE:N	2.12	0.64
1:A:925:ALA:O	1:A:929:ILE:HG13	1.98	0.64
2:D:225:GLY:HA2	2:D:265:ASN:HB3	1.79	0.64
1:A:493:GLU:O	1:A:493:GLU:HG2	1.97	0.64
2:B:112:TYR:HE2	2:B:255:LEU:HB3	1.62	0.64
1:C:795:LEU:CD1	1:C:915:PHE:HB3	2.25	0.64
2:D:40:VAL:CG2	2:D:41:ILE:H	2.09	0.64
1:A:56:LEU:HD13	1:A:182:ASP:CA	2.28	0.64
1:A:238:PHE:HD2	1:A:258:THR:HG21	1.62	0.64
1:C:166:ARG:O	1:C:168:GLY:N	2.30	0.64
1:A:52:LEU:HD23	1:A:199:ILE:HD13	1.79	0.64
1:A:110:ILE:HG21	1:A:311:LEU:CD2	2.26	0.64
1:A:934:ARG:O	1:A:1003:ARG:HD3	1.97	0.64
1:C:129:LEU:HD23	1:C:801:LEU:HD11	1.79	0.64
1:C:288:ILE:HG22	1:C:289:THR:N	2.13	0.64
2:D:83:SER:HB3	2:D:86:THR:H	1.63	0.64
1:C:608:MET:HB3	1:C:682:VAL:HG13	1.78	0.64
1:C:774:THR:CG2	1:C:846:ALA:HA	2.27	0.64
2:D:177:ILE:HD12	2:D:258:LEU:HD23	1.80	0.64
1:A:125:LEU:HD21	1:A:797:THR:CG2	2.26	0.64
1:A:199:ILE:O	1:A:222:PRO:HG3	1.98	0.64
1:A:308:TYR:HB3	1:A:312:GLU:HB3	1.79	0.64
1:A:531:PHE:CD1	1:A:531:PHE:C	2.71	0.64
1:A:769:ILE:HG22	1:A:770:ALA:N	2.13	0.64
1:C:295:LEU:HD12	1:C:324:ASN:HD21	1.60	0.64
1:C:493:GLU:O	1:C:493:GLU:HG2	1.98	0.64
1:C:863:PHE:HB3	2:D:54:ILE:HD11	1.78	0.64
2:D:295:PHE:HD1	2:D:296:ASP:H	1.46	0.64
1:C:569:VAL:CG1	1:C:570:ASN:H	2.05	0.64
1:A:225:THR:OG1	1:A:226:ASN:HB2	1.98	0.63
1:C:871:PHE:CD1	1:C:871:PHE:N	2.67	0.63
1:A:778:PRO:HG2	1:A:919:ILE:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:THR:HG22	1:C:266:LEU:N	2.13	0.63
1:A:618:LYS:HD3	1:A:657:VAL:HG21	1.80	0.63
1:A:854:GLN:HG2	1:A:991:ILE:HD11	1.80	0.63
1:A:929:ILE:HB	1:A:995:ASP:OD2	1.98	0.63
1:C:508:LEU:C	1:C:510:ARG:H	2.00	0.63
1:C:875:HIS:O	1:C:879:LEU:HD21	1.98	0.63
2:D:40:VAL:CG2	2:D:41:ILE:N	2.61	0.63
1:A:111:GLN:HE22	1:A:122:ASN:HD22	1.45	0.63
1:A:569:VAL:CG1	1:A:570:ASN:H	2.10	0.63
1:A:774:THR:CG2	1:A:846:ALA:HA	2.28	0.63
2:B:40:VAL:HG23	2:B:41:ILE:N	2.13	0.63
2:B:60:THR:CG2	2:B:61:ILE:H	1.97	0.63
2:B:177:ILE:HD12	2:B:258:LEU:HD23	1.80	0.63
1:C:206:VAL:HG23	1:C:242:CYS:HA	1.81	0.63
1:A:117:GLU:C	1:A:119:GLN:H	2.02	0.63
2:B:225:GLY:HA2	2:B:265:ASN:CB	2.29	0.63
1:C:984:ALA:O	1:C:987:TYR:HB2	1.98	0.63
2:D:213:CYS:HB3	2:D:274:ILE:HD11	1.81	0.63
1:A:275:THR:HG1	1:A:277:ILE:HG22	1.61	0.63
2:B:83:SER:HB3	2:B:86:THR:H	1.63	0.63
2:B:213:CYS:HB3	2:B:274:ILE:HD11	1.81	0.63
1:C:611:GLY:HA2	1:C:686:THR:H	1.62	0.63
1:C:769:ILE:HG22	1:C:770:ALA:N	2.14	0.63
1:A:202:ASN:OD1	1:A:202:ASN:C	2.35	0.63
1:A:508:LEU:C	1:A:510:ARG:H	2.00	0.63
2:B:140:ASN:HB3	2:B:142:GLU:HG3	1.80	0.63
2:D:170:LYS:HB3	2:D:174:PRO:HA	1.81	0.63
1:A:492:ALA:CA	1:A:493:GLU:HB2	2.28	0.62
1:A:755:VAL:HG13	1:A:825:MET:SD	2.39	0.62
1:A:789:ALA:O	1:A:791:ILE:N	2.31	0.62
2:B:295:PHE:HD1	2:B:296:ASP:H	1.47	0.62
1:C:166:ARG:C	1:C:168:GLY:N	2.53	0.62
1:C:429:ASN:O	1:C:430:GLN:HG2	1.99	0.62
1:C:618:LYS:HD3	1:C:657:VAL:HG21	1.80	0.62
1:A:225:THR:HG21	1:A:233:ARG:HD2	1.81	0.62
2:B:21:LYS:CG	2:B:22:LYS:HB2	2.30	0.62
1:C:153:SER:O	1:C:156:ASN:HB2	1.98	0.62
1:C:207:ASP:HB3	1:C:241:ASN:ND2	2.14	0.62
1:C:227:GLU:OE1	1:C:227:GLU:HA	1.99	0.62
1:C:873:PRO:HA	1:C:876:LEU:HD12	1.81	0.62
1:A:48:TYR:HB2	1:A:50:THR:CG2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:O	1:A:280:GLU:N	2.31	0.62
1:A:404:PHE:O	1:A:405:ASP:CB	2.47	0.62
1:A:429:ASN:O	1:A:430:GLN:HG2	2.00	0.62
1:A:857:GLY:CA	1:A:987:TYR:CD1	2.81	0.62
2:B:37:LEU:HD12	2:B:37:LEU:O	2.00	0.62
1:C:370:LYS:HB2	1:C:608:MET:CE	2.30	0.62
1:C:492:ALA:CA	1:C:493:GLU:HB2	2.29	0.62
2:D:170:LYS:HD3	2:D:175:CYS:CB	2.28	0.62
1:A:142:TYR:CE2	1:A:338:THR:CG2	2.82	0.62
1:A:462:GLU:C	1:A:464:ARG:H	2.02	0.62
1:C:174:ASN:HB3	1:C:177:GLU:HG3	1.79	0.62
1:C:747:ASN:HD21	1:C:749:ALA:HB3	1.65	0.62
1:C:873:PRO:O	1:C:876:LEU:HB2	1.98	0.62
1:A:284:PHE:CD1	1:A:284:PHE:C	2.72	0.62
2:B:23:GLU:C	2:B:25:LEU:N	2.53	0.62
2:B:157:GLY:HA3	2:B:230:PHE:CD1	2.35	0.62
1:C:48:TYR:CB	1:C:50:THR:HG22	2.29	0.62
1:C:139:PHE:CD1	1:C:331:ALA:HB1	2.34	0.62
1:C:182:ASP:O	1:C:251:VAL:HG22	2.00	0.62
1:C:443:ASP:O	1:C:444:ALA:C	2.37	0.62
1:C:637:ILE:HG12	1:C:640:ARG:NH1	2.14	0.62
1:C:96:LEU:O	1:C:99:ILE:HG13	2.00	0.62
1:C:103:LEU:CD2	1:C:317:LEU:HD12	2.30	0.62
1:C:893:ASP:CG	1:C:894:SER:H	2.03	0.62
2:D:225:GLY:HA2	2:D:265:ASN:CB	2.29	0.62
1:A:48:TYR:CB	1:A:50:THR:HG22	2.30	0.62
1:A:224:PHE:C	1:A:224:PHE:HD2	2.03	0.62
1:A:893:ASP:CG	1:A:894:SER:H	2.02	0.62
1:A:918:THR:O	1:A:922:VAL:HG13	2.00	0.62
2:B:170:LYS:HB3	2:B:174:PRO:HA	1.82	0.62
1:C:255:GLY:O	1:C:258:THR:HG23	1.98	0.62
1:C:793:LEU:HD12	1:C:794:PRO:HD2	1.82	0.62
1:A:281:ILE:O	1:A:283:HIS:N	2.33	0.62
1:A:645:VAL:O	1:A:647:GLN:N	2.33	0.62
1:A:747:ASN:HD21	1:A:749:ALA:CB	2.13	0.62
1:A:860:PHE:CE1	2:B:53:THR:O	2.52	0.62
1:A:992:PHE:C	1:A:992:PHE:CD1	2.73	0.62
1:C:299:PHE:CD2	1:C:784:LEU:HD22	2.34	0.62
1:A:120:ASN:O	1:A:124:TYR:HD1	1.82	0.62
1:A:411:TRP:O	1:A:413:ALA:N	2.33	0.62
1:A:608:MET:HB3	1:A:682:VAL:HG13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:TYR:HB2	2:B:169:TYR:CE1	2.35	0.62
1:C:790:ASN:HB3	1:C:880:ARG:HG2	1.81	0.62
1:A:304:LEU:CD1	1:A:310:TRP:HZ3	2.11	0.61
1:A:747:ASN:ND2	1:A:747:ASN:C	2.47	0.61
1:A:982:PHE:CD2	1:A:982:PHE:N	2.68	0.61
1:A:151:MET:C	1:A:153:SER:H	2.03	0.61
1:A:545:VAL:HG22	1:A:583:SER:HB3	1.82	0.61
1:C:373:THR:HG21	1:C:708:THR:HB	1.82	0.61
1:C:886:ARG:HA	1:C:901:TYR:CD1	2.35	0.61
2:D:170:LYS:HG2	2:D:174:PRO:C	2.21	0.61
1:A:224:PHE:HD2	1:A:224:PHE:O	1.83	0.61
2:B:40:VAL:CG2	2:B:41:ILE:N	2.63	0.61
2:B:152:ARG:O	2:B:155:TRP:CD1	2.54	0.61
2:D:37:LEU:HD12	2:D:37:LEU:O	2.00	0.61
1:A:284:PHE:HD1	1:A:284:PHE:C	2.04	0.61
1:A:340:THR:CG2	1:A:343:ARG:HH21	2.09	0.61
1:A:386:SER:HB2	1:A:391:HIS:NE2	2.14	0.61
1:A:795:LEU:CD1	1:A:915:PHE:HB3	2.28	0.61
1:A:898:GLN:HG3	2:B:182:ARG:HG3	1.81	0.61
2:B:73:ALA:HB1	2:B:74:PRO:HD2	1.83	0.61
2:B:78:THR:HG22	2:B:181:ASN:OD1	1.99	0.61
2:B:170:LYS:HD3	2:B:175:CYS:CB	2.31	0.61
2:D:78:THR:HG22	2:D:181:ASN:OD1	2.01	0.61
2:D:157:GLY:HA3	2:D:230:PHE:CD1	2.34	0.61
2:D:167:TYR:HB2	2:D:169:TYR:CE1	2.35	0.61
1:A:38:LYS:HG2	1:A:224:PHE:CE1	2.34	0.61
1:A:790:ASN:HB3	1:A:880:ARG:HG2	1.82	0.61
1:C:172:SER:O	1:C:173:ILE:HG23	1.99	0.61
1:C:531:PHE:HD1	1:C:532:GLN:N	1.99	0.61
1:C:747:ASN:HD22	1:C:748:PHE:N	1.99	0.61
2:D:73:ALA:HB1	2:D:74:PRO:HD2	1.83	0.61
2:D:130:PRO:HB2	2:D:204:TYR:OH	2.00	0.61
1:A:277:ILE:HG23	1:A:278:ALA:N	2.15	0.61
1:A:284:PHE:HZ	1:A:330:LEU:HD21	1.66	0.61
1:A:993:VAL:O	1:A:997:VAL:HG23	2.00	0.61
1:A:995:ASP:OD1	1:A:998:ARG:NH1	2.33	0.61
1:A:172:SER:O	1:A:173:ILE:HG23	2.00	0.61
1:A:565:ASP:N	1:A:570:ASN:HD22	1.99	0.61
1:C:288:ILE:O	1:C:290:GLY:N	2.34	0.61
1:C:925:ALA:O	1:C:929:ILE:HG13	1.99	0.61
1:C:993:VAL:O	1:C:997:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ILE:HG22	1:A:135:ILE:N	2.15	0.61
1:A:288:ILE:HD11	1:A:773:LEU:HD21	1.82	0.61
1:A:637:ILE:HG12	1:A:640:ARG:NH1	2.16	0.61
2:B:123:PHE:HD2	2:B:123:PHE:H	1.49	0.61
1:C:165:ILE:O	1:C:166:ARG:HG3	2.00	0.61
1:C:462:GLU:C	1:C:464:ARG:H	2.03	0.61
1:C:781:THR:HA	1:C:784:LEU:HB2	1.83	0.61
1:A:300:PHE:HA	1:A:303:SER:HB3	1.83	0.61
1:A:747:ASN:HD22	1:A:748:PHE:N	1.97	0.61
1:A:876:LEU:O	1:A:878:GLY:N	2.29	0.61
1:A:878:GLY:O	1:A:881:VAL:HG23	1.99	0.61
1:C:252:VAL:O	1:C:253:TYR:CD1	2.54	0.61
1:C:982:PHE:CD2	1:C:982:PHE:N	2.68	0.61
2:D:239:PRO:HG2	2:D:242:TYR:HE1	1.66	0.61
1:A:206:VAL:HG23	1:A:242:CYS:HA	1.83	0.61
1:C:299:PHE:CE2	1:C:784:LEU:HD13	2.36	0.61
1:A:142:TYR:HE2	1:A:338:THR:HG21	1.61	0.60
1:A:886:ARG:HA	1:A:901:TYR:CD1	2.36	0.60
1:A:913:THR:OG1	1:A:973:MET:HA	2.00	0.60
1:A:495:ARG:O	1:A:496:HIS:CB	2.50	0.60
1:C:132:VAL:HA	1:C:135:ILE:HG22	1.82	0.60
1:C:992:PHE:CD1	1:C:992:PHE:C	2.75	0.60
1:A:226:ASN:HD22	1:A:226:ASN:C	2.03	0.60
1:A:227:GLU:OE1	1:A:227:GLU:HA	2.01	0.60
2:B:83:SER:OG	2:B:86:THR:HA	2.01	0.60
2:B:272:ILE:HD13	2:B:272:ILE:H	1.65	0.60
1:C:354:LEU:O	1:C:356:ALA:N	2.35	0.60
1:C:506:ARG:HG3	1:C:506:ARG:NH1	2.10	0.60
1:C:734:VAL:O	1:C:735:SER:C	2.39	0.60
1:A:370:LYS:HB2	1:A:608:MET:CE	2.31	0.60
1:A:940:GLN:O	1:A:940:GLN:HG3	2.00	0.60
1:C:187:LYS:O	1:C:242:CYS:SG	2.60	0.60
2:D:152:ARG:O	2:D:155:TRP:CD1	2.55	0.60
1:A:47:LYS:HE2	1:A:48:TYR:OH	2.01	0.60
1:A:493:GLU:H	1:A:494:PRO:CD	2.15	0.60
1:A:748:PHE:CD2	1:A:748:PHE:O	2.54	0.60
1:C:186:VAL:HG11	1:C:192:ILE:HD13	1.82	0.60
1:C:194:ALA:HB1	1:C:253:TYR:O	2.02	0.60
1:A:300:PHE:O	1:A:303:SER:HB3	2.01	0.60
1:C:288:ILE:C	1:C:290:GLY:N	2.55	0.60
2:D:59:LEU:N	2:D:60:THR:CA	2.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:LYS:HG2	2:D:175:CYS:HB2	1.84	0.60
2:B:130:PRO:HB2	2:B:204:TYR:OH	2.01	0.60
2:B:201:VAL:O	2:B:202:MET:HB2	2.01	0.60
1:C:111:GLN:HE22	1:C:122:ASN:HD22	1.50	0.60
1:C:645:VAL:O	1:C:647:GLN:N	2.33	0.60
1:A:252:VAL:O	1:A:253:TYR:CD1	2.55	0.60
1:C:52:LEU:CD2	1:C:199:ILE:HD13	2.31	0.60
1:C:149:LYS:HB2	1:C:737:GLN:OE1	2.02	0.60
1:A:232:THR:OG1	1:A:234:ASN:OD1	2.12	0.60
1:C:58:PRO:O	1:C:61:ALA:HB3	2.02	0.60
1:C:853:ILE:HD13	2:D:46:LEU:HD21	1.83	0.60
1:A:166:ARG:C	1:A:168:GLY:N	2.55	0.60
1:C:470:ILE:HG12	1:C:485:ILE:O	2.01	0.60
1:C:531:PHE:CD1	1:C:532:GLN:N	2.69	0.60
1:C:912:HIS:O	1:C:914:PRO:N	2.35	0.60
2:D:71:ARG:NH1	3:H:23:TYR:OH	2.35	0.60
1:A:174:ASN:HB3	1:A:177:GLU:HG3	1.82	0.59
2:B:40:VAL:CG2	2:B:41:ILE:H	2.14	0.59
1:C:189:GLY:N	1:C:242:CYS:O	2.29	0.59
1:A:443:ASP:O	1:A:444:ALA:C	2.39	0.59
1:C:241:ASN:N	1:C:241:ASN:ND2	2.47	0.59
1:C:296:GLY:HA2	1:C:320:ILE:HG21	1.84	0.59
1:C:778:PRO:HG2	1:C:919:ILE:HD11	1.82	0.59
1:C:860:PHE:HE1	2:D:53:THR:O	1.85	0.59
2:D:73:ALA:CB	2:D:74:PRO:CD	2.81	0.59
2:D:272:ILE:HD13	2:D:272:ILE:H	1.67	0.59
1:A:110:ILE:CG2	1:A:311:LEU:HD13	2.32	0.59
1:A:710:ASP:O	1:A:731:GLY:HA2	2.03	0.59
1:C:181:GLY:H	1:C:251:VAL:HG23	1.68	0.59
1:C:195:ASP:HB2	1:C:253:TYR:HB2	1.84	0.59
1:C:216:GLU:HG3	1:C:216:GLU:O	2.01	0.59
1:A:56:LEU:CD1	1:A:182:ASP:HA	2.32	0.59
1:A:337:LEU:O	1:A:339:LEU:N	2.35	0.59
1:A:504:PRO:HG2	1:A:535:TYR:HE1	1.67	0.59
2:D:60:THR:CG2	2:D:61:ILE:H	1.97	0.59
1:C:755:VAL:HG13	1:C:825:MET:SD	2.43	0.59
1:C:789:ALA:O	1:C:791:ILE:N	2.35	0.59
1:A:73:LEU:H	1:A:73:LEU:CD1	2.11	0.59
1:A:265:THR:HG22	1:A:266:LEU:N	2.17	0.59
1:C:253:TYR:HB3	1:C:258:THR:HA	1.83	0.59
1:C:473:ILE:HD12	1:C:483:LEU:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:PRO:O	1:C:495:ARG:O	2.19	0.59
1:C:748:PHE:CD2	1:C:748:PHE:O	2.55	0.59
2:D:285:TYR:HB3	2:D:294:ARG:HH21	1.68	0.59
1:A:61:ALA:O	1:A:64:ILE:N	2.35	0.59
2:B:278:ALA:O	2:B:283:ILE:HG21	2.03	0.59
2:D:57:MET:HG3	2:D:58:LEU:HG	1.83	0.59
2:D:201:VAL:O	2:D:202:MET:HB2	2.01	0.59
1:A:260:MET:O	1:A:263:ILE:HB	2.03	0.59
1:C:328:GLY:H	1:C:804:ASP:HB2	1.68	0.59
1:C:339:LEU:O	1:C:341:ALA:N	2.35	0.59
1:C:854:GLN:HG2	1:C:991:ILE:HD11	1.84	0.59
1:C:1001:ILE:HG21	1:C:1010:VAL:CG2	2.30	0.59
1:A:285:ILE:HD11	1:A:330:LEU:HD11	1.85	0.59
1:A:338:THR:HG23	1:A:354:LEU:CD2	2.33	0.59
1:A:880:ARG:HG3	1:A:881:VAL:H	1.68	0.58
1:C:288:ILE:HD11	1:C:773:LEU:CD1	2.33	0.58
1:C:756:GLU:HG2	1:C:757:GLU:N	2.17	0.58
1:C:918:THR:HB	1:C:984:ALA:HB2	1.85	0.58
2:D:56:VAL:HA	2:D:59:LEU:HG	1.85	0.58
1:A:60:ARG:O	1:A:60:ARG:HG3	2.03	0.58
1:A:189:GLY:N	1:A:242:CYS:O	2.30	0.58
1:A:905:LYS:O	1:A:908:GLU:N	2.36	0.58
1:A:913:THR:CG2	1:A:976:LEU:HD21	2.30	0.58
1:A:936:SER:HB3	1:A:939:GLN:HG3	1.85	0.58
2:B:73:ALA:CB	2:B:74:PRO:CD	2.81	0.58
1:C:633:THR:OG1	1:C:634:VAL:N	2.36	0.58
1:C:861:THR:CG2	1:C:983:CYS:HB3	2.34	0.58
1:A:309:THR:N	1:A:312:GLU:HB2	2.17	0.58
1:A:708:THR:HG21	1:A:748:PHE:HE1	1.67	0.58
2:B:272:ILE:HD13	2:B:272:ILE:N	2.18	0.58
1:C:878:GLY:O	1:C:881:VAL:HG23	2.02	0.58
1:C:909:PHE:CD2	1:C:972:ARG:HB3	2.38	0.58
1:A:58:PRO:O	1:A:61:ALA:HB3	2.04	0.58
1:A:309:THR:H	1:A:312:GLU:HB2	1.69	0.58
1:A:756:GLU:HG2	1:A:757:GLU:N	2.18	0.58
1:A:873:PRO:O	1:A:876:LEU:HB2	2.03	0.58
1:C:225:THR:HG21	1:C:233:ARG:HD2	1.85	0.58
1:C:275:THR:HG21	1:C:355:GLU:OE2	2.03	0.58
1:C:276:PRO:CG	1:C:359:THR:HG23	2.34	0.58
1:C:800:ILE:C	1:C:802:CYS:H	2.07	0.58
1:C:897:GLN:HA	2:D:182:ARG:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:TYR:HE2	7:D:3001:CLR:C18	2.16	0.58
1:A:194:ALA:HB3	1:A:251:VAL:HG12	1.85	0.58
2:B:57:MET:HG3	2:B:58:LEU:HG	1.84	0.58
2:B:245:TYR:CD1	2:B:246:TYR:N	2.63	0.58
1:C:103:LEU:HB3	1:C:318:ILE:HD11	1.85	0.58
1:C:570:ASN:OD1	1:C:570:ASN:O	2.21	0.58
1:A:238:PHE:CD1	1:A:239:SER:N	2.71	0.58
2:B:21:LYS:CD	2:B:22:LYS:CD	2.81	0.58
2:B:34:LYS:H	2:B:34:LYS:HD2	1.67	0.58
1:C:495:ARG:O	1:C:496:HIS:CB	2.51	0.58
1:C:918:THR:O	1:C:922:VAL:HG13	2.04	0.58
1:C:980:TRP:HA	1:C:980:TRP:HE3	1.68	0.58
1:A:793:LEU:HD12	1:A:794:PRO:HD2	1.85	0.58
1:C:232:THR:OG1	1:C:234:ASN:OD1	2.12	0.58
1:C:277:ILE:CG2	1:C:278:ALA:N	2.66	0.58
1:C:876:LEU:O	1:C:878:GLY:N	2.34	0.58
2:D:83:SER:OG	2:D:86:THR:HA	2.03	0.58
2:D:178:ILE:HG12	2:D:179:LYS:N	2.19	0.58
1:A:23:ARG:HA	1:A:27:GLU:OE2	2.03	0.58
1:A:51:ASP:OD1	1:A:52:LEU:N	2.37	0.58
1:A:216:GLU:HG3	1:A:216:GLU:O	2.02	0.58
1:A:734:VAL:O	1:A:735:SER:C	2.40	0.58
2:B:76:GLY:HA3	2:B:291:PHE:O	2.04	0.58
1:C:238:PHE:HD2	1:C:258:THR:HG21	1.68	0.58
2:D:272:ILE:HD13	2:D:272:ILE:N	2.18	0.58
1:A:56:LEU:HD13	1:A:182:ASP:CB	2.34	0.58
1:A:56:LEU:HD13	1:A:182:ASP:HB3	1.86	0.58
1:A:166:ARG:O	1:A:168:GLY:N	2.37	0.58
1:A:338:THR:HG23	1:A:354:LEU:HD21	1.85	0.58
1:A:145:ALA:C	1:A:146:LYS:CG	2.73	0.58
1:A:194:ALA:HB1	1:A:253:TYR:O	2.04	0.58
1:A:778:PRO:HG3	1:A:854:GLN:HB3	1.86	0.58
1:A:795:LEU:HD13	1:A:915:PHE:CB	2.29	0.58
1:C:339:LEU:C	1:C:341:ALA:H	2.06	0.58
1:C:493:GLU:H	1:C:494:PRO:HD3	1.69	0.58
1:A:299:PHE:N	1:A:299:PHE:CD1	2.71	0.57
2:B:59:LEU:N	2:B:60:THR:CA	2.66	0.57
2:B:80:ILE:H	2:B:81:PRO:CD	2.17	0.57
1:C:187:LYS:CG	1:C:188:GLY:N	2.66	0.57
1:C:201:ALA:HA	1:C:247:ALA:HA	1.85	0.57
1:C:209:SER:O	1:C:211:LEU:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:TYR:O	1:A:309:THR:O	2.22	0.57
1:A:984:ALA:O	1:A:987:TYR:HB2	2.03	0.57
2:B:179:LYS:HD2	2:B:256:GLN:OE1	2.03	0.57
1:C:778:PRO:HG3	1:C:854:GLN:HB3	1.85	0.57
1:A:73:LEU:N	1:A:73:LEU:CD1	2.66	0.57
1:A:831:ASN:O	1:A:833:LYS:N	2.37	0.57
1:A:980:TRP:HA	1:A:980:TRP:HE3	1.69	0.57
2:B:245:TYR:HD1	2:B:245:TYR:C	2.06	0.57
1:C:39:LEU:HD22	1:C:43:GLU:HB3	1.86	0.57
1:C:534:ALA:O	1:C:538:LEU:HB2	2.03	0.57
1:C:565:ASP:N	1:C:570:ASN:HD22	2.00	0.57
2:D:21:LYS:CD	2:D:22:LYS:CD	2.82	0.57
1:A:37:HIS:HB3	1:A:235:ILE:HD11	1.84	0.57
2:B:92:PRO:HD2	2:B:303:SER:HA	1.86	0.57
2:B:170:LYS:HD2	2:B:170:LYS:H	1.70	0.57
1:C:144:GLU:O	1:C:146:LYS:HE3	2.05	0.57
1:C:493:GLU:N	1:C:494:PRO:CD	2.68	0.57
2:D:278:ALA:O	2:D:283:ILE:HG21	2.04	0.57
1:A:304:LEU:HD13	1:A:310:TRP:CH2	2.40	0.57
1:A:747:ASN:HD21	1:A:749:ALA:HB3	1.69	0.57
1:A:992:PHE:C	1:A:992:PHE:HD1	2.08	0.57
2:B:21:LYS:CG	2:B:22:LYS:HG3	2.35	0.57
1:C:23:ARG:HA	1:C:27:GLU:OE2	2.04	0.57
1:C:365:THR:HB	1:C:705:VAL:CG1	2.35	0.57
1:C:867:ALA:HB3	2:D:57:MET:HE1	1.87	0.57
1:C:913:THR:OG1	1:C:973:MET:HA	2.04	0.57
2:D:76:GLY:HA3	2:D:291:PHE:O	2.05	0.57
1:A:186:VAL:HG11	1:A:192:ILE:HD13	1.86	0.57
1:C:341:ALA:HB2	1:C:357:VAL:HG21	1.86	0.57
1:C:1009:TRP:CZ2	1:C:1013:GLU:HG3	2.38	0.57
1:A:165:ILE:O	1:A:166:ARG:HG3	2.05	0.57
1:A:253:TYR:HB3	1:A:258:THR:HA	1.86	0.57
1:A:516:ILE:C	1:A:518:GLY:H	2.07	0.57
1:A:800:ILE:C	1:A:802:CYS:H	2.07	0.57
1:A:873:PRO:HA	1:A:876:LEU:HD12	1.85	0.57
1:A:912:HIS:O	1:A:914:PRO:N	2.38	0.57
1:A:1009:TRP:CZ2	1:A:1013:GLU:HG3	2.38	0.57
2:B:170:LYS:HG2	2:B:174:PRO:C	2.25	0.57
2:B:285:TYR:HB3	2:B:294:ARG:HH21	1.70	0.57
1:C:209:SER:C	1:C:211:LEU:H	2.07	0.57
1:C:226:ASN:HD22	1:C:226:ASN:C	2.08	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:VAL:HG23	1:C:448:ALA:O	2.04	0.57
1:A:164:VAL:HA	1:A:183:LEU:O	2.04	0.57
1:A:907:VAL:CG2	2:B:71:ARG:HD3	2.33	0.57
2:D:238:PHE:CD1	2:D:257:PRO:HB2	2.39	0.57
1:A:138:CYS:O	1:A:141:TYR:N	2.37	0.57
1:A:531:PHE:HD1	1:A:532:GLN:N	2.03	0.57
2:B:191:PRO:HB2	2:B:196:LEU:HD11	1.87	0.57
2:B:204:TYR:HD1	2:B:235:TYR:CZ	2.23	0.57
1:C:48:TYR:HB2	1:C:50:THR:CG2	2.34	0.57
1:C:982:PHE:N	1:C:982:PHE:HD2	2.03	0.57
2:B:173:LYS:HB3	2:B:264:THR:HA	1.87	0.57
1:C:94:SER:HB3	1:C:98:TRP:CD1	2.40	0.57
1:C:299:PHE:HE2	1:C:784:LEU:HD13	1.69	0.57
2:D:80:ILE:HD11	2:D:108:PHE:CB	2.35	0.57
2:D:179:LYS:HD2	2:D:256:GLN:OE1	2.05	0.57
1:A:475:PHE:C	1:A:475:PHE:CD2	2.78	0.56
1:C:38:LYS:HG2	1:C:224:PHE:HE1	1.70	0.56
1:A:284:PHE:CZ	1:A:330:LEU:HD21	2.39	0.56
1:A:767:LYS:HD3	1:A:931:LYS:O	2.05	0.56
1:A:980:TRP:HA	1:A:980:TRP:CE3	2.40	0.56
2:B:170:LYS:HG2	2:B:175:CYS:HB2	1.86	0.56
2:B:239:PRO:HG2	2:B:242:TYR:HE1	1.68	0.56
1:C:173:ILE:HD12	1:C:177:GLU:HB2	1.87	0.56
1:C:463:MET:O	1:C:463:MET:HG2	2.05	0.56
1:C:493:GLU:N	1:C:494:PRO:HD3	2.20	0.56
2:D:80:ILE:H	2:D:81:PRO:CD	2.19	0.56
1:A:185:GLU:OE1	1:A:248:ARG:NH1	2.39	0.56
1:A:241:ASN:N	1:A:241:ASN:ND2	2.45	0.56
1:A:565:ASP:H	1:A:570:ASN:HD22	1.51	0.56
1:A:727:MET:HE3	1:A:746:ASP:HA	1.87	0.56
1:A:982:PHE:N	1:A:982:PHE:HD2	2.03	0.56
2:B:80:ILE:HD11	2:B:108:PHE:CB	2.35	0.56
2:B:238:PHE:CD1	2:B:257:PRO:HB2	2.39	0.56
1:C:37:HIS:HB3	1:C:235:ILE:HD11	1.87	0.56
1:C:61:ALA:O	1:C:64:ILE:N	2.37	0.56
1:C:565:ASP:H	1:C:570:ASN:HD22	1.52	0.56
1:C:980:TRP:HA	1:C:980:TRP:CE3	2.39	0.56
2:D:34:LYS:H	2:D:34:LYS:HD2	1.70	0.56
2:D:204:TYR:HD1	2:D:235:TYR:CZ	2.23	0.56
2:D:224:VAL:HG22	2:D:267:THR:CB	2.36	0.56
3:H:27:ARG:O	3:H:31:LEU:HG	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:C	1:A:90:PHE:CD2	2.79	0.56
1:C:134:ILE:HG22	1:C:135:ILE:N	2.20	0.56
1:C:880:ARG:HG3	1:C:881:VAL:H	1.70	0.56
1:A:97:LEU:CG	1:A:325:VAL:HG11	2.31	0.56
1:A:120:ASN:HB3	1:A:124:TYR:CE1	2.40	0.56
2:B:56:VAL:HA	2:B:59:LEU:HG	1.87	0.56
1:C:440:VAL:CG1	1:C:447:SER:HB2	2.23	0.56
1:A:224:PHE:CD2	1:A:225:THR:N	2.73	0.56
1:A:238:PHE:O	1:A:239:SER:CB	2.53	0.56
1:A:308:TYR:H	1:A:308:TYR:HD2	1.53	0.56
1:A:432:ASN:HB2	1:A:433:LEU:HD23	1.86	0.56
1:A:736:LYS:O	1:A:738:ALA:N	2.39	0.56
1:A:870:GLY:O	1:A:872:LEU:N	2.39	0.56
1:C:185:GLU:OE1	1:C:248:ARG:NH1	2.37	0.56
2:D:23:GLU:C	2:D:25:LEU:N	2.55	0.56
2:D:112:TYR:CE2	2:D:255:LEU:HB3	2.40	0.56
1:A:781:THR:HA	1:A:784:LEU:HB2	1.87	0.56
1:A:865:ILE:HD13	1:A:980:TRP:CZ2	2.40	0.56
1:A:977:LYS:HD2	2:B:68:TYR:HE1	1.66	0.56
1:C:198:ILE:HG22	1:C:200:SER:O	2.06	0.56
1:C:865:ILE:HD13	1:C:980:TRP:CZ2	2.41	0.56
2:D:170:LYS:CD	2:D:175:CYS:HB2	2.34	0.56
2:D:191:PRO:HB2	2:D:196:LEU:HD11	1.87	0.56
1:A:611:GLY:HA2	1:A:685:ARG:HA	1.88	0.56
2:B:201:VAL:O	2:B:202:MET:CB	2.54	0.56
2:B:257:PRO:C	2:B:258:LEU:HD12	2.26	0.56
2:D:135:GLU:O	2:D:137:GLY:N	2.39	0.56
1:A:633:THR:OG1	1:A:634:VAL:N	2.38	0.56
1:C:143:GLN:HG3	1:C:354:LEU:HD23	1.88	0.56
1:C:200:SER:O	1:C:201:ALA:HB2	2.05	0.56
1:C:383:HIS:O	1:C:384:MET:HG3	2.06	0.56
1:C:886:ARG:HB2	1:C:886:ARG:NH1	2.21	0.56
1:A:349:CYS:SG	1:A:741:MET:HG2	2.46	0.56
2:B:245:TYR:CD1	2:B:245:TYR:C	2.79	0.56
1:C:284:PHE:CD1	1:C:285:ILE:N	2.74	0.56
1:C:411:TRP:O	1:C:412:LEU:C	2.42	0.56
1:C:831:ASN:O	1:C:833:LYS:N	2.39	0.56
1:A:434:PRO:HG2	1:A:437:LYS:HE2	1.87	0.55
1:A:886:ARG:NH1	1:A:886:ARG:HB2	2.21	0.55
1:C:339:LEU:C	1:C:341:ALA:N	2.60	0.55
1:C:504:PRO:HG2	1:C:535:TYR:HE1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:992:PHE:C	1:C:992:PHE:HD1	2.10	0.55
1:A:195:ASP:HB2	1:A:253:TYR:HB2	1.89	0.55
1:A:440:VAL:HG13	1:A:451:LYS:HE3	1.88	0.55
1:A:834:THR:HG22	1:A:835:ASP:N	2.17	0.55
1:A:946:ILE:HG22	1:A:947:LEU:N	2.21	0.55
1:C:508:LEU:C	1:C:510:ARG:N	2.60	0.55
1:C:648:VAL:O	1:C:650:PRO:HD3	2.06	0.55
1:C:727:MET:HE3	1:C:746:ASP:HA	1.87	0.55
2:D:245:TYR:HD1	2:D:245:TYR:C	2.09	0.55
1:A:411:TRP:O	1:A:412:LEU:C	2.43	0.55
1:A:793:LEU:HD12	1:A:794:PRO:CD	2.37	0.55
1:C:238:PHE:CD1	1:C:239:SER:N	2.72	0.55
1:C:475:PHE:C	1:C:475:PHE:CD2	2.78	0.55
2:D:78:THR:OG1	2:D:79:GLN:N	2.39	0.55
2:D:257:PRO:C	2:D:258:LEU:HD12	2.27	0.55
1:A:150:ILE:HD11	1:A:738:ALA:HB2	1.89	0.55
1:A:216:GLU:HG3	1:A:218:GLN:HE22	1.70	0.55
1:A:531:PHE:CD1	1:A:532:GLN:N	2.74	0.55
2:B:21:LYS:HG2	2:B:27:ARG:HG2	1.89	0.55
1:C:194:ALA:HB3	1:C:251:VAL:HG12	1.88	0.55
1:C:955:THR:HG22	1:C:956:ALA:N	2.22	0.55
2:D:201:VAL:O	2:D:202:MET:CB	2.54	0.55
1:A:715:SER:CB	1:A:716:PRO:HD3	2.37	0.55
1:A:747:ASN:HD22	1:A:749:ALA:N	1.94	0.55
2:B:74:PRO:HB2	2:B:292:GLN:HE21	1.71	0.55
1:C:61:ALA:C	1:C:63:GLU:N	2.58	0.55
2:D:74:PRO:HB2	2:D:292:GLN:HE21	1.70	0.55
2:D:123:PHE:HD2	2:D:123:PHE:H	1.50	0.55
1:A:198:ILE:HG22	1:A:200:SER:O	2.07	0.55
1:A:495:ARG:O	1:A:496:HIS:HB2	2.05	0.55
1:C:238:PHE:O	1:C:239:SER:CB	2.55	0.55
1:C:304:LEU:HD11	1:C:310:TRP:CZ3	2.41	0.55
1:C:663:LEU:CA	1:C:666:MET:HE2	2.31	0.55
2:D:224:VAL:HG13	2:D:224:VAL:O	2.06	0.55
1:A:179:VAL:O	1:A:181:GLY:N	2.40	0.55
1:A:563:GLN:HA	1:A:563:GLN:OE1	2.07	0.55
3:G:27:ARG:O	3:G:31:LEU:HG	2.06	0.55
1:C:327:GLU:CB	1:C:805:LEU:HD11	2.36	0.55
1:A:207:ASP:HB3	1:A:241:ASN:HD21	1.70	0.55
2:B:135:GLU:O	2:B:137:GLY:N	2.40	0.55
1:C:40:SER:H	1:C:43:GLU:HB2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:HD21	1:C:199:ILE:HD13	1.88	0.55
1:C:918:THR:CB	1:C:984:ALA:HB2	2.37	0.55
1:C:982:PHE:HA	1:C:985:PHE:CD2	2.42	0.55
2:D:21:LYS:HG2	2:D:27:ARG:HG2	1.88	0.55
