Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2023 – 09:02 PM EST

PDB ID	:	1UKJ
Title	:	Detailed structure of L-Methionine-Lyase from Pseudomonas putida
Authors	:	Misaki, S.; Takimoto, A.; Takakura, T.; Yoshioka, T.; Yamashita, M.; Tamura, T.; Tanaka, H.; Inagaki, K.
Deposited on	:	2003-08-24
Resolution	:	1.80 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:

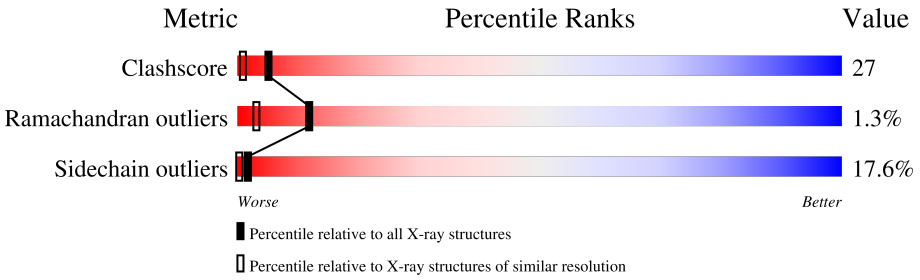
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	398	51% 38% 12%
1	B	398	53% 37% 10% .
1	C	398	56% 36% 8%
1	D	398	57% 35% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13148 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.

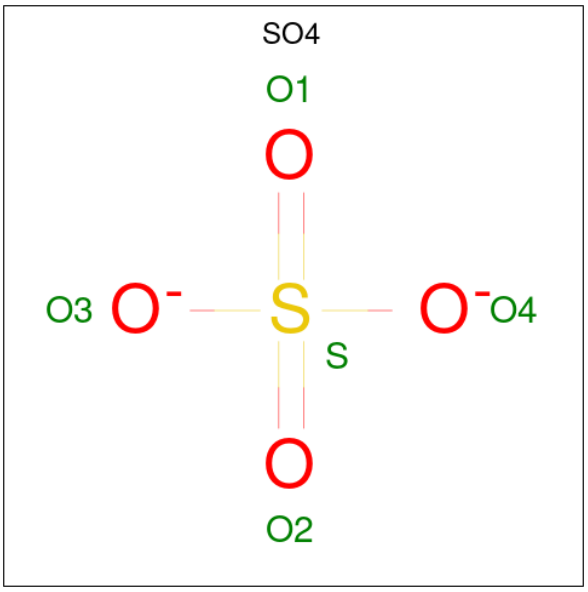
- Molecule 1 is a protein called Methionine gamma-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	P	S	0	0	0
			3011	1897	533	562	1	18			
1	B	398	Total	C	N	O	P	S	0	0	0
			3011	1897	533	562	1	18			
1	C	398	Total	C	N	O	P	S	0	0	0
			3011	1897	533	562	1	18			
1	D	398	Total	C	N	O	P	S	0	0	0
			3011	1897	533	562	1	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	LLP	LYS	modified residue	UNP P13254
B	711	LLP	LYS	modified residue	UNP P13254
C	1211	LLP	LYS	modified residue	UNP P13254
D	1711	LLP	LYS	modified residue	UNP P13254

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	243	Total O 243 243	0	0
3	B	251	Total O 251 251	0	0
3	C	297	Total O 297 297	0	0
3	D	288	Total O 288 288	0	0

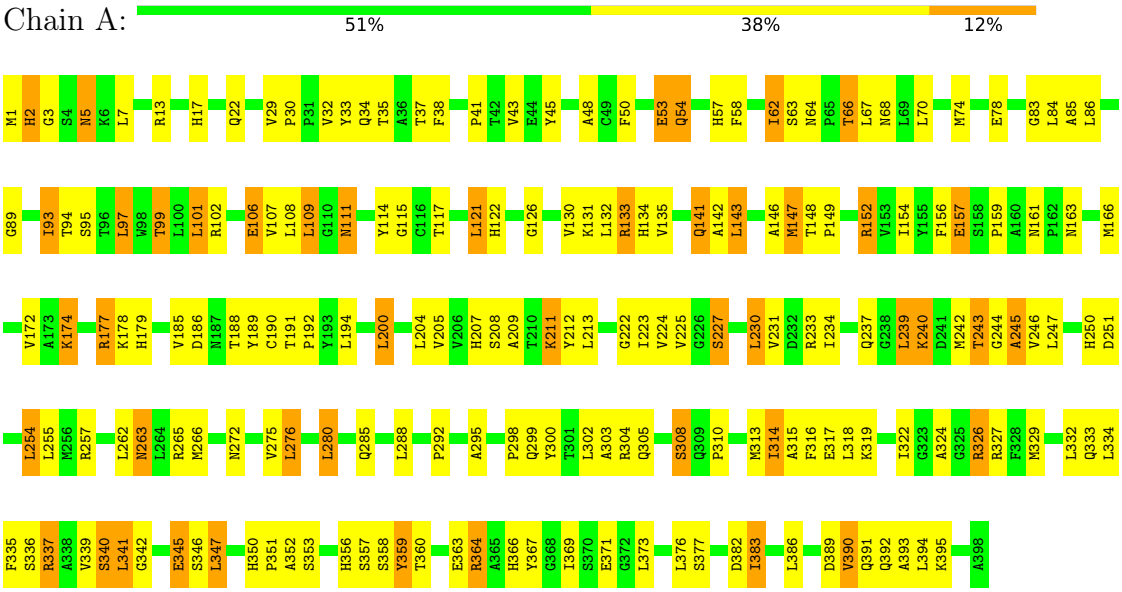
3 Residue-property plots (i)

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

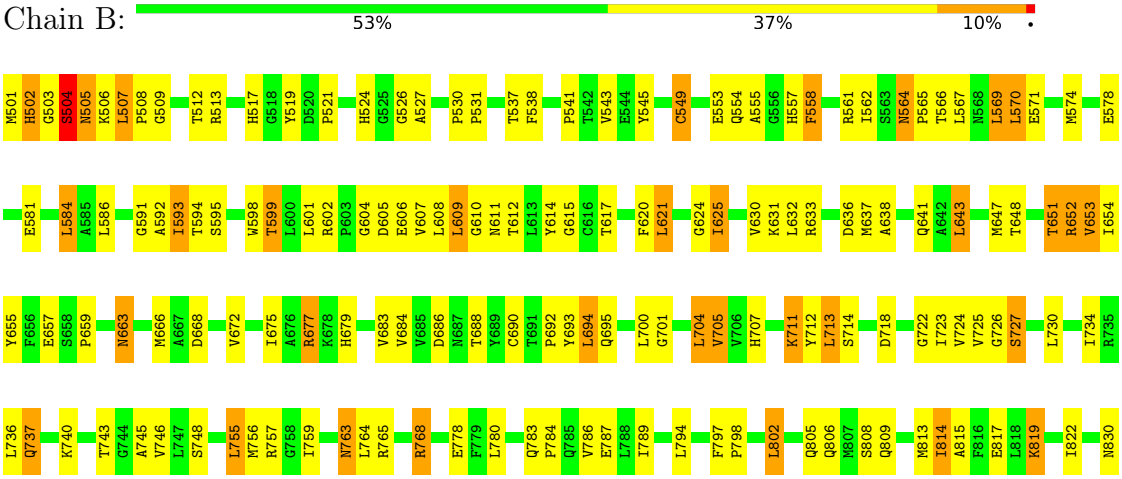
• Molecule 1: Methionine gamma-lyase

Chain A:



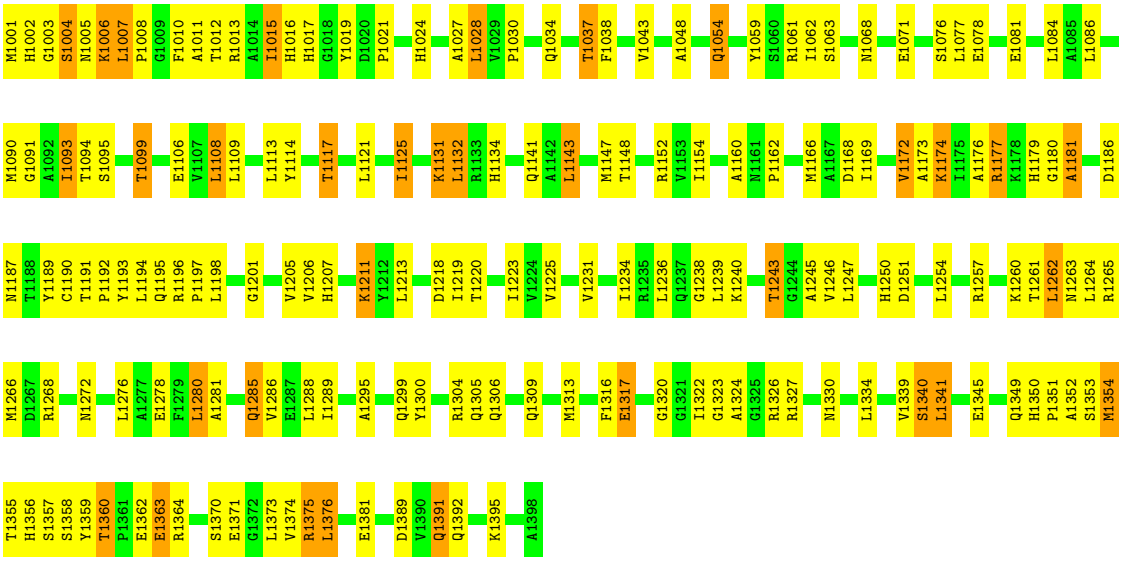
• Molecule 1: Methionine gamma-lyase

Chain B:



