



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2024 – 01:08 PM EST

PDB ID : 2EYQ
Title : Crystal structure of Escherichia coli transcription-repair coupling factor
Authors : Deaconescu, A.M.; Darst, S.A.
Deposited on : 2005-11-09
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

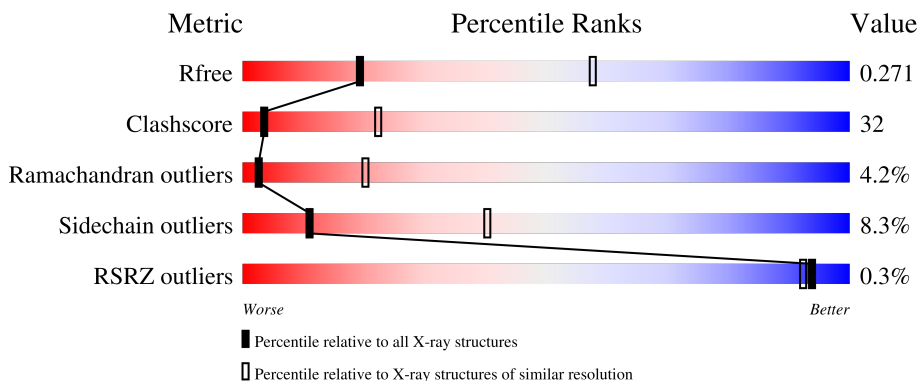
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 $\leq 5\%$. 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	1151	
1	B	1151	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EPE	A	1151	-	-	X	-
3	EPE	B	1150	-	-	X	-
3	EPE	B	1151	-	-	X	X
3	EPE	B	1152	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18063 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.

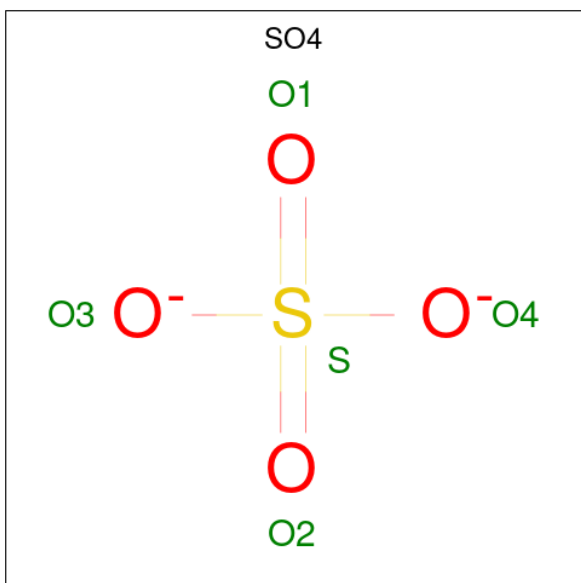
- Molecule 1 is a protein called Transcription-repair coupling factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1146	8980	5683	1605	1656	36	0	0	0
1	B	1143	8873	5611	1584	1642	36	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

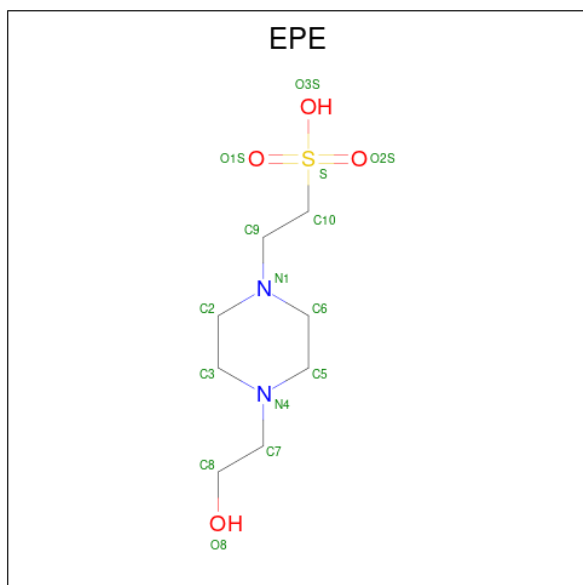
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P30958
A	-1	PRO	-	cloning artifact	UNP P30958
A	0	HIS	-	cloning artifact	UNP P30958
B	-2	GLY	-	cloning artifact	UNP P30958
B	-1	PRO	-	cloning artifact	UNP P30958
B	0	HIS	-	cloning artifact	UNP P30958

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 15 8 2 4 1	0	0
3	A	1	Total C N O S 15 8 2 4 1	0	0
3	B	1	Total C N O S 15 8 2 4 1	0	0
3	B	1	Total C N O S 15 8 2 4 1	0	0
3	B	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	68	Total O 68 68	0	0

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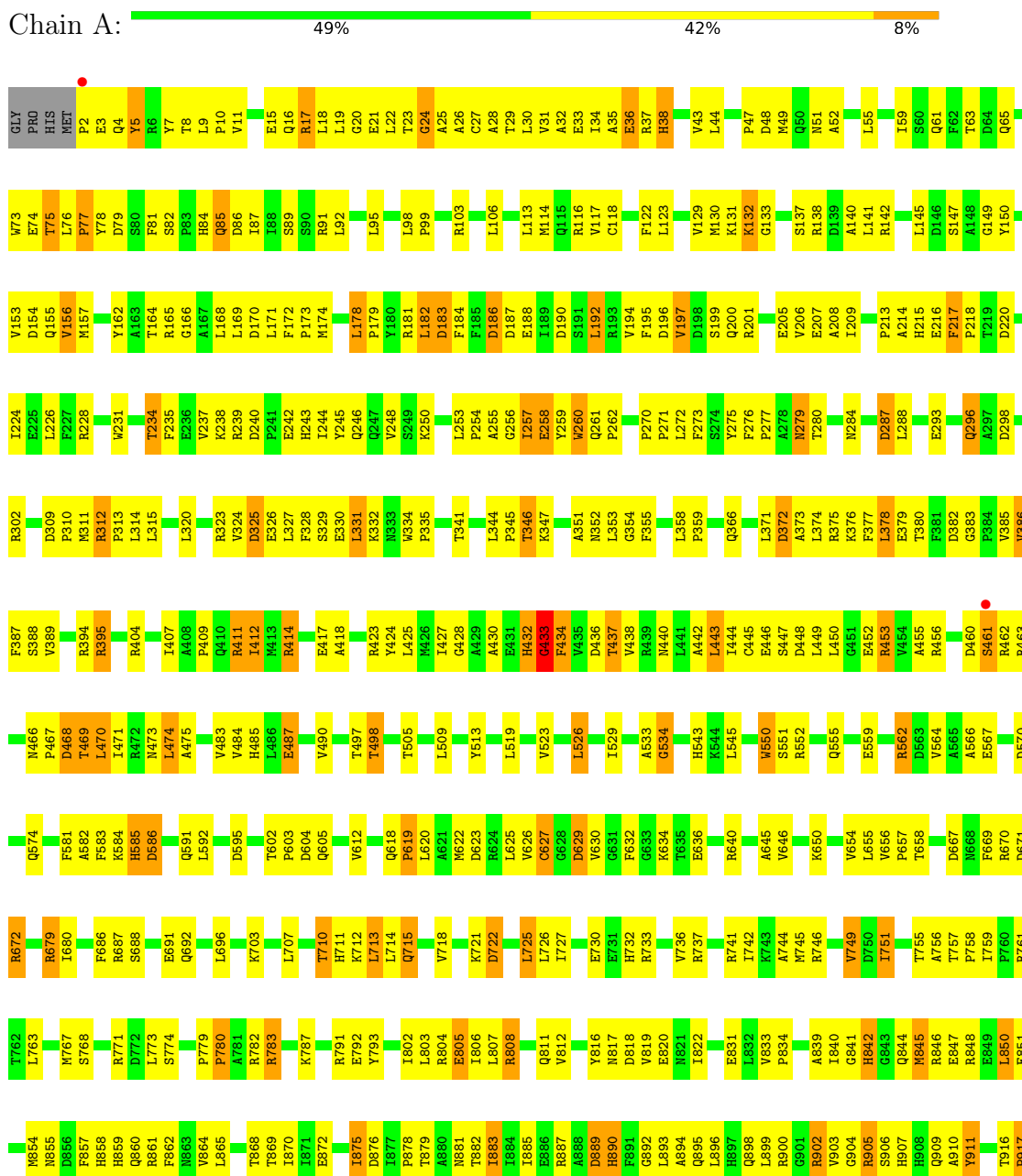
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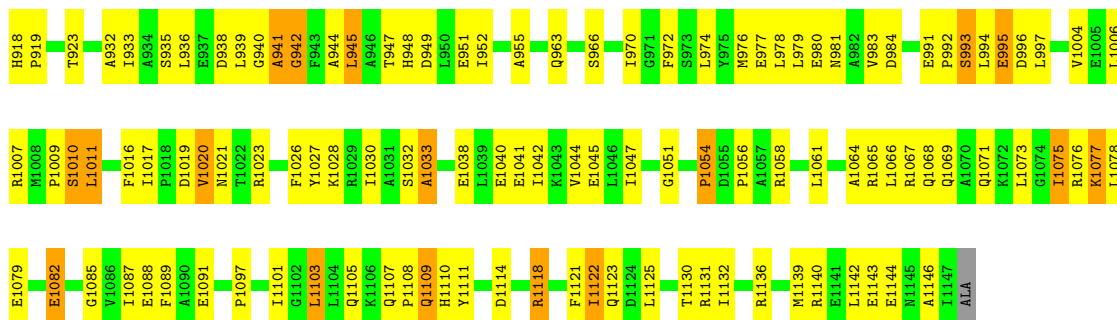
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	52	Total	O	0	0
			52	52		

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.

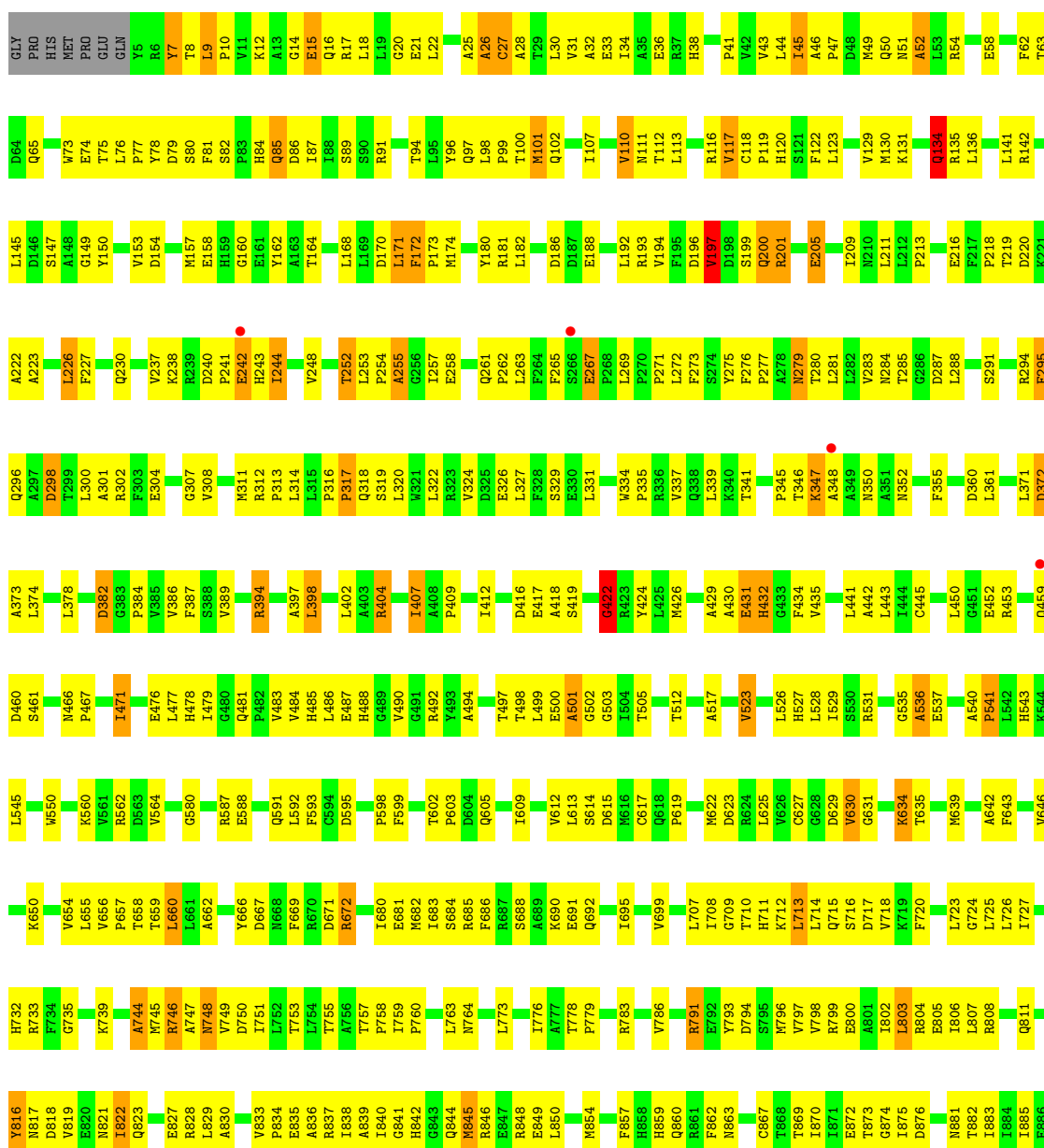
• Molecule 1: Transcription-repair coupling factor

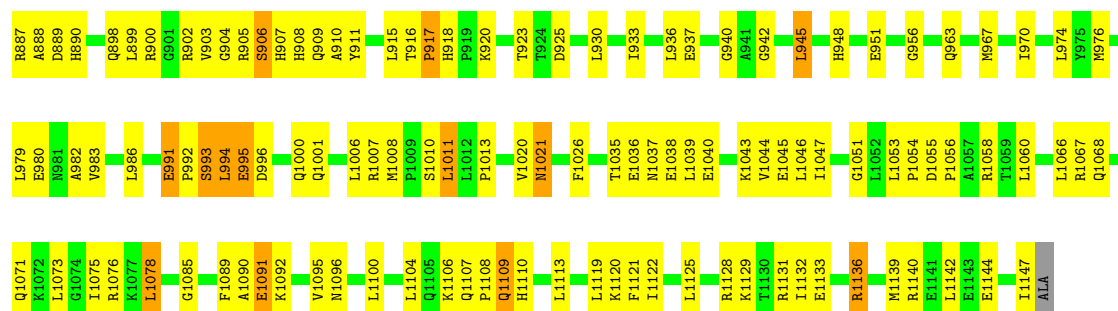




• Molecule 1: Transcription-repair coupling factor

Chain B: 50% 43% 6%





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.87Å 161.99Å 161.73Å 90.00° 105.09° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 29.91 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 98.0 (29.91-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.18Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.295 0.212 , 0.271	Depositor DCC
R_{free} test set	3095 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	63.1	Xtrriage
Anisotropy	0.045	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18063	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: EPE, SO4

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	0.49	0/9162	0.74	3/12429 (0.0%)
1	B	0.47	0/9051	0.69	1/12284 (0.0%)
All	All	0.48	0/18213	0.72	4/24713 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	ARG	NE-CZ-NH2	-11.19	114.70	120.30
1	A	414	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	B	422	GLY	N-CA-C	8.52	134.41	113.10
1	A	433	GLY	N-CA-C	5.70	127.34	113.10

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	8980	0	8865	583	0
1	B	8873	0	8675	551	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	30	0	36	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	45	0	54	26	0
4	A	68	0	0	5	0
4	B	52	0	0	3	0
All	All	18063	0	17630	1130	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 32.

