



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2022 – 12:15 PM JST

PDB ID : 6KFV
Title : GroEL from *Xanthomonas oryzae* pv. *oryzae*
Authors : Tran, H.T.; Lee, J.H.; Kang, L.W.
Deposited on : 2019-07-08
Resolution : 3.22 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 : 2.25
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) : 2.25

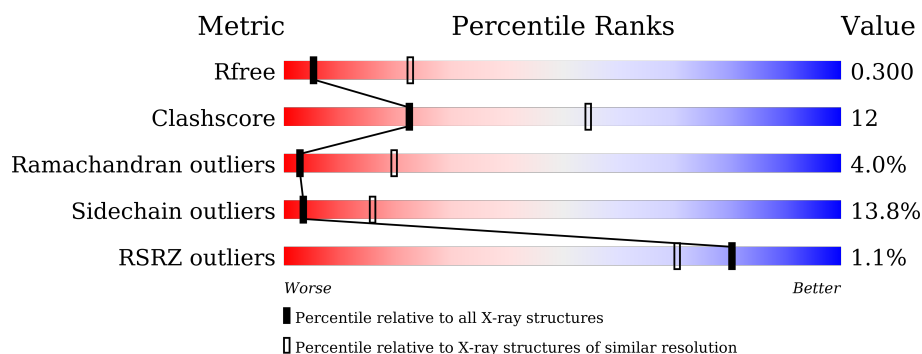
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	525	<div> <div>73%</div> <div>23%</div> <div>• •</div> </div>
1	B	525	<div> <div>%</div> <div>68%</div> <div>27%</div> <div>5%</div> </div>
1	C	525	<div> <div>%</div> <div>70%</div> <div>26%</div> <div>• •</div> </div>
1	D	525	<div> <div>%</div> <div>76%</div> <div>21%</div> <div>•</div> </div>
1	E	525	<div> <div>%</div> <div>74%</div> <div>22%</div> <div>•</div> </div>
1	F	525	<div> <div>%</div> <div>67%</div> <div>26%</div> <div>6%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	525	<div><div></div><div>73%22%5%</div></div>
1	H	525	<div><div>%</div><div>68%25%6%•</div></div>
1	I	525	<div><div></div><div>65%29%6%</div></div>
1	J	525	<div><div>2%</div><div>72%25%•</div></div>
1	K	525	<div><div>2%</div><div>69%24%6%•</div></div>
1	L	525	<div><div>%</div><div>68%26%6%•</div></div>
1	M	525	<div><div>3%</div><div>71%24%••</div></div>
1	N	525	<div><div>2%</div><div>63%29%7%•</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 53933 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 60 kDa chaperonin.

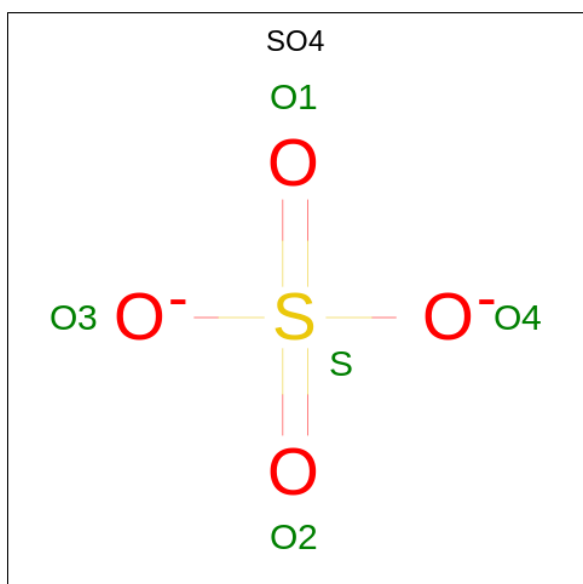
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			3862	2396	677	775	14			
1	B	525	Total	C	N	O	S	0	0	0
			3858	2393	676	775	14			
1	C	525	Total	C	N	O	S	0	0	0
			3862	2396	677	775	14			
1	D	525	Total	C	N	O	S	0	0	0
			3854	2392	677	771	14			
1	E	525	Total	C	N	O	S	0	0	0
			3854	2392	677	771	14			
1	F	525	Total	C	N	O	S	0	0	0
			3839	2383	672	770	14			
1	G	525	Total	C	N	O	S	0	0	0
			3858	2393	676	775	14			
1	H	525	Total	C	N	O	S	0	0	0
			3856	2393	674	775	14			
1	I	525	Total	C	N	O	S	0	0	0
			3842	2384	669	775	14			
1	J	525	Total	C	N	O	S	0	0	0
			3854	2391	675	774	14			
1	K	518	Total	C	N	O	S	0	0	0
			3809	2364	667	764	14			
1	L	525	Total	C	N	O	S	0	0	0
			3859	2393	677	775	14			
1	M	525	Total	C	N	O	S	0	0	0
			3854	2390	675	775	14			
1	N	524	Total	C	N	O	S	0	0	0
			3811	2362	668	767	14			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0

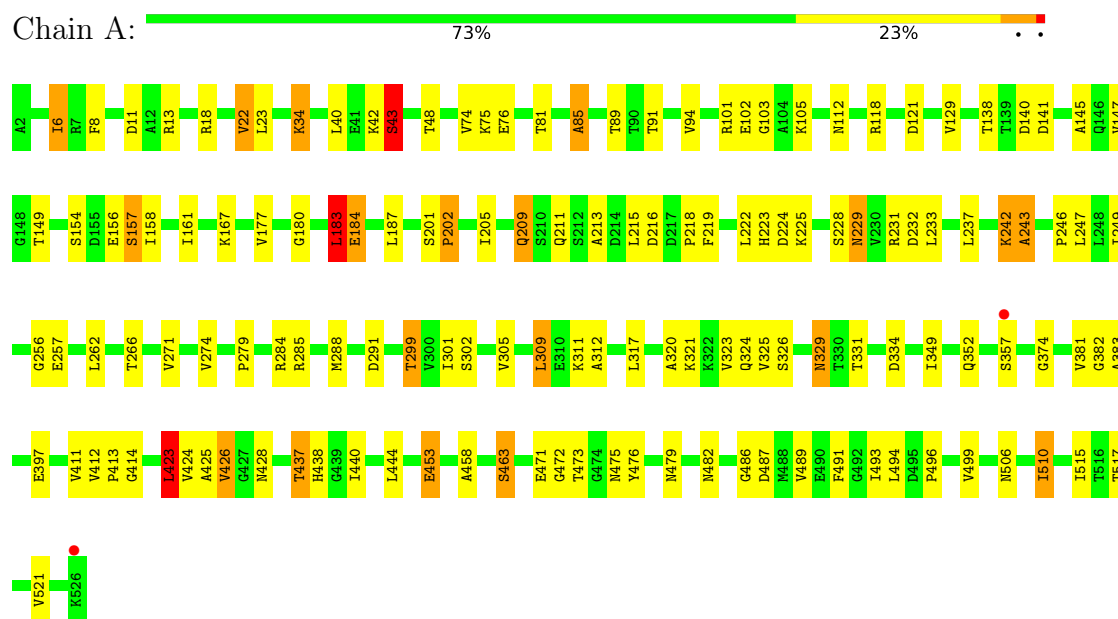
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total O 6 6	0	0
4	C	3	Total O 3 3	0	0
4	D	3	Total O 3 3	0	0
4	E	2	Total O 2 2	0	0
4	F	1	Total O 1 1	0	0
4	G	4	Total O 4 4	0	0
4	H	1	Total O 1 1	0	0
4	I	2	Total O 2 2	0	0
4	J	2	Total O 2 2	0	0
4	K	3	Total O 3 3	0	0
4	M	5	Total O 5 5	0	0
4	N	1	Total O 1 1	0	0

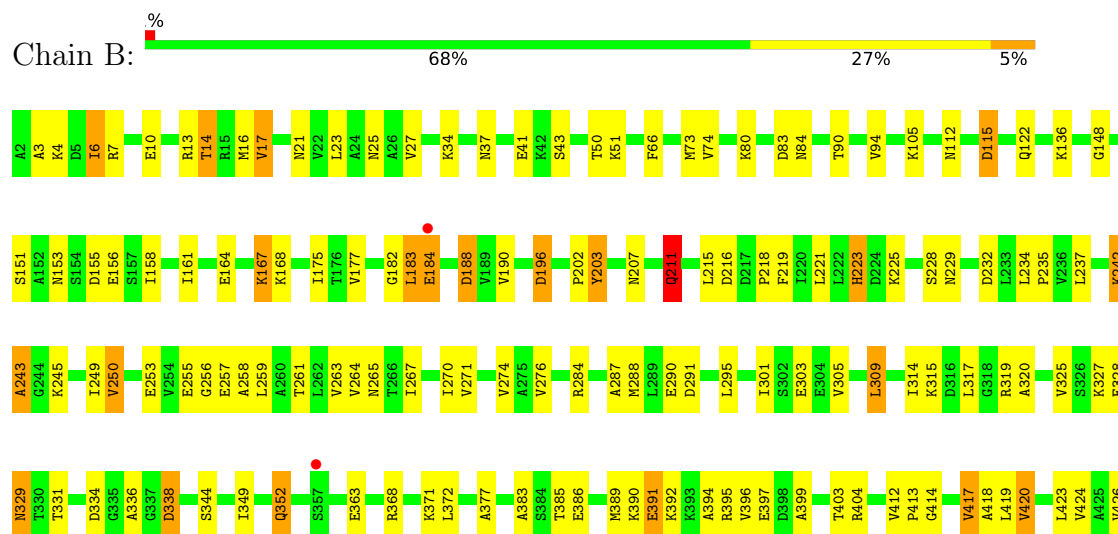
3 Residue-property plots

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

- Molecule 1: 60 kDa chaperonin

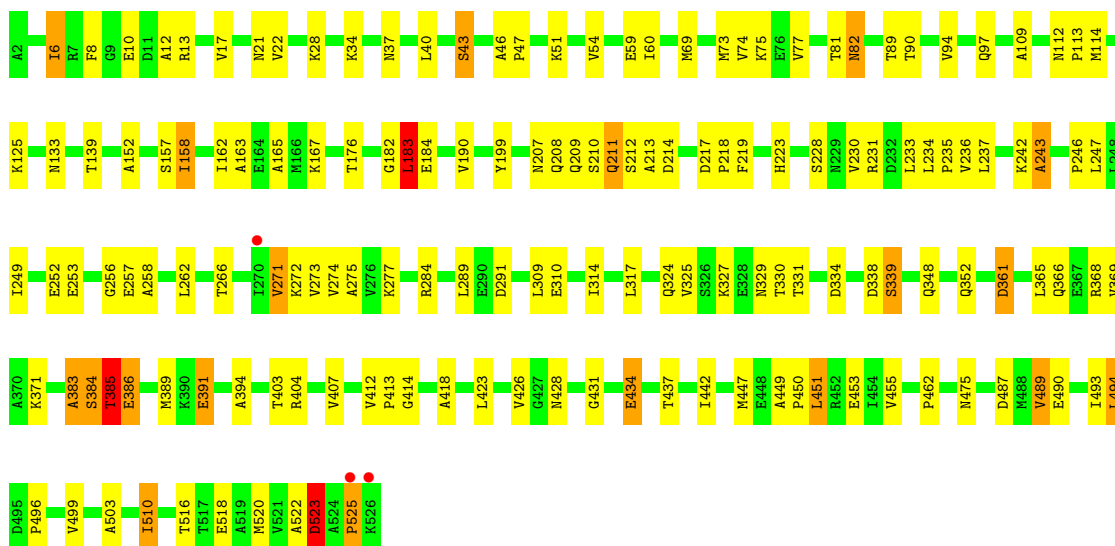


- Molecule 1: 60 kDa chaperonin

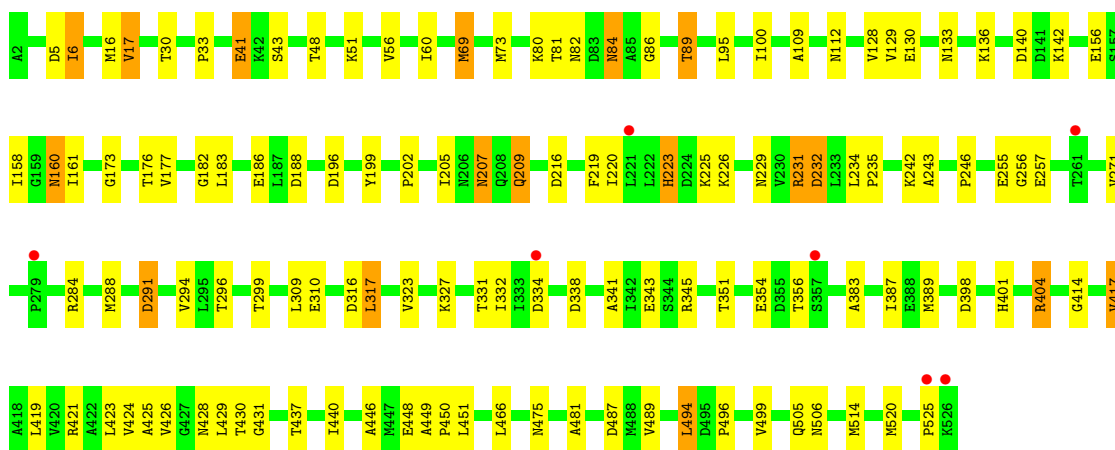
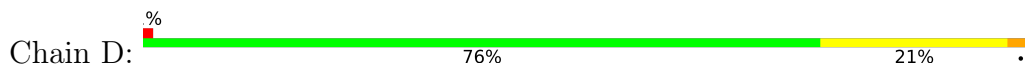




