



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:40 am BST

PDB ID : 1MMF
Title : Crystal structure of substrate free form of glycerol dehydratase
Authors : Liao, D.I.; Dotson, G.; Turner, I.; Reiss, L.; Emptage, M.
Deposited on : 2002-09-03
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

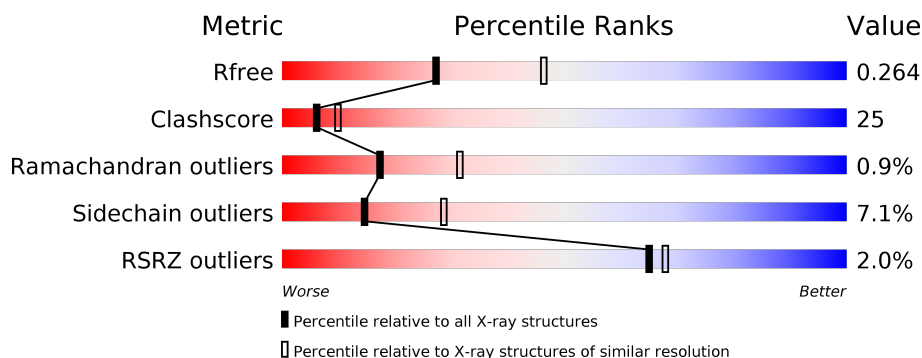
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	555	<div> <div>0.5%</div> <div>57%</div> <div>38%</div> <div>• •</div> </div>
1	L	555	<div> <div>0.5%</div> <div>63%</div> <div>33%</div> <div>5%</div> </div>
2	B	194	<div> <div>4%</div> <div>47%</div> <div>41%</div> <div>5%</div> <div>7%</div> </div>
2	E	194	<div> <div>2%</div> <div>47%</div> <div>44%</div> <div>•</div> <div>5%</div> </div>
3	G	141	<div> <div>4%</div> <div>62%</div> <div>28%</div> <div>•</div> <div>6%</div> </div>
3	M	141	<div> <div>3%</div> <div>60%</div> <div>30%</div> <div>• •</div> <div>7%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13782 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 glycerol dehydrase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4220	2624	734	832	30			
1	L	555	Total	C	N	O	S	0	0	0
			4245	2639	737	839	30			

- Molecule 2 is a protein called glycerol dehydrase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1396	883	251	258	4			
2	E	184	Total	C	N	O	S	0	0	0
			1420	897	257	262	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	VAL	MET	CONFLICT	UNP O08505
E	1	VAL	MET	CONFLICT	UNP O08505

- Molecule 3 is a protein called glycerol dehydrase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	132	Total	C	N	O	S	0	0	0
			1059	662	198	197	2			
3	M	131	Total	C	N	O	S	0	0	0
			1051	658	197	194	2			

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

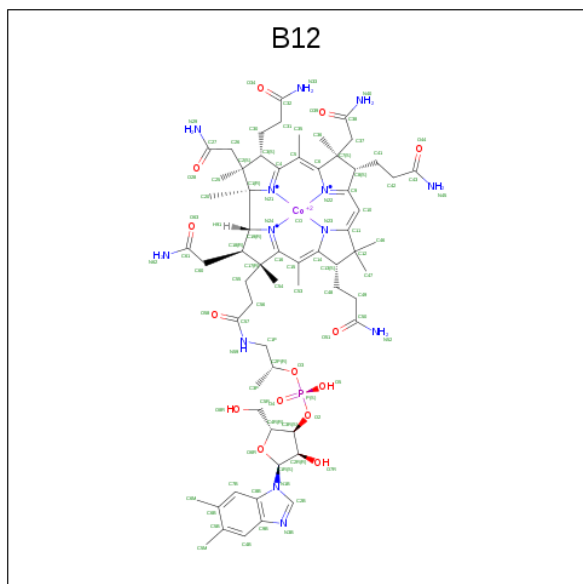
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total K 1 1	0	0

- Molecule 5 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
5	E	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

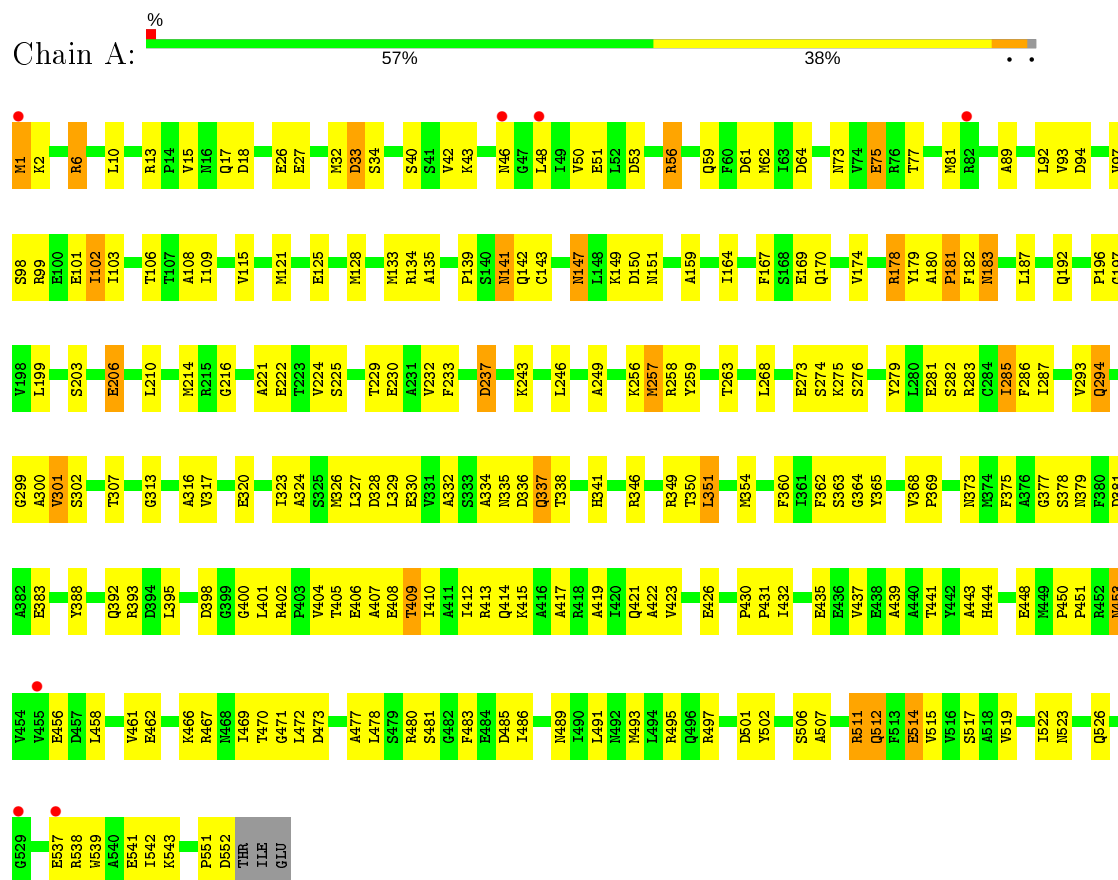
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	55	Total O 55 55	0	0
6	B	17	Total O 17 17	0	0
6	G	20	Total O 20 20	0	0
6	L	71	Total O 71 71	0	0
6	E	25	Total O 25 25	0	0
6	M	19	Total O 19 19	0	0

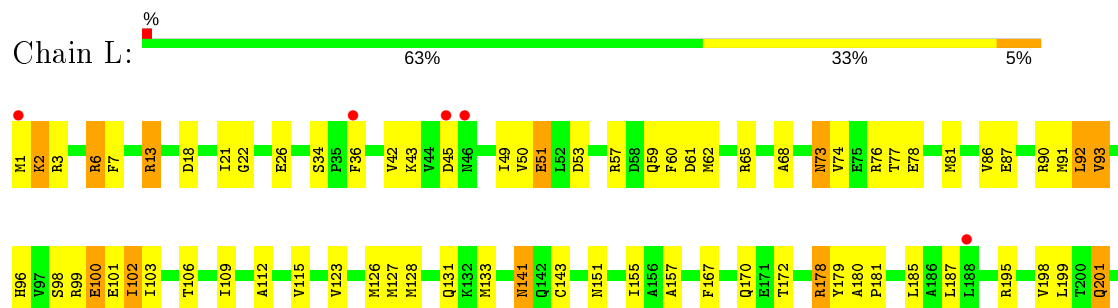
3 Residue-property plots

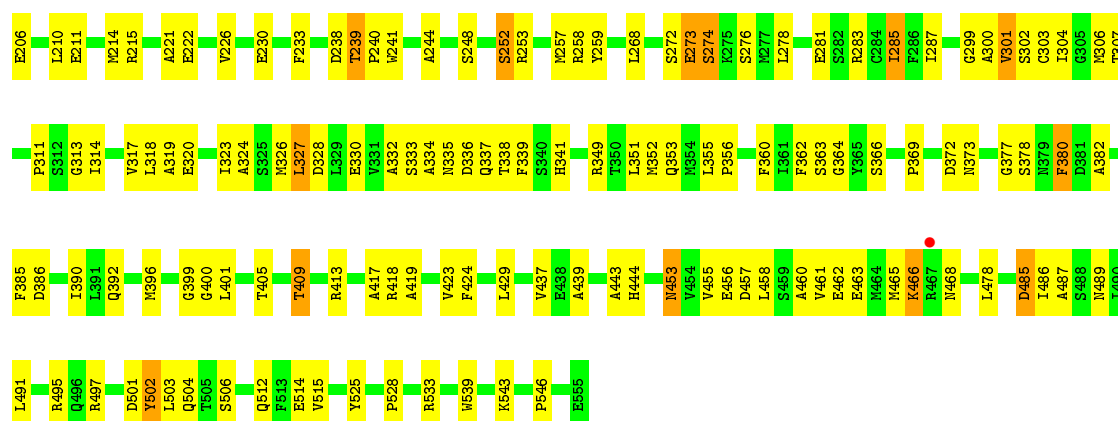
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: glycerol dehydrase alpha subunit

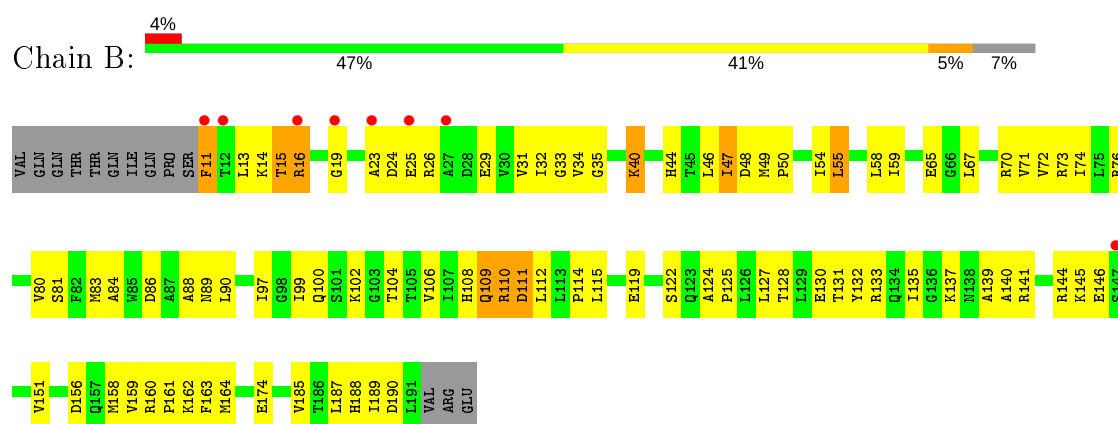


- Molecule 1: glycerol dehydrase alpha subunit

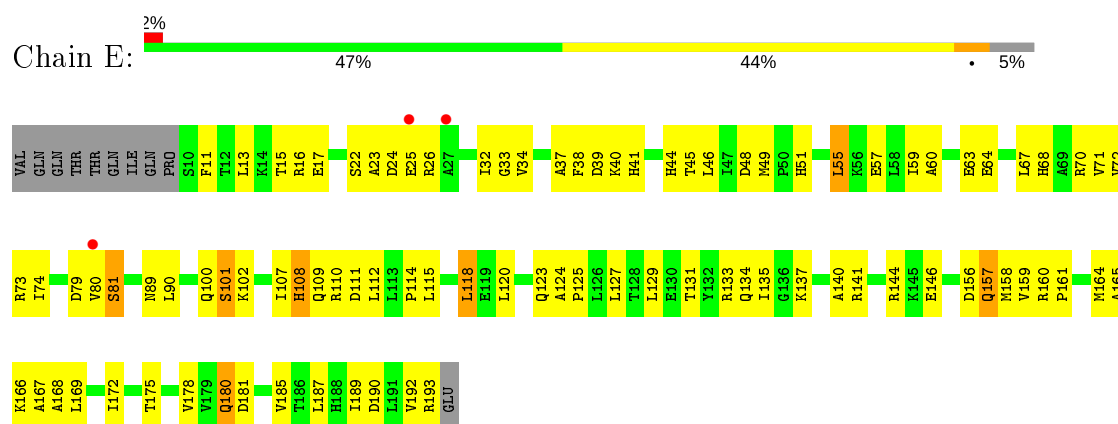




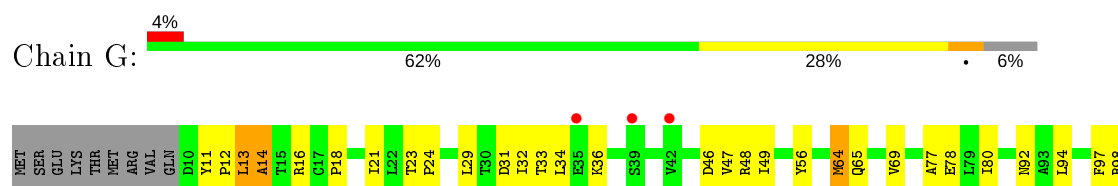
- Molecule 2: glycerol dehydrogenase beta subunit