All (1130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:PRO:HD2	1:B:257:ILE:HD12	1.17	1.15
1:A:474:LEU:HD21	1:A:1028:LYS:HG3	1.31	1.07
1:B:117:VAL:HG12	1:B:118:CYS:H	1.16	1.05
1:A:116:ARG:HG3	1:A:320:LEU:O	1.57	1.04
1:B:386:VAL:HB	1:B:443:LEU:HD12	1.39	1.03
1:B:659:THR:HG22	1:B:684:SER:HB2	1.39	1.01
1:B:562:ARG:HG3	1:B:992:PRO:HG3	1.04	1.00
1:B:20:GLY:HA3	1:B:352:ASN:HA	1.42	0.99
1:B:490:VAL:H	1:B:543:HIS:HD2	1.07	0.98
1:A:279:ASN:HD22	1:A:279:ASN:H	1.01	0.97
1:A:822:ILE:HD12	1:A:868:THR:CG2	1.97	0.95
1:B:791:ARG:HG3	1:B:791:ARG:HH11	1.31	0.95
1:A:991:GLU:CD	1:A:992:PRO:HD2	1.87	0.94
1:A:991:GLU:CG	1:A:992:PRO:HD2	1.98	0.93
1:B:562:ARG:CG	1:B:992:PRO:HG3	1.95	0.93
1:B:18:LEU:HD12	1:B:350:ASN:HB3	1.49	0.93
1:B:710:THR:HG23	1:B:712:LYS:H	1.31	0.93
1:A:409:PRO:HB2	1:A:425:LEU:HD23	1.50	0.92
1:B:605:GLN:HE21	1:B:634:LYS:HD2	1.33	0.92
1:B:726:LEU:HD23	1:B:751:ILE:HD11	1.51	0.92
1:A:155:GLN:O	1:A:156:VAL:HG12	1.69	0.91
1:B:63:THR:HG22	1:B:65:GLN:H	1.31	0.91
1:B:1136:ARG:HG3	1:B:1136:ARG:HH11	1.35	0.91
1:B:384:PRO:HG2	1:B:441:LEU:HD13	1.53	0.91
1:A:178:LEU:HD23	1:A:178:LEU:H	1.36	0.90
1:A:473:ASN:C	1:A:474:LEU:HD23	1.92	0.90
1:B:182:LEU:CD2	1:B:192:LEU:HD13	2.02	0.90
1:B:562:ARG:HG3	1:B:992:PRO:CG	1.98	0.87
1:A:170:ASP:OD1	1:A:181:ARG:HG3	1.75	0.87
1:A:412:ILE:HG22	1:A:417:GLU:HB2	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:ARG:HD2	1:A:992:PRO:HG3	1.53	0.86
1:A:344:LEU:HB2	1:A:352:ASN:ND2	1.91	0.86
1:A:279:ASN:H	1:A:279:ASN:ND2	1.74	0.84
1:B:481:GLN:HE22	1:B:531:ARG:HH12	1.25	0.84
1:B:389:VAL:CG1	1:B:394:ARG:HB3	2.06	0.84
1:B:940:GLY:N	3:B:1151:EPE:O1S	2.11	0.84
1:A:881:ASN:HA	1:A:903:VAL:HG13	1.58	0.84
1:A:887:ARG:HG2	1:A:890:HIS:CE1	2.12	0.84
1:B:117:VAL:HG12	1:B:118:CYS:N	1.93	0.83
1:B:113:LEU:HD12	1:B:272:LEU:HD23	1.60	0.83
1:A:627:CYS:SG	1:A:773:LEU:HD11	2.18	0.82
1:A:279:ASN:HD22	1:A:279:ASN:N	1.69	0.82
1:B:182:LEU:HD21	1:B:192:LEU:HD13	1.61	0.82
1:A:276:PHE:HB3	1:A:280:THR:HG21	1.61	0.82
1:B:490:VAL:H	1:B:543:HIS:CD2	1.95	0.82
1:A:7:TYR:CE1	1:A:37:ARG:NH1	2.48	0.82
1:A:787:LYS:HG3	1:A:909:GLN:NE2	1.94	0.82
1:A:1091:GLU:CD	1:A:1091:GLU:H	1.83	0.82
1:B:157:MET:HA	1:B:197:VAL:HG12	1.62	0.82
1:B:31:VAL:HA	1:B:34:ILE:HG22	1.61	0.81
1:B:937:GLU:HG2	3:B:1151:EPE:H31	1.61	0.81
1:B:389:VAL:HG13	1:B:394:ARG:HB3	1.63	0.80
1:A:277:PRO:O	1:A:280:THR:HG22	1.81	0.80
1:B:78:TYR:CD2	1:B:314:LEU:HD13	2.16	0.79
1:A:63:THR:HG22	1:A:65:GLN:H	1.47	0.79
1:A:296:GLN:HE22	1:A:323:ARG:HA	1.46	0.79
1:B:1035:THR:HB	1:B:1038:GLU:HG3	1.64	0.79
1:B:936:LEU:HB3	3:B:1151:EPE:H101	1.63	0.78
1:A:497:THR:HG22	1:A:498:THR:N	1.98	0.78
1:A:273:PHE:CD1	1:A:330:GLU:HG2	2.20	0.77
1:B:982:ALA:O	1:B:986:LEU:HD13	1.82	0.77
1:B:302:ARG:HH11	1:B:302:ARG:HB3	1.48	0.77
1:A:903:VAL:HG12	1:A:910:ALA:HB1	1.66	0.77
1:B:602:THR:HB	1:B:605:GLN:HB2	1.65	0.77
1:A:21:GLU:HA	1:A:341:THR:O	1.84	0.76
1:B:170:ASP:OD1	1:B:181:ARG:HG3	1.86	0.76
1:B:903:VAL:CG1	1:B:910:ALA:HB1	2.15	0.76
1:B:1035:THR:HG22	1:B:1037:ASN:H	1.48	0.76
1:B:726:LEU:HD23	1:B:751:ILE:CD1	2.15	0.76
1:B:970:ILE:HB	1:B:974:LEU:HD23	1.67	0.76
1:B:98:LEU:HB3	1:B:99:PRO:HD3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ARG:HH21	1:A:427:ILE:HD11	1.51	0.76
1:B:659:THR:HG21	1:B:685:ARG:HB2	1.68	0.76
1:A:730:GLU:OE2	1:A:755:THR:HA	1.86	0.75
1:B:490:VAL:N	1:B:543:HIS:HD2	1.83	0.75
1:A:65:GLN:HE22	1:A:103:ARG:HG2	1.51	0.75
1:B:791:ARG:HH11	1:B:791:ARG:CG	2.00	0.75
1:A:254:PRO:HD2	1:A:257:ILE:HD12	1.67	0.75
1:B:994:LEU:C	1:B:996:ASP:H	1.91	0.75
1:B:298:ASP:O	1:B:302:ARG:HG3	1.87	0.74
1:A:373:ALA:HA	1:A:376:LYS:HE2	1.68	0.74
1:A:994:LEU:C	1:A:996:ASP:H	1.89	0.74
1:A:936:LEU:HD22	3:A:1151:EPE:H62	1.70	0.74
1:A:562:ARG:CD	1:A:992:PRO:HG3	2.18	0.74
1:B:942:GLY:N	3:B:1151:EPE:O2S	2.21	0.74
1:A:4:GLN:HB2	1:A:5:TYR:CE1	2.23	0.74
1:A:425:LEU:HD12	1:A:425:LEU:O	1.87	0.73
1:A:991:GLU:HG3	1:A:992:PRO:HD2	1.69	0.73
1:A:726:LEU:HD23	1:A:751:ILE:HD11	1.70	0.73
1:B:481:GLN:NE2	1:B:531:ARG:HH12	1.86	0.73
1:B:839:ALA:HB2	1:B:862:PHE:CD2	2.23	0.73
1:A:178:LEU:HD23	1:A:178:LEU:N	2.04	0.72
1:A:848:ARG:NH2	1:B:685:ARG:O	2.23	0.72
1:B:96:TYR:O	1:B:99:PRO:HD2	1.90	0.72
1:A:434:PHE:HD1	1:A:434:PHE:C	1.92	0.72
1:B:117:VAL:CG1	1:B:118:CYS:H	1.99	0.72
1:A:156:VAL:HG11	1:A:170:ASP:HB3	1.72	0.72
1:A:899:LEU:O	1:A:902:ARG:HG3	1.89	0.72
1:A:242:GLU:HB2	1:A:311:MET:HE2	1.72	0.72
1:B:630:VAL:HG12	1:B:630:VAL:O	1.89	0.72
1:B:1136:ARG:HH11	1:B:1136:ARG:CG	2.02	0.71
1:A:378:LEU:HD12	1:A:407:ILE:CD1	2.21	0.71
1:A:474:LEU:HD23	1:A:474:LEU:N	2.04	0.71
1:A:181:ARG:HG3	1:A:181:ARG:HH11	1.55	0.71
1:B:91:ARG:HD3	1:B:216:GLU:OE1	1.91	0.71
1:B:386:VAL:HG11	1:B:426:MET:HE2	1.72	0.71
1:B:685:ARG:HG3	3:B:1150:EPE:H61	1.71	0.71
1:A:707:LEU:HD21	1:A:713:LEU:HD21	1.73	0.71
1:B:994:LEU:O	1:B:996:ASP:N	2.23	0.71
1:B:31:VAL:HA	1:B:34:ILE:CG2	2.20	0.71
1:B:1125:LEU:HB3	1:B:1131:ARG:HB2	1.72	0.71
1:A:497:THR:CG2	1:A:498:THR:N	2.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:ARG:O	1:B:591:GLN:HG2	1.91	0.70
1:B:386:VAL:HB	1:B:443:LEU:CD1	2.19	0.70
1:B:699:VAL:HG21	1:B:707:LEU:HD22	1.73	0.70
1:A:174:MET:HG3	1:A:214:ALA:HA	1.74	0.70
1:A:375:ARG:O	1:A:379:GLU:HG2	1.92	0.70
1:A:655:LEU:HD11	1:A:714:LEU:HD21	1.73	0.70
1:B:1140:ARG:O	1:B:1144:GLU:HG3	1.90	0.70
1:A:47:PRO:HG2	1:A:51:ASN:HD22	1.56	0.70
1:B:131:LYS:H	1:B:134:GLN:HG3	1.55	0.70
1:A:76:LEU:O	1:A:79:ASP:HB2	1.91	0.70
1:A:940:GLY:N	3:A:1151:EPE:O1S	2.25	0.70
1:A:377:PHE:HD2	1:A:378:LEU:HD23	1.55	0.70
1:A:260:TRP:HH2	1:A:312:ARG:HG2	1.56	0.70
1:A:903:VAL:CG1	1:A:910:ALA:HB1	2.21	0.70
1:B:27:CYS:SG	1:B:339:LEU:HD13	2.31	0.70
1:B:76:LEU:O	1:B:79:ASP:HB2	1.92	0.70
1:A:20:GLY:N	1:A:344:LEU:HD11	2.07	0.70
1:A:117:VAL:HG12	1:A:118:CYS:O	1.92	0.69
1:A:20:GLY:HA3	1:A:344:LEU:HG	1.73	0.69
1:A:98:LEU:HB3	1:A:99:PRO:HD3	1.73	0.69
1:B:307:GLY:HA2	1:B:314:LEU:HG	1.75	0.69
1:A:344:LEU:HB2	1:A:352:ASN:HD21	1.56	0.69
1:B:612:VAL:HA	1:B:622:MET:CE	2.23	0.69
1:A:612:VAL:O	1:A:622:MET:HE3	1.93	0.69
1:B:196:ASP:HB3	1:B:199:SER:HB3	1.74	0.69
1:A:178:LEU:N	1:A:178:LEU:CD2	2.56	0.69
1:A:936:LEU:HD13	3:A:1151:EPE:H102	1.74	0.69
1:B:903:VAL:HG12	1:B:910:ALA:HB1	1.74	0.69
1:A:992:PRO:C	1:A:994:LEU:H	1.96	0.68
1:A:36:GLU:OE2	1:A:63:THR:HG23	1.93	0.68
1:A:63:THR:HG21	1:A:65:GLN:HB2	1.76	0.68
1:A:1082:GLU:HA	1:A:1125:LEU:O	1.93	0.68
1:A:73:TRP:CH2	1:A:258:GLU:HB3	2.29	0.68
1:A:1038:GLU:O	1:A:1042:ILE:HG13	1.94	0.68
1:B:378:LEU:HD21	1:B:407:ILE:HD13	1.75	0.68
1:A:490:VAL:H	1:A:543:HIS:CD2	2.12	0.68
1:B:182:LEU:HD23	1:B:192:LEU:HD13	1.74	0.68
1:B:634:LYS:HE2	1:B:776:ILE:HG21	1.76	0.68
1:A:37:ARG:O	1:A:37:ARG:HG3	1.93	0.68
1:A:114:MET:HG2	1:A:327:LEU:HD22	1.76	0.68
1:B:116:ARG:HD2	1:B:319:SER:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:992:PRO:C	1:B:994:LEU:H	1.98	0.68
1:A:679:ARG:HD3	1:A:703:LYS:O	1.94	0.67
1:B:937:GLU:CG	3:B:1151:EPE:H31	2.23	0.67
1:B:905:ARG:HD3	1:B:908:HIS:CD2	2.29	0.67
1:B:1119:LEU:HD12	1:B:1120:LYS:H	1.57	0.67
1:A:1073:LEU:HD11	1:A:1143:GLU:HB3	1.74	0.67
1:A:434:PHE:C	1:A:434:PHE:CD1	2.67	0.67
1:A:842:HIS:CE1	3:B:1150:EPE:H62	2.30	0.67
1:A:916:THR:HB	1:A:917:PRO:HD2	1.76	0.67
1:A:182:LEU:O	1:A:183:ASP:HB3	1.95	0.67
1:A:842:HIS:NE2	3:B:1150:EPE:H62	2.09	0.67
1:A:1122:ILE:O	1:A:1123:GLN:HG2	1.95	0.67
1:B:7:TYR:HD2	1:B:8:THR:H	1.41	0.67
1:B:136:LEU:HD13	1:B:141:LEU:HB2	1.75	0.67
1:B:688:SER:OG	1:B:691:GLU:HG3	1.95	0.67
1:B:134:GLN:O	1:B:188:GLU:HG2	1.95	0.67
1:B:153:VAL:HG12	1:B:154:ASP:H	1.59	0.67
1:B:153:VAL:HG12	1:B:154:ASP:N	2.08	0.67
1:A:872:GLU:O	1:A:875:ILE:HG13	1.95	0.67
1:B:936:LEU:HD22	3:B:1151:EPE:H62	1.76	0.67
1:B:1107:GLN:HA	1:B:1109:GLN:HE22	1.60	0.67
1:A:47:PRO:HG2	1:A:48:ASP:OD1	1.96	0.66
1:A:153:VAL:HG12	1:A:154:ASP:N	2.10	0.66
1:B:135:ARG:HG2	1:B:188:GLU:HG3	1.76	0.66
1:B:378:LEU:HD21	1:B:407:ILE:CD1	2.25	0.66
1:B:523:VAL:HA	1:B:526:LEU:HD23	1.77	0.66
1:A:490:VAL:H	1:A:543:HIS:HD2	1.41	0.66
1:A:585:HIS:O	1:A:586:ASP:HB3	1.94	0.66
1:B:171:LEU:HG	1:B:173:PRO:HD3	1.77	0.66
1:A:434:PHE:HD1	1:A:434:PHE:O	1.78	0.66
1:B:10:PRO:HB2	1:B:15:GLU:HB3	1.76	0.66
1:A:612:VAL:HG13	1:A:622:MET:HE1	1.77	0.66
1:A:24:GLY:C	1:A:26:ALA:H	1.99	0.66
1:A:386:VAL:HA	1:A:424:TYR:O	1.96	0.66
1:B:930:LEU:O	1:B:933:ILE:HG22	1.96	0.66
1:B:46:ALA:O	1:B:110:VAL:HG23	1.96	0.65
1:B:612:VAL:HA	1:B:622:MET:HE3	1.78	0.65
1:B:629:ASP:OD1	1:B:634:LYS:CE	2.43	0.65
1:B:817:ASN:O	1:B:818:ASP:HB2	1.95	0.65
1:A:244:ILE:O	1:A:248:VAL:HG23	1.97	0.65
1:B:629:ASP:OD1	1:B:634:LYS:HG2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ASP:O	1:A:462:ARG:N	2.29	0.65
1:A:411:ARG:NH2	1:A:427:ILE:HD11	2.11	0.65
1:B:117:VAL:HG21	1:B:272:LEU:HD13	1.79	0.65
1:A:10:PRO:HB3	1:A:15:GLU:O	1.96	0.65
1:A:122:PHE:CE1	1:A:218:PRO:HD3	2.31	0.65
1:A:1073:LEU:HD13	1:A:1142:LEU:HG	1.77	0.65
1:B:145:LEU:HD21	1:B:211:LEU:HD11	1.77	0.65
1:B:625:LEU:HD13	1:B:753:THR:HG22	1.79	0.65
1:A:467:PRO:O	1:A:471:ILE:HG13	1.97	0.65
1:B:671:ASP:CG	1:B:848:ARG:HH11	1.99	0.65
1:A:199:SER:O	1:A:200:GLN:HB2	1.97	0.65
1:B:157:MET:HA	1:B:197:VAL:CG1	2.26	0.65
1:A:10:PRO:HG3	1:A:17:ARG:HB2	1.78	0.65
1:A:63:THR:CG2	1:A:65:GLN:HB2	2.26	0.65
1:A:1107:GLN:N	1:A:1108:PRO:HD3	2.10	0.65
1:A:432:HIS:HA	1:A:445:CYS:HB2	1.77	0.64
1:B:605:GLN:HE21	1:B:634:LYS:CD	2.10	0.64
1:A:896:LEU:HA	1:A:899:LEU:HD12	1.79	0.64
1:B:302:ARG:HB3	1:B:302:ARG:NH1	2.12	0.64
1:A:630:VAL:HG12	1:A:630:VAL:O	1.97	0.64
1:A:881:ASN:CA	1:A:903:VAL:HG13	2.27	0.64
1:B:38:HIS:CD2	1:B:281:LEU:HD23	2.33	0.64
1:A:181:ARG:NH2	1:A:200:GLN:O	2.30	0.64
1:A:1017:ILE:O	1:A:1023:ARG:HD3	1.98	0.64
1:A:1078:LEU:C	1:A:1078:LEU:HD23	2.18	0.64
1:B:794:ASP:HB3	1:B:797:VAL:HG23	1.78	0.64
1:B:180:TYR:HB3	1:B:192:LEU:HD11	1.78	0.64
1:B:725:LEU:HD12	1:B:726:LEU:H	1.63	0.64
1:A:170:ASP:OD1	1:A:181:ARG:NH1	2.31	0.64
1:A:170:ASP:OD2	1:A:181:ARG:NH1	2.31	0.64
1:B:220:ASP:OD1	1:B:222:ALA:HB3	1.98	0.64
1:B:254:PRO:HD2	1:B:257:ILE:CD1	2.12	0.64
1:A:30:LEU:HD11	1:A:353:LEU:CD1	2.28	0.64
1:B:869:THR:H	1:B:872:GLU:HG2	1.61	0.64
1:B:211:LEU:HD23	1:B:211:LEU:O	1.98	0.63
1:B:466:ASN:OD1	1:B:467:PRO:HD2	1.98	0.63
1:A:432:HIS:HB2	1:A:448:ASP:OD1	1.96	0.63
1:A:1132:ILE:O	1:A:1136:ARG:HG3	1.99	0.63
1:B:492:ARG:NH2	1:B:540:ALA:O	2.31	0.63
1:B:523:VAL:HA	1:B:526:LEU:CD2	2.27	0.63
1:B:1106:LYS:C	1:B:1108:PRO:HD3	2.18	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:685:ARG:HD2	3:B:1150:EPE:H61	1.80	0.63
1:B:936:LEU:HA	3:B:1151:EPE:H51	1.81	0.63
1:A:1040:GLU:O	1:A:1044:VAL:HG23	1.99	0.63
1:B:484:VAL:HG22	1:B:490:VAL:HG22	1.80	0.63
1:A:78:TYR:CD2	1:A:314:LEU:HD13	2.34	0.63
1:A:936:LEU:HA	3:A:1151:EPE:H51	1.81	0.63
1:A:870:ILE:CD1	1:A:895:GLN:HB3	2.29	0.63
1:B:386:VAL:HA	1:B:424:TYR:CB	2.29	0.63
1:B:936:LEU:HB3	3:B:1151:EPE:C10	2.29	0.63
1:A:386:VAL:HG22	1:A:424:TYR:HB2	1.80	0.63
1:A:436:ASP:O	1:A:440:ASN:N	2.32	0.62
1:A:942:GLY:N	3:A:1151:EPE:O2S	2.32	0.62
1:B:802:ILE:O	1:B:806:ILE:HG13	1.99	0.62
1:A:10:PRO:CG	1:A:17:ARG:HB2	2.30	0.62
1:A:254:PRO:HD2	1:A:257:ILE:CD1	2.30	0.62
1:B:1000:GLN:O	1:B:1071:GLN:NE2	2.32	0.62
1:B:945:LEU:O	1:B:948:HIS:HB3	1.99	0.62
1:A:155:GLN:O	1:A:156:VAL:CG1	2.46	0.62
1:A:468:ASP:O	1:A:469:THR:C	2.38	0.62
1:A:156:VAL:HG13	1:A:156:VAL:O	2.00	0.62
1:A:885:ILE:HD13	1:A:899:LEU:HD13	1.81	0.62
1:A:570:ASP:O	1:A:574:GLN:HG3	1.99	0.62
1:B:692:GLN:HE22	1:B:712:LYS:HD3	1.64	0.62
1:A:30:LEU:O	1:A:34:ILE:HG13	2.00	0.62
1:A:117:VAL:HG12	1:A:118:CYS:N	2.15	0.62
1:B:494:ALA:HB2	1:B:512:THR:HG23	1.81	0.62
1:A:47:PRO:CG	1:A:51:ASN:HD22	2.12	0.62
1:A:298:ASP:O	1:A:302:ARG:HG3	1.99	0.62
1:A:870:ILE:HD11	1:A:895:GLN:HB3	1.82	0.61
1:B:430:ALA:HB1	1:B:445:CYS:SG	2.40	0.61
1:A:688:SER:OG	1:A:691:GLU:HG3	2.00	0.61
1:A:474:LEU:CD2	1:A:1028:LYS:HG3	2.20	0.61
1:A:629:ASP:O	1:A:634:LYS:HG3	2.01	0.61
1:B:906:SER:O	1:B:907:HIS:HB2	2.00	0.61
1:A:811:GLN:HG2	1:A:857:PHE:CD2	2.35	0.61
1:A:1016:PHE:CD2	1:A:1017:ILE:HG13	2.35	0.61
1:B:262:PRO:HG3	1:B:269:LEU:HD12	1.83	0.61
1:B:881:ASN:HA	1:B:903:VAL:HG13	1.82	0.61
1:B:1011:LEU:HD22	1:B:1056:PRO:HB3	1.82	0.61
1:A:117:VAL:CG1	1:A:118:CYS:N	2.63	0.61
1:A:358:LEU:HD21	1:A:444:ILE:HG12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:THR:HG23	1:B:712:LYS:N	2.12	0.61
1:B:811:GLN:HG2	1:B:857:PHE:CD2	2.35	0.61
1:A:131:LYS:O	1:A:133:GLY:N	2.33	0.61