2:D:22:LYS:HG2	2:D:23:GLU:H	1.71	0.55
1:A:51:ASP:O	1:A:52:LEU:HB2	2.05	0.55
1:A:493:GLU:N	1:A:494:PRO:CD	2.70	0.55
2:B:243:TYR:N	2:B:243:TYR:CD2	2.71	0.55
1:C:51:ASP:OD1	1:C:52:LEU:N	2.40	0.55
1:C:111:GLN:HB3	1:C:117:GLU:HB2	1.87	0.55
1:C:853:ILE:HG21	1:C:990:LEU:HD13	1.88	0.55
3:H:39:ILE:O	3:H:43:ILE:HG12	2.07	0.55
3:H:48:LYS:O	3:H:49:ARG:HB2	2.07	0.55
1:A:209:SER:O	1:A:211:LEU:N	2.40	0.55
2:B:80:ILE:HD11	2:B:108:PHE:CG	2.41	0.55
2:B:224:VAL:HG22	2:B:267:THR:CB	2.37	0.55
2:B:254:TYR:CD1	2:B:254:TYR:C	2.81	0.54
2:D:92:PRO:HD2	2:D:303:SER:HA	1.88	0.54
2:D:170:LYS:CB	2:D:174:PRO:HA	2.37	0.54
2:D:182:ARG:HE	2:D:245:TYR:HE2	1.56	0.54
1:A:104:CYS:SG	1:A:318:ILE:HD13	2.47	0.54
1:A:626:ILE:O	1:A:680:GLU:HB3	2.07	0.54
1:A:663:LEU:CA	1:A:666:MET:HE2	2.34	0.54
1:C:514:ILE:CD1	1:C:527:LEU:HD12	2.38	0.54
1:C:640:ARG:C	1:C:641:LEU:HD12	2.27	0.54
1:C:793:LEU:HD12	1:C:794:PRO:CD	2.36	0.54
1:C:912:HIS:O	1:C:915:PHE:N	2.37	0.54
1:C:918:THR:HG22	1:C:984:ALA:H	1.73	0.54
2:D:39:TYR:CE2	7:D:3001:CLR:H182	2.42	0.54
1:A:93:PHE:CD2	1:A:326:PRO:HD2	2.43	0.54
1:A:94:SER:O	1:A:98:TRP:HD1	1.89	0.54
1:A:562:PHE:HE2	1:A:570:ASN:HD21	1.53	0.54
1:A:663:LEU:HB3	1:A:690:GLN:NE2	2.21	0.54
1:A:714:ASP:O	1:A:715:SER:C	2.46	0.54
1:A:918:THR:HB	1:A:984:ALA:HB2	1.88	0.54
1:C:48:TYR:OH	1:C:252:VAL:HG12	2.07	0.54
1:C:199:ILE:O	1:C:222:PRO:CG	2.55	0.54
1:C:460:VAL:HG11	1:C:464:ARG:HH11	1.71	0.54
1:C:763:ASP:O	1:C:766:LYS:HB2	2.07	0.54
1:A:86:CYS:C	1:A:88:GLN:N	2.59	0.54
1:A:209:SER:C	1:A:211:LEU:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:THR:O	1:A:267:ALA:N	2.41	0.54
1:A:624:VAL:HG23	1:A:625:GLY:N	2.21	0.54
1:A:982:PHE:HA	1:A:985:PHE:CD2	2.42	0.54
2:B:170:LYS:CD	2:B:175:CYS:HB2	2.37	0.54
2:B:170:LYS:CB	2:B:174:PRO:HA	2.38	0.54
1:C:440:VAL:HG13	1:C:451:LYS:HE3	1.88	0.54
2:D:130:PRO:HG2	2:D:204:TYR:CE1	2.42	0.54
1:A:302:LEU:O	1:A:302:LEU:HD23	2.07	0.54
1:A:648:VAL:O	1:A:650:PRO:HD3	2.08	0.54
1:A:875:HIS:O	1:A:879:LEU:HD21	2.06	0.54
2:B:109:LEU:O	2:B:112:TYR:HB2	2.08	0.54
1:C:351:VAL:HG11	1:C:357:VAL:HG22	1.88	0.54
1:C:507:ILE:O	1:C:507:ILE:CG2	2.55	0.54
1:C:940:GLN:HG3	1:C:940:GLN:O	2.06	0.54
2:D:80:ILE:HD11	2:D:108:PHE:CG	2.43	0.54
2:D:109:LEU:O	2:D:112:TYR:HB2	2.07	0.54
2:D:170:LYS:HD2	2:D:170:LYS:H	1.72	0.54
2:D:245:TYR:C	2:D:245:TYR:CD1	2.81	0.54
1:A:199:ILE:HD12	1:A:200:SER:H	1.73	0.54
1:A:277:ILE:CG2	1:A:278:ALA:N	2.71	0.54
1:A:707:VAL:HG21	1:A:717:ALA:HB1	1.89	0.54
1:C:56:LEU:HD13	1:C:182:ASP:CA	2.38	0.54
1:C:165:ILE:C	1:C:166:ARG:HG3	2.27	0.54
2:D:173:LYS:HB3	2:D:264:THR:HA	1.90	0.54
1:A:191:ARG:O	1:A:193:PRO:HD3	2.07	0.54
1:A:645:VAL:C	1:A:647:GLN:N	2.60	0.54
2:D:117:GLN:OE1	2:D:150:ARG:HB2	2.08	0.54
1:A:514:ILE:CD1	1:A:527:LEU:HD12	2.37	0.54
1:C:432:ASN:HB2	1:C:433:LEU:HD23	1.90	0.54
2:D:90:PHE:CD2	2:D:98:TYR:HB3	2.42	0.54
1:A:354:LEU:O	1:A:356:ALA:N	2.41	0.54
1:A:433:LEU:HD23	1:A:433:LEU:N	2.23	0.54
1:A:861:THR:CG2	1:A:983:CYS:HB3	2.38	0.54
1:A:900:THR:O	1:A:904:ARG:HG2	2.08	0.54
2:B:112:TYR:CE2	2:B:255:LEU:HB3	2.40	0.54
2:B:275:GLU:CD	2:B:277:LYS:HG3	2.28	0.54
3:G:48:LYS:O	3:G:49:ARG:HB2	2.07	0.54
1:C:180:VAL:HG22	1:C:254:THR:CG2	2.37	0.54
1:C:516:ILE:C	1:C:518:GLY:H	2.08	0.54
2:D:21:LYS:HD2	2:D:22:LYS:CD	2.31	0.54
2:B:272:ILE:O	2:B:272:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:GLU:HB2	1:C:805:LEU:HD11	1.90	0.53
1:C:611:GLY:HA2	1:C:685:ARG:HA	1.89	0.53
1:C:802:CYS:HB3	1:C:916:PHE:HE2	1.74	0.53
1:C:876:LEU:HA	1:C:879:LEU:HG	1.90	0.53
1:A:508:LEU:C	1:A:510:ARG:N	2.61	0.53
2:B:61:ILE:HG22	2:B:67:THR:CG2	2.38	0.53
1:C:874:ILE:C	1:C:876:LEU:N	2.62	0.53
2:D:76:GLY:HA2	2:D:293:GLY:N	2.19	0.53
1:A:61:ALA:C	1:A:63:GLU:N	2.61	0.53
1:A:329:LEU:HB2	1:A:772:THR:HG21	1.90	0.53
1:A:893:ASP:CG	1:A:894:SER:N	2.61	0.53
1:C:56:LEU:HD13	1:C:182:ASP:CB	2.39	0.53
1:C:288:ILE:C	1:C:290:GLY:H	2.10	0.53
1:C:742:ILE:HG22	1:C:742:ILE:O	2.08	0.53
1:C:856:LEU:CD1	2:D:46:LEU:HD13	2.38	0.53
1:C:910:THR:O	1:C:914:PRO:CD	2.56	0.53
2:D:275:GLU:CD	2:D:277:LYS:HG3	2.28	0.53
1:A:165:ILE:HG22	1:A:170:LYS:HA	1.89	0.53
1:A:195:ASP:OD2	1:A:259:VAL:HG23	2.08	0.53
1:A:699:GLN:O	1:A:700:ARG:C	2.46	0.53
1:C:56:LEU:HD13	1:C:182:ASP:HB3	1.89	0.53
1:C:150:ILE:HG21	1:C:268:SER:HB2	1.89	0.53
1:C:187:LYS:HG3	1:C:188:GLY:N	2.22	0.53
1:C:865:ILE:O	1:C:869:ASN:HB2	2.07	0.53
1:A:274:GLN:CD	1:A:279:ALA:HB2	2.28	0.53
1:A:640:ARG:C	1:A:641:LEU:HD12	2.29	0.53
1:A:955:THR:HG22	1:A:956:ALA:N	2.24	0.53
2:B:90:PHE:CD2	2:B:98:TYR:HB3	2.43	0.53
2:B:203:LYS:O	2:B:205:ASN:N	2.41	0.53
1:C:103:LEU:HD21	1:C:317:LEU:HD12	1.90	0.53
1:C:324:ASN:O	1:C:326:PRO:HD3	2.08	0.53
1:C:708:THR:HG21	1:C:748:PHE:CE1	2.43	0.53
1:A:299:PHE:N	1:A:299:PHE:HD1	2.06	0.53
1:A:317:LEU:HA	1:A:320:ILE:HG22	1.89	0.53
1:A:556:GLU:H	1:A:556:GLU:CD	2.11	0.53
1:A:961:LEU:HD11	1:A:971:LEU:HD12	1.91	0.53
1:C:590:ALA:O	1:C:593:PRO:HD2	2.09	0.53
1:A:281:ILE:C	1:A:283:HIS:H	2.12	0.53
1:A:311:LEU:O	1:A:315:ILE:HB	2.08	0.53
1:A:440:VAL:CG1	1:A:447:SER:HB2	2.27	0.53
1:A:736:LYS:C	1:A:738:ALA:N	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:CYS:HB3	1:A:916:PHE:HE2	1.73	0.53
2:B:178:ILE:HG12	2:B:179:LYS:N	2.23	0.53
1:C:300:PHE:CD2	1:C:300:PHE:O	2.61	0.53
1:C:715:SER:OG	1:C:716:PRO:HD3	2.09	0.53
1:C:961:LEU:HD11	1:C:971:LEU:HD12	1.91	0.53
1:A:742:ILE:O	1:A:744:LEU:N	2.42	0.53
1:C:44:LEU:O	1:C:45:HIS:C	2.47	0.53
1:C:118:PRO:O	1:C:119:GLN:C	2.47	0.53
1:C:165:ILE:HG22	1:C:170:LYS:HA	1.91	0.53
1:C:637:ILE:HG12	1:C:640:ARG:HH12	1.74	0.53
1:C:663:LEU:HB3	1:C:690:GLN:NE2	2.24	0.53
1:C:849:GLN:O	1:C:851:GLY:N	2.42	0.53
2:D:254:TYR:C	2:D:254:TYR:CD1	2.82	0.53
1:A:637:ILE:HG12	1:A:640:ARG:HH12	1.74	0.53
1:A:849:GLN:O	1:A:851:GLY:N	2.42	0.53
1:A:865:ILE:O	1:A:869:ASN:HB2	2.08	0.53
2:B:37:LEU:HD12	2:B:37:LEU:C	2.29	0.53
2:B:78:THR:OG1	2:B:79:GLN:N	2.41	0.53
2:B:286:SER:HB3	2:B:289:ASP:HB3	1.91	0.53
1:C:35:ASP:HB2	1:C:229:PRO:CG	2.39	0.53
1:C:265:THR:O	1:C:267:ALA:N	2.42	0.53
1:C:404:PHE:O	1:C:405:ASP:CB	2.47	0.53
1:C:908:GLU:O	1:C:911:CYS:N	2.37	0.53
2:D:203:LYS:O	2:D:205:ASN:N	2.41	0.53
1:A:305:ILE:C	1:A:306:LEU:HD23	2.30	0.53
1:A:329:LEU:O	1:A:333:VAL:HG23	2.08	0.53
1:A:618:LYS:O	1:A:622:LYS:HG3	2.09	0.53
1:A:977:LYS:O	1:A:978:PRO:C	2.47	0.53
1:A:982:PHE:HD2	1:A:982:PHE:H	1.57	0.53
2:B:117:GLN:OE1	2:B:150:ARG:HB2	2.09	0.53
1:C:56:LEU:CD1	1:C:182:ASP:HA	2.37	0.53
1:C:340:THR:OG1	1:C:761:ILE:HD13	2.09	0.53
1:C:411:TRP:C	1:C:413:ALA:N	2.61	0.53
1:C:1015:TYR:O	1:C:1016:TYR:C	2.48	0.53
1:A:530:ALA:HA	1:A:533:ASN:CB	2.38	0.52
1:C:225:THR:OG1	1:C:226:ASN:HB2	2.09	0.52
1:C:434:PRO:HG2	1:C:437:LYS:HE2	1.91	0.52
1:C:556:GLU:CD	1:C:556:GLU:H	2.11	0.52
2:D:31:SER:HA	2:D:32:TRP:CB	2.35	0.52
2:D:37:LEU:HD12	2:D:37:LEU:C	2.29	0.52
1:A:834:THR:O	1:A:835:ASP:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:PHE:C	1:C:224:PHE:HD2	2.10	0.52
1:C:370:LYS:HA	1:C:374:LEU:HB2	1.90	0.52
1:C:900:THR:O	1:C:904:ARG:HG2	2.09	0.52
1:A:879:LEU:O	1:A:880:ARG:C	2.47	0.52
2:B:245:TYR:CE1	2:B:247:GLY:N	2.78	0.52
1:C:207:ASP:HB3	1:C:241:ASN:HD21	1.74	0.52
1:C:320:ILE:HD11	1:C:784:LEU:HD23	1.91	0.52
1:C:683:PHE:CG	1:C:694:ILE:HD13	2.45	0.52
1:A:893:ASP:OD2	1:A:894:SER:N	2.43	0.52
2:B:130:PRO:HG2	2:B:204:TYR:CE1	2.44	0.52
2:B:152:ARG:C	2:B:154:GLU:H	2.13	0.52
2:B:216:LYS:HD2	2:B:216:LYS:N	2.24	0.52
1:C:22:GLU:C	1:C:24:ASP:H	2.13	0.52
1:C:337:LEU:O	1:C:339:LEU:N	2.42	0.52
1:C:771:TYR:CE1	1:C:927:LEU:HB2	2.44	0.52
1:C:870:GLY:O	1:C:872:LEU:N	2.42	0.52
2:D:61:ILE:O	2:D:62:SER:O	2.27	0.52
1:A:22:GLU:C	1:A:24:ASP:H	2.13	0.52
1:C:645:VAL:C	1:C:647:GLN:N	2.62	0.52
1:A:558:PHE:HA	1:A:562:PHE:HD1	1.74	0.52
1:C:108:TYR:CG	1:C:123:LEU:HB2	2.45	0.52
1:C:736:LYS:O	1:C:738:ALA:N	2.42	0.52
1:C:879:LEU:O	1:C:880:ARG:C	2.48	0.52
1:C:946:ILE:HG22	1:C:947:LEU:N	2.24	0.52
2:D:156:LEU:HD13	2:D:159:CYS:HB2	1.92	0.52
1:A:370:LYS:HA	1:A:374:LEU:HB2	1.92	0.52
1:A:687:SER:OG	1:A:690:GLN:HG3	2.09	0.52
1:A:910:THR:O	1:A:914:PRO:CD	2.57	0.52
1:C:81:GLU:OE1	1:C:81:GLU:HA	2.10	0.52
1:C:982:PHE:HD2	1:C:982:PHE:H	1.57	0.52
1:A:153:SER:OG	1:A:733:ASP:HB3	2.08	0.52
2:B:22:LYS:HG2	2:B:23:GLU:H	1.74	0.52
1:C:316:PHE:HE1	1:C:783:PHE:O	1.93	0.52
1:C:699:GLN:O	1:C:700:ARG:C	2.48	0.52
1:A:356:ALA:HA	1:A:359:THR:OG1	2.10	0.52
2:B:271:GLU:OE1	2:B:298:LYS:HD3	2.10	0.52
1:C:65:LEU:O	1:C:69:GLY:N	2.37	0.52
1:C:97:LEU:CD2	1:C:325:VAL:HG11	2.38	0.52
1:C:433:LEU:HD23	1:C:433:LEU:N	2.25	0.52
1:C:453:ILE:O	1:C:454:GLU:C	2.48	0.52
1:C:530:ALA:HA	1:C:533:ASN:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:736:LYS:C	1:C:738:ALA:N	2.63	0.52
1:A:978:PRO:O	1:A:980:TRP:N	2.42	0.52
1:C:210:SER:HA	1:C:712:VAL:HG13	1.92	0.52
1:C:450:LEU:C	1:C:450:LEU:CD2	2.78	0.52
1:C:495:ARG:O	1:C:496:HIS:HB2	2.09	0.52
1:C:558:PHE:HD1	1:C:562:PHE:CE1	2.28	0.52
2:D:251:GLN:OE1	2:D:254:TYR:CD2	2.63	0.52
1:A:208:ASN:HB3	1:A:212:THR:HG23	1.92	0.51
1:A:308:TYR:N	1:A:308:TYR:CD2	2.78	0.51
1:A:335:VAL:HG11	1:A:813:ILE:HG13	1.92	0.51
1:A:374:LEU:O	1:A:592:VAL:HG21	2.11	0.51
1:A:398:ASN:O	1:A:399:GLN:HB2	2.10	0.51
1:A:876:LEU:HA	1:A:879:LEU:HG	1.91	0.51
1:A:909:PHE:CD2	1:A:972:ARG:HB3	2.45	0.51
2:B:22:LYS:O	2:B:24:PHE:N	2.44	0.51
2:B:58:LEU:O	2:B:60:THR:HB	2.10	0.51
1:C:936:SER:HB3	1:C:939:GLN:HG3	1.91	0.51
2:D:61:ILE:HG22	2:D:67:THR:CG2	2.40	0.51
2:D:198:THR:HG23	2:D:203:LYS:CE	2.39	0.51
1:A:65:LEU:O	1:A:69:GLY:N	2.38	0.51
1:A:88:GLN:C	1:A:90:PHE:H	2.14	0.51
1:A:97:LEU:HB3	1:A:133:VAL:HG23	1.92	0.51
1:A:226:ASN:ND2	1:A:227:GLU:H	2.03	0.51
1:A:493:GLU:N	1:A:494:PRO:HD3	2.25	0.51
1:A:1015:TYR:O	1:A:1016:TYR:C	2.48	0.51
2:B:52:GLY:O	2:B:55:GLN:N	2.40	0.51
3:G:39:ILE:O	3:G:43:ILE:HG12	2.09	0.51
1:C:93:PHE:CZ	1:C:288:ILE:HG21	2.45	0.51
1:C:110:ILE:HG21	1:C:311:LEU:CB	2.38	0.51
1:C:344:MET:O	1:C:347:LYS:N	2.42	0.51
1:C:803:ILE:O	1:C:808:ASP:HB2	2.11	0.51
1:C:905:LYS:O	1:C:908:GLU:N	2.43	0.51
2:D:152:ARG:C	2:D:154:GLU:H	2.14	0.51
2:D:271:GLU:OE1	2:D:298:LYS:HD3	2.10	0.51
1:A:44:LEU:O	1:A:45:HIS:C	2.49	0.51
2:B:61:ILE:O	2:B:62:SER:O	2.27	0.51
1:C:51:ASP:O	1:C:52:LEU:HB2	2.10	0.51
1:C:725:VAL:HG11	1:C:751:ILE:HD11	1.92	0.51
2:D:53:THR:O	2:D:57:MET:HB3	2.10	0.51
1:A:203:GLY:O	1:A:245:GLY:HA3	2.10	0.51
1:A:824:ILE:C	1:A:826:LYS:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:843:ILE:C	1:A:845:MET:H	2.11	0.51
1:C:490:ASN:HB3	1:C:492:ALA:H	1.73	0.51
1:C:563:GLN:OE1	1:C:563:GLN:HA	2.10	0.51
1:C:626:ILE:O	1:C:680:GLU:HB3	2.10	0.51
2:D:245:TYR:CE1	2:D:247:GLY:N	2.78	0.51
1:A:475:PHE:C	1:A:475:PHE:HD2	2.13	0.51
1:A:538:LEU:HD11	1:A:583:SER:OG	2.10	0.51
1:A:962:SER:C	1:A:963:TYR:CD1	2.84	0.51
1:C:71:ASN:O	1:C:72:ALA:HB2	2.11	0.51
1:C:157:MET:O	1:C:191:ARG:HD3	2.10	0.51
1:C:260:MET:O	1:C:263:ILE:HB	2.09	0.51
1:C:893:ASP:CG	1:C:894:SER:N	2.63	0.51
1:C:948:ILE:O	1:C:951:LEU:HB2	2.11	0.51
2:D:272:ILE:O	2:D:272:ILE:HG12	2.10	0.51
2:D:286:SER:HB3	2:D:289:ASP:HB3	1.91	0.51
1:A:715:SER:OG	1:A:716:PRO:HD3	2.10	0.51
1:A:863:PHE:HB3	2:B:54:ILE:HD11	1.91	0.51
2:B:156:LEU:HD13	2:B:159:CYS:HB2	1.91	0.51
1:C:367:CYS:HB2	1:C:707:VAL:HG22	1.92	0.51
1:A:86:CYS:C	1:A:88:GLN:H	2.14	0.51
1:A:139:PHE:O	1:A:334:THR:OG1	2.23	0.51
1:A:304:LEU:HD22	1:A:310:TRP:CE3	2.45	0.51
1:A:316:PHE:HE1	1:A:783:PHE:O	1.93	0.51
1:A:570:ASN:O	1:A:570:ASN:OD1	2.29	0.51
1:A:734:VAL:O	1:A:736:LYS:N	2.43	0.51
1:A:803:ILE:O	1:A:808:ASP:HB2	2.10	0.51
1:A:908:GLU:O	1:A:911:CYS:N	2.41	0.51
1:C:57:THR:HG22	1:C:58:PRO:HD2	1.93	0.51
1:C:475:PHE:C	1:C:475:PHE:HD2	2.13	0.51
1:C:538:LEU:HD11	1:C:583:SER:OG	2.10	0.51
2:D:226:THR:H	2:D:265:ASN:HB3	1.76	0.51
1:A:106:LEU:O	1:A:107:ALA:C	2.48	0.51
1:A:624:VAL:CG2	1:A:625:GLY:N	2.74	0.51
1:A:803:ILE:HG22	1:A:804:ASP:N	2.25	0.51
2:B:112:TYR:CD2	2:B:255:LEU:HD13	2.46	0.51
1:C:195:ASP:OD2	1:C:259:VAL:HG23	2.10	0.51
1:C:670:GLN:O	1:C:674:ILE:HG13	2.10	0.51
2:D:38:PHE:O	2:D:38:PHE:CD2	2.64	0.51
2:D:112:TYR:CD2	2:D:255:LEU:HD13	2.45	0.51
1:A:656:CYS:HG	1:A:678:HIS:CE1	2.29	0.51
1:A:918:THR:CB	1:A:984:ALA:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:GLY:O	2:B:31:SER:CB	2.54	0.51
2:B:38:PHE:CD2	2:B:38:PHE:O	2.64	0.51
1:C:316:PHE:CZ	1:C:787:ILE:HG13	2.46	0.51
1:C:1000:LEU:N	1:C:1000:LEU:HD23	2.26	0.51
1:A:263:ILE:CD1	1:A:688:PRO:HB2	2.41	0.51
1:A:321:ILE:HG22	1:A:322:VAL:N	2.26	0.51
1:A:564:PHE:HA	1:A:570:ASN:ND2	2.26	0.51
1:A:590:ALA:O	1:A:593:PRO:HD2	2.11	0.51
1:A:874:ILE:C	1:A:876:LEU:N	2.64	0.51
2:B:198:THR:HG23	2:B:203:LYS:CE	2.38	0.51
1:C:52:LEU:C	1:C:54:ARG:N	2.63	0.51
1:C:286:HIS:O	1:C:287:ILE:C	2.46	0.51
2:D:216:LYS:HD2	2:D:216:LYS:N	2.25	0.51
1:A:93:PHE:HZ	1:A:288:ILE:HD12	1.76	0.50
1:A:165:ILE:C	1:A:166:ARG:HG3	2.31	0.50
1:A:918:THR:HG22	1:A:984:ALA:H	1.74	0.50
1:A:961:LEU:HD11	1:A:971:LEU:CD1	2.41	0.50
2:B:39:TYR:CE2	7:B:3001:CLR:H182	2.47	0.50
2:B:182:ARG:HE	2:B:245:TYR:HE2	1.58	0.50
1:C:61:ALA:C	1:C:63:GLU:H	2.14	0.50
1:C:89:LEU:C	1:C:90:PHE:CD2	2.85	0.50
1:C:191:ARG:HG2	1:C:191:ARG:HH11	1.76	0.50
1:C:374:LEU:O	1:C:592:VAL:HG21	2.11	0.50
1:C:427:GLN:HA	1:C:427:GLN:NE2	2.26	0.50
1:C:860:PHE:CE1	2:D:53:THR:O	2.64	0.50
1:C:977:LYS:O	1:C:978:PRO:C	2.50	0.50
2:D:201:VAL:O	2:D:201:VAL:HG22	2.11	0.50
2:B:80:ILE:H	2:B:81:PRO:HD3	1.76	0.50
1:C:96:LEU:O	1:C:98:TRP:N	2.44	0.50
1:C:224:PHE:CD2	1:C:225:THR:N	2.78	0.50
1:C:300:PHE:CE1	1:C:313:ALA:HB1	2.46	0.50
1:C:340:THR:O	1:C:340:THR:HG22	2.10	0.50
1:C:618:LYS:O	1:C:622:LYS:HG3	2.10	0.50
1:C:843:ILE:C	1:C:845:MET:H	2.15	0.50
2:D:243:TYR:N	2:D:243:TYR:CD2	2.73	0.50
1:A:110:ILE:HD12	1:A:311:LEU:HD22	1.92	0.50
1:A:551:LEU:HG	1:A:553:LEU:HD23	1.93	0.50
1:A:725:VAL:HG11	1:A:751:ILE:HD11	1.93	0.50
1:A:853:ILE:HG21	1:A:990:LEU:HD13	1.93	0.50
1:C:183:LEU:HD12	1:C:249:GLY:O	2.11	0.50
1:C:417:ILE:HG21	1:C:548:PHE:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:ARG:O	1:C:496:HIS:CG	2.64	0.50
1:C:803:ILE:HG22	1:C:804:ASP:N	2.25	0.50
1:C:892:GLU:OE2	2:D:248:LYS:HD2	2.11	0.50
1:A:284:PHE:HZ	1:A:330:LEU:CD2	2.25	0.50
1:A:303:SER:OG	1:A:313:ALA:HB2	2.12	0.50
1:A:909:PHE:CD1	1:A:909:PHE:N	2.77	0.50
1:A:977:LYS:O	1:A:980:TRP:HB2	2.11	0.50
2:B:76:GLY:HA2	2:B:293:GLY:N	2.19	0.50
2:B:226:THR:H	2:B:265:ASN:HB3	1.76	0.50
1:C:216:GLU:HG3	1:C:218:GLN:HE22	1.75	0.50
1:C:332:THR:HG23	1:C:813:ILE:HD12	1.92	0.50
1:C:398:ASN:O	1:C:399:GLN:HB2	2.11	0.50
1:C:687:SER:OG	1:C:690:GLN:HG3	2.11	0.50
1:C:786:PHE:CD1	1:C:793:LEU:HB2	2.46	0.50
2:D:21:LYS:CG	2:D:22:LYS:HG3	2.41	0.50
1:A:200:SER:O	1:A:201:ALA:HB2	2.11	0.50
1:A:503:ALA:O	1:A:507:ILE:HB	2.11	0.50
1:A:766:LYS:HE2	1:A:837:LEU:O	2.11	0.50
1:A:858:GLY:HA3	1:A:915:PHE:CE2	2.47	0.50
1:C:277:ILE:O	1:C:279:ALA:N	2.44	0.50
1:C:558:PHE:CD1	1:C:562:PHE:CE1	2.99	0.50
2:D:88:ILE:HG22	2:D:101:TYR:CD1	2.46	0.50
1:A:180:VAL:HG22	1:A:254:THR:CG2	2.42	0.50
1:C:110:ILE:CG2	1:C:311:LEU:HB3	2.36	0.50
1:A:316:PHE:CG	1:A:316:PHE:O	2.65	0.50
1:A:529:ASP:O	1:A:533:ASN:HB2	2.12	0.50
1:A:755:VAL:O	1:A:759:ARG:HG3	2.12	0.50
1:A:948:ILE:O	1:A:951:LEU:HB2	2.11	0.50
2:B:40:VAL:O	2:B:41:ILE:C	2.48	0.50
2:B:137:GLY:HA3	2:B:146:ARG:HH21	1.76	0.50
2:B:201:VAL:O	2:B:201:VAL:HG22	2.12	0.50
1:C:529:ASP:O	1:C:533:ASN:HB2	2.12	0.50
1:A:40:SER:N	1:A:43:GLU:HB2	2.26	0.50
1:A:453:ILE:O	1:A:454:GLU:C	2.50	0.50
1:A:641:LEU:O	1:A:642:ASN:C	2.50	0.50
1:C:96:LEU:HD11	1:C:292:ALA:CB	2.41	0.50
1:C:960:PHE:C	1:C:960:PHE:CD2	2.85	0.50
2:D:74:PRO:O	2:D:292:GLN:HG3	2.11	0.50
2:D:170:LYS:HG2	2:D:174:PRO:O	2.12	0.50
1:A:122:ASN:ND2	1:A:315:ILE:HD11	2.27	0.50
1:A:300:PHE:HA	1:A:303:SER:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:GLY:O	1:A:881:VAL:CG2	2.60	0.50
2:B:21:LYS:HD3	2:B:22:LYS:CE	2.42	0.50
2:B:60:THR:O	2:B:61:ILE:HG23	2.12	0.50
1:C:226:ASN:ND2	1:C:227:GLU:N	2.39	0.50
1:C:856:LEU:HD12	2:D:46:LEU:HD13	1.93	0.50
1:C:900:THR:OG1	1:C:903:GLN:HB2	2.11	0.50
1:A:201:ALA:HB3	1:A:222:PRO:HD3	1.94	0.49
1:A:238:PHE:HD1	1:A:238:PHE:C	2.15	0.49
1:A:336:CYS:SG	1:A:816:ALA:HB2	2.52	0.49
1:A:775:SER:HB3	1:A:923:GLN:NE2	2.27	0.49
1:A:790:ASN:HD22	1:A:880:ARG:CG	2.25	0.49
1:A:792:PRO:HD2	1:A:862:TYR:OH	2.12	0.49
2:B:188:PRO:HG2	2:B:243:TYR:CE1	2.47	0.49
1:C:132:VAL:O	1:C:136:THR:HB	2.12	0.49
1:C:288:ILE:HG22	1:C:289:THR:H	1.77	0.49
1:C:416:ARG:HD2	1:C:467:TYR:CZ	2.47	0.49
1:C:495:ARG:O	1:C:496:HIS:CD2	2.65	0.49
1:C:707:VAL:HG21	1:C:717:ALA:HB1	1.94	0.49
1:C:767:LYS:HD3	1:C:931:LYS:O	2.11	0.49
1:C:834:THR:HG22	1:C:835:ASP:N	2.20	0.49
1:C:962:SER:C	1:C:963:TYR:CD1	2.85	0.49
2:D:60:THR:O	2:D:61:ILE:HG23	2.12	0.49
1:A:450:LEU:CD2	1:A:450:LEU:C	2.80	0.49
2:B:31:SER:HA	2:B:32:TRP:CB	2.36	0.49
1:C:451:LYS:O	1:C:452:CYS:C	2.48	0.49
1:C:893:ASP:OD2	1:C:894:SER:N	2.45	0.49
2:D:73:ALA:O	2:D:74:PRO:C	2.51	0.49
1:A:238:PHE:CD1	1:A:238:PHE:C	2.85	0.49
1:A:473:ILE:HD12	1:A:483:LEU:HD11	1.94	0.49
2:B:74:PRO:O	2:B:292:GLN:HG3	2.11	0.49
1:C:374:LEU:CD2	1:C:592:VAL:HG11	2.42	0.49
1:C:374:LEU:HD22	1:C:592:VAL:HG11	1.94	0.49
1:C:655:ALA:HB2	1:C:680:GLU:HB2	1.94	0.49
2:D:40:VAL:O	2:D:41:ILE:C	2.50	0.49
2:D:224:VAL:HG22	2:D:267:THR:HB	1.94	0.49
1:A:266:LEU:O	1:A:266:LEU:HG	2.11	0.49
1:A:856:LEU:HD13	2:B:50:PHE:HB2	1.93	0.49
1:C:327:GLU:HB2	1:C:805:LEU:CD1	2.42	0.49
1:C:417:ILE:HG22	1:C:548:PHE:HD2	1.78	0.49
1:C:564:PHE:HA	1:C:570:ASN:ND2	2.27	0.49
1:C:953:GLU:O	1:C:954:GLU:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ALA:HA	1:A:65:LEU:HB2	1.93	0.49
1:A:900:THR:OG1	1:A:903:GLN:HB2	2.12	0.49
1:C:288:ILE:CG2	1:C:289:THR:N	2.76	0.49
1:C:356:ALA:HA	1:C:359:THR:OG1	2.12	0.49
1:C:435:ILE:HD13	1:C:438:ARG:CZ	2.43	0.49
1:C:551:LEU:HG	1:C:553:LEU:HD23	1.95	0.49
1:C:715:SER:CB	1:C:716:PRO:HD3	2.42	0.49
1:C:755:VAL:O	1:C:759:ARG:HG3	2.12	0.49
1:C:856:LEU:HD13	2:D:50:PHE:HB2	1.94	0.49
1:C:864:VAL:HG22	2:D:57:MET:SD	2.52	0.49
2:D:188:PRO:HD2	2:D:243:TYR:HD1	1.77	0.49
1:A:47:LYS:HG3	1:A:47:LYS:O	2.11	0.49
1:A:163:LEU:HG	1:C:169:GLU:OE2	2.12	0.49
1:A:301:ILE:HD12	1:A:301:ILE:C	2.33	0.49
1:A:383:HIS:HB2	1:A:538:LEU:HD11	1.94	0.49
1:A:598:LYS:CB	1:A:752:VAL:HG21	2.42	0.49
1:A:633:THR:HG23	1:A:636:ASP:H	1.78	0.49
2:B:152:ARG:H	2:B:155:TRP:HE1	1.60	0.49
2:B:222:GLU:O	2:B:223:LYS:C	2.51	0.49
1:C:44:LEU:O	1:C:47:LYS:N	2.46	0.49
1:C:150:ILE:HG22	1:C:268:SER:HB2	1.93	0.49
1:C:320:ILE:HD11	1:C:784:LEU:CD2	2.42	0.49
1:C:369:ASP:O	1:C:373:THR:HB	2.12	0.49
1:C:977:LYS:O	1:C:980:TRP:HB2	2.13	0.49
2:D:50:PHE:O	2:D:54:ILE:HG22	2.13	0.49
1:A:592:VAL:HB	1:A:593:PRO:HD3	1.95	0.49
1:A:655:ALA:HB2	1:A:680:GLU:HB2	1.94	0.49
1:A:917:VAL:O	1:A:918:THR:C	2.50	0.49
1:C:52:LEU:C	1:C:54:ARG:H	2.16	0.49
1:C:104:CYS:SG	1:C:318:ILE:HD13	2.53	0.49
1:C:747:ASN:HD21	1:C:749:ALA:N	2.10	0.49
1:C:841:GLN:HG2	1:C:1012:LYS:O	2.13	0.49
2:D:22:LYS:O	2:D:24:PHE:N	2.45	0.49
2:D:245:TYR:CD1	2:D:246:TYR:N	2.66	0.49
1:A:411:TRP:C	1:A:413:ALA:N	2.64	0.49
1:A:797:THR:O	1:A:800:ILE:N	2.45	0.49
1:C:306:LEU:O	1:C:307:GLU:C	2.51	0.49
1:C:909:PHE:N	1:C:909:PHE:CD1	2.81	0.49
1:A:258:THR:OG1	1:A:259:VAL:N	2.46	0.49
1:A:365:THR:HB	1:A:705:VAL:CG1	2.41	0.49
1:A:683:PHE:CG	1:A:694:ILE:HD13	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ILE:HG23	2:B:80:ILE:O	2.13	0.49
2:B:188:PRO:HD2	2:B:243:TYR:HD1	1.76	0.49
1:C:734:VAL:O	1:C:736:LYS:N	2.45	0.49
1:C:792:PRO:HD2	1:C:862:TYR:OH	2.13	0.49
1:C:907:VAL:HA	1:C:910:THR:HB	1.94	0.49
2:B:224:VAL:HG13	2:B:224:VAL:O	2.13	0.49
2:B:251:GLN:OE1	2:B:254:TYR:CD2	2.65	0.49
1:C:125:LEU:CD1	1:C:798:VAL:HG23	2.42	0.49
1:C:637:ILE:O	1:C:638:ALA:C	2.50	0.49
1:A:103:LEU:C	1:A:318:ILE:HD11	2.33	0.48
1:A:727:MET:HE3	1:A:746:ASP:CA	2.43	0.48
1:A:905:LYS:C	1:A:907:VAL:N	2.67	0.48
1:A:953:GLU:O	1:A:954:GLU:C	2.50	0.48
1:A:990:LEU:O	1:A:991:ILE:C	2.51	0.48
2:B:144:GLY:O	2:B:146:ARG:N	2.46	0.48
2:B:199:TYR:CG	2:B:200:PRO:HD2	2.48	0.48
1:C:28:LEU:C	1:C:30:LYS:H	2.16	0.48
1:C:842:LEU:O	1:C:845:MET:HB2	2.13	0.48
1:C:858:GLY:HA3	1:C:915:PHE:CE2	2.48	0.48
1:C:978:PRO:O	1:C:980:TRP:N	2.45	0.48
2:D:52:GLY:O	2:D:55:GLN:N	2.43	0.48
2:D:222:GLU:O	2:D:223:LYS:C	2.52	0.48
1:A:515:LEU:O	1:A:516:ILE:HG13	2.14	0.48
1:A:960:PHE:C	1:A:960:PHE:CD2	2.86	0.48
2:B:88:ILE:HG22	2:B:101:TYR:CD1	2.47	0.48
1:C:38:LYS:HG2	1:C:224:PHE:CE1	2.47	0.48
1:C:47:LYS:HE2	1:C:48:TYR:OH	2.12	0.48
1:C:917:VAL:O	1:C:918:THR:C	2.50	0.48
1:A:115:GLU:HB3	2:B:85:LYS:CE	2.38	0.48
1:A:241:ASN:H	1:A:241:ASN:ND2	1.97	0.48
2:B:36:LEU:O	2:B:39:TYR:HB2	2.13	0.48
1:C:73:LEU:H	1:C:73:LEU:CD1	2.11	0.48
1:C:200:SER:OG	1:C:201:ALA:N	2.46	0.48
1:C:671:LEU:HD22	1:C:675:LEU:HD22	1.94	0.48
1:C:824:ILE:C	1:C:826:LYS:H	2.17	0.48
2:D:61:ILE:HG22	2:D:67:THR:HG21	1.94	0.48
2:D:152:ARG:H	2:D:155:TRP:HE1	1.61	0.48
2:D:199:TYR:CG	2:D:200:PRO:HD2	2.48	0.48
1:A:417:ILE:HD11	1:A:550:HIS:HB3	1.95	0.48
1:A:534:ALA:O	1:A:538:LEU:HB2	2.12	0.48
1:A:912:HIS:O	1:A:915:PHE:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:THR:O	2:B:57:MET:HB3	2.13	0.48
2:B:61:ILE:HG22	2:B:67:THR:HG21	1.96	0.48
1:C:124:TYR:C	1:C:126:GLY:H	2.17	0.48