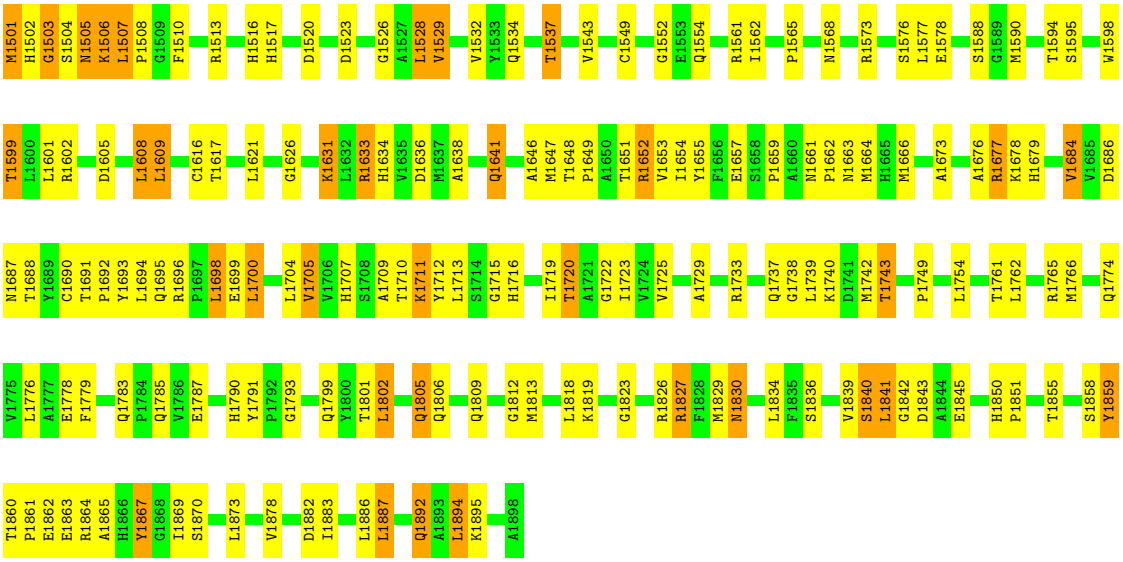
• Molecule 1: Methionine gamma-lyase

Chain C:



• Molecule 1: Methionine gamma-lyase

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	133.09Å 133.09Å 215.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 98.0	Depositor
R, R_{free}	0.177 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13148	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, LLP

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	0.35	0/3051	0.60	1/4139 (0.0%)
1	B	0.33	0/3051	0.61	0/4139
1	C	0.35	0/3051	0.61	0/4139
1	D	0.34	0/3051	0.59	0/4139
All	All	0.34	0/12204	0.60	1/16556 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	208	SER	N-CA-C	-5.30	96.70	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	3011	0	2970	164	0
1	B	3011	0	2967	181	0
1	C	3011	0	2967	179	0
1	D	3011	0	2967	153	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	243	0	0	13	0
3	B	251	0	0	17	0
3	C	297	0	0	34	0
3	D	288	0	0	23	0
All	All	13148	0	11871	643	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 27.