- Molecule 2: glycerol dehydrogenase beta subunit

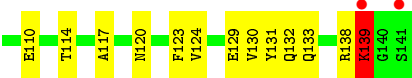


- Molecule 3: glycerol dehydrogenase gamma subunit





● Molecule 3: glycerol dehydrase gamma subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.70Å 110.07Å 114.69Å 90.00° 107.64° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 28.82 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.50) 85.1 (28.82-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.269 0.226 , 0.264	Depositor DCC
R_{free} test set	3316 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.998	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.59$, $\langle L^2 \rangle = 0.45$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13782	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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: K, B12

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	0.39	0/4283	0.65	0/5798
1	L	0.48	2/4308 (0.0%)	0.70	5/5831 (0.1%)
2	B	0.45	1/1423 (0.1%)	0.68	1/1928 (0.1%)
2	E	0.38	0/1447	0.68	0/1960
3	G	0.36	0/1079	0.62	0/1462
3	M	0.40	0/1071	0.62	0/1451
All	All	0.42	3/13611 (0.0%)	0.67	6/18430 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	380	PHE	CE1-CZ	13.75	1.63	1.37
1	L	380	PHE	CE2-CZ	-5.96	1.26	1.37
2	B	111	ASP	N-CA	-5.03	1.36	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	274	SER	O-C-N	8.50	136.30	122.70
1	L	273	GLU	O-C-N	7.03	133.95	122.70
1	L	380	PHE	CZ-CE2-CD2	5.84	127.11	120.10
1	L	274	SER	CA-C-N	-5.63	104.82	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	110	ARG	C-N-CA	-5.33	108.37	121.70
1	L	273	GLU	CA-C-N	-5.31	105.52	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	380	PHE	Sidechain

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	4220	0	4171	243	0
1	L	4245	0	4195	176	0
2	B	1396	0	1418	97	0
2	E	1420	0	1445	107	0
3	G	1059	0	1061	34	0
3	M	1051	0	1057	46	0
4	A	1	0	0	0	0
4	L	1	0	0	0	0
5	B	91	0	88	5	0
5	E	91	0	87	11	0
6	A	55	0	0	1	0
6	B	17	0	0	1	0
6	E	25	0	0	1	0
6	G	20	0	0	0	0
6	L	71	0	0	3	0
6	M	19	0	0	4	0
All	All	13782	0	13522	666	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 25.