1:C:961:LEU:HD11	1:C:971:LEU:CD1	2.44	0.48
2:D:122:ILE:HG22	2:D:122:ILE:O	2.14	0.48
1:A:117:GLU:C	1:A:119:GLN:N	2.67	0.48
1:A:224:PHE:CD2	1:A:224:PHE:O	2.62	0.48
1:A:301:ILE:O	1:A:305:ILE:HB	2.13	0.48
1:A:367:CYS:HB2	1:A:707:VAL:HG22	1.94	0.48
1:A:558:PHE:HD1	1:A:562:PHE:CE1	2.32	0.48
1:A:616:THR:O	1:A:617:ALA:C	2.50	0.48
2:B:152:ARG:O	2:B:155:TRP:HD1	1.97	0.48
1:C:32:VAL:HG12	1:C:33:SER:H	1.78	0.48
1:C:62:ALA:HA	1:C:65:LEU:HB2	1.96	0.48
1:C:108:TYR:CD1	1:C:123:LEU:HB2	2.48	0.48
1:C:224:PHE:HD2	1:C:224:PHE:O	1.95	0.48
1:A:86:CYS:HA	1:A:89:LEU:HG	1.96	0.48
1:A:107:ALA:O	1:A:110:ILE:HB	2.13	0.48
1:A:340:THR:HG21	1:A:761:ILE:HD13	1.96	0.48
1:A:427:GLN:NE2	1:A:427:GLN:HA	2.28	0.48
1:A:558:PHE:CD1	1:A:562:PHE:CE1	3.01	0.48
1:A:1000:LEU:N	1:A:1000:LEU:HD23	2.27	0.48
1:C:197:ARG:HD3	1:C:234:ASN:ND2	2.28	0.48
1:C:329:LEU:HA	1:C:332:THR:HB	1.95	0.48
1:C:624:VAL:CG2	1:C:626:ILE:HG13	2.44	0.48
1:C:640:ARG:O	1:C:640:ARG:HG2	2.14	0.48
1:A:51:ASP:O	1:A:52:LEU:CB	2.61	0.48
1:A:94:SER:O	1:A:98:TRP:CD1	2.66	0.48
1:A:99:ILE:HA	1:A:102:ILE:HG22	1.95	0.48
1:A:864:VAL:HG22	2:B:57:MET:SD	2.53	0.48
1:A:916:PHE:O	1:A:916:PHE:CG	2.67	0.48
2:B:104:SER:HA	2:B:107:ARG:HB2	1.96	0.48
2:B:170:LYS:N	2:B:170:LYS:CD	2.71	0.48
2:B:257:PRO:O	2:B:258:LEU:HD12	2.13	0.48
1:C:281:ILE:HD13	1:C:281:ILE:N	2.28	0.48
1:C:503:ALA:O	1:C:507:ILE:HB	2.14	0.48
1:C:609:VAL:HG11	1:C:691:LYS:HG2	1.93	0.48
1:C:641:LEU:O	1:C:642:ASN:C	2.51	0.48
1:C:705:VAL:O	1:C:722:ASP:HB2	2.14	0.48
1:C:862:TYR:HD1	1:C:863:PHE:CD1	2.31	0.48
2:D:143:ARG:HH11	2:D:143:ARG:CG	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LYS:HE2	1:A:692:LEU:HD21	1.95	0.48
1:A:37:HIS:HD2	1:A:232:THR:CG2	2.20	0.48
1:A:39:LEU:HD12	1:A:44:LEU:HD12	1.96	0.48
1:A:39:LEU:HD22	1:A:43:GLU:HB3	1.95	0.48
1:A:103:LEU:HD21	1:A:317:LEU:CD1	2.39	0.48
1:A:353:ASN:O	1:A:356:ALA:HB3	2.13	0.48
1:A:405:ASP:O	1:A:406:LYS:HB2	2.14	0.48
1:A:631:ASN:OD1	1:A:654:LYS:HB2	2.14	0.48
1:A:842:LEU:O	1:A:845:MET:HB2	2.14	0.48
1:A:917:VAL:C	1:A:919:ILE:N	2.65	0.48
2:B:21:LYS:HD3	2:B:22:LYS:HE3	1.95	0.48
1:C:238:PHE:CD1	1:C:238:PHE:C	2.87	0.48
2:D:58:LEU:O	2:D:60:THR:HB	2.13	0.48
1:A:841:GLN:HG2	1:A:1012:LYS:O	2.13	0.48
2:B:73:ALA:O	2:B:74:PRO:C	2.52	0.48
2:B:85:LYS:HB3	2:B:87:GLU:OE2	2.14	0.48
1:C:154:PHE:CE1	1:C:264:ALA:HB2	2.45	0.48
1:C:277:ILE:C	1:C:279:ALA:N	2.65	0.48
1:C:285:ILE:HD11	1:C:330:LEU:HD11	1.96	0.48
2:D:22:LYS:CG	2:D:23:GLU:H	2.26	0.48
2:D:137:GLY:HA3	2:D:146:ARG:HH21	1.78	0.48
1:A:321:ILE:HD13	1:A:321:ILE:N	2.28	0.48
1:A:670:GLN:O	1:A:674:ILE:HG13	2.14	0.48
1:A:687:SER:CB	1:A:690:GLN:HG3	2.43	0.48
1:A:899:TRP:CH2	2:B:72:VAL:HG22	2.48	0.48
1:C:164:VAL:HG12	1:C:184:VAL:HG22	1.96	0.48
2:D:21:LYS:HD3	2:D:22:LYS:HE3	1.96	0.48
2:D:71:ARG:HH12	3:H:23:TYR:HE1	1.60	0.48
2:D:80:ILE:H	2:D:81:PRO:HD3	1.78	0.48
2:D:206:PRO:HB2	2:D:207:TYR:CE2	2.49	0.48
1:A:150:ILE:HG22	1:A:151:MET:N	2.29	0.47
1:A:550:HIS:HD2	1:A:577:CYS:HB3	1.79	0.47
1:A:795:LEU:CD1	1:A:799:THR:HG21	2.43	0.47
1:A:862:TYR:HD1	1:A:863:PHE:CD1	2.31	0.47
1:C:238:PHE:HD1	1:C:238:PHE:C	2.17	0.47
1:C:550:HIS:HD2	1:C:577:CYS:HB3	1.79	0.47
1:C:752:VAL:O	1:C:755:VAL:HG12	2.13	0.47
2:D:21:LYS:CG	2:D:22:LYS:HB2	2.41	0.47
2:D:58:LEU:O	2:D:59:LEU:HD23	2.14	0.47
2:D:101:TYR:O	2:D:105:ILE:HG13	2.14	0.47
1:A:181:GLY:H	1:A:251:VAL:HG23	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LEU:O	1:A:332:THR:N	2.47	0.47
1:A:742:ILE:O	1:A:742:ILE:HG22	2.13	0.47
2:B:101:TYR:O	2:B:105:ILE:HG13	2.14	0.47
1:C:469:LYS:CB	1:C:486:HIS:CE1	2.97	0.47
1:C:530:ALA:HA	1:C:533:ASN:HB3	1.96	0.47
1:C:727:MET:HE3	1:C:746:ASP:CA	2.44	0.47
1:C:774:THR:HG23	1:C:846:ALA:CA	2.40	0.47
1:C:916:PHE:CZ	1:C:961:LEU:HD23	2.49	0.47
1:A:299:PHE:CE2	1:A:784:LEU:HD13	2.50	0.47
1:A:460:VAL:HG11	1:A:464:ARG:HH11	1.79	0.47
1:A:469:LYS:HB2	1:A:486:HIS:CE1	2.50	0.47
1:A:504:PRO:HG2	1:A:535:TYR:CE1	2.49	0.47
1:A:898:GLN:OE1	2:B:182:ARG:HD3	2.15	0.47
1:C:22:GLU:OE1	1:C:22:GLU:HA	2.15	0.47
1:C:166:ARG:O	1:C:167:ASN:CB	2.60	0.47
1:C:369:ASP:OD1	4:C:2001:MF4:F2	2.22	0.47
1:C:374:LEU:CD2	1:C:592:VAL:CG1	2.92	0.47
1:C:714:ASP:O	1:C:715:SER:C	2.52	0.47
1:C:834:THR:O	1:C:835:ASP:C	2.53	0.47
1:C:990:LEU:O	1:C:991:ILE:C	2.52	0.47
1:A:48:TYR:OH	1:A:252:VAL:HG12	2.14	0.47
1:A:293:VAL:HG23	1:A:294:PHE:N	2.29	0.47
1:A:394:ASP:OD2	1:A:399:GLN:HA	2.14	0.47
1:A:598:LYS:C	1:A:600:ARG:H	2.17	0.47
1:A:715:SER:CB	1:A:716:PRO:CD	2.92	0.47
1:A:984:ALA:O	1:A:987:TYR:N	2.46	0.47
2:B:224:VAL:HG22	2:B:267:THR:HB	1.96	0.47
1:C:786:PHE:CE1	1:C:793:LEU:HB2	2.49	0.47
1:A:383:HIS:O	1:A:384:MET:HG3	2.14	0.47
1:A:524:ASP:OD1	1:A:524:ASP:N	2.47	0.47
1:A:562:PHE:C	1:A:562:PHE:CD2	2.87	0.47
1:A:562:PHE:CD2	1:A:563:GLN:N	2.82	0.47
2:B:21:LYS:HD3	2:B:22:LYS:CD	2.44	0.47
2:B:240:LEU:HD12	2:B:240:LEU:N	2.30	0.47
1:C:609:VAL:HG12	1:C:691:LYS:HG2	1.95	0.47
1:C:613:HIS:CE1	1:C:685:ARG:CZ	2.97	0.47
1:C:654:LYS:HE2	1:C:654:LYS:CA	2.36	0.47
1:C:815:LEU:HD22	1:C:815:LEU:H	1.80	0.47
1:A:216:GLU:HG3	1:A:218:GLN:NE2	2.28	0.47
1:A:288:ILE:O	1:A:290:GLY:N	2.48	0.47
1:A:328:GLY:HA3	1:A:804:ASP:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:HE3	1:A:412:LEU:HD21	1.96	0.47
1:A:624:VAL:CG2	1:A:626:ILE:HG13	2.45	0.47
2:B:61:ILE:O	2:B:61:ILE:HD12	2.14	0.47
1:C:60:ARG:HG3	1:C:60:ARG:O	2.13	0.47
1:C:117:GLU:C	1:C:119:GLN:N	2.67	0.47
1:C:381:VAL:CG2	1:C:452:CYS:HB2	2.42	0.47
1:C:568:ASP:C	1:C:569:VAL:O	2.51	0.47
1:C:831:ASN:HA	1:C:832:PRO:HD2	1.63	0.47
1:A:39:LEU:CD1	1:A:44:LEU:HD12	2.45	0.47
1:A:50:THR:HB	1:A:56:LEU:HD12	1.90	0.47
1:A:341:ALA:C	1:A:343:ARG:H	2.17	0.47
1:A:435:ILE:HD13	1:A:438:ARG:CZ	2.45	0.47
1:A:451:LYS:O	1:A:452:CYS:C	2.50	0.47
1:A:455:LEU:HD23	1:A:456:CYS:HB3	1.97	0.47
1:A:514:ILE:HD12	1:A:527:LEU:HD12	1.97	0.47
1:A:717:ALA:C	1:A:719:LYS:N	2.67	0.47
2:B:22:LYS:CG	2:B:23:GLU:H	2.28	0.47
2:B:182:ARG:H	2:B:182:ARG:HG2	1.50	0.47
1:C:285:ILE:O	1:C:289:THR:HB	2.14	0.47
1:C:405:ASP:O	1:C:406:LYS:HB2	2.14	0.47
1:C:453:ILE:O	1:C:456:CYS:N	2.48	0.47
1:C:598:LYS:C	1:C:600:ARG:H	2.18	0.47
1:C:790:ASN:CB	1:C:880:ARG:HG2	2.44	0.47
1:C:810:VAL:HB	1:C:811:PRO:HD3	1.97	0.47
1:C:898:GLN:HG3	2:D:182:ARG:CG	2.44	0.47
1:C:909:PHE:CG	1:C:972:ARG:HB3	2.50	0.47
2:D:66:PRO:HD2	2:D:69:GLN:NE2	2.29	0.47
1:A:38:LYS:CG	1:A:224:PHE:HE1	2.27	0.47
1:A:68:ASP:OD2	1:A:180:VAL:HG21	2.15	0.47
1:A:637:ILE:HG22	1:A:638:ALA:N	2.30	0.47
1:A:866:LEU:HD13	1:A:876:LEU:HD21	1.96	0.47
1:A:867:ALA:C	1:A:869:ASN:H	2.17	0.47
1:A:907:VAL:HA	1:A:910:THR:HB	1.97	0.47
2:B:103:VAL:O	2:B:106:VAL:HB	2.14	0.47
1:C:32:VAL:HG12	1:C:33:SER:N	2.30	0.47
1:C:354:LEU:C	1:C:356:ALA:H	2.18	0.47
2:D:104:SER:HA	2:D:107:ARG:HB2	1.96	0.47
2:D:188:PRO:HG2	2:D:243:TYR:CE1	2.49	0.47
1:A:470:ILE:HG12	1:A:470:ILE:H	1.61	0.47
1:A:613:HIS:CE1	1:A:685:ARG:CZ	2.98	0.47
1:A:699:GLN:O	1:A:701:GLN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:VAL:HB	1:A:811:PRO:HD3	1.96	0.47
2:B:105:ILE:HG23	2:B:109:LEU:HD23	1.97	0.47
2:B:204:TYR:CD2	2:B:206:PRO:HD2	2.49	0.47
1:C:86:CYS:O	1:C:88:GLN:N	2.47	0.47
1:C:558:PHE:HA	1:C:562:PHE:HD1	1.80	0.47
1:C:624:VAL:HG23	1:C:625:GLY:N	2.29	0.47
2:D:85:LYS:HB3	2:D:87:GLU:OE2	2.15	0.47
2:D:204:TYR:CE2	2:D:207:TYR:HB2	2.49	0.47
1:A:143:GLN:HG2	1:A:144:GLU:OE2	2.15	0.47
1:A:187:LYS:CG	1:A:188:GLY:N	2.77	0.47
1:A:329:LEU:O	1:A:331:ALA:N	2.48	0.47
1:A:815:LEU:H	1:A:815:LEU:HD22	1.80	0.47
2:B:80:ILE:N	2:B:81:PRO:CD	2.78	0.47
2:B:167:TYR:HB2	2:B:169:TYR:CD1	2.50	0.47
1:C:99:ILE:O	1:C:103:LEU:HB2	2.14	0.47
1:C:411:TRP:C	1:C:413:ALA:H	2.18	0.47
1:C:562:PHE:CD2	1:C:562:PHE:C	2.88	0.47
2:D:30:GLY:O	2:D:31:SER:CB	2.61	0.47
1:A:142:TYR:O	1:A:142:TYR:HD2	1.86	0.46
1:A:349:CYS:SG	1:A:741:MET:CE	3.03	0.46
1:A:493:GLU:H	1:A:494:PRO:HD3	1.80	0.46
1:A:660:GLY:HA3	1:A:685:ARG:O	2.13	0.46
1:A:786:PHE:CD1	1:A:793:LEU:HB2	2.50	0.46
2:B:224:VAL:HG11	2:B:272:ILE:HG21	1.96	0.46
2:B:249:LEU:HD13	2:B:250:LEU:HD13	1.97	0.46
2:B:287:GLU:O	2:B:290:ARG:NH1	2.48	0.46
1:C:394:ASP:OD2	1:C:399:GLN:HA	2.15	0.46
1:C:620:ILE:HD13	1:C:620:ILE:HA	1.71	0.46
1:C:916:PHE:CG	1:C:916:PHE:O	2.68	0.46
2:D:79:GLN:CB	2:D:295:PHE:HZ	2.18	0.46
2:D:80:ILE:HG23	2:D:80:ILE:O	2.15	0.46
2:D:235:TYR:HA	2:D:236:PRO:HD3	1.81	0.46
1:A:57:THR:HG22	1:A:58:PRO:HD2	1.98	0.46
1:A:104:CYS:N	1:A:318:ILE:HD11	2.30	0.46
1:A:688:PRO:O	1:A:689:GLN:C	2.52	0.46
1:A:717:ALA:C	1:A:719:LYS:H	2.19	0.46
1:A:1000:LEU:O	1:A:1001:ILE:C	2.53	0.46
2:B:88:ILE:HD13	2:B:88:ILE:N	2.30	0.46
1:C:514:ILE:HD13	1:C:527:LEU:HD12	1.98	0.46
2:D:170:LYS:CG	2:D:175:CYS:HB2	2.45	0.46
2:D:240:LEU:HD12	2:D:240:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:ALA:HA	1:A:533:ASN:HB3	1.96	0.46
1:A:640:ARG:O	1:A:640:ARG:HG2	2.16	0.46
1:A:794:PRO:O	1:A:912:HIS:HD2	1.98	0.46
1:A:944:ASN:C	1:A:946:ILE:H	2.19	0.46
2:B:206:PRO:HB2	2:B:207:TYR:CE2	2.49	0.46
1:C:35:ASP:HB2	1:C:229:PRO:HG3	1.98	0.46
1:C:125:LEU:HD21	1:C:797:THR:HG21	1.97	0.46
1:C:254:THR:HG23	1:C:254:THR:O	2.14	0.46
1:C:258:THR:OG1	1:C:259:VAL:N	2.48	0.46
1:C:265:THR:HG22	1:C:266:LEU:H	1.80	0.46
1:C:795:LEU:CD1	1:C:799:THR:HG21	2.45	0.46
1:C:797:THR:O	1:C:800:ILE:N	2.48	0.46
2:D:36:LEU:O	2:D:39:TYR:HB2	2.15	0.46
2:D:287:GLU:O	2:D:290:ARG:NH1	2.49	0.46
1:A:311:LEU:CD2	1:A:311:LEU:H	2.28	0.46
1:A:336:CYS:CB	1:A:765:LEU:HD21	2.45	0.46
1:A:917:VAL:O	1:A:919:ILE:N	2.47	0.46
2:B:204:TYR:CE2	2:B:207:TYR:HB2	2.50	0.46
1:C:187:LYS:CG	1:C:188:GLY:H	2.28	0.46
1:C:226:ASN:ND2	1:C:228:ASN:H	2.13	0.46
1:C:561:GLY:O	1:C:562:PHE:C	2.54	0.46
1:C:775:SER:HB3	1:C:923:GLN:NE2	2.30	0.46
1:A:97:LEU:CD2	1:A:325:VAL:HG11	2.46	0.46
1:A:117:GLU:N	1:A:118:PRO:HD3	2.31	0.46
1:A:191:ARG:HH11	1:A:191:ARG:HG2	1.80	0.46
1:C:341:ALA:C	1:C:343:ARG:H	2.18	0.46
1:A:351:VAL:HG11	1:A:357:VAL:HG22	1.97	0.46
2:B:22:LYS:O	2:B:25:LEU:N	2.49	0.46
2:B:66:PRO:HD2	2:B:69:GLN:NE2	2.30	0.46
1:C:64:ILE:O	1:C:64:ILE:CG2	2.64	0.46
1:C:354:LEU:C	1:C:356:ALA:N	2.67	0.46
1:C:536:LEU:O	1:C:537:GLU:C	2.54	0.46
1:C:546:LEU:HD23	1:C:546:LEU:HA	1.74	0.46
1:C:753:THR:HG22	1:C:754:GLY:N	2.29	0.46
1:C:853:ILE:CG2	1:C:990:LEU:HD13	2.46	0.46
1:C:906:ILE:O	1:C:906:ILE:HG22	2.16	0.46
1:C:917:VAL:O	1:C:919:ILE:N	2.48	0.46
2:D:105:ILE:HG23	2:D:109:LEU:HD23	1.97	0.46
1:A:378:ARG:CZ	1:A:436:LEU:CD2	2.92	0.46
1:A:495:ARG:O	1:A:496:HIS:CG	2.68	0.46
1:C:284:PHE:O	1:C:288:ILE:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:LEU:O	1:C:302:LEU:HD23	2.15	0.46
1:C:779:GLU:OE1	1:C:800:ILE:HG23	2.15	0.46
2:D:180:LEU:HB2	2:D:238:PHE:CE2	2.51	0.46
2:D:257:PRO:O	2:D:258:LEU:HD12	2.14	0.46
1:A:107:ALA:O	1:A:108:TYR:C	2.54	0.46
1:A:142:TYR:O	1:A:142:TYR:CG	2.67	0.46
1:A:254:THR:O	1:A:254:THR:HG23	2.16	0.46
1:A:320:ILE:HG23	1:A:321:ILE:HD13	1.97	0.46
1:A:453:ILE:O	1:A:456:CYS:N	2.49	0.46
1:A:761:ILE:O	1:A:765:LEU:HG	2.16	0.46
1:A:790:ASN:CB	1:A:880:ARG:HG2	2.45	0.46
1:C:23:ARG:O	1:C:27:GLU:HB2	2.15	0.46
1:C:74:THR:HA	1:C:75:PRO:HD3	1.70	0.46
1:C:97:LEU:HG	1:C:325:VAL:HG11	1.98	0.46
1:C:202:ASN:O	1:C:203:GLY:C	2.54	0.46
1:C:286:HIS:CD2	1:C:286:HIS:N	2.82	0.46
1:C:699:GLN:O	1:C:701:GLN:N	2.48	0.46
1:C:766:LYS:HE2	1:C:837:LEU:O	2.16	0.46
1:C:794:PRO:O	1:C:912:HIS:HD2	1.98	0.46
1:A:81:GLU:OE2	1:A:84:LYS:HD3	2.15	0.46
1:A:86:CYS:O	1:A:88:GLN:N	2.48	0.46
1:A:210:SER:HA	1:A:712:VAL:HG13	1.98	0.46
1:A:633:THR:H	1:A:636:ASP:HB2	1.80	0.46
1:A:786:PHE:CE1	1:A:793:LEU:HB2	2.51	0.46
1:A:845:MET:SD	1:A:1014:THR:HG22	2.56	0.46
1:C:97:LEU:HB3	1:C:133:VAL:HG23	1.97	0.46
1:C:349:CYS:SG	1:C:741:MET:HG2	2.55	0.46
1:C:687:SER:CB	1:C:690:GLN:HG3	2.46	0.46
1:C:688:PRO:O	1:C:689:GLN:C	2.53	0.46
1:C:708:THR:HG21	1:C:748:PHE:HE1	1.79	0.46
1:C:732:SER:O	1:C:736:LYS:HG2	2.16	0.46
1:C:812:ALA:C	1:C:814:SER:N	2.68	0.46
2:D:144:GLY:O	2:D:146:ARG:N	2.48	0.46
2:D:186:PHE:CZ	2:D:282:ASN:HB3	2.51	0.46
2:D:249:LEU:HD13	2:D:250:LEU:HD13	1.98	0.46
1:A:44:LEU:O	1:A:47:LYS:N	2.49	0.46
1:A:71:ASN:OD1	1:A:255:GLY:N	2.49	0.46
1:C:360:LEU:O	1:C:755:VAL:HG23	2.15	0.46
1:C:365:THR:HG23	1:C:605:LYS:HB3	1.97	0.46
2:D:224:VAL:HG11	2:D:272:ILE:HG21	1.97	0.46
2:D:251:GLN:OE1	2:D:254:TYR:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ILE:HG21	1:A:311:LEU:HD13	1.97	0.45
1:A:116:GLU:C	1:A:118:PRO:HD3	2.36	0.45
1:A:157:MET:O	1:A:191:ARG:HD3	2.15	0.45
1:A:370:LYS:CB	1:A:608:MET:HE3	2.44	0.45
1:A:986:PRO:HG2	1:A:987:TYR:HD2	1.81	0.45
1:C:154:PHE:HE2	1:C:734:VAL:HG11	1.82	0.45
1:C:275:THR:CG2	1:C:355:GLU:OE2	2.63	0.45
1:C:309:THR:OG1	1:C:312:GLU:OE1	2.34	0.45
1:C:481:TYR:CD1	1:C:481:TYR:C	2.90	0.45
1:C:857:GLY:HA2	1:C:987:TYR:CD1	2.51	0.45
1:C:919:ILE:HA	1:C:919:ILE:HD13	1.70	0.45
2:D:103:VAL:O	2:D:106:VAL:HB	2.16	0.45
1:A:151:MET:C	1:A:153:SER:N	2.70	0.45
1:A:222:PRO:O	1:A:224:PHE:N	2.49	0.45
1:A:753:THR:HG22	1:A:754:GLY:N	2.31	0.45
1:A:815:LEU:O	1:A:818:GLU:N	2.49	0.45
2:B:177:ILE:CD1	2:B:258:LEU:HD23	2.47	0.45
1:C:61:ALA:O	1:C:63:GLU:N	2.49	0.45
1:C:68:ASP:OD2	1:C:180:VAL:HG21	2.16	0.45
1:C:410:THR:HG23	1:C:515:LEU:HD13	1.99	0.45
1:C:414:LEU:HD12	1:C:414:LEU:C	2.35	0.45
2:D:80:ILE:N	2:D:81:PRO:CD	2.79	0.45
2:D:164:ASP:HB3	2:D:165:GLU:H	1.59	0.45
1:A:205:LYS:HA	1:A:218:GLN:O	2.17	0.45
1:A:831:ASN:C	1:A:831:ASN:OD1	2.54	0.45
2:B:251:GLN:C	2:B:252:PRO:O	2.54	0.45
1:C:57:THR:HB	1:C:60:ARG:H	1.81	0.45
1:C:254:THR:HG23	1:C:257:ARG:HE	1.82	0.45
1:C:329:LEU:O	1:C:332:THR:N	2.49	0.45
1:C:406:LYS:HE3	1:C:412:LEU:HD21	1.98	0.45
1:C:692:LEU:O	1:C:694:ILE:N	2.49	0.45
1:C:736:LYS:HG3	1:C:737:GLN:H	1.81	0.45
1:C:850:ILE:O	1:C:854:GLN:HG3	2.16	0.45
1:C:1001:ILE:O	1:C:1002:ILE:C	2.54	0.45
1:A:174:ASN:O	1:A:176:GLU:N	2.50	0.45
1:A:226:ASN:ND2	1:A:228:ASN:H	2.14	0.45
1:A:312:GLU:OE2	1:A:880:ARG:NH2	2.50	0.45
1:A:586:ASP:HA	1:A:587:PRO:HD3	1.56	0.45
1:A:959:ALA:O	1:A:963:TYR:HD1	1.99	0.45
2:B:180:LEU:HB2	2:B:238:PHE:CE2	2.51	0.45
1:C:86:CYS:O	1:C:87:ARG:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:ILE:CG2	1:C:322:VAL:N	2.78	0.45
1:C:383:HIS:CD2	1:C:392:GLU:HB3	2.52	0.45
1:C:880:ARG:O	1:C:881:VAL:C	2.54	0.45
1:C:1000:LEU:HA	1:C:1000:LEU:HD22	1.45	0.45
2:D:21:LYS:HD3	2:D:22:LYS:CE	2.47	0.45
1:A:202:ASN:O	1:A:203:GLY:C	2.54	0.45
1:A:216:GLU:O	1:A:218:GLN:NE2	2.50	0.45
1:A:469:LYS:CB	1:A:486:HIS:CE1	2.99	0.45
1:A:732:SER:O	1:A:734:VAL:N	2.50	0.45
1:A:802:CYS:O	1:A:807:THR:HG23	2.17	0.45
2:B:238:PHE:HA	2:B:239:PRO:HD3	1.70	0.45
1:C:241:ASN:H	1:C:241:ASN:ND2	1.98	0.45
1:C:295:LEU:HD12	1:C:324:ASN:ND2	2.28	0.45
1:C:435:ILE:CD1	1:C:438:ARG:NH2	2.77	0.45
1:C:624:VAL:CG2	1:C:625:GLY:N	2.79	0.45
1:C:715:SER:CB	1:C:716:PRO:CD	2.94	0.45
1:C:860:PHE:C	1:C:860:PHE:CD2	2.90	0.45
1:C:867:ALA:C	1:C:869:ASN:H	2.18	0.45
1:C:894:SER:O	1:C:895:TYR:CD1	2.70	0.45
2:D:61:ILE:O	2:D:61:ILE:HD12	2.16	0.45
2:D:61:ILE:CG2	2:D:67:THR:OG1	2.65	0.45
1:A:173:ILE:HD12	1:A:177:GLU:HB2	1.98	0.45
1:A:238:PHE:O	1:A:239:SER:HB3	2.16	0.45
1:A:663:LEU:HA	1:A:663:LEU:HD23	1.78	0.45
1:C:263:ILE:HD12	1:C:688:PRO:HB2	1.98	0.45
1:C:667:THR:O	1:C:668:SER:C	2.54	0.45
1:C:732:SER:O	1:C:734:VAL:N	2.50	0.45
1:C:799:THR:O	1:C:802:CYS:HB2	2.17	0.45
1:C:802:CYS:O	1:C:807:THR:HG23	2.16	0.45
1:C:862:TYR:CD1	1:C:863:PHE:CD1	3.05	0.45
1:A:288:ILE:HD13	1:A:326:PRO:CG	2.47	0.45
1:A:369:ASP:O	1:A:373:THR:HB	2.17	0.45
1:A:880:ARG:O	1:A:881:VAL:C	2.54	0.45
1:A:1000:LEU:HD22	1:A:1000:LEU:HA	1.52	0.45
1:C:39:LEU:HB3	1:C:43:GLU:CB	2.47	0.45
1:C:120:ASN:O	1:C:124:TYR:HD1	1.99	0.45
1:C:274:GLN:C	1:C:275:THR:O	2.54	0.45
1:A:138:CYS:O	1:A:139:PHE:C	2.56	0.45
1:A:201:ALA:HA	1:A:247:ALA:HA	1.97	0.45
1:A:299:PHE:O	1:A:316:PHE:CE2	2.57	0.45
1:A:344:MET:O	1:A:347:LYS:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:TYR:CD2	1:A:467:TYR:N	2.85	0.45
1:A:568:ASP:C	1:A:569:VAL:O	2.54	0.45
1:A:732:SER:O	1:A:736:LYS:HG2	2.17	0.45
1:A:850:ILE:O	1:A:854:GLN:HG3	2.17	0.45
1:C:52:LEU:HD23	1:C:199:ILE:HD13	1.98	0.45
1:C:97:LEU:HD21	1:C:325:VAL:HG11	1.99	0.45
1:C:450:LEU:CD2	1:C:450:LEU:O	2.64	0.45
1:C:469:LYS:HB2	1:C:486:HIS:CE1	2.51	0.45
1:C:524:ASP:OD1	1:C:524:ASP:N	2.49	0.45
1:C:592:VAL:HB	1:C:593:PRO:HD3	1.98	0.45
1:C:598:LYS:CB	1:C:752:VAL:HG21	2.46	0.45
2:D:167:TYR:HB2	2:D:169:TYR:CD1	2.51	0.45
2:D:170:LYS:N	2:D:170:LYS:CD	2.73	0.45
2:D:209:LEU:O	2:D:237:GLY:HA3	2.17	0.45
2:D:290:ARG:NE	2:D:290:ARG:HA	2.31	0.45
1:A:57:THR:HB	1:A:60:ARG:H	1.82	0.45
1:A:86:CYS:O	1:A:89:LEU:N	2.46	0.45
1:A:743:LEU:HD11	1:A:751:ILE:CD1	2.47	0.45
1:A:842:LEU:HD23	1:A:843:ILE:N	2.32	0.45
1:A:856:LEU:HD12	2:B:46:LEU:HD13	1.98	0.45
1:A:860:PHE:C	1:A:860:PHE:CD2	2.90	0.45
2:B:60:THR:OG1	2:B:61:ILE:N	2.50	0.45
2:B:290:ARG:NE	2:B:290:ARG:HA	2.32	0.45
1:C:266:LEU:O	1:C:266:LEU:HG	2.16	0.45
1:C:377:ASN:O	1:C:377:ASN:ND2	2.50	0.45
1:C:410:THR:HG1	1:C:517:HIS:H	1.65	0.45
1:C:476:ASN:HB2	1:C:479:ASN:OD1	2.17	0.45
1:C:761:ILE:O	1:C:765:LEU:HG	2.17	0.45
1:C:791:ILE:HG23	1:C:792:PRO:N	2.32	0.45
1:A:369:ASP:OD1	4:A:2001:MF4:F2	2.24	0.45
1:A:471:VAL:HG12	1:A:485:ILE:HG13	1.99	0.45
1:A:691:LYS:HE3	1:A:713:ASN:ND2	2.32	0.45
1:A:774:THR:HG23	1:A:846:ALA:CA	2.42	0.45
1:C:277:ILE:CG2	1:C:278:ALA:H	2.30	0.45
1:C:303:SER:O	1:C:308:TYR:CD2	2.62	0.45
1:C:790:ASN:HD22	1:C:880:ARG:CG	2.29	0.45
1:A:93:PHE:CZ	1:A:288:ILE:HG21	2.52	0.44
1:A:374:LEU:CD2	1:A:592:VAL:HG11	2.48	0.44
1:A:490:ASN:HB3	1:A:492:ALA:H	1.81	0.44
2:B:170:LYS:HG2	2:B:174:PRO:O	2.17	0.44
2:B:170:LYS:CG	2:B:175:CYS:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ASN:O	1:C:72:ALA:CB	2.65	0.44
1:C:163:LEU:HD23	1:C:163:LEU:HA	1.58	0.44
1:C:222:PRO:O	1:C:224:PHE:N	2.50	0.44
1:C:660:GLY:HA3	1:C:685:ARG:O	2.18	0.44
1:C:761:ILE:HD12	1:C:761:ILE:HA	1.70	0.44
1:C:765:LEU:HD23	1:C:765:LEU:HA	1.74	0.44
1:A:28:LEU:C	1:A:30:LYS:H	2.19	0.44
1:A:47:LYS:HG2	1:A:48:TYR:CE2	2.53	0.44
1:A:52:LEU:C	1:A:54:ARG:N	2.67	0.44
1:A:530:ALA:HA	1:A:533:ASN:HB2	1.98	0.44
1:A:771:TYR:CE1	1:A:927:LEU:HB2	2.51	0.44
1:C:462:GLU:C	1:C:464:ARG:N	2.68	0.44
1:C:586:ASP:HA	1:C:587:PRO:HD3	1.53	0.44
1:C:866:LEU:HD13	1:C:876:LEU:HD21	1.99	0.44
1:C:969:VAL:O	1:C:969:VAL:CG1	2.65	0.44
1:A:22:GLU:OE1	1:A:22:GLU:HA	2.16	0.44
1:A:197:ARG:HD3	1:A:234:ASN:ND2	2.32	0.44
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.55	0.44
1:A:288:ILE:O	1:A:289:THR:C	2.55	0.44
1:A:462:GLU:C	1:A:464:ARG:N	2.67	0.44
1:A:483:LEU:HD23	1:A:500:MET:CE	2.48	0.44
1:A:521:GLN:HB3	1:A:522:PRO:CD	2.43	0.44
1:A:916:PHE:CZ	1:A:961:LEU:HD23	2.52	0.44
2:B:39:TYR:HE2	7:B:3001:CLR:H182	1.81	0.44
1:C:305:ILE:HD13	1:C:305:ILE:HA	1.69	0.44
1:C:383:HIS:HB2	1:C:538:LEU:HD11	2.00	0.44
1:C:510:ARG:HH11	1:C:510:ARG:CB	2.21	0.44
1:C:573:LEU:C	1:C:574:ASP:OD1	2.56	0.44
1:C:789:ALA:O	1:C:790:ASN:C	2.56	0.44
1:A:61:ALA:C	1:A:63:GLU:H	2.19	0.44
1:A:228:ASN:HA	1:A:229:PRO:HD3	1.85	0.44
1:C:267:ALA:C	1:C:269:GLY:N	2.70	0.44
1:C:308:TYR:CZ	1:C:787:ILE:HD13	2.51	0.44
1:C:318:ILE:HG22	1:C:318:ILE:O	2.16	0.44
1:C:747:ASN:ND2	1:C:749:ALA:HB3	2.32	0.44
1:A:314:VAL:HG23	1:A:314:VAL:O	2.16	0.44
1:A:485:ILE:HD11	1:A:571:PHE:CE2	2.52	0.44
1:C:179:VAL:O	1:C:181:GLY:N	2.50	0.44
1:C:187:LYS:HD2	1:C:188:GLY:N	2.17	0.44
1:C:276:PRO:HG3	1:C:359:THR:HG23	1.99	0.44
1:A:329:LEU:HA	1:A:332:THR:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:ILE:O	1:A:1002:ILE:C	2.55	0.44
2:B:122:ILE:HG22	2:B:122:ILE:O	2.17	0.44
1:C:174:ASN:O	1:C:176:GLU:N	2.51	0.44
1:C:717:ALA:C	1:C:719:LYS:N	2.70	0.44
1:C:802:CYS:HB3	1:C:916:PHE:CE2	2.52	0.44
1:C:857:GLY:N	1:C:987:TYR:CD1	2.86	0.44
1:C:878:GLY:O	1:C:881:VAL:CG2	2.66	0.44
1:C:986:PRO:HG2	1:C:987:TYR:HD2	1.81	0.44
1:C:1000:LEU:O	1:C:1001:ILE:C	2.55	0.44
2:D:252:PRO:C	2:D:254:TYR:H	2.21	0.44
1:A:143:GLN:HG3	1:A:355:GLU:HG2	1.99	0.44
1:A:154:PHE:CE1	1:A:264:ALA:HB2	2.48	0.44
1:A:288:ILE:CG2	1:A:289:THR:N	2.78	0.44
1:A:336:CYS:HB2	1:A:765:LEU:HD21	2.00	0.44
1:A:752:VAL:O	1:A:755:VAL:HG12	2.16	0.44
1:A:797:THR:C	1:A:799:THR:N	2.71	0.44
2:B:51:ILE:HA	2:B:54:ILE:HG22	2.00	0.44
2:B:112:TYR:CE2	2:B:255:LEU:HD13	2.53	0.44
2:B:156:LEU:HD23	2:B:156:LEU:HA	1.51	0.44
2:B:157:GLY:HA3	2:B:230:PHE:CZ	2.53	0.44
1:C:455:LEU:HD23	1:C:456:CYS:HB3	1.99	0.44
1:C:467:TYR:CD2	1:C:467:TYR:N	2.85	0.44
1:C:570:ASN:OD1	1:C:570:ASN:C	2.55	0.44
1:C:874:ILE:O	1:C:876:LEU:N	2.51	0.44
2:D:182:ARG:H	2:D:182:ARG:HG2	1.48	0.44
2:D:204:TYR:CD2	2:D:206:PRO:HD2	2.53	0.44
1:A:63:GLU:O	1:A:63:GLU:HG2	2.16	0.44
1:A:115:GLU:O	1:A:116:GLU:C	2.55	0.44
1:A:379:MET:SD	1:A:584:MET:HG3	2.58	0.44
1:A:416:ARG:HD2	1:A:467:TYR:CZ	2.52	0.44
1:A:510:ARG:HH11	1:A:510:ARG:CB	2.25	0.44
1:A:799:THR:O	1:A:802:CYS:HB2	2.16	0.44
1:A:921:VAL:O	1:A:988:SER:OG	2.35	0.44
1:A:963:TYR:CD1	1:A:963:TYR:N	2.86	0.44
2:B:209:LEU:HA	2:B:210:PRO:HD3	1.81	0.44
2:B:214:THR:O	2:B:274:ILE:HG13	2.18	0.44
1:C:327:GLU:HB3	1:C:805:LEU:HD11	2.00	0.44
1:C:375:THR:HB	1:C:587:PRO:O	2.17	0.44
1:C:530:ALA:HA	1:C:533:ASN:HB2	1.98	0.44
1:C:791:ILE:HG23	1:C:862:TYR:HH	1.83	0.44