All (643) 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:A:174:LYS:HE2	1:A:177:ARG:HH11	1.26	1.00
1:A:303:ALA:HB1	1:A:304:ARG:HH21	1.24	1.00
1:A:152:ARG:HH22	1:A:233:ARG:HH22	1.13	0.97
1:C:1219:ILE:HD11	1:C:1254:LEU:HD23	1.45	0.96
1:A:313:MET:HE1	1:A:377:SER:HB2	1.47	0.95
1:C:1330:ASN:HD21	1:D:1543:VAL:H	1.09	0.95
1:C:1121:LEU:HD23	1:C:1125:ILE:HD11	1.49	0.94
1:A:93:ILE:HG13	1:A:94:THR:N	1.82	0.94
1:C:1043:VAL:H	1:D:1830:ASN:HD21	0.96	0.90
1:C:1231:VAL:HA	3:C:2706:HOH:O	1.71	0.89
1:A:108:LEU:HD23	1:A:133:ARG:HB3	1.54	0.89
1:B:787:GLU:HB2	1:B:819:LYS:HG3	1.54	0.88
1:B:527:ALA:HA	3:C:2714:HOH:O	1.75	0.87
1:C:1234:ILE:HB	3:C:2706:HOH:O	1.75	0.85
1:D:1698:LEU:HD13	3:D:2820:HOH:O	1.78	0.84
1:D:1549:CYS:HB3	3:D:2723:HOH:O	1.78	0.83
1:D:1595:SER:O	1:D:1599:THR:HG23	1.77	0.83
1:D:1705:VAL:HB	3:D:2820:HOH:O	1.79	0.83
1:B:743:THR:HG22	1:B:745:ALA:H	1.43	0.83
1:A:300:TYR:O	1:A:304:ARG:HG2	1.78	0.83
1:A:339:VAL:O	1:A:340:SER:HB2	1.81	0.78
1:B:864:ARG:HG3	1:B:869:ILE:HD12	1.66	0.78
1:C:1061:ARG:HG3	1:C:1246:VAL:CG2	2.15	0.77
1:C:1169:ILE:H	1:C:1306:GLN:HE22	1.32	0.77
1:D:1698:LEU:HB2	3:D:2091:HOH:O	1.83	0.77
1:C:1043:VAL:H	1:D:1830:ASN:ND2	1.79	0.77
1:C:1062:ILE:HA	3:C:2017:HOH:O	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1633:ARG:HH11	1:D:1646:ALA:HA	1.51	0.76
1:A:263:ASN:H	1:A:263:ASN:HD22	1.31	0.76
1:A:111:ASN:HB2	3:A:2984:HOH:O	1.84	0.76
1:C:1004:SER:HA	1:C:1008:PRO:HD2	1.67	0.76
1:A:152:ARG:HH22	1:A:233:ARG:NH2	1.83	0.75
1:A:174:LYS:HE2	1:A:177:ARG:NH1	2.01	0.75
1:C:1003:GLY:HA2	1:C:1017:HIS:HA	1.69	0.75
1:B:578:GLU:OE2	1:B:707:HIS:HE1	1.69	0.75
1:C:1360:THR:HG23	1:C:1362:GLU:H	1.52	0.75
1:D:1504:SER:HB2	1:D:1517:HIS:NE2	2.02	0.75
1:A:43:VAL:HG22	1:B:830:ASN:HD21	1.52	0.75
1:B:505:ASN:HA	1:B:513:ARG:HD3	1.67	0.75
1:C:1015:ILE:HG21	3:C:2728:HOH:O	1.87	0.74
1:C:1207:HIS:HB2	1:C:1223:ILE:HB	1.70	0.74
1:A:298:PRO:HB2	3:A:2989:HOH:O	1.87	0.73
1:C:1093:ILE:HG13	1:C:1094:THR:N	2.04	0.73
1:C:1330:ASN:ND2	1:D:1543:VAL:H	1.84	0.73
1:B:621:LEU:HA	1:B:625:ILE:CD1	2.18	0.72
1:C:1345:GLU:HG2	3:C:2677:HOH:O	1.89	0.72
1:B:713:LEU:HG	3:B:2726:HOH:O	1.90	0.72
1:B:538:PHE:HB2	1:B:558:PHE:HA	1.71	0.72
1:A:43:VAL:H	1:B:830:ASN:HD21	1.34	0.72
1:B:504:SER:N	1:B:508:PRO:HG2	2.05	0.72
1:C:1001:MET:N	1:C:1008:PRO:HG3	2.06	0.71
1:C:1043:VAL:N	1:D:1830:ASN:HD21	1.81	0.71
1:D:1578:GLU:OE1	1:D:1707:HIS:HE1	1.73	0.71
1:A:329:MET:O	1:A:337:ARG:HD3	1.91	0.70
1:B:574:MET:SD	3:B:2726:HOH:O	2.50	0.70
1:D:1859:TYR:HB2	1:D:1864:ARG:HG3	1.73	0.70
1:B:545:TYR:O	1:B:549:CYS:HB2	1.92	0.70
1:C:1339:VAL:O	1:C:1340:SER:HB3	1.90	0.70
1:A:3:GLY:C	1:A:17:HIS:HD2	1.94	0.70
1:C:1001:MET:N	1:C:1006:LYS:H	1.90	0.69
1:B:564:ASN:ND2	1:B:566:THR:H	1.90	0.69
1:C:1095:SER:OG	1:C:1243:THR:HG21	1.93	0.69
1:A:66:THR:HB	3:A:2183:HOH:O	1.92	0.69
1:A:265:ARG:HD2	3:A:2093:HOH:O	1.92	0.69
1:A:108:LEU:CD2	1:A:133:ARG:HD2	2.22	0.69
1:C:1048:ALA:HB1	1:C:1054:GLN:HB2	1.75	0.68
1:D:1520:ASP:HB3	1:D:1523:ASP:OD2	1.93	0.68
1:A:243:THR:HG23	1:A:245:ALA:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:PRO:O	1:B:819:LYS:HE2	1.94	0.68
1:A:3:GLY:HA2	1:A:13:ARG:HG3	1.76	0.68
1:A:43:VAL:HG22	1:B:830:ASN:ND2	2.09	0.68
1:C:1121:LEU:HD23	1:C:1125:ILE:CD1	2.23	0.68
1:A:303:ALA:HB1	1:A:304:ARG:NH2	2.06	0.68
1:B:743:THR:HG22	1:B:745:ALA:N	2.08	0.67
1:A:239:LEU:O	1:A:240:LYS:HB2	1.95	0.67
1:A:33:TYR:HB2	1:A:66:THR:CG2	2.24	0.67
1:C:1280:LEU:HD12	1:C:1286:VAL:HG21	1.77	0.67
1:C:1240:LYS:HB2	3:C:2017:HOH:O	1.94	0.67
1:C:1391:GLN:O	1:C:1395:LYS:HG2	1.94	0.67
1:A:280:LEU:HD23	1:A:314:ILE:HD11	1.75	0.67
1:C:1243:THR:CG2	1:C:1245:ALA:H	2.08	0.67
1:C:1262:LEU:HD22	1:C:1266:MET:HG2	1.76	0.67
1:D:1504:SER:C	1:D:1506:LYS:H	1.97	0.67
1:D:1504:SER:O	1:D:1508:PRO:HD2	1.95	0.66
1:A:345:GLU:HG3	1:C:1028:LEU:HD11	1.78	0.66
1:C:1173:ALA:O	1:C:1177:ARG:HG2	1.95	0.66
1:C:1350:HIS:HD1	1:C:1353:SER:HG	1.44	0.66
1:A:360:THR:OG1	1:A:363:GLU:HG3	1.94	0.66
1:C:1147:MET:CE	1:C:1179:HIS:HB2	2.26	0.66
1:C:1194:LEU:HD22	1:C:1309:GLN:HB2	1.77	0.66
1:D:1733:ARG:O	1:D:1737:GLN:HB2	1.96	0.66
1:D:1694:LEU:HD22	1:D:1809:GLN:HB2	1.78	0.66
1:A:33:TYR:H	1:A:66:THR:HG21	1.61	0.65
1:A:389:ASP:O	1:A:392:GLN:HG3	1.95	0.65
1:D:1710:THR:O	3:D:2137:HOH:O	2.15	0.65
1:A:33:TYR:HB2	1:A:66:THR:HG22	1.78	0.65
1:C:1169:ILE:H	1:C:1306:GLN:NE2	1.94	0.65
1:B:860:THR:O	1:B:862:GLU:HG3	1.97	0.64
1:D:1652:ARG:HG2	3:D:2959:HOH:O	1.96	0.64
1:C:1117:THR:HG21	3:C:2189:HOH:O	1.96	0.64
1:C:1147:MET:HE2	1:C:1179:HIS:HB2	1.78	0.64
1:A:161:ASN:ND2	1:A:189:TYR:OH	2.28	0.64
1:B:765:ARG:HD2	3:B:2020:HOH:O	1.98	0.64
1:D:1504:SER:HB2	1:D:1517:HIS:CD2	2.32	0.64
1:B:621:LEU:HA	1:B:625:ILE:HD11	1.79	0.64
1:C:1288:LEU:HB3	1:C:1317:GLU:HG3	1.80	0.64
1:A:383:ILE:HG13	3:A:2581:HOH:O	1.97	0.64
1:B:783:GLN:HB2	1:B:786:VAL:HG23	1.78	0.64
1:B:704:LEU:HD12	1:B:726:GLY:HA3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:THR:H	1:B:651:THR:CG2	2.10	0.64
1:B:852:ALA:HA	1:B:864:ARG:HD2	1.80	0.64
1:C:1095:SER:O	1:C:1099:THR:HG23	1.98	0.64
1:C:1353:SER:C	1:C:1357:SER:HB2	2.18	0.64
1:C:1003:GLY:O	1:C:1013:ARG:HG2	1.98	0.63
1:A:339:VAL:O	1:A:340:SER:CB	2.46	0.63
1:C:1043:VAL:HG22	1:D:1830:ASN:ND2	2.13	0.63
1:B:612:THR:HG22	3:B:2854:HOH:O	1.98	0.63
1:C:1007:LEU:N	1:C:1008:PRO:HD3	2.13	0.63
1:C:1168:ASP:O	1:C:1172:VAL:HG13	1.99	0.63
1:D:1799:GLN:HB2	3:D:2209:HOH:O	1.98	0.63
1:A:86:LEU:HD23	1:A:239:LEU:HD13	1.81	0.62
1:D:1851:PRO:HB2	1:D:1869:ILE:HG21	1.81	0.62
1:A:93:ILE:HD13	1:A:117:THR:HG23	1.79	0.62
1:A:2:HIS:HB2	1:C:1334:LEU:HD13	1.80	0.62
1:A:363:GLU:O	1:A:366:HIS:HB3	2.00	0.62
1:B:505:ASN:HA	1:B:513:ARG:CD	2.30	0.62
1:B:759:ILE:HD11	3:B:2726:HOH:O	1.99	0.62
1:D:1823:GLY:HA2	1:D:1826:ARG:NH2	2.15	0.62
1:B:607:VAL:HG22	1:B:609:LEU:HD13	1.82	0.62
1:D:1762:LEU:HB3	3:D:2269:HOH:O	1.99	0.62
1:B:648:THR:H	1:B:651:THR:HG22	1.65	0.61
1:C:1114:TYR:HD2	1:C:1117:THR:HG22	1.65	0.61
1:C:1281:ALA:HA	1:C:1289:ILE:CD1	2.30	0.61
1:A:64:ASN:HB3	1:A:67:LEU:HB2	1.81	0.61
1:D:1561:ARG:HH11	1:D:1561:ARG:HG2	1.64	0.61
1:A:237:GLN:HB3	3:A:3072:HOH:O	2.00	0.61
1:B:502:HIS:HB2	1:D:1834:LEU:HD13	1.82	0.61
1:B:561:ARG:HH11	1:B:561:ARG:HG2	1.64	0.61
1:B:598:TRP:CZ3	1:B:625:ILE:HG23	2.35	0.61
1:C:1114:TYR:HB3	1:C:1117:THR:CG2	2.30	0.61
1:A:316:PHE:HE2	1:A:318:LEU:HD13	1.66	0.61
1:B:860:THR:O	1:B:862:GLU:N	2.33	0.61
1:C:1300:TYR:O	1:C:1304:ARG:HG2	2.01	0.60
1:D:1860:THR:H	1:D:1863:GLU:HB2	1.65	0.60
1:A:122:HIS:NE2	1:A:134:HIS:HE1	1.99	0.60
1:A:351:PRO:HG2	3:A:2744:HOH:O	2.00	0.60
1:D:1738:GLY:O	1:D:1742:MET:O	2.18	0.60
1:A:109:LEU:HB2	1:A:134:HIS:CD2	2.36	0.60
1:A:250:HIS:HD2	1:A:251:ASP:OD2	1.83	0.60
1:C:1132:LEU:H	1:C:1132:LEU:HD22	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1648:THR:HB	1:D:1649:PRO:HD2	1.82	0.60
1:D:1855:THR:HG23	3:D:2743:HOH:O	2.02	0.60
1:B:502:HIS:O	1:B:512:THR:HG22	2.02	0.60
1:D:1802:LEU:HD22	1:D:1802:LEU:O	2.02	0.60
1:B:503:GLY:O	1:B:517:HIS:ND1	2.35	0.60
1:D:1823:GLY:HA2	1:D:1826:ARG:CZ	2.32	0.60
1:D:1621:LEU:O	1:D:1626:GLY:HA3	2.02	0.60
1:C:1243:THR:OG1	1:D:1743:THR:HA	2.03	0.59
1:D:1504:SER:C	1:D:1506:LYS:N	2.54	0.59
1:B:501:MET:HG2	3:B:2168:HOH:O	2.01	0.59
1:B:746:VAL:HA	3:B:2196:HOH:O	2.00	0.59