- Molecule 1: 60 kDa chaperonin

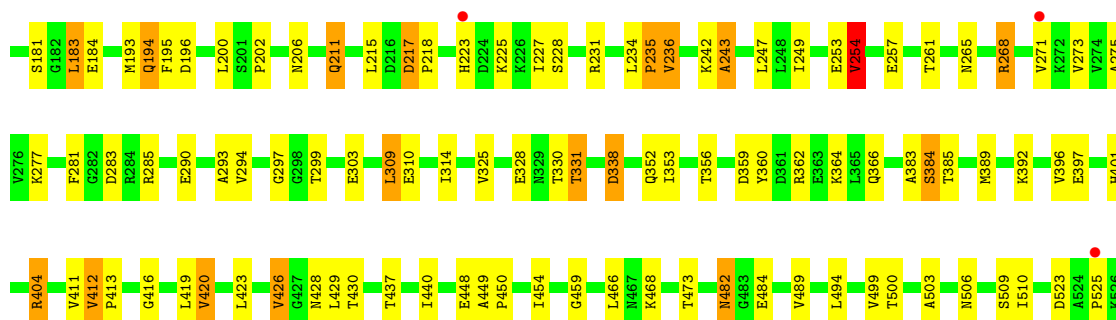


- Molecule 1: 60 kDa chaperonin

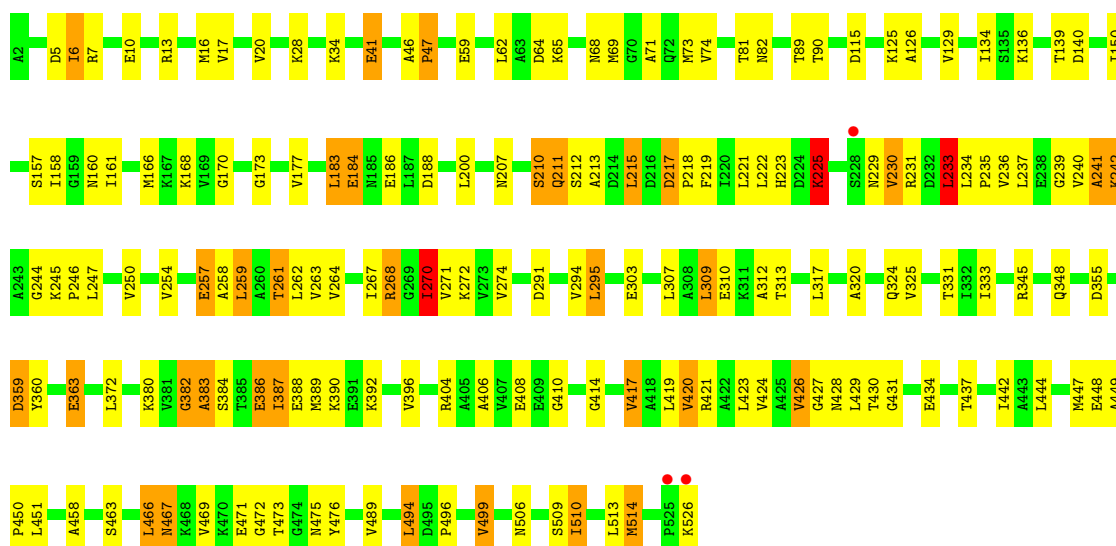


- Molecule 1: 60 kDa chaperonin

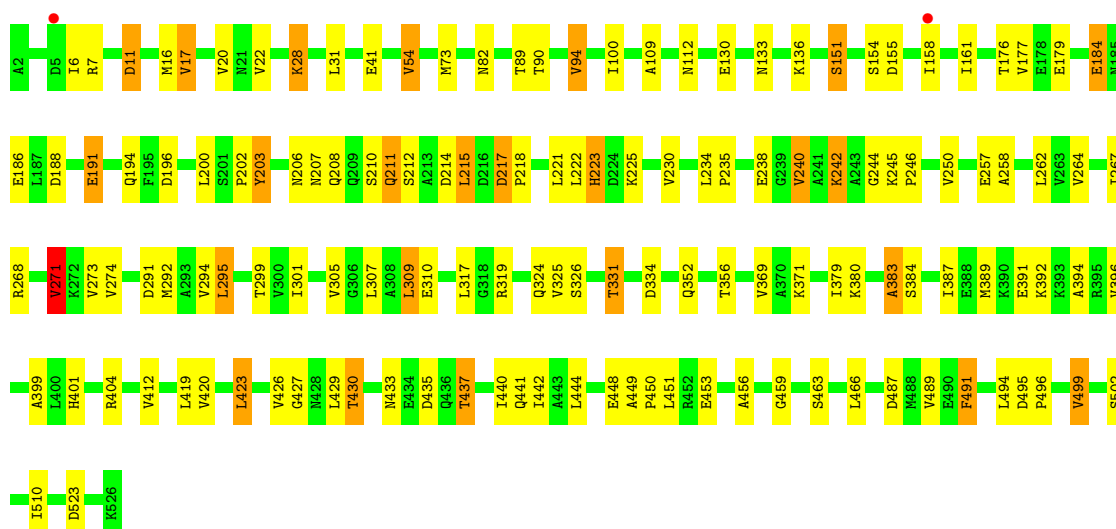




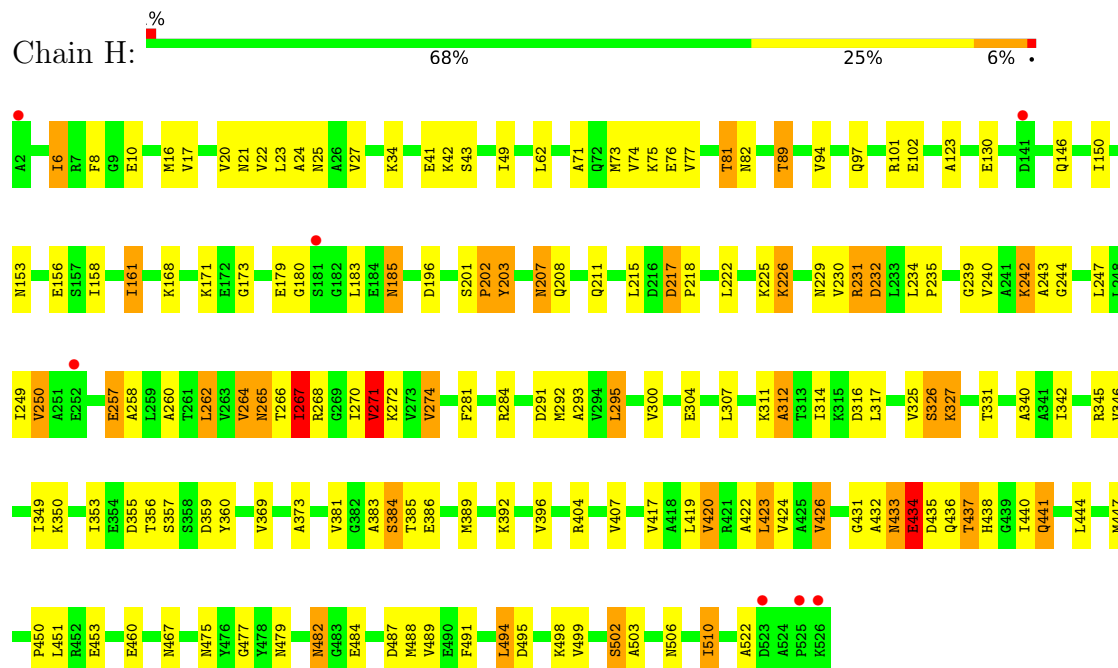
● Molecule 1: 60 kDa chaperonin



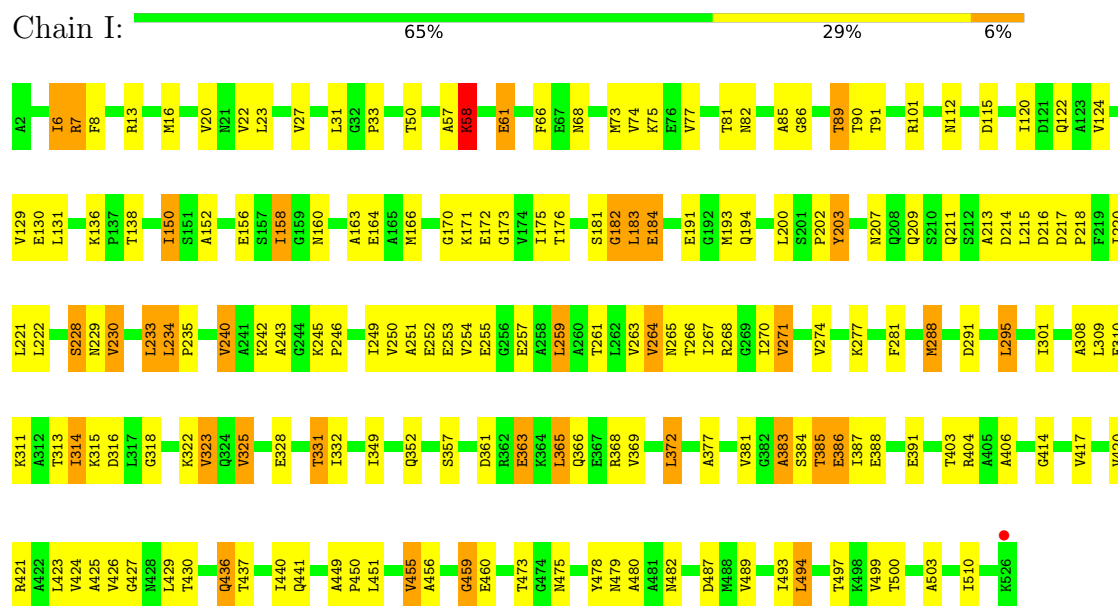
● Molecule 1: 60 kDa chaperonin



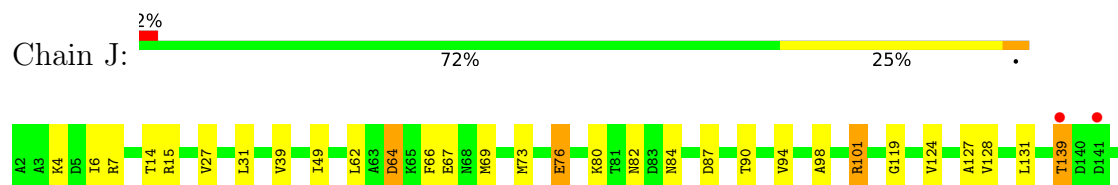
- Molecule 1: 60 kDa chaperonin

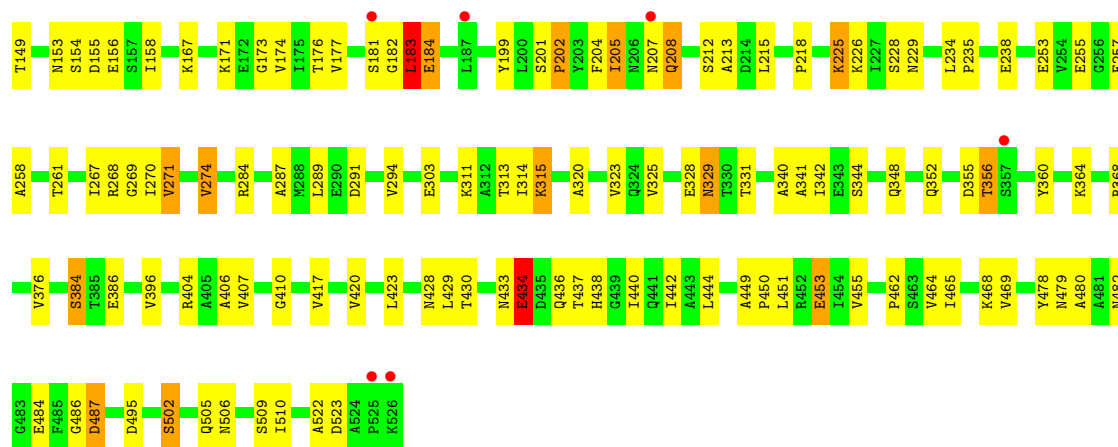


- Molecule 1: 60 kDa chaperonin

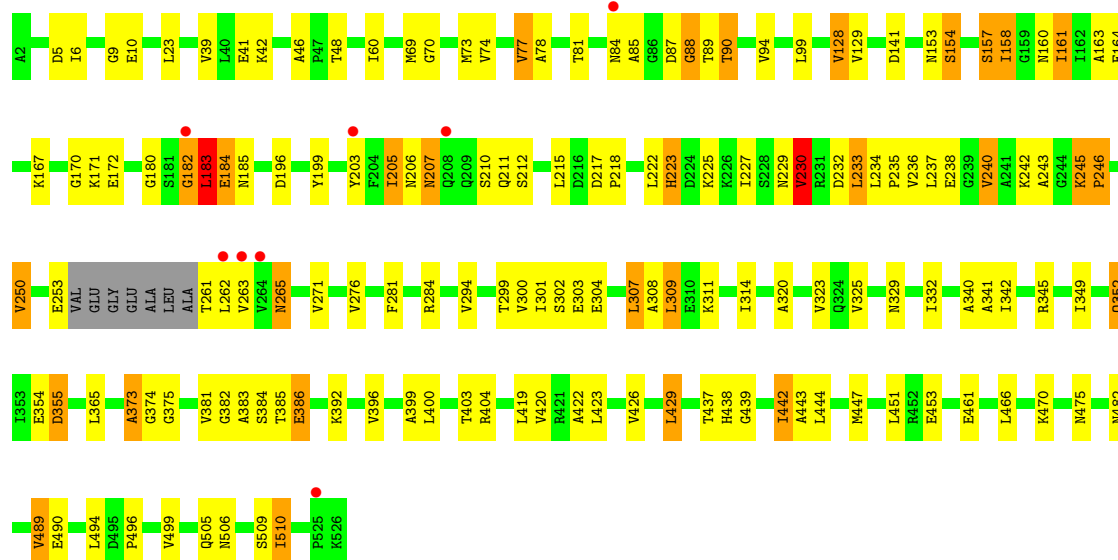


- Molecule 1: 60 kDa chaperonin

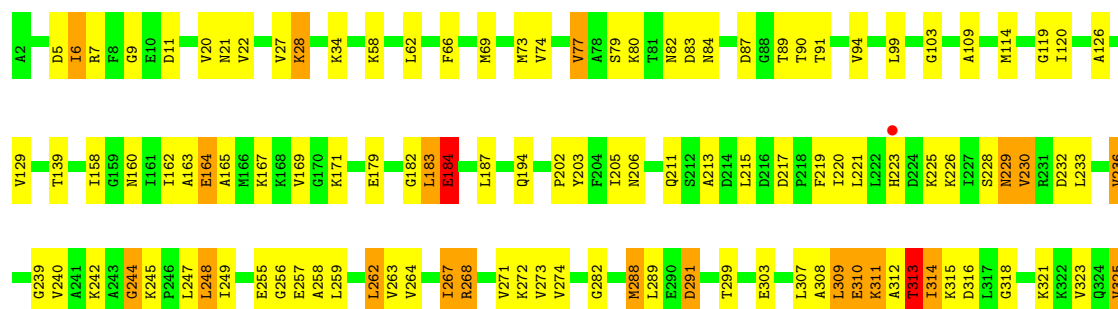


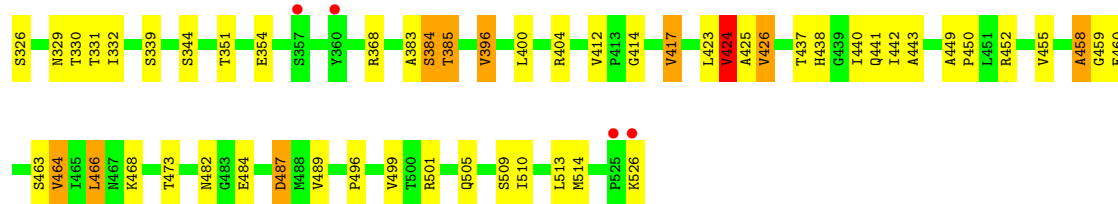


• Molecule 1: 60 kDa chaperonin

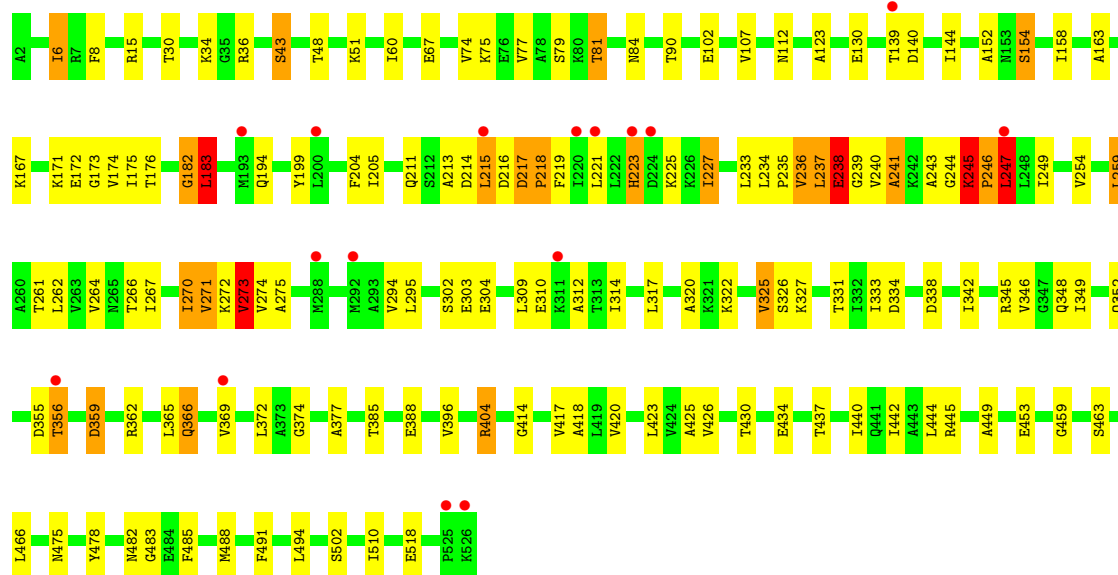


• Molecule 1: 60 kDa chaperonin

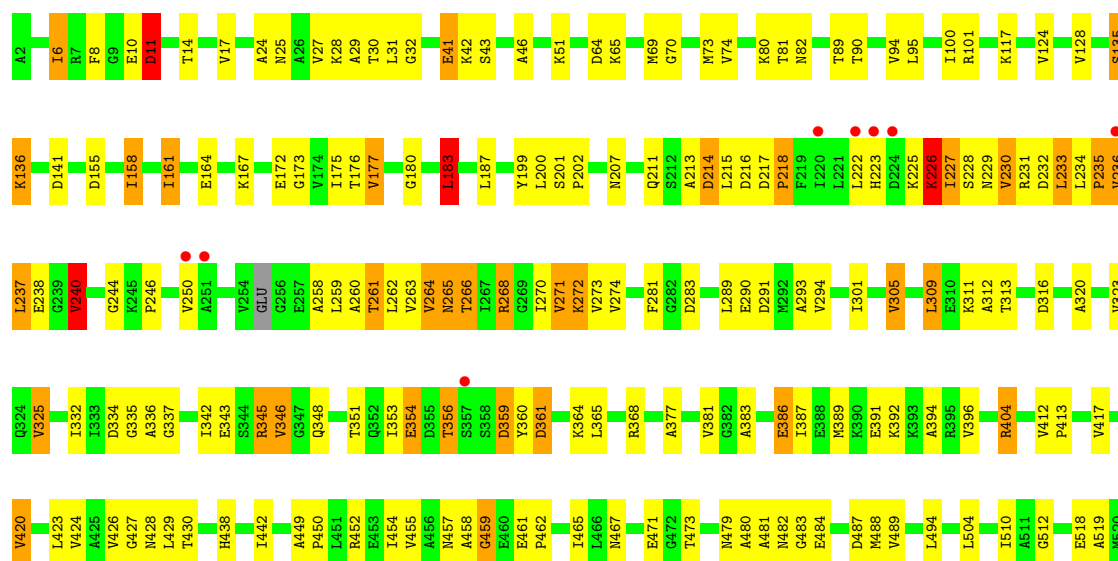




• Molecule 1: 60 kDa chaperonin



• Molecule 1: 60 kDa chaperonin





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.09Å 239.50Å 278.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.36 – 3.22 47.36 – 3.22	Depositor EDS
% Data completeness (in resolution range)	91.7 (47.36-3.22) 91.8 (47.36-3.22)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.219 , 0.304 0.215 , 0.300	Depositor DCC
R_{free} test set	6843 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	68.9	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	53933	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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

5.1 Standard geometry

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

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	0.71	0/3892	0.82	1/5251 (0.0%)
1	B	0.70	0/3888	0.82	0/5247
1	C	0.71	0/3892	0.82	0/5251
1	D	0.72	0/3884	0.82	0/5241
1	E	0.71	0/3884	0.83	0/5241
1	F	0.71	0/3869	0.83	0/5223
1	G	0.71	0/3888	0.83	0/5247
1	H	0.71	0/3886	0.83	0/5244
1	I	0.71	0/3872	0.83	0/5229
1	J	0.72	0/3884	0.80	0/5242
1	K	0.72	0/3838	0.83	0/5177
1	L	0.72	0/3889	0.82	0/5247
1	M	0.73	0/3884	0.85	1/5243 (0.0%)
1	N	0.72	0/3840	0.82	0/5184
All	All	0.72	0/54290	0.83	2/73267 (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	M	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	245	LYS	C-N-CD	-15.61	86.26	120.60
1	A	453	GLU	CB-CA-C	5.65	121.69	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	245	LYS	Mainchain

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	3862	0	3973	71	0
1	B	3858	0	3962	94	0
1	C	3862	0	3973	84	0
1	D	3854	0	3965	66	0
1	E	3854	0	3965	69	0
1	F	3839	0	3932	112	0
1	G	3858	0	3962	76	0
1	H	3856	0	3962	101	0
1	I	3842	0	3929	109	0
1	J	3854	0	3956	73	0
1	K	3809	0	3916	95	0
1	L	3859	0	3964	83	0
1	M	3854	0	3951	129	0
1	N	3811	0	3874	152	0
2	B	6	0	8	3	0
2	F	12	0	16	0	0
3	I	5	0	0	0	0
3	K	5	0	0	0	0
4	A	6	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	4	0	0	0	0
4	H	1	0	0	0	0
4	I	2	0	0	1	0
4	J	2	0	0	0	0
4	K	3	0	0	1	0
4	M	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	1	0	0	0	0
All	All	53933	0	55308	1262	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 12.