2:D:88:ILE:HD13	2:D:88:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:112:TYR:CE2	2:D:255:LEU:HD13	2.53	0.44
1:A:383:HIS:CD2	1:A:392:GLU:HB3	2.53	0.44
1:A:440:VAL:CG1	1:A:451:LYS:HE3	2.48	0.44
2:B:23:GLU:O	2:B:25:LEU:N	2.50	0.44
2:B:32:TRP:H	2:B:35:ILE:HG13	1.82	0.44
2:B:79:GLN:CB	2:B:295:PHE:HZ	2.19	0.44
2:B:88:ILE:HG22	2:B:101:TYR:HE1	1.77	0.44
2:B:186:PHE:CZ	2:B:282:ASN:HB3	2.53	0.44
2:B:216:LYS:HD3	2:B:222:GLU:OE2	2.18	0.44
1:C:132:VAL:O	1:C:132:VAL:HG12	2.18	0.44
1:C:164:VAL:HA	1:C:183:LEU:O	2.17	0.44
1:C:917:VAL:C	1:C:919:ILE:N	2.67	0.44
2:D:114:ASP:OD1	2:D:114:ASP:N	2.50	0.44
1:A:187:LYS:CD	1:A:188:GLY:H	2.23	0.43
1:A:204:CYS:HB2	1:A:246:THR:O	2.17	0.43
1:A:329:LEU:HD11	1:A:769:ILE:CG1	2.48	0.43
1:A:598:LYS:HB3	1:A:752:VAL:HG21	1.99	0.43
1:A:671:LEU:HD22	1:A:675:LEU:HD22	2.00	0.43
1:A:736:LYS:O	1:A:739:ALA:N	2.47	0.43
1:A:769:ILE:O	1:A:770:ALA:C	2.56	0.43
2:B:225:GLY:HA2	2:B:265:ASN:HB2	2.00	0.43
1:C:337:LEU:HD12	1:C:337:LEU:HA	1.79	0.43
1:C:460:VAL:HG13	1:C:464:ARG:HD3	1.98	0.43
1:C:504:PRO:HG2	1:C:535:TYR:CE1	2.53	0.43
1:A:74:THR:HA	1:A:75:PRO:HD3	1.69	0.43
1:A:289:THR:HA	1:A:292:ALA:HB3	1.98	0.43
1:A:481:TYR:CD1	1:A:481:TYR:C	2.90	0.43
1:A:672:ASP:O	1:A:676:LYS:HB2	2.17	0.43
1:A:802:CYS:HB3	1:A:916:PHE:CE2	2.52	0.43
1:A:905:LYS:O	1:A:907:VAL:N	2.51	0.43
1:C:205:LYS:HA	1:C:218:GLN:O	2.18	0.43
1:C:756:GLU:HB2	1:C:825:MET:CG	2.48	0.43
2:D:31:SER:HA	2:D:33:PHE:N	2.30	0.43
1:A:98:TRP:CE2	1:A:133:VAL:HG11	2.53	0.43
1:A:165:ILE:HG12	1:A:183:LEU:HB3	2.00	0.43
1:A:288:ILE:CD1	1:A:326:PRO:HG2	2.48	0.43
1:A:398:ASN:O	1:A:399:GLN:CB	2.67	0.43
1:A:512:SER:CB	1:A:575:ASN:HA	2.48	0.43
1:A:667:THR:O	1:A:668:SER:C	2.56	0.43
1:A:791:ILE:HG23	1:A:862:TYR:HH	1.83	0.43
1:A:862:TYR:CD1	1:A:863:PHE:CD1	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:926:ASP:C	1:A:928:VAL:H	2.21	0.43
1:A:994:TYR:CE2	2:B:42:PHE:HE1	2.36	0.43
2:B:229:TYR:O	2:B:230:PHE:CD1	2.72	0.43
1:C:208:ASN:HB3	1:C:212:THR:HG23	1.98	0.43
1:C:348:ASN:O	1:C:744:LEU:HB2	2.18	0.43
1:C:633:THR:HG23	1:C:636:ASP:H	1.83	0.43
2:D:157:GLY:HA3	2:D:230:PHE:CZ	2.52	0.43
2:D:238:PHE:HA	2:D:239:PRO:HD3	1.68	0.43
1:A:35:ASP:HB2	1:A:229:PRO:CG	2.49	0.43
1:A:275:THR:HG21	1:A:355:GLU:OE2	2.19	0.43
1:A:747:ASN:HD21	1:A:749:ALA:N	2.14	0.43
1:A:795:LEU:HD12	1:A:795:LEU:HA	1.80	0.43
2:B:290:ARG:HH21	2:B:294:ARG:NH1	2.17	0.43
1:C:311:LEU:O	1:C:315:ILE:HB	2.18	0.43
1:C:385:TRP:HB2	1:C:581:LEU:HB2	1.99	0.43
1:C:431:GLU:CD	1:C:431:GLU:H	2.22	0.43
1:C:899:TRP:CH2	2:D:72:VAL:HG22	2.52	0.43
2:D:88:ILE:HD11	2:D:299:ILE:CG2	2.44	0.43
1:A:23:ARG:O	1:A:27:GLU:HB2	2.18	0.43
1:A:687:SER:HB2	1:A:690:GLN:HG3	1.99	0.43
2:B:21:LYS:CG	2:B:22:LYS:CG	2.96	0.43
2:B:51:ILE:O	2:B:54:ILE:HG22	2.19	0.43
2:B:156:LEU:CD1	2:B:159:CYS:HB3	2.46	0.43
1:C:158:VAL:HG23	1:C:159:PRO:CD	2.48	0.43
1:C:488:ASN:OD1	1:C:489:PRO:CD	2.66	0.43
1:C:562:PHE:CD2	1:C:563:GLN:N	2.86	0.43
1:C:872:LEU:O	1:C:873:PRO:C	2.57	0.43
2:D:60:THR:OG1	2:D:61:ILE:N	2.49	0.43
2:D:225:GLY:HA2	2:D:265:ASN:HB2	2.00	0.43
1:A:374:LEU:HA	1:A:374:LEU:HD23	1.67	0.43
1:A:562:PHE:HD2	1:A:563:GLN:N	2.17	0.43
1:A:717:ALA:O	1:A:719:LYS:N	2.52	0.43
1:C:216:GLU:HG3	1:C:218:GLN:NE2	2.34	0.43
1:C:263:ILE:CD1	1:C:688:PRO:HB2	2.48	0.43
1:C:270:LEU:HD23	1:C:270:LEU:HA	1.63	0.43
1:C:655:ALA:CB	1:C:680:GLU:HB2	2.49	0.43
1:A:165:ILE:HG22	1:A:170:LYS:CA	2.49	0.43
1:A:311:LEU:H	1:A:311:LEU:HD23	1.81	0.43
1:A:354:LEU:C	1:A:356:ALA:N	2.71	0.43
1:A:414:LEU:HD12	1:A:414:LEU:C	2.37	0.43
1:A:570:ASN:OD1	1:A:570:ASN:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:TYR:HA	2:B:101:TYR:HD2	1.84	0.43
2:B:179:LYS:HD2	2:B:256:GLN:CD	2.39	0.43
1:C:65:LEU:HD13	1:C:70:PRO:HD3	2.01	0.43
1:C:609:VAL:HG12	1:C:609:VAL:O	2.19	0.43
1:C:633:THR:H	1:C:636:ASP:HB2	1.83	0.43
2:D:106:VAL:O	2:D:110:GLU:HB2	2.19	0.43
1:A:263:ILE:HD12	1:A:688:PRO:HB2	2.00	0.43
2:B:37:LEU:C	2:B:39:TYR:H	2.22	0.43
2:B:61:ILE:CG2	2:B:67:THR:OG1	2.67	0.43
1:C:60:ARG:HA	1:C:63:GLU:HB3	2.01	0.43
1:C:158:VAL:HG23	1:C:159:PRO:N	2.33	0.43
1:C:450:LEU:C	1:C:450:LEU:HD22	2.38	0.43
1:C:905:LYS:C	1:C:907:VAL:N	2.72	0.43
2:D:79:GLN:NE2	2:D:83:SER:OG	2.50	0.43
1:A:89:LEU:O	1:A:90:PHE:CD2	2.72	0.43
1:A:319:GLY:HA3	1:A:783:PHE:CE1	2.53	0.43
1:A:411:TRP:C	1:A:413:ALA:H	2.22	0.43
1:A:637:ILE:O	1:A:638:ALA:C	2.57	0.43
1:A:667:THR:O	1:A:669:GLU:N	2.52	0.43
2:B:80:ILE:HD12	2:B:80:ILE:HA	1.89	0.43
2:B:252:PRO:C	2:B:254:TYR:H	2.21	0.43
1:C:483:LEU:HD23	1:C:500:MET:CE	2.48	0.43
1:C:485:ILE:HD11	1:C:571:PHE:CE2	2.53	0.43
1:C:668:SER:O	1:C:671:LEU:HB3	2.18	0.43
1:C:815:LEU:O	1:C:818:GLU:N	2.52	0.43
1:A:128:VAL:O	1:A:129:LEU:C	2.57	0.43
1:A:304:LEU:CD1	1:A:310:TRP:CZ3	2.87	0.43
1:A:409:ALA:O	1:A:410:THR:C	2.57	0.43
1:A:885:ASP:CG	1:A:888:ILE:HG13	2.39	0.43
1:C:40:SER:N	1:C:43:GLU:HB2	2.34	0.43
1:C:349:CYS:SG	1:C:741:MET:CE	3.07	0.43
1:C:631:ASN:OD1	1:C:654:LYS:HB2	2.18	0.43
2:D:226:THR:HB	2:D:265:ASN:HA	2.00	0.43
1:A:121:ASP:HB3	1:A:122:ASN:H	1.58	0.42
1:A:129:LEU:HD23	1:A:129:LEU:HA	1.83	0.42
1:A:237:PHE:O	1:A:240:THR:OG1	2.34	0.42
1:A:328:GLY:H	1:A:804:ASP:HB2	1.84	0.42
1:A:694:ILE:O	1:A:695:VAL:C	2.56	0.42
1:A:732:SER:C	1:A:734:VAL:N	2.72	0.42
1:A:843:ILE:C	1:A:845:MET:N	2.72	0.42
1:A:898:GLN:HG3	2:B:182:ARG:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:PHE:CG	1:A:972:ARG:HB3	2.55	0.42
1:A:986:PRO:HG2	1:A:987:TYR:CD2	2.54	0.42
2:B:58:LEU:O	2:B:59:LEU:HD23	2.19	0.42
2:B:74:PRO:HB2	2:B:292:GLN:NE2	2.34	0.42
1:C:63:GLU:O	1:C:63:GLU:HG2	2.19	0.42
1:C:341:ALA:C	1:C:343:ARG:N	2.72	0.42
1:C:909:PHE:CZ	1:C:972:ARG:NE	2.88	0.42
1:C:959:ALA:O	1:C:963:TYR:HD1	2.01	0.42
2:D:196:LEU:HB3	2:D:197:GLU:H	1.57	0.42
2:D:209:LEU:O	2:D:237:GLY:CA	2.67	0.42
2:D:216:LYS:HD3	2:D:222:GLU:OE2	2.18	0.42
7:D:3001:CLR:H211	7:D:3001:CLR:H231	1.73	0.42
1:A:88:GLN:O	1:A:90:PHE:N	2.46	0.42
1:A:111:GLN:NE2	1:A:122:ASN:HD22	2.15	0.42
1:A:410:THR:HG1	1:A:517:HIS:H	1.67	0.42
1:A:872:LEU:O	1:A:873:PRO:C	2.56	0.42
1:A:969:VAL:O	1:A:969:VAL:CG1	2.67	0.42
2:B:50:PHE:O	2:B:54:ILE:HG22	2.19	0.42
2:B:79:GLN:NE2	2:B:83:SER:OG	2.51	0.42
2:B:128:ASN:CG	2:B:155:TRP:HH2	2.23	0.42
2:B:209:LEU:O	2:B:237:GLY:HA3	2.18	0.42
1:C:142:TYR:C	1:C:142:TYR:CD2	2.91	0.42
1:C:667:THR:O	1:C:669:GLU:N	2.52	0.42
1:C:831:ASN:OD1	1:C:831:ASN:C	2.57	0.42
2:D:128:ASN:CG	2:D:155:TRP:HH2	2.22	0.42
1:A:71:ASN:O	1:A:72:ALA:HB2	2.19	0.42
1:A:779:GLU:OE1	1:A:800:ILE:HG23	2.19	0.42
1:A:793:LEU:HD12	1:A:793:LEU:C	2.40	0.42
1:A:831:ASN:HA	1:A:832:PRO:HD2	1.66	0.42
1:A:886:ARG:HB2	1:A:886:ARG:HH11	1.84	0.42
2:B:21:LYS:CA	2:B:22:LYS:HB2	2.44	0.42
2:B:209:LEU:O	2:B:237:GLY:CA	2.67	0.42
1:C:245:GLY:C	1:C:246:THR:HG22	2.40	0.42
1:C:295:LEU:O	1:C:296:GLY:C	2.55	0.42
1:C:301:ILE:O	1:C:305:ILE:HB	2.19	0.42
1:C:384:MET:HG2	1:C:582:ILE:HG12	2.01	0.42
1:C:808:ASP:OD2	1:C:923:GLN:NE2	2.51	0.42
2:D:60:THR:OG1	2:D:61:ILE:HG13	2.20	0.42
1:A:32:VAL:HG12	1:A:33:SER:H	1.85	0.42
1:A:52:LEU:C	1:A:54:ARG:H	2.23	0.42
1:A:64:ILE:O	1:A:64:ILE:CG2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:VAL:HG12	1:A:184:VAL:HG22	2.00	0.42
1:A:187:LYS:HG3	1:A:188:GLY:N	2.35	0.42
1:A:293:VAL:O	1:A:294:PHE:C	2.57	0.42
1:A:800:ILE:O	1:A:802:CYS:N	2.51	0.42
1:A:866:LEU:CD1	1:A:876:LEU:HD21	2.48	0.42
2:B:164:ASP:HB3	2:B:165:GLU:H	1.58	0.42
2:B:197:GLU:CD	2:B:279:TYR:OH	2.58	0.42
1:C:54:ARG:NH2	1:C:167:ASN:O	2.52	0.42
1:C:71:ASN:HB3	1:C:176:GLU:HA	2.02	0.42
1:C:100:GLY:O	1:C:101:ALA:C	2.57	0.42
1:C:795:LEU:HD13	1:C:915:PHE:CG	2.55	0.42
1:A:93:PHE:CZ	1:A:288:ILE:HD12	2.54	0.42
1:A:267:ALA:C	1:A:269:GLY:N	2.73	0.42
1:A:306:LEU:HD23	1:A:306:LEU:N	2.33	0.42
1:A:736:LYS:HG3	1:A:737:GLN:H	1.84	0.42
1:A:789:ALA:O	1:A:790:ASN:C	2.57	0.42
1:A:901:TYR:C	1:A:903:GLN:N	2.73	0.42
2:B:106:VAL:O	2:B:110:GLU:HB2	2.20	0.42
1:C:134:ILE:O	1:C:135:ILE:C	2.58	0.42
1:C:172:SER:O	1:C:173:ILE:CG2	2.64	0.42
1:C:514:ILE:HD12	1:C:527:LEU:HD12	2.02	0.42
1:C:926:ASP:C	1:C:928:VAL:H	2.23	0.42
2:D:21:LYS:CA	2:D:22:LYS:HB2	2.47	0.42
2:D:179:LYS:HD2	2:D:256:GLN:CD	2.40	0.42
1:A:120:ASN:O	1:A:121:ASP:O	2.38	0.42
1:A:551:LEU:HB2	1:A:576:LEU:HD23	2.02	0.42
1:A:893:ASP:OD2	1:A:895:TYR:N	2.49	0.42
1:C:506:ARG:NH1	1:C:506:ARG:CG	2.77	0.42
1:C:691:LYS:HE3	1:C:713:ASN:ND2	2.35	0.42
1:C:815:LEU:O	1:C:818:GLU:HB2	2.20	0.42
1:C:823:ASP:O	1:C:826:LYS:HB3	2.20	0.42
2:D:31:SER:CA	2:D:32:TRP:CB	2.86	0.42
1:A:329:LEU:HD11	1:A:769:ILE:HG13	2.01	0.42
1:A:360:LEU:O	1:A:363:THR:OG1	2.38	0.42
1:A:365:THR:HG23	1:A:605:LYS:HB3	2.00	0.42
1:A:435:ILE:CD1	1:A:438:ARG:NH2	2.80	0.42
1:A:705:VAL:O	1:A:722:ASP:HB2	2.20	0.42
1:A:812:ALA:C	1:A:814:SER:N	2.71	0.42
1:A:917:VAL:O	1:A:920:VAL:N	2.53	0.42
1:A:988:SER:O	1:A:991:ILE:HB	2.18	0.42
2:B:114:ASP:N	2:B:114:ASP:OD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:ASN:HA	1:C:229:PRO:HD3	1.93	0.42
1:C:318:ILE:O	1:C:318:ILE:CG2	2.67	0.42
1:C:453:ILE:HG23	1:C:457:CYS:HB2	2.01	0.42
1:C:944:ASN:C	1:C:946:ILE:H	2.21	0.42
2:D:23:GLU:O	2:D:25:LEU:N	2.52	0.42
2:D:74:PRO:HB2	2:D:292:GLN:NE2	2.34	0.42
2:D:80:ILE:HD12	2:D:80:ILE:HA	1.88	0.42
2:D:197:GLU:CD	2:D:279:TYR:OH	2.58	0.42
1:A:199:ILE:O	1:A:222:PRO:CG	2.65	0.42
1:A:263:ILE:HD11	1:A:688:PRO:HB2	2.02	0.42
1:A:329:LEU:HD12	1:A:332:THR:CG2	2.50	0.42
1:A:374:LEU:CD2	1:A:592:VAL:CG1	2.97	0.42
1:A:556:GLU:O	1:A:558:PHE:N	2.53	0.42
1:A:937:VAL:O	1:A:937:VAL:HG12	2.20	0.42
2:B:132:GLU:HA	2:B:207:TYR:CE1	2.54	0.42
1:C:94:SER:O	1:C:98:TRP:CD1	2.73	0.42
1:C:148:SER:O	1:C:148:SER:OG	2.31	0.42
1:C:265:THR:O	1:C:266:LEU:C	2.58	0.42
1:C:699:GLN:HG2	1:C:705:VAL:CG2	2.50	0.42
2:D:40:VAL:HG22	2:D:41:ILE:H	1.83	0.42
2:D:156:LEU:CD1	2:D:159:CYS:HB3	2.47	0.42
1:A:32:VAL:HG12	1:A:33:SER:N	2.35	0.42
1:A:60:ARG:O	1:A:60:ARG:CG	2.67	0.42
1:A:132:VAL:O	1:A:136:THR:HB	2.20	0.42
1:A:134:ILE:O	1:A:137:GLY:N	2.50	0.42
1:A:274:GLN:NE2	1:A:279:ALA:HB2	2.35	0.42
1:A:433:LEU:HD23	1:A:433:LEU:H	1.85	0.42
1:A:856:LEU:CD1	2:B:46:LEU:HD13	2.50	0.42
1:A:985:PHE:N	1:A:986:PRO:HD2	2.35	0.42
2:B:40:VAL:HG23	2:B:41:ILE:HD13	2.02	0.42
1:C:93:PHE:CE1	1:C:288:ILE:HG22	2.55	0.42
1:C:460:VAL:CG1	1:C:464:ARG:CD	2.94	0.42
1:C:637:ILE:HG22	1:C:638:ALA:N	2.34	0.42
1:C:960:PHE:C	1:C:962:SER:H	2.23	0.42
1:C:963:TYR:CD1	1:C:963:TYR:N	2.88	0.42
1:A:196:LEU:HA	1:A:196:LEU:HD23	1.72	0.42
1:A:341:ALA:C	1:A:343:ARG:N	2.72	0.42
1:A:354:LEU:C	1:A:356:ALA:H	2.23	0.42
1:A:385:TRP:CZ3	1:A:531:PHE:HB2	2.54	0.42
1:A:793:LEU:HD12	1:A:794:PRO:N	2.34	0.42
2:B:170:LYS:H	2:B:170:LYS:CD	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:GLY:O	1:C:138:CYS:C	2.57	0.42
1:C:662:ASP:O	1:C:666:MET:HG3	2.19	0.42
2:D:26:GLY:O	2:D:27:ARG:HB2	2.20	0.42
2:D:224:VAL:O	2:D:267:THR:CG2	2.68	0.42
1:A:82:TRP:O	1:A:83:VAL:C	2.58	0.41
1:A:514:ILE:HD13	1:A:527:LEU:HD12	2.02	0.41
1:A:889:ASN:O	1:A:899:TRP:O	2.37	0.41
2:B:188:PRO:CD	2:B:243:TYR:CD1	2.94	0.41
2:B:226:THR:HB	2:B:265:ASN:HA	2.00	0.41
1:C:119:GLN:C	1:C:121:ASP:N	2.74	0.41
1:C:325:VAL:O	1:C:325:VAL:HG12	2.20	0.41
1:C:385:TRP:CZ3	1:C:531:PHE:HB2	2.54	0.41
1:C:409:ALA:O	1:C:410:THR:C	2.58	0.41
1:C:521:GLN:HB3	1:C:522:PRO:CD	2.42	0.41
1:C:615:ILE:H	1:C:615:ILE:HG12	1.63	0.41
1:C:800:ILE:O	1:C:802:CYS:N	2.51	0.41
1:C:886:ARG:HB2	1:C:886:ARG:HH11	1.83	0.41
1:C:928:VAL:O	1:C:928:VAL:CG1	2.68	0.41
1:C:985:PHE:N	1:C:986:PRO:HD2	2.35	0.41
1:A:265:THR:HG22	1:A:266:LEU:H	1.82	0.41
1:A:329:LEU:C	1:A:331:ALA:N	2.73	0.41
1:A:654:LYS:HE2	1:A:654:LYS:CA	2.39	0.41
1:C:93:PHE:HZ	1:C:288:ILE:HG21	1.85	0.41
1:C:327:GLU:CD	1:C:327:GLU:H	2.24	0.41
1:C:508:LEU:O	1:C:510:ARG:N	2.52	0.41
1:C:512:SER:CB	1:C:575:ASN:HA	2.50	0.41
1:C:918:THR:HG22	1:C:984:ALA:HB2	2.02	0.41
1:A:622:LYS:HG2	1:A:627:ILE:HB	2.02	0.41
1:A:867:ALA:C	1:A:869:ASN:N	2.74	0.41
1:A:960:PHE:C	1:A:962:SER:H	2.23	0.41
2:B:21:LYS:HD2	2:B:22:LYS:CD	2.37	0.41
2:B:21:LYS:CD	2:B:22:LYS:CG	2.98	0.41
2:B:118:LYS:O	2:B:121:MET:O	2.39	0.41
1:C:203:GLY:O	1:C:245:GLY:HA3	2.20	0.41
1:C:283:HIS:O	1:C:286:HIS:N	2.53	0.41
1:C:523:LEU:HD22	1:C:528:LYS:CE	2.49	0.41
1:C:687:SER:HB2	1:C:690:GLN:HG3	2.02	0.41
1:C:723:ILE:O	1:C:723:ILE:HG23	2.19	0.41
1:C:872:LEU:HD23	1:C:872:LEU:HA	1.75	0.41
1:C:918:THR:O	1:C:922:VAL:HG22	2.19	0.41
2:D:208:VAL:HA	2:D:238:PHE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:SER:C	1:A:211:LEU:N	2.74	0.41
1:A:450:LEU:C	1:A:450:LEU:HD22	2.40	0.41
1:A:501:LYS:HA	1:A:547:GLY:O	2.20	0.41
1:A:573:LEU:C	1:A:574:ASP:OD1	2.59	0.41
1:A:857:GLY:N	1:A:987:TYR:CD1	2.88	0.41
1:A:926:ASP:O	1:A:928:VAL:N	2.52	0.41
1:C:180:VAL:CG2	1:C:254:THR:HG21	2.50	0.41
1:C:370:LYS:CB	1:C:608:MET:HE3	2.47	0.41
2:D:37:LEU:HG	2:D:38:PHE:N	2.34	0.41
2:D:130:PRO:HB2	2:D:204:TYR:CZ	2.56	0.41
2:D:178:ILE:HD12	2:D:259:MET:CE	2.51	0.41
2:D:209:LEU:HA	2:D:210:PRO:HD3	1.81	0.41
2:D:229:TYR:O	2:D:230:PHE:CD1	2.73	0.41
1:A:35:ASP:HB3	1:A:36:ASP:H	1.70	0.41
1:A:117:GLU:O	1:A:119:GLN:N	2.41	0.41
1:A:493:GLU:O	1:A:493:GLU:CG	2.66	0.41
1:A:523:LEU:HD22	1:A:528:LYS:CE	2.51	0.41
1:A:815:LEU:C	1:A:817:TYR:N	2.73	0.41
1:A:876:LEU:HD23	1:A:879:LEU:HD12	2.01	0.41
1:A:889:ASN:OD1	1:A:900:THR:HB	2.21	0.41
1:C:209:SER:C	1:C:211:LEU:N	2.73	0.41
1:C:216:GLU:O	1:C:218:GLN:NE2	2.54	0.41
1:C:374:LEU:HA	1:C:374:LEU:HD23	1.69	0.41
1:C:378:ARG:NH2	1:C:436:LEU:HD22	2.35	0.41
1:C:442:GLY:O	1:C:443:ASP:HB3	2.20	0.41
1:C:952:PHE:HB3	3:H:37:ALA:O	2.20	0.41
1:A:154:PHE:HE2	1:A:734:VAL:HG11	1.84	0.41
1:A:329:LEU:HD12	1:A:332:THR:HG22	2.02	0.41
1:A:476:ASN:HB2	1:A:479:ASN:OD1	2.20	0.41
1:A:854:GLN:HG2	1:A:991:ILE:CD1	2.49	0.41
1:A:978:PRO:O	1:A:979:THR:C	2.59	0.41
2:B:198:THR:O	2:B:203:LYS:HE2	2.20	0.41
1:C:50:THR:O	1:C:51:ASP:O	2.38	0.41
1:C:162:ALA:O	1:C:172:SER:HA	2.20	0.41
1:C:199:ILE:H	1:C:199:ILE:HG13	1.66	0.41
1:C:440:VAL:CG1	1:C:451:LYS:HE3	2.50	0.41
1:C:616:THR:O	1:C:617:ALA:C	2.59	0.41
1:C:743:LEU:HD11	1:C:751:ILE:CD1	2.50	0.41
1:C:845:MET:SD	1:C:1014:THR:HG22	2.61	0.41
1:C:855:ALA:O	1:C:858:GLY:N	2.52	0.41
1:C:921:VAL:O	1:C:988:SER:OG	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:117:GLN:HG2	2:D:123:PHE:HE1	1.86	0.41
1:A:106:LEU:HG	1:A:107:ALA:N	2.35	0.41
1:A:110:ILE:HD12	1:A:311:LEU:CD2	2.51	0.41
1:A:159:PRO:HG3	1:A:191:ARG:HB2	2.02	0.41
1:A:500:MET:HG3	1:A:549:CYS:SG	2.60	0.41
1:A:571:PHE:HB2	1:A:572:PRO:CD	2.50	0.41
1:A:853:ILE:CG2	1:A:990:LEU:HD13	2.50	0.41
1:A:872:LEU:HD23	1:A:872:LEU:HA	1.75	0.41
2:B:38:PHE:O	2:B:39:TYR:HD1	2.04	0.41
1:C:616:THR:O	1:C:619:ALA:N	2.53	0.41
1:C:627:ILE:HA	1:C:680:GLU:OE1	2.20	0.41
1:C:788:ILE:HD13	1:C:788:ILE:HA	1.84	0.41
2:D:38:PHE:O	2:D:39:TYR:HD1	2.03	0.41
2:D:98:TYR:HA	2:D:101:TYR:HD2	1.84	0.41
2:D:214:THR:O	2:D:274:ILE:HG13	2.20	0.41
2:D:245:TYR:CD1	2:D:247:GLY:N	2.89	0.41
1:A:83:VAL:HG13	1:A:87:ARG:CG	2.51	0.41
1:A:162:ALA:O	1:A:172:SER:HA	2.21	0.41
1:A:374:LEU:HD22	1:A:592:VAL:HG11	2.02	0.41
1:A:460:VAL:CG1	1:A:464:ARG:CD	2.95	0.41
1:A:633:THR:HG22	1:A:636:ASP:OD2	2.20	0.41
2:B:272:ILE:HD11	2:B:299:ILE:HG13	2.02	0.41
1:C:769:ILE:O	1:C:770:ALA:C	2.58	0.41
1:C:885:ASP:CG	1:C:888:ILE:HG13	2.41	0.41
1:C:893:ASP:OD2	1:C:895:TYR:N	2.48	0.41
1:C:928:VAL:O	1:C:928:VAL:HG12	2.20	0.41
2:D:83:SER:HB3	2:D:86:THR:N	2.34	0.41
1:A:47:LYS:HG2	1:A:48:TYR:CD2	2.55	0.41
1:A:142:TYR:HE2	1:A:338:THR:HG23	1.78	0.41
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.62	0.41
1:A:174:ASN:O	1:A:177:GLU:HG3	2.20	0.41
1:A:254:THR:HG23	1:A:257:ARG:HE	1.86	0.41
1:A:321:ILE:O	1:A:324:ASN:N	2.35	0.41
1:A:361:GLY:C	1:A:363:THR:H	2.23	0.41
1:A:445:SER:O	1:A:446:GLU:C	2.59	0.41
1:A:609:VAL:HG12	1:A:691:LYS:HG2	1.99	0.41
1:A:699:GLN:HG2	1:A:705:VAL:CG2	2.51	0.41
1:A:742:ILE:HG22	1:A:744:LEU:HD23	2.02	0.41
1:A:796:GLY:O	1:A:799:THR:HG22	2.21	0.41
1:A:815:LEU:O	1:A:818:GLU:HB2	2.21	0.41
1:A:874:ILE:O	1:A:876:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:TYR:O	1:A:903:GLN:N	2.54	0.41
2:B:133:LEU:CD2	2:B:240:LEU:HB3	2.50	0.41
2:B:152:ARG:C	2:B:154:GLU:N	2.73	0.41
1:C:71:ASN:OD1	1:C:255:GLY:N	2.54	0.41
1:C:95:MET:O	1:C:99:ILE:HG12	2.21	0.41
1:C:96:LEU:HD11	1:C:292:ALA:HB1	2.01	0.41
1:C:98:TRP:CZ2	1:C:133:VAL:CG1	2.95	0.41
1:C:129:LEU:CD2	1:C:801:LEU:HD11	2.49	0.41
1:C:158:VAL:CG2	1:C:159:PRO:N	2.83	0.41
1:C:277:ILE:C	1:C:279:ALA:H	2.22	0.41
1:C:353:ASN:O	1:C:356:ALA:HB3	2.21	0.41
1:C:571:PHE:HE1	1:C:573:LEU:HD21	1.86	0.41
1:C:628:SER:O	1:C:631:ASN:HB2	2.21	0.41
1:C:715:SER:O	1:C:719:LYS:N	2.54	0.41
1:C:918:THR:CG2	1:C:984:ALA:HB2	2.51	0.41
2:D:21:LYS:HD3	2:D:22:LYS:CD	2.50	0.41
2:D:51:ILE:HA	2:D:54:ILE:HG22	2.02	0.41
2:D:61:ILE:O	2:D:62:SER:C	2.59	0.41
2:D:138:GLU:C	2:D:140:ASN:H	2.24	0.41
2:D:198:THR:O	2:D:203:LYS:HE2	2.21	0.41
2:D:247:GLY:C	2:D:249:LEU:H	2.24	0.41
2:D:251:GLN:C	2:D:252:PRO:O	2.58	0.41
1:A:54:ARG:NH2	1:A:167:ASN:O	2.54	0.41
1:A:82:TRP:O	1:A:84:LYS:N	2.54	0.41
1:A:115:GLU:O	1:A:117:GLU:HG3	2.21	0.41
1:A:793:LEU:HD11	1:A:795:LEU:O	2.21	0.41
1:A:865:ILE:HD13	1:A:980:TRP:CE2	2.56	0.41
1:A:919:ILE:HA	1:A:922:VAL:HG22	2.03	0.41
1:A:932:THR:HG23	1:A:999:LYS:NZ	2.35	0.41
2:B:88:ILE:HD11	2:B:299:ILE:CG2	2.46	0.41
2:B:138:GLU:C	2:B:140:ASN:H	2.24	0.41
1:C:291:VAL:HG23	1:C:324:ASN:OD1	2.21	0.41
1:C:319:GLY:O	1:C:320:ILE:C	2.60	0.41
1:C:501:LYS:HA	1:C:547:GLY:O	2.21	0.41
1:C:502:GLY:O	1:C:503:ALA:C	2.59	0.41
1:C:504:PRO:HG2	1:C:545:VAL:HG12	2.03	0.41
1:C:569:VAL:CG1	1:C:570:ASN:N	2.69	0.41
1:C:692:LEU:O	1:C:693:ILE:C	2.57	0.41
1:C:776:ASN:O	1:C:779:GLU:HB2	2.21	0.41
1:A:172:SER:O	1:A:173:ILE:CG2	2.67	0.40
1:A:195:ASP:C	1:A:196:LEU:HD23	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:VAL:HA	1:A:338:THR:OG1	2.21	0.40
1:A:431:GLU:H	1:A:431:GLU:CD	2.24	0.40
1:A:460:VAL:HG13	1:A:464:ARG:HD3	2.01	0.40
1:A:808:ASP:OD2	1:A:923:GLN:NE2	2.54	0.40
2:B:119:ASP:C	2:B:121:MET:N	2.73	0.40
3:G:45:LEU:C	3:G:47:SER:H	2.25	0.40
1:C:119:GLN:C	1:C:121:ASP:H	2.23	0.40
1:C:493:GLU:O	1:C:495:ARG:HG3	2.21	0.40
1:C:755:VAL:HG13	1:C:825:MET:CE	2.51	0.40
1:C:793:LEU:HA	1:C:794:PRO:HD3	1.94	0.40
1:C:865:ILE:HD13	1:C:980:TRP:CE2	2.57	0.40
2:D:46:LEU:HD22	2:D:46:LEU:HA	1.93	0.40
2:D:152:ARG:C	2:D:154:GLU:N	2.74	0.40
1:A:61:ALA:O	1:A:63:GLU:N	2.54	0.40
1:A:93:PHE:HB3	1:A:325:VAL:HG13	2.04	0.40
1:A:104:CYS:SG	1:A:125:LEU:HB3	2.61	0.40
1:A:288:ILE:HG22	1:A:289:THR:H	1.83	0.40
1:A:385:TRP:HB2	1:A:581:LEU:HB2	2.03	0.40
1:A:546:LEU:HD23	1:A:546:LEU:HA	1.76	0.40
1:A:919:ILE:HA	1:A:919:ILE:HD13	1.78	0.40
2:B:251:GLN:OE1	2:B:254:TYR:HD2	2.03	0.40
2:B:272:ILE:N	2:B:272:ILE:CD1	2.84	0.40
1:C:93:PHE:HE1	1:C:288:ILE:HG22	1.87	0.40
1:C:117:GLU:O	1:C:119:GLN:N	2.54	0.40
1:C:288:ILE:CD1	1:C:773:LEU:HD11	2.49	0.40
1:C:613:HIS:HA	1:C:614:PRO:HD3	1.90	0.40
1:C:633:THR:HG22	1:C:636:ASP:OD2	2.22	0.40
1:C:697:GLY:HA2	1:C:700:ARG:HB2	2.03	0.40
1:C:777:ILE:HA	1:C:777:ILE:HD13	1.64	0.40
1:C:778:PRO:HG3	1:C:919:ILE:HD11	2.03	0.40
1:C:895:TYR:HE2	2:D:66:PRO:HA	1.86	0.40
1:C:984:ALA:O	1:C:987:TYR:N	2.53	0.40
1:A:857:GLY:HA2	1:A:987:TYR:CD1	2.56	0.40
2:B:245:TYR:CD1	2:B:247:GLY:N	2.89	0.40
1:C:165:ILE:H	1:C:165:ILE:HG12	1.65	0.40
1:C:574:ASP:C	1:C:576:LEU:H	2.24	0.40
1:C:895:TYR:O	2:D:248:LYS:N	2.43	0.40
2:D:132:GLU:O	2:D:241:GLN:HA	2.22	0.40
1:A:791:ILE:HG23	1:A:792:PRO:N	2.37	0.40
1:A:864:VAL:O	1:A:868:GLU:HB2	2.21	0.40
1:A:905:LYS:C	1:A:907:VAL:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:906:ILE:O	1:A:906:ILE:HG22	2.22	0.40
2:B:61:ILE:O	2:B:62:SER:C	2.60	0.40
2:B:79:GLN:HB2	2:B:81:PRO:HD2	2.03	0.40
2:B:81:PRO:CG	2:B:176:VAL:HG13	2.52	0.40
1:C:90:PHE:CD2	1:C:90:PHE:N	2.89	0.40
1:C:123:LEU:HD23	1:C:123:LEU:C	2.42	0.40
1:C:129:LEU:HD11	1:C:322:VAL:HG21	2.02	0.40
1:C:159:PRO:HG3	1:C:191:ARG:HB2	2.03	0.40
1:C:290:GLY:O	1:C:291:VAL:C	2.59	0.40
1:C:515:LEU:O	1:C:516:ILE:HG13	2.21	0.40
1:A:139:PHE:HD1	1:A:331:ALA:HB1	1.79	0.40
1:A:332:THR:HG22	1:A:333:VAL:N	2.35	0.40
1:A:384:MET:HG2	1:A:582:ILE:HG12	2.04	0.40
1:A:495:ARG:O	1:A:496:HIS:CD2	2.75	0.40
1:A:550:HIS:CD2	1:A:577:CYS:HB3	2.55	0.40
1:A:598:LYS:O	1:A:600:ARG:N	2.55	0.40
1:A:982:PHE:HA	1:A:985:PHE:CE2	2.56	0.40
2:B:183:VAL:HB	2:B:186:PHE:HB2	2.04	0.40
2:B:270:THR:HG22	2:B:272:ILE:HG23	2.04	0.40
1:C:114:THR:HG22	1:C:115:GLU:H	1.87	0.40
1:C:165:ILE:HG13	1:C:183:LEU:CD2	2.40	0.40
1:C:370:LYS:HG3	1:C:620:ILE:HG21	2.02	0.40
1:C:550:HIS:CD2	1:C:577:CYS:HB3	2.56	0.40
1:C:609:VAL:HG22	1:C:694:ILE:HD12	2.03	0.40
1:C:637:ILE:O	1:C:640:ARG:N	2.34	0.40
1:C:906:ILE:O	1:C:906:ILE:CG2	2.69	0.40
2:D:51:ILE:O	2:D:54:ILE:HG22	2.22	0.40
2:D:152:ARG:O	2:D:155:TRP:HD1	1.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	996/998 (100%)	665 (67%)	199 (20%)	132 (13%)	0	4
1	C	996/998 (100%)	671 (67%)	196 (20%)	129 (13%)	0	4
2	B	284/286 (99%)	182 (64%)	68 (24%)	34 (12%)	0	5
2	D	284/286 (99%)	183 (64%)	70 (25%)	31 (11%)	0	6
3	G	25/27 (93%)	22 (88%)	3 (12%)	0	100	100
3	H	25/27 (93%)	21 (84%)	4 (16%)	0	100	100
All	All	2610/2622 (100%)	1744 (67%)	540 (21%)	326 (12%)	0	5