1:C:1109:LEU:HD22	1:C:1121:LEU:HD13	1.84	0.59
1:C:1174:LYS:HD2	1:C:1174:LYS:N	2.17	0.59
1:B:864:ARG:O	1:B:869:ILE:HG13	2.02	0.59
1:B:636:ASP:OD1	1:B:638:ALA:HB3	2.02	0.59
1:B:863:GLU:O	1:B:863:GLU:HG3	2.02	0.59
1:C:1048:ALA:CB	1:C:1054:GLN:HB2	2.33	0.59
1:A:322:ILE:HB	1:A:371:GLU:HG3	1.85	0.59
1:A:263:ASN:H	1:A:263:ASN:ND2	2.01	0.58
1:D:1715:GLY:HA2	1:D:1842:GLY:O	2.03	0.58
1:B:780:LEU:HD12	1:B:814:ILE:HD11	1.85	0.58
1:A:223:ILE:HG23	3:A:2087:HOH:O	2.02	0.58
1:C:1353:SER:HB2	1:D:1543:VAL:HG11	1.85	0.58
1:C:1353:SER:HB2	1:D:1543:VAL:CG1	2.33	0.58
1:D:1517:HIS:CE1	1:D:1576:SER:HB2	2.38	0.58
1:A:48:ALA:HB1	1:A:54:GLN:HB2	1.85	0.58
1:D:1590:MET:O	1:D:1594:THR:HG23	2.04	0.58
1:D:1869:ILE:HD12	1:D:1869:ILE:H	1.67	0.58
1:A:314:ILE:HG13	1:A:315:ALA:N	2.19	0.58
1:B:570:LEU:HA	3:B:2701:HOH:O	2.04	0.58
1:B:657:GLU:HG2	1:B:686:ASP:HB3	1.84	0.58
1:B:860:THR:C	1:B:862:GLU:H	2.05	0.58
1:A:33:TYR:H	1:A:66:THR:CG2	2.17	0.58
1:A:108:LEU:HD21	1:A:133:ARG:HD2	1.86	0.58
1:A:326:ARG:HE	1:A:353:SER:HB2	1.67	0.58
1:B:504:SER:H	1:B:508:PRO:HG2	1.68	0.58
1:C:1261:THR:O	1:C:1265:ARG:HG3	2.04	0.58
1:A:304:ARG:NH1	3:A:2242:HOH:O	2.36	0.58
1:C:1061:ARG:NH2	1:D:1616:CYS:SG	2.77	0.58
1:A:174:LYS:HA	1:A:177:ARG:NH1	2.19	0.57
1:A:239:LEU:O	1:A:240:LYS:CB	2.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1015:ILE:HG12	3:C:2728:HOH:O	2.05	0.57
1:D:1709:ALA:HB3	3:D:2693:HOH:O	2.05	0.57
1:A:156:PHE:CZ	1:A:185:VAL:HG22	2.39	0.57
1:B:501:MET:HG3	1:B:521:PRO:CD	2.35	0.57
1:B:595:SER:O	1:B:599:THR:CG2	2.53	0.57
1:A:223:ILE:HD13	3:A:2087:HOH:O	2.05	0.57
1:B:595:SER:O	1:B:599:THR:HG23	2.04	0.57
1:B:503:GLY:HA2	1:B:513:ARG:HG2	1.86	0.57
1:B:584:LEU:HD13	1:B:586:LEU:HD11	1.87	0.56
1:C:1019:TYR:CE1	1:C:1030:PRO:HB3	2.40	0.56
1:C:1160:ALA:HB1	3:C:2489:HOH:O	2.05	0.56
1:A:359:TYR:HB2	1:A:364:ARG:HG3	1.87	0.56
1:C:1061:ARG:HG3	1:C:1246:VAL:HG22	1.87	0.56
1:C:1196:ARG:HG3	1:C:1196:ARG:HH11	1.69	0.56
1:D:1712:TYR:CE1	1:D:1842:GLY:HA2	2.40	0.56
1:A:303:ALA:HB3	1:A:304:ARG:HE	1.71	0.56
1:C:1076:SER:HB3	3:C:2697:HOH:O	2.05	0.56
1:A:299:GLN:HE21	1:A:302:LEU:HD23	1.70	0.56
1:A:29:VAL:HG13	1:A:30:PRO:HD2	1.88	0.56
1:B:648:THR:O	1:B:651:THR:HG22	2.06	0.56
1:C:1243:THR:HG22	1:C:1245:ALA:H	1.69	0.56
1:B:768:ARG:NH1	3:B:2795:HOH:O	2.39	0.56
1:B:862:GLU:OE1	1:B:863:GLU:HB3	2.06	0.56
1:D:1565:PRO:O	1:D:1568:ASN:HB2	2.05	0.55
1:A:141:GLN:HG3	1:A:142:ALA:N	2.21	0.55
1:A:152:ARG:NH2	1:A:233:ARG:HH22	1.93	0.55
1:A:114:TYR:CE2	1:A:211:LLP:H5'1	2.42	0.55
1:C:1095:SER:O	1:C:1099:THR:CG2	2.54	0.55
1:C:1015:ILE:CG2	3:C:2728:HOH:O	2.48	0.55
1:A:74:MET:HG3	1:A:223:ILE:HD12	1.87	0.55
1:C:1180:GLY:O	1:C:1181:ALA:O	2.25	0.55
1:A:93:ILE:HD12	1:A:97:LEU:HD22	1.89	0.55
1:B:574:MET:CE	1:B:713:LEU:HD21	2.36	0.55
1:C:1247:LEU:N	3:C:2022:HOH:O	2.39	0.55
1:D:1608:LEU:HD12	1:D:1633:ARG:HB3	1.88	0.55
1:A:316:PHE:CE2	1:A:318:LEU:HD13	2.42	0.54
1:C:1196:ARG:HG3	1:C:1196:ARG:NH1	2.22	0.54
1:D:1688:THR:HB	1:D:1711:LLP:H2'2	1.88	0.54
1:D:1712:TYR:CD1	1:D:1842:GLY:HA2	2.42	0.54
1:D:1812:GLY:O	1:D:1878:VAL:HG12	2.07	0.54
1:A:89:GLY:O	1:A:93:ILE:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1166:MET:HE3	3:C:2807:HOH:O	2.06	0.54
1:D:1813:MET:SD	1:D:1841:LEU:HD13	2.48	0.54
1:C:1349:GLN:HB2	1:C:1354:MET:CE	2.38	0.54
1:B:578:GLU:HG2	1:B:692:PRO:HB3	1.90	0.54
1:B:501:MET:HG3	1:B:521:PRO:HD2	1.90	0.54
1:C:1043:VAL:HG22	1:D:1830:ASN:HD21	1.72	0.54
1:C:1071:GLU:HG2	1:C:1084:LEU:HA	1.90	0.54
1:C:1353:SER:O	1:C:1357:SER:HB2	2.08	0.53
1:D:1673:ALA:O	1:D:1677:ARG:HB2	2.07	0.53
1:A:107:VAL:HG12	1:A:131:LYS:O	2.08	0.53
1:A:359:TYR:N	1:A:359:TYR:CD1	2.74	0.53
1:D:1839:VAL:O	1:D:1840:SER:CB	2.56	0.53
1:A:211:LLP:HD3	1:A:341:LEU:HG	1.90	0.53
1:D:1684:VAL:HA	1:D:1704:LEU:O	2.09	0.53
1:B:856:HIS:O	1:B:859:TYR:HB2	2.07	0.53
1:C:1037:THR:O	3:C:2714:HOH:O	2.18	0.53
1:C:1061:ARG:HG3	1:C:1246:VAL:HG21	1.91	0.53
1:C:1349:GLN:HB2	1:C:1354:MET:HE2	1.90	0.53
1:C:1262:LEU:CD2	1:C:1266:MET:HG2	2.39	0.53
1:A:295:ALA:HA	1:A:300:TYR:CD1	2.43	0.53
1:C:1106:GLU:HA	1:C:1131:LYS:O	2.09	0.53
1:D:1504:SER:HA	1:D:1513:ARG:HD3	1.90	0.53
1:A:95:SER:O	1:A:99:THR:CG2	2.56	0.52
1:C:1001:MET:HG3	1:C:1006:LYS:HB3	1.91	0.52
1:B:562:ILE:HD13	1:B:740:LYS:HG3	1.92	0.52
1:B:705:VAL:HG23	1:B:725:VAL:HB	1.91	0.52
1:B:860:THR:C	1:B:862:GLU:N	2.62	0.52
1:C:1109:LEU:HD22	1:C:1121:LEU:CD1	2.40	0.52
1:D:1504:SER:CB	1:D:1517:HIS:NE2	2.73	0.52
1:D:1561:ARG:HG2	1:D:1561:ARG:NH1	2.24	0.52
1:D:1895:LYS:HE3	3:D:2260:HOH:O	2.10	0.52
1:B:780:LEU:CD1	1:B:814:ILE:HD11	2.39	0.52
1:D:1843:ASP:HB3	3:D:2916:HOH:O	2.09	0.52
1:B:569:LEU:HD13	1:B:756:MET:SD	2.50	0.52
1:D:1562:ILE:CG1	1:D:1740:LYS:HD2	2.40	0.52
1:C:1198:LEU:CD1	3:C:2702:HOH:O	2.58	0.52
1:A:211:LLP:O3	1:A:211:LLP:NZ	2.43	0.52
1:A:227:SER:O	1:A:231:VAL:HG23	2.10	0.52
1:D:1588:SER:O	1:D:1722:GLY:HA3	2.10	0.52
1:B:802:LEU:HB2	3:B:2257:HOH:O	2.09	0.52
1:B:704:LEU:CD1	1:B:726:GLY:HA3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1198:LEU:HD12	3:C:2702:HOH:O	2.10	0.52
1:C:1339:VAL:O	1:C:1340:SER:CB	2.58	0.52
1:D:1503:GLY:O	1:D:1508:PRO:HG2	2.10	0.52
1:D:1505:ASN:HB2	1:D:1507:LEU:HG	1.92	0.52
1:B:809:GLN:HG2	3:B:2034:HOH:O	2.09	0.51
1:A:122:HIS:NE2	1:A:134:HIS:CE1	2.77	0.51
1:C:1078:GLU:HG2	1:C:1192:PRO:HB3	1.92	0.51
1:D:1504:SER:N	1:D:1517:HIS:CD2	2.78	0.51
1:A:106:GLU:HA	1:A:131:LYS:HB2	1.92	0.51
1:D:1508:PRO:HB2	1:D:1513:ARG:HG3	1.92	0.51
1:A:205:VAL:CG2	1:A:225:VAL:HB	2.41	0.51
1:A:212:TYR:CD1	1:A:342:GLY:HA2	2.46	0.51
1:B:713:LEU:HB3	1:B:755:LEU:HD21	1.93	0.51
1:B:867:TYR:HB3	1:B:869:ILE:HG12	1.91	0.51
1:D:1709:ALA:HB2	1:D:1713:LEU:HD12	1.92	0.51
1:A:352:ALA:HA	1:A:364:ARG:HD2	1.91	0.51
1:B:505:ASN:C	1:B:507:LEU:H	2.13	0.51
1:B:561:ARG:HG2	1:B:561:ARG:NH1	2.24	0.51
1:D:1602:ARG:N	1:D:1605:ASP:OD1	2.43	0.51
1:D:1710:THR:O	1:D:1710:THR:HG22	2.11	0.51
1:C:1295:ALA:HA	1:C:1300:TYR:CE1	2.46	0.51
1:D:1690:CYS:C	1:D:1691:THR:HG23	2.31	0.51
1:A:322:ILE:O	1:A:326:ARG:HG3	2.10	0.51
1:B:688:THR:HB	1:B:711:LLP:H2'2	1.92	0.51
1:C:1243:THR:HG23	1:C:1245:ALA:H	1.76	0.51
1:A:121:LEU:O	1:A:126:GLY:HA3	2.10	0.51
1:A:32:VAL:HB	1:D:1532:VAL:CG1	2.41	0.51
1:B:860:THR:OG1	1:B:862:GLU:HG2	2.10	0.51
1:A:285:GLN:O	1:A:319:LYS:HB3	2.11	0.50
1:D:1802:LEU:O	1:D:1805:GLN:HG3	2.11	0.50
1:A:86:LEU:O	1:A:247:LEU:HD13	2.10	0.50
1:A:191:THR:HB	1:A:192:PRO:HD2	1.93	0.50
1:A:345:GLU:HG3	1:C:1028:LEU:CD1	2.41	0.50
1:B:813:MET:SD	1:B:841:LEU:HD13	2.51	0.50
1:C:1059:TYR:HE2	1:C:1061:ARG:NH1	2.09	0.50
1:B:505:ASN:O	1:B:507:LEU:N	2.41	0.50
1:B:756:MET:HG2	3:B:2701:HOH:O	2.10	0.50
1:C:1108:LEU:HD23	1:C:1143:LEU:CD2	2.41	0.50
1:A:204:LEU:HD11	1:A:230:LEU:HG	1.92	0.50
1:A:212:TYR:CE1	1:A:342:GLY:HA2	2.46	0.50
1:A:356:HIS:O	1:A:364:ARG:HD3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:GLY:C	1:B:505:ASN:H	2.15	0.50
1:B:860:THR:HG23	1:B:862:GLU:HG2	1.93	0.50
1:B:501:MET:SD	1:B:501:MET:N	2.84	0.50
1:D:1595:SER:O	1:D:1599:THR:CG2	2.56	0.50
1:D:1801:THR:O	1:D:1805:GLN:HG2	2.12	0.50
1:A:159:PRO:HB3	1:A:166:MET:HE2	1.94	0.49
1:B:663:ASN:H	1:B:663:ASN:ND2	2.09	0.49
1:B:591:GLY:O	1:B:595:SER:HB2	2.11	0.49
1:C:1177:ARG:NH2	1:C:1201:GLY:O	2.45	0.49
1:A:174:LYS:O	1:A:174:LYS:HD3	2.12	0.49