All (1262) 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:M:234:LEU:HA	1:M:237:LEU:CD2	1.34	1.55
1:N:228:SER:O	1:N:258:ALA:CB	1.63	1.42
1:F:234:LEU:CD2	1:F:235:PRO:HD3	1.52	1.40
1:M:234:LEU:CA	1:M:237:LEU:CD2	2.00	1.39
1:F:234:LEU:HD23	1:F:235:PRO:CD	1.53	1.38
1:M:234:LEU:N	1:M:237:LEU:HD21	1.41	1.33
1:N:343:GLU:C	1:N:346:VAL:CG2	1.99	1.31
1:N:290:GLU:CD	1:N:345:ARG:NH1	1.86	1.28
1:M:246:PRO:O	1:M:273:VAL:CA	1.82	1.28
1:M:233:LEU:C	1:M:237:LEU:HD21	1.52	1.27
1:N:343:GLU:O	1:N:346:VAL:HG23	1.16	1.26
1:I:385:THR:O	1:I:387:ILE:N	1.69	1.22
1:M:234:LEU:CA	1:M:237:LEU:HD23	1.60	1.22
1:E:482:ASN:OD1	1:E:484:GLU:CG	1.88	1.19
1:N:214:ASP:C	1:N:215:LEU:HD23	1.63	1.18
1:M:246:PRO:O	1:M:273:VAL:HA	1.03	1.18
1:N:343:GLU:O	1:N:346:VAL:CG2	1.91	1.16
1:N:343:GLU:CA	1:N:346:VAL:CG2	2.25	1.15
1:E:482:ASN:OD1	1:E:484:GLU:HG2	1.45	1.15
1:H:267:ILE:HG22	1:H:268:ARG:N	1.58	1.13
1:N:343:GLU:CA	1:N:346:VAL:HG21	1.80	1.11
1:N:343:GLU:HA	1:N:346:VAL:CG2	1.82	1.10
1:H:267:ILE:HG22	1:H:268:ARG:H	0.94	1.09
1:N:228:SER:O	1:N:258:ALA:HB3	1.49	1.08
1:F:240:VAL:O	1:F:242:LYS:O	1.70	1.07
1:K:217:ASP:HB3	1:K:245:LYS:HZ2	1.14	1.05
1:N:343:GLU:HA	1:N:346:VAL:HG21	1.14	1.05
1:N:228:SER:O	1:N:258:ALA:HB2	1.58	1.03
1:M:215:LEU:HD13	1:M:246:PRO:HB2	1.37	1.03
1:M:239:GLY:HA2	1:M:271:VAL:CG1	1.89	1.02
1:N:343:GLU:C	1:N:346:VAL:HG23	1.73	1.01
1:N:214:ASP:O	1:N:215:LEU:HD23	1.61	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:482:ASN:OD1	1:E:484:GLU:HG3	1.62	0.99
1:N:290:GLU:CD	1:N:345:ARG:HH11	1.60	0.99
1:G:429:LEU:HD12	1:G:430:THR:N	1.79	0.98
1:M:233:LEU:HB3	1:M:237:LEU:HD11	1.45	0.98
1:H:267:ILE:CG2	1:H:268:ARG:H	1.74	0.98
1:M:246:PRO:HA	1:M:273:VAL:H	1.30	0.97
1:N:290:GLU:OE2	1:N:345:ARG:NH1	1.98	0.96
1:N:343:GLU:C	1:N:346:VAL:HG22	1.87	0.91
1:H:267:ILE:CG2	1:H:268:ARG:N	2.30	0.91
1:N:29:ALA:O	1:N:457:ASN:ND2	2.04	0.91
1:M:234:LEU:CA	1:M:237:LEU:HD21	1.83	0.89
1:F:386:GLU:O	1:F:389:MET:N	2.04	0.89
1:N:6:ILE:HD11	1:N:8:PHE:CZ	2.08	0.89
1:L:259:LEU:HA	1:L:262:LEU:HB2	1.55	0.88
1:N:228:SER:O	1:N:258:ALA:HB1	1.73	0.88
1:N:232:ASP:OD2	1:N:309:LEU:HB3	1.74	0.88
1:K:217:ASP:HB3	1:K:245:LYS:NZ	1.90	0.87
1:F:234:LEU:HD23	1:F:235:PRO:HD3	0.87	0.87
1:N:290:GLU:CD	1:N:345:ARG:HH12	1.71	0.87
1:N:262:LEU:O	1:N:265:ASN:ND2	2.07	0.86
1:N:343:GLU:CA	1:N:346:VAL:HG22	2.05	0.86
1:K:245:LYS:O	1:K:246:PRO:O	1.92	0.86
1:F:386:GLU:O	1:F:388:GLU:N	2.09	0.84
1:M:233:LEU:C	1:M:237:LEU:CD2	2.42	0.84
1:L:158:ILE:HD11	1:L:396:VAL:HG22	1.60	0.83
1:B:506:ASN:HD21	2:B:601:GOL:H31	1.43	0.82
1:F:234:LEU:HD23	1:F:235:PRO:HD2	1.60	0.82
1:M:234:LEU:N	1:M:237:LEU:CD2	2.24	0.81
1:M:245:LYS:O	1:M:247:LEU:N	2.12	0.81
1:M:215:LEU:HB3	1:M:246:PRO:CG	2.11	0.80
1:B:506:ASN:ND2	2:B:601:GOL:H31	1.97	0.80
1:I:263:VAL:HA	1:I:266:THR:OG1	1.81	0.79
1:M:239:GLY:HA2	1:M:271:VAL:HG11	1.64	0.79
1:M:233:LEU:CB	1:M:237:LEU:HD11	2.12	0.79
1:G:6:ILE:HD11	1:I:22:VAL:HG13	1.64	0.79
1:B:459:GLY:HA3	1:M:112:ASN:HD21	1.45	0.79
1:K:234:LEU:N	1:K:235:PRO:HD2	1.99	0.78
1:G:429:LEU:HD12	1:G:430:THR:H	1.47	0.77
1:N:215:LEU:HD11	1:N:274:VAL:HG12	1.66	0.77
1:E:158:ILE:HD13	1:E:396:VAL:HG22	1.68	0.76
1:N:231:ARG:HA	1:N:234:LEU:HD12	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:228:SER:O	1:I:257:GLU:HB3	1.85	0.75
1:M:246:PRO:O	1:M:247:LEU:O	2.06	0.74
1:N:234:LEU:N	1:N:235:PRO:HD2	2.03	0.74
1:N:228:SER:C	1:N:258:ALA:HB3	2.08	0.74
1:N:342:ILE:O	1:N:346:VAL:HG22	1.86	0.74
1:A:13:ARG:NH1	1:A:517:THR:O	2.22	0.73
1:I:385:THR:O	1:I:386:GLU:C	2.26	0.73
1:M:246:PRO:HA	1:M:273:VAL:N	2.03	0.73
1:M:219:PHE:HE1	1:M:314:ILE:HD12	1.52	0.73
1:N:218:PRO:HB3	1:N:246:PRO:HG2	1.70	0.73
1:H:264:VAL:C	1:H:266:THR:H	1.91	0.72
1:N:246:PRO:HA	1:N:272:LYS:HB2	1.72	0.72
1:N:261:THR:O	1:N:265:ASN:OD1	2.06	0.72
1:I:385:THR:HG22	1:I:387:ILE:HG22	1.70	0.72
1:A:209:GLN:HE21	1:A:209:GLN:HA	1.53	0.72
1:G:7:ARG:NH1	1:G:11:ASP:OD2	2.22	0.72
1:C:383:ALA:HB1	1:C:389:MET:HB2	1.70	0.72
1:K:205:ILE:CG2	1:K:211:GLN:C	2.59	0.71
1:M:215:LEU:HD11	1:M:274:VAL:HG12	1.71	0.71
1:F:386:GLU:HG2	1:F:387:ILE:N	2.05	0.71
1:N:353:ILE:HA	1:N:356:THR:HG23	1.72	0.71
1:I:173:GLY:O	1:I:404:ARG:NH2	2.23	0.71
1:M:345:ARG:HA	1:M:348:GLN:HE21	1.56	0.71
1:N:17:VAL:HG23	1:N:100:ILE:HG22	1.73	0.71
1:B:182:GLY:HA2	1:B:383:ALA:HB2	1.73	0.70
1:I:414:GLY:O	1:I:417:VAL:HG13	1.90	0.70
1:G:309:LEU:HD23	1:G:309:LEU:N	2.06	0.70
1:B:182:GLY:CA	1:B:383:ALA:HB2	2.22	0.70
1:D:199:TYR:CZ	1:D:327:LYS:HA	2.27	0.70
1:B:228:SER:O	1:B:258:ALA:HB2	1.91	0.70
1:D:207:ASN:HD22	1:D:209:GLN:HE22	1.40	0.70
1:H:234:LEU:N	1:H:235:PRO:HD2	2.07	0.70
1:H:434:GLU:HG3	1:I:441:GLN:HE21	1.57	0.69
1:L:264:VAL:O	1:L:268:ARG:HB3	1.91	0.69
1:M:246:PRO:HB3	1:M:272:LYS:HB3	1.73	0.69
1:F:183:LEU:HB2	1:F:384:SER:HB2	1.74	0.69
1:I:385:THR:C	1:I:387:ILE:N	2.45	0.69
1:I:228:SER:HB3	1:I:255:GLU:HB3	1.74	0.69
1:M:216:ASP:HA	1:M:322:LYS:HA	1.74	0.69
1:N:90:THR:O	1:N:94:VAL:HG13	1.93	0.68
1:H:264:VAL:O	1:H:267:ILE:HD12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:302:SER:C	1:K:309:LEU:HD22	2.13	0.68
1:F:382:GLY:O	1:F:383:ALA:HB3	1.93	0.68
1:A:437:THR:O	1:A:440:ILE:HB	1.94	0.68
1:F:414:GLY:O	1:F:417:VAL:HG13	1.93	0.68
1:N:222:LEU:CD1	1:N:293:ALA:HA	2.23	0.68
1:M:239:GLY:O	1:M:271:VAL:HG12	1.94	0.68
1:K:426:VAL:O	1:K:426:VAL:HG22	1.93	0.68
1:E:6:ILE:HD11	1:E:8:PHE:CZ	2.29	0.68
1:N:361:ASP:O	1:N:365:LEU:HG	1.94	0.68
1:A:262:LEU:O	1:A:266:THR:HG23	1.94	0.67
1:K:373:ALA:O	1:K:375:GLY:N	2.27	0.67
1:D:84:ASN:C	1:D:84:ASN:HD22	1.98	0.67
1:K:87:ASP:O	1:K:499:VAL:HG21	1.93	0.67
1:L:501:ARG:NH1	1:L:505:GLN:OE1	2.28	0.67
1:N:263:VAL:CG2	1:N:264:VAL:N	2.56	0.67
1:L:228:SER:HA	1:L:258:ALA:HB2	1.76	0.67
1:N:290:GLU:OE1	1:N:345:ARG:NH1	2.26	0.67
1:F:382:GLY:O	1:F:383:ALA:CB	2.43	0.67
1:N:226:LYS:HD3	1:N:226:LYS:C	2.16	0.67
1:C:383:ALA:CB	1:C:389:MET:HB2	2.25	0.66
1:D:235:PRO:HG3	1:D:310:GLU:HA	1.75	0.66
1:M:246:PRO:CA	1:M:273:VAL:H	2.07	0.66
1:N:354:GLU:OE1	1:N:354:GLU:HA	1.95	0.66
1:H:158:ILE:HD13	1:H:396:VAL:HG22	1.76	0.66
1:I:194:GLN:HB2	1:I:331:THR:HB	1.77	0.66
1:N:259:LEU:O	1:N:262:LEU:CB	2.43	0.66
1:I:130:GLU:HG2	1:I:425:ALA:CB	2.26	0.66
1:D:496:PRO:O	1:D:499:VAL:HG12	1.96	0.66
1:F:13:ARG:O	1:F:17:VAL:HG12	1.95	0.66
1:I:366:GLN:O	1:I:369:VAL:HG22	1.96	0.66
1:L:217:ASP:O	1:L:245:LYS:HE2	1.96	0.66
1:I:251:ALA:O	1:I:253:GLU:N	2.28	0.65
1:L:229:ASN:O	1:L:230:VAL:HG22	1.97	0.65
1:F:16:MET:HB3	1:F:514:MET:HE1	1.77	0.65
1:F:230:VAL:HG21	1:F:261:THR:OG1	1.97	0.65
1:H:353:ILE:HG22	1:H:353:ILE:O	1.95	0.65
1:I:385:THR:O	1:I:387:ILE:CA	2.44	0.65
1:N:217:ASP:N	1:N:218:PRO:HD3	2.12	0.65
1:I:233:LEU:HD22	1:I:233:LEU:H	1.62	0.65
1:F:309:LEU:N	1:F:309:LEU:HD22	2.12	0.65
1:B:4:LYS:HG3	1:C:59:GLU:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:194:GLN:HB2	1:E:331:THR:HB	1.77	0.65
1:I:385:THR:O	1:I:387:ILE:HG22	1.97	0.65
1:N:438:HIS:O	1:N:442:ILE:HG23	1.97	0.65
1:H:434:GLU:CG	1:I:441:GLN:HE21	2.10	0.64
1:M:234:LEU:HA	1:M:237:LEU:HD23	0.66	0.64
1:E:223:HIS:ND1	1:E:227:ILE:HD11	2.11	0.64
1:K:233:LEU:C	1:K:235:PRO:HD2	2.18	0.64
1:F:386:GLU:CG	1:F:387:ILE:N	2.56	0.64
1:M:215:LEU:HB3	1:M:246:PRO:HG3	1.78	0.64
1:L:384:SER:O	1:L:385:THR:OG1	2.12	0.64
1:A:440:ILE:O	1:A:444:LEU:HG	1.95	0.64
1:J:417:VAL:HA	1:J:420:VAL:HG22	1.78	0.64
1:E:200:LEU:HD13	1:E:254:VAL:CG2	2.28	0.64
1:J:352:GLN:O	1:J:356:THR:HG23	1.98	0.64
1:B:215:LEU:HD11	1:B:274:VAL:HG12	1.79	0.64
1:F:234:LEU:CG	1:F:235:PRO:HD3	2.28	0.63
1:H:432:ALA:HB3	1:H:436:GLN:NE2	2.13	0.63
1:L:158:ILE:CD1	1:L:396:VAL:HG22	2.29	0.63
1:N:233:LEU:HD12	1:N:233:LEU:N	2.13	0.63
1:M:239:GLY:HA2	1:M:271:VAL:HG13	1.80	0.63
1:N:233:LEU:HD12	1:N:233:LEU:H	1.62	0.63
1:D:173:GLY:O	1:D:404:ARG:NH2	2.31	0.63
1:H:432:ALA:HB3	1:H:436:GLN:HE21	1.64	0.63
1:L:239:GLY:O	1:L:314:ILE:HG21	1.98	0.63
1:D:128:VAL:HG21	1:D:505:GLN:HE21	1.63	0.63
1:H:264:VAL:O	1:H:266:THR:N	2.31	0.62
1:J:212:SER:OG	1:J:213:ALA:N	2.32	0.62
1:M:223:HIS:NE2	1:M:309:LEU:HD22	2.14	0.62
1:M:238:GLU:HB2	1:M:241:ALA:HB3	1.81	0.62
1:F:158:ILE:HG12	1:F:396:VAL:HG22	1.80	0.62
1:K:237:LEU:HA	1:K:240:VAL:HG23	1.81	0.62
1:N:263:VAL:HG23	1:N:264:VAL:N	2.12	0.62
1:C:383:ALA:HB2	1:C:389:MET:CG	2.29	0.62
1:L:313:THR:O	1:L:315:LYS:N	2.31	0.62
1:M:217:ASP:N	1:M:218:PRO:HD3	2.13	0.62
1:N:215:LEU:HD23	1:N:215:LEU:N	2.08	0.62
1:N:173:GLY:O	1:N:404:ARG:NH2	2.32	0.62
1:I:150:ILE:HD13	1:I:494:LEU:HD11	1.80	0.62
1:N:228:SER:CA	1:N:258:ALA:HB3	2.30	0.62
1:N:262:LEU:C	1:N:265:ASN:OD1	2.38	0.62
1:M:362:ARG:HG2	1:M:366:GLN:HE22	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:228:SER:C	1:N:258:ALA:CB	2.60	0.62
1:D:475:ASN:HD22	1:D:489:VAL:HG12	1.64	0.61
1:G:223:HIS:CD2	1:G:225:LYS:HD3	2.35	0.61
1:K:303:GLU:HG3	1:K:309:LEU:HD13	1.82	0.61
1:G:392:LYS:O	1:G:396:VAL:HG23	2.01	0.61
1:N:320:ALA:HA	1:N:335:GLY:HA2	1.82	0.61
1:G:215:LEU:HD11	1:G:274:VAL:HG12	1.82	0.61
1:M:238:GLU:CB	1:M:241:ALA:HB3	2.30	0.61
1:M:246:PRO:O	1:M:273:VAL:N	2.33	0.61
1:B:223:HIS:NE2	1:B:225:LYS:HD3	2.16	0.61
1:H:482:ASN:HD21	1:H:484:GLU:HB2	1.65	0.61
1:L:82:ASN:HB2	1:L:89:THR:CG2	2.31	0.61
1:M:218:PRO:HD2	1:M:320:ALA:O	2.01	0.61
1:A:425:ALA:O	1:A:426:VAL:HB	2.01	0.60
1:F:240:VAL:CG1	1:F:245:LYS:O	2.49	0.60
1:L:423:LEU:O	1:L:425:ALA:N	2.34	0.60
1:M:219:PHE:CE1	1:M:314:ILE:HD12	2.36	0.60
1:H:262:LEU:O	1:H:266:THR:OG1	2.18	0.60
1:B:34:LYS:CB	1:B:458:ALA:HA	2.32	0.60
1:C:73:MET:HB3	1:C:510:ILE:HD11	1.83	0.60
1:E:200:LEU:HD13	1:E:254:VAL:HG22	1.81	0.60
1:K:245:LYS:C	1:K:246:PRO:O	2.37	0.60
1:M:423:LEU:HD21	1:M:444:LEU:O	2.01	0.60
1:B:183:LEU:N	1:B:383:ALA:HB2	2.17	0.60
1:K:223:HIS:HA	1:K:301:ILE:O	2.02	0.60
1:N:135:SER:OG	1:N:136:LYS:N	2.35	0.60
1:B:202:PRO:O	1:B:203:TYR:HB2	2.02	0.60
1:J:479:ASN:ND2	1:J:482:ASN:ND2	2.50	0.60
1:L:213:ALA:HB3	1:L:325:VAL:HG13	1.83	0.60
1:M:270:ILE:O	1:M:271:VAL:HG22	2.02	0.60
1:B:223:HIS:HE2	1:B:309:LEU:HD22	1.67	0.59
1:D:232:ASP:HB3	1:D:309:LEU:HB2	1.84	0.59
1:I:234:LEU:N	1:I:235:PRO:HD2	2.17	0.59
1:M:215:LEU:HB3	1:M:246:PRO:CB	2.32	0.59
1:G:223:HIS:NE2	1:G:309:LEU:HD22	2.17	0.59
1:N:234:LEU:C	1:N:236:VAL:H	2.05	0.59
1:G:73:MET:HB3	1:G:510:ILE:HD11	1.83	0.59
1:B:309:LEU:HD23	1:B:309:LEU:N	2.17	0.59
1:G:158:ILE:HD11	1:G:396:VAL:HG13	1.84	0.59
1:K:205:ILE:HG23	1:K:211:GLN:C	2.23	0.59
1:C:348:GLN:O	1:C:352:GLN:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:264:VAL:O	1:G:268:ARG:HG3	2.03	0.59
1:D:219:PHE:HB3	1:D:317:LEU:HD23	1.85	0.59
1:F:210:SER:O	1:F:212:SER:N	2.35	0.59
1:G:158:ILE:CD1	1:G:396:VAL:HG22	2.32	0.59
1:J:438:HIS:O	1:J:442:ILE:HG23	2.03	0.59
1:N:262:LEU:O	1:N:265:ASN:CG	2.41	0.59
1:J:155:ASP:O	1:J:158:ILE:HG22	2.02	0.59
1:L:423:LEU:O	1:L:424:VAL:C	2.41	0.59
1:A:177:VAL:HG21	1:A:397:GLU:HG3	1.85	0.58
1:B:80:LYS:O	1:B:84:ASN:HB3	2.02	0.58
1:M:215:LEU:CD1	1:M:246:PRO:HB2	2.25	0.58
1:A:81:THR:HG22	1:A:506:ASN:OD1	2.02	0.58
1:I:182:GLY:O	1:I:183:LEU:HB2	2.03	0.58
1:K:157:SER:O	1:K:161:ILE:HG23	2.03	0.58
1:L:438:HIS:O	1:L:442:ILE:HG23	2.03	0.58
1:D:80:LYS:O	1:D:84:ASN:CB	2.51	0.58
1:J:479:ASN:HD22	1:J:482:ASN:ND2	2.01	0.58
1:B:37:ASN:HD21	1:B:51:LYS:HE2	1.69	0.58
1:E:281:PHE:CZ	1:K:182:GLY:HA2	2.39	0.58
1:D:431:GLY:N	1:D:437:THR:HG22	2.18	0.58
1:L:90:THR:O	1:L:94:VAL:HG13	2.04	0.58
1:M:414:GLY:O	1:M:417:VAL:HG22	2.04	0.58
1:N:213:ALA:HB3	1:N:325:VAL:HG13	1.85	0.58
1:D:234:LEU:N	1:D:235:PRO:HD2	2.18	0.58
1:M:219:PHE:HE1	1:M:314:ILE:CD1	2.17	0.58
1:M:234:LEU:C	1:M:237:LEU:CD2	2.72	0.58
1:D:288:MET:HA	1:D:291:ASP:HB2	1.85	0.57
1:I:220:ILE:N	1:I:318:GLY:O	2.35	0.57
1:B:221:LEU:CD1	1:B:301:ILE:HD12	2.34	0.57
1:C:46:ALA:HB1	1:C:47:PRO:CD	2.34	0.57
1:H:161:ILE:HD13	1:H:185:ASN:HD22	1.69	0.57
1:I:449:ALA:HB3	1:I:450:PRO:HD3	1.87	0.57
1:K:77:VAL:HG21	1:K:510:ILE:HB	1.86	0.57
1:N:290:GLU:CG	1:N:345:ARG:HH12	2.16	0.57
1:B:218:PRO:HD2	1:B:320:ALA:O	2.05	0.57
1:K:234:LEU:N	1:K:235:PRO:CD	2.68	0.57
1:M:302:SER:O	1:M:304:GLU:N	2.37	0.57
1:F:259:LEU:HA	1:F:262:LEU:HD21	1.86	0.57
1:I:207:ASN:HB3	1:I:209:GLN:HE22	1.69	0.57
1:K:90:THR:O	1:K:94:VAL:HG13	2.05	0.57
1:N:25:ASN:OD1	1:N:28:LYS:HE2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:369:VAL:O	1:H:373:ALA:HB3	2.05	0.57
1:L:414:GLY:O	1:L:417:VAL:HG13	2.04	0.57
1:M:240:VAL:HG12	1:M:240:VAL:O	2.05	0.57
1:D:383:ALA:HB2	1:D:389:MET:HG3	1.87	0.57
1:I:130:GLU:HG2	1:I:425:ALA:HB3	1.85	0.57
1:I:385:THR:CG2	1:I:387:ILE:HG22	2.34	0.57
1:F:386:GLU:HG2	1:F:387:ILE:H	1.68	0.57
1:N:73:MET:HB3	1:N:510:ILE:HD11	1.86	0.57
1:F:430:THR:HA	1:F:437:THR:HG22	1.86	0.56
1:C:431:GLY:N	1:C:437:THR:HG22	2.20	0.56
1:B:506:ASN:HD21	2:B:601:GOL:C3	2.17	0.56
1:M:240:VAL:CG2	1:M:270:ILE:HG23	2.34	0.56
1:N:8:PHE:CD1	1:N:519:ALA:HB2	2.40	0.56
1:B:423:LEU:HD21	1:B:447:MET:HB2	1.87	0.56
1:F:423:LEU:HD21	1:F:447:MET:HB2	1.87	0.56
1:D:338:ASP:HB2	1:D:341:ALA:HB3	1.88	0.56
1:H:264:VAL:C	1:H:266:THR:N	2.59	0.56
1:B:426:VAL:O	1:B:426:VAL:HG22	2.06	0.56
1:E:70:GLY:HA2	1:E:73:MET:HE3	1.88	0.56
1:B:413:PRO:O	1:B:418:ALA:HB2	2.05	0.56
1:C:109:ALA:HB2	1:L:109:ALA:HB2	1.87	0.56
1:G:440:ILE:O	1:G:444:LEU:HG	2.05	0.56
1:C:423:LEU:HD21	1:C:447:MET:HB2	1.87	0.56
1:L:217:ASP:N	1:L:321:LYS:O	2.35	0.56
1:A:349:ILE:O	1:A:352:GLN:N	2.35	0.56
1:E:426:VAL:HG22	1:E:429:LEU:HB2	1.88	0.56
1:F:234:LEU:HD21	1:F:235:PRO:HD3	1.75	0.56
1:G:112:ASN:ND2	1:I:459:GLY:HA3	2.21	0.56
1:H:24:ALA:HB3	1:H:97:GLN:HE21	1.71	0.56
1:D:449:ALA:HB3	1:D:450:PRO:HD3	1.87	0.55
1:E:32:GLY:HA3	1:E:454:ILE:HG23	1.89	0.55
1:G:82:ASN:HB2	1:G:89:THR:HG23	1.87	0.55
1:L:194:GLN:HA	1:L:330:THR:O	2.07	0.55
1:C:413:PRO:O	1:C:418:ALA:HB2	2.07	0.55
1:D:423:LEU:O	1:D:425:ALA:N	2.39	0.55
1:L:247:LEU:HB3	1:L:273:VAL:HG13	1.88	0.55
1:M:102:GLU:OE1	1:M:445:ARG:NH1	2.39	0.55
1:G:223:HIS:NE2	1:G:309:LEU:CD2	2.69	0.55
1:E:211:GLN:HG3	1:E:211:GLN:O	2.07	0.55
1:G:158:ILE:HD13	1:G:396:VAL:HG22	1.88	0.55