All (326) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	45	HIS
1	A	51	ASP
1	A	70	PRO
1	A	83	VAL
1	A	106	LEU
1	A	107	ALA
1	A	121	ASP
1	A	146	LYS
1	A	210	SER
1	A	258	THR
1	A	265	THR
1	A	268	SER
1	A	288	ILE
1	A	289	THR
1	A	309	THR
1	A	321	ILE
1	A	338	THR
1	A	403	SER
1	A	405	ASP
1	A	406	LYS
1	A	444	ALA
1	A	463	MET
1	A	493	GLU
1	A	495	ARG
1	A	524	ASP
1	A	557	GLN
1	A	685	ARG
1	A	700	ARG
1	A	737	GLN

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Mol	Chain	Res	Type
1	A	743	LEU
1	A	790	ASN
1	A	832	PRO
1	A	871	PHE
1	A	913	THR
2	B	23	GLU
2	B	31	SER
2	B	62	SER
2	B	73	ALA
2	B	74	PRO
2	B	93	ASN
2	B	136	ARG
2	B	202	MET
2	B	204	TYR
2	B	302	LYS
1	C	44	LEU
1	C	45	HIS
1	C	51	ASP
1	C	70	PRO
1	C	121	ASP
1	C	210	SER
1	C	258	THR
1	C	265	THR
1	C	268	SER
1	C	403	SER
1	C	405	ASP
1	C	406	LYS
1	C	444	ALA
1	C	463	MET
1	C	493	GLU
1	C	495	ARG
1	C	496	HIS
1	C	524	ASP
1	C	685	ARG
1	C	700	ARG
1	C	737	GLN
1	C	790	ASN
1	C	832	PRO
1	C	871	PHE
1	C	913	THR
2	D	23	GLU
2	D	31	SER