1:A:304:ARG:HD3	3:A:2808:HOH:O	2.13	0.49
1:C:1090:MET:O	1:C:1094:THR:HG23	2.12	0.49
1:D:1883:ILE:HG13	1:D:1887:LEU:HD22	1.94	0.49
1:A:257:ARG:HG3	3:C:2067:HOH:O	2.12	0.49
1:B:695:GLN:HG3	1:B:806:GLN:O	2.12	0.49
1:D:1647:MET:HG2	1:D:1679:HIS:CD2	2.48	0.49
1:D:1655:TYR:CD1	1:D:1684:VAL:HG22	2.47	0.49
1:A:102:ARG:NH1	3:A:2394:HOH:O	2.41	0.49
1:A:43:VAL:H	1:B:830:ASN:ND2	2.06	0.49
1:A:326:ARG:NE	1:A:353:SER:HB2	2.28	0.49
1:B:581:GLU:HB2	1:B:727:SER:HA	1.93	0.49
1:C:1349:GLN:HG3	1:C:1351:PRO:HD3	1.93	0.49
1:D:1578:GLU:OE1	1:D:1707:HIS:CE1	2.59	0.49
1:A:78:GLU:OE2	1:A:207:HIS:HE1	1.95	0.49
1:A:209:ALA:HB1	1:A:255:LEU:HD11	1.95	0.49
1:B:557:HIS:HD2	3:B:3062:HOH:O	1.95	0.49
1:C:1238:GLY:O	1:C:1243:THR:HB	2.13	0.49
1:D:1779:PHE:O	1:D:1783:GLN:HG2	2.13	0.49
1:B:743:THR:CG2	1:B:745:ALA:HB2	2.43	0.49
1:A:147:MET:CE	1:A:154:ILE:HD11	2.43	0.49
1:B:780:LEU:HD12	1:B:814:ILE:CD1	2.43	0.49
1:B:867:TYR:HB3	1:B:869:ILE:CG1	2.42	0.49
1:A:148:THR:HB	1:A:149:PRO:HD2	1.95	0.48
1:A:359:TYR:N	1:A:359:TYR:HD1	2.11	0.48
1:D:1505:ASN:HA	3:D:2926:HOH:O	2.14	0.48
1:A:262:LEU:O	1:A:266:MET:HG2	2.13	0.48
1:A:78:GLU:OE2	1:A:207:HIS:CE1	2.67	0.48
1:A:324:ALA:HA	1:A:327:ARG:NH2	2.27	0.48
1:C:1078:GLU:CD	1:C:1192:PRO:HB3	2.33	0.48
1:D:1695:GLN:HE21	1:D:1806:GLN:HB3	1.78	0.48
1:A:133:ARG:NH2	1:A:146:ALA:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:863:GLU:HA	1:B:866:HIS:HB3	1.93	0.48
1:C:1162:PRO:HA	3:C:2827:HOH:O	2.13	0.48
1:D:1859:TYR:HB3	1:D:1863:GLU:HB2	1.96	0.48
1:A:190:CYS:O	1:A:194:LEU:HB2	2.12	0.48
1:A:174:LYS:HD3	1:A:174:LYS:C	2.33	0.48
1:D:1659:PRO:HB3	1:D:1666:MET:HE2	1.96	0.48
1:A:308:SER:HB3	3:A:2810:HOH:O	2.14	0.48
1:B:620:PHE:O	1:B:624:GLY:HA3	2.13	0.48
1:B:643:LEU:O	1:B:647:MET:HG2	2.14	0.48
1:C:1281:ALA:HA	1:C:1289:ILE:HD11	1.94	0.48
1:A:292:PRO:HB2	1:A:310:PRO:HB3	1.95	0.48
1:B:538:PHE:HB2	1:B:558:PHE:CA	2.42	0.48
1:B:611:ASN:OD1	1:B:636:ASP:HA	2.13	0.48
1:D:1641:GLN:H	1:D:1641:GLN:NE2	2.12	0.47
1:B:601:LEU:HD21	1:B:653:VAL:HG13	1.96	0.47
1:B:707:HIS:HB2	1:B:723:ILE:HB	1.96	0.47
1:B:863:GLU:C	1:B:865:ALA:N	2.67	0.47
1:C:1071:GLU:HG2	1:C:1084:LEU:CA	2.43	0.47
1:B:519:TYR:CE2	1:B:524:HIS:CD2	3.03	0.47
1:B:564:ASN:ND2	1:B:566:THR:N	2.61	0.47
1:C:1061:ARG:NH1	1:D:1711:LLP:OP2	2.47	0.47
1:A:230:LEU:O	1:A:234:ILE:HG13	2.14	0.47
1:B:617:THR:O	1:B:621:LEU:HD23	2.15	0.47
1:B:712:TYR:CE1	1:B:842:GLY:HA2	2.49	0.47
1:B:763:ASN:N	1:B:763:ASN:HD22	2.11	0.47
1:C:1030:PRO:HG2	3:C:3014:HOH:O	2.13	0.47
1:D:1865:ALA:C	1:D:1867:TYR:H	2.18	0.47
1:A:242:MET:HA	1:B:620:PHE:CD1	2.49	0.47
1:B:620:PHE:CZ	1:B:625:ILE:HG13	2.50	0.47
1:C:1132:LEU:HD22	1:C:1132:LEU:N	2.28	0.47
1:C:1326:ARG:HH11	1:C:1353:SER:CB	2.28	0.47
1:D:1529:VAL:HA	3:D:2423:HOH:O	2.13	0.47
1:D:1673:ALA:HB1	1:D:1677:ARG:HH21	1.79	0.47
1:B:574:MET:HE1	1:B:713:LEU:HD21	1.97	0.47
1:B:614:TYR:HB3	1:B:617:THR:OG1	2.15	0.47
1:B:621:LEU:O	1:B:632:LEU:HD11	2.14	0.47
1:B:526:GLY:O	1:C:1038:PHE:HA	2.15	0.47
1:C:1078:GLU:CG	1:C:1192:PRO:HB3	2.45	0.47
1:A:188:THR:HG21	1:A:211:LLP:HG2	1.97	0.46
1:B:507:LEU:CB	1:B:508:PRO:HD3	2.45	0.46
1:B:541:PRO:HD2	1:B:545:TYR:CD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:PHE:O	1:B:798:PRO:C	2.53	0.46
1:B:864:ARG:HA	1:B:869:ILE:HD12	1.95	0.46
1:C:1081:GLU:HB2	3:C:2241:HOH:O	2.14	0.46
1:C:1109:LEU:O	1:C:1134:HIS:HA	2.14	0.46
1:A:147:MET:HG2	1:A:179:HIS:CG	2.50	0.46
1:B:505:ASN:CA	1:B:513:ARG:HD3	2.40	0.46
1:B:864:ARG:HA	1:B:869:ILE:CD1	2.45	0.46
1:D:1696:ARG:HD2	1:D:1699:GLU:OE2	2.15	0.46
1:B:574:MET:HE2	1:B:713:LEU:HD21	1.97	0.46
1:C:1077:LEU:O	1:C:1196:ARG:HD3	2.16	0.46
1:C:1195:GLN:HG2	1:C:1197:PRO:HD3	1.96	0.46
1:C:1320:GLY:HA3	1:C:1324:ALA:HB2	1.98	0.46
1:B:859:TYR:CE1	1:B:863:GLU:HG2	2.50	0.46
1:C:1004:SER:HA	1:C:1008:PRO:CD	2.41	0.46
1:A:333:GLN:O	1:C:1002:HIS:HD2	1.99	0.46
1:B:637:MET:CE	1:B:654:ILE:HG23	2.46	0.46
1:C:1326:ARG:HH11	1:C:1353:SER:HB3	1.81	0.46
1:B:814:ILE:HG13	1:B:815:ALA:N	2.26	0.46
1:B:839:VAL:O	1:B:840:SER:CB	2.63	0.46
1:C:1391:GLN:NE2	3:C:2008:HOH:O	2.46	0.46
1:A:58:PHE:CE2	1:A:62:ILE:HD13	2.50	0.46
1:A:244:GLY:O	1:A:246:VAL:N	2.46	0.46
1:B:503:GLY:O	1:B:505:ASN:N	2.49	0.46
1:B:677:ARG:NH1	1:B:701:GLY:O	2.47	0.46
1:C:1211:LLP:HD3	1:C:1341:LEU:HD13	1.97	0.46
1:C:1360:THR:HG23	1:C:1362:GLU:N	2.26	0.46
1:C:1389:ASP:O	1:C:1392:GLN:HG3	2.15	0.46
1:A:336:SER:HB2	1:A:347:LEU:HD12	1.98	0.46
1:C:1001:MET:HG3	1:C:1006:LYS:CB	2.46	0.46
1:C:1323:GLY:O	1:C:1327:ARG:HG3	2.16	0.46
3:C:2102:HOH:O	1:D:1537:THR:HG22	2.15	0.46
1:D:1859:TYR:CD2	1:D:1863:GLU:HB3	2.50	0.46
1:B:675:ILE:O	1:B:679:HIS:HD2	1.98	0.46
1:A:222:GLY:C	1:A:223:ILE:HG12	2.36	0.45
1:C:1352:ALA:HA	1:C:1364:ARG:HD3	1.97	0.45
1:D:1647:MET:HE1	1:D:1654:ILE:HD11	1.98	0.45
1:D:1661:ASN:HB3	1:D:1662:PRO:HA	1.98	0.45
1:D:1720:THR:HG23	3:D:2356:HOH:O	2.15	0.45
1:A:332:LEU:HD23	1:A:393:ALA:HB2	1.98	0.45
1:B:578:GLU:CD	1:B:692:PRO:HB3	2.36	0.45
1:C:1186:ASP:HA	1:C:1206:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1219:ILE:HD12	1:C:1251:ASP:CB	2.47	0.45
1:A:58:PHE:HE2	1:A:62:ILE:HD13	1.81	0.45
1:A:329:MET:HB2	1:B:543:VAL:HG11	1.99	0.45
1:C:1001:MET:CA	1:C:1008:PRO:HG3	2.45	0.45
1:D:1504:SER:CB	1:D:1576:SER:HG	2.29	0.45
1:D:1713:LEU:HG	3:D:2073:HOH:O	2.16	0.45
1:D:1765:ARG:HD2	3:D:2076:HOH:O	2.16	0.45
1:C:1078:GLU:OE2	1:C:1207:HIS:NE2	2.35	0.45
1:A:313:MET:HE1	1:A:377:SER:CB	2.32	0.45
1:B:509:GLY:HA3	1:D:1882:ASP:OD1	2.16	0.45
1:C:1078:GLU:HB3	3:C:2702:HOH:O	2.16	0.45
1:B:607:VAL:HG22	1:B:609:LEU:CD1	2.47	0.45
1:B:668:ASP:O	1:B:672:VAL:HG13	2.16	0.45
3:B:2146:HOH:O	1:D:1528:LEU:HD12	2.17	0.45
1:C:1189:TYR:OH	1:C:1375:ARG:NH1	2.49	0.45
1:A:335:PHE:CD1	1:A:346:SER:HB3	2.51	0.45
1:C:1109:LEU:CD2	1:C:1121:LEU:HD13	2.47	0.45
1:D:1609:LEU:O	1:D:1634:HIS:HA	2.17	0.45
1:A:38:PHE:HA	1:D:1526:GLY:O	2.17	0.45
1:B:501:MET:HG3	1:B:521:PRO:HD3	1.97	0.45
1:C:1010:PHE:CZ	1:C:1193:TYR:HB2	2.52	0.45
1:C:1109:LEU:HB3	1:C:1113:LEU:HD11	1.98	0.45
1:D:1892:GLN:HE21	1:D:1892:GLN:HB3	1.56	0.45
1:A:386:LEU:O	1:A:390:VAL:HG13	2.17	0.45
1:B:592:ALA:HB1	1:B:724:VAL:CG2	2.48	0.45
1:B:783:GLN:HB2	1:B:786:VAL:CG2	2.44	0.45
1:C:1114:TYR:HB3	1:C:1117:THR:HG23	1.97	0.45
1:C:1166:MET:HB3	1:C:1166:MET:HE2	1.69	0.45
1:A:233:ARG:O	1:A:237:GLN:HG3	2.16	0.44
1:C:1141:GLN:HG3	3:C:2605:HOH:O	2.17	0.44
1:C:1246:VAL:HA	3:C:2022:HOH:O	2.17	0.44
1:D:1534:GLN:HA	1:D:1749:PRO:HG2	1.99	0.44
1:A:272:ASN:O	1:A:276:LEU:HB2	2.17	0.44
1:B:562:ILE:CD1	1:B:740:LYS:HG3	2.46	0.44
1:B:602:ARG:O	1:B:630:VAL:HG22	2.17	0.44
1:D:1690:CYS:O	1:D:1691:THR:HG23	2.17	0.44
1:D:1501:MET:HA	1:D:1516:HIS:HB3	1.99	0.44
1:A:57:HIS:NE2	1:A:68:ASN:ND2	2.65	0.44
1:A:95:SER:OG	1:A:243:THR:HG21	2.17	0.44
1:B:567:LEU:O	1:B:571:GLU:HG3	2.18	0.44
3:C:2117:HOH:O	1:D:1839:VAL:HG22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1147:MET:HE3	1:C:1179:HIS:HB2	1.97	0.44
1:D:1659:PRO:HB3	1:D:1666:MET:CE	2.47	0.44
1:B:593:ILE:HG12	1:B:655:TYR:OH	2.17	0.44
1:B:722:GLY:C	1:B:723:ILE:HG12	2.38	0.44
1:B:768:ARG:HA	1:B:768:ARG:HD3	1.68	0.44
1:C:1219:ILE:HG22	1:C:1220:THR:N	2.32	0.44
1:D:1507:LEU:CG	1:D:1508:PRO:HD3	2.48	0.44
1:D:1791:TYR:CE2	1:D:1793:GLY:HA3	2.52	0.44
1:B:610:GLY:O	1:B:611:ASN:C	2.56	0.44