1:A:214:ALA:O	1:A:215:HIS:CG	2.53	0.61
1:B:747:ALA:O	1:B:748:ASN:CB	2.48	0.61
1:B:874:GLY:HA2	1:B:902:ARG:NH1	2.16	0.61
1:B:1108:PRO:HD2	1:B:1109:GLN:HE21	1.65	0.61
1:A:763:LEU:O	1:A:767:MET:HG2	2.01	0.61
1:B:237:VAL:HG12	1:B:238:LYS:N	2.16	0.60
1:A:629:ASP:OD1	1:A:634:LYS:HE3	1.99	0.60
1:A:802:ILE:HD12	1:A:833:VAL:HG21	1.83	0.60
1:A:822:ILE:HD12	1:A:868:THR:HG23	1.80	0.60
1:B:498:THR:O	1:B:499:LEU:HD23	2.01	0.60
1:A:78:TYR:HD2	1:A:314:LEU:HD22	1.67	0.60
1:B:168:LEU:CD2	1:B:181:ARG:HD3	2.31	0.60
1:B:386:VAL:HG11	1:B:426:MET:CE	2.30	0.60
1:A:9:LEU:HD11	1:A:37:ARG:HG3	1.82	0.60
1:B:147:SER:C	1:B:149:GLY:H	2.03	0.60
1:A:235:PHE:HZ	1:A:315:LEU:HD23	1.66	0.60
1:A:911:TYR:N	1:A:911:TYR:CD1	2.69	0.60
1:B:17:ARG:HB2	1:B:337:VAL:HG13	1.83	0.60
1:B:80:SER:O	1:B:255:ALA:HB1	2.02	0.60
1:B:412:ILE:HD13	1:B:418:ALA:HB2	1.83	0.60
1:A:24:GLY:O	1:A:26:ALA:N	2.35	0.60
1:A:497:THR:CG2	1:A:498:THR:H	2.14	0.60
1:A:562:ARG:CG	1:A:992:PRO:HG3	2.31	0.60
1:B:432:HIS:CD2	1:B:432:HIS:H	2.19	0.60
1:A:562:ARG:HG3	1:A:992:PRO:HG3	1.84	0.60
1:A:584:LYS:O	1:A:585:HIS:HB2	2.01	0.60
1:A:1009:PRO:HD2	4:A:1207:HOH:O	2.01	0.60
1:B:1129:LYS:O	1:B:1132:ILE:HG22	2.02	0.60
1:A:73:TRP:HE1	1:A:91:ARG:HH11	1.50	0.59
1:B:794:ASP:C	1:B:796:MET:H	2.05	0.59
1:A:456:ARG:HE	1:A:876:ASP:CG	2.05	0.59
1:B:659:THR:H	3:B:1150:EPE:H92	1.66	0.59
1:B:659:THR:CG2	1:B:684:SER:HB2	2.23	0.59
1:A:1078:LEU:HD23	1:A:1078:LEU:O	2.01	0.59
1:B:991:GLU:CD	1:B:992:PRO:HD2	2.23	0.59
1:A:840:ILE:HG22	1:A:841:GLY:N	2.18	0.59
1:B:119:PRO:HD2	1:B:265:PHE:CE2	2.37	0.59
1:A:412:ILE:CG2	1:A:417:GLU:HB2	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:GLN:HE22	1:A:712:LYS:HE2	1.67	0.59
1:A:1103:LEU:HD21	1:A:1111:TYR:CE1	2.37	0.59
1:B:49:MET:O	1:B:52:ALA:HB3	2.02	0.59
1:A:966:SER:O	1:A:970:ILE:HG12	2.02	0.59
1:A:244:ILE:HD13	1:A:311:MET:O	2.01	0.59
1:B:291:SER:O	1:B:294:ARG:HB3	2.03	0.59
1:B:778:THR:HG22	1:B:779:PRO:HD2	1.83	0.59
1:A:434:PHE:CE1	1:A:443:LEU:HB2	2.38	0.58
1:A:1011:LEU:HD23	1:A:1056:PRO:HB3	1.85	0.58
1:B:642:ALA:O	1:B:646:VAL:HG23	2.02	0.58
1:A:224:ILE:O	1:A:228:ARG:HG3	2.03	0.58
1:B:63:THR:HG22	1:B:65:GLN:N	2.11	0.58
1:A:555:GLN:HE21	1:A:559:GLU:HG3	1.68	0.58
1:B:629:ASP:OD1	1:B:634:LYS:CD	2.51	0.58
1:B:1035:THR:HG22	1:B:1036:GLU:N	2.17	0.58
1:B:1109:GLN:H	1:B:1109:GLN:NE2	2.02	0.58
1:A:192:LEU:N	1:A:192:LEU:HD22	2.19	0.58
1:B:122:PHE:CE1	1:B:218:PRO:HD3	2.39	0.58
1:B:873:THR:O	1:B:902:ARG:HD2	2.02	0.58
1:A:73:TRP:NE1	1:A:91:ARG:NH1	2.52	0.58
1:A:444:ILE:CG2	1:A:449:LEU:HD13	2.33	0.58
1:A:1109:GLN:H	1:A:1109:GLN:NE2	2.01	0.58
1:A:52:ALA:HA	1:A:55:LEU:HD12	1.86	0.58
1:A:196:ASP:HB3	1:A:199:SER:HB3	1.85	0.58
1:A:323:ARG:HB2	1:A:326:GLU:HG3	1.85	0.58
1:A:261:GLN:HB3	1:A:262:PRO:HD3	1.85	0.57
1:A:1069:GLN:HB2	1:A:1139:MET:HE2	1.86	0.57
1:B:394:ARG:O	1:B:397:ALA:HB3	2.05	0.57
1:B:659:THR:HG21	1:B:685:ARG:H	1.69	0.57
1:A:82:SER:OG	1:A:255:ALA:O	2.17	0.57
1:A:899:LEU:O	1:A:902:ARG:CG	2.52	0.57
1:B:31:VAL:CA	1:B:34:ILE:HG22	2.35	0.57
1:A:116:ARG:HG3	1:A:320:LEU:C	2.25	0.57
1:A:216:GLU:O	1:A:217:PHE:HB3	2.04	0.57
1:B:435:VAL:HA	1:B:442:ALA:HA	1.85	0.57
1:B:218:PRO:HB2	1:B:223:ALA:HB2	1.85	0.57
1:A:745:MET:HG2	1:A:745:MET:O	2.04	0.57
1:A:412:ILE:HG12	1:A:424:TYR:HB3	1.86	0.57
1:A:467:PRO:HG2	1:A:468:ASP:H	1.70	0.57
1:A:783:ARG:HD2	4:A:1186:HOH:O	2.03	0.57
1:B:145:LEU:CD2	1:B:211:LEU:HD11	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:VAL:HG12	1:A:130:MET:N	2.20	0.56
1:B:21:GLU:O	1:B:355:PHE:HB2	2.05	0.56
1:B:749:VAL:HG12	1:B:750:ASP:N	2.20	0.56
1:A:279:ASN:ND2	1:A:279:ASN:N	2.42	0.56
1:B:73:TRP:CH2	1:B:258:GLU:HB3	2.40	0.56
1:B:710:THR:CG2	1:B:712:LYS:H	2.12	0.56
1:B:869:THR:HG22	1:B:870:ILE:N	2.20	0.56
1:A:726:LEU:HD23	1:A:751:ILE:CD1	2.35	0.56
1:B:18:LEU:CD1	1:B:350:ASN:HB3	2.30	0.56
1:B:180:TYR:CE2	1:B:194:VAL:HG22	2.41	0.56
1:B:432:HIS:CD2	1:B:432:HIS:N	2.73	0.56
1:A:296:GLN:OE1	1:A:324:VAL:HG23	2.04	0.56
1:B:823:GLN:O	1:B:827:GLU:HG3	2.06	0.56
1:B:98:LEU:HD23	1:B:275:TYR:CB	2.36	0.56
1:B:441:LEU:HD12	1:B:442:ALA:H	1.70	0.56
1:A:78:TYR:CG	1:A:314:LEU:HD13	2.40	0.56
1:A:284:ASN:OD1	1:A:288:LEU:HD11	2.06	0.56
1:B:710:THR:HG23	1:B:711:HIS:N	2.21	0.56
1:A:667:ASP:OD1	1:A:670:ARG:NH2	2.39	0.56
1:B:432:HIS:H	1:B:432:HIS:HD2	1.51	0.56
1:B:744:ALA:O	1:B:746:ARG:N	2.38	0.56
1:B:1119:LEU:HD12	1:B:1120:LYS:N	2.21	0.56
1:A:5:TYR:N	1:A:5:TYR:CD1	2.73	0.56
1:A:351:ALA:O	1:A:352:ASN:HB2	2.05	0.56
1:A:802:ILE:HG22	1:A:806:ILE:CD1	2.36	0.56
1:A:18:LEU:O	1:A:19:LEU:HD23	2.05	0.56
1:A:889:ASP:OD1	1:A:889:ASP:N	2.37	0.56
1:A:939:LEU:HA	3:A:1151:EPE:O1S	2.06	0.56
1:A:1010:SER:O	1:A:1011:LEU:HB3	2.06	0.56
1:B:89:SER:HB2	1:B:174:MET:HE1	1.88	0.56
1:B:725:LEU:HD12	1:B:726:LEU:N	2.20	0.56
1:B:786:VAL:HG22	1:B:910:ALA:HB3	1.88	0.56
1:B:992:PRO:O	1:B:994:LEU:N	2.39	0.56
1:A:171:LEU:HG	1:A:173:PRO:HD3	1.88	0.55
1:A:168:LEU:HD23	1:A:181:ARG:HD3	1.88	0.55
1:A:714:LEU:HB3	1:A:741:ARG:HG2	1.86	0.55
1:B:27:CYS:O	1:B:30:LEU:HB3	2.05	0.55
1:B:32:ALA:O	1:B:36:GLU:HG3	2.06	0.55
1:B:44:LEU:O	1:B:107:ILE:HA	2.05	0.55
1:B:244:ILE:O	1:B:248:VAL:HG23	2.06	0.55
1:B:261:GLN:N	1:B:262:PRO:CD	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:VAL:HG12	1:A:904:GLY:N	2.22	0.55
1:B:791:ARG:O	1:B:915:LEU:HA	2.06	0.55
1:A:153:VAL:HG12	1:A:154:ASP:H	1.70	0.55
1:A:181:ARG:HG3	1:A:181:ARG:NH1	2.22	0.55
1:A:629:ASP:OD1	1:A:629:ASP:N	2.40	0.55
1:B:625:LEU:HD13	1:B:753:THR:CG2	2.37	0.55
1:B:625:LEU:HB3	1:B:773:LEU:HD23	1.89	0.55
1:A:840:ILE:CG2	1:A:841:GLY:N	2.69	0.55
1:B:7:TYR:HD2	1:B:8:THR:N	2.04	0.55
1:B:916:THR:OG1	1:B:917:PRO:HD2	2.07	0.55
1:A:564:VAL:HG21	1:A:963:GLN:CD	2.27	0.55
1:B:91:ARG:NH1	1:B:216:GLU:OE1	2.40	0.55
1:B:157:MET:O	1:B:197:VAL:HG11	2.06	0.55
1:A:463:ARG:O	1:A:782:ARG:HA	2.07	0.54
1:A:10:PRO:HB2	1:A:335:PRO:HB2	1.89	0.54
1:A:585:HIS:O	1:A:586:ASP:CB	2.55	0.54
1:B:1107:GLN:HA	1:B:1109:GLN:NE2	2.22	0.54
1:A:994:LEU:O	1:A:996:ASP:N	2.41	0.54
1:B:170:ASP:OD2	1:B:181:ARG:NH1	2.40	0.54
1:B:244:ILE:HD13	1:B:312:ARG:HG2	1.89	0.54
1:B:685:ARG:CG	3:B:1150:EPE:H61	2.36	0.54
1:A:164:THR:O	1:A:165:ARG:HG3	2.08	0.54
1:A:846:ARG:NH2	1:B:686:PHE:CE2	2.76	0.54
1:B:244:ILE:CD1	1:B:312:ARG:HG2	2.38	0.54
1:B:685:ARG:HG3	3:B:1150:EPE:H22	1.89	0.54
1:B:273:PHE:HA	1:B:276:PHE:CD1	2.43	0.54
1:B:483:VAL:HG12	1:B:484:VAL:N	2.23	0.54
1:B:22:LEU:O	1:B:341:THR:HG22	2.07	0.54
1:B:89:SER:HB2	1:B:174:MET:CE	2.37	0.54
1:B:662:ALA:O	1:B:682:MET:HE3	2.08	0.54
1:B:887:ARG:HG2	1:B:887:ARG:HH11	1.71	0.54
1:A:182:LEU:O	1:A:183:ASP:CB	2.56	0.54
1:A:242:GLU:HB2	1:A:311:MET:CE	2.37	0.54
1:A:377:PHE:CD2	1:A:378:LEU:HD23	2.41	0.54
1:A:868:THR:N	1:A:872:GLU:OE1	2.25	0.54
1:A:896:LEU:O	1:A:899:LEU:N	2.41	0.54
1:B:976:MET:O	1:B:980:GLU:HG3	2.08	0.54
1:B:1132:ILE:HG23	1:B:1133:GLU:N	2.23	0.54
1:A:387:PHE:N	1:A:424:TYR:O	2.37	0.54
1:A:994:LEU:C	1:A:996:ASP:N	2.61	0.54
1:B:994:LEU:C	1:B:996:ASP:N	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ASP:O	1:A:376:LYS:HG2	2.08	0.53
1:B:629:ASP:OD1	1:B:634:LYS:HE2	2.08	0.53
1:A:707:LEU:CD2	1:A:713:LEU:HD21	2.37	0.53
1:A:1076:ARG:O	1:A:1077:LYS:HB2	2.08	0.53
1:B:174:MET:HG3	1:B:213:PRO:O	2.08	0.53
1:A:48:ASP:OD1	1:A:48:ASP:N	2.41	0.53
1:A:327:LEU:O	1:A:331:LEU:HB2	2.08	0.53
1:A:447:SER:OG	1:A:453:ARG:HG3	2.07	0.53
1:A:733:ARG:HB2	1:B:821:ASN:ND2	2.24	0.53
1:A:76:LEU:HD12	1:A:807:LEU:HD12	1.90	0.53
1:B:284:ASN:CB	1:B:288:LEU:HD11	2.39	0.53
1:B:500:GLU:OE2	1:B:505:THR:HG23	2.08	0.53
1:B:1089:PHE:CE2	1:B:1095:VAL:HG21	2.43	0.53
1:A:460:ASP:CB	1:A:782:ARG:HD3	2.37	0.53
1:A:758:PRO:O	1:A:759:ILE:HD12	2.09	0.53
1:A:841:GLY:O	1:A:842:HIS:O	2.26	0.53
1:A:671:ASP:OD1	1:B:688:SER:HB3	2.09	0.53
1:A:842:HIS:O	1:A:845:MET:HG2	2.08	0.53
1:A:378:LEU:HD12	1:A:407:ILE:HD13	1.91	0.53
1:A:1085:GLY:HA3	1:A:1121:PHE:CZ	2.44	0.53
1:B:486:LEU:O	1:B:550:TRP:NE1	2.41	0.53
1:A:1077:LYS:HG3	1:A:1078:LEU:N	2.23	0.52
1:A:385:VAL:O	1:A:442:ALA:O	2.27	0.52
1:B:91:ARG:O	1:B:94:THR:N	2.36	0.52
1:B:181:ARG:NH2	1:B:200:GLN:O	2.42	0.52
1:A:76:LEU:HD13	1:A:804:ARG:HA	1.90	0.52
1:A:715:GLN:OE1	1:A:737:ARG:NH2	2.43	0.52
1:B:34:ILE:HD13	1:B:283:VAL:HG21	1.90	0.52
1:B:450:LEU:HB3	1:B:598:PRO:HB2	1.90	0.52
1:B:615:ASP:HB2	1:B:622:MET:HE3	1.91	0.52
1:A:77:PRO:O	1:A:302:ARG:NH1	2.41	0.52
1:B:281:LEU:HD12	1:B:281:LEU:C	2.29	0.52
1:B:1055:ASP:HB2	1:B:1056:PRO:HD3	1.91	0.52
1:B:1078:LEU:HD12	1:B:1078:LEU:C	2.30	0.52
1:A:763:LEU:HA	1:A:976:MET:HE1	1.90	0.52
1:A:859:HIS:CD2	1:A:861:ARG:NH2	2.77	0.52
1:A:875:ILE:HG22	1:A:876:ASP:N	2.24	0.52
1:B:147:SER:C	1:B:149:GLY:N	2.60	0.52
1:B:830:ALA:HB2	1:B:838:ILE:HD12	1.92	0.52
1:B:1091:GLU:CD	1:B:1092:LYS:H	2.13	0.52
1:A:26:ALA:O	1:A:29:THR:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:PHE:HB3	1:B:680:ILE:HD13	1.92	0.52
1:A:456:ARG:NE	1:A:876:ASP:OD1	2.42	0.52
1:A:612:VAL:HA	1:A:622:MET:CE	2.39	0.52
1:A:622:MET:HG2	1:A:623:ASP:N	2.25	0.52
1:B:1006:LEU:O	1:B:1131:ARG:NH1	2.43	0.52
1:A:206:VAL:HG12	1:A:207:GLU:N	2.24	0.52
1:A:385:VAL:HA	1:A:442:ALA:HB3	1.92	0.52
1:B:459:GLN:C	1:B:461:SER:H	2.14	0.52
1:A:30:LEU:HD11	1:A:353:LEU:HD12	1.91	0.51
1:B:62:PHE:HE2	1:B:426:MET:CE	2.23	0.51
1:A:376:LYS:O	1:A:380:THR:HG22	2.10	0.51
1:B:254:PRO:CD	1:B:257:ILE:HD12	2.12	0.51
1:B:898:GLN:HE21	1:B:902:ARG:NH2	2.07	0.51
1:A:974:LEU:O	1:A:977:GLU:HB3	2.10	0.51
1:B:50:GLN:HG2	1:B:860:GLN:NE2	2.26	0.51
1:A:1077:LYS:HB3	1:A:1088:GLU:HB3	1.91	0.51
1:B:535:GLY:O	1:B:536:ALA:HB2	2.09	0.51
1:A:178:LEU:H	1:A:178:LEU:CD2	2.11	0.51
1:A:382:ASP:CG	1:A:383:GLY:N	2.64	0.51
1:A:526:LEU:HD22	1:A:1027:TYR:HB3	1.93	0.51
1:A:992:PRO:O	1:A:994:LEU:N	2.43	0.51
1:A:1114:ASP:OD2	1:A:1118:ARG:HD3	2.10	0.51
1:B:564:VAL:HG21	1:B:963:GLN:CD	2.31	0.51
1:B:656:VAL:HG21	1:B:662:ALA:HA	1.91	0.51
1:B:887:ARG:HG2	1:B:887:ARG:NH1	2.26	0.51
1:A:436:ASP:O	1:A:440:ASN:HA	2.10	0.51
1:A:822:ILE:HD12	1:A:868:THR:HG21	1.88	0.51
1:B:10:PRO:CB	1:B:15:GLU:HB3	2.40	0.51
1:B:43:VAL:HG12	1:B:43:VAL:O	2.10	0.51
1:B:794:ASP:OD2	1:B:796:MET:HB3	2.10	0.51
1:A:170:ASP:CG	1:A:181:ARG:NH1	2.63	0.51
1:A:625:LEU:HD23	1:A:773:LEU:HD13	1.93	0.51
1:B:100:THR:O	1:B:101:MET:C	2.48	0.51
1:B:540:ALA:O	1:B:541:PRO:O	2.28	0.51
1:B:593:PHE:CD1	1:B:643:PHE:CD1	2.98	0.51
1:B:1136:ARG:CG	1:B:1136:ARG:NH1	2.65	0.51
1:A:37:ARG:O	1:A:38:HIS:HB2	2.11	0.51
1:A:261:GLN:N	1:A:262:PRO:CD	2.74	0.51
1:B:31:VAL:HG12	1:B:31:VAL:O	2.10	0.51
1:B:1026:PHE:CD2	1:B:1046:LEU:HD21	2.46	0.51
1:A:324:VAL:O	1:A:328:PHE:HD1	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ALA:HB3	1:B:434:PHE:CD2	2.45	0.51
1:B:416:ASP:C	1:B:418:ALA:H	2.14	0.51
1:B:501:ALA:HB2	4:B:1176:HOH:O	2.10	0.51
1:B:791:ARG:CG	1:B:791:ARG:NH1	2.67	0.51
1:B:835:GLU:OE1	1:B:835:GLU:N	2.36	0.51
1:A:686:PHE:O	1:A:687:ARG:HG2	2.11	0.51
1:B:74:GLU:HG2	1:B:808:ARG:HD3	1.92	0.51
1:B:501:ALA:C	1:B:503:GLY:H	2.14	0.51
1:A:509:LEU:HD23	1:A:529:ILE:HD12	1.92	0.50
1:B:685:ARG:CD	3:B:1150:EPE:H61	2.40	0.50
1:B:713:LEU:CD2	1:B:718:VAL:HG21	2.41	0.50
1:B:873:THR:CG2	1:B:902:ARG:HG3	2.41	0.50
1:B:992:PRO:C	1:B:994:LEU:N	2.64	0.50
1:A:1091:GLU:OE1	1:A:1091:GLU:N	2.41	0.50
1:B:430:ALA:HB1	1:B:445:CYS:HB3	1.93	0.50
1:A:602:THR:HB	1:A:605:GLN:HB2	1.93	0.50
1:A:893:LEU:O	1:A:894:ALA:C	2.49	0.50
1:A:895:GLN:O	1:A:896:LEU:C	2.49	0.50
1:A:916:THR:HB	1:A:917:PRO:CD	2.42	0.50
1:A:1114:ASP:O	1:A:1118:ARG:HB2	2.11	0.50
1:B:17:ARG:O	1:B:18:LEU:HD23	2.10	0.50
1:B:47:PRO:HD3	1:B:285:THR:HB	1.93	0.50
1:B:316:PRO:C	1:B:318:GLN:H	2.15	0.50
1:B:936:LEU:HA	3:B:1151:EPE:C5	2.41	0.50
1:B:1096:ASN:OD1	1:B:1147:ILE:HD11	2.11	0.50
1:B:63:THR:CG2	1:B:65:GLN:HB2	2.40	0.50
1:A:22:LEU:HD23	1:A:355:PHE:HD1	1.77	0.50
1:A:141:LEU:O	1:A:145:LEU:HG	2.10	0.50
1:A:1082:GLU:OE1	1:A:1131:ARG:NH2	2.44	0.50
1:B:33:GLU:HG3	1:B:34:ILE:N	2.26	0.50
1:B:605:GLN:NE2	1:B:634:LYS:HD2	2.15	0.50
1:A:519:LEU:HB2	1:A:545:LEU:HD21	1.94	0.50
1:A:1140:ARG:O	1:A:1144:GLU:HG3	2.12	0.50
1:B:117:VAL:HG21	1:B:272:LEU:CD1	2.40	0.50
1:A:195:PHE:HB2	1:A:201:ARG:O	2.12	0.50
1:A:258:GLU:OE1	1:A:258:GLU:N	2.33	0.50
1:A:452:GLU:HG2	1:A:855:ASN:OD1	2.12	0.50
1:A:460:ASP:O	1:A:461:SER:C	2.50	0.50
1:A:483:VAL:HG12	1:A:484:VAL:N	2.27	0.50
1:B:346:THR:O	1:B:347:LYS:C	2.49	0.50
1:B:827:GLU:C	1:B:829:LEU:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1107:GLN:N	1:B:1108:PRO:HD3	2.25	0.50