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Mol	Chain	Res	Type
2	D	62	SER
2	D	73	ALA
2	D	74	PRO
2	D	93	ASN
2	D	136	ARG
2	D	202	MET
2	D	204	TYR
1	A	21	LYS
1	A	52	LEU
1	A	72	ALA
1	A	82	TRP
1	A	115	GLU
1	A	135	ILE
1	A	138	CYS
1	A	139	PHE
1	A	142	TYR
1	A	223	ASP
1	A	239	SER
1	A	266	LEU
1	A	282	GLU
1	A	296	GLY
1	A	327	GLU
1	A	355	GLU
1	A	399	GLN
1	A	400	SER
1	A	401	GLY
1	A	412	LEU
1	A	453	ILE
1	A	492	ALA
1	A	496	HIS
1	A	642	ASN
1	A	646	SER
1	A	731	GLY
1	A	734	VAL
1	A	735	SER
1	A	801	LEU
1	A	809	MET
1	A	844	SER
1	A	850	ILE
1	A	860	PHE
1	A	877	LEU
1	A	916	PHE

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Mol	Chain	Res	Type
1	A	954	GLU
1	A	979	THR
1	A	991	ILE
2	B	22	LYS
2	B	60	THR
2	B	61	ILE
2	B	82	GLN
2	B	145	GLU
2	B	170	LYS
2	B	174	PRO
2	B	220	ASP
2	B	296	ASP
1	C	21	LYS
1	C	52	LEU
1	C	72	ALA
1	C	82	TRP
1	C	91	GLY
1	C	97	LEU
1	C	114	THR
1	C	152	GLU
1	C	223	ASP
1	C	239	SER
1	C	266	LEU
1	C	275	THR
1	C	289	THR
1	C	296	GLY
1	C	307	GLU
1	C	308	TYR
1	C	340	THR
1	C	355	GLU
1	C	399	GLN
1	C	400	SER
1	C	401	GLY
1	C	412	LEU
1	C	492	ALA
1	C	557	GLN
1	C	570	ASN
1	C	617	ALA
1	C	642	ASN
1	C	646	SER
1	C	731	GLY
1	C	734	VAL