1:H:215:LEU:HD11	1:H:274:VAL:CG1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:270:ILE:O	1:H:271:VAL:HG22	2.06	0.55
1:C:234:LEU:N	1:C:235:PRO:HD2	2.22	0.55
1:G:6:ILE:HD11	1:I:22:VAL:CG1	2.36	0.55
1:G:234:LEU:N	1:G:235:PRO:HD2	2.22	0.55
1:C:247:LEU:HB3	1:C:273:VAL:HG22	1.89	0.55
1:I:194:GLN:HA	1:I:331:THR:HA	1.88	0.55
1:I:281:PHE:CZ	1:M:182:GLY:HA2	2.42	0.55
1:I:403:THR:O	1:I:406:ALA:HB3	2.06	0.55
1:N:32:GLY:HA3	1:N:454:ILE:HG23	1.89	0.55
1:B:223:HIS:CD2	1:B:225:LYS:HD3	2.42	0.55
1:C:366:GLN:O	1:C:369:VAL:HG22	2.07	0.55
1:D:16:MET:HB3	1:D:514:MET:HE1	1.87	0.55
1:D:69:MET:O	1:D:73:MET:HG3	2.07	0.55
1:F:234:LEU:N	1:F:235:PRO:HD2	2.21	0.55
1:L:496:PRO:O	1:L:499:VAL:HG12	2.06	0.55
1:N:214:ASP:O	1:N:215:LEU:CD2	2.47	0.55
1:N:260:ALA:O	1:N:263:VAL:HG13	2.06	0.55
1:I:253:GLU:HG2	1:I:277:LYS:HE2	1.89	0.55
1:I:455:VAL:HG13	1:I:460:GLU:HB2	1.89	0.55
1:K:158:ILE:HD13	1:K:396:VAL:HG22	1.88	0.55
1:K:236:VAL:O	1:K:240:VAL:HG22	2.07	0.55
1:L:233:LEU:O	1:L:236:VAL:HG12	2.06	0.55
1:E:81:THR:HG21	1:E:503:ALA:HA	1.89	0.54
1:M:259:LEU:C	1:M:259:LEU:HD22	2.27	0.54
1:B:250:VAL:HA	1:B:276:VAL:O	2.07	0.54
1:D:223:HIS:NE2	1:D:309:LEU:HD22	2.22	0.54
1:E:223:HIS:NE2	1:E:309:LEU:HD22	2.22	0.54
1:G:194:GLN:HB2	1:G:331:THR:HB	1.89	0.54
1:A:423:LEU:HD21	1:A:444:LEU:O	2.08	0.54
1:D:207:ASN:ND2	1:D:209:GLN:HE22	2.04	0.54
1:H:81:THR:HG22	1:H:506:ASN:OD1	2.07	0.54
1:J:15:ARG:O	1:J:67:GLU:HA	2.06	0.54
1:A:215:LEU:HD12	1:A:323:VAL:HG22	1.90	0.54
1:B:287:ALA:HB1	1:B:368:ARG:NH1	2.23	0.54
1:F:262:LEU:HD23	1:F:262:LEU:H	1.73	0.54
1:I:156:GLU:O	1:I:160:ASN:HB2	2.08	0.54
1:J:440:ILE:O	1:J:444:LEU:HG	2.08	0.54
1:K:217:ASP:CB	1:K:245:LYS:NZ	2.68	0.54
1:K:261:THR:O	1:K:262:LEU:HD23	2.07	0.54
1:L:215:LEU:HD11	1:L:274:VAL:HG12	1.88	0.54
1:N:262:LEU:O	1:N:265:ASN:OD1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:449:ALA:HB3	1:F:450:PRO:HD3	1.90	0.54
1:I:214:ASP:OD1	1:I:322:LYS:HE2	2.07	0.54
1:B:188:ASP:OD1	1:B:188:ASP:N	2.41	0.54
1:B:219:PHE:HB3	1:B:317:LEU:HD23	1.90	0.54
1:F:270:ILE:HD13	1:J:229:ASN:ND2	2.23	0.54
1:L:73:MET:HB3	1:L:510:ILE:HD11	1.89	0.54
1:I:200:LEU:HD21	1:I:277:LYS:HE3	1.90	0.54
1:M:234:LEU:HD23	1:M:237:LEU:HD23	1.90	0.54
1:A:496:PRO:O	1:A:499:VAL:HG12	2.08	0.54
1:B:183:LEU:N	1:B:383:ALA:CB	2.70	0.54
1:B:183:LEU:HB2	1:B:383:ALA:HB3	1.89	0.54
1:G:496:PRO:O	1:G:499:VAL:HG13	2.08	0.54
1:I:215:LEU:HD22	1:I:246:PRO:HB2	1.90	0.54
1:J:269:GLY:O	1:J:271:VAL:N	2.41	0.54
1:F:386:GLU:C	1:F:388:GLU:N	2.60	0.54
1:H:242:LYS:O	1:H:244:GLY:N	2.35	0.54
1:I:361:ASP:O	1:I:365:LEU:HD12	2.08	0.54
1:L:119:GLY:O	1:L:440:ILE:HG13	2.08	0.54
1:M:317:LEU:N	1:M:317:LEU:HD12	2.23	0.54
1:E:81:THR:HG22	1:E:506:ASN:OD1	2.07	0.53
1:N:164:GLU:HA	1:N:167:LYS:HB2	1.90	0.53
1:F:62:LEU:HB2	1:F:68:ASN:HB2	1.89	0.53
1:I:202:PRO:O	1:I:203:TYR:HB2	2.08	0.53
1:K:438:HIS:O	1:K:442:ILE:HG22	2.08	0.53
1:B:414:GLY:O	1:B:417:VAL:HG13	2.08	0.53
1:H:207:ASN:N	1:H:207:ASN:HD22	2.05	0.53
1:M:475:ASN:O	1:M:488:MET:HG2	2.07	0.53
1:N:265:ASN:O	1:N:270:ILE:O	2.27	0.53
1:F:270:ILE:O	1:F:272:LYS:N	2.37	0.53
1:H:180:GLY:HA3	1:H:381:VAL:O	2.08	0.53
1:N:260:ALA:O	1:N:263:VAL:HG22	2.08	0.53
1:N:429:LEU:HD12	1:N:430:THR:H	1.72	0.53
1:C:383:ALA:HB2	1:C:389:MET:HG3	1.90	0.53
1:F:231:ARG:O	1:F:234:LEU:HD22	2.08	0.53
1:M:219:PHE:HD2	1:M:219:PHE:N	2.06	0.53
1:N:223:HIS:CD2	1:N:301:ILE:HB	2.44	0.53
1:F:219:PHE:CE2	1:F:245:LYS:CB	2.92	0.53
1:C:199:TYR:CZ	1:C:327:LYS:HA	2.44	0.53
1:F:506:ASN:O	1:F:509:SER:HB3	2.08	0.53
1:G:215:LEU:HD13	1:G:246:PRO:HB2	1.91	0.53
1:L:239:GLY:HA2	1:L:242:LYS:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:222:LEU:HD23	1:K:250:VAL:HG13	1.91	0.53
1:L:288:MET:HA	1:L:291:ASP:HB2	1.90	0.53
1:A:157:SER:O	1:A:161:ILE:HG13	2.09	0.52
1:E:362:ARG:HG2	1:E:366:GLN:HE21	1.73	0.52
1:L:165:ALA:O	1:L:169:VAL:HG22	2.09	0.52
1:N:225:LYS:O	1:N:226:LYS:CB	2.57	0.52
1:C:455:VAL:HG11	1:C:462:PRO:HA	1.91	0.52
1:N:228:SER:HA	1:N:258:ALA:HB3	1.91	0.52
1:B:183:LEU:HA	1:B:383:ALA:H	1.75	0.52
1:J:226:LYS:HA	1:J:253:GLU:O	2.10	0.52
1:M:239:GLY:CA	1:M:271:VAL:CG1	2.76	0.52
1:D:494:LEU:N	1:D:494:LEU:HD12	2.24	0.52
1:H:423:LEU:HD21	1:H:447:MET:HB2	1.91	0.52
1:K:323:VAL:HG12	1:K:332:ILE:HA	1.90	0.52
1:M:219:PHE:N	1:M:219:PHE:CD2	2.77	0.52
1:B:158:ILE:CD1	1:B:396:VAL:HG22	2.40	0.52
1:C:252:GLU:O	1:C:277:LYS:HG3	2.09	0.52
1:C:291:ASP:OD1	1:C:368:ARG:NH1	2.43	0.52
1:C:210:SER:O	1:C:212:SER:N	2.43	0.52
1:C:496:PRO:O	1:C:499:VAL:HG12	2.10	0.52
1:D:323:VAL:HG12	1:D:332:ILE:HA	1.91	0.52
1:I:230:VAL:HG11	1:I:261:THR:HG21	1.92	0.52
1:E:309:LEU:HD23	1:E:309:LEU:N	2.24	0.52
1:G:17:VAL:HG23	1:G:100:ILE:HG22	1.91	0.52
1:J:62:LEU:HD12	1:J:67:GLU:HB3	1.92	0.52
1:M:81:THR:HA	1:M:84:ASN:HB2	1.92	0.52
1:N:234:LEU:O	1:N:236:VAL:N	2.43	0.52
1:C:28:LYS:HB2	1:C:453:GLU:OE2	2.10	0.52
1:D:383:ALA:CB	1:D:389:MET:HG3	2.40	0.52
1:G:186:GLU:HB2	1:G:380:LYS:HB2	1.92	0.52
1:H:23:LEU:O	1:H:27:VAL:HG23	2.10	0.52
1:L:247:LEU:HB3	1:L:273:VAL:CG1	2.40	0.52
1:F:239:GLY:O	1:F:242:LYS:O	2.28	0.52
1:K:355:ASP:OD1	1:K:355:ASP:N	2.43	0.52
1:A:218:PRO:HD2	1:A:320:ALA:O	2.09	0.51
1:B:242:LYS:O	1:B:243:ALA:CB	2.58	0.51
1:F:219:PHE:CD2	1:F:245:LYS:CB	2.94	0.51
1:G:429:LEU:HD12	1:G:429:LEU:C	2.26	0.51
1:M:173:GLY:O	1:M:404:ARG:NH2	2.44	0.51
1:B:328:GLU:O	1:B:329:ASN:HB2	2.09	0.51
1:E:173:GLY:O	1:E:404:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:GLU:HB2	1:F:380:LYS:HB2	1.92	0.51
1:K:203:TYR:CB	1:K:263:VAL:HG13	2.40	0.51
1:M:144:ILE:HG22	1:M:163:ALA:HB2	1.91	0.51
1:M:246:PRO:O	1:M:273:VAL:CB	2.57	0.51
1:B:432:ALA:CB	1:B:436:GLN:OE1	2.59	0.51
1:F:259:LEU:O	1:F:263:VAL:HG23	2.11	0.51
1:J:183:LEU:HD23	1:J:384:SER:HB3	1.92	0.51
1:F:158:ILE:CD1	1:F:396:VAL:HG22	2.41	0.51
1:F:384:SER:OG	1:J:360:TYR:OH	2.23	0.51
1:B:23:LEU:HD23	1:B:74:VAL:HG13	1.92	0.51
1:E:281:PHE:CE2	1:K:182:GLY:HA2	2.45	0.51
1:H:73:MET:O	1:H:76:GLU:HB2	2.11	0.51
1:D:156:GLU:O	1:D:160:ASN:HB2	2.11	0.51
1:E:419:LEU:HD13	1:E:450:PRO:HG2	1.92	0.51
1:F:254:VAL:O	1:F:259:LEU:HD22	2.11	0.51
1:F:383:ALA:HB2	1:F:389:MET:HA	1.93	0.51
1:J:479:ASN:ND2	1:J:482:ASN:HD22	2.07	0.51
1:K:303:GLU:HA	1:K:309:LEU:HD13	1.92	0.51
1:C:217:ASP:N	1:C:218:PRO:CD	2.74	0.51
1:J:455:VAL:HG11	1:J:462:PRO:HA	1.93	0.51
1:A:223:HIS:CE1	1:A:225:LYS:HB2	2.45	0.51
1:E:448:GLU:HB3	1:E:466:LEU:HD11	1.93	0.51
1:L:449:ALA:HB3	1:L:450:PRO:HD3	1.91	0.51
1:A:223:HIS:HD2	1:A:301:ILE:O	1.94	0.51
1:D:220:ILE:HD13	1:D:296:THR:HG21	1.93	0.51
1:H:270:ILE:O	1:H:270:ILE:HG22	2.11	0.51
1:I:385:THR:O	1:I:388:GLU:N	2.39	0.51
1:J:158:ILE:HD11	1:J:396:VAL:HG13	1.93	0.51
1:N:391:GLU:O	1:N:394:ALA:HB3	2.11	0.51
1:N:417:VAL:HA	1:N:420:VAL:HG13	1.92	0.51
1:D:294:VAL:HG11	1:D:345:ARG:HG2	1.92	0.51
1:M:294:VAL:HG11	1:M:345:ARG:HG2	1.92	0.51
1:B:392:LYS:O	1:B:396:VAL:HG23	2.11	0.50
1:F:240:VAL:O	1:F:241:ALA:C	2.50	0.50
1:G:31:LEU:HD13	1:G:90:THR:HG22	1.91	0.50
1:I:385:THR:O	1:I:387:ILE:CG2	2.58	0.50
1:A:201:SER:OG	1:A:202:PRO:O	2.21	0.50
1:F:264:VAL:O	1:F:268:ARG:HD3	2.11	0.50
1:G:208:GLN:C	1:G:210:SER:H	2.14	0.50
1:H:225:LYS:HG3	1:H:226:LYS:HE2	1.93	0.50
1:J:328:GLU:O	1:J:329:ASN:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ASP:HB3	1:A:309:LEU:HG	1.93	0.50
1:D:80:LYS:O	1:D:84:ASN:HB2	2.12	0.50
1:M:234:LEU:N	1:M:235:PRO:HD2	2.26	0.50
1:B:6:ILE:HD11	1:C:22:VAL:HG13	1.93	0.50
1:E:69:MET:HE2	1:K:39:VAL:HG12	1.92	0.50
1:J:437:THR:HA	1:J:440:ILE:HD12	1.94	0.50
1:K:475:ASN:HD22	1:K:489:VAL:HB	1.77	0.50
1:N:259:LEU:O	1:N:262:LEU:N	2.42	0.50
1:N:479:ASN:O	1:N:481:ALA:N	2.44	0.50
1:C:449:ALA:HB3	1:C:450:PRO:HD3	1.93	0.50
1:F:234:LEU:N	1:F:235:PRO:CD	2.74	0.50
1:H:475:ASN:HD22	1:H:489:VAL:CG1	2.23	0.50
1:I:112:ASN:ND2	1:M:459:GLY:HA3	2.26	0.50
1:L:160:ASN:O	1:L:163:ALA:HB3	2.11	0.50
1:N:392:LYS:O	1:N:396:VAL:HG23	2.11	0.50
1:A:140:ASP:C	1:A:140:ASP:OD1	2.50	0.50
1:B:34:LYS:HB3	1:B:458:ALA:HA	1.94	0.50
1:D:16:MET:HG3	1:D:520:MET:HE1	1.92	0.50
1:F:158:ILE:CG1	1:F:396:VAL:HG22	2.42	0.50
1:F:236:VAL:HG23	1:F:312:ALA:O	2.11	0.50
1:K:230:VAL:HG21	1:K:261:THR:HG21	1.94	0.50
1:L:219:PHE:O	1:L:247:LEU:O	2.30	0.50
1:A:309:LEU:HD23	1:A:309:LEU:H	1.77	0.50
1:B:338:ASP:N	1:B:338:ASP:OD1	2.45	0.50
1:J:482:ASN:OD1	1:J:484:GLU:N	2.44	0.50
1:K:203:TYR:HD2	1:K:263:VAL:CG1	2.25	0.50
1:K:294:VAL:HG11	1:K:345:ARG:HG2	1.93	0.50
1:N:234:LEU:N	1:N:235:PRO:CD	2.75	0.50
1:F:449:ALA:HB3	1:F:450:PRO:CD	2.42	0.50
1:J:407:VAL:CG1	1:J:407:VAL:O	2.60	0.50
1:L:126:ALA:O	1:L:129:VAL:HG12	2.12	0.50
1:I:158:ILE:HD12	1:I:158:ILE:C	2.32	0.50
1:N:158:ILE:HD13	1:N:396:VAL:HG22	1.94	0.50
1:B:389:MET:SD	1:B:389:MET:O	2.70	0.49
1:C:37:ASN:ND2	1:C:51:LYS:HE2	2.26	0.49
1:F:59:GLU:O	1:J:4:LYS:HG3	2.12	0.49
1:G:28:LYS:HB2	1:G:453:GLU:CD	2.32	0.49
1:G:223:HIS:NE2	1:G:225:LYS:HD3	2.27	0.49
1:K:423:LEU:HD21	1:K:447:MET:HB2	1.94	0.49
1:M:175:ILE:HA	1:M:377:ALA:O	2.12	0.49
1:E:194:GLN:HA	1:E:331:THR:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:265:ASN:O	1:I:271:VAL:O	2.29	0.49
1:L:99:LEU:CD2	1:L:443:ALA:HA	2.42	0.49
1:L:449:ALA:O	1:L:450:PRO:C	2.51	0.49
1:N:413:PRO:HB2	1:N:417:VAL:CG2	2.42	0.49
1:B:328:GLU:O	1:B:329:ASN:CB	2.60	0.49
1:F:242:LYS:N	1:F:242:LYS:CD	2.74	0.49
1:F:257:GLU:O	1:F:261:THR:OG1	2.30	0.49
1:H:435:ASP:O	1:H:438:HIS:N	2.45	0.49
1:K:128:VAL:HG21	1:K:505:GLN:HE21	1.76	0.49
1:M:449:ALA:O	1:M:453:GLU:HB2	2.13	0.49
1:N:290:GLU:CB	1:N:345:ARG:HH12	2.25	0.49
1:I:385:THR:HG22	1:I:387:ILE:CG2	2.39	0.49
1:I:437:THR:O	1:I:440:ILE:N	2.46	0.49
1:N:335:GLY:O	1:N:337:GLY:N	2.38	0.49
1:E:437:THR:HA	1:E:440:ILE:HD12	1.94	0.49
1:F:223:HIS:CE1	1:F:225:LYS:HG3	2.47	0.49
1:G:449:ALA:HB3	1:G:450:PRO:HD3	1.93	0.49
1:M:213:ALA:HB3	1:M:325:VAL:HG13	1.94	0.49
1:B:164:GLU:O	1:B:167:LYS:HB3	2.12	0.49
1:B:177:VAL:HG11	1:B:396:VAL:HG12	1.95	0.49
1:C:361:ASP:O	1:C:365:LEU:HG	2.12	0.49
1:C:434:GLU:CD	1:L:441:GLN:HG3	2.33	0.49
1:C:475:ASN:O	1:C:487:ASP:HA	2.13	0.49
1:I:349:ILE:HA	1:I:352:GLN:HB2	1.95	0.49
1:K:205:ILE:HG21	1:K:211:GLN:C	2.31	0.49
1:N:70:GLY:HA2	1:N:73:MET:HE3	1.94	0.49
1:A:219:PHE:HB3	1:A:317:LEU:HD23	1.95	0.49
1:D:16:MET:HB3	1:D:514:MET:CE	2.43	0.49
1:F:240:VAL:C	1:F:242:LYS:O	2.46	0.49
1:L:437:THR:O	1:L:440:ILE:HB	2.13	0.49
1:E:360:TYR:CZ	1:E:364:LYS:HE2	2.48	0.49
1:A:299:THR:O	1:A:301:ILE:HD12	2.13	0.49
1:B:259:LEU:O	1:B:263:VAL:HG23	2.12	0.49
1:G:223:HIS:CE1	1:G:309:LEU:HD22	2.48	0.49
1:D:448:GLU:HG2	1:D:466:LEU:HD21	1.94	0.49
1:E:81:THR:CG2	1:E:506:ASN:OD1	2.61	0.49
1:I:77:VAL:HG21	1:I:510:ILE:HB	1.95	0.49
1:J:464:VAL:O	1:J:468:LYS:HB2	2.13	0.49
1:K:183:LEU:HD22	1:K:184:GLU:N	2.28	0.49
1:F:230:VAL:CG2	1:F:261:THR:OG1	2.60	0.48
1:H:173:GLY:O	1:H:404:ARG:NH2	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:346:VAL:HG12	1:H:350:LYS:HE2	1.95	0.48
1:H:383:ALA:HB1	1:N:281:PHE:CZ	2.48	0.48
1:I:215:LEU:HD11	1:I:274:VAL:HG12	1.95	0.48
1:I:221:LEU:HD23	1:I:249:ILE:HD12	1.95	0.48
1:K:294:VAL:HG23	1:K:341:ALA:HB1	1.95	0.48
1:M:223:HIS:ND1	1:M:227:ILE:HD11	2.28	0.48
1:H:21:ASN:O	1:H:25:ASN:ND2	2.46	0.48
1:K:78:ALA:O	1:K:89:THR:HG22	2.14	0.48
1:K:496:PRO:O	1:K:499:VAL:HG12	2.13	0.48
1:L:425:ALA:O	1:L:426:VAL:HB	2.13	0.48
1:A:22:VAL:HG22	1:L:6:ILE:HD11	1.93	0.48
1:B:242:LYS:O	1:B:243:ALA:HB3	2.12	0.48
1:B:391:GLU:OE2	1:B:395:ARG:NH2	2.46	0.48
1:D:81:THR:HA	1:D:84:ASN:HB3	1.95	0.48
1:E:247:LEU:HD21	1:E:249:ILE:HD11	1.95	0.48
1:G:235:PRO:HG3	1:G:310:GLU:HA	1.94	0.48
1:M:123:ALA:HB2	1:M:440:ILE:HG23	1.95	0.48
1:N:8:PHE:HD1	1:N:519:ALA:HB2	1.77	0.48
1:H:433:ASN:O	1:H:437:THR:HG23	2.13	0.48
1:L:309:LEU:O	1:L:311:LYS:N	2.40	0.48
1:M:233:LEU:O	1:M:237:LEU:CD2	2.59	0.48
1:M:482:ASN:OD1	1:M:483:GLY:N	2.46	0.48
1:E:122:GLN:NE2	1:E:430:THR:O	2.47	0.48
1:I:213:ALA:HB3	1:I:325:VAL:HG13	1.95	0.48
1:J:202:PRO:HB3	1:J:205:ILE:HD12	1.95	0.48
1:K:245:LYS:O	1:K:246:PRO:C	2.51	0.48
1:M:254:VAL:HG12	1:M:259:LEU:HB3	1.94	0.48
1:B:182:GLY:C	1:B:383:ALA:HB2	2.33	0.48
1:A:74:VAL:HA	1:A:510:ILE:HD12	1.94	0.48
1:H:311:LYS:O	1:H:312:ALA:HB2	2.14	0.48
1:I:13:ARG:HA	1:I:16:MET:HE3	1.95	0.48
1:I:73:MET:HB3	1:I:510:ILE:HD11	1.94	0.48
1:I:170:GLY:C	1:I:172:GLU:H	2.16	0.48
1:N:294:VAL:HG11	1:N:345:ARG:HD3	1.95	0.48
1:B:37:ASN:ND2	1:B:51:LYS:HE2	2.29	0.48
1:C:152:ALA:CB	1:C:158:ILE:HG12	2.44	0.48
1:F:41:GLU:HB2	1:J:522:ALA:HA	1.96	0.48
1:H:222:LEU:HD23	1:H:250:VAL:HG13	1.96	0.48
1:L:230:VAL:HG12	1:L:258:ALA:HA	1.95	0.48
1:N:266:THR:HG23	1:N:273:VAL:HG22	1.96	0.48
1:A:479:ASN:ND2	1:A:482:ASN:HB2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LEU:N	1:B:235:PRO:HD2	2.29	0.48
1:C:383:ALA:CB	1:C:389:MET:CB	2.90	0.48
1:D:431:GLY:H	1:D:437:THR:HG22	1.79	0.48
1:F:421:ARG:O	1:F:424:VAL:HG12	2.14	0.48
1:G:151:SER:HB3	1:G:399:ALA:HA	1.96	0.48
1:H:22:VAL:HG11	1:H:62:LEU:HD21	1.96	0.48
1:K:261:THR:O	1:K:261:THR:HG22	2.13	0.48
1:K:475:ASN:HD21	1:K:489:VAL:HG23	1.79	0.48
1:M:174:VAL:HG21	1:M:194:GLN:HB3	1.95	0.48
1:M:420:VAL:HA	1:M:423:LEU:HB2	1.96	0.48
1:N:215:LEU:HD11	1:N:274:VAL:CG1	2.40	0.48
1:C:125:LYS:HD2	1:C:125:LYS:HA	1.74	0.47
1:D:414:GLY:O	1:D:417:VAL:HG13	2.14	0.47
1:F:233:LEU:C	1:F:233:LEU:HD23	2.34	0.47
1:G:179:GLU:HG3	1:G:389:MET:SD	2.54	0.47
1:H:234:LEU:N	1:H:235:PRO:CD	2.76	0.47
1:N:263:VAL:O	1:N:264:VAL:C	2.51	0.47
1:B:10:GLU:O	1:B:14:THR:HB	2.14	0.47
1:E:177:VAL:HG21	1:E:397:GLU:HG3	1.96	0.47
1:E:449:ALA:HB3	1:E:450:PRO:HD3	1.95	0.47
1:H:342:ILE:O	1:H:345:ARG:HB3	2.14	0.47
1:L:164:GLU:HA	1:L:167:LYS:HB3	1.96	0.47
1:M:266:THR:HA	1:M:271:VAL:O	2.14	0.47
1:E:225:LYS:HD3	1:E:309:LEU:HD21	1.95	0.47
1:F:217:ASP:N	1:F:218:PRO:CD	2.77	0.47
1:F:383:ALA:CB	1:F:389:MET:HA	2.44	0.47
1:G:161:ILE:HD12	1:G:379:ILE:HG23	1.95	0.47
1:G:176:THR:HG23	1:G:324:GLN:NE2	2.29	0.47
1:H:326:SER:O	1:H:327:LYS:C	2.53	0.47
1:K:229:ASN:O	1:K:230:VAL:HG13	2.14	0.47
1:L:221:LEU:HD23	1:L:249:ILE:HG12	1.96	0.47
1:A:472:GLY:HA3	1:A:476:TYR:HD2	1.78	0.47