1:C:1225:VAL:CG1	3:C:2702:HOH:O	2.66	0.44
1:C:1285:GLN:HE21	1:C:1285:GLN:HB2	1.62	0.44
1:D:1774:GLN:O	1:D:1778:GLU:HG3	2.18	0.44
1:A:335:PHE:CE1	1:A:346:SER:HB3	2.53	0.44
1:B:599:THR:HB	1:B:737:GLN:HE21	1.82	0.44
1:B:620:PHE:O	1:B:624:GLY:CA	2.65	0.44
1:C:1341:LEU:HD13	1:C:1341:LEU:N	2.32	0.44
1:D:1761:THR:HA	3:D:2044:HOH:O	2.17	0.44
1:D:1860:THR:O	1:D:1861:PRO:C	2.55	0.44
1:B:643:LEU:HD13	1:B:675:ILE:HG21	2.00	0.44
1:C:1176:ALA:O	1:C:1180:GLY:O	2.36	0.44
1:C:1313:MET:CE	1:C:1375:ARG:HD2	2.48	0.44
1:D:1631:LYS:HB3	3:D:2799:HOH:O	2.18	0.44
1:A:41:PRO:HD2	1:A:45:TYR:CG	2.53	0.43
1:A:356:HIS:CG	1:A:369:ILE:HD13	2.53	0.43
1:D:1513:ARG:O	1:D:1517:HIS:HB2	2.18	0.43
1:D:1663:ASN:HB3	1:D:1790:HIS:CD2	2.53	0.43
1:C:1003:GLY:O	1:C:1008:PRO:HG2	2.19	0.43
1:C:1012:THR:O	1:C:1016:HIS:HB2	2.18	0.43
1:C:1356:HIS:HD2	1:C:1359:TYR:CE1	2.35	0.43
1:D:1617:THR:O	1:D:1621:LEU:HD12	2.19	0.43
1:D:1823:GLY:O	1:D:1827:ARG:HB2	2.18	0.43
1:A:95:SER:O	1:A:99:THR:HG23	2.17	0.43
1:B:501:MET:CG	1:B:521:PRO:HD2	2.48	0.43
1:C:1218:ASP:O	1:C:1219:ILE:HD13	2.18	0.43
1:C:1355:THR:HG21	3:C:2352:HOH:O	2.17	0.43
1:A:143:LEU:CD1	1:A:172:VAL:HG22	2.48	0.43
1:A:390:VAL:O	1:A:394:LEU:HG	2.19	0.43
1:C:1148:THR:HG21	3:C:2935:HOH:O	2.18	0.43
1:C:1257:ARG:O	1:C:1260:LYS:HB2	2.18	0.43
1:C:1295:ALA:HA	1:C:1300:TYR:CD1	2.54	0.43
1:D:1785:GLN:NE2	1:D:1894:LEU:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:THR:HG21	1:A:234:ILE:HA	2.00	0.43
1:B:530:PRO:HA	1:B:531:PRO:HD3	1.94	0.43
1:B:817:GLU:HA	1:B:872:GLY:O	2.18	0.43
1:D:1636:ASP:OD2	1:D:1638:ALA:HB3	2.19	0.43
1:D:1710:THR:OG1	1:D:1720:THR:HA	2.19	0.43
1:B:564:ASN:HD21	1:B:566:THR:H	1.63	0.43
1:B:853:SER:C	1:B:857:SER:HB2	2.38	0.43
1:A:257:ARG:HH21	1:C:1218:ASP:CG	2.21	0.43
1:B:570:LEU:HD21	1:B:755:LEU:HD13	2.01	0.43
1:B:501:MET:HE3	3:D:2473:HOH:O	2.19	0.43
1:D:1654:ILE:HD13	1:D:1676:ALA:HB2	2.01	0.43
1:B:621:LEU:HD13	1:B:625:ILE:CD1	2.48	0.43
1:C:1211:LLP:NZ	1:C:1211:LLP:O3	2.52	0.43
1:C:1213:LEU:HG	3:C:2055:HOH:O	2.19	0.43
1:D:1754:LEU:HD23	1:D:1754:LEU:HA	1.91	0.43
1:A:190:CYS:HB3	1:A:194:LEU:HB3	2.01	0.43
1:B:834:LEU:HD12	1:D:1501:MET:N	2.33	0.43
1:A:70:LEU:HD21	1:A:255:LEU:HD23	1.99	0.42
1:B:605:ASP:HB3	1:B:652:ARG:HB2	2.01	0.42
1:B:606:GLU:HB3	1:B:651:THR:HA	2.00	0.42
1:C:1359:TYR:HB3	1:C:1363:GLU:HB3	2.01	0.42
1:A:254:LEU:HD12	1:A:254:LEU:HA	1.75	0.42
1:B:621:LEU:HD13	1:B:625:ILE:HD11	2.01	0.42
1:B:693:TYR:CD2	1:B:694:LEU:HD13	2.54	0.42
1:D:1647:MET:CE	1:D:1654:ILE:HD11	2.49	0.42
1:B:690:CYS:O	1:B:694:LEU:HB2	2.20	0.42
1:B:757:ARG:NH2	1:D:1716:HIS:HB2	2.34	0.42
3:B:2767:HOH:O	1:C:1024:HIS:HB3	2.19	0.42
1:C:1001:MET:N	1:C:1006:LYS:N	2.63	0.42
1:C:1190:CYS:C	1:C:1191:THR:HG23	2.39	0.42
1:C:1364:ARG:HG3	1:C:1364:ARG:NH1	2.34	0.42
1:D:1510:PHE:CE1	1:D:1577:LEU:HD22	2.54	0.42
1:D:1517:HIS:ND1	1:D:1576:SER:HB2	2.35	0.42
1:C:1078:GLU:CB	3:C:2702:HOH:O	2.68	0.42
1:D:1700:LEU:HD12	1:D:1700:LEU:HA	1.89	0.42
1:D:1710:THR:HG23	1:D:1720:THR:HA	2.00	0.42
1:C:1352:ALA:O	1:C:1357:SER:HA	2.19	0.42
1:D:1663:ASN:HB3	1:D:1790:HIS:CG	2.54	0.42
1:D:1691:THR:HB	1:D:1692:PRO:HD2	2.01	0.42
1:A:48:ALA:HA	1:A:53:GLU:HG2	2.02	0.42
1:B:648:THR:H	1:B:651:THR:HG21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1313:MET:HE3	1:C:1375:ARG:HD2	2.01	0.42
1:D:1742:MET:C	1:D:1743:THR:HG23	2.40	0.42
1:D:1818:LEU:HB3	3:D:2195:HOH:O	2.19	0.42
1:A:35:THR:OG1	1:D:1529:VAL:HG13	2.20	0.42
1:A:353:SER:C	1:A:357:SER:HB2	2.39	0.42
1:B:564:ASN:HA	1:B:565:PRO:HD3	1.89	0.42
1:B:655:TYR:CD1	1:B:684:VAL:HG22	2.54	0.42
1:B:862:GLU:CG	1:B:863:GLU:H	2.32	0.42
1:C:1350:HIS:HD2	1:C:1373:LEU:O	2.02	0.42
1:D:1729:ALA:O	1:D:1733:ARG:HG3	2.20	0.42
1:A:34:GLN:HG3	1:B:718:ASP:O	2.20	0.42
1:A:83:GLY:HA2	1:A:224:VAL:O	2.20	0.42
1:A:345:GLU:H	1:A:345:GLU:HG2	1.47	0.42
1:D:1693:TYR:CD2	1:D:1766:MET:HB2	2.55	0.42
1:A:280:LEU:HD23	1:A:314:ILE:CD1	2.45	0.42
1:B:712:TYR:CD1	1:B:842:GLY:HA2	2.55	0.42
1:C:1219:ILE:CG2	1:C:1220:THR:N	2.82	0.42
1:D:1705:VAL:HG12	1:D:1725:VAL:HB	2.02	0.42
1:B:593:ILE:HG22	1:B:594:THR:N	2.35	0.41
1:B:813:MET:HE3	1:B:876:LEU:O	2.20	0.41
1:D:1505:ASN:HB2	1:D:1507:LEU:CD2	2.50	0.41
1:D:1505:ASN:HB2	1:D:1507:LEU:CG	2.50	0.41
1:A:337:ARG:HE	1:A:337:ARG:HB2	1.61	0.41
1:B:578:GLU:OE2	1:B:707:HIS:CE1	2.60	0.41
1:B:591:GLY:O	1:B:595:SER:CB	2.67	0.41
1:B:743:THR:CG2	1:B:745:ALA:CB	2.98	0.41
1:B:894:LEU:HD12	1:B:894:LEU:HA	1.96	0.41
1:C:1360:THR:HG22	1:C:1363:GLU:H	1.84	0.41
1:D:1507:LEU:CB	1:D:1508:PRO:HD3	2.49	0.41
1:A:288:LEU:HB3	1:A:317:GLU:HG3	2.03	0.41
1:A:200:LEU:HD12	1:A:200:LEU:HA	1.86	0.41
1:B:503:GLY:C	1:B:505:ASN:N	2.73	0.41
1:B:763:ASN:ND2	1:B:764:LEU:H	2.17	0.41
1:B:873:LEU:HB3	3:B:2803:HOH:O	2.20	0.41
1:C:1021:PRO:HB3	1:C:1027:ALA:O	2.21	0.41
1:C:1268:ARG:O	1:C:1272:ASN:HB2	2.21	0.41
1:D:1723:ILE:HG12	3:D:2693:HOH:O	2.20	0.41
1:D:1787:GLU:HG3	3:D:3061:HOH:O	2.20	0.41
1:A:2:HIS:HB2	1:C:1334:LEU:CD1	2.50	0.41
1:A:383:ILE:HG13	1:A:383:ILE:H	1.47	0.41
1:C:1187:ASN:ND2	1:C:1195:GLN:HE21	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:TYR:HE2	1:B:524:HIS:CD2	2.38	0.41
1:B:599:THR:HG21	1:B:734:ILE:HA	2.02	0.41
1:D:1504:SER:N	1:D:1517:HIS:HD2	2.17	0.41
1:C:1091:GLY:HA2	1:D:1743:THR:O	2.20	0.41
1:D:1677:ARG:HD3	1:D:1677:ARG:HA	1.72	0.41
1:B:659:PRO:HG3	1:B:666:MET:CE	2.51	0.41
1:A:85:ALA:O	1:A:86:LEU:HG	2.21	0.41
1:A:101:LEU:HG	1:A:130:VAL:HG11	2.03	0.41
1:A:114:TYR:O	1:A:117:THR:N	2.52	0.41
1:B:507:LEU:HD22	1:B:507:LEU:HA	1.83	0.41
1:B:554:GLN:HG3	1:B:555:ALA:N	2.35	0.41
1:B:604:GLY:O	1:B:631:LYS:HE2	2.21	0.41
1:B:677:ARG:NH2	1:B:683:VAL:HG23	2.36	0.41
1:C:1034:GLN:HE22	1:C:1250:HIS:N	2.18	0.41
1:C:1280:LEU:HD13	1:C:1280:LEU:HA	1.94	0.41
1:C:1373:LEU:HD13	1:C:1374:VAL:N	2.36	0.41
1:B:768:ARG:HB3	1:B:880:LEU:CD2	2.51	0.41
1:C:1001:MET:HA	1:C:1008:PRO:HG3	2.02	0.41
1:A:205:VAL:HG23	1:A:225:VAL:HB	2.02	0.40
1:C:1364:ARG:HG3	1:C:1364:ARG:HH11	1.86	0.40
1:A:157:GLU:HB3	1:A:186:ASP:HB3	2.02	0.40
1:A:174:LYS:NZ	1:A:177:ARG:HB3	2.37	0.40
1:B:578:GLU:CG	1:B:692:PRO:HB3	2.49	0.40
1:B:705:VAL:CG2	1:B:725:VAL:HB	2.50	0.40
1:B:833:GLN:NE2	3:B:2535:HOH:O	2.53	0.40
1:C:1086:LEU:HA	3:C:2022:HOH:O	2.21	0.40
1:C:1316:PHE:HE1	1:C:1376:LEU:HD22	1.86	0.40
1:D:1501:MET:N	1:D:1516:HIS:CG	2.89	0.40
1:A:366:HIS:HD2	1:A:367:TYR:CD2	2.40	0.40
1:C:1001:MET:N	1:C:1006:LYS:HB2	2.36	0.40
1:C:1011:ALA:HB2	1:C:1263:ASN:ND2	2.37	0.40
1:A:102:ARG:HD3	1:A:102:ARG:HA	1.87	0.40
1:A:329:MET:HG3	1:A:350:HIS:HB2	2.02	0.40
1:C:1068:ASN:HA	1:C:1071:GLU:OE2	2.21	0.40
1:D:1647:MET:HE1	1:D:1651:THR:HG21	2.02	0.40
1:D:1657:GLU:HG2	1:D:1686:ASP:HB3	2.04	0.40
1:B:507:LEU:HB3	1:B:508:PRO:HD3	2.04	0.40
1:B:614:TYR:O	1:B:615:GLY:C	2.60	0.40
1:C:1375:ARG:HG3	3:C:2827:HOH:O	2.20	0.40
1:D:1505:ASN:HB2	1:D:1507:LEU:HD21	2.04	0.40
1:D:1621:LEU:O	1:D:1626:GLY:CA	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1829:MET:HG3	1:D:1850:HIS:HB2	2.04	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	395/398 (99%)	365 (92%)	24 (6%)	6 (2%)	10	2
1	B	395/398 (99%)	357 (90%)	32 (8%)	6 (2%)	10	2
1	C	395/398 (99%)	367 (93%)	25 (6%)	3 (1%)	19	7
1	D	395/398 (99%)	357 (90%)	33 (8%)	5 (1%)	12	3
All	All	1580/1592 (99%)	1446 (92%)	114 (7%)	20 (1%)	12	3