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Mol	Chain	Res	Type
1	C	735	SER
1	C	743	LEU
1	C	801	LEU
1	C	830	ARG
1	C	850	ILE
1	C	877	LEU
1	C	954	GLU
1	C	979	THR
1	C	991	ILE
2	D	22	LYS
2	D	60	THR
2	D	61	ILE
2	D	82	GLN
2	D	145	GLU
2	D	170	LYS
2	D	174	PRO
2	D	220	ASP
2	D	302	LYS
1	A	89	LEU
1	A	116	GLU
1	A	128	VAL
1	A	295	LEU
1	A	300	PHE
1	A	330	LEU
1	A	342	LYS
1	A	404	PHE
1	A	454	GLU
1	A	504	PRO
1	A	509	ASP
1	A	570	ASN
1	A	599	CYS
1	A	617	ALA
1	A	629	GLU
1	A	668	SER
1	A	830	ARG
1	A	835	ASP
1	A	875	HIS
1	A	912	HIS
1	A	914	PRO
1	A	953	GLU
1	A	978	PRO
2	B	24	PHE

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Mol	Chain	Res	Type
2	B	158	ASN
2	B	200	PRO
1	C	29	LYS
1	C	87	ARG
1	C	92	GLY
1	C	115	GLU
1	C	119	GLN
1	C	146	LYS
1	C	175	ALA
1	C	276	PRO
1	C	404	PHE
1	C	504	PRO
1	C	509	ASP
1	C	599	CYS
1	C	629	GLU
1	C	668	SER
1	C	715	SER
1	C	809	MET
1	C	816	ALA
1	C	835	ASP
1	C	860	PHE
1	C	875	HIS
1	C	912	HIS
1	C	914	PRO
1	C	916	PHE
1	C	951	LEU
1	C	978	PRO
2	D	24	PHE
2	D	158	ASN
2	D	200	PRO
2	D	223	LYS
2	D	296	ASP
1	A	23	ARG
1	A	359	THR
1	A	387	ASP
1	A	490	ASN
1	A	554	PRO
1	A	816	ALA
1	A	945	LYS
2	B	53	THR
2	B	206	PRO
2	B	223	LYS

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Mol	Chain	Res	Type
2	B	251	GLN
1	C	23	ARG
1	C	62	ALA
1	C	116	GLU
1	C	201	ALA
1	C	453	ILE
1	C	454	GLU
1	C	710	ASP
1	C	788	ILE
1	C	819	GLN
1	C	945	LYS
1	C	953	GLU
2	D	206	PRO
1	A	322	VAL
1	A	489	PRO
1	A	715	SER
1	A	730	ALA
1	A	788	ILE
1	A	823	ASP
1	A	951	LEU
1	A	1001	ILE
2	B	41	ILE
2	B	42	PHE
2	B	80	ILE
2	B	139	TYR
1	C	321	ILE
1	C	359	THR
1	C	387	ASP
1	C	422	ASN
1	C	489	PRO
1	C	554	PRO
1	C	730	ALA
1	C	893	ASP
1	C	900	THR
1	C	1001	ILE
2	D	42	PHE
2	D	80	ILE
2	D	139	TYR
2	D	251	GLN
1	A	47	LYS
1	A	80	PRO
1	A	825	MET

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Mol	Chain	Res	Type
1	A	893	ASP
1	A	900	THR
1	A	906	ILE
1	A	965	PRO
1	C	47	LYS
1	C	125	LEU
1	C	287	ILE
1	C	649	ASN
1	C	965	PRO
2	D	41	ILE
1	A	180	VAL
1	A	873	PRO
1	A	888	ILE
1	C	135	ILE
1	C	569	VAL
1	C	1002	ILE
2	D	66	PRO
1	A	134	ILE
1	C	318	ILE
1	C	693	ILE
1	C	873	PRO
1	C	888	ILE
1	A	92	GLY
1	A	118	PRO
1	A	269	GLY
1	A	435	ILE
1	A	742	ILE
1	A	1002	ILE
2	B	173	LYS
1	C	435	ILE
1	C	593	PRO
2	D	173	LYS
1	A	318	ILE
1	A	569	VAL
1	A	782	PRO
2	B	29	GLY
2	B	52	GLY
1	C	180	VAL
1	C	660	GLY
1	C	695	VAL
1	C	742	ILE
1	C	906	ILE

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Mol	Chain	Res	Type
1	A	649	ASN
2	B	66	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	848/848 (100%)	654 (77%)	194 (23%)	1 4
1	C	848/848 (100%)	653 (77%)	195 (23%)	1 4
2	B	256/256 (100%)	213 (83%)	43 (17%)	2 12
2	D	256/256 (100%)	214 (84%)	42 (16%)	2 13
3	G	21/21 (100%)	20 (95%)	1 (5%)	25 60
3	H	21/21 (100%)	20 (95%)	1 (5%)	25 60
All	All	2250/2250 (100%)	1774 (79%)	476 (21%)	1 5

All (476) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	MET
1	A	26	ASP
1	A	27	GLU
1	A	33	SER
1	A	34	MET
1	A	37	HIS
1	A	46	ARG
1	A	50	THR
1	A	52	LEU
1	A	57	THR
1	A	60	ARG
1	A	64	ILE
1	A	65	LEU
1	A	68	ASP
1	A	70	PRO
1	A	73	LEU

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Mol	Chain	Res	Type
1	A	74	THR
1	A	78	THR
1	A	87	ARG
1	A	110	ILE
1	A	114	THR
1	A	115	GLU
1	A	123	LEU
1	A	125	LEU
1	A	133	VAL
1	A	134	ILE
1	A	136	THR
1	A	143	GLN
1	A	144	GLU
1	A	146	LYS
1	A	150	ILE
1	A	151	MET
1	A	153	SER
1	A	158	VAL
1	A	161	GLN
1	A	163	LEU
1	A	165	ILE
1	A	169	GLU
1	A	187	LYS
1	A	197	ARG
1	A	198	ILE
1	A	199	ILE
1	A	200	SER
1	A	206	VAL
1	A	210	SER
1	A	211	LEU
1	A	214	GLU
1	A	224	PHE
1	A	225	THR
1	A	226	ASN
1	A	227	GLU
1	A	232	THR
1	A	233	ARG
1	A	238	PHE
1	A	241	ASN
1	A	243	VAL
1	A	246	THR
1	A	251	VAL

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Mol	Chain	Res	Type
1	A	256	ASP
1	A	260	MET
1	A	266	LEU
1	A	268	SER
1	A	271	GLU
1	A	275	THR
1	A	284	PHE
1	A	297	VAL
1	A	298	SER
1	A	299	PHE
1	A	304	LEU
1	A	305	ILE
1	A	309	THR
1	A	310	TRP
1	A	311	LEU
1	A	315	ILE
1	A	321	ILE
1	A	324	ASN
1	A	330	LEU
1	A	332	THR
1	A	333	VAL
1	A	334	THR
1	A	335	VAL
1	A	337	LEU
1	A	338	THR
1	A	365	THR
1	A	371	THR
1	A	376	GLN
1	A	380	THR
1	A	384	MET
1	A	385	TRP
1	A	395	THR
1	A	397	GLU
1	A	402	VAL
1	A	412	LEU
1	A	415	SER
1	A	420	LEU
1	A	433	LEU
1	A	436	LEU
1	A	450	LEU
1	A	468	THR
1	A	469	LYS

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Mol	Chain	Res	Type
1	A	470	ILE
1	A	471	VAL
1	A	475	PHE
1	A	477	SER
1	A	478	THR
1	A	479	ASN
1	A	481	TYR
1	A	485	ILE
1	A	490	ASN
1	A	491	THR
1	A	498	LEU
1	A	501	LYS
1	A	505	GLU
1	A	506	ARG
1	A	507	ILE
1	A	510	ARG
1	A	515	LEU
1	A	526	GLU
1	A	531	PHE
1	A	533	ASN
1	A	537	GLU
1	A	538	LEU
1	A	550	HIS
1	A	566	THR
1	A	584	MET
1	A	596	VAL
1	A	605	LYS
1	A	606	VAL
1	A	615	ILE
1	A	620	ILE
1	A	633	THR
1	A	634	VAL
1	A	635	GLU
1	A	637	ILE
1	A	646	SER
1	A	663	LEU
1	A	667	THR
1	A	671	LEU
1	A	673	ASP
1	A	675	LEU
1	A	686	THR
1	A	700	ARG