All (666) 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)
3:M:139:LYS:HD2	3:M:139:LYS:H	1.08	1.06
2:B:16:ARG:HA	2:B:16:ARG:HE	1.19	1.04
1:L:285:ILE:HD12	1:L:324:ALA:HA	1.39	1.02
1:L:272:SER:C	1:L:274:SER:H	1.44	1.01
1:A:285:ILE:HD13	1:A:324:ALA:HA	1.43	0.99
2:B:49:MET:HE3	2:B:54:ILE:HG12	1.43	0.98
2:E:89:ASN:ND2	2:E:110:ARG:HB2	1.78	0.97
3:G:24:PRO:HB3	3:G:80:ILE:HD11	1.42	0.97
1:A:147:ASN:HD21	1:A:151:ASN:H	1.13	0.93
1:A:1:MET:HG3	1:A:2:LYS:N	1.84	0.92
2:E:157:GLN:H	2:E:157:GLN:HE21	1.11	0.92
1:L:272:SER:O	1:L:274:SER:N	2.02	0.92
1:A:470:THR:HG22	1:A:472:LEU:H	1.32	0.92
1:L:272:SER:C	1:L:274:SER:N	2.19	0.90
1:A:1:MET:CG	1:A:2:LYS:H	1.82	0.89
3:G:139:LYS:HD2	3:G:140:GLY:H	1.38	0.89
1:A:511:ARG:HB3	1:A:511:ARG:HH21	1.35	0.89
1:A:1:MET:HG3	1:A:2:LYS:H	1.36	0.89
1:A:551:PRO:HG3	1:L:21:ILE:HB	1.53	0.89
3:G:78:GLU:CD	3:G:119:VAL:HG12	1.94	0.88
3:M:139:LYS:N	3:M:139:LYS:HD2	1.87	0.87
1:A:224:VAL:HG12	1:A:243:LYS:HD2	1.56	0.86
1:L:338:THR:H	2:E:160:ARG:HH21	1.24	0.85
1:L:239:THR:HG22	1:L:241:TRP:H	1.42	0.84
2:E:109:GLN:NE2	2:E:111:ASP:H	1.76	0.83
1:A:373:ASN:HD22	1:A:377:GLY:H	1.25	0.82
1:A:426:GLU:HG3	1:A:480:ARG:HH21	1.43	0.82
2:E:32:ILE:HG13	2:E:32:ILE:O	1.79	0.82
1:A:453:ASN:HD22	1:A:456:GLU:H	1.25	0.82
2:E:124:ALA:HA	2:E:127:LEU:HD23	1.63	0.81
1:A:373:ASN:HD21	1:A:375:PHE:HB2	1.47	0.80
1:A:453:ASN:ND2	1:A:456:GLU:H	1.79	0.80
2:E:160:ARG:HB3	2:E:161:PRO:HD3	1.63	0.80
2:E:60:ALA:O	2:E:64:GLU:HG3	1.80	0.80
1:A:373:ASN:ND2	1:A:377:GLY:H	1.79	0.80
1:A:405:THR:O	1:A:409:THR:HG22	1.82	0.79
3:G:78:GLU:OE2	3:G:119:VAL:HG12	1.83	0.79
2:E:157:GLN:H	2:E:157:GLN:NE2	1.80	0.78
2:E:46:LEU:HD21	2:E:167:ALA:HA	1.65	0.78
1:A:462:GLU:O	1:A:466:LYS:HD3	1.83	0.78
1:L:285:ILE:HD11	1:L:327:LEU:HD12	1.65	0.78
2:E:109:GLN:HE22	2:E:111:ASP:H	1.28	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:NH2	1:A:59:GLN:HB2	1.99	0.77
1:L:306:MET:HG2	2:E:164:MET:HE3	1.65	0.77
1:A:103:ILE:HD12	1:A:328:ASP:HB2	1.65	0.77
1:A:192:GLN:HE22	1:A:197:GLY:H	1.31	0.76
1:A:56:ARG:H	1:A:56:ARG:HH21	1.32	0.76
2:B:35:GLY:HA3	2:B:174:GLU:OE1	1.85	0.76
3:M:129:GLU:HG2	3:M:133:GLN:NE2	2.00	0.76
1:A:73:ASN:OD1	1:A:75:GLU:HG3	1.84	0.76
2:B:23:ALA:HA	2:B:90:LEU:HD12	1.67	0.76
1:A:351:LEU:HD12	1:A:354:MET:HE3	1.66	0.76
2:B:109:GLN:HG2	2:B:112:LEU:HD13	1.68	0.76
3:G:139:LYS:HD2	3:G:140:GLY:N	2.01	0.75
1:L:302:SER:HA	1:L:337:GLN:HG3	1.68	0.74
1:L:306:MET:HG2	2:E:164:MET:CE	2.17	0.73
2:B:80:VAL:HG22	2:B:106:VAL:HG12	1.70	0.73
2:E:175:THR:O	2:E:178:VAL:HG22	1.87	0.73
1:A:332:ALA:HA	1:A:360:PHE:HB2	1.70	0.73
1:A:6:ARG:HD3	1:L:444:HIS:ND1	2.03	0.72
1:L:466:LYS:N	1:L:466:LYS:HE3	2.04	0.72
1:A:302:SER:HA	1:A:337:GLN:HG3	1.70	0.72
1:A:522:ILE:HD12	1:A:522:ILE:H	1.53	0.72
2:E:89:ASN:HD22	2:E:110:ARG:HB2	1.55	0.71
1:A:337:GLN:HA	1:A:337:GLN:HE21	1.56	0.71
1:A:486:ILE:HD12	1:A:486:ILE:H	1.56	0.71
1:A:539:TRP:CE2	1:A:543:LYS:HD2	2.24	0.71
1:A:180:ALA:HB3	1:A:181:PRO:HD3	1.71	0.71
2:B:40:LYS:HD2	2:B:73:ARG:HH22	1.56	0.70
2:E:32:ILE:HD11	2:E:55:LEU:HD21	1.73	0.70
1:L:528:PRO:HA	1:L:533:ARG:NH2	2.06	0.70
1:A:92:LEU:HD21	1:A:102:ILE:HD13	1.72	0.70
1:A:373:ASN:ND2	1:A:375:PHE:H	1.88	0.70
2:B:128:THR:HG23	2:B:131:THR:H	1.54	0.70
1:L:405:THR:O	1:L:409:THR:HG23	1.91	0.70
1:A:368:VAL:CG2	1:A:369:PRO:HD2	2.21	0.70
2:E:168:ALA:O	2:E:172:ILE:HG13	1.92	0.69
3:G:138:ARG:HG2	3:G:139:LYS:HG3	1.73	0.69
1:L:180:ALA:HB3	1:L:181:PRO:HD3	1.74	0.69
1:A:273:GLU:O	1:A:275:LYS:HD2	1.92	0.69
1:A:405:THR:HG22	1:A:407:ALA:H	1.57	0.69
1:L:65:ARG:HH12	3:M:133:GLN:HE22	1.39	0.69
2:B:71:VAL:HG21	2:B:189:ILE:HD11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:MET:HE3	2:B:54:ILE:CG1	2.22	0.69
1:A:92:LEU:CD2	1:A:102:ILE:HD13	2.23	0.69
2:B:124:ALA:HB3	2:B:125:PRO:HD3	1.73	0.69
3:G:92:ASN:O	3:G:98:ARG:HG3	1.91	0.69
1:A:368:VAL:HG22	1:A:369:PRO:HD2	1.74	0.68
1:L:239:THR:HG22	1:L:241:TRP:N	2.07	0.68
1:L:285:ILE:CD1	1:L:324:ALA:HA	2.19	0.68
1:A:99:ARG:O	1:A:103:ILE:HG12	1.93	0.68
1:A:409:THR:HG21	1:L:7:PHE:CE1	2.29	0.68
2:E:157:GLN:HE21	2:E:157:GLN:N	1.89	0.68
1:L:45:ASP:OD2	1:L:50:VAL:HG21	1.94	0.68
1:A:56:ARG:HH21	1:A:56:ARG:N	1.90	0.68
1:A:141:ASN:ND2	1:A:362:PHE:HB2	2.08	0.67
1:A:102:ILE:HD11	1:A:326:MET:HB2	1.77	0.67
2:E:81:SER:OG	5:E:602:B12:HM62	1.95	0.67
2:E:17:GLU:HG3	2:E:185:VAL:HG11	1.77	0.67
1:L:1:MET:O	1:L:2:LYS:HB2	1.95	0.66
3:M:14:ALA:O	3:M:18:PRO:HG3	1.96	0.66
1:A:17:GLN:HB2	1:A:341:HIS:CD2	2.31	0.66
1:A:56:ARG:HD3	1:A:56:ARG:H	1.60	0.66
2:B:32:ILE:HD11	2:B:71:VAL:HG22	1.77	0.66
2:E:72:VAL:HG12	2:E:73:ARG:N	2.11	0.66
2:E:13:LEU:HD21	2:E:59:ILE:HD12	1.78	0.65
1:A:141:ASN:HD21	1:A:362:PHE:HB2	1.59	0.65
1:A:486:ILE:N	1:A:486:ILE:HD12	2.10	0.65
1:A:77:THR:HG23	1:A:108:ALA:O	1.97	0.65
1:A:134:ARG:NH1	1:A:139:PRO:HG3	2.12	0.65
2:B:49:MET:CE	2:B:54:ILE:HG12	2.23	0.65
1:A:1:MET:CG	1:A:2:LYS:N	2.48	0.64
1:A:346:ARG:HB2	1:A:379:ASN:HD21	1.60	0.64
1:A:26:GLU:O	1:A:274:SER:HB3	1.97	0.64
1:A:337:GLN:NE2	2:B:160:ARG:HH22	1.95	0.64
1:L:201:GLN:NE2	6:L:1014:HOH:O	2.31	0.64
1:L:501:ASP:HB3	1:L:515:VAL:HG21	1.79	0.64
3:G:139:LYS:CD	3:G:140:GLY:H	2.08	0.63
1:A:159:ALA:HB1	1:A:170:GLN:HE22	1.63	0.63
2:E:156:ASP:HB3	2:E:159:VAL:HG23	1.79	0.63
2:B:47:ILE:HG23	2:B:47:ILE:O	1.97	0.63
1:A:539:TRP:NE1	1:A:543:LYS:HD2	2.13	0.63
1:A:18:ASP:OD1	1:A:341:HIS:HD2	1.82	0.63
1:A:56:ARG:CZ	1:A:59:GLN:HB2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:MET:HE1	2:B:99:ILE:O	1.99	0.63
1:L:285:ILE:HD13	1:L:323:ILE:HG22	1.80	0.63
1:L:332:ALA:HA	1:L:360:PHE:HB2	1.80	0.63
1:A:330:GLU:OE2	1:A:506:SER:HA	1.99	0.62
1:L:18:ASP:OD1	1:L:341:HIS:HD2	1.82	0.62
1:A:300:ALA:HB2	1:A:307:THR:HG21	1.81	0.62
1:A:42:VAL:HG11	1:A:77:THR:HG22	1.80	0.62
5:E:602:B12:H531	5:E:602:B12:H552	1.82	0.62
3:M:129:GLU:HG2	3:M:133:GLN:HE21	1.63	0.62
3:M:11:TYR:N	3:M:12:PRO:CD	2.62	0.62
1:A:336:ASP:O	1:A:378:SER:HA	1.99	0.62
2:B:97:ILE:HD11	2:B:139:ALA:CB	2.29	0.61
1:L:239:THR:CG2	1:L:241:TRP:H	2.12	0.61
1:A:285:ILE:CD1	1:A:324:ALA:HA	2.27	0.61
2:B:156:ASP:HB3	2:B:159:VAL:HG23	1.83	0.61
2:B:109:GLN:CG	2:B:112:LEU:HD13	2.30	0.61
1:A:40:SER:HA	1:A:53:ASP:OD1	2.00	0.61
3:G:49:ILE:O	3:G:80:ILE:HD12	2.00	0.61
1:L:453:ASN:HD22	1:L:453:ASN:C	2.02	0.61
1:L:102:ILE:HD12	1:L:133:MET:HE2	1.83	0.61
3:M:48:ARG:HB3	6:M:148:HOH:O	2.01	0.61
1:A:285:ILE:HD11	1:A:327:LEU:CD2	2.30	0.61
1:A:491:LEU:O	1:A:495:ARG:HG3	2.01	0.60
2:E:109:GLN:HE22	2:E:111:ASP:N	1.99	0.60
1:A:426:GLU:CG	1:A:480:ARG:HH21	2.14	0.60
2:B:127:LEU:HD22	2:B:127:LEU:N	2.16	0.60
1:L:123:VAL:HG11	1:L:352:MET:SD	2.42	0.60
2:E:89:ASN:HD21	2:E:110:ARG:HB2	1.63	0.60
1:L:157:ALA:HB1	1:L:413:ARG:HD3	1.84	0.60
1:A:470:THR:HG22	1:A:472:LEU:N	2.11	0.60
1:L:87:GLU:O	1:L:91:MET:HG3	2.02	0.60
1:A:346:ARG:HB2	1:A:379:ASN:ND2	2.17	0.60
2:B:13:LEU:C	2:B:13:LEU:HD23	2.22	0.60
5:B:601:B12:H473	5:B:601:B12:H491	1.84	0.60
2:E:169:LEU:HA	2:E:172:ILE:HD12	1.82	0.60
3:M:13:LEU:HB3	3:M:21:ILE:HD11	1.83	0.60
2:B:67:LEU:HD11	2:B:144:ARG:HD2	1.83	0.60
1:A:537:GLU:CD	1:A:537:GLU:H	2.06	0.59
3:M:52:GLN:HB2	6:M:147:HOH:O	2.02	0.59
1:A:1:MET:O	1:A:2:LYS:HB3	2.03	0.59
1:A:437:VAL:O	1:A:441:THR:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ALA:O	1:A:423:VAL:HG23	2.03	0.59
2:B:65:GLU:OE1	2:B:137:LYS:HE2	2.02	0.59