1:B:13:ARG:O	1:B:17:VAL:HG12	2.15	0.47
1:F:215:LEU:HD11	1:F:274:VAL:CG1	2.44	0.47
1:F:236:VAL:HG12	1:F:236:VAL:O	2.13	0.47
1:G:82:ASN:HB2	1:G:89:THR:CG2	2.44	0.47
1:I:363:GLU:N	1:I:363:GLU:OE2	2.48	0.47
1:K:215:LEU:HD22	1:K:246:PRO:CB	2.44	0.47
1:L:183:LEU:HD23	1:L:384:SER:HB2	1.96	0.47
1:M:15:ARG:O	1:M:67:GLU:HA	2.14	0.47
1:A:23:LEU:HD21	1:A:75:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:LEU:HD21	1:B:504:LEU:HD22	1.96	0.47
1:E:69:MET:CE	1:K:39:VAL:HG12	2.45	0.47
1:G:242:LYS:C	1:G:244:GLY:H	2.17	0.47
1:I:414:GLY:HA3	1:I:493:ILE:HG22	1.96	0.47
1:D:80:LYS:O	1:D:84:ASN:HB3	2.15	0.47
1:F:427:GLY:O	1:F:429:LEU:N	2.38	0.47
1:N:237:LEU:C	1:N:237:LEU:HD12	2.35	0.47
1:N:455:VAL:HG13	1:N:465:ILE:HD12	1.96	0.47
1:A:209:GLN:HE21	1:A:209:GLN:CA	2.23	0.47
1:A:329:ASN:HD22	1:A:329:ASN:HA	1.57	0.47
1:G:202:PRO:O	1:G:203:TYR:HB2	2.15	0.47
1:G:391:GLU:O	1:G:394:ALA:HB3	2.15	0.47
1:K:196:ASP:OD1	1:K:329:ASN:ND2	2.48	0.47
1:M:238:GLU:HB3	1:M:241:ALA:HB3	1.97	0.47
1:C:10:GLU:HG2	1:C:13:ARG:HH21	1.80	0.47
1:G:262:LEU:HD13	1:G:273:VAL:HG11	1.97	0.47
1:H:81:THR:HG21	1:H:503:ALA:HA	1.97	0.47
1:I:170:GLY:O	1:I:172:GLU:N	2.47	0.47
1:L:7:ARG:HG3	1:L:66:PHE:CZ	2.50	0.47
1:L:312:ALA:O	1:L:313:THR:C	2.52	0.47
1:M:238:GLU:HB3	1:M:241:ALA:CB	2.45	0.47
1:M:417:VAL:HA	1:M:420:VAL:HG13	1.96	0.47
1:E:281:PHE:CA	1:E:285:ARG:HB2	2.45	0.47
1:I:222:LEU:HD23	1:I:250:VAL:CG1	2.44	0.47
1:J:64:ASP:OD1	1:J:66:PHE:N	2.48	0.47
1:A:103:GLY:HA3	1:A:515:ILE:HD11	1.96	0.47
1:J:344:SER:OG	1:J:348:GLN:NE2	2.48	0.47
1:K:419:LEU:O	1:K:422:ALA:HB3	2.15	0.47
1:M:295:LEU:HB2	1:M:372:LEU:HD11	1.97	0.47
1:N:6:ILE:C	1:N:6:ILE:HD12	2.36	0.47
1:B:264:VAL:HG12	1:B:265:ASN:HD22	1.79	0.46
1:E:423:LEU:C	1:E:423:LEU:HD23	2.35	0.46
1:M:158:ILE:HD13	1:M:396:VAL:HG22	1.96	0.46
1:B:431:GLY:N	1:B:437:THR:HG22	2.30	0.46
1:B:452:ARG:NH2	1:N:461:GLU:OE2	2.47	0.46
1:E:437:THR:O	1:E:440:ILE:HB	2.15	0.46
1:G:221:LEU:CD1	1:G:301:ILE:HD12	2.45	0.46
1:I:152:ALA:CB	1:I:158:ILE:HG12	2.45	0.46
1:I:352:GLN:HB3	1:I:365:LEU:HD22	1.97	0.46
1:A:180:GLY:HA3	1:A:381:VAL:O	2.14	0.46
1:E:265:ASN:HD22	1:E:268:ARG:HD2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:426:VAL:HG13	1:E:426:VAL:O	2.14	0.46
1:J:174:VAL:HG12	1:J:376:VAL:HG13	1.97	0.46
1:K:88:GLY:HA2	4:K:702:HOH:O	2.14	0.46
1:M:437:THR:O	1:M:440:ILE:HB	2.15	0.46
1:N:31:LEU:HD13	1:N:90:THR:CG2	2.45	0.46
1:N:386:GLU:O	1:N:389:MET:N	2.42	0.46
1:N:467:ASN:O	1:N:471:GLU:HB2	2.15	0.46
1:C:28:LYS:HB2	1:C:453:GLU:CD	2.36	0.46
1:D:207:ASN:HD22	1:D:209:GLN:NE2	2.08	0.46
1:F:233:LEU:HG	1:F:233:LEU:O	2.16	0.46
1:H:353:ILE:O	1:H:353:ILE:CG2	2.61	0.46
1:H:489:VAL:HG23	1:H:494:LEU:CD2	2.45	0.46
1:I:308:ALA:HB3	1:I:311:LYS:HB3	1.96	0.46
1:J:313:THR:O	1:J:315:LYS:N	2.49	0.46
1:M:237:LEU:O	1:M:239:GLY:N	2.48	0.46
1:N:155:ASP:O	1:N:158:ILE:HG23	2.16	0.46
1:B:7:ARG:HD2	1:B:66:PHE:CE1	2.50	0.46
1:B:221:LEU:HD23	1:B:249:ILE:HD13	1.97	0.46
1:B:243:ALA:O	1:B:245:LYS:HG2	2.16	0.46
1:H:217:ASP:N	1:H:218:PRO:CD	2.78	0.46
1:K:160:ASN:O	1:K:163:ALA:HB3	2.15	0.46
1:M:342:ILE:O	1:M:346:VAL:HG23	2.16	0.46
1:G:191:GLU:O	1:G:334:ASP:HA	2.15	0.46
1:I:263:VAL:HA	1:I:266:THR:HG1	1.78	0.46
1:G:194:GLN:O	1:G:371:LYS:HE3	2.16	0.46
1:G:433:ASN:O	1:G:437:THR:HG23	2.16	0.46
1:I:259:LEU:O	1:I:263:VAL:HG23	2.16	0.46
1:K:185:ASN:OD1	1:K:382:GLY:N	2.42	0.46
1:L:69:MET:O	1:L:73:MET:HG3	2.16	0.46
1:L:220:ILE:N	1:L:318:GLY:O	2.49	0.46
1:L:452:ARG:HG3	1:L:466:LEU:HD13	1.97	0.46
1:M:215:LEU:HD11	1:M:274:VAL:CG1	2.41	0.46
1:N:386:GLU:HG3	1:N:387:ILE:N	2.31	0.46
1:C:21:ASN:HA	1:C:97:GLN:HE21	1.80	0.46
1:C:385:THR:O	1:C:386:GLU:C	2.54	0.46
1:D:41:GLU:HB2	1:H:522:ALA:HA	1.97	0.46
1:H:240:VAL:HG21	1:H:247:LEU:HD22	1.96	0.46
1:I:6:ILE:HD11	1:I:8:PHE:CZ	2.50	0.46
1:J:173:GLY:O	1:J:404:ARG:NH2	2.46	0.46
1:K:281:PHE:CE2	1:L:182:GLY:HA2	2.50	0.46
1:B:349:ILE:HA	1:B:352:GLN:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:ALA:O	1:C:384:SER:HB3	2.16	0.46
1:E:281:PHE:CZ	1:K:383:ALA:HB1	2.51	0.46
1:F:240:VAL:HG12	1:F:245:LYS:O	2.15	0.46
1:H:150:ILE:HD13	1:H:494:LEU:HD11	1.97	0.46
1:J:98:ALA:HA	1:J:101:ARG:CZ	2.45	0.46
1:L:351:THR:HA	1:L:354:GLU:HG2	1.97	0.46
1:M:77:VAL:HG21	1:M:510:ILE:HB	1.97	0.46
1:N:180:GLY:HA3	1:N:381:VAL:O	2.16	0.46
1:A:321:LYS:HB2	1:A:334:ASP:HB2	1.98	0.46
1:A:349:ILE:O	1:A:352:GLN:HB2	2.15	0.46
1:H:392:LYS:O	1:H:396:VAL:HG23	2.16	0.46
1:N:10:GLU:O	1:N:11:ASP:C	2.54	0.46
1:A:183:LEU:O	1:A:184:GLU:CB	2.64	0.45
1:F:345:ARG:HA	1:F:348:GLN:HE21	1.81	0.45
1:I:160:ASN:O	1:I:163:ALA:HB3	2.16	0.45
1:I:497:THR:O	1:I:497:THR:HG22	2.16	0.45
1:J:149:THR:HG23	1:J:156:GLU:HA	1.99	0.45
1:K:230:VAL:C	1:K:232:ASP:H	2.20	0.45
1:L:27:VAL:CG1	1:L:90:THR:HG23	2.46	0.45
1:L:28:LYS:HB3	1:L:94:VAL:HG12	1.97	0.45
1:L:510:ILE:HA	1:L:513:LEU:HD12	1.98	0.45
1:N:359:ASP:N	1:N:359:ASP:OD1	2.49	0.45
1:N:420:VAL:O	1:N:424:VAL:HG12	2.15	0.45
1:B:21:ASN:O	1:B:25:ASN:ND2	2.49	0.45
1:B:288:MET:CE	1:B:371:LYS:HE2	2.47	0.45
1:C:407:VAL:O	1:C:407:VAL:HG12	2.15	0.45
1:C:489:VAL:HG22	1:C:489:VAL:O	2.16	0.45
1:F:173:GLY:O	1:F:404:ARG:NH2	2.50	0.45
1:K:237:LEU:HA	1:K:240:VAL:CG2	2.46	0.45
1:B:432:ALA:HB3	1:B:436:GLN:OE1	2.16	0.45
1:E:195:PHE:N	1:E:330:THR:O	2.43	0.45
1:H:386:GLU:O	1:H:389:MET:N	2.49	0.45
1:H:431:GLY:H	1:H:437:THR:HG22	1.81	0.45
1:M:233:LEU:O	1:M:237:LEU:HD21	2.03	0.45
1:A:215:LEU:HD22	1:A:246:PRO:HB2	1.97	0.45
1:B:16:MET:HG3	1:B:520:MET:SD	2.56	0.45
1:B:112:ASN:HB3	1:B:115:ASP:HB2	1.98	0.45
1:C:176:THR:HG23	1:C:324:GLN:NE2	2.31	0.45
1:J:31:LEU:HD23	1:J:453:GLU:HB3	1.99	0.45
1:J:183:LEU:HD13	1:J:184:GLU:N	2.30	0.45
1:M:247:LEU:O	1:M:273:VAL:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:485:PHE:O	1:M:491:PHE:HZ	1.99	0.45
1:B:80:LYS:O	1:B:84:ASN:CB	2.65	0.45
1:B:232:ASP:HB2	1:B:309:LEU:HD12	1.98	0.45
1:E:416:GLY:O	1:E:420:VAL:HG13	2.15	0.45
1:F:240:VAL:C	1:F:242:LYS:N	2.69	0.45
1:G:90:THR:O	1:G:94:VAL:HG13	2.17	0.45
1:L:248:LEU:HA	1:L:274:VAL:O	2.17	0.45
1:E:126:ALA:HA	1:E:129:VAL:HG12	1.99	0.45
1:E:426:VAL:CG2	1:E:429:LEU:HB2	2.47	0.45
1:F:73:MET:HB3	1:F:510:ILE:HD11	1.98	0.45
1:K:205:ILE:HG23	1:K:212:SER:N	2.31	0.45
1:K:301:ILE:HG23	1:K:309:LEU:HD23	1.98	0.45
1:L:313:THR:C	1:L:315:LYS:N	2.70	0.45
1:C:230:VAL:CG1	1:C:258:ALA:HA	2.47	0.45
1:F:240:VAL:HG13	1:F:245:LYS:O	2.15	0.45
1:H:16:MET:SD	1:H:73:MET:HE1	2.57	0.45
1:H:230:VAL:O	1:H:232:ASP:N	2.50	0.45
1:H:384:SER:HA	1:N:360:TYR:OH	2.16	0.45
1:I:221:LEU:CD1	1:I:301:ILE:HD12	2.46	0.45
1:J:73:MET:O	1:J:76:GLU:HB2	2.16	0.45
1:K:74:VAL:HA	1:K:510:ILE:HD12	1.98	0.45
1:M:60:ILE:O	1:M:75:LYS:NZ	2.50	0.45
1:M:272:LYS:O	1:M:273:VAL:O	2.35	0.45
1:D:199:TYR:CE1	1:D:327:LYS:HA	2.52	0.45
1:D:255:GLU:O	1:D:257:GLU:N	2.49	0.45
1:E:242:LYS:O	1:E:243:ALA:CB	2.65	0.45
1:J:127:ALA:O	1:J:131:LEU:HB2	2.17	0.45
1:J:208:GLN:HE21	1:J:208:GLN:HB3	1.65	0.45
1:M:245:LYS:HA	1:M:246:PRO:HD3	1.54	0.45
1:N:264:VAL:O	1:N:268:ARG:HB2	2.17	0.45
1:C:158:ILE:CD1	1:C:162:ILE:HD11	2.47	0.45
1:C:414:GLY:HA3	1:C:493:ILE:HG22	1.98	0.45
1:E:217:ASP:N	1:E:218:PRO:HD3	2.32	0.45
1:F:496:PRO:HD2	1:F:499:VAL:HG11	1.99	0.45
1:C:6:ILE:HD11	1:C:8:PHE:CZ	2.52	0.45
1:C:46:ALA:HB1	1:C:47:PRO:HD2	1.98	0.45
1:C:182:GLY:O	1:C:183:LEU:O	2.34	0.45
1:F:245:LYS:HA	1:F:246:PRO:HD2	1.84	0.45
1:J:4:LYS:HD2	1:J:522:ALA:O	2.17	0.45
1:N:222:LEU:HD23	1:N:250:VAL:CG1	2.47	0.45
1:A:34:LYS:HB3	1:A:458:ALA:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:PRO:O	1:A:285:ARG:HG3	2.17	0.44
1:E:194:GLN:HA	1:E:330:THR:O	2.16	0.44
1:G:54:VAL:CG2	1:G:89:THR:HG21	2.47	0.44
1:G:301:ILE:HG23	1:G:307:LEU:HB3	1.99	0.44
1:H:355:ASP:O	1:H:357:SER:N	2.50	0.44
1:I:475:ASN:HD22	1:I:489:VAL:CG1	2.30	0.44
1:N:6:ILE:HB	1:N:521:VAL:HG22	1.99	0.44
1:N:225:LYS:O	1:N:226:LYS:HB3	2.17	0.44
1:A:242:LYS:O	1:A:243:ALA:CB	2.65	0.44
1:B:122:GLN:NE2	1:B:430:THR:O	2.48	0.44
1:B:196:ASP:OD1	1:B:196:ASP:N	2.50	0.44
1:C:249:ILE:O	1:C:275:ALA:HA	2.17	0.44
1:G:271:VAL:HG12	1:G:271:VAL:O	2.17	0.44
1:K:205:ILE:HG21	1:K:211:GLN:HA	2.00	0.44
1:M:238:GLU:H	1:M:238:GLU:HG3	1.54	0.44
1:C:162:ILE:O	1:C:163:ALA:C	2.56	0.44
1:D:33:PRO:HG2	1:D:481:ALA:HB2	2.00	0.44
1:D:112:ASN:HD21	1:E:459:GLY:HA3	1.82	0.44
1:D:383:ALA:HB3	1:H:281:PHE:CE2	2.52	0.44
1:F:472:GLY:HA3	1:F:476:TYR:CD2	2.52	0.44
1:G:292:MET:HA	1:G:295:LEU:HB2	1.99	0.44
1:H:267:ILE:HB	1:H:270:ILE:CD1	2.47	0.44
1:I:31:LEU:HD13	1:I:90:THR:HG22	1.98	0.44
1:I:215:LEU:HD11	1:I:274:VAL:CG1	2.47	0.44
1:I:429:LEU:HD12	1:I:429:LEU:HA	1.68	0.44
1:J:267:ILE:HG13	1:J:268:ARG:N	2.32	0.44
1:K:85:ALA:HB1	1:K:499:VAL:HB	1.99	0.44
1:K:423:LEU:HD21	1:K:444:LEU:O	2.18	0.44
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.98	0.44
1:C:207:ASN:O	1:C:209:GLN:N	2.51	0.44
1:H:24:ALA:HB3	1:H:97:GLN:NE2	2.32	0.44
1:I:263:VAL:O	1:I:264:VAL:HG23	2.16	0.44
1:I:421:ARG:O	1:I:424:VAL:HG12	2.17	0.44
1:A:229:ASN:OD1	1:N:270:ILE:HD12	2.16	0.44
1:A:475:ASN:HB3	1:A:487:ASP:OD1	2.18	0.44
1:B:34:LYS:CG	1:B:458:ALA:HA	2.48	0.44
1:B:472:GLY:HA3	1:B:476:TYR:CD2	2.53	0.44
1:C:213:ALA:HB3	1:C:325:VAL:CG1	2.47	0.44
1:G:271:VAL:O	1:G:271:VAL:CG1	2.66	0.44
1:G:487:ASP:O	1:G:491:PHE:CD1	2.70	0.44
1:H:202:PRO:O	1:H:203:TYR:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:182:GLY:O	1:I:183:LEU:CB	2.63	0.44
1:I:217:ASP:N	1:I:218:PRO:HD3	2.32	0.44
1:K:205:ILE:CG2	1:K:212:SER:N	2.80	0.44
1:N:426:VAL:O	1:N:428:ASN:N	2.51	0.44
1:A:187:LEU:O	1:A:187:LEU:HG	2.18	0.44
1:B:431:GLY:H	1:B:437:THR:HG22	1.83	0.44
1:I:257:GLU:HA	1:I:257:GLU:OE1	2.17	0.44
1:J:234:LEU:N	1:J:235:PRO:HD2	2.32	0.44
1:K:23:LEU:HD22	1:K:74:VAL:HG13	2.00	0.44
1:M:30:THR:HB	1:M:51:LYS:O	2.18	0.44
1:C:162:ILE:HG21	1:C:403:THR:HG21	1.99	0.44
1:C:209:GLN:H	1:C:209:GLN:CD	2.21	0.44
1:E:69:MET:SD	1:K:41:GLU:HG3	2.58	0.44
1:E:338:ASP:OD1	1:E:338:ASP:N	2.47	0.44
1:F:166:MET:O	1:F:170:GLY:N	2.51	0.44
1:L:34:LYS:CB	1:L:458:ALA:HA	2.48	0.44
1:L:230:VAL:HG13	1:L:257:GLU:HG3	1.99	0.44
1:M:6:ILE:HD11	1:M:8:PHE:CZ	2.53	0.44
1:M:182:GLY:O	1:M:183:LEU:CB	2.65	0.44
1:M:249:ILE:HB	1:M:275:ALA:HA	1.99	0.44
1:N:236:VAL:HG22	1:N:312:ALA:O	2.17	0.44
1:C:383:ALA:CB	1:C:389:MET:CG	2.95	0.44
1:E:392:LYS:O	1:E:396:VAL:HG23	2.17	0.44
1:G:89:THR:OG1	1:G:90:THR:N	2.51	0.44
1:H:419:LEU:HD13	1:H:450:PRO:HG2	2.00	0.44
1:J:80:LYS:HD2	1:J:506:ASN:ND2	2.32	0.44
1:J:201:SER:O	1:J:202:PRO:O	2.35	0.44
1:N:231:ARG:CA	1:N:234:LEU:HD12	2.41	0.44
1:C:112:ASN:OD1	1:C:114:MET:N	2.50	0.44
1:C:219:PHE:HB3	1:C:317:LEU:HB3	2.00	0.44
1:D:109:ALA:HB2	1:G:109:ALA:HB2	1.98	0.44
1:E:76:GLU:HG3	1:K:46:ALA:CB	2.47	0.44
1:F:386:GLU:C	1:F:388:GLU:H	2.20	0.44
1:K:182:GLY:O	1:K:183:LEU:CB	2.65	0.44
1:L:202:PRO:HA	1:L:205:ILE:HG13	2.00	0.44
1:M:225:LYS:HE2	1:M:309:LEU:HD11	2.00	0.44
1:N:65:LYS:O	1:N:69:MET:HG3	2.18	0.44
1:N:223:HIS:ND1	1:N:225:LYS:HG3	2.32	0.44
1:N:237:LEU:O	1:N:240:VAL:HG12	2.18	0.44
1:F:431:GLY:H	1:F:437:THR:CG2	2.31	0.43
1:J:406:ALA:O	1:J:410:GLY:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:449:ALA:N	1:J:450:PRO:CD	2.81	0.43
1:K:203:TYR:CD2	1:K:263:VAL:HG13	2.53	0.43
1:L:20:VAL:HG11	1:L:514:MET:HE1	2.00	0.43
1:N:31:LEU:HD13	1:N:90:THR:HG22	2.00	0.43
1:N:117:LYS:HG3	1:N:512:GLY:HA2	2.00	0.43
1:A:40:LEU:HB2	1:A:48:THR:HB	1.99	0.43
1:A:412:VAL:HB	1:A:413:PRO:HD2	1.99	0.43
1:C:158:ILE:HD11	1:C:162:ILE:HD11	1.99	0.43
1:E:142:LYS:HG2	1:E:146:GLN:HE22	1.82	0.43
1:E:235:PRO:HG2	1:E:310:GLU:O	2.18	0.43
1:H:201:SER:C	1:H:202:PRO:O	2.54	0.43
1:H:433:ASN:O	1:H:434:GLU:C	2.57	0.43
1:I:57:ALA:O	1:I:58:LYS:C	2.56	0.43
1:I:175:ILE:HA	1:I:377:ALA:O	2.18	0.43
1:K:99:LEU:CD2	1:K:443:ALA:HA	2.48	0.43
1:L:77:VAL:O	1:L:80:LYS:N	2.50	0.43
1:M:215:LEU:CB	1:M:246:PRO:CG	2.91	0.43
1:A:34:LYS:HD3	1:L:114:MET:HG3	2.00	0.43
1:A:475:ASN:CB	1:A:487:ASP:OD1	2.66	0.43
1:C:475:ASN:OD1	1:C:489:VAL:CG1	2.67	0.43
1:D:80:LYS:CE	1:D:506:ASN:HD21	2.31	0.43
1:F:320:ALA:HB1	1:F:333:ILE:O	2.18	0.43
1:J:128:VAL:HG21	1:J:505:GLN:HE21	1.82	0.43
1:J:465:ILE:O	1:J:469:VAL:HG23	2.17	0.43
1:K:392:LYS:O	1:K:396:VAL:HG23	2.19	0.43
1:L:229:ASN:O	1:L:229:ASN:ND2	2.48	0.43
1:M:219:PHE:CE1	1:M:314:ILE:HB	2.53	0.43
1:M:317:LEU:N	1:M:317:LEU:CD1	2.81	0.43
1:N:237:LEU:HG	1:N:238:GLU:N	2.33	0.43
1:N:323:VAL:HG12	1:N:332:ILE:HA	2.00	0.43
1:N:351:THR:HA	1:N:354:GLU:HB2	1.99	0.43
1:A:81:THR:O	1:A:85:ALA:HB3	2.18	0.43
1:A:177:VAL:HG21	1:A:397:GLU:CG	2.49	0.43
1:B:202:PRO:O	1:B:203:TYR:CB	2.65	0.43
1:C:176:THR:HG23	1:C:324:GLN:HE22	1.83	0.43
1:D:437:THR:HA	1:D:440:ILE:HD12	1.99	0.43
1:F:150:ILE:HG21	1:F:494:LEU:HD11	1.99	0.43
1:F:392:LYS:O	1:F:396:VAL:HG23	2.18	0.43
1:F:510:ILE:HA	1:F:513:LEU:HD12	2.00	0.43
1:G:222:LEU:HD23	1:G:250:VAL:CG1	2.49	0.43
1:I:313:THR:OG1	1:I:314:ILE:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:451:LEU:C	1:J:451:LEU:HD23	2.38	0.43
1:K:180:GLY:HA3	1:K:381:VAL:O	2.18	0.43
1:M:221:LEU:HD23	1:M:249:ILE:CD1	2.48	0.43
1:N:227:ILE:HD12	1:N:228:SER:H	1.84	0.43
1:B:7:ARG:HD2	1:B:66:PHE:CZ	2.54	0.43
1:D:17:VAL:HG23	1:D:100:ILE:HG22	2.00	0.43
1:D:223:HIS:CE1	1:D:309:LEU:HD22	2.53	0.43
1:G:16:MET:SD	1:G:73:MET:HE1	2.58	0.43
1:G:419:LEU:O	1:G:423:LEU:HB2	2.18	0.43
1:H:73:MET:HB2	1:H:73:MET:HE3	1.86	0.43
1:M:356:THR:HG21	1:M:365:LEU:CD1	2.48	0.43
1:N:345:ARG:HA	1:N:348:GLN:NE2	2.34	0.43
1:C:60:ILE:O	1:C:75:LYS:NZ	2.45	0.43
1:C:233:LEU:O	1:C:236:VAL:N	2.49	0.43
1:C:385:THR:O	1:C:385:THR:OG1	2.29	0.43
1:E:68:ASN:O	1:E:72:GLN:HG2	2.18	0.43
1:E:106:ALA:O	1:E:111:MET:HB2	2.18	0.43
1:H:71:ALA:O	1:H:75:LYS:HB2	2.18	0.43
1:H:479:ASN:ND2	1:H:482:ASN:HD22	2.17	0.43
1:I:218:PRO:HG3	1:I:323:VAL:HG13	2.00	0.43
1:J:183:LEU:CD2	1:J:384:SER:HB3	2.49	0.43
1:K:439:GLY:HA2	1:K:442:ILE:HG23	1.99	0.43
1:L:21:ASN:O	1:L:22:VAL:C	2.57	0.43
1:B:151:SER:HB3	1:B:399:ALA:HA	2.00	0.43
1:F:222:LEU:HD23	1:F:250:VAL:HG13	2.00	0.43
1:F:420:VAL:O	1:F:423:LEU:HB2	2.18	0.43