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	ALA
1	A	340	SER
1	B	862	GLU
1	C	1181	ALA
1	A	240	LYS
1	B	840	SER
1	C	1381	GLU
1	D	1859	TYR
1	A	5	ASN
1	B	504	SER
1	B	505	ASN
1	B	558	PHE
1	D	1840	SER
1	A	115	GLY

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Mol	Chain	Res	Type
1	B	861	PRO
1	D	1664	MET
1	A	359	TYR
1	C	1340	SER
1	D	1503	GLY
1	D	1552	GLY

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	306/306 (100%)	244 (80%)	62 (20%)	1	0
1	B	306/306 (100%)	248 (81%)	58 (19%)	1	0
1	C	306/306 (100%)	260 (85%)	46 (15%)	3	0
1	D	306/306 (100%)	257 (84%)	49 (16%)	2	0
All	All	1224/1224 (100%)	1009 (82%)	215 (18%)	2	0

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	HIS
1	A	5	ASN
1	A	7	LEU
1	A	22	GLN
1	A	37	THR
1	A	50	PHE
1	A	53	GLU
1	A	54	GLN
1	A	62	ILE
1	A	63	SER
1	A	66	THR
1	A	84	LEU
1	A	93	ILE
1	A	97	LEU

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Mol	Chain	Res	Type
1	A	99	THR
1	A	101	LEU
1	A	106	GLU
1	A	109	LEU
1	A	111	ASN
1	A	121	LEU
1	A	132	LEU
1	A	133	ARG
1	A	135	VAL
1	A	141	GLN
1	A	143	LEU
1	A	147	MET
1	A	152	ARG
1	A	157	GLU
1	A	163	ASN
1	A	174	LYS
1	A	177	ARG
1	A	178	LYS
1	A	200	LEU
1	A	213	LEU
1	A	227	SER
1	A	230	LEU
1	A	239	LEU
1	A	243	THR
1	A	254	LEU
1	A	263	ASN
1	A	275	VAL
1	A	276	LEU
1	A	280	LEU
1	A	305	GLN
1	A	308	SER
1	A	314	ILE
1	A	326	ARG
1	A	334	LEU
1	A	337	ARG
1	A	341	LEU
1	A	345	GLU
1	A	347	LEU
1	A	358	SER
1	A	364	ARG
1	A	373	LEU
1	A	376	LEU

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Mol	Chain	Res	Type
1	A	382	ASP
1	A	383	ILE
1	A	390	VAL
1	A	391	GLN
1	A	395	LYS
1	B	502	HIS
1	B	504	SER
1	B	506	LYS
1	B	507	LEU
1	B	537	THR
1	B	549	CYS
1	B	553	GLU
1	B	564	ASN
1	B	569	LEU
1	B	570	LEU
1	B	584	LEU
1	B	593	ILE
1	B	599	THR
1	B	608	LEU
1	B	609	LEU
1	B	621	LEU
1	B	625	ILE
1	B	633	ARG
1	B	641	GLN
1	B	643	LEU
1	B	651	THR
1	B	652	ARG
1	B	653	VAL
1	B	663	ASN
1	B	677	ARG
1	B	694	LEU
1	B	700	LEU
1	B	704	LEU
1	B	705	VAL
1	B	713	LEU
1	B	714	SER
1	B	727	SER
1	B	730	LEU
1	B	736	LEU
1	B	737	GLN
1	B	748	SER
1	B	755	LEU