2:E:16:ARG:NH1	2:E:190:ASP:OD2	2.36	0.59
1:L:300:ALA:HB2	1:L:307:THR:HG21	1.83	0.59
1:L:528:PRO:HA	1:L:533:ARG:HH22	1.67	0.59
2:B:141:ARG:O	2:B:146:GLU:HB2	2.03	0.59
1:L:485:ASP:OD1	1:L:486:ILE:HG13	2.03	0.59
1:A:192:GLN:HE21	1:A:489:ASN:HB3	1.68	0.58
1:L:453:ASN:HD21	1:L:455:VAL:HB	1.69	0.58
1:L:330:GLU:OE2	1:L:506:SER:HA	2.03	0.58
5:B:601:B12:H552	5:B:601:B12:H531	1.85	0.58
1:A:470:THR:CG2	1:A:471:GLY:N	2.65	0.58
2:B:80:VAL:HG22	2:B:106:VAL:CG1	2.34	0.58
2:B:16:ARG:NE	2:B:16:ARG:HA	2.01	0.58
1:A:206:GLU:OE2	1:A:243:LYS:NZ	2.37	0.58
2:B:23:ALA:CA	2:B:90:LEU:HD12	2.33	0.58
1:A:164:ILE:HG23	1:A:404:VAL:HG11	1.84	0.57
2:E:123:GLN:HG2	5:E:602:B12:O58	2.04	0.57
1:L:26:GLU:O	1:L:274:SER:OG	2.14	0.57
3:M:70:ALA:O	3:M:74:ARG:HG2	2.04	0.57
2:E:180:GLN:H	2:E:180:GLN:CD	2.07	0.57
1:A:470:THR:HG22	1:A:471:GLY:N	2.19	0.57
1:A:237:ASP:CG	3:G:98:ARG:HH22	2.07	0.57
1:A:102:ILE:HD11	1:A:133:MET:HE2	1.86	0.57
1:A:341:HIS:CE1	2:B:162:LYS:NZ	2.72	0.57
1:L:501:ASP:CB	1:L:515:VAL:HG21	2.35	0.57
1:A:210:LEU:O	1:A:214:MET:HG3	2.04	0.57
2:B:72:VAL:HG12	2:B:73:ARG:N	2.18	0.57
2:B:74:ILE:HD12	2:B:74:ILE:N	2.19	0.57
1:L:126:MET:CE	1:L:319:ALA:HB2	2.34	0.57
1:L:128:MET:O	1:L:131:GLN:HG2	2.05	0.57
1:A:414:GLN:HA	1:A:441:THR:HG22	1.86	0.56
1:L:102:ILE:HD11	1:L:326:MET:HB2	1.87	0.56
3:M:74:ARG:NH2	6:M:151:HOH:O	2.19	0.56
2:B:67:LEU:HD13	2:B:140:ALA:HB1	1.87	0.56
1:A:519:VAL:O	1:A:522:ILE:HD11	2.04	0.56
2:B:16:ARG:HE	2:B:16:ARG:CA	2.02	0.56
1:L:334:ALA:O	1:L:335:ASN:HB2	2.05	0.56
1:L:334:ALA:HA	1:L:363:SER:OG	2.04	0.56
1:L:98:SER:OG	1:L:101:GLU:HG3	2.06	0.56
1:L:400:GLY:O	1:L:401:LEU:HD12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:PHE:CD1	1:A:461:VAL:HG22	2.40	0.56
1:A:341:HIS:HE1	2:B:162:LYS:NZ	2.03	0.56
1:L:539:TRP:O	1:L:543:LYS:HG2	2.04	0.56
5:E:602:B12:H351	5:E:602:B12:H362	1.87	0.56
2:E:79:ASP:OD1	2:E:81:SER:HB2	2.05	0.56
1:L:143:CYS:SG	1:L:170:GLN:HG2	2.45	0.56
3:M:78:GLU:HB2	3:M:120:ASN:ND2	2.21	0.56
3:G:129:GLU:O	3:G:133:GLN:HG3	2.05	0.56
1:L:337:GLN:HB3	2:E:160:ARG:CZ	2.36	0.56
1:A:10:LEU:O	1:A:13:ARG:HB2	2.06	0.55
1:A:444:HIS:ND1	1:L:6:ARG:HD3	2.21	0.55
1:L:301:VAL:HG12	1:L:302:SER:N	2.22	0.55
2:B:84:ALA:HB2	2:B:106:VAL:HG13	1.87	0.55
2:E:72:VAL:CG1	2:E:73:ARG:N	2.70	0.55
2:E:37:ALA:HB1	2:E:41:HIS:HB2	1.89	0.55
2:E:16:ARG:NH1	2:E:190:ASP:CG	2.60	0.55
1:A:285:ILE:HD11	1:A:327:LEU:HD22	1.88	0.55
1:L:338:THR:N	2:E:160:ARG:HH21	2.00	0.55
1:A:395:LEU:HD23	1:L:314:ILE:HB	1.88	0.55
1:A:256:LYS:NZ	1:A:507:ALA:O	2.36	0.55
1:L:338:THR:H	2:E:160:ARG:NH2	1.99	0.55
1:A:147:ASN:C	1:A:147:ASN:HD22	2.10	0.55
1:A:56:ARG:HH22	1:A:59:GLN:HB2	1.71	0.55
1:L:172:THR:HG22	1:L:187:LEU:HD22	1.89	0.55
1:A:552:ASP:OD1	1:A:552:ASP:O	2.25	0.55
1:L:419:ALA:O	1:L:423:VAL:HG23	2.06	0.55
1:A:203:SER:HB3	6:A:1045:HOH:O	2.06	0.54
1:A:486:ILE:H	1:A:486:ILE:CD1	2.21	0.54
1:L:353:GLN:O	1:L:356:PRO:HD2	2.06	0.54
1:L:141:ASN:ND2	1:L:362:PHE:HB2	2.23	0.54
1:A:98:SER:OG	1:A:101:GLU:HG3	2.06	0.54
1:L:201:GLN:HE22	1:L:222:GLU:HB3	1.73	0.54
1:L:299:GLY:HA2	1:L:320:GLU:CD	2.28	0.54
1:A:467:ARG:HB3	1:A:469:ILE:HD13	1.88	0.54
2:B:80:VAL:CG2	2:B:106:VAL:HG12	2.37	0.54
1:L:313:GLY:O	1:L:317:VAL:HG23	2.07	0.54
2:B:160:ARG:HB3	2:B:161:PRO:HD3	1.89	0.54
2:B:33:GLY:HA3	2:B:74:ILE:CD1	2.38	0.54
2:E:32:ILE:HD11	2:E:71:VAL:HG22	1.89	0.54
1:L:285:ILE:CD1	1:L:323:ILE:HG22	2.38	0.54
2:B:29:GLU:OE1	2:B:70:ARG:NE	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:108:HIS:CD2	2:E:109:GLN:H	2.26	0.54
2:B:158:MET:C	2:B:161:PRO:HD2	2.28	0.53
2:B:71:VAL:CG2	2:B:189:ILE:HD11	2.37	0.53
1:L:304:ILE:HG23	1:L:339:PHE:HB3	1.91	0.53
2:E:38:PHE:CE1	2:E:51:HIS:HB3	2.42	0.53
2:B:32:ILE:CD1	2:B:71:VAL:HG22	2.38	0.53
5:B:601:B12:H362	5:B:601:B12:H351	1.90	0.53
1:L:222:GLU:HG3	1:L:258:ARG:HD2	1.90	0.53
1:L:239:THR:HG23	1:L:240:PRO:HD2	1.91	0.53
1:A:56:ARG:H	1:A:56:ARG:CD	2.22	0.53
1:L:6:ARG:HB2	1:L:6:ARG:HH11	1.73	0.53
1:A:102:ILE:HG13	1:A:103:ILE:N	2.22	0.53
2:E:127:LEU:HD22	2:E:127:LEU:N	2.23	0.53
2:E:73:ARG:HB2	2:E:187:LEU:HD11	1.90	0.53
1:A:283:ARG:O	1:A:287:ILE:HG13	2.08	0.53
1:L:466:LYS:CA	1:L:466:LYS:HE3	2.38	0.53
1:A:501:ASP:CB	1:A:515:VAL:HG21	2.39	0.53
1:L:61:ASP:HB2	1:L:230:GLU:OE2	2.09	0.53
1:L:90:ARG:HB3	1:L:90:ARG:NH1	2.23	0.53
1:A:282:SER:O	1:A:286:PHE:HD1	1.92	0.52
1:A:483:PHE:HB3	1:A:486:ILE:HD13	1.92	0.52
1:L:1:MET:HG2	1:L:2:LYS:O	2.09	0.52
1:A:143:CYS:HB3	1:A:167:PHE:CD1	2.44	0.52
1:A:368:VAL:HG22	1:A:369:PRO:CD	2.39	0.52
1:A:388:TYR:O	1:A:392:GLN:HG3	2.09	0.52
1:A:495:ARG:NH2	3:G:29:LEU:HG	2.25	0.52
1:A:317:VAL:HA	1:A:320:GLU:OE1	2.09	0.52
2:B:80:VAL:HB	2:B:100:GLN:HG3	1.90	0.52
1:A:421:GLN:HA	1:A:432:ILE:HD12	1.91	0.52
2:B:19:GLY:O	2:B:185:VAL:HG22	2.08	0.52
3:G:100:SER:HB3	3:G:138:ARG:NH2	2.24	0.52
3:G:13:LEU:HG	3:G:56:TYR:CE2	2.45	0.52
3:G:97:PHE:O	3:G:138:ARG:HA	2.09	0.52
1:A:133:MET:HE2	1:A:326:MET:HA	1.91	0.52
2:E:46:LEU:HG	2:E:102:LYS:HB2	1.91	0.52
1:A:42:VAL:HG11	1:A:81:MET:HG3	1.92	0.52
3:G:14:ALA:O	3:G:18:PRO:HB3	2.09	0.52
1:L:178:ARG:HB3	1:L:458:LEU:HD22	1.91	0.52
2:B:145:LYS:HE2	6:B:616:HOH:O	2.09	0.52
1:L:328:ASP:OD2	3:M:66:ARG:HD3	2.10	0.52
1:A:102:ILE:HG12	1:A:133:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLN:HA	1:A:441:THR:CG2	2.41	0.51
1:L:491:LEU:O	1:L:495:ARG:HG3	2.10	0.51
1:L:49:ILE:HD12	1:L:68:ALA:O	2.09	0.51
2:B:40:LYS:HD2	2:B:73:ARG:NH2	2.23	0.51
2:E:112:LEU:HD11	2:E:118:LEU:HD13	1.92	0.51
1:L:337:GLN:NE2	2:E:160:ARG:HH12	2.08	0.51
3:M:59:GLN:O	3:M:63:GLN:HG3	2.10	0.51
1:L:92:LEU:CD1	1:L:102:ILE:HG13	2.41	0.51
1:A:237:ASP:OD1	3:G:98:ARG:NH2	2.43	0.51
1:L:253:ARG:HG3	3:M:48:ARG:NH1	2.24	0.51
2:B:130:GLU:O	2:B:133:ARG:HB3	2.11	0.51
1:L:102:ILE:HD11	1:L:106:THR:HG21	1.92	0.51
1:L:453:ASN:ND2	1:L:456:GLU:H	2.09	0.51
1:A:106:THR:O	1:A:109:ILE:HG12	2.11	0.51
2:E:34:VAL:HB	2:E:38:PHE:CB	2.41	0.51
3:M:11:TYR:O	3:M:12:PRO:C	2.49	0.51
5:E:602:B12:H491	5:E:602:B12:H473	1.93	0.51
1:L:210:LEU:O	1:L:214:MET:HG3	2.11	0.51
1:L:307:THR:O	1:L:313:GLY:HA3	2.11	0.51
1:L:465:MET:HB2	1:L:466:LYS:NZ	2.25	0.51
2:B:58:LEU:HD23	2:B:132:TYR:O	2.11	0.51
1:L:306:MET:N	2:E:164:MET:HE2	2.26	0.51
1:L:462:GLU:O	1:L:466:LYS:HD2	2.11	0.51
1:L:65:ARG:NH1	3:M:133:GLN:HE22	2.07	0.51
2:B:31:VAL:HG22	2:B:70:ARG:HG3	1.93	0.51
1:L:439:ALA:O	1:L:443:ALA:HB2	2.11	0.51
2:E:158:MET:C	2:E:161:PRO:HD2	2.32	0.50
2:E:38:PHE:O	2:E:73:ARG:NH1	2.44	0.50
3:G:103:GLU:O	3:G:107:ILE:HG13	2.11	0.50
2:E:15:THR:HB	2:E:39:ASP:OD2	2.11	0.50
1:A:426:GLU:HG3	1:A:480:ARG:NH2	2.19	0.50
2:E:127:LEU:HD12	2:E:131:THR:HG21	1.92	0.50
1:A:406:GLU:O	1:A:409:THR:HG23	2.10	0.50
2:B:44:HIS:HB2	2:B:48:ASP:HA	1.92	0.50
2:E:34:VAL:HB	2:E:38:PHE:HB3	1.93	0.50
2:E:89:ASN:ND2	2:E:110:ARG:CB	2.65	0.50
1:L:1:MET:O	1:L:2:LYS:CB	2.59	0.50
1:L:460:ALA:O	1:L:463:GLU:HB2	2.11	0.50
2:B:109:GLN:CD	2:B:111:ASP:H	2.14	0.50
1:A:257:MET:HE3	1:A:293:VAL:HG13	1.94	0.50
1:A:402:ARG:HD2	1:A:541:GLU:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ARG:NH2	1:A:511:ARG:HB3	2.15	0.50
2:B:72:VAL:HG12	2:B:73:ARG:H	1.74	0.50
1:L:170:GLN:NE2	1:L:198:VAL:HG11	2.27	0.50
3:M:17:CYS:N	3:M:18:PRO:HD3	2.27	0.50
1:A:337:GLN:NE2	2:B:160:ARG:NH2	2.59	0.50
2:E:108:HIS:HD2	2:E:109:GLN:H	1.59	0.50
2:E:40:LYS:HD2	2:E:73:ARG:NH2	2.27	0.50