1:G:383:ALA:HB2	1:G:389:MET:HB2	2.00	0.43
1:H:101:ARG:NH1	1:H:102:GLU:OE2	2.51	0.43
1:J:64:ASP:OD1	1:J:64:ASP:C	2.57	0.43
1:J:486:GLY:O	1:J:487:ASP:C	2.57	0.43
1:M:199:TYR:CZ	1:M:327:LYS:HA	2.54	0.43
1:A:112:ASN:ND2	1:N:458:ALA:O	2.41	0.43
1:D:423:LEU:C	1:D:425:ALA:N	2.72	0.43
1:H:426:VAL:O	1:H:426:VAL:CG2	2.66	0.43
1:I:240:VAL:CG1	1:I:245:LYS:O	2.67	0.43
1:J:158:ILE:HD13	1:J:396:VAL:HG22	2.01	0.43
1:N:417:VAL:HG21	1:N:488:MET:HG3	2.00	0.43
1:C:210:SER:O	1:C:211:GLN:C	2.56	0.43
1:L:206:ASN:C	1:L:206:ASN:OD1	2.57	0.43
1:L:263:VAL:O	1:L:267:ILE:HD13	2.19	0.43
1:B:155:ASP:CG	1:B:158:ILE:HG22	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:LYS:HD2	1:C:453:GLU:OE1	2.19	0.43
1:F:448:GLU:HG2	1:F:466:LEU:HD11	2.01	0.43
1:I:288:MET:O	1:I:291:ASP:HB2	2.19	0.43
1:I:473:THR:CG2	4:I:702:HOH:O	2.66	0.43
1:K:23:LEU:HD12	1:K:60:ILE:HG13	2.01	0.43
1:A:233:LEU:HB3	1:A:237:LEU:HD12	2.01	0.42
1:D:82:ASN:OD1	1:D:86:GLY:O	2.38	0.42
1:F:68:ASN:O	1:F:71:ALA:HB3	2.19	0.42
1:F:240:VAL:O	1:F:242:LYS:C	2.51	0.42
1:F:419:LEU:HD13	1:F:450:PRO:HG2	2.01	0.42
1:G:240:VAL:HG13	1:G:245:LYS:O	2.19	0.42
1:G:487:ASP:O	1:G:491:PHE:HD1	2.02	0.42
1:I:120:ILE:O	1:I:124:VAL:HG23	2.19	0.42
1:J:434:GLU:OE2	1:K:438:HIS:HA	2.18	0.42
1:L:162:ILE:HG12	1:L:400:LEU:HD13	2.01	0.42
1:L:311:LYS:HG3	1:L:316:ASP:OD2	2.19	0.42
1:M:356:THR:HG21	1:M:365:LEU:HD12	2.01	0.42
1:N:175:ILE:HA	1:N:377:ALA:O	2.18	0.42
1:A:242:LYS:O	1:A:243:ALA:HB2	2.20	0.42
1:C:162:ILE:O	1:C:165:ALA:N	2.52	0.42
1:D:423:LEU:C	1:D:425:ALA:H	2.23	0.42
1:H:342:ILE:O	1:H:345:ARG:N	2.52	0.42
1:I:385:THR:CG2	1:I:387:ILE:CG2	2.97	0.42
1:M:130:GLU:HG2	1:M:425:ALA:HB3	2.01	0.42
1:M:314:ILE:HA	1:M:317:LEU:HD13	1.99	0.42
1:N:30:THR:HB	1:N:51:LYS:O	2.19	0.42
1:N:226:LYS:C	1:N:226:LYS:CD	2.86	0.42
1:N:482:ASN:OD1	1:N:483:GLY:N	2.52	0.42
1:A:23:LEU:HD23	1:A:74:VAL:CG2	2.49	0.42
1:A:229:ASN:OD1	1:N:270:ILE:CD1	2.68	0.42
1:B:148:GLY:HA2	1:B:403:THR:OG1	2.19	0.42
1:C:69:MET:HE1	1:J:39:VAL:HG12	2.00	0.42
1:D:229:ASN:ND2	1:D:231:ARG:HB2	2.35	0.42
1:D:351:THR:HA	1:D:354:GLU:HG2	2.00	0.42
1:H:311:LYS:O	1:H:312:ALA:CB	2.67	0.42
1:H:437:THR:O	1:H:440:ILE:HB	2.20	0.42
1:I:365:LEU:O	1:I:368:ARG:N	2.52	0.42
1:K:70:GLY:HA2	1:K:73:MET:HE2	2.02	0.42
1:K:426:VAL:HG23	1:K:429:LEU:HD13	2.01	0.42
1:K:475:ASN:ND2	1:K:489:VAL:HG23	2.34	0.42
1:L:229:ASN:O	1:L:230:VAL:CG2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:309:LEU:HG	1:L:310:GLU:OE1	2.19	0.42
1:M:182:GLY:O	1:M:183:LEU:HB2	2.19	0.42
1:M:218:PRO:CD	1:M:320:ALA:O	2.66	0.42
1:M:246:PRO:CA	1:M:273:VAL:N	2.75	0.42
1:B:417:VAL:HA	1:B:420:VAL:HG13	2.01	0.42
1:C:475:ASN:OD1	1:C:489:VAL:HG11	2.19	0.42
1:E:131:LEU:HD21	1:E:500:THR:HG22	2.01	0.42
1:F:386:GLU:O	1:F:387:ILE:C	2.55	0.42
1:G:202:PRO:O	1:G:203:TYR:CB	2.68	0.42
1:G:423:LEU:HD21	1:G:444:LEU:HB3	2.00	0.42
1:H:489:VAL:HG23	1:H:494:LEU:HD23	2.02	0.42
1:J:7:ARG:HD2	1:J:66:PHE:CE2	2.55	0.42
1:J:464:VAL:HG22	1:L:464:VAL:HA	2.01	0.42
1:K:199:TYR:HA	1:K:276:VAL:HG12	2.01	0.42
1:N:449:ALA:HA	1:N:452:ARG:HB2	2.01	0.42
1:N:449:ALA:HB3	1:N:450:PRO:HD3	2.01	0.42
1:F:406:ALA:O	1:F:410:GLY:N	2.52	0.42
1:F:467:ASN:C	1:F:467:ASN:HD22	2.22	0.42
1:L:455:VAL:HG13	1:L:460:GLU:HB2	2.02	0.42
1:N:290:GLU:CG	1:N:345:ARG:NH1	2.73	0.42
1:A:414:GLY:HA3	1:A:493:ILE:HG22	2.01	0.42
1:C:383:ALA:CB	1:C:389:MET:HG3	2.49	0.42
1:D:56:VAL:O	1:D:60:ILE:HG12	2.19	0.42
1:E:27:VAL:HG12	1:E:90:THR:HG23	2.02	0.42
1:E:277:LYS:NZ	1:K:386:GLU:OE2	2.52	0.42
1:F:6:ILE:CD1	1:G:22:VAL:HG13	2.50	0.42
1:F:242:LYS:HA	1:F:242:LYS:HD2	1.89	0.42
1:G:448:GLU:HB3	1:G:466:LEU:HD11	2.02	0.42
1:G:456:ALA:O	1:G:459:GLY:N	2.52	0.42
1:H:423:LEU:CD2	1:H:444:LEU:HA	2.50	0.42
1:J:215:LEU:HD11	1:J:274:VAL:HG12	2.00	0.42
1:J:218:PRO:HD2	1:J:320:ALA:O	2.19	0.42
1:K:227:ILE:HD12	1:K:227:ILE:N	2.34	0.42
1:K:245:LYS:HA	1:K:246:PRO:HD2	1.67	0.42
1:L:323:VAL:HG12	1:L:332:ILE:HA	2.00	0.42
1:A:145:ALA:O	1:A:149:THR:OG1	2.23	0.42
1:B:232:ASP:CB	1:B:309:LEU:HD12	2.49	0.42
1:C:426:VAL:HG22	1:C:426:VAL:O	2.20	0.42
1:C:489:VAL:HG23	1:C:494:LEU:CD2	2.49	0.42
1:H:437:THR:O	1:H:441:GLN:HG2	2.20	0.42
1:H:498:LYS:O	1:H:502:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:82:ASN:HB2	1:I:89:THR:HG23	2.02	0.42
1:I:200:LEU:CD1	1:I:254:VAL:HB	2.50	0.42
1:K:164:GLU:O	1:K:167:LYS:HB3	2.19	0.42
1:M:123:ALA:HB2	1:M:440:ILE:HG12	2.02	0.42
1:N:455:VAL:HG11	1:N:462:PRO:HA	2.02	0.42
1:B:27:VAL:HG12	1:B:90:THR:HG23	2.02	0.42
1:G:217:ASP:N	1:G:218:PRO:CD	2.83	0.42
1:H:477:GLY:HA3	1:H:488:MET:SD	2.60	0.42
1:L:120:ILE:HG12	1:L:443:ALA:HB2	2.01	0.42
1:L:183:LEU:HD13	1:L:184:GLU:N	2.35	0.42
1:L:240:VAL:O	1:L:244:GLY:HA2	2.19	0.42
1:M:236:VAL:HG21	1:M:312:ALA:O	2.18	0.42
1:C:310:GLU:N	1:C:310:GLU:OE2	2.52	0.42
1:D:84:ASN:C	1:D:84:ASN:ND2	2.71	0.42
1:E:293:ALA:O	1:E:297:GLY:N	2.53	0.42
1:F:183:LEU:O	1:F:184:GLU:HB3	2.20	0.42
1:F:307:LEU:H	1:F:307:LEU:HD23	1.84	0.42
1:H:82:ASN:HB2	1:H:89:THR:HG23	2.02	0.42
1:H:229:ASN:O	1:H:231:ARG:N	2.43	0.42
1:I:7:ARG:HD2	1:I:66:PHE:CD2	2.55	0.42
1:I:131:LEU:HD21	1:I:500:THR:HG22	2.01	0.42
1:J:7:ARG:CZ	1:J:15:ARG:NH2	2.83	0.42
1:J:119:GLY:HA3	1:J:436:GLN:O	2.20	0.42
1:J:202:PRO:O	1:J:204:PHE:N	2.52	0.42
1:K:69:MET:O	1:K:73:MET:HG3	2.19	0.42
1:A:472:GLY:HA3	1:A:476:TYR:CD2	2.55	0.42
1:C:262:LEU:O	1:C:266:THR:HG23	2.20	0.42
1:G:206:ASN:OD1	1:G:207:ASN:N	2.53	0.42
1:G:258:ALA:O	1:G:262:LEU:HG	2.20	0.42
1:H:6:ILE:HD11	1:H:8:PHE:CZ	2.55	0.42
1:H:208:GLN:HA	1:H:211:GLN:HA	2.02	0.42
1:H:232:ASP:N	1:H:232:ASP:OD1	2.52	0.42
1:M:217:ASP:N	1:M:217:ASP:OD1	2.53	0.42
1:N:124:VAL:O	1:N:128:VAL:HG23	2.20	0.42
1:N:364:LYS:O	1:N:368:ARG:HG3	2.19	0.42
1:G:433:ASN:OD1	1:G:435:ASP:HB2	2.19	0.41
1:H:435:ASP:O	1:H:436:GLN:C	2.58	0.41
1:J:27:VAL:HG13	1:J:90:THR:HG23	2.02	0.41
1:A:324:GLN:HG3	1:A:331:THR:CG2	2.50	0.41
1:C:391:GLU:O	1:C:394:ALA:N	2.52	0.41
1:D:225:LYS:NZ	1:D:309:LEU:HD21	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:VAL:HG12	1:E:314:ILE:HG22	2.01	0.41
1:F:229:ASN:O	1:F:258:ALA:HB2	2.20	0.41
1:F:434:GLU:HA	1:F:437:THR:OG1	2.21	0.41
1:I:27:VAL:HG12	1:I:90:THR:HG23	2.01	0.41
1:I:183:LEU:HD13	1:I:184:GLU:N	2.35	0.41
1:I:372:LEU:HD12	1:I:372:LEU:HA	1.85	0.41
1:N:64:ASP:OD1	1:N:64:ASP:C	2.57	0.41
1:A:138:THR:HG21	1:A:147:VAL:HG21	2.01	0.41
1:A:426:VAL:HG22	1:A:426:VAL:O	2.20	0.41
1:H:81:THR:HB	1:H:502:SER:HB3	2.02	0.41
1:H:437:THR:HA	1:H:440:ILE:HD12	2.02	0.41
1:K:466:LEU:HD21	1:K:470:LYS:HE2	2.02	0.41
1:K:506:ASN:HD22	1:K:506:ASN:HA	1.66	0.41
1:M:216:ASP:HB3	1:M:322:LYS:HG3	2.01	0.41
1:A:215:LEU:HD12	1:A:323:VAL:CG2	2.50	0.41
1:A:486:GLY:HA3	1:A:491:PHE:CZ	2.55	0.41
1:D:419:LEU:HD13	1:D:450:PRO:HG2	2.02	0.41
1:E:234:LEU:N	1:E:235:PRO:CD	2.84	0.41
1:E:412:VAL:HB	1:E:413:PRO:HD2	2.03	0.41
1:F:46:ALA:CB	1:J:76:GLU:HG3	2.50	0.41
1:G:240:VAL:O	1:G:242:LYS:O	2.37	0.41
1:H:123:ALA:HB2	1:H:440:ILE:HA	2.02	0.41
1:I:115:ASP:OD1	1:I:436:GLN:NE2	2.54	0.41
1:I:281:PHE:HZ	1:M:182:GLY:HA2	1.82	0.41
1:K:349:ILE:HA	1:K:352:GLN:HB2	2.03	0.41
1:K:423:LEU:HD22	1:K:444:LEU:HB3	2.02	0.41
1:M:204:PHE:CG	1:M:274:VAL:HG23	2.55	0.41
1:M:352:GLN:O	1:M:356:THR:HG23	2.19	0.41
1:N:342:ILE:C	1:N:346:VAL:HG22	2.41	0.41
1:C:12:ALA:HB1	1:C:520:MET:HG3	2.03	0.41
1:C:522:ALA:O	1:C:523:ASP:C	2.58	0.41
1:H:77:VAL:HG11	1:H:510:ILE:HB	2.01	0.41
1:K:349:ILE:HG23	1:K:365:LEU:HD22	2.01	0.41
1:L:164:GLU:HB3	1:L:187:LEU:CD2	2.50	0.41
1:M:152:ALA:C	1:M:154:SER:H	2.24	0.41
1:M:237:LEU:N	1:M:237:LEU:HD22	2.35	0.41
1:A:6:ILE:HG22	1:A:521:VAL:HG22	2.02	0.41
1:B:211:GLN:HE22	1:B:327:LYS:HB2	1.84	0.41
1:C:431:GLY:H	1:C:437:THR:HG22	1.85	0.41
1:D:448:GLU:CG	1:D:466:LEU:HD21	2.51	0.41
1:E:249:ILE:O	1:E:275:ALA:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:383:ALA:HB2	1:E:389:MET:HG3	2.02	0.41
1:F:221:LEU:HD12	1:F:222:LEU:N	2.35	0.41
1:L:482:ASN:HD22	1:L:484:GLU:HB2	1.85	0.41
1:M:320:ALA:HB1	1:M:333:ILE:O	2.20	0.41
1:M:349:ILE:HA	1:M:352:GLN:HG2	2.02	0.41
1:M:366:GLN:HA	1:M:369:VAL:HG22	2.02	0.41
1:N:95:LEU:HD13	1:N:504:LEU:HA	2.01	0.41
1:A:76:GLU:HG3	1:N:46:ALA:CB	2.51	0.41
1:B:386:GLU:O	1:B:390:LYS:HG2	2.21	0.41
1:C:54:VAL:HG22	1:C:89:THR:OG1	2.21	0.41
1:C:113:PRO:HB2	1:C:516:THR:HG22	2.03	0.41
1:C:167:LYS:HA	1:C:167:LYS:HD2	1.86	0.41
1:C:246:PRO:HB3	1:C:272:LYS:O	2.21	0.41
1:D:16:MET:SD	1:D:73:MET:HE1	2.60	0.41
1:D:112:ASN:ND2	1:E:459:GLY:HA3	2.35	0.41
1:F:213:ALA:HB3	1:F:325:VAL:HG13	2.02	0.41
1:F:295:LEU:HD22	1:F:295:LEU:O	2.21	0.41
1:F:360:TYR:HA	1:F:363:GLU:HG2	2.03	0.41
1:H:257:GLU:O	1:H:260:ALA:HB3	2.20	0.41
1:K:207:ASN:N	1:K:207:ASN:HD22	2.17	0.41
1:A:218:PRO:HG3	1:A:323:VAL:HG13	2.02	0.41
1:B:151:SER:CB	1:B:399:ALA:HA	2.50	0.41
1:B:521:VAL:HB	1:C:40:LEU:HD23	2.03	0.41
1:D:30:THR:HB	1:D:51:LYS:O	2.21	0.41
1:F:34:LYS:HG3	1:F:458:ALA:CB	2.51	0.41
1:F:69:MET:HE1	1:G:41:GLU:N	2.35	0.41
1:F:126:ALA:O	1:F:129:VAL:HG12	2.21	0.41
1:F:158:ILE:HD11	1:F:396:VAL:HG22	2.02	0.41
1:H:291:ASP:O	1:H:295:LEU:HB2	2.21	0.41
1:H:422:ALA:O	1:H:423:LEU:C	2.58	0.41
1:H:475:ASN:HD22	1:H:489:VAL:HG12	1.86	0.41
1:J:478:TYR:CE2	1:J:480:ALA:HA	2.56	0.41
1:L:487:ASP:OD1	1:L:489:VAL:HG12	2.21	0.41
1:M:359:ASP:OD1	1:M:359:ASP:N	2.54	0.41
1:M:478:TYR:N	1:M:488:MET:SD	2.91	0.41
1:A:23:LEU:CD2	1:A:75:LYS:HG3	2.51	0.41
1:A:224:ASP:OD2	1:A:302:SER:HB2	2.21	0.41
1:B:16:MET:SD	1:B:73:MET:HE1	2.61	0.41
1:B:175:ILE:HG12	1:B:377:ALA:HB3	2.03	0.41
1:B:223:HIS:CE1	1:B:309:LEU:HD13	2.56	0.41
1:B:256:GLY:HA2	1:B:259:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:ASN:HD22	1:B:506:ASN:HA	1.58	0.41
1:C:82:ASN:HB2	1:C:89:THR:CG2	2.51	0.41
1:D:317:LEU:N	1:D:317:LEU:CD1	2.84	0.41
1:D:383:ALA:CB	1:H:281:PHE:CE2	3.04	0.41
1:E:247:LEU:O	1:E:273:VAL:HA	2.20	0.41
1:F:64:ASP:OD1	1:F:65:LYS:N	2.54	0.41
1:F:421:ARG:NH2	1:F:469:VAL:O	2.50	0.41
1:H:293:ALA:HB2	1:H:300:VAL:HG23	2.02	0.41
1:I:7:ARG:HD2	1:I:66:PHE:CE2	2.56	0.41
1:I:61:GLU:HG2	1:I:68:ASN:OD1	2.21	0.41
1:I:263:VAL:HG12	1:I:267:ILE:HD12	2.03	0.41
1:J:176:THR:HG22	1:J:177:VAL:N	2.36	0.41
1:J:228:SER:C	1:J:258:ALA:HB2	2.41	0.41
1:J:267:ILE:HG13	1:J:268:ARG:H	1.85	0.41
1:J:287:ALA:HB1	1:J:368:ARG:CZ	2.50	0.41
1:K:399:ALA:O	1:K:403:THR:OG1	2.28	0.41
1:L:232:ASP:HB3	1:L:309:LEU:HD11	2.03	0.41
1:M:199:TYR:CE2	1:M:327:LYS:HA	2.56	0.41
1:A:438:HIS:HD2	1:B:434:GLU:OE1	2.04	0.41
1:B:263:VAL:O	1:B:267:ILE:HG12	2.21	0.41
1:C:242:LYS:O	1:C:243:ALA:CB	2.69	0.41
1:D:95:LEU:HD23	1:D:446:ALA:O	2.21	0.41
1:F:219:PHE:O	1:F:247:LEU:HA	2.21	0.41
1:F:222:LEU:HD23	1:F:250:VAL:CG1	2.50	0.41
1:G:207:ASN:HD22	1:G:210:SER:HB3	1.86	0.41
1:M:174:VAL:CG2	1:M:194:GLN:HB3	2.51	0.41
1:N:265:ASN:HD22	1:N:271:VAL:HG11	1.86	0.41
1:A:8:PHE:O	1:A:11:ASP:HB3	2.21	0.40
1:A:42:LYS:O	1:A:43:SER:C	2.59	0.40
1:B:190:VAL:HG21	1:B:334:ASP:HB2	2.03	0.40
1:B:391:GLU:O	1:B:394:ALA:HB3	2.20	0.40
1:C:237:LEU:HD22	1:C:271:VAL:HG11	2.04	0.40
1:C:451:LEU:CD2	1:C:455:VAL:HG23	2.52	0.40
1:F:259:LEU:CA	1:F:262:LEU:HD21	2.50	0.40
1:G:54:VAL:HG23	1:G:89:THR:HG21	2.03	0.40
1:H:488:MET:O	1:H:491:PHE:HB2	2.21	0.40
1:I:183:LEU:HD23	1:I:383:ALA:O	2.20	0.40
1:I:295:LEU:HD23	1:I:372:LEU:HD12	2.02	0.40
1:I:478:TYR:CE2	1:I:480:ALA:HA	2.57	0.40
1:I:479:ASN:ND2	1:I:482:ASN:HD21	2.19	0.40
1:J:294:VAL:HG23	1:J:341:ALA:HB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:218:PRO:HD2	1:K:320:ALA:O	2.22	0.40
1:N:24:ALA:O	1:N:28:LYS:HB3	2.21	0.40
1:N:183:LEU:HA	1:N:383:ALA:H	1.85	0.40
1:N:265:ASN:OD1	1:N:265:ASN:N	2.53	0.40
1:B:223:HIS:CD2	1:B:225:LYS:CD	3.03	0.40
1:D:421:ARG:HD3	1:D:421:ARG:HA	1.92	0.40
1:E:193:MET:HE3	1:E:193:MET:HB3	1.84	0.40
1:H:185:ASN:OD1	1:H:185:ASN:N	2.54	0.40
1:I:235:PRO:HG3	1:I:310:GLU:O	2.21	0.40
1:M:130:GLU:HG2	1:M:425:ALA:CB	2.51	0.40
1:N:158:ILE:O	1:N:161:ILE:HG13	2.20	0.40
1:N:263:VAL:HG22	1:N:264:VAL:H	1.86	0.40
1:F:423:LEU:CD2	1:F:447:MET:HB2	2.52	0.40
1:H:239:GLY:HA3	1:H:314:ILE:HG23	2.03	0.40
1:H:420:VAL:O	1:H:423:LEU:HB2	2.22	0.40
1:J:433:ASN:N	1:J:433:ASN:OD1	2.55	0.40
1:N:234:LEU:C	1:N:236:VAL:N	2.71	0.40
1:A:247:LEU:CD2	1:A:249:ILE:HD11	2.51	0.40
1:D:6:ILE:HD11	1:E:22:VAL:HG13	2.02	0.40
1:F:431:GLY:H	1:F:437:THR:HG23	1.86	0.40
1:G:301:ILE:O	1:G:301:ILE:HG22	2.21	0.40
1:H:229:ASN:C	1:H:230:VAL:HG13	2.42	0.40
1:I:193:MET:O	1:I:332:ILE:N	2.41	0.40
1:I:385:THR:CB	1:I:387:ILE:HG22	2.52	0.40
1:J:69:MET:O	1:J:73:MET:HB2	2.21	0.40
1:J:149:THR:O	1:J:154:SER:N	2.52	0.40
1:L:233:LEU:HD11	1:L:262:LEU:HD21	2.03	0.40
1:N:260:ALA:C	1:N:262:LEU:N	2.75	0.40
1:A:112:ASN:ND2	1:N:459:GLY:HA3	2.37	0.40
1:A:247:LEU:HG	1:A:249:ILE:HD13	2.03	0.40
1:G:155:ASP:O	1:G:158:ILE:HG22	2.22	0.40
1:H:49:ILE:HD11	1:N:73:MET:SD	2.61	0.40
1:H:345:ARG:O	1:H:349:ILE:HG13	2.22	0.40
1:I:33:PRO:CG	1:I:480:ALA:HB3	2.52	0.40
1:I:81:THR:HG21	1:I:503:ALA:HA	2.03	0.40
1:J:73:MET:HB3	1:J:510:ILE:HD11	2.02	0.40
1:K:302:SER:C	1:K:309:LEU:CD2	2.88	0.40
1:K:438:HIS:O	1:K:442:ILE:CG2	2.69	0.40
1:M:236:VAL:O	1:M:237:LEU:HD13	2.22	0.40
1:N:177:VAL:HG11	1:N:396:VAL:HG12	2.02	0.40
1:N:263:VAL:CG2	1:N:264:VAL:H	2.32	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	523/525 (100%)	438 (84%)	65 (12%)	20 (4%)	3	21
1	B	523/525 (100%)	441 (84%)	66 (13%)	16 (3%)	4	26
1	C	523/525 (100%)	441 (84%)	59 (11%)	23 (4%)	2	18
1	D	523/525 (100%)	451 (86%)	60 (12%)	12 (2%)	6	33
1	E	523/525 (100%)	434 (83%)	72 (14%)	17 (3%)	4	24
1	F	523/525 (100%)	432 (83%)	69 (13%)	22 (4%)	3	19
1	G	523/525 (100%)	452 (86%)	62 (12%)	9 (2%)	9	40
1	H	523/525 (100%)	424 (81%)	75 (14%)	24 (5%)	2	17
1	I	523/525 (100%)	436 (83%)	62 (12%)	25 (5%)	2	16
1	J	523/525 (100%)	437 (84%)	65 (12%)	21 (4%)	3	20
1	K	514/525 (98%)	420 (82%)	69 (13%)	25 (5%)	2	16
1	L	523/525 (100%)	409 (78%)	86 (16%)	28 (5%)	2	13
1	M	523/525 (100%)	433 (83%)	65 (12%)	25 (5%)	2	16
1	N	520/525 (99%)	403 (78%)	90 (17%)	27 (5%)	2	14
All	All	7310/7350 (100%)	6051 (83%)	965 (13%)	294 (4%)	3	20