1:A:87:ILE:O	1:A:91:ARG:HG3	2.12	0.50
1:A:326:GLU:HA	1:A:329:SER:HB3	1.94	0.50
1:A:436:ASP:O	1:A:440:ASN:CA	2.60	0.50
1:A:629:ASP:CG	1:A:634:LYS:HE3	2.31	0.50
1:A:473:ASN:O	1:A:474:LEU:C	2.49	0.50
1:B:629:ASP:OD1	1:B:634:LYS:CG	2.59	0.50
1:B:936:LEU:CD2	3:B:1151:EPE:H62	2.40	0.50
1:A:153:VAL:CG1	1:A:154:ASP:N	2.74	0.49
1:A:260:TRP:C	1:A:262:PRO:HD2	2.32	0.49
1:A:474:LEU:N	1:A:474:LEU:CD2	2.73	0.49
1:A:645:ALA:O	1:A:650:LYS:HB2	2.10	0.49
1:A:78:TYR:CD2	1:A:314:LEU:HD22	2.46	0.49
1:A:382:ASP:CG	1:A:383:GLY:H	2.16	0.49
1:A:732:HIS:CE1	1:A:733:ARG:HD3	2.47	0.49
1:A:802:ILE:HG22	1:A:806:ILE:HD11	1.94	0.49
1:A:949:ASP:O	1:A:952:ILE:HB	2.12	0.49
1:B:28:ALA:HB2	1:B:58:GLU:HG2	1.93	0.49
1:B:481:GLN:NE2	1:B:531:ARG:NH1	2.59	0.49
1:A:61:GLN:OE1	1:A:430:ALA:HB2	2.12	0.49
1:B:98:LEU:HD23	1:B:275:TYR:HB3	1.95	0.49
1:B:691:GLU:O	1:B:695:ILE:HG13	2.12	0.49
1:A:182:LEU:HD22	1:A:192:LEU:HD13	1.93	0.49
1:A:237:VAL:HG12	1:A:238:LYS:N	2.27	0.49
1:A:805:GLU:OE2	1:A:881:ASN:HB2	2.12	0.49
1:B:84:HIS:CD2	1:B:86:ASP:HB2	2.47	0.49
1:B:98:LEU:HD23	1:B:275:TYR:HB2	1.95	0.49
1:A:22:LEU:HD21	1:A:353:LEU:HD12	1.93	0.49
1:A:309:ASP:OD1	1:A:310:PRO:HD2	2.11	0.49
1:A:749:VAL:HA	4:A:1199:HOH:O	2.12	0.49
1:A:1061:LEU:O	1:A:1064:ALA:HB3	2.12	0.49
1:A:1121:PHE:C	1:A:1122:ILE:HD13	2.33	0.49
1:B:10:PRO:HA	1:B:15:GLU:OE1	2.12	0.49
1:B:1076:ARG:HE	1:B:1090:ALA:CB	2.24	0.49
1:B:227:PHE:HA	1:B:263:LEU:O	2.12	0.49
1:A:2:PRO:HG2	1:A:3:GLU:H	1.77	0.49
1:A:387:PHE:CD2	1:A:444:ILE:HB	2.48	0.49
1:A:805:GLU:HG2	1:A:882:THR:OG1	2.13	0.49
1:A:869:THR:HG22	1:A:870:ILE:N	2.26	0.49
1:B:300:LEU:O	1:B:304:GLU:HG2	2.13	0.49
1:B:993:SER:O	1:B:995:GLU:N	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:PHE:CD2	1:A:313:PRO:HB2	2.47	0.49
1:A:388:SER:HB3	1:A:445:CYS:SG	2.53	0.49
1:A:455:ALA:O	1:A:878:PRO:HG2	2.13	0.49
1:A:636:GLU:O	1:A:640:ARG:HG3	2.13	0.49
1:A:899:LEU:HA	1:A:902:ARG:HD2	1.94	0.49
1:B:477:LEU:O	1:B:1021:ASN:ND2	2.43	0.49
1:B:923:THR:HG22	1:B:925:ASP:H	1.77	0.49
1:A:1103:LEU:HD22	1:A:1111:TYR:CD1	2.48	0.49
1:B:75:THR:HG22	1:B:76:LEU:H	1.78	0.49
1:A:129:VAL:C	1:A:130:MET:HG3	2.34	0.49
1:A:287:ASP:OD1	1:A:287:ASP:O	2.31	0.49
1:A:418:ALA:HA	1:A:424:TYR:CE1	2.47	0.49
1:A:467:PRO:HG2	1:A:468:ASP:N	2.26	0.49
1:A:626:VAL:HA	1:A:774:SER:O	2.13	0.49
1:A:1016:PHE:CE1	1:A:1054:PRO:HD3	2.47	0.49
1:B:634:LYS:CE	1:B:776:ILE:HG21	2.41	0.49
1:A:24:GLY:C	1:A:26:ALA:N	2.66	0.48
1:A:533:ALA:O	1:A:534:GLY:C	2.51	0.48
1:A:533:ALA:CB	1:A:972:PHE:HB3	2.44	0.48
1:B:869:THR:HG22	1:B:870:ILE:H	1.77	0.48
1:A:394:ARG:HD3	1:A:446:GLU:OE1	2.13	0.48
1:A:811:GLN:HG2	1:A:857:PHE:HD2	1.78	0.48
1:A:869:THR:HB	1:A:872:GLU:HG3	1.94	0.48
1:B:77:PRO:HG2	1:B:302:ARG:HD3	1.95	0.48
1:B:660:LEU:HD13	1:B:844:GLN:NE2	2.28	0.48
1:B:850:LEU:HB3	1:B:854:MET:CE	2.42	0.48
1:A:887:ARG:HG2	1:A:890:HIS:NE2	2.28	0.48
1:B:158:GLU:C	1:B:172:PHE:HD1	2.16	0.48
1:B:262:PRO:HG2	1:B:319:SER:HB3	1.95	0.48
1:B:842:HIS:O	1:B:845:MET:HG2	2.12	0.48
1:A:32:ALA:O	1:A:36:GLU:HG2	2.13	0.48
1:A:201:ARG:CD	1:A:1045:GLU:HG3	2.44	0.48
1:B:798:VAL:O	1:B:802:ILE:HG13	2.13	0.48
1:B:805:GLU:CG	1:B:882:THR:OG1	2.61	0.48
1:A:27:CYS:O	1:A:28:ALA:C	2.52	0.48
1:B:30:LEU:O	1:B:33:GLU:HG2	2.12	0.48
1:B:85:GLN:CD	1:B:158:GLU:HB3	2.34	0.48
1:B:816:TYR:CZ	1:B:822:ILE:HG23	2.47	0.48
1:B:888:ALA:O	1:B:889:ASP:C	2.50	0.48
1:A:179:PRO:HG2	1:A:195:PHE:O	2.14	0.48
1:A:498:THR:O	1:A:498:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:PHE:CZ	1:A:650:LYS:HE3	2.49	0.48
1:A:11:VAL:HG12	1:A:11:VAL:O	2.14	0.48
1:A:859:HIS:O	1:A:861:ARG:N	2.46	0.48
1:A:992:PRO:C	1:A:994:LEU:N	2.65	0.48
1:B:82:SER:OG	1:B:258:GLU:OE1	2.31	0.48
1:B:517:ALA:HB1	1:B:545:LEU:HD12	1.96	0.48
1:B:537:GLU:O	1:B:537:GLU:HG2	2.14	0.48
1:B:867:CYS:HB3	1:B:872:GLU:HB2	1.94	0.48
1:A:271:PRO:O	1:A:272:LEU:C	2.49	0.48
1:B:97:GLN:O	1:B:97:GLN:HG2	2.13	0.48
1:B:180:TYR:HB3	1:B:192:LEU:CD1	2.41	0.48
1:B:1085:GLY:HA3	1:B:1121:PHE:CZ	2.48	0.48
1:A:18:LEU:C	1:A:19:LEU:HD23	2.34	0.48
1:A:906:SER:O	1:A:907:HIS:HB2	2.13	0.48
1:B:833:VAL:O	1:B:836:ALA:HB3	2.14	0.48
1:B:1008:MET:HE1	1:B:1128:ARG:HG2	1.96	0.48
1:B:316:PRO:O	1:B:318:GLN:N	2.45	0.48
1:B:1047:ILE:HA	1:B:1051:GLY:O	2.13	0.48
1:A:73:TRP:CZ3	1:A:258:GLU:HB3	2.48	0.47
1:A:592:LEU:HD23	1:A:595:ASP:OD2	2.14	0.47
1:B:62:PHE:HE2	1:B:426:MET:HE1	1.78	0.47
1:B:168:LEU:HD21	1:B:181:ARG:HD3	1.96	0.47
1:B:523:VAL:O	1:B:526:LEU:HD23	2.14	0.47
1:A:654:VAL:HA	1:A:727:ILE:O	2.14	0.47
1:B:25:ALA:HB3	1:B:434:PHE:HD2	1.79	0.47
1:B:168:LEU:HD23	1:B:181:ARG:HD3	1.95	0.47
1:B:833:VAL:N	1:B:834:PRO:HD3	2.29	0.47
1:B:899:LEU:HA	1:B:902:ARG:HG2	1.96	0.47
1:B:986:LEU:N	1:B:986:LEU:HD12	2.29	0.47
1:B:1040:GLU:O	1:B:1043:LYS:HB3	2.14	0.47
1:A:153:VAL:CG1	1:A:154:ASP:H	2.27	0.47
1:B:612:VAL:HA	1:B:622:MET:HE1	1.94	0.47
1:B:683:ILE:HD12	1:B:692:GLN:HG2	1.96	0.47
1:A:328:PHE:O	1:A:332:LYS:HG3	2.14	0.47
1:A:940:GLY:H	3:A:1151:EPE:H92	1.79	0.47
1:B:588:GLU:O	1:B:592:LEU:HD23	2.15	0.47
1:B:659:THR:HA	1:B:662:ALA:HB3	1.97	0.47
1:A:696:LEU:HD22	1:A:718:VAL:HG13	1.97	0.47
1:B:459:GLN:OE1	1:B:459:GLN:HA	2.15	0.47
1:B:903:VAL:HG12	1:B:904:GLY:N	2.29	0.47
1:B:1100:LEU:HD11	1:B:1119:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:VAL:HG12	1:A:43:VAL:O	2.13	0.47
1:A:95:LEU:HD13	1:A:117:VAL:HG13	1.96	0.47
1:A:206:VAL:CG1	1:A:207:GLU:N	2.77	0.47
1:A:550:TRP:O	1:A:552:ARG:N	2.47	0.47
1:B:74:GLU:HG2	1:B:808:ARG:CD	2.43	0.47
1:B:227:PHE:CE2	1:B:248:VAL:HG21	2.49	0.47
1:B:271:PRO:HB3	1:B:322:LEU:HD21	1.97	0.47
1:B:710:THR:CG2	1:B:712:LYS:HB2	2.43	0.47
1:B:881:ASN:CA	1:B:903:VAL:HG13	2.45	0.47
1:A:118:CYS:O	1:A:275:TYR:OH	2.21	0.47
1:A:287:ASP:O	1:A:287:ASP:CG	2.52	0.47
1:A:386:VAL:HG13	1:A:412:ILE:HD11	1.97	0.47
1:A:471:ILE:HD13	1:A:948:HIS:CD2	2.49	0.47
1:A:945:LEU:O	1:A:948:HIS:HB3	2.15	0.47
1:A:1132:ILE:O	1:A:1136:ARG:CG	2.61	0.47
1:B:129:VAL:HG12	1:B:130:MET:N	2.29	0.47
1:B:307:GLY:HA2	1:B:314:LEU:CG	2.44	0.47
1:B:347:LYS:HB2	1:B:350:ASN:HD22	1.79	0.47
1:B:564:VAL:CG2	1:B:963:GLN:NE2	2.78	0.47
1:B:936:LEU:HD13	3:B:1151:EPE:O3S	2.15	0.47
1:B:956:GLY:HA2	1:B:967:MET:HE3	1.96	0.47
1:B:1040:GLU:O	1:B:1044:VAL:HG23	2.14	0.47
1:A:377:PHE:HA	1:A:380:THR:CG2	2.44	0.47
1:A:432:HIS:HA	1:A:445:CYS:CB	2.44	0.47
1:B:237:VAL:CG1	1:B:238:LYS:N	2.78	0.47
1:B:312:ARG:O	1:B:314:LEU:HD23	2.15	0.47
1:B:478:HIS:O	1:B:481:GLN:HG3	2.15	0.47
1:B:655:LEU:HA	1:B:655:LEU:HD23	1.72	0.47
1:B:760:PRO:HG3	1:B:951:GLU:HB3	1.97	0.47
1:B:991:GLU:CB	1:B:992:PRO:HD2	2.44	0.47
1:A:1097:PRO:O	1:A:1101:ILE:HG22	2.14	0.47
1:B:526:LEU:HD13	1:B:529:ILE:HG13	1.97	0.47
1:A:783:ARG:HA	1:A:939:LEU:O	2.15	0.47
1:A:792:GLU:O	1:A:793:TYR:C	2.53	0.47
1:B:316:PRO:HA	1:B:317:PRO:HD3	1.77	0.47
1:B:326:GLU:O	1:B:329:SER:HB3	2.15	0.47
1:B:805:GLU:HG3	1:B:882:THR:HB	1.96	0.47
1:A:92:LEU:HD22	1:A:123:LEU:HD21	1.97	0.46
1:A:817:ASN:O	1:A:818:ASP:HB2	2.15	0.46
1:B:41:PRO:HD2	1:B:279:ASN:O	2.15	0.46
1:B:279:ASN:O	1:B:280:THR:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:LYS:HB3	1:B:963:GLN:HE22	1.80	0.46
1:B:807:LEU:HD13	1:B:807:LEU:C	2.35	0.46
1:A:147:SER:C	1:A:149:GLY:N	2.69	0.46
1:A:206:VAL:HG12	1:A:208:ALA:H	1.79	0.46
1:A:484:VAL:O	1:A:529:ILE:HA	2.15	0.46
1:B:911:TYR:N	1:B:911:TYR:CD1	2.83	0.46
1:B:1121:PHE:C	1:B:1122:ILE:HD12	2.35	0.46
1:A:162:TYR:HA	1:A:170:ASP:O	2.16	0.46
1:A:201:ARG:HD3	1:A:1045:GLU:HG3	1.97	0.46
1:A:371:LEU:HD11	1:A:404:ARG:HE	1.79	0.46
1:A:742:ILE:C	1:A:744:ALA:N	2.69	0.46
1:A:805:GLU:CG	1:A:882:THR:OG1	2.63	0.46
1:A:1082:GLU:H	1:A:1082:GLU:HG2	1.46	0.46
1:B:262:PRO:HG3	1:B:269:LEU:CD1	2.46	0.46
1:B:799:ARG:O	1:B:803:LEU:HB2	2.15	0.46
1:B:1008:MET:CE	1:B:1128:ARG:HG2	2.45	0.46
1:A:132:LYS:O	1:A:132:LYS:HG3	2.15	0.46
1:A:412:ILE:HG22	1:A:417:GLU:OE1	2.16	0.46
1:B:625:LEU:HB3	1:B:773:LEU:CD2	2.45	0.46
1:A:182:LEU:HD22	1:A:192:LEU:CD1	2.46	0.46
1:A:377:PHE:HA	1:A:380:THR:HG22	1.97	0.46
1:B:97:GLN:OE1	1:B:101:MET:HE2	2.16	0.46
1:B:98:LEU:HB3	1:B:99:PRO:CD	2.42	0.46
1:B:153:VAL:CG1	1:B:154:ASP:N	2.77	0.46
1:B:242:GLU:HG3	1:B:311:MET:HE2	1.96	0.46
1:B:605:GLN:O	1:B:609:ILE:HG13	2.15	0.46
1:B:629:ASP:C	1:B:631:GLY:H	2.19	0.46
1:B:711:HIS:HA	1:B:714:LEU:HD12	1.98	0.46
1:B:120:HIS:HD1	1:B:275:TYR:HE2	1.62	0.46
1:B:683:ILE:HD11	1:B:695:ILE:HB	1.98	0.46
1:A:150:TYR:CE1	1:A:214:ALA:HB2	2.50	0.46
1:A:256:GLY:H	1:A:312:ARG:HH22	1.63	0.46
1:A:485:HIS:CE1	1:A:487:GLU:HB2	2.51	0.46
1:A:831:GLU:O	1:A:834:PRO:HD3	2.15	0.46
1:A:1006:LEU:HD12	1:A:1132:ILE:HD11	1.97	0.46
1:A:1122:ILE:C	1:A:1123:GLN:HG2	2.36	0.46
1:B:1011:LEU:HD23	1:B:1011:LEU:C	2.36	0.46
1:A:277:PRO:O	1:A:280:THR:CG2	2.57	0.46
1:A:839:ALA:HB2	1:A:862:PHE:CD2	2.51	0.46
1:A:1109:GLN:H	1:A:1109:GLN:HE21	1.62	0.46
1:B:30:LEU:C	1:B:32:ALA:H	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1125:LEU:HB3	1:B:1131:ARG:CB	2.44	0.46
1:A:433:GLY:HA3	1:A:443:LEU:O	2.15	0.46
1:B:226:LEU:HD22	1:B:230:GLN:NE2	2.31	0.46
1:B:361:LEU:HD22	1:B:374:LEU:HD12	1.98	0.46
1:B:827:GLU:O	1:B:829:LEU:N	2.49	0.46
1:A:602:THR:HG22	1:A:604:ASP:H	1.81	0.45
1:A:859:HIS:C	1:A:861:ARG:N	2.70	0.45
1:A:1032:SER:O	1:A:1033:ALA:C	2.54	0.45
1:B:7:TYR:OH	1:B:17:ARG:CZ	2.64	0.45
1:B:662:ALA:C	1:B:682:MET:CE	2.85	0.45
1:B:711:HIS:C	1:B:713:LEU:H	2.19	0.45
1:B:712:LYS:CD	3:B:1150:EPE:H72	2.46	0.45
1:B:805:GLU:HG2	1:B:882:THR:OG1	2.16	0.45
1:A:359:PRO:HG2	1:A:377:PHE:CE1	2.52	0.45
1:A:533:ALA:O	1:A:534:GLY:O	2.33	0.45
1:A:692:GLN:NE2	1:A:712:LYS:HE2	2.31	0.45
1:A:1103:LEU:HD21	1:A:1111:TYR:CZ	2.51	0.45
1:B:598:PRO:HD2	1:B:599:PHE:CE1	2.51	0.45
1:B:659:THR:HG23	3:B:1150:EPE:H21	1.97	0.45
1:B:778:THR:CG2	1:B:779:PRO:HD2	2.46	0.45
1:A:328:PHE:HA	1:A:331:LEU:HB2	1.98	0.45
1:A:903:VAL:CG1	1:A:904:GLY:N	2.79	0.45
1:A:244:ILE:CD1	1:A:312:ARG:HG3	2.47	0.45
1:B:327:LEU:O	1:B:331:LEU:HB2	2.16	0.45
1:B:1108:PRO:CD	1:B:1109:GLN:HE21	2.27	0.45
1:A:19:LEU:HD22	1:A:351:ALA:HB3	1.99	0.45
1:A:37:ARG:O	1:A:37:ARG:CG	2.64	0.45
1:A:201:ARG:NH1	1:A:201:ARG:HB3	2.31	0.45
1:A:446:GLU:HG2	1:A:450:LEU:HD12	1.98	0.45
1:A:859:HIS:C	1:A:861:ARG:H	2.18	0.45
1:B:384:PRO:O	1:B:441:LEU:HD12	2.17	0.45
1:A:9:LEU:HA	1:A:10:PRO:HD3	1.79	0.45
1:A:257:ILE:O	1:A:260:TRP:HB2	2.16	0.45
1:A:1054:PRO:O	1:A:1058:ARG:HG3	2.17	0.45
1:B:873:THR:HG22	1:B:902:ARG:HG3	1.99	0.45
1:B:110:VAL:O	1:B:112:THR:N	2.49	0.45
1:B:295:PHE:C	1:B:295:PHE:CD2	2.89	0.45
1:B:384:PRO:HA	1:B:422:GLY:N	2.31	0.45
1:B:800:GLU:O	1:B:804:ARG:N	2.45	0.45
1:A:23:THR:O	1:A:24:GLY:O	2.35	0.45
1:A:271:PRO:O	1:A:273:PHE:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:LEU:O	1:A:595:ASP:HB2	2.17	0.45
1:A:1078:LEU:HG	1:A:1087:ILE:HD13	1.97	0.45
1:B:14:GLY:O	1:B:16:GLN:HG2	2.17	0.45
1:B:25:ALA:O	1:B:26:ALA:C	2.54	0.45
1:B:254:PRO:O	1:B:257:ILE:HB	2.16	0.45
1:A:952:ILE:O	1:A:955:ALA:HB3	2.16	0.45
1:A:1103:LEU:CD2	1:A:1111:TYR:CE1	3.00	0.45
1:B:193:ARG:NH1	1:B:205:GLU:HG2	2.32	0.45
1:B:279:ASN:C	1:B:279:ASN:ND2	2.69	0.45
1:B:654:VAL:HA	1:B:727:ILE:O	2.17	0.45
1:B:720:PHE:CD1	1:B:723:LEU:HD22	2.52	0.45
1:B:909:GLN:HG3	1:B:910:ALA:N	2.32	0.45
1:A:404:ARG:NH1	1:A:591:GLN:HG2	2.32	0.45
1:B:170:ASP:OD1	1:B:181:ARG:NH1	2.50	0.45
1:B:452:GLU:OE2	1:B:859:HIS:CE1	2.70	0.45
1:B:760:PRO:HA	1:B:951:GLU:OE1	2.16	0.45
1:B:794:ASP:C	1:B:796:MET:N	2.70	0.45
1:B:1104:LEU:HD13	1:B:1113:LEU:HD11	1.99	0.45
1:A:61:GLN:CD	1:A:428:GLY:HA3	2.38	0.44
1:A:244:ILE:HD11	1:A:312:ARG:HG3	2.00	0.44
1:A:455:ALA:HB2	1:A:858:HIS:ND1	2.32	0.44
1:A:710:THR:HG22	1:A:711:HIS:ND1	2.31	0.44
1:B:113:LEU:CD1	1:B:272:LEU:HD23	2.40	0.44
1:B:666:TYR:HA	1:B:708:ILE:CD1	2.47	0.44
1:B:1013:PRO:HG2	1:B:1054:PRO:HB2	1.98	0.44
1:B:1035:THR:CB	1:B:1038:GLU:HG3	2.41	0.44
1:A:1006:LEU:CD1	1:A:1132:ILE:HD13	2.48	0.44
1:A:1107:GLN:N	1:A:1108:PRO:CD	2.80	0.44
1:B:150:TYR:CD2	1:B:160:GLY:HA2	2.51	0.44
1:B:710:THR:HG21	3:B:1150:EPE:H32	1.98	0.44
1:B:1075:ILE:HD12	1:B:1139:MET:CE	2.46	0.44
1:A:325:ASP:OD1	1:A:325:ASP:N	2.50	0.44
1:B:153:VAL:CG1	1:B:154:ASP:H	2.28	0.44
1:B:412:ILE:HD12	1:B:424:TYR:CB	2.48	0.44
1:B:713:LEU:HD23	1:B:718:VAL:HG21	1.99	0.44
1:A:84:HIS:CD2	1:A:86:ASP:H	2.36	0.44
1:A:280:THR:HG23	1:A:334:TRP:CD1	2.51	0.44
1:A:1019:ASP:O	1:A:1020:VAL:C	2.54	0.44
1:B:12:LYS:C	1:B:335:PRO:HG3	2.38	0.44
1:B:710:THR:HG21	3:B:1150:EPE:C3	2.48	0.44