2:E:74:ILE:N	2:E:74:ILE:HD12	2.27	0.50
2:E:71:VAL:HG21	2:E:189:ILE:HD11	1.94	0.49
1:L:99:ARG:O	1:L:103:ILE:HG13	2.12	0.49
3:M:47:VAL:O	3:M:47:VAL:HG23	2.11	0.49
1:L:497:ARG:O	3:M:49:ILE:HB	2.12	0.49
1:A:102:ILE:HG12	1:A:133:MET:CE	2.42	0.49
1:A:174:VAL:HG12	1:A:183:ASN:OD1	2.12	0.49
1:A:334:ALA:O	1:A:335:ASN:HB2	2.11	0.49
3:M:51:ARG:HD2	3:M:52:GLN:N	2.27	0.49
1:A:507:ALA:HA	1:A:517:SER:HB3	1.93	0.49
1:L:382:ALA:HA	1:L:385:PHE:CE2	2.48	0.49
3:M:98:ARG:HH11	3:M:98:ARG:HG2	1.77	0.49
1:A:332:ALA:HB1	1:A:363:SER:HB2	1.94	0.49
1:A:373:ASN:ND2	1:A:375:PHE:N	2.60	0.49
1:L:73:ASN:C	1:L:73:ASN:HD22	2.16	0.49
1:A:299:GLY:HA2	1:A:320:GLU:CD	2.33	0.49
1:A:42:VAL:CG1	1:A:81:MET:HG3	2.42	0.49
1:A:511:ARG:HH21	1:A:511:ARG:CB	2.17	0.49
3:G:77:ALA:O	3:G:80:ILE:HG22	2.13	0.49
1:L:115:VAL:HG23	1:L:278:LEU:HD23	1.94	0.49
2:E:100:GLN:NE2	2:E:102:LYS:NZ	2.61	0.48
2:E:26:ARG:HH22	2:E:68:HIS:CE1	2.31	0.48
1:L:369:PRO:HG3	1:L:444:HIS:NE2	2.28	0.48
1:A:102:ILE:HD12	1:A:106:THR:HG21	1.94	0.48
1:A:398:ASP:C	1:A:398:ASP:OD1	2.52	0.48
1:A:56:ARG:HD3	1:A:56:ARG:N	2.25	0.48
2:E:124:ALA:HA	2:E:127:LEU:CD2	2.37	0.48
1:A:147:ASN:HD21	1:A:151:ASN:N	1.96	0.48
1:A:406:GLU:O	1:A:410:ILE:HG13	2.12	0.48
1:A:538:ARG:NH1	1:A:542:ILE:HG13	2.28	0.48
2:E:26:ARG:NH2	2:E:68:HIS:CE1	2.81	0.48
3:G:31:ASP:O	3:G:36:LYS:HD2	2.13	0.48
1:L:151:ASN:O	1:L:155:ILE:HG12	2.12	0.48
1:L:226:VAL:HG21	1:L:259:TYR:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ILE:O	1:A:327:LEU:HB2	2.12	0.48
2:E:124:ALA:HB3	2:E:125:PRO:HD3	1.95	0.48
1:A:229:THR:OG1	1:A:232:VAL:HG23	2.13	0.48
2:B:24:ASP:HB2	2:B:70:ARG:NH1	2.29	0.48
1:L:355:LEU:HB2	1:L:356:PRO:HD3	1.96	0.48
1:A:15:VAL:HG22	1:L:390:ILE:HD13	1.95	0.48
1:A:285:ILE:HD12	1:A:329:LEU:HD12	1.96	0.48
1:L:301:VAL:HG12	1:L:302:SER:H	1.79	0.48
1:L:306:MET:N	2:E:164:MET:CE	2.76	0.48
1:L:77:THR:HG23	1:L:78:GLU:N	2.28	0.48
2:B:100:GLN:HE21	2:B:104:THR:HB	1.77	0.48
2:E:108:HIS:HE1	2:E:114:PRO:O	1.96	0.48
2:E:33:GLY:HA3	2:E:74:ILE:HD13	1.95	0.48
1:L:468:ASN:HB3	6:L:1059:HOH:O	2.12	0.48
2:B:106:VAL:HG23	2:B:119:GLU:O	2.14	0.48
3:G:23:THR:HB	3:G:24:PRO:HD2	1.95	0.48
1:L:333:SER:HB2	1:L:353:GLN:HG2	1.95	0.48
1:L:304:ILE:CG2	1:L:339:PHE:HB3	2.44	0.48
3:M:120:ASN:O	3:M:124:VAL:HG23	2.12	0.48
2:B:97:ILE:HD11	2:B:139:ALA:HB2	1.94	0.47
1:L:336:ASP:O	1:L:378:SER:HA	2.15	0.47
1:A:405:THR:HB	1:A:408:GLU:HG3	1.95	0.47
1:L:504:GLN:NE2	3:M:57:GLN:HB3	2.28	0.47
1:A:99:ARG:NH2	1:A:135:ALA:HA	2.28	0.47
2:E:45:THR:HG22	2:E:101:SER:O	2.13	0.47
1:A:409:THR:O	1:A:412:ILE:HG22	2.14	0.47
2:B:16:ARG:HB2	2:B:188:HIS:HB2	1.95	0.47
3:G:139:LYS:NZ	3:G:141:SER:OXT	2.47	0.47
2:E:51:HIS:HE1	2:E:101:SER:HB3	1.79	0.47
1:L:34:SER:HB2	1:L:276:SER:HB3	1.96	0.47
2:E:124:ALA:O	2:E:127:LEU:HD23	2.13	0.47
3:G:112:GLU:O	3:G:116:HIS:HA	2.15	0.47
3:G:139:LYS:CG	3:G:140:GLY:H	2.27	0.47
1:L:299:GLY:N	1:L:320:GLU:OE2	2.45	0.47
3:G:18:PRO:HA	3:G:21:ILE:HG13	1.97	0.47
2:E:107:ILE:HD11	2:E:135:ILE:HG23	1.96	0.47
1:A:180:ALA:HB3	1:A:181:PRO:CD	2.44	0.47
1:A:301:VAL:HG12	1:A:302:SER:N	2.29	0.47
1:A:199:LEU:HD23	1:A:493:MET:CE	2.44	0.47
1:A:501:ASP:HB2	1:A:515:VAL:HG21	1.97	0.47
1:A:93:VAL:HG23	1:A:128:MET:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:OE2	1:A:258:ARG:NH2	2.43	0.47
2:E:26:ARG:NH2	2:E:68:HIS:ND1	2.62	0.47
1:L:306:MET:HG2	2:E:164:MET:HE2	1.94	0.47
1:L:86:VAL:O	1:L:90:ARG:HG3	2.15	0.47
1:A:313:GLY:O	1:A:316:ALA:HB3	2.14	0.47
1:A:393:ARG:NH2	1:L:311:PRO:HD3	2.30	0.47
1:A:467:ARG:HB3	1:A:469:ILE:CD1	2.45	0.47
2:B:119:GLU:OE2	2:B:151:VAL:N	2.46	0.47
2:E:109:GLN:NE2	2:E:111:ASP:N	2.56	0.47
1:A:317:VAL:O	1:A:320:GLU:HG2	2.15	0.46
1:A:409:THR:O	1:A:413:ARG:HG3	2.15	0.46
1:A:400:GLY:O	1:A:401:LEU:HD23	2.15	0.46
1:A:453:ASN:ND2	1:A:456:GLU:HB2	2.30	0.46
2:B:46:LEU:HG	2:B:102:LYS:HB2	1.96	0.46
2:E:55:LEU:O	2:E:59:ILE:HG13	2.16	0.46
1:L:283:ARG:O	1:L:287:ILE:HG13	2.15	0.46
1:A:351:LEU:HD23	1:L:351:LEU:HD23	1.97	0.46
3:M:58:ALA:O	3:M:62:GLU:HG3	2.16	0.46
1:A:143:CYS:HB3	1:A:167:PHE:CE1	2.51	0.46
1:A:335:ASN:OD1	1:A:350:THR:HA	2.15	0.46
1:A:147:ASN:ND2	1:A:150:ASP:N	2.64	0.46
1:A:221:ALA:O	1:A:257:MET:HA	2.16	0.46
2:E:67:LEU:N	2:E:67:LEU:HD12	2.31	0.46
1:L:126:MET:HE1	1:L:319:ALA:HB2	1.97	0.46
1:L:377:GLY:O	2:E:160:ARG:NH2	2.49	0.46
1:A:381:ASP:OD1	1:A:381:ASP:C	2.52	0.46
1:A:422:ALA:HB1	1:A:481:SER:HB3	1.98	0.46
2:B:124:ALA:O	2:B:127:LEU:HD23	2.15	0.46
2:B:55:LEU:O	2:B:59:ILE:HG13	2.15	0.46
1:L:468:ASN:HD22	1:L:468:ASN:N	2.13	0.46
2:B:50:PRO:O	2:B:54:ILE:HG13	2.15	0.46
1:L:93:VAL:CG2	1:L:128:MET:HG2	2.46	0.46
3:M:30:THR:HG22	3:M:30:THR:O	2.15	0.46
1:A:102:ILE:O	1:A:106:THR:HG23	2.15	0.46
1:A:115:VAL:HG21	1:A:279:TYR:HA	1.97	0.46
1:A:294:GLN:C	1:A:294:GLN:NE2	2.69	0.46
1:A:417:ALA:CB	1:A:437:VAL:HG13	2.45	0.46
2:E:13:LEU:HG	2:E:189:ILE:HG23	1.98	0.46
1:A:42:VAL:HG22	1:A:43:LYS:N	2.30	0.46
2:E:131:THR:O	2:E:135:ILE:HG13	2.16	0.46
2:E:141:ARG:O	2:E:146:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ILE:HA	1:A:473:ASP:OD2	2.16	0.45
2:E:102:LYS:HZ1	5:E:602:B12:H5R2	1.81	0.45
2:E:180:GLN:N	2:E:180:GLN:CD	2.70	0.45
3:G:78:GLU:OE1	3:G:119:VAL:HG12	2.15	0.45
1:L:123:VAL:HG13	1:L:318:LEU:CD2	2.45	0.45
1:L:221:ALA:O	1:L:257:MET:HA	2.15	0.45
1:A:551:PRO:HG2	1:L:22:GLY:O	2.16	0.45
2:B:14:LYS:HG2	2:B:15:THR:H	1.81	0.45
1:A:341:HIS:CE1	2:B:162:LYS:HZ3	2.34	0.45
1:A:281:GLU:HA	1:A:281:GLU:OE2	2.16	0.45
2:B:124:ALA:HA	2:B:127:LEU:HD23	1.99	0.45
1:L:201:GLN:NE2	1:L:222:GLU:HB3	2.31	0.45
3:M:20:HIS:O	3:M:22:LEU:HG	2.16	0.45
1:A:149:LYS:O	1:A:150:ASP:C	2.55	0.45
1:A:351:LEU:HD12	1:A:354:MET:CE	2.42	0.45
1:A:426:GLU:HG2	1:A:477:ALA:HA	1.99	0.45
1:L:418:ARG:HG3	1:L:437:VAL:HG11	1.99	0.45
3:M:110:GLU:O	3:M:114:THR:HB	2.17	0.45
2:B:89:ASN:OD1	2:B:110:ARG:HB2	2.17	0.45
2:B:127:LEU:CD2	2:B:127:LEU:N	2.79	0.45
1:L:195:ARG:O	1:L:198:VAL:HG23	2.17	0.45
3:M:78:GLU:HB2	3:M:120:ASN:HD22	1.80	0.45
1:L:100:GLU:H	1:L:100:GLU:CD	2.19	0.45
1:L:317:VAL:O	1:L:320:GLU:HG2	2.16	0.45
3:M:139:LYS:CD	3:M:139:LYS:H	1.95	0.45
1:A:46:ASN:O	1:A:48:LEU:HD12	2.17	0.45
1:A:56:ARG:HH22	1:A:59:GLN:CB	2.28	0.45
1:L:323:ILE:O	1:L:327:LEU:HB2	2.16	0.45
2:B:25:GLU:HA	2:B:25:GLU:OE1	2.15	0.45
2:B:32:ILE:HG22	2:B:97:ILE:HB	1.99	0.45
1:L:244:ALA:HB3	3:M:123:PHE:HZ	1.82	0.45
5:E:602:B12:H5R1	5:E:602:B12:O51	2.17	0.45
3:G:64:MET:O	3:G:65:GLN:HB2	2.17	0.45
2:B:109:GLN:OE1	2:B:110:ARG:N	2.50	0.44
1:L:248:SER:O	1:L:252:SER:HB3	2.17	0.44
1:L:366:SER:HB2	1:L:373:ASN:ND2	2.32	0.44
1:A:486:ILE:N	1:A:486:ILE:CD1	2.80	0.44
2:E:44:HIS:HA	2:E:49:MET:O	2.18	0.44
1:A:430:PRO:HA	1:A:431:PRO:HD2	1.88	0.44
1:L:299:GLY:O	1:L:300:ALA:HB3	2.16	0.44
1:L:525:TYR:HB2	6:L:1060:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:THR:HG22	1:A:407:ALA:N	2.29	0.44
1:A:522:ILE:HG22	1:A:523:ASN:O	2.18	0.44
1:A:97:VAL:HG13	1:A:101:GLU:OE2	2.17	0.44
2:B:29:GLU:CD	2:B:70:ARG:HE	2.20	0.44
1:L:366:SER:HB2	1:L:373:ASN:HD22	1.83	0.44
1:L:392:GLN:CD	1:L:399:GLY:H	2.17	0.44
1:L:465:MET:C	1:L:466:LYS:HE3	2.37	0.44
3:M:20:HIS:CE1	3:M:21:ILE:HG12	2.52	0.44
2:B:14:LYS:HG2	2:B:15:THR:N	2.33	0.44
2:E:23:ALA:HA	2:E:90:LEU:HD12	2.00	0.44
1:L:112:ALA:HA	1:L:115:VAL:HG12	2.00	0.44
1:L:123:VAL:HG12	1:L:127:MET:CE	2.48	0.44