All (294) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	LEU
1	A	184	GLU
1	A	256	GLY
1	A	383	ALA
1	A	426	VAL
1	A	428	ASN

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Mol	Chain	Res	Type
1	B	229	ASN
1	B	329	ASN
1	C	183	LEU
1	C	211	GLN
1	D	89	THR
1	D	205	ILE
1	D	271	VAL
1	E	183	LEU
1	E	211	GLN
1	E	426	VAL
1	F	183	LEU
1	F	211	GLN
1	F	237	LEU
1	F	244	GLY
1	F	383	ALA
1	F	386	GLU
1	F	387	ILE
1	F	428	ASN
1	G	154	SER
1	G	211	GLN
1	G	427	GLY
1	H	183	LEU
1	H	242	LYS
1	H	258	ALA
1	H	312	ALA
1	H	356	THR
1	I	171	LYS
1	I	183	LEU
1	I	242	LYS
1	I	252	GLU
1	I	264	VAL
1	I	386	GLU
1	I	427	GLY
1	J	202	PRO
1	J	255	GLU
1	J	270	ILE
1	J	314	ILE
1	J	329	ASN
1	J	429	LEU
1	K	183	LEU
1	K	205	ILE
1	K	230	VAL

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Mol	Chain	Res	Type
1	K	246	PRO
1	K	304	GLU
1	K	307	LEU
1	K	374	GLY
1	L	211	GLN
1	L	256	GLY
1	L	308	ALA
1	L	329	ASN
1	L	383	ALA
1	L	424	VAL
1	L	426	VAL
1	M	183	LEU
1	M	211	GLN
1	M	238	GLU
1	M	243	ALA
1	M	246	PRO
1	M	247	LEU
1	M	271	VAL
1	M	273	VAL
1	M	303	GLU
1	M	356	THR
1	M	385	THR
1	N	43	SER
1	N	135	SER
1	N	230	VAL
1	N	264	VAL
1	N	427	GLY
1	A	154	SER
1	A	211	GLN
1	A	243	ALA
1	A	271	VAL
1	A	423	LEU
1	B	203	TYR
1	B	211	GLN
1	B	270	ILE
1	B	271	VAL
1	B	427	GLY
1	C	43	SER
1	C	243	ALA
1	C	329	ASN
1	C	334	ASP
1	C	339	SER