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Mol	Chain	Res	Type
1	A	705	VAL
1	A	708	THR
1	A	712	VAL
1	A	715	SER
1	A	718	SER
1	A	719	LYS
1	A	723	ILE
1	A	729	ILE
1	A	747	ASN
1	A	753	THR
1	A	756	GLU
1	A	761	ILE
1	A	774	THR
1	A	776	ASN
1	A	780	ILE
1	A	781	THR
1	A	784	LEU
1	A	785	ILE
1	A	791	ILE
1	A	798	VAL
1	A	799	THR
1	A	803	ILE
1	A	804	ASP
1	A	807	THR
1	A	814	SER
1	A	824	ILE
1	A	825	MET
1	A	835	ASP
1	A	853	ILE
1	A	862	TYR
1	A	869	ASN
1	A	871	PHE
1	A	880	ARG
1	A	881	VAL
1	A	894	SER
1	A	911	CYS
1	A	915	PHE
1	A	919	ILE
1	A	932	THR
1	A	933	ARG
1	A	934	ARG
1	A	946	ILE

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Mol	Chain	Res	Type
1	A	947	LEU
1	A	957	LEU
1	A	972	ARG
1	A	979	THR
1	A	980	TRP
1	A	982	PHE
1	A	990	LEU
1	A	992	PHE
1	A	1000	LEU
1	A	1015	TYR
2	B	28	THR
2	B	37	LEU
2	B	39	TYR
2	B	46	LEU
2	B	51	ILE
2	B	56	VAL
2	B	57	MET
2	B	60	THR
2	B	67	THR
2	B	72	VAL
2	B	77	LEU
2	B	78	THR
2	B	82	GLN
2	B	83	SER
2	B	88	ILE
2	B	94	ASP
2	B	123	PHE
2	B	145	GLU
2	B	153	LEU
2	B	156	LEU
2	B	162	LEU
2	B	170	LYS
2	B	173	LYS
2	B	177	ILE
2	B	178	ILE
2	B	182	ARG
2	B	184	LEU
2	B	198	THR
2	B	204	TYR
2	B	216	LYS
2	B	221	LYS
2	B	222	GLU

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Mol	Chain	Res	Type
2	B	245	TYR
2	B	249	LEU
2	B	250	LEU
2	B	251	GLN
2	B	256	GLN
2	B	267	THR
2	B	272	ILE
2	B	276	CYS
2	B	294	ARG
2	B	295	PHE
2	B	299	ILE
3	G	23	TYR
1	C	25	MET
1	C	26	ASP
1	C	27	GLU
1	C	33	SER
1	C	34	MET
1	C	37	HIS
1	C	46	ARG
1	C	50	THR
1	C	52	LEU
1	C	57	THR
1	C	60	ARG
1	C	64	ILE
1	C	65	LEU
1	C	68	ASP
1	C	70	PRO
1	C	73	LEU
1	C	74	THR
1	C	78	THR
1	C	79	THR
1	C	87	ARG
1	C	99	ILE
1	C	114	THR
1	C	115	GLU
1	C	125	LEU
1	C	129	LEU
1	C	136	THR
1	C	139	PHE
1	C	141	TYR
1	C	142	TYR
1	C	144	GLU

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Mol	Chain	Res	Type
1	C	146	LYS
1	C	150	ILE
1	C	151	MET
1	C	158	VAL
1	C	163	LEU
1	C	165	ILE
1	C	169	GLU
1	C	187	LYS
1	C	197	ARG
1	C	198	ILE
1	C	199	ILE
1	C	200	SER
1	C	206	VAL
1	C	210	SER
1	C	211	LEU
1	C	214	GLU
1	C	216	GLU
1	C	224	PHE
1	C	225	THR
1	C	226	ASN
1	C	227	GLU
1	C	232	THR
1	C	233	ARG
1	C	238	PHE
1	C	241	ASN
1	C	243	VAL
1	C	246	THR
1	C	251	VAL
1	C	256	ASP
1	C	260	MET
1	C	266	LEU
1	C	268	SER
1	C	271	GLU
1	C	276	PRO
1	C	284	PHE
1	C	287	ILE
1	C	288	ILE
1	C	289	THR
1	C	293	VAL
1	C	305	ILE
1	C	309	THR
1	C	311	LEU

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Mol	Chain	Res	Type
1	C	315	ILE
1	C	320	ILE
1	C	324	ASN
1	C	330	LEU
1	C	336	CYS
1	C	337	LEU
1	C	338	THR
1	C	365	THR
1	C	371	THR
1	C	376	GLN
1	C	380	THR
1	C	384	MET
1	C	385	TRP
1	C	395	THR
1	C	397	GLU
1	C	402	VAL
1	C	412	LEU
1	C	415	SER
1	C	420	LEU
1	C	433	LEU
1	C	436	LEU
1	C	450	LEU
1	C	468	THR
1	C	469	LYS
1	C	470	ILE
1	C	471	VAL
1	C	475	PHE
1	C	477	SER
1	C	478	THR
1	C	479	ASN
1	C	481	TYR
1	C	485	ILE
1	C	490	ASN
1	C	491	THR
1	C	498	LEU
1	C	501	LYS
1	C	505	GLU
1	C	506	ARG
1	C	507	ILE
1	C	510	ARG
1	C	515	LEU
1	C	526	GLU

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Mol	Chain	Res	Type
1	C	531	PHE
1	C	533	ASN
1	C	537	GLU
1	C	538	LEU
1	C	550	HIS
1	C	558	PHE
1	C	566	THR
1	C	574	ASP
1	C	584	MET
1	C	596	VAL
1	C	605	LYS
1	C	606	VAL
1	C	615	ILE
1	C	620	ILE
1	C	633	THR
1	C	634	VAL
1	C	635	GLU
1	C	637	ILE
1	C	643	ILE
1	C	646	SER
1	C	663	LEU
1	C	667	THR
1	C	671	LEU
1	C	673	ASP
1	C	675	LEU
1	C	686	THR
1	C	700	ARG
1	C	705	VAL
1	C	707	VAL
1	C	708	THR
1	C	712	VAL
1	C	715	SER
1	C	718	SER
1	C	719	LYS
1	C	723	ILE
1	C	729	ILE
1	C	747	ASN
1	C	753	THR
1	C	756	GLU
1	C	761	ILE
1	C	774	THR
1	C	776	ASN

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Mol	Chain	Res	Type
1	C	777	ILE
1	C	780	ILE
1	C	784	LEU
1	C	785	ILE
1	C	791	ILE
1	C	798	VAL
1	C	799	THR
1	C	803	ILE
1	C	804	ASP
1	C	807	THR
1	C	814	SER
1	C	824	ILE
1	C	825	MET
1	C	835	ASP
1	C	853	ILE
1	C	862	TYR
1	C	869	ASN
1	C	871	PHE
1	C	880	ARG
1	C	881	VAL
1	C	894	SER
1	C	911	CYS
1	C	915	PHE
1	C	919	ILE
1	C	932	THR
1	C	933	ARG
1	C	934	ARG
1	C	946	ILE
1	C	947	LEU
1	C	957	LEU
1	C	972	ARG
1	C	979	THR
1	C	980	TRP
1	C	982	PHE
1	C	990	LEU
1	C	992	PHE
1	C	1000	LEU
1	C	1014	THR
1	C	1015	TYR
2	D	28	THR
2	D	37	LEU
2	D	39	TYR

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Mol	Chain	Res	Type
2	D	46	LEU
2	D	51	ILE
2	D	56	VAL
2	D	57	MET
2	D	60	THR
2	D	67	THR
2	D	72	VAL
2	D	77	LEU
2	D	78	THR
2	D	82	GLN
2	D	83	SER
2	D	88	ILE
2	D	94	ASP
2	D	123	PHE
2	D	145	GLU
2	D	153	LEU
2	D	156	LEU
2	D	162	LEU
2	D	170	LYS
2	D	173	LYS
2	D	177	ILE
2	D	178	ILE
2	D	182	ARG
2	D	184	LEU
2	D	198	THR
2	D	204	TYR
2	D	216	LYS
2	D	221	LYS
2	D	222	GLU
2	D	245	TYR
2	D	249	LEU
2	D	250	LEU
2	D	251	GLN
2	D	256	GLN
2	D	267	THR
2	D	272	ILE
2	D	276	CYS
2	D	295	PHE
2	D	299	ILE
3	H	23	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	218	GLN
1	A	226	ASN
1	A	241	ASN
1	A	427	GLN
1	A	432	ASN
1	A	533	ASN
1	A	550	HIS
1	A	570	ASN
1	A	613	HIS
1	A	713	ASN
1	A	747	ASN
1	A	790	ASN
1	A	875	HIS
1	A	912	HIS
2	B	79	GLN
2	B	82	GLN
2	B	84	GLN
2	B	158	ASN
2	B	256	GLN
2	B	262	GLN
2	B	265	ASN
2	B	292	GLN
1	C	111	GLN
1	C	218	GLN
1	C	226	ASN
1	C	241	ASN
1	C	286	HIS
1	C	324	ASN
1	C	427	GLN
1	C	432	ASN
1	C	496	HIS
1	C	533	ASN
1	C	550	HIS
1	C	570	ASN
1	C	613	HIS
1	C	713	ASN
1	C	747	ASN
1	C	790	ASN
1	C	875	HIS
1	C	912	HIS
2	D	82	GLN
2	D	84	GLN

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Mol	Chain	Res	Type
2	D	158	ASN
2	D	256	GLN
2	D	262	GLN
2	D	265	ASN
2	D	292	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	MF4	C	2001	1	0,4,4	-	-	-		
7	CLR	D	3001	-	31,31,31	1.91	3 (9%)	48,48,48	2.25	13 (27%)
4	MF4	A	2001	1	0,4,4	-	-	-		
7	CLR	B	3001	-	31,31,31	1.88	2 (6%)	48,48,48	2.26	13 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CLR	D	3001	-	-	4/10/68/68	0/4/4/4
7	CLR	B	3001	-	-	3/10/68/68	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	3001	CLR	C6-C5	9.65	1.52	1.33
7	B	3001	CLR	C6-C5	9.46	1.52	1.33
7	D	3001	CLR	C4-C5	2.16	1.56	1.51
7	D	3001	CLR	C4-C3	2.11	1.55	1.52
7	B	3001	CLR	C4-C5	2.01	1.55	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	3001	CLR	C7-C6-C5	-6.94	113.30	125.02
7	B	3001	CLR	C4-C5-C6	-6.90	111.21	120.57
7	D	3001	CLR	C3-C4-C5	6.37	122.19	112.05
7	B	3001	CLR	C3-C4-C5	5.96	121.54	112.05
7	D	3001	CLR	C10-C5-C6	-5.80	114.45	122.93
7	D	3001	CLR	C7-C6-C5	-5.36	115.97	125.02
7	D	3001	CLR	C4-C5-C6	-5.14	113.60	120.57
7	D	3001	CLR	C1-C2-C3	5.05	117.18	110.48
7	B	3001	CLR	C10-C5-C6	-4.69	116.08	122.93
7	B	3001	CLR	C19-C10-C9	-3.48	107.76	111.66
7	D	3001	CLR	C19-C10-C5	-3.42	103.16	108.38
7	D	3001	CLR	C12-C11-C9	3.19	118.55	113.14
7	B	3001	CLR	C1-C2-C3	3.07	114.54	110.48
7	D	3001	CLR	C4-C5-C10	-3.01	112.57	116.42
7	B	3001	CLR	C9-C10-C5	2.91	113.91	109.65
7	D	3001	CLR	C2-C1-C10	2.74	118.62	112.78
7	D	3001	CLR	C15-C14-C13	2.63	106.94	103.84
7	D	3001	CLR	C14-C8-C9	-2.52	105.80	109.09
7	D	3001	CLR	C7-C8-C9	-2.50	106.84	109.72
7	B	3001	CLR	C7-C8-C14	-2.46	107.45	110.93
7	D	3001	CLR	C9-C10-C5	2.44	113.22	109.65
7	B	3001	CLR	C16-C17-C20	-2.39	108.55	112.18
7	B	3001	CLR	C13-C14-C8	2.25	117.61	114.41
7	B	3001	CLR	C13-C17-C20	2.18	122.87	119.50
7	B	3001	CLR	C11-C9-C8	-2.10	108.85	111.78
7	B	3001	CLR	C8-C7-C6	2.01	115.55	112.76

There are no chirality outliers.

All (7) torsion outliers are listed below:

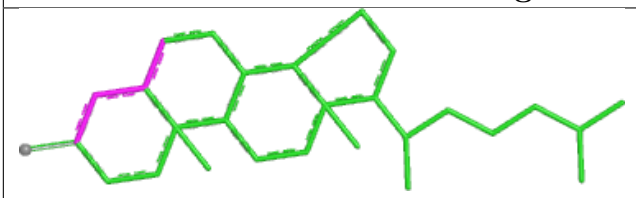
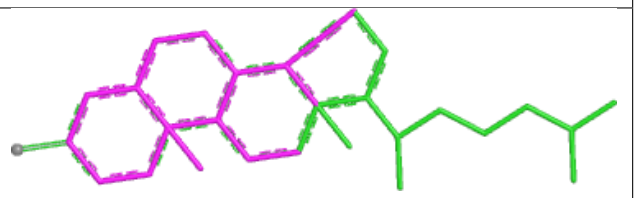
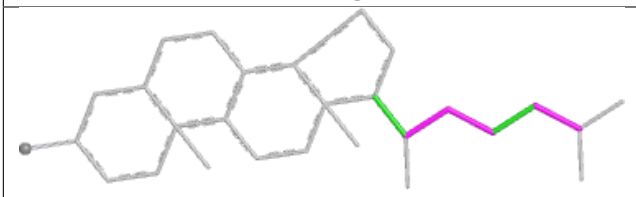
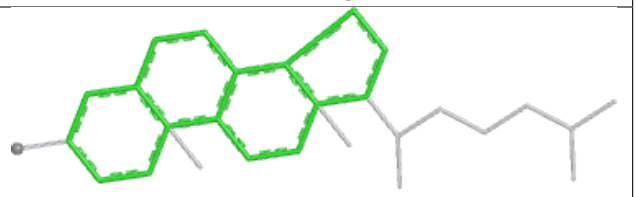
Mol	Chain	Res	Type	Atoms
7	B	3001	CLR	C20-C22-C23-C24
7	B	3001	CLR	C23-C24-C25-C27
7	D	3001	CLR	C23-C24-C25-C26
7	D	3001	CLR	C21-C20-C22-C23
7	B	3001	CLR	C23-C24-C25-C26
7	D	3001	CLR	C23-C24-C25-C27
7	D	3001	CLR	C20-C22-C23-C24

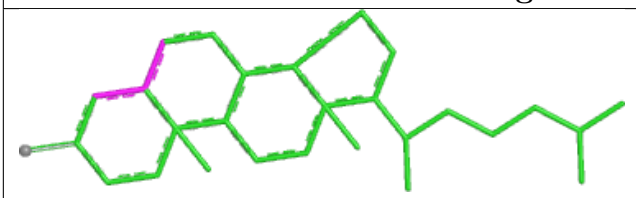
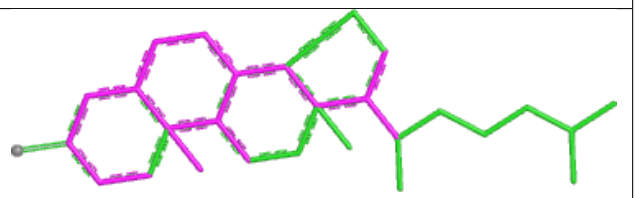
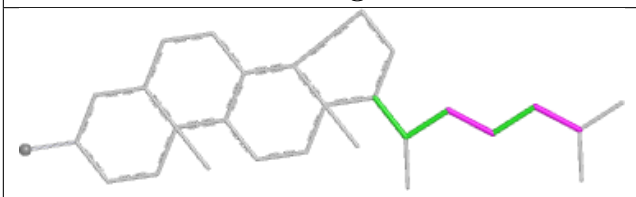
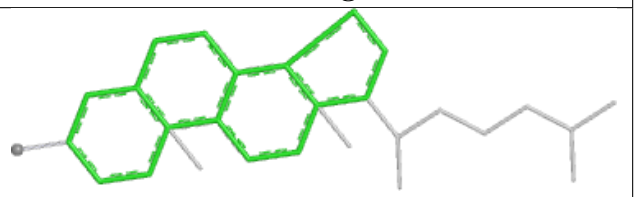
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2001	MF4	1	0
7	D	3001	CLR	4	0
4	A	2001	MF4	1	0
7	B	3001	CLR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CLR D 3001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLR B 3001	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	998/998 (100%)	-0.47	5 (0%)	91	88	39, 106, 197, 356	0
1	C	998/998 (100%)	-0.48	3 (0%)	94	91	39, 105, 195, 363	0
2	B	286/286 (100%)	0.12	18 (6%)	20	18	79, 190, 320, 582	0
2	D	286/286 (100%)	0.51	36 (12%)	3	5	66, 217, 341, 579	0
3	G	27/27 (100%)	1.91	10 (37%)	0	0	194, 246, 345, 447	0
3	H	27/27 (100%)	1.42	5 (18%)	1	1	151, 232, 301, 353	0
All	All	2622/2622 (100%)	-0.26	77 (2%)	51	45	39, 119, 270, 582	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	166	THR	10.1
2	B	166	THR	7.5
2	D	167	TYR	7.2
3	G	33	PHE	7.1
2	B	201	VAL	6.2
2	B	165	GLU	6.1
2	B	200	PRO	5.6
2	B	217	ARG	5.5
2	D	165	GLU	5.3
2	B	163	ASN	5.2
2	B	219	GLU	5.2
2	D	236	PRO	5.2
1	C	19	ALA	5.0
3	G	32	ILE	5.0
2	B	164	ASP	4.7
2	D	218	ASP	4.6
2	D	176	VAL	4.5
2	D	164	ASP	4.5
2	D	244	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
2	D	178	ILE	4.0
2	D	260	ALA	4.0
3	G	45	LEU	4.0
2	D	303	SER	4.0
2	D	246	TYR	3.9
2	B	162	LEU	3.9
2	B	199	TYR	3.8
1	A	115	GLU	3.6
2	D	175	CYS	3.6
2	D	262	GLN	3.5
2	D	163	ASN	3.4
3	G	34	ALA	3.4
2	D	219	GLU	3.3
3	G	36	LEU	3.1
2	B	208	VAL	3.1
1	A	943	LYS	3.0
1	A	19	ALA	3.0
2	D	250	LEU	2.9
2	D	145	GLU	2.9
2	D	258	LEU	2.9
3	G	31	LEU	2.8
2	B	218	ASP	2.8
2	D	237	GLY	2.8
2	D	197	GLU	2.8
2	D	273	ARG	2.7
2	D	243	TYR	2.7
2	D	271	GLU	2.7
2	D	139	TYR	2.7
1	A	931	LYS	2.6
2	D	220	ASP	2.6
3	H	49	ARG	2.5
3	G	38	PHE	2.5
1	C	115	GLU	2.5
2	B	205	ASN	2.5
3	G	44	ILE	2.5
2	D	259	MET	2.5
3	H	26	VAL	2.5
3	G	41	GLY	2.5
3	G	30	GLY	2.4
2	D	227	MET	2.4
2	D	302	LYS	2.4
3	H	38	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	259	MET	2.3
2	D	184	LEU	2.3
2	B	260	ALA	2.3
2	D	277	LYS	2.2
3	H	44	ILE	2.2
2	D	217	ARG	2.2
2	B	236	PRO	2.2
2	D	272	ILE	2.1
2	B	267	THR	2.1
2	D	93	ASN	2.1
1	A	113	ALA	2.1
2	D	266	LEU	2.1
2	B	197	GLU	2.1
3	H	27	ARG	2.1
1	C	461	LYS	2.0
2	D	223	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CLR	D	3001	28/28	0.86	0.32	101,102,102,102	0
7	CLR	B	3001	28/28	0.89	0.28	103,103,104,104	0
6	RB	A	2005	1/1	0.94	0.33	182,182,182,182	0
6	RB	A	2003	1/1	0.97	0.18	127,127,127,127	0
6	RB	C	2003	1/1	0.98	0.22	134,134,134,134	0
6	RB	C	2005	1/1	0.98	0.27	194,194,194,194	0
4	MF4	A	2001	5/5	0.98	0.28	88,91,93,97	0

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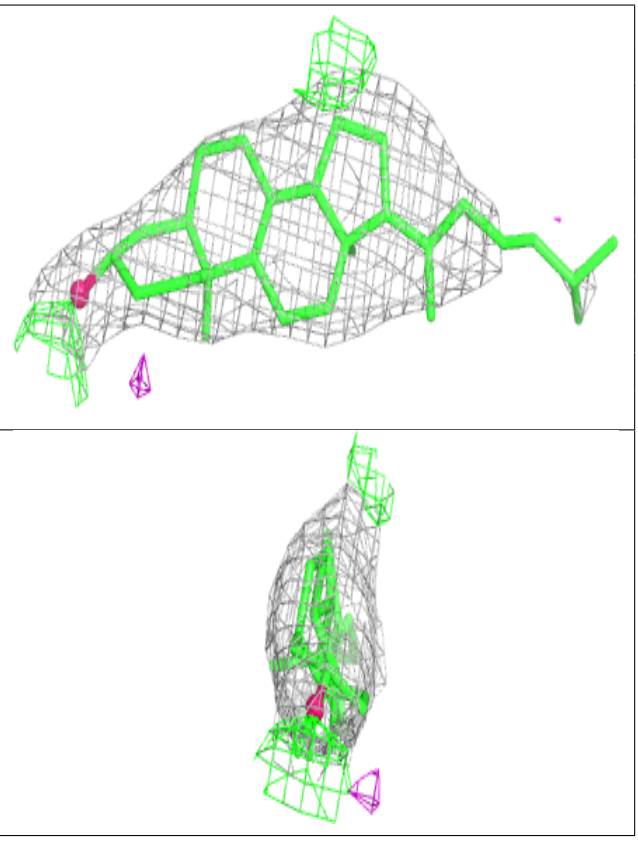
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MF4	C	2001	5/5	0.98	0.26	91,95,99,102	0
6	RB	C	2004	1/1	0.99	0.17	122,122,122,122	0
6	RB	A	2004	1/1	0.99	0.23	121,121,121,121	0
5	MG	C	2002	1/1	0.99	0.33	32,32,32,32	0
5	MG	A	2002	1/1	0.99	0.23	33,33,33,33	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

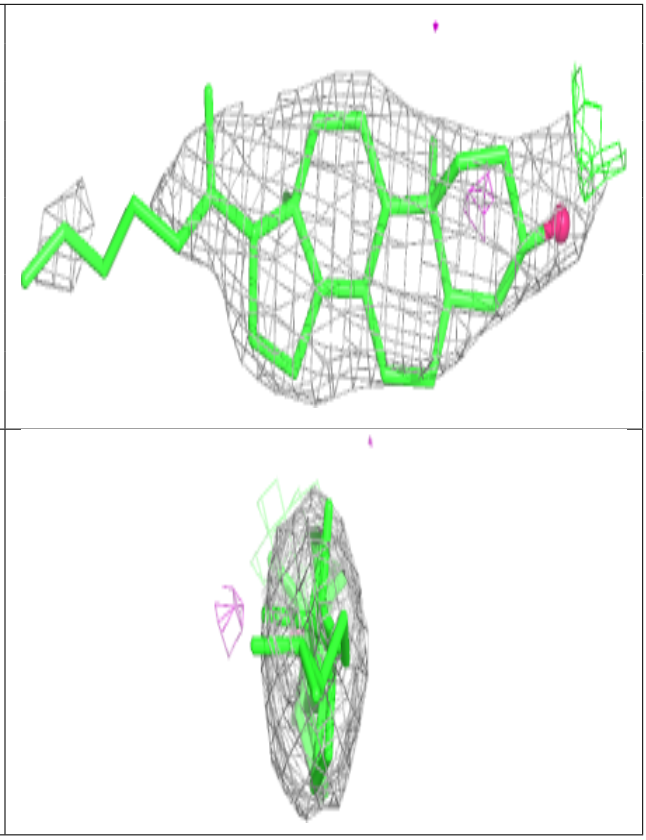
Electron density around CLR D 3001:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLR B 3001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.