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Mol	Chain	Res	Type
1	B	763	ASN
1	B	768	ARG
1	B	778	GLU
1	B	789	ILE
1	B	794	LEU
1	B	802	LEU
1	B	805	GLN
1	B	808	SER
1	B	814	ILE
1	B	819	LYS
1	B	822	ILE
1	B	841	LEU
1	B	855	THR
1	B	858	SER
1	B	860	THR
1	B	862	GLU
1	B	863	GLU
1	B	869	ILE
1	B	870	SER
1	B	887	LEU
1	B	894	LEU
1	C	1004	SER
1	C	1005	ASN
1	C	1006	LYS
1	C	1007	LEU
1	C	1015	ILE
1	C	1028	LEU
1	C	1037	THR
1	C	1054	GLN
1	C	1063	SER
1	C	1093	ILE
1	C	1099	THR
1	C	1108	LEU
1	C	1117	THR
1	C	1125	ILE
1	C	1131	LYS
1	C	1132	LEU
1	C	1143	LEU
1	C	1152	ARG
1	C	1154	ILE
1	C	1172	VAL
1	C	1174	LYS

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Mol	Chain	Res	Type
1	C	1177	ARG
1	C	1205	VAL
1	C	1236	LEU
1	C	1239	LEU
1	C	1243	THR
1	C	1262	LEU
1	C	1264	LEU
1	C	1276	LEU
1	C	1278	GLU
1	C	1280	LEU
1	C	1285	GLN
1	C	1299	GLN
1	C	1305	GLN
1	C	1317	GLU
1	C	1322	ILE
1	C	1341	LEU
1	C	1354	MET
1	C	1358	SER
1	C	1360	THR
1	C	1363	GLU
1	C	1370	SER
1	C	1371	GLU
1	C	1375	ARG
1	C	1376	LEU
1	C	1391	GLN
1	D	1501	MET
1	D	1502	HIS
1	D	1505	ASN
1	D	1506	LYS
1	D	1507	LEU
1	D	1528	LEU
1	D	1529	VAL
1	D	1537	THR
1	D	1554	GLN
1	D	1573	ARG
1	D	1598	TRP
1	D	1599	THR
1	D	1601	LEU
1	D	1608	LEU
1	D	1609	LEU
1	D	1631	LYS
1	D	1633	ARG

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Mol	Chain	Res	Type
1	D	1641	GLN
1	D	1652	ARG
1	D	1653	VAL
1	D	1677	ARG
1	D	1678	LYS
1	D	1684	VAL
1	D	1687	ASN
1	D	1698	LEU
1	D	1700	LEU
1	D	1705	VAL
1	D	1719	ILE
1	D	1720	THR
1	D	1739	LEU
1	D	1743	THR
1	D	1776	LEU
1	D	1802	LEU
1	D	1805	GLN
1	D	1819	LYS
1	D	1827	ARG
1	D	1830	ASN
1	D	1836	SER
1	D	1841	LEU
1	D	1845	GLU
1	D	1858	SER
1	D	1862	GLU
1	D	1867	TYR
1	D	1870	SER
1	D	1873	LEU
1	D	1886	LEU
1	D	1887	LEU
1	D	1892	GLN
1	D	1894	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	68	ASN
1	A	111	ASN
1	A	134	HIS
1	A	141	GLN
1	A	161	ASN

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Mol	Chain	Res	Type
1	A	207	HIS
1	A	228	GLN
1	A	237	GLN
1	A	250	HIS
1	A	263	ASN
1	A	274	GLN
1	A	309	GLN
1	A	349	GLN
1	A	366	HIS
1	B	522	GLN
1	B	524	HIS
1	B	557	HIS
1	B	564	ASN
1	B	641	GLN
1	B	661	ASN
1	B	663	ASN
1	B	707	HIS
1	B	737	GLN
1	B	763	ASN
1	B	790	HIS
1	B	799	GLN
1	B	830	ASN
1	B	833	GLN
1	C	1002	HIS
1	C	1034	GLN
1	C	1068	ASN
1	C	1161	ASN
1	C	1165	HIS
1	C	1179	HIS
1	C	1187	ASN
1	C	1274	GLN
1	C	1285	GLN
1	C	1306	GLN
1	C	1309	GLN
1	C	1330	ASN
1	C	1356	HIS
1	D	1505	ASN
1	D	1516	HIS
1	D	1517	HIS
1	D	1534	GLN
1	D	1641	GLN
1	D	1661	ASN

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Mol	Chain	Res	Type
1	D	1687	ASN
1	D	1695	GLN
1	D	1707	HIS
1	D	1774	GLN
1	D	1790	HIS
1	D	1830	ASN
1	D	1849	GLN
1	D	1892	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	LLP	B	711	1	23,24,25	2.92	6 (26%)	25,32,34	1.72	6 (24%)
1	LLP	D	1711	1	23,24,25	2.89	6 (26%)	25,32,34	1.69	6 (24%)
1	LLP	A	211	1	23,24,25	2.90	6 (26%)	25,32,34	1.73	5 (20%)
1	LLP	C	1211	1	23,24,25	2.88	7 (30%)	25,32,34	1.65	5 (20%)

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
1	LLP	B	711	1	-	7/16/17/19	0/1/1/1
1	LLP	D	1711	1	-	4/16/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	211	1	-	5/16/17/19	0/1/1/1
1	LLP	C	1211	1	-	5/16/17/19	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	711	LLP	C6-C5	7.54	1.53	1.37
1	A	211	LLP	C6-C5	7.23	1.52	1.37
1	C	1211	LLP	C6-C5	7.13	1.52	1.37
1	D	1711	LLP	C6-C5	7.11	1.52	1.37
1	D	1711	LLP	C6-N1	5.92	1.46	1.34
1	C	1211	LLP	O3-C3	-5.86	1.23	1.37
1	B	711	LLP	C6-N1	5.80	1.46	1.34
1	C	1211	LLP	C4'-NZ	5.77	1.46	1.27
1	B	711	LLP	O3-C3	-5.75	1.23	1.37
1	B	711	LLP	C4'-NZ	5.74	1.46	1.27
1	A	211	LLP	O3-C3	-5.72	1.23	1.37
1	D	1711	LLP	C4'-NZ	5.70	1.46	1.27
1	A	211	LLP	C6-N1	5.69	1.46	1.34
1	D	1711	LLP	O3-C3	-5.67	1.23	1.37
1	C	1211	LLP	C6-N1	5.64	1.46	1.34
1	A	211	LLP	C4'-NZ	5.60	1.46	1.27
1	A	211	LLP	P-OP4	-3.73	1.48	1.60
1	C	1211	LLP	P-OP4	-3.57	1.48	1.60
1	D	1711	LLP	C4-C4'	3.54	1.53	1.46
1	D	1711	LLP	P-OP4	-3.53	1.48	1.60
1	B	711	LLP	P-OP4	-3.52	1.48	1.60
1	A	211	LLP	C4-C4'	3.47	1.53	1.46
1	C	1211	LLP	C4-C4'	3.45	1.53	1.46
1	B	711	LLP	C4-C4'	3.42	1.53	1.46
1	C	1211	LLP	C2'-C2	2.05	1.53	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	211	LLP	C5-C6-N1	-5.98	113.85	123.82
1	B	711	LLP	C5-C6-N1	-5.87	114.05	123.82
1	D	1711	LLP	C5-C6-N1	-5.83	114.10	123.82
1	C	1211	LLP	C5-C6-N1	-5.83	114.11	123.82
1	A	211	LLP	C4-C4'-NZ	-2.97	110.67	124.31
1	D	1711	LLP	C4-C4'-NZ	-2.89	111.05	124.31
1	B	711	LLP	C4-C4'-NZ	-2.87	111.15	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1211	LLP	C4-C3-C2	2.76	121.89	120.19
1	B	711	LLP	C4-C3-C2	2.54	121.76	120.19
1	C	1211	LLP	C4-C4'-NZ	-2.47	112.96	124.31
1	A	211	LLP	C4-C3-C2	2.40	121.68	120.19
1	D	1711	LLP	C2'-C2-C3	-2.33	118.02	120.89
1	B	711	LLP	C3-C4-C5	2.31	120.03	118.26
1	B	711	LLP	C2'-C2-C3	-2.26	118.10	120.89
1	A	211	LLP	C2'-C2-C3	-2.24	118.12	120.89
1	A	211	LLP	C6-N1-C2	2.20	123.24	119.17
1	D	1711	LLP	C6-N1-C2	2.17	123.19	119.17
1	D	1711	LLP	C4-C3-C2	2.15	121.52	120.19
1	C	1211	LLP	C6-N1-C2	2.13	123.11	119.17
1	B	711	LLP	C6-N1-C2	2.11	123.08	119.17
1	C	1211	LLP	C2'-C2-C3	-2.10	118.30	120.89
1	D	1711	LLP	C3-C4-C5	2.00	119.80	118.26

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	211	LLP	O-C-CA-CB
1	B	711	LLP	O-C-CA-CB
1	C	1211	LLP	C4-C4'-NZ-CE
1	C	1211	LLP	N-CA-CB-CG
1	C	1211	LLP	O-C-CA-CB
1	C	1211	LLP	CG-CD-CE-NZ
1	D	1711	LLP	O-C-CA-CB
1	D	1711	LLP	C4-C4'-NZ-CE
1	A	211	LLP	C4-C4'-NZ-CE
1	B	711	LLP	CG-CD-CE-NZ
1	C	1211	LLP	CA-CB-CG-CD
1	B	711	LLP	C3-C4-C4'-NZ
1	A	211	LLP	CD-CE-NZ-C4'
1	D	1711	LLP	CD-CE-NZ-C4'
1	B	711	LLP	C4-C5-C5'-OP4
1	A	211	LLP	N-CA-CB-CG
1	B	711	LLP	CD-CE-NZ-C4'
1	A	211	LLP	CA-CB-CG-CD
1	D	1711	LLP	C3-C4-C4'-NZ
1	B	711	LLP	C5-C4-C4'-NZ
1	B	711	LLP	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	711	LLP	1	0
1	D	1711	LLP	2	0
1	A	211	LLP	4	0
1	C	1211	LLP	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	400	-	4,4,4	0.42	0	6,6,6	0.05	0
2	SO4	D	1900	-	4,4,4	0.37	0	6,6,6	0.05	0
2	SO4	B	1901	-	4,4,4	0.45	0	6,6,6	0.04	0
2	SO4	C	1400	-	4,4,4	0.39	0	6,6,6	0.05	0
2	SO4	B	900	-	4,4,4	0.39	0	6,6,6	0.05	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.