1:A:94:ASP:OD2	1:L:96:HIS:NE2	2.51	0.44
2:E:34:VAL:HG22	2:E:72:VAL:O	2.18	0.43
1:L:123:VAL:HG12	1:L:127:MET:HE2	2.00	0.43
2:E:11:PHE:HB3	2:E:192:VAL:O	2.18	0.43
2:E:46:LEU:CD2	2:E:166:LYS:HG2	2.48	0.43
1:L:400:GLY:O	1:L:401:LEU:CD1	2.65	0.43
1:L:178:ARG:CB	1:L:458:LEU:HD22	2.47	0.43
3:M:92:ASN:O	3:M:98:ARG:HG3	2.18	0.43
1:A:263:THR:HG23	1:A:320:GLU:CD	2.38	0.43
2:E:120:LEU:CD2	5:E:602:B12:H311	2.48	0.43
2:E:22:SER:O	2:E:70:ARG:NH2	2.52	0.43
1:L:281:GLU:HA	1:L:281:GLU:OE1	2.18	0.43
1:A:368:VAL:HG23	1:A:369:PRO:HD2	1.99	0.43
1:A:92:LEU:HD21	1:A:102:ILE:CD1	2.43	0.43
2:E:193:ARG:HH11	2:E:193:ARG:HG2	1.82	0.43
1:L:143:CYS:HB3	1:L:167:PHE:CD1	2.54	0.43
1:L:42:VAL:HA	1:L:51:GLU:O	2.18	0.43
1:A:246:LEU:O	1:A:249:ALA:HB3	2.19	0.43
1:A:426:GLU:CG	1:A:480:ARG:NH2	2.81	0.43
2:E:74:ILE:N	2:E:74:ILE:CD1	2.82	0.43
1:L:285:ILE:HD12	1:L:324:ALA:CA	2.29	0.43
1:A:93:VAL:HG23	1:A:128:MET:CG	2.48	0.43
2:B:34:VAL:HG12	2:B:99:ILE:CG2	2.49	0.43
3:M:95:ARG:HB3	3:M:98:ARG:NH1	2.33	0.43
2:E:51:HIS:CE1	2:E:101:SER:HB3	2.54	0.43
1:L:323:ILE:HA	1:L:326:MET:HG2	2.01	0.43
1:L:181:PRO:HB2	1:L:461:VAL:HG13	2.00	0.43
1:L:478:LEU:HB2	1:L:487:ALA:HB2	2.00	0.43
1:A:199:LEU:HD23	1:A:493:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LYS:HE2	1:A:486:ILE:HD11	2.01	0.43
3:M:97:PHE:O	3:M:138:ARG:HA	2.18	0.43
1:A:147:ASN:C	1:A:147:ASN:ND2	2.72	0.43
1:A:180:ALA:O	1:A:181:PRO:C	2.56	0.43
2:E:44:HIS:HB3	2:E:48:ASP:HA	2.00	0.43
2:E:72:VAL:CG1	2:E:73:ARG:H	2.31	0.43
2:E:24:ASP:OD2	2:E:26:ARG:HB2	2.19	0.43
3:G:33:THR:HG22	3:G:34:LEU:N	2.33	0.43
1:L:43:LYS:HA	1:L:43:LYS:HD2	1.85	0.43
1:A:439:ALA:HB1	1:A:448:GLU:O	2.18	0.42
1:A:56:ARG:NH1	1:A:59:GLN:HB2	2.33	0.42
1:A:6:ARG:NH1	1:L:444:HIS:O	2.52	0.42
2:B:11:PHE:CD2	2:B:11:PHE:N	2.87	0.42
2:E:127:LEU:HD22	2:E:127:LEU:H	1.82	0.42
1:L:18:ASP:OD1	1:L:341:HIS:CD2	2.69	0.42
1:A:279:TYR:O	1:A:282:SER:HB3	2.19	0.42
1:A:522:ILE:N	1:A:522:ILE:HD12	2.27	0.42
2:B:33:GLY:HA3	2:B:74:ILE:HD13	2.00	0.42
1:A:6:ARG:HD3	1:L:444:HIS:CE1	2.53	0.42
2:B:84:ALA:CB	2:B:106:VAL:HG13	2.49	0.42
2:B:115:LEU:HD13	5:B:601:B12:H412	2.02	0.42
2:E:180:GLN:HB2	2:E:181:ASP:H	1.64	0.42
1:A:216:GLY:HA2	1:A:497:ARG:NH2	2.33	0.42
2:B:74:ILE:CD1	2:B:74:ILE:N	2.82	0.42
1:A:149:LYS:C	1:A:151:ASN:N	2.70	0.42
1:A:27:GLU:HA	1:A:27:GLU:OE1	2.19	0.42
1:L:303:CYS:HA	2:E:164:MET:CE	2.49	0.42
2:E:32:ILE:CD1	2:E:71:VAL:HG22	2.49	0.42
3:M:120:ASN:O	3:M:123:PHE:HB3	2.20	0.42
3:M:20:HIS:C	3:M:20:HIS:ND1	2.70	0.42
1:A:143:CYS:SG	1:A:170:GLN:HG2	2.59	0.42
1:A:178:ARG:CB	1:A:458:LEU:HD22	2.49	0.42
1:A:539:TRP:CD1	1:A:543:LYS:HD2	2.54	0.42
1:L:424:PHE:CD2	1:L:429:LEU:HB2	2.54	0.42
1:L:57:ARG:HG3	1:L:60:PHE:CD1	2.54	0.42
1:L:62:MET:HG2	3:M:130:VAL:CG1	2.50	0.42
1:A:501:ASP:HB3	1:A:515:VAL:HG21	2.01	0.42
1:A:61:ASP:H	1:A:64:ASP:HB2	1.85	0.42
2:B:16:ARG:HG3	2:B:190:ASP:OD1	2.20	0.42
2:B:47:ILE:CG2	2:B:47:ILE:O	2.67	0.42
2:B:35:GLY:N	2:B:83:MET:HE1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ASP:O	2:B:90:LEU:HB2	2.20	0.42
1:A:522:ILE:CD1	1:A:522:ILE:H	2.28	0.42
1:L:42:VAL:CG1	1:L:81:MET:HG3	2.49	0.42
1:L:57:ARG:HG3	1:L:60:PHE:CE1	2.55	0.42
1:A:192:GLN:NE2	1:A:196:PRO:HA	2.35	0.42
1:A:178:ARG:HB2	1:A:458:LEU:HD22	2.02	0.42
2:B:24:ASP:OD2	2:B:26:ARG:CB	2.68	0.42
2:E:100:GLN:HE22	2:E:102:LYS:HZ1	1.68	0.42
3:G:11:TYR:CE1	3:G:12:PRO:HG3	2.54	0.42
1:L:239:THR:HG21	3:M:131:TYR:CE1	2.55	0.42
1:A:206:GLU:HG3	1:A:246:LEU:HD21	2.02	0.41
1:A:268:LEU:HD12	1:A:268:LEU:O	2.20	0.41
1:A:439:ALA:O	1:A:443:ALA:HB2	2.20	0.41
2:E:45:THR:HB	2:E:102:LYS:O	2.20	0.41
2:E:80:VAL:HB	2:E:100:GLN:CG	2.50	0.41
1:L:106:THR:O	1:L:109:ILE:HG12	2.20	0.41
1:L:353:GLN:C	1:L:356:PRO:HD2	2.41	0.41
1:L:502:TYR:CD1	1:L:502:TYR:C	2.94	0.41
2:E:137:LYS:HB3	2:E:137:LYS:HE3	1.87	0.41
2:E:120:LEU:HD23	5:E:602:B12:H311	2.01	0.41
1:A:1:MET:O	1:A:2:LYS:CB	2.68	0.41
1:A:373:ASN:ND2	1:A:377:GLY:N	2.58	0.41
2:B:122:SER:HB2	5:B:601:B12:O7R	2.21	0.41
2:B:163:PHE:O	2:B:164:MET:C	2.59	0.41
1:L:396:MET:HE2	1:L:539:TRP:CE2	2.55	0.41
2:B:76:ARG:NE	2:B:86:ASP:OD2	2.50	0.41
2:E:140:ALA:O	2:E:144:ARG:HG3	2.19	0.41
2:E:165:ALA:HB3	6:E:615:HOH:O	2.21	0.41
3:G:31:ASP:O	3:G:33:THR:N	2.50	0.41
1:A:383:GLU:O	1:L:13:ARG:CZ	2.68	0.41
3:M:78:GLU:HB3	3:M:117:ALA:HA	2.02	0.41
3:M:11:TYR:N	3:M:12:PRO:HD3	2.35	0.41
1:A:34:SER:HB2	1:A:276:SER:HB3	2.03	0.41
1:L:300:ALA:HB1	1:L:304:ILE:HA	2.01	0.41
3:M:74:ARG:NH1	6:M:151:HOH:O	2.48	0.41
1:A:225:SER:O	1:A:243:LYS:HE3	2.21	0.41
1:A:206:GLU:HG3	1:A:246:LEU:CD2	2.49	0.41
1:A:42:VAL:HG21	1:A:77:THR:HG21	2.03	0.41
1:A:56:ARG:NH2	1:A:56:ARG:H	2.07	0.41
1:A:93:VAL:CG2	1:A:128:MET:HG2	2.50	0.41
2:B:24:ASP:O	2:B:25:GLU:OE1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:57:GLU:HG3	2:E:129:LEU:HB3	2.02	0.41
5:E:602:B12:H291	5:E:602:B12:H91	1.86	0.41
1:A:92:LEU:HD23	1:A:102:ILE:HD13	1.99	0.41
2:B:131:THR:O	2:B:135:ILE:HG13	2.20	0.41
1:L:332:ALA:HB1	1:L:363:SER:HB3	2.02	0.41
1:L:457:ASP:O	1:L:461:VAL:HG23	2.20	0.41
3:M:138:ARG:O	3:M:139:LYS:C	2.57	0.41
1:A:147:ASN:HD22	1:A:149:LYS:N	2.18	0.41
1:A:229:THR:HG1	1:A:232:VAL:HG23	1.85	0.41
2:B:88:ALA:C	2:B:90:LEU:H	2.24	0.41
3:M:20:HIS:CE1	3:M:56:TYR:HE1	2.39	0.41
1:A:478:LEU:HD13	1:A:486:ILE:HB	2.03	0.41
1:A:341:HIS:CE1	2:B:162:LYS:HZ1	2.37	0.41
2:B:16:ARG:O	2:B:187:LEU:HA	2.21	0.41
1:L:62:MET:HE2	1:L:230:GLU:HG2	2.03	0.41
1:L:417:ALA:CB	1:L:437:VAL:HG13	2.51	0.41
1:A:121:MET:HA	1:A:125:GLU:OE2	2.21	0.41
1:A:237:ASP:CG	3:G:98:ARG:NH2	2.73	0.41
1:A:450:PRO:HA	1:A:451:PRO:HD3	1.88	0.41
1:A:89:ALA:O	1:A:92:LEU:HB2	2.21	0.41
2:B:67:LEU:HD12	2:B:67:LEU:N	2.36	0.41
1:A:13:ARG:HA	1:A:13:ARG:HD3	1.86	0.40
1:A:512:GLN:HB2	1:A:514:GLU:OE2	2.20	0.40
1:A:62:MET:HG2	3:G:130:VAL:CG1	2.51	0.40
2:B:109:GLN:HG3	2:B:109:GLN:O	2.21	0.40
2:E:120:LEU:HD13	5:E:602:B12:HM63	2.03	0.40
3:G:46:ASP:O	3:G:48:ARG:N	2.52	0.40
1:L:36:PHE:HB2	1:L:274:SER:O	2.21	0.40
1:A:62:MET:HG3	1:A:230:GLU:OE2	2.21	0.40
1:A:332:ALA:HB1	1:A:363:SER:CB	2.51	0.40
1:A:50:VAL:HG22	1:A:50:VAL:O	2.22	0.40
2:B:33:GLY:HA3	2:B:74:ILE:HD11	2.03	0.40
3:G:138:ARG:O	3:G:139:LYS:C	2.58	0.40
1:L:53:ASP:OD1	1:L:112:ALA:HB3	2.22	0.40
1:A:170:GLN:HE21	1:A:187:LEU:HD11	1.85	0.40
1:A:259:TYR:CZ	1:A:293:VAL:HG21	2.56	0.40
1:A:32:MET:O	1:A:33:ASP:C	2.60	0.40
2:B:71:VAL:HG12	2:B:187:LEU:HD12	2.03	0.40
2:B:16:ARG:CB	2:B:188:HIS:HB2	2.51	0.40
1:L:211:GLU:O	1:L:215:ARG:HG3	2.22	0.40
1:L:239:THR:HG23	1:L:240:PRO:CD	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:27:LYS:HA	3:M:28:PRO:HD3	1.94	0.40
1:A:301:VAL:HG12	1:A:302:SER:H	1.86	0.40
2:B:108:HIS:HE1	2:B:114:PRO:O	2.04	0.40
1:A:462:GLU:HG2	1:A:466:LYS:HE3	2.02	0.40
1:A:517:SER:C	1:A:519:VAL:H	2.24	0.40
2:E:13:LEU:HD12	2:E:13:LEU:N	2.37	0.40
2:E:37:ALA:CB	2:E:41:HIS:HB2	2.50	0.40
1:L:486:ILE:HA	1:L:489:ASN:HD22	1.86	0.40
1:L:49:ILE:HG13	1:L:74:VAL:HG12	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	550/555 (99%)	499 (91%)	47 (8%)	4 (1%)	22	39
1	L	553/555 (100%)	504 (91%)	45 (8%)	4 (1%)	22	39
2	B	179/194 (92%)	162 (90%)	16 (9%)	1 (1%)	25	43
2	E	182/194 (94%)	165 (91%)	16 (9%)	1 (0%)	29	48
3	G	130/141 (92%)	120 (92%)	5 (4%)	5 (4%)	3	4
3	M	129/141 (92%)	116 (90%)	12 (9%)	1 (1%)	19	35
All	All	1723/1780 (97%)	1566 (91%)	141 (8%)	16 (1%)	17	31