1:B:827:GLU:C	1:B:829:LEU:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:VAL:HG13	1:A:622:MET:CE	2.45	0.44
1:A:771:ARG:HG3	1:A:771:ARG:HH11	1.83	0.44
1:A:812:VAL:HB	1:A:864:VAL:HG22	1.98	0.44
1:B:174:MET:HB3	1:B:174:MET:HE3	1.92	0.44
1:A:626:VAL:HG22	1:A:774:SER:HB2	1.99	0.44
1:A:1065:ARG:O	1:A:1069:GLN:HG3	2.17	0.44
1:B:116:ARG:HD3	1:B:269:LEU:O	2.18	0.44
1:A:84:HIS:HD2	1:A:86:ASP:N	2.15	0.44
1:A:387:PHE:HD2	1:A:444:ILE:HB	1.81	0.44
1:A:1006:LEU:CD1	1:A:1132:ILE:CD1	2.95	0.44
1:B:119:PRO:HG2	1:B:265:PHE:CD2	2.52	0.44
1:B:346:THR:O	1:B:346:THR:HG22	2.18	0.44
1:B:564:VAL:HG21	1:B:963:GLN:NE2	2.33	0.44
1:B:746:ARG:HG3	1:B:751:ILE:HG13	1.98	0.44
1:A:257:ILE:CG2	1:A:258:GLU:N	2.79	0.44
1:A:812:VAL:HG22	1:A:882:THR:HB	1.99	0.44
1:B:8:THR:O	1:B:9:LEU:CB	2.65	0.44
1:B:660:LEU:HD23	1:B:660:LEU:HA	1.68	0.44
1:A:34:ILE:HG22	1:A:34:ILE:O	2.18	0.44
1:A:138:ARG:NH1	1:A:166:GLY:O	2.49	0.44
1:A:470:LEU:HD23	1:A:475:ALA:HB3	2.00	0.44
1:A:552:ARG:O	1:A:555:GLN:N	2.41	0.44
1:A:632:PHE:CE1	1:A:851:GLU:HB3	2.53	0.44
1:A:756:ALA:O	1:A:757:THR:C	2.55	0.44
1:A:1032:SER:O	1:A:1033:ALA:O	2.35	0.44
1:B:488:HIS:O	1:B:550:TRP:CG	2.71	0.44
1:A:239:ARG:O	1:A:240:ASP:C	2.55	0.43
1:A:1077:LYS:HE3	1:A:1079:GLU:HG2	2.01	0.43
1:A:33:GLU:HA	1:A:36:GLU:HG3	1.99	0.43
1:A:43:VAL:HG22	1:A:106:LEU:HD23	1.99	0.43
1:A:654:VAL:HG13	1:A:727:ILE:HB	1.99	0.43
1:A:1103:LEU:CD2	1:A:1111:TYR:CD1	3.01	0.43
1:B:25:ALA:HB2	1:B:432:HIS:O	2.18	0.43
1:B:592:LEU:O	1:B:595:ASP:HB2	2.17	0.43
1:B:657:PRO:C	1:B:658:THR:HG23	2.38	0.43
1:B:936:LEU:HD22	3:B:1151:EPE:H102	1.99	0.43
1:A:31:VAL:HG11	1:A:44:LEU:HD22	2.01	0.43
1:A:98:LEU:HD12	1:A:98:LEU:O	2.18	0.43
1:A:138:ARG:HG3	1:A:184:PHE:CE1	2.53	0.43
1:A:257:ILE:O	1:A:259:TYR:N	2.51	0.43
1:A:791:ARG:HD2	4:A:1156:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:GLU:O	1:B:267:GLU:HG3	2.18	0.43
1:B:899:LEU:O	1:B:902:ARG:HG2	2.17	0.43
1:A:117:VAL:CG1	1:A:118:CYS:H	2.31	0.43
1:A:583:PHE:O	1:A:584:LYS:HB2	2.18	0.43
1:A:883:ILE:HG22	1:A:903:VAL:HG21	2.00	0.43
1:A:883:ILE:CD1	1:A:885:ILE:HD11	2.48	0.43
1:A:938:ASP:O	3:A:1151:EPE:H101	2.18	0.43
1:B:30:LEU:C	1:B:32:ALA:N	2.72	0.43
1:B:84:HIS:O	1:B:87:ILE:HB	2.18	0.43
1:B:295:PHE:HD2	1:B:295:PHE:O	2.01	0.43
1:B:453:ARG:CZ	1:B:453:ARG:CB	2.96	0.43
1:B:816:TYR:CZ	1:B:818:ASP:HA	2.53	0.43
1:A:169:LEU:HD13	1:A:170:ASP:N	2.34	0.43
1:A:425:LEU:HD12	1:A:425:LEU:C	2.38	0.43
1:A:618:GLN:HA	1:A:619:PRO:HD3	1.83	0.43
1:A:627:CYS:HA	1:A:755:THR:O	2.19	0.43
1:A:713:LEU:HA	1:A:713:LEU:HD23	1.75	0.43
1:A:978:LEU:O	1:A:981:ASN:HB3	2.19	0.43
1:A:1007:ARG:O	1:A:1007:ARG:HG2	2.17	0.43
1:B:120:HIS:C	1:B:122:PHE:H	2.22	0.43
1:B:483:VAL:CG1	1:B:484:VAL:N	2.81	0.43
1:A:21:GLU:O	1:A:21:GLU:HG3	2.18	0.43
1:A:216:GLU:O	1:A:217:PHE:CB	2.67	0.43
1:A:583:PHE:CE2	1:A:645:ALA:HA	2.54	0.43
1:A:932:ALA:O	1:A:935:SER:HB3	2.19	0.43
1:B:38:HIS:HD2	1:B:281:LEU:HD23	1.79	0.43
1:B:122:PHE:HB2	1:B:265:PHE:HE2	1.83	0.43
1:B:272:LEU:O	1:B:272:LEU:HD12	2.18	0.43
1:B:899:LEU:O	1:B:900:ARG:C	2.56	0.43
1:A:75:THR:HG21	1:A:81:PHE:O	2.18	0.43
1:A:1032:SER:C	1:A:1033:ALA:O	2.56	0.43
1:B:634:LYS:HD2	1:B:634:LYS:HA	1.82	0.43
1:B:667:ASP:OD2	1:B:846:ARG:NE	2.51	0.43
1:A:231:TRP:CZ2	1:A:243:HIS:HE1	2.37	0.43
1:A:840:ILE:HG21	1:A:842:HIS:CE1	2.53	0.43
1:A:995:GLU:C	1:A:997:LEU:N	2.71	0.43
1:A:1004:VAL:O	1:A:1004:VAL:HG12	2.18	0.43
1:B:683:ILE:HD13	1:B:683:ILE:HA	1.94	0.43
1:B:1053:LEU:HA	1:B:1054:PRO:HD3	1.86	0.43
1:A:602:THR:HG22	1:A:603:PRO:N	2.33	0.43
1:A:905:ARG:HD3	3:A:1152:EPE:O3S	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979:LEU:O	1:A:980:GLU:C	2.57	0.43
1:B:117:VAL:O	1:B:269:LEU:HD22	2.18	0.43
1:B:312:ARG:N	1:B:313:PRO:HD3	2.34	0.43
1:B:850:LEU:HB3	1:B:854:MET:HE1	2.00	0.43
1:B:873:THR:O	1:B:873:THR:HG22	2.18	0.43
1:B:1001:GLN:HA	4:B:1195:HOH:O	2.18	0.43
1:A:95:LEU:HD13	1:A:117:VAL:CG1	2.49	0.43
1:A:842:HIS:NE2	3:B:1150:EPE:C6	2.81	0.43
1:A:1105:GLN:O	1:A:1108:PRO:HD3	2.19	0.43
1:A:1110:HIS:C	1:A:1111:TYR:CD1	2.92	0.43
1:B:20:GLY:HA3	1:B:352:ASN:CA	2.30	0.43
1:B:51:ASN:O	1:B:54:ARG:HB3	2.19	0.43
1:B:85:GLN:NE2	1:B:158:GLU:HB3	2.34	0.43
1:B:759:ILE:HG23	1:B:763:LEU:HD23	2.00	0.43
1:A:8:THR:O	1:A:17:ARG:HG2	2.19	0.42
1:A:76:LEU:CD1	1:A:807:LEU:HD12	2.48	0.42
1:A:257:ILE:HG22	1:A:258:GLU:N	2.34	0.42
1:A:354:GLY:HA3	1:A:437:THR:HB	2.01	0.42
1:B:630:VAL:O	1:B:630:VAL:CG1	2.61	0.42
1:B:692:GLN:HE22	1:B:712:LYS:CD	2.32	0.42
1:B:758:PRO:HG2	1:B:951:GLU:HG2	2.01	0.42
1:A:33:GLU:C	1:A:35:ALA:N	2.72	0.42
1:A:91:ARG:O	1:A:92:LEU:C	2.55	0.42
1:A:618:GLN:C	1:A:620:LEU:H	2.22	0.42
1:A:1011:LEU:CD2	1:A:1056:PRO:HB3	2.49	0.42
1:A:1068:GLN:O	1:A:1071:GLN:N	2.52	0.42
1:B:296:GLN:OE1	1:B:324:VAL:HG23	2.19	0.42
1:B:580:GLY:N	1:B:619:PRO:O	2.52	0.42
1:B:692:GLN:NE2	1:B:712:LYS:HD3	2.31	0.42
1:B:1045:GLU:O	1:B:1046:LEU:C	2.57	0.42
1:A:113:LEU:HD12	1:A:272:LEU:HD23	2.01	0.42
1:A:636:GLU:CD	1:A:672:ARG:HH21	2.22	0.42
1:A:885:ILE:CD1	1:A:899:LEU:HD13	2.48	0.42
1:B:372:ASP:O	1:B:373:ALA:C	2.57	0.42
1:B:650:LYS:HB3	1:B:724:GLY:HA3	2.01	0.42
1:B:1010:SER:OG	1:B:1060:LEU:HA	2.19	0.42
1:B:1073:LEU:HD13	1:B:1142:LEU:CD2	2.49	0.42
1:B:1110:HIS:O	1:B:1121:PHE:HA	2.19	0.42
1:A:33:GLU:C	1:A:35:ALA:H	2.22	0.42
1:B:158:GLU:C	1:B:172:PHE:CD1	2.93	0.42
1:B:162:TYR:CD1	1:B:162:TYR:C	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1100:LEU:CD1	1:B:1119:LEU:HD22	2.49	0.42
1:A:23:THR:HG22	1:A:24:GLY:N	2.35	0.42
1:A:169:LEU:HD13	1:A:169:LEU:C	2.40	0.42
1:A:186:ASP:O	1:A:188:GLU:N	2.53	0.42
1:A:246:GLN:HE21	1:A:250:LYS:HE3	1.85	0.42
1:A:467:PRO:CG	1:A:468:ASP:H	2.33	0.42
1:A:895:GLN:O	1:A:898:GLN:HB3	2.19	0.42
1:B:301:ALA:O	1:B:304:GLU:HB2	2.19	0.42
1:B:398:LEU:O	1:B:402:LEU:HG	2.20	0.42
1:B:681:GLU:HG3	1:B:682:MET:N	2.35	0.42
1:B:793:TYR:CE1	1:B:798:VAL:HG21	2.54	0.42
1:B:1035:THR:CG2	1:B:1036:GLU:N	2.83	0.42
1:B:1066:LEU:O	1:B:1067:ARG:C	2.58	0.42
1:A:61:GLN:NE2	1:A:428:GLY:HA3	2.35	0.42
1:A:742:ILE:O	1:A:744:ALA:N	2.53	0.42
1:B:81:PHE:CD2	1:B:911:TYR:HE2	2.38	0.42
1:B:371:LEU:HD11	1:B:404:ARG:HE	1.84	0.42
1:B:711:HIS:C	1:B:713:LEU:N	2.73	0.42
1:B:732:HIS:CE1	1:B:733:ARG:HG3	2.54	0.42
1:B:1076:ARG:HE	1:B:1090:ALA:HB1	1.85	0.42
1:B:1132:ILE:CG2	1:B:1133:GLU:N	2.82	0.42
1:A:293:GLU:HG3	1:A:324:VAL:HG21	2.02	0.42
1:B:201:ARG:HD3	1:B:1045:GLU:HG3	2.02	0.42
1:B:846:ARG:O	1:B:849:GLU:HB2	2.20	0.42
1:B:903:VAL:CG1	1:B:904:GLY:N	2.83	0.42
1:B:1020:VAL:HB	4:B:1187:HOH:O	2.19	0.42
1:B:1109:GLN:HE21	1:B:1109:GLN:H	1.67	0.42
1:A:707:LEU:HD23	1:A:713:LEU:HD11	2.02	0.42
1:B:147:SER:O	1:B:149:GLY:N	2.53	0.42
1:A:17:ARG:HA	1:A:17:ARG:HD2	1.85	0.42
1:A:1041:GLU:HA	1:A:1041:GLU:OE1	2.20	0.42
1:A:1069:GLN:HB2	1:A:1139:MET:CE	2.48	0.42
1:B:690:LYS:O	1:B:691:GLU:C	2.56	0.42
1:B:993:SER:C	1:B:995:GLU:H	2.20	0.42
1:A:395:ARG:NH1	1:A:425:LEU:HD21	2.35	0.41
1:A:669:PHE:HB3	1:A:680:ILE:HD13	2.01	0.41
1:A:933:ILE:C	1:A:935:SER:N	2.73	0.41
1:B:243:HIS:O	1:B:244:ILE:C	2.58	0.41
1:A:76:LEU:O	1:A:79:ASP:N	2.54	0.41
1:A:150:TYR:CD1	1:A:214:ALA:HB2	2.55	0.41
1:A:228:ARG:NH1	1:A:245:TYR:OH	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:PHE:CD2	1:A:276:PHE:HE2	2.37	0.41
1:A:618:GLN:O	1:A:620:LEU:N	2.52	0.41
1:A:721:LYS:O	1:A:722:ASP:HB2	2.21	0.41
1:A:870:ILE:HD13	1:A:895:GLN:HB3	2.02	0.41
1:A:941:ALA:O	1:A:944:ALA:N	2.53	0.41
1:B:615:ASP:HB2	1:B:622:MET:CE	2.51	0.41
1:A:270:PRO:HA	1:A:271:PRO:HD3	1.88	0.41
1:A:280:THR:HG23	1:A:334:TRP:NE1	2.36	0.41
1:A:385:VAL:O	1:A:386:VAL:O	2.37	0.41
1:B:135:ARG:HG2	1:B:188:GLU:CG	2.46	0.41
1:B:837:ARG:NH1	1:B:837:ARG:HG3	2.35	0.41
1:A:389:VAL:HG11	1:A:395:ARG:N	2.35	0.41
1:A:566:ALA:O	1:A:567:GLU:C	2.58	0.41
1:A:725:LEU:CD2	1:A:726:LEU:N	2.83	0.41
1:A:761:ARG:HG3	1:A:761:ARG:HH11	1.85	0.41
1:A:1026:PHE:O	1:A:1030:ILE:HG13	2.21	0.41
1:B:430:ALA:HB1	1:B:445:CYS:CB	2.50	0.41
1:B:430:ALA:O	1:B:431:GLU:O	2.38	0.41
1:B:527:HIS:CE1	1:B:528:LEU:HD21	2.55	0.41
1:B:840:ILE:HG22	1:B:841:GLY:N	2.36	0.41
1:A:686:PHE:C	1:A:687:ARG:HG2	2.40	0.41
1:A:850:LEU:HD22	1:A:854:MET:HE2	2.03	0.41
1:A:875:ILE:CG2	1:A:876:ASP:N	2.84	0.41
1:B:131:LYS:N	1:B:134:GLN:HG3	2.27	0.41
1:B:918:HIS:HB3	1:B:920:LYS:HG2	2.02	0.41
1:A:85:GLN:H	1:A:85:GLN:HG3	1.43	0.41
1:A:137:SER:O	1:A:140:ALA:HB3	2.21	0.41
1:A:377:PHE:C	1:A:380:THR:HG22	2.41	0.41
1:A:805:GLU:HG3	1:A:882:THR:HB	2.02	0.41
1:B:45:ILE:HD12	1:B:113:LEU:HD22	2.02	0.41
1:A:55:LEU:O	1:A:59:ILE:HG13	2.20	0.41
1:A:581:PHE:CD2	1:A:582:ALA:O	2.74	0.41
1:A:763:LEU:HA	1:A:976:MET:CE	2.49	0.41
1:B:244:ILE:CD1	1:B:244:ILE:H	2.33	0.41
1:B:347:LYS:O	1:B:350:ASN:N	2.54	0.41
1:B:627:CYS:HA	1:B:755:THR:O	2.20	0.41
1:A:74:GLU:HG2	1:A:808:ARG:HB2	2.03	0.41
1:A:911:TYR:N	1:A:911:TYR:HD1	2.17	0.41
1:A:1047:ILE:O	1:A:1051:GLY:HA2	2.20	0.41
1:B:49:MET:O	1:B:52:ALA:CB	2.67	0.41
1:B:614:SER:O	1:B:617:CYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:VAL:HG22	1:B:709:GLY:O	2.19	0.41
1:A:9:LEU:CD1	1:A:37:ARG:O	2.69	0.41
1:A:21:GLU:HG3	1:A:353:LEU:O	2.21	0.41
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.82	0.41
1:A:656:VAL:HA	1:A:657:PRO:HD3	1.83	0.41
1:A:710:THR:HB	1:A:712:LYS:H	1.86	0.41
1:A:726:LEU:HB3	1:A:751:ILE:HG12	2.02	0.41
1:A:763:LEU:O	1:A:763:LEU:HG	2.20	0.41
1:A:983:VAL:O	1:A:984:ASP:C	2.59	0.41
1:B:73:TRP:HB3	1:B:75:THR:OG1	2.21	0.41
1:B:76:LEU:O	1:B:77:PRO:C	2.56	0.41
1:B:77:PRO:HG2	1:B:302:ARG:CD	2.51	0.41
1:B:96:TYR:HA	1:B:123:LEU:HD21	2.02	0.41
1:B:196:ASP:O	1:B:200:GLN:N	2.36	0.41
1:B:430:ALA:CB	1:B:445:CYS:HB3	2.51	0.41
1:B:659:THR:HG23	3:B:1150:EPE:C2	2.51	0.41
1:B:710:THR:O	1:B:713:LEU:HB2	2.21	0.41
1:B:791:ARG:HG3	1:B:791:ARG:NH1	2.12	0.41
1:B:874:GLY:O	1:B:876:ASP:N	2.54	0.41
1:B:883:ILE:HG12	1:B:885:ILE:HD12	2.02	0.41
1:B:1039:LEU:HD23	1:B:1039:LEU:HA	1.82	0.41
1:A:456:ARG:HG2	1:A:876:ASP:OD2	2.21	0.41
1:A:1078:LEU:O	1:A:1078:LEU:CD2	2.68	0.41
1:B:312:ARG:O	1:B:313:PRO:C	2.59	0.41
1:B:485:HIS:HD2	1:B:486:LEU:N	2.19	0.41
1:B:499:LEU:O	1:B:505:THR:HA	2.20	0.41
1:B:811:GLN:HG3	1:B:863:ASN:HA	2.03	0.41
1:B:979:LEU:O	1:B:983:VAL:HG23	2.20	0.41
1:A:178:LEU:HB2	1:A:179:PRO:HD2	2.02	0.40
1:A:779:PRO:HA	1:A:780:PRO:HD3	1.83	0.40
1:A:1066:LEU:O	1:A:1067:ARG:C	2.59	0.40
1:A:1075:ILE:HA	1:A:1089:PHE:HA	2.02	0.40
1:B:276:PHE:HA	1:B:277:PRO:HD3	1.93	0.40
1:B:471:ILE:H	1:B:471:ILE:HG13	1.58	0.40
1:B:613:LEU:HA	1:B:613:LEU:HD23	1.77	0.40
1:B:873:THR:HG22	1:B:902:ARG:CG	2.51	0.40
1:B:1047:ILE:HG12	1:B:1053:LEU:HD13	2.03	0.40
1:A:157:MET:O	1:A:197:VAL:HG11	2.21	0.40
1:A:345:PRO:O	1:A:347:LYS:N	2.54	0.40
1:A:377:PHE:CA	1:A:380:THR:HG22	2.51	0.40
1:A:513:TYR:CD1	1:A:545:LEU:HD13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:LEU:HA	1:A:595:ASP:OD2	2.20	0.40
1:A:892:GLY:O	1:A:893:LEU:C	2.60	0.40
1:A:936:LEU:HD13	3:A:1151:EPE:C10	2.48	0.40
1:A:1142:LEU:HD12	1:A:1142:LEU:O	2.21	0.40
1:B:45:ILE:HD12	1:B:113:LEU:CD2	2.50	0.40
1:B:257:ILE:O	1:B:257:ILE:HG12	2.22	0.40
1:B:416:ASP:C	1:B:418:ALA:N	2.74	0.40
1:B:416:ASP:O	1:B:418:ALA:N	2.54	0.40
1:B:735:GLY:O	1:B:739:LYS:HE3	2.22	0.40
1:B:991:GLU:CG	1:B:992:PRO:HD2	2.51	0.40
1:A:16:GLN:O	1:A:17:ARG:CD	2.69	0.40
1:A:117:VAL:HG21	1:A:272:LEU:HD13	2.04	0.40
1:A:129:VAL:CG1	1:A:130:MET:N	2.84	0.40
1:A:209:ILE:O	1:A:209:ILE:HG23	2.22	0.40
1:A:466:ASN:HB2	1:A:469:THR:CB	2.51	0.40
1:A:505:THR:HB	4:A:1208:HOH:O	2.20	0.40
1:A:1047:ILE:O	1:A:1051:GLY:N	2.52	0.40
1:A:1068:GLN:O	1:A:1069:GLN:C	2.59	0.40
1:B:75:THR:HG22	1:B:79:ASP:CB	2.52	0.40
1:B:502:GLY:HA3	1:B:1007:ARG:HH12	1.86	0.40
1:B:602:THR:HG23	1:B:603:PRO:HD2	2.03	0.40
1:B:906:SER:O	1:B:907:HIS:CB	2.69	0.40
1:A:48:ASP:OD1	1:A:51:ASN:ND2	2.54	0.40
1:A:231:TRP:O	1:A:234:THR:N	2.44	0.40
1:A:526:LEU:CD2	1:A:1027:TYR:HB3	2.51	0.40
1:A:562:ARG:HG3	1:A:992:PRO:CG	2.50	0.40
1:B:387:PHE:HB2	1:B:424:TYR:O	2.21	0.40
1:A:156:VAL:CG1	1:A:156:VAL:O	2.69	0.40
1:A:385:VAL:HG23	1:A:423:ARG:NH1	2.36	0.40
1:A:947:THR:O	1:A:951:GLU:HG3	2.21	0.40
1:A:993:SER:C	1:A:995:GLU:H	2.25	0.40
1:B:252:THR:O	1:B:253:LEU:HD23	2.22	0.40
1:B:639:MET:HE3	1:B:672:ARG:HB2	2.03	0.40
1:B:744:ALA:C	1:B:746:ARG:N	2.75	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	1144/1151 (99%)	941 (82%)	153 (13%)	50 (4%)	2	19
1	B	1141/1151 (99%)	942 (83%)	153 (13%)	46 (4%)	3	21
All	All	2285/2302 (99%)	1883 (82%)	306 (13%)	96 (4%)	3	20