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	139	LYS
1	L	273	GLU
2	E	180	GLN

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Mol	Chain	Res	Type
1	A	364	GLY
1	L	178	ARG
3	M	139	LYS
1	A	178	ARG
2	B	40	LYS
1	L	364	GLY
1	A	33	ASP
3	G	14	ALA
1	A	301	VAL
1	L	301	VAL
3	G	32	ILE
3	G	47	VAL
3	G	140	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	450/453 (99%)	417 (93%)	33 (7%)	14	27
1	L	453/453 (100%)	416 (92%)	37 (8%)	11	22
2	B	150/163 (92%)	143 (95%)	7 (5%)	26	49
2	E	153/163 (94%)	142 (93%)	11 (7%)	14	28
3	G	111/120 (92%)	105 (95%)	6 (5%)	22	42
3	M	110/120 (92%)	102 (93%)	8 (7%)	14	27
All	All	1427/1472 (97%)	1325 (93%)	102 (7%)	14	28

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	ARG
1	A	51	GLU
1	A	56	ARG
1	A	75	GLU

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Mol	Chain	Res	Type
1	A	102	ILE
1	A	141	ASN
1	A	142	GLN
1	A	147	ASN
1	A	179	TYR
1	A	181	PRO
1	A	183	ASN
1	A	206	GLU
1	A	222	GLU
1	A	233	PHE
1	A	237	ASP
1	A	257	MET
1	A	285	ILE
1	A	294	GLN
1	A	337	GLN
1	A	338	THR
1	A	349	ARG
1	A	351	LEU
1	A	365	TYR
1	A	409	THR
1	A	435	GLU
1	A	453	ASN
1	A	485	ASP
1	A	502	TYR
1	A	511	ARG
1	A	512	GLN
1	A	514	GLU
1	A	526	GLN
2	B	11	PHE
2	B	15	THR
2	B	16	ARG
2	B	47	ILE
2	B	55	LEU
2	B	81	SER
2	B	109	GLN
3	G	13	LEU
3	G	16	ARG
3	G	64	MET
3	G	69	VAL
3	G	94	LEU
3	G	111	LEU
1	L	2	LYS

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Mol	Chain	Res	Type
1	L	3	ARG
1	L	6	ARG
1	L	13	ARG
1	L	51	GLU
1	L	59	GLN
1	L	73	ASN
1	L	76	ARG
1	L	92	LEU
1	L	93	VAL
1	L	100	GLU
1	L	102	ILE
1	L	141	ASN
1	L	179	TYR
1	L	185	LEU
1	L	199	LEU
1	L	201	GLN
1	L	206	GLU
1	L	233	PHE
1	L	238	ASP
1	L	239	THR
1	L	252	SER
1	L	268	LEU
1	L	285	ILE
1	L	327	LEU
1	L	349	ARG
1	L	372	ASP
1	L	386	ASP
1	L	409	THR
1	L	453	ASN
1	L	466	LYS
1	L	485	ASP
1	L	502	TYR
1	L	503	LEU
1	L	512	GLN
1	L	514	GLU
1	L	546	PRO
2	E	25	GLU
2	E	55	LEU
2	E	63	GLU
2	E	81	SER
2	E	101	SER
2	E	108	HIS

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Mol	Chain	Res	Type
2	E	115	LEU
2	E	118	LEU
2	E	133	ARG
2	E	134	GLN
2	E	157	GLN
3	M	20	HIS
3	M	31	ASP
3	M	41	GLU
3	M	51	ARG
3	M	64	MET
3	M	74	ARG
3	M	132	GLN
3	M	139	LYS

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

Mol	Chain	Res	Type
1	A	12	GLN
1	A	16	ASN
1	A	79	GLN
1	A	120	GLN
1	A	141	ASN
1	A	147	ASN
1	A	154	GLN
1	A	170	GLN
1	A	192	GLN
1	A	201	GLN
1	A	294	GLN
1	A	321	ASN
1	A	337	GLN
1	A	341	HIS
1	A	373	ASN
1	A	379	ASN
1	A	447	ASN
1	A	453	ASN
1	A	468	ASN
1	A	489	ASN
1	A	512	GLN
1	A	526	GLN
2	B	42	GLN
2	B	100	GLN
2	B	108	HIS

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Mol	Chain	Res	Type
3	G	59	GLN
1	L	46	ASN
1	L	59	GLN
1	L	141	ASN
1	L	201	GLN
1	L	337	GLN
1	L	341	HIS
1	L	453	ASN
1	L	468	ASN
1	L	489	ASN
1	L	504	GLN
1	L	512	GLN
1	L	544	ASN
2	E	89	ASN
2	E	100	GLN
2	E	108	HIS
2	E	109	GLN
2	E	134	GLN
2	E	157	GLN
3	M	59	GLN
3	M	120	ASN
3	M	132	GLN
3	M	133	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	B12	B	601	-	80,101,101	1.53	13 (16%)	101,166,166	1.86	29 (28%)
5	B12	E	602	-	80,101,101	1.55	10 (12%)	101,166,166	1.82	27 (26%)

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
5	B12	B	601	-	-	12/51/223/223	0/3/11/11
5	B12	E	602	-	-	12/51/223/223	0/3/11/11

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	602	B12	C17-C18	5.12	1.61	1.54
5	B	601	B12	CO-N24	-4.78	1.77	1.89
5	E	602	B12	CO-N24	-4.60	1.77	1.89
5	B	601	B12	C17-C18	4.59	1.60	1.54
5	E	602	B12	C11-C10	-4.53	1.33	1.40
5	B	601	B12	C11-C10	-4.12	1.34	1.40
5	B	601	B12	O58-C57	3.85	1.31	1.23
5	E	602	B12	O58-C57	3.22	1.29	1.23
5	B	601	B12	C48-C49	2.81	1.61	1.52
5	B	601	B12	C7B-C6B	2.60	1.44	1.37
5	E	602	B12	CO-N23	-2.59	1.81	1.94
5	E	602	B12	O7R-C2R	-2.56	1.36	1.43
5	B	601	B12	CO-N23	-2.54	1.82	1.94
5	B	601	B12	O7R-C2R	-2.40	1.37	1.43
5	B	601	B12	C6B-C5B	2.38	1.46	1.40
5	E	602	B12	C6B-C5B	2.38	1.46	1.40
5	E	602	B12	C48-C49	2.31	1.60	1.52
5	E	602	B12	CO-N22	2.24	2.05	1.94
5	B	601	B12	CO-N22	2.21	2.04	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	602	B12	P-O5	-2.19	1.45	1.55
5	B	601	B12	P-O5	-2.08	1.45	1.55
5	B	601	B12	C18-C19	2.08	1.58	1.53
5	B	601	B12	C37-C38	2.02	1.58	1.51

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	B12	O58-C57-C56	-5.99	111.06	122.02
5	E	602	B12	O58-C57-C56	-5.90	111.22	122.02
5	B	601	B12	C26-C2-C1	4.61	117.19	110.02
5	B	601	B12	C7B-C8B-C9B	-4.25	116.34	120.54
5	E	602	B12	O5-P-O2	4.23	123.46	106.78
5	B	601	B12	O5-P-O2	4.14	123.11	106.78
5	E	602	B12	C7B-C8B-C9B	-3.99	116.60	120.54
5	E	602	B12	C6-C5-C4	-3.75	118.41	124.27
5	B	601	B12	C47-C12-C46	-3.63	102.12	109.73
5	B	601	B12	C2-C26-C27	3.57	125.27	115.22
5	B	601	B12	C6-C5-C4	-3.49	118.83	124.27
5	E	602	B12	C20-C1-C19	-3.45	106.03	109.36
5	E	602	B12	C47-C12-C46	-3.42	102.55	109.73
5	E	602	B12	C56-C57-N59	3.40	122.14	116.42
5	B	601	B12	C56-C57-N59	3.36	122.07	116.42
5	E	602	B12	C30-C3-C2	3.32	126.17	119.13
5	B	601	B12	C20-C1-C19	-3.10	106.36	109.36
5	E	602	B12	C2P-C1P-N59	3.08	117.48	112.93
5	B	601	B12	C3P-C2P-C1P	3.02	117.25	111.39
5	B	601	B12	C8-C9-N22	2.99	114.86	111.12
5	E	602	B12	C55-C17-C16	2.95	119.76	109.92
5	B	601	B12	C55-C17-C16	2.90	119.59	109.92
5	E	602	B12	C2-C26-C27	2.84	123.21	115.22
5	B	601	B12	C4B-C9B-C8B	2.84	124.01	121.10
5	E	602	B12	C8-C9-N22	2.78	114.59	111.12
5	B	601	B12	C25-C2-C1	-2.74	109.73	113.80
5	E	602	B12	C26-C2-C1	2.73	114.27	110.02
5	E	602	B12	C4B-C9B-C8B	2.65	123.82	121.10
5	E	602	B12	O44-C43-C42	-2.62	113.39	121.07
5	B	601	B12	O44-C43-C42	-2.61	113.41	121.07
5	E	602	B12	C2-C1-C19	2.57	122.65	118.60
5	B	601	B12	C3-C4-C5	-2.52	122.55	131.68
5	B	601	B12	C2-C1-C19	2.45	122.47	118.60
5	E	602	B12	C37-C7-C8	-2.43	101.86	108.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	602	B12	O6R-C4R-C5R	-2.40	104.02	109.21
5	E	602	B12	C7-C37-C38	2.37	121.26	114.20
5	E	602	B12	C3-C4-C5	-2.36	123.13	131.68
5	B	601	B12	C7-C37-C38	2.33	121.14	114.20
5	B	601	B12	C25-C2-C26	-2.27	105.11	109.71
5	E	602	B12	C3P-C2P-C1P	2.27	115.80	111.39
5	B	601	B12	O6R-C4R-C5R	-2.22	104.41	109.21
5	E	602	B12	C25-C2-C1	-2.20	110.53	113.80
5	E	602	B12	C19-C1-N21	2.20	104.41	102.16
5	B	601	B12	C2P-C1P-N59	2.19	116.17	112.93
5	B	601	B12	C48-C49-C50	2.18	119.98	112.59
5	B	601	B12	C42-C43-N45	2.17	123.27	116.51
5	B	601	B12	C17-C18-C19	-2.10	99.17	102.37
5	B	601	B12	C41-C8-C7	2.08	119.72	114.08
5	E	602	B12	C1-C2-C3	2.06	104.16	101.59
5	E	602	B12	C41-C8-C7	2.05	119.64	114.08
5	B	601	B12	O58-C57-N59	2.04	126.87	123.01
5	B	601	B12	C56-C55-C17	2.04	119.45	115.50
5	E	602	B12	C31-C32-N33	2.04	122.85	116.51
5	B	601	B12	C54-C17-C55	-2.02	105.93	109.26
5	B	601	B12	C26-C2-C3	2.01	111.18	107.47
5	E	602	B12	C42-C43-N45	2.00	122.75	116.51

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	601	B12	C12-C13-C48-C49
5	E	602	B12	C12-C13-C48-C49
5	B	601	B12	O6R-C4R-C5R-O8R
5	B	601	B12	C3R-C4R-C5R-O8R
5	E	602	B12	C8-C41-C42-C43
5	B	601	B12	C1-C2-C26-C27
5	B	601	B12	C25-C2-C26-C27
5	E	602	B12	C1-C2-C26-C27
5	E	602	B12	C25-C2-C26-C27
5	E	602	B12	C41-C42-C43-O44
5	B	601	B12	C17-C18-C60-C61
5	E	602	B12	C17-C18-C60-C61
5	E	602	B12	O6R-C4R-C5R-O8R
5	B	601	B12	C41-C42-C43-O44
5	E	602	B12	C3R-C4R-C5R-O8R