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLY
1	A	25	ALA
1	A	38	HIS
1	A	132	LYS
1	A	187	ASP
1	A	346	THR
1	A	386	VAL
1	A	461	SER
1	A	469	THR
1	A	585	HIS
1	A	736	VAL
1	A	842	HIS
1	A	1146	ALA
1	B	244	ILE
1	B	255	ALA
1	B	419	SER
1	B	422	GLY
1	B	431	GLU
1	B	541	PRO
1	B	745	MET
1	B	819	VAL
1	B	993	SER
1	B	995	GLU
1	A	217	PHE
1	A	433	GLY

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Mol	Chain	Res	Type
1	A	438	VAL
1	A	534	GLY
1	A	551	SER
1	A	586	ASP
1	A	820	GLU
1	A	942	GLY
1	A	993	SER
1	A	995	GLU
1	A	1075	ILE
1	B	52	ALA
1	B	241	PRO
1	B	317	PRO
1	B	360	ASP
1	B	372	ASP
1	B	429	ALA
1	B	875	ILE
1	B	994	LEU
1	A	183	ASP
1	A	220	ASP
1	A	470	LEU
1	A	550	TRP
1	A	619	PRO
1	A	722	ASP
1	A	1033	ALA
1	A	1077	LYS
1	B	101	MET
1	B	111	ASN
1	B	347	LYS
1	B	348	ALA
1	B	409	PRO
1	B	417	GLU
1	B	501	ALA
1	B	630	VAL
1	B	715	GLN
1	B	746	ARG
1	B	828	ARG
1	A	182	LEU
1	A	186	ASP
1	A	190	ASP
1	A	258	GLU
1	A	437	THR
1	A	468	ASP