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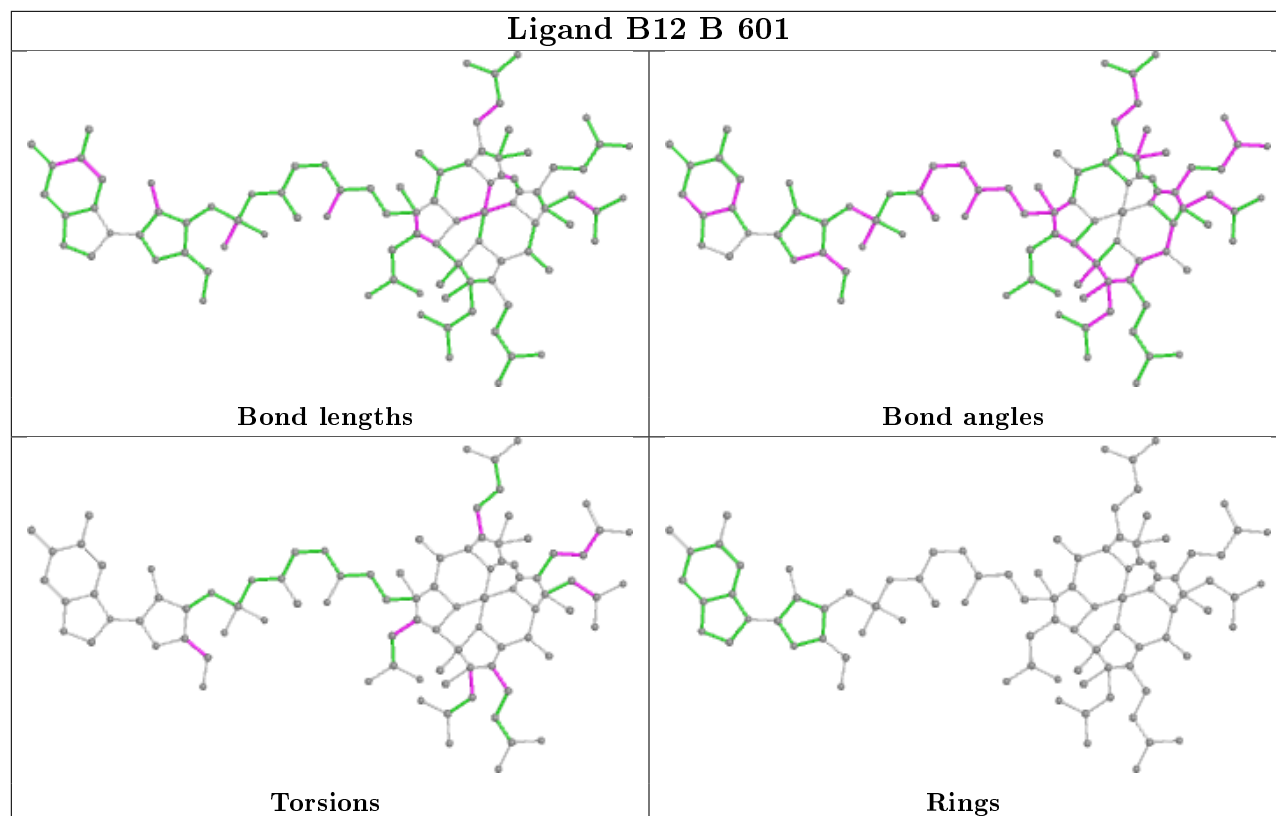
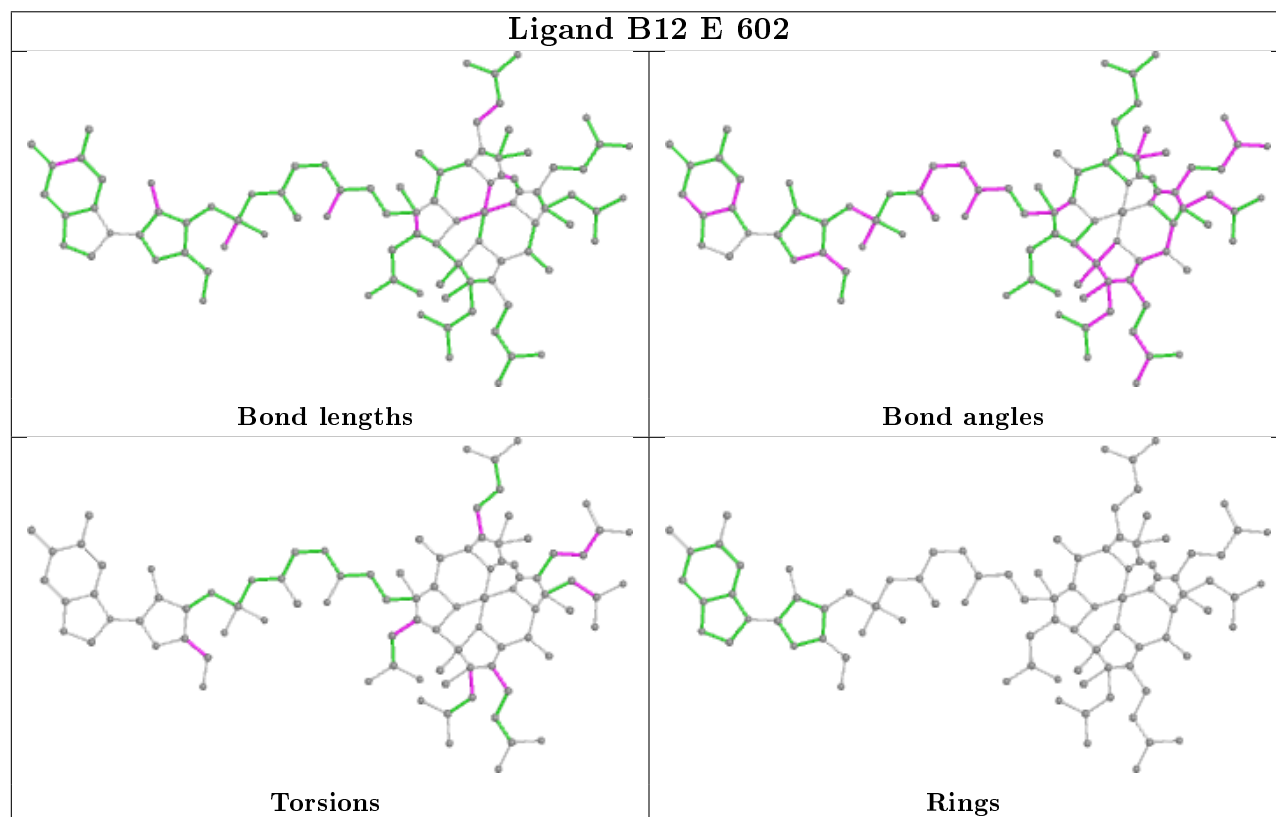
Mol	Chain	Res	Type	Atoms
5	B	601	B12	C4-C3-C30-C31
5	E	602	B12	C4-C3-C30-C31
5	B	601	B12	C8-C41-C42-C43
5	E	602	B12	C41-C42-C43-N45
5	B	601	B12	C19-C18-C60-C61
5	E	602	B12	C19-C18-C60-C61
5	B	601	B12	C41-C42-C43-N45
5	B	601	B12	C7-C37-C38-N40
5	E	602	B12	C7-C37-C38-N40

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	601	B12	5	0
5	E	602	B12	11	0

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

Ligand B12 B 601**Ligand B12 E 602**

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	552/555 (99%)	-0.15	7 (1%) 77 79	24, 38, 55, 69	0
1	L	555/555 (100%)	-0.14	6 (1%) 80 82	21, 36, 54, 72	0
2	B	181/194 (93%)	0.25	8 (4%) 34 37	30, 48, 66, 77	0
2	E	184/194 (94%)	0.05	3 (1%) 72 74	32, 45, 61, 75	0
3	G	132/141 (93%)	-0.04	6 (4%) 33 36	31, 47, 66, 80	0
3	M	131/141 (92%)	-0.01	4 (3%) 49 52	28, 43, 67, 75	0
All	All	1735/1780 (97%)	-0.07	34 (1%) 65 68	21, 41, 60, 80	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	25	GLU	4.7
3	M	141	SER	4.5
1	L	1	MET	4.5
2	E	25	GLU	4.3
1	A	529	GLY	4.2
2	B	11	PHE	3.8
3	M	56	TYR	3.8
1	L	45	ASP	3.6
3	M	20	HIS	3.5
2	B	19	GLY	3.3
1	L	46	ASN	3.1
2	B	27	ALA	3.0
2	B	16	ARG	3.0
1	A	455	VAL	2.9
1	L	36	PHE	2.9
3	G	35	GLU	2.6
1	A	82	ARG	2.6
3	G	42	VAL	2.6
3	G	141	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	46	ASN	2.6
1	A	537	GLU	2.6
1	A	48	LEU	2.4
1	A	1	MET	2.4
2	B	12	THR	2.4
3	M	139	LYS	2.4
1	L	188	LEU	2.3
3	G	139	LYS	2.3
3	G	39	SER	2.2
2	E	27	ALA	2.1
1	L	467	ARG	2.1
2	B	147	SER	2.1
2	B	23	ALA	2.0
2	E	80	VAL	2.0
3	G	140	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

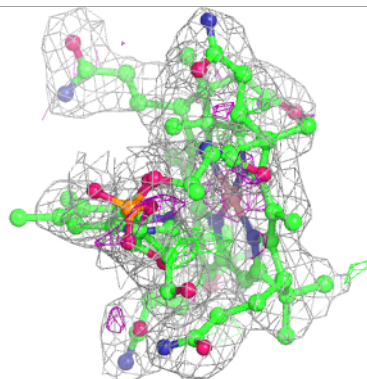
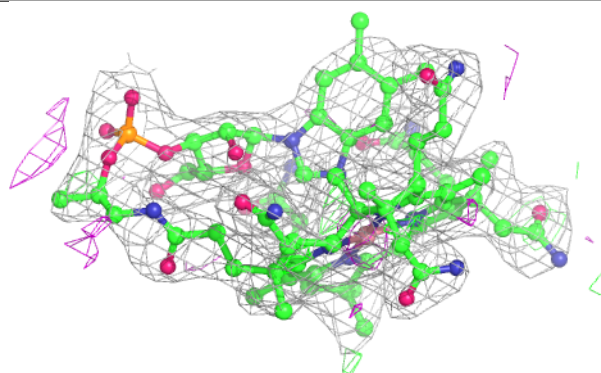
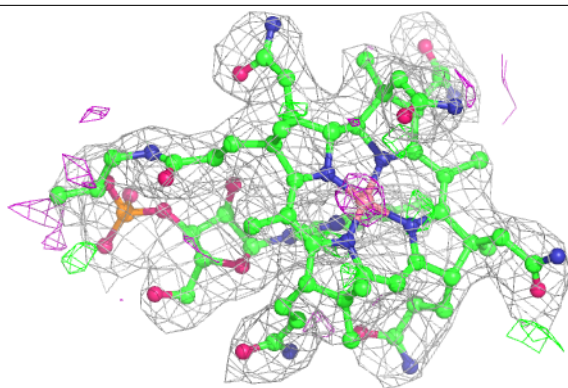
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	B12	B	601	91/91	0.95	0.16	20,34,45,48	0
5	B12	E	602	91/91	0.95	0.15	22,31,38,46	0
4	K	A	1001	1/1	0.99	0.19	40,40,40,40	0
4	K	L	1002	1/1	0.99	0.07	34,34,34,34	0

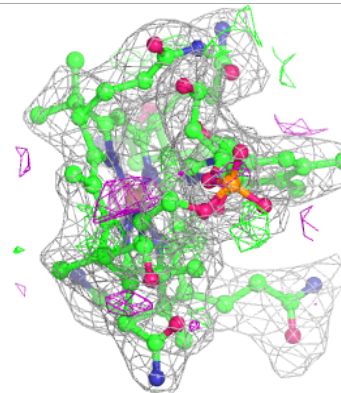
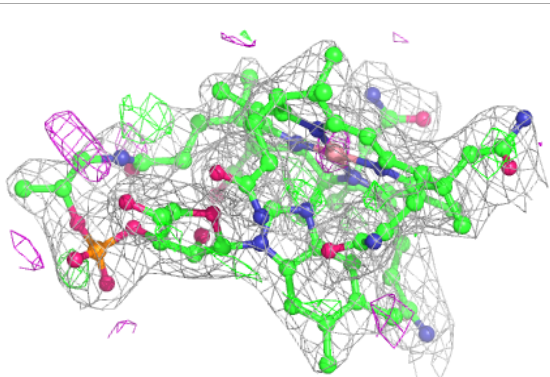
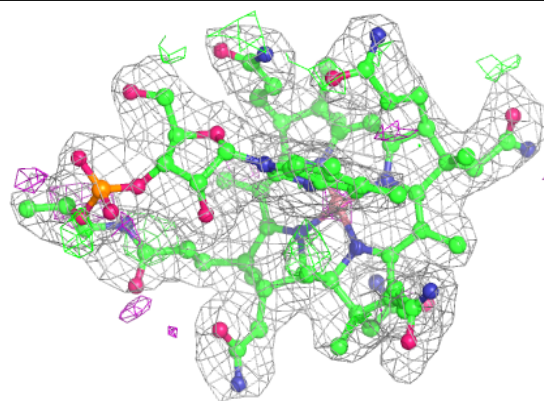
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B12 B 601:

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

**Electron density around B12 E 602:**

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



6.5 Other polymers

There are no such residues in this entry.