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Mol	Chain	Res	Type
1	A	941	ALA
1	B	9	LEU
1	B	345	PRO
1	B	382	ASP
1	B	479	ILE
1	B	536	ALA
1	B	748	ASN
1	A	213	PRO
1	A	768	SER
1	A	780	PRO
1	A	860	GLN
1	A	919	PRO
1	A	1054	PRO
1	B	26	ALA
1	B	744	ALA
1	B	917	PRO
1	A	156	VAL
1	A	819	VAL
1	B	134	GLN
1	B	242	GLU
1	B	308	VAL
1	B	460	ASP
1	B	623	ASP
1	B	117	VAL
1	A	875	ILE
1	A	917	PRO
1	B	110	VAL
1	B	197	VAL
1	A	1020	VAL

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	930/975 (95%)	843 (91%)	87 (9%)	8 33
1	B	904/975 (93%)	838 (93%)	66 (7%)	14 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1834/1950 (94%)	1681 (92%)	153 (8%)	11	40

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	TYR
1	A	17	ARG
1	A	36	GLU
1	A	49	MET
1	A	75	THR
1	A	77	PRO
1	A	85	GLN
1	A	89	SER
1	A	142	ARG
1	A	172	PHE
1	A	178	LEU
1	A	192	LEU
1	A	194	VAL
1	A	197	VAL
1	A	205	GLU
1	A	226	LEU
1	A	234	THR
1	A	257	ILE
1	A	260	TRP
1	A	279	ASN
1	A	287	ASP
1	A	296	GLN
1	A	312	ARG
1	A	325	ASP
1	A	331	LEU
1	A	346	THR
1	A	366	GLN
1	A	372	ASP
1	A	374	LEU
1	A	378	LEU
1	A	395	ARG
1	A	411	ARG
1	A	412	ILE
1	A	414	ARG
1	A	432	HIS
1	A	434	PHE
1	A	443	LEU

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Mol	Chain	Res	Type
1	A	453	ARG
1	A	474	LEU
1	A	487	GLU
1	A	498	THR
1	A	523	VAL
1	A	526	LEU
1	A	562	ARG
1	A	627	CYS
1	A	629	ASP
1	A	646	VAL
1	A	658	THR
1	A	672	ARG
1	A	679	ARG
1	A	710	THR
1	A	713	LEU
1	A	715	GLN
1	A	725	LEU
1	A	746	ARG
1	A	749	VAL
1	A	751	ILE
1	A	783	ARG
1	A	803	LEU
1	A	805	GLU
1	A	808	ARG
1	A	816	TYR
1	A	844	GLN
1	A	845	MET
1	A	847	GLU
1	A	850	LEU
1	A	865	LEU
1	A	879	THR
1	A	883	ILE
1	A	889	ASP
1	A	890	HIS
1	A	900	ARG
1	A	902	ARG
1	A	905	ARG
1	A	911	TYR
1	A	918	HIS
1	A	923	THR
1	A	945	LEU
1	A	1010	SER

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Mol	Chain	Res	Type
1	A	1011	LEU
1	A	1021	ASN
1	A	1082	GLU
1	A	1103	LEU
1	A	1109	GLN
1	A	1118	ARG
1	A	1122	ILE
1	A	1130	THR
1	B	7	TYR
1	B	15	GLU
1	B	27	CYS
1	B	45	ILE
1	B	85	GLN
1	B	102	GLN
1	B	134	GLN
1	B	142	ARG
1	B	164	THR
1	B	171	LEU
1	B	172	PHE
1	B	186	ASP
1	B	197	VAL
1	B	200	GLN
1	B	201	ARG
1	B	205	GLU
1	B	209	ILE
1	B	219	THR
1	B	226	LEU
1	B	240	ASP
1	B	252	THR
1	B	267	GLU
1	B	279	ASN
1	B	287	ASP
1	B	295	PHE
1	B	298	ASP
1	B	320	LEU
1	B	334	TRP
1	B	382	ASP
1	B	394	ARG
1	B	398	LEU
1	B	404	ARG
1	B	407	ILE
1	B	432	HIS

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Mol	Chain	Res	Type
1	B	471	ILE
1	B	476	GLU
1	B	487	GLU
1	B	497	THR
1	B	523	VAL
1	B	634	LYS
1	B	635	THR
1	B	660	LEU
1	B	672	ARG
1	B	713	LEU
1	B	716	SER
1	B	717	ASP
1	B	757	THR
1	B	764	ASN
1	B	783	ARG
1	B	791	ARG
1	B	803	LEU
1	B	816	TYR
1	B	822	ILE
1	B	845	MET
1	B	890	HIS
1	B	906	SER
1	B	945	LEU
1	B	991	GLU
1	B	1011	LEU
1	B	1021	ASN
1	B	1058	ARG
1	B	1068	GLN
1	B	1078	LEU
1	B	1091	GLU
1	B	1109	GLN
1	B	1136	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	51	ASN
1	A	56	HIS
1	A	65	GLN
1	A	84	HIS
1	A	115	GLN

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Mol	Chain	Res	Type
1	A	246	GLN
1	A	279	ASN
1	A	338	GLN
1	A	527	HIS
1	A	543	HIS
1	A	555	GLN
1	A	668	ASN
1	A	811	GLN
1	A	859	HIS
1	A	909	GLN
1	A	1071	GLN
1	A	1107	GLN
1	A	1109	GLN
1	B	84	HIS
1	B	134	GLN
1	B	230	GLN
1	B	279	ASN
1	B	338	GLN
1	B	350	ASN
1	B	432	HIS
1	B	485	HIS
1	B	527	HIS
1	B	543	HIS
1	B	664	GLN
1	B	692	GLN
1	B	764	ASN
1	B	821	ASN
1	B	844	GLN
1	B	855	ASN
1	B	890	HIS
1	B	898	GLN
1	B	909	GLN
1	B	927	GLN
1	B	948	HIS
1	B	963	GLN
1	B	1105	GLN
1	B	1109	GLN

5.3.3 RNA

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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EPE	B	1150	-	15,15,15	0.93	0	18,20,20	1.59	2 (11%)
3	EPE	A	1152	-	15,15,15	1.03	0	18,20,20	1.59	3 (16%)
3	EPE	B	1151	-	15,15,15	1.35	1 (6%)	18,20,20	1.57	2 (11%)
2	SO4	A	1150	-	4,4,4	0.22	0	6,6,6	0.21	0
2	SO4	B	1149	-	4,4,4	0.28	0	6,6,6	0.22	0
2	SO4	A	1149	-	4,4,4	0.25	0	6,6,6	0.27	0
3	EPE	B	1152	-	15,15,15	1.04	0	18,20,20	1.41	2 (11%)
3	EPE	A	1151	-	15,15,15	1.11	0	18,20,20	1.58	2 (11%)

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
3	EPE	B	1150	-	-	1/9/19/19	0/1/1/1
3	EPE	A	1152	-	-	1/9/19/19	0/1/1/1
3	EPE	B	1151	-	-	1/9/19/19	0/1/1/1
3	EPE	B	1152	-	-	0/9/19/19	0/1/1/1
3	EPE	A	1151	-	-	1/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1151	EPE	C10-S	2.85	1.81	1.77

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1152	EPE	O1S-S-C10	5.23	113.21	106.92
3	A	1151	EPE	O1S-S-C10	5.16	113.13	106.92
3	B	1151	EPE	O1S-S-C10	4.76	112.65	106.92
3	B	1150	EPE	O1S-S-C10	4.71	112.59	106.92
3	B	1152	EPE	O1S-S-C10	4.41	112.23	106.92
3	B	1151	EPE	O3S-S-O1S	-3.59	102.50	111.27
3	A	1151	EPE	O3S-S-O1S	-2.95	104.06	111.27
3	B	1150	EPE	O3S-S-O2S	-2.63	104.84	111.27
3	A	1152	EPE	O3S-S-O2S	-2.26	105.76	111.27
3	B	1152	EPE	O3S-S-O1S	-2.19	105.93	111.27
3	A	1152	EPE	O3S-S-O1S	-2.07	106.22	111.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1151	EPE	N4-C7-C8-O8
3	A	1151	EPE	N4-C7-C8-O8
3	A	1152	EPE	N4-C7-C8-O8
3	B	1150	EPE	N4-C7-C8-O8

There are no ring outliers.

4 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1150	EPE	14	0
3	A	1152	EPE	1	0
3	B	1151	EPE	12	0
3	A	1151	EPE	9	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	1146/1151 (99%)	-0.58	2 (0%) 95 94	4, 44, 83, 109	0
1	B	1143/1151 (99%)	-0.46	4 (0%) 94 92	4, 53, 105, 123	0
All	All	2289/2302 (99%)	-0.52	6 (0%) 94 92	4, 48, 100, 123	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	PRO	5.4
1	A	461	SER	3.7
1	B	348	ALA	3.0
1	B	266	SER	2.7
1	B	459	GLN	2.4
1	B	242	GLU	2.1

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(\AA^2)	Q<0.9
3	EPE	B	1152	15/15	0.73	0.47	95,95,98,98	0
3	EPE	B	1151	15/15	0.75	0.45	105,108,109,109	0
3	EPE	B	1150	15/15	0.84	0.34	81,89,91,92	0
3	EPE	A	1152	15/15	0.87	0.38	88,89,91,92	0
2	SO4	B	1149	5/5	0.87	0.21	120,120,120,121	0
3	EPE	A	1151	15/15	0.89	0.40	104,105,105,106	0
2	SO4	A	1149	5/5	0.91	0.16	89,89,89,89	0
2	SO4	A	1150	5/5	0.95	0.13	104,104,105,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.