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Mol	Chain	Res	Type
1	C	383	ALA
1	C	385	THR
1	C	386	GLU
1	C	490	GLU
1	D	243	ALA
1	D	256	GLY
1	D	356	THR
1	D	424	VAL
1	D	525	PRO
1	E	243	ALA
1	E	254	VAL
1	E	356	THR
1	E	384	SER
1	E	428	ASN
1	F	225	LYS
1	G	305	VAL
1	H	43	SER
1	H	168	LYS
1	H	203	TYR
1	H	265	ASN
1	H	267	ILE
1	H	423	LEU
1	I	58	LYS
1	I	230	VAL
1	I	259	LEU
1	I	270	ILE
1	J	84	ASN
1	J	205	ILE
1	J	225	LYS
1	J	271	VAL
1	J	434	GLU
1	J	502	SER
1	K	9	GLY
1	K	84	ASN
1	K	154	SER
1	K	243	ALA
1	K	265	ASN
1	K	308	ALA
1	L	9	GLY
1	L	84	ASN
1	L	183	LEU
1	L	230	VAL

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Mol	Chain	Res	Type
1	L	271	VAL
1	L	313	THR
1	L	314	ILE
1	L	385	THR
1	M	172	GLU
1	M	218	PRO
1	M	264	VAL
1	N	207	ASN
1	N	211	GLN
1	N	218	PRO
1	N	226	LYS
1	N	244	GLY
1	N	265	ASN
1	N	311	LYS
1	N	336	ALA
1	N	386	GLU
1	N	480	ALA
1	A	85	ALA
1	A	374	GLY
1	B	3	ALA
1	B	153	ASN
1	B	243	ALA
1	C	208	GLN
1	C	228	SER
1	C	434	GLU
1	C	525	PRO
1	E	181	SER
1	E	303	GLU
1	F	134	ILE
1	F	241	ALA
1	G	184	GLU
1	G	383	ALA
1	G	384	SER
1	H	304	GLU
1	H	385	THR
1	H	487	ASP
1	I	85	ALA
1	I	182	GLY
1	I	203	TYR
1	I	383	ALA
1	J	139	THR
1	J	487	ASP

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Mol	Chain	Res	Type
1	K	157	SER
1	K	182	GLY
1	K	271	VAL
1	K	385	THR
1	L	87	ASP
1	L	384	SER
1	L	396	VAL
1	L	458	ALA
1	L	463	SER
1	M	182	GLY
1	N	14	THR
1	N	187	LEU
1	N	271	VAL
1	A	43	SER
1	A	202	PRO
1	A	229	ASN
1	A	463	SER
1	C	523	ASP
1	D	183	LEU
1	D	202	PRO
1	D	246	PRO
1	E	9	GLY
1	E	385	THR
1	F	359	ASP
1	G	203	TYR
1	H	202	PRO
1	H	243	ALA
1	H	271	VAL
1	H	434	GLU
1	I	243	ALA
1	J	183	LEU
1	J	340	ALA
1	J	386	GLU
1	K	245	LYS
1	K	340	ALA
1	K	373	ALA
1	L	184	GLU
1	L	203	TYR
1	L	311	LYS
1	M	43	SER
1	M	154	SER
1	M	374	GLY

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Mol	Chain	Res	Type
1	N	183	LEU
1	N	202	PRO
1	N	235	PRO
1	A	213	ALA
1	B	184	GLU
1	B	336	ALA
1	B	424	VAL
1	C	184	GLU
1	C	271	VAL
1	C	384	SER
1	C	503	ALA
1	E	184	GLU
1	E	271	VAL
1	E	525	PRO
1	F	184	GLU
1	F	233	LEU
1	F	270	ILE
1	G	271	VAL
1	H	231	ARG
1	H	327	LYS
1	H	340	ALA
1	H	433	ASN
1	I	181	SER
1	I	184	GLU
1	I	271	VAL
1	I	381	VAL
1	J	87	ASP
1	K	184	GLU
1	K	384	SER
1	L	248	LEU
1	M	205	ILE
1	M	241	ALA
1	M	326	SER
1	M	418	ALA
1	N	11	ASP
1	A	312	ALA
1	B	183	LEU
1	B	385	THR
1	B	519	ALA
1	F	230	VAL
1	F	313	THR
1	F	382	GLY

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Mol	Chain	Res	Type
1	F	426	VAL
1	H	217	ASP
1	I	456	ALA
1	J	384	SER
1	K	88	GLY
1	K	342	ILE
1	M	107	VAL
1	N	41	GLU
1	C	314	ILE
1	I	86	GLY
1	L	244	GLY
1	N	459	GLY
1	D	182	GLY
1	F	217	ASP
1	I	455	VAL
1	N	236	VAL
1	N	240	VAL
1	F	271	VAL
1	L	103	GLY
1	L	282	GLY
1	L	459	GLY
1	M	236	VAL
1	M	244	GLY
1	A	382	GLY
1	C	256	GLY
1	C	489	VAL
1	F	47	PRO
1	I	150	ILE
1	J	342	ILE
1	K	170	GLY
1	E	202	PRO
1	E	235	PRO
1	H	264	VAL
1	I	459	GLY
1	J	182	GLY
1	N	305	VAL

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	404/404 (100%)	353 (87%)	51 (13%)	4	20
1	B	403/404 (100%)	339 (84%)	64 (16%)	2	11
1	C	404/404 (100%)	361 (89%)	43 (11%)	6	27
1	D	402/404 (100%)	351 (87%)	51 (13%)	4	19
1	E	402/404 (100%)	348 (87%)	54 (13%)	4	17
1	F	398/404 (98%)	327 (82%)	71 (18%)	2	9
1	G	403/404 (100%)	341 (85%)	62 (15%)	2	12
1	H	403/404 (100%)	341 (85%)	62 (15%)	2	12
1	I	400/404 (99%)	345 (86%)	55 (14%)	3	16
1	J	402/404 (100%)	357 (89%)	45 (11%)	6	24
1	K	399/404 (99%)	341 (86%)	58 (14%)	3	14
1	L	403/404 (100%)	351 (87%)	52 (13%)	4	19
1	M	402/404 (100%)	354 (88%)	48 (12%)	5	22
1	N	392/404 (97%)	333 (85%)	59 (15%)	3	13
All	All	5617/5656 (99%)	4842 (86%)	775 (14%)	3	16

All (775) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	18	ARG
1	A	22	VAL
1	A	34	LYS
1	A	43	SER
1	A	89	THR
1	A	91	THR
1	A	94	VAL
1	A	101	ARG
1	A	102	GLU
1	A	105	LYS
1	A	118	ARG
1	A	121	ASP
1	A	129	VAL
1	A	141	ASP
1	A	156	GLU

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Mol	Chain	Res	Type
1	A	157	SER
1	A	158	ILE
1	A	167	LYS
1	A	183	LEU
1	A	205	ILE
1	A	209	GLN
1	A	216	ASP
1	A	222	LEU
1	A	228	SER
1	A	231	ARG
1	A	242	LYS
1	A	257	GLU
1	A	274	VAL
1	A	284	ARG
1	A	288	MET
1	A	291	ASP
1	A	299	THR
1	A	305	VAL
1	A	309	LEU
1	A	311	LYS
1	A	325	VAL
1	A	326	SER
1	A	329	ASN
1	A	357	SER
1	A	411	VAL
1	A	423	LEU
1	A	424	VAL
1	A	437	THR
1	A	453	GLU
1	A	463	SER
1	A	471	GLU
1	A	473	THR
1	A	489	VAL
1	A	494	LEU
1	A	510	ILE
1	B	6	ILE
1	B	14	THR
1	B	17	VAL
1	B	41	GLU
1	B	43	SER
1	B	50	THR
1	B	83	ASP

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Mol	Chain	Res	Type
1	B	94	VAL
1	B	105	LYS
1	B	115	ASP
1	B	136	LYS
1	B	156	GLU
1	B	161	ILE
1	B	167	LYS
1	B	168	LYS
1	B	184	GLU
1	B	188	ASP
1	B	196	ASP
1	B	207	ASN
1	B	211	GLN
1	B	216	ASP
1	B	223	HIS
1	B	237	LEU
1	B	242	LYS
1	B	250	VAL
1	B	253	GLU
1	B	255	GLU
1	B	257	GLU
1	B	261	THR
1	B	284	ARG
1	B	290	GLU
1	B	291	ASP
1	B	295	LEU
1	B	303	GLU
1	B	305	VAL
1	B	309	LEU
1	B	314	ILE
1	B	315	LYS
1	B	319	ARG
1	B	325	VAL
1	B	331	THR
1	B	338	ASP
1	B	344	SER
1	B	352	GLN
1	B	363	GLU
1	B	372	LEU
1	B	391	GLU
1	B	397	GLU
1	B	404	ARG

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Mol	Chain	Res	Type
1	B	412	VAL
1	B	417	VAL
1	B	420	VAL
1	B	430	THR
1	B	434	GLU
1	B	451	LEU
1	B	463	SER
1	B	468	LYS
1	B	494	LEU
1	B	499	VAL
1	B	502	SER
1	B	506	ASN
1	B	510	ILE
1	B	518	GLU
1	B	526	LYS
1	C	6	ILE
1	C	17	VAL
1	C	34	LYS
1	C	43	SER
1	C	74	VAL
1	C	77	VAL
1	C	81	THR
1	C	82	ASN
1	C	90	THR
1	C	94	VAL
1	C	133	ASN
1	C	139	THR
1	C	157	SER
1	C	158	ILE
1	C	183	LEU
1	C	190	VAL
1	C	214	ASP
1	C	223	HIS
1	C	231	ARG
1	C	253	GLU
1	C	257	GLU
1	C	274	VAL
1	C	284	ARG
1	C	289	LEU
1	C	309	LEU
1	C	330	THR
1	C	331	THR

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Mol	Chain	Res	Type
1	C	338	ASP
1	C	339	SER
1	C	361	ASP
1	C	371	LYS
1	C	385	THR
1	C	391	GLU
1	C	404	ARG
1	C	412	VAL
1	C	428	ASN
1	C	442	ILE
1	C	451	LEU
1	C	494	LEU
1	C	510	ILE
1	C	518	GLU
1	C	523	ASP
1	C	525	PRO
1	D	5	ASP
1	D	6	ILE
1	D	17	VAL
1	D	41	GLU
1	D	43	SER
1	D	48	THR
1	D	69	MET
1	D	84	ASN
1	D	89	THR
1	D	129	VAL
1	D	130	GLU
1	D	133	ASN
1	D	136	LYS
1	D	140	ASP
1	D	142	LYS
1	D	158	ILE
1	D	160	ASN
1	D	161	ILE
1	D	176	THR
1	D	177	VAL
1	D	186	GLU
1	D	188	ASP
1	D	196	ASP
1	D	207	ASN
1	D	209	GLN
1	D	216	ASP

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Mol	Chain	Res	Type
1	D	223	HIS
1	D	226	LYS
1	D	231	ARG
1	D	232	ASP
1	D	242	LYS
1	D	284	ARG
1	D	291	ASP
1	D	299	THR
1	D	316	ASP
1	D	317	LEU
1	D	331	THR
1	D	334	ASP
1	D	343	GLU
1	D	387	ILE
1	D	398	ASP
1	D	401	HIS
1	D	404	ARG
1	D	417	VAL
1	D	426	VAL
1	D	428	ASN
1	D	429	LEU
1	D	430	THR
1	D	451	LEU
1	D	487	ASP
1	D	494	LEU
1	E	6	ILE
1	E	11	ASP
1	E	17	VAL
1	E	76	GLU
1	E	77	VAL
1	E	101	ARG
1	E	125	LYS
1	E	132	LYS
1	E	133	ASN
1	E	141	ASP
1	E	146	GLN
1	E	158	ILE
1	E	160	ASN
1	E	183	LEU
1	E	194	GLN
1	E	196	ASP
1	E	206	ASN

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Mol	Chain	Res	Type
1	E	215	LEU
1	E	217	ASP
1	E	228	SER
1	E	231	ARG
1	E	236	VAL
1	E	253	GLU
1	E	254	VAL
1	E	257	GLU
1	E	261	THR
1	E	268	ARG
1	E	283	ASP
1	E	290	GLU
1	E	294	VAL
1	E	299	THR
1	E	309	LEU
1	E	325	VAL
1	E	328	GLU
1	E	331	THR
1	E	338	ASP
1	E	352	GLN
1	E	353	ILE
1	E	359	ASP
1	E	384	SER
1	E	401	HIS
1	E	404	ARG
1	E	411	VAL
1	E	412	VAL
1	E	420	VAL
1	E	468	LYS
1	E	473	THR
1	E	482	ASN
1	E	489	VAL
1	E	494	LEU
1	E	499	VAL
1	E	509	SER
1	E	510	ILE
1	E	523	ASP
1	F	5	ASP
1	F	6	ILE
1	F	7	ARG
1	F	10	GLU
1	F	20	VAL

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Mol	Chain	Res	Type
1	F	28	LYS
1	F	41	GLU
1	F	47	PRO
1	F	74	VAL
1	F	81	THR
1	F	82	ASN
1	F	89	THR
1	F	90	THR
1	F	115	ASP
1	F	125	LYS
1	F	136	LYS
1	F	139	THR
1	F	140	ASP
1	F	157	SER
1	F	160	ASN
1	F	161	ILE
1	F	168	LYS
1	F	177	VAL
1	F	188	ASP
1	F	200	LEU
1	F	207	ASN
1	F	210	SER
1	F	211	GLN
1	F	215	LEU
1	F	225	LYS
1	F	233	LEU
1	F	242	LYS
1	F	257	GLU
1	F	259	LEU
1	F	261	THR
1	F	267	ILE
1	F	268	ARG
1	F	270	ILE
1	F	291	ASP
1	F	294	VAL
1	F	295	LEU
1	F	303	GLU
1	F	309	LEU
1	F	310	GLU
1	F	317	LEU
1	F	324	GLN
1	F	331	THR

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Mol	Chain	Res	Type
1	F	355	ASP
1	F	359	ASP
1	F	363	GLU
1	F	372	LEU
1	F	390	LYS
1	F	408	GLU
1	F	417	VAL
1	F	420	VAL
1	F	426	VAL
1	F	442	ILE
1	F	444	LEU
1	F	451	LEU
1	F	463	SER
1	F	466	LEU
1	F	467	ASN
1	F	471	GLU
1	F	473	THR
1	F	475	ASN
1	F	489	VAL
1	F	494	LEU
1	F	499	VAL
1	F	510	ILE
1	F	514	MET
1	F	526	LYS
1	G	11	ASP
1	G	17	VAL
1	G	20	VAL
1	G	28	LYS
1	G	54	VAL
1	G	94	VAL
1	G	130	GLU
1	G	133	ASN
1	G	136	LYS
1	G	151	SER
1	G	177	VAL
1	G	184	GLU
1	G	188	ASP
1	G	191	GLU
1	G	196	ASP
1	G	200	LEU
1	G	211	GLN
1	G	212	SER

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Mol	Chain	Res	Type
1	G	214	ASP
1	G	215	LEU
1	G	217	ASP
1	G	223	HIS
1	G	230	VAL
1	G	238	GLU
1	G	240	VAL
1	G	242	LYS
1	G	257	GLU
1	G	267	ILE
1	G	271	VAL
1	G	291	ASP
1	G	294	VAL
1	G	295	LEU
1	G	299	THR
1	G	309	LEU
1	G	317	LEU
1	G	319	ARG
1	G	325	VAL
1	G	326	SER
1	G	331	THR
1	G	352	GLN
1	G	356	THR
1	G	369	VAL
1	G	387	ILE
1	G	401	HIS
1	G	404	ARG
1	G	412	VAL
1	G	420	VAL
1	G	423	LEU
1	G	426	VAL
1	G	430	THR
1	G	437	THR
1	G	441	GLN
1	G	442	ILE
1	G	451	LEU
1	G	463	SER
1	G	489	VAL
1	G	491	PHE
1	G	494	LEU
1	G	495	ASP
1	G	499	VAL

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Mol	Chain	Res	Type
1	G	502	SER
1	G	523	ASP
1	H	6	ILE
1	H	10	GLU
1	H	17	VAL
1	H	20	VAL
1	H	34	LYS
1	H	41	GLU
1	H	42	LYS
1	H	74	VAL
1	H	81	THR
1	H	89	THR
1	H	94	VAL
1	H	130	GLU
1	H	146	GLN
1	H	153	ASN
1	H	156	GLU
1	H	161	ILE
1	H	171	LYS
1	H	179	GLU
1	H	185	ASN
1	H	196	ASP
1	H	207	ASN
1	H	226	LYS
1	H	232	ASP
1	H	249	ILE
1	H	250	VAL
1	H	257	GLU
1	H	262	LEU
1	H	265	ASN
1	H	267	ILE
1	H	271	VAL
1	H	272	LYS
1	H	274	VAL
1	H	284	ARG
1	H	292	MET
1	H	295	LEU
1	H	307	LEU
1	H	316	ASP
1	H	317	LEU
1	H	325	VAL
1	H	326	SER

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Mol	Chain	Res	Type
1	H	331	THR
1	H	359	ASP
1	H	360	TYR
1	H	384	SER
1	H	407	VAL
1	H	417	VAL
1	H	420	VAL
1	H	424	VAL
1	H	426	VAL
1	H	434	GLU
1	H	437	THR
1	H	441	GLN
1	H	451	LEU
1	H	453	GLU
1	H	460	GLU
1	H	467	ASN
1	H	482	ASN
1	H	494	LEU
1	H	495	ASP
1	H	499	VAL
1	H	502	SER
1	H	510	ILE
1	I	6	ILE
1	I	7	ARG
1	I	20	VAL
1	I	23	LEU
1	I	50	THR
1	I	58	LYS
1	I	61	GLU
1	I	74	VAL
1	I	75	LYS
1	I	89	THR
1	I	91	THR
1	I	101	ARG
1	I	122	GLN
1	I	129	VAL
1	I	136	LYS
1	I	138	THR
1	I	158	ILE
1	I	164	GLU
1	I	166	MET
1	I	176	THR

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Mol	Chain	Res	Type
1	I	191	GLU
1	I	211	GLN
1	I	216	ASP
1	I	228	SER
1	I	229	ASN
1	I	233	LEU
1	I	234	LEU
1	I	240	VAL
1	I	268	ARG
1	I	288	MET
1	I	295	LEU
1	I	309	LEU
1	I	314	ILE
1	I	315	LYS
1	I	316	ASP
1	I	323	VAL
1	I	325	VAL
1	I	328	GLU
1	I	331	THR
1	I	357	SER
1	I	363	GLU
1	I	365	LEU
1	I	372	LEU
1	I	384	SER
1	I	385	THR
1	I	391	GLU
1	I	420	VAL
1	I	423	LEU
1	I	426	VAL
1	I	430	THR
1	I	436	GLN
1	I	451	LEU
1	I	487	ASP
1	I	494	LEU
1	I	499	VAL
1	J	6	ILE
1	J	14	THR
1	J	49	ILE
1	J	64	ASP
1	J	76	GLU
1	J	82	ASN
1	J	94	VAL

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Mol	Chain	Res	Type
1	J	101	ARG
1	J	124	VAL
1	J	139	THR
1	J	153	ASN
1	J	167	LYS
1	J	171	LYS
1	J	181	SER
1	J	183	LEU
1	J	184	GLU
1	J	199	TYR
1	J	207	ASN
1	J	208	GLN
1	J	225	LYS
1	J	238	GLU
1	J	257	GLU
1	J	261	THR
1	J	274	VAL
1	J	284	ARG
1	J	289	LEU
1	J	291	ASP
1	J	303	GLU
1	J	311	LYS
1	J	315	LYS
1	J	323	VAL
1	J	325	VAL
1	J	331	THR
1	J	355	ASP
1	J	356	THR
1	J	364	LYS
1	J	423	LEU
1	J	428	ASN
1	J	430	THR
1	J	434	GLU
1	J	453	GLU
1	J	495	ASP
1	J	502	SER
1	J	509	SER
1	J	523	ASP
1	K	5	ASP
1	K	6	ILE
1	K	10	GLU
1	K	42	LYS

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Mol	Chain	Res	Type
1	K	48	THR
1	K	77	VAL
1	K	81	THR
1	K	90	THR
1	K	128	VAL
1	K	129	VAL
1	K	141	ASP
1	K	153	ASN
1	K	154	SER
1	K	158	ILE
1	K	161	ILE
1	K	171	LYS
1	K	172	GLU
1	K	183	LEU
1	K	206	ASN
1	K	207	ASN
1	K	210	SER
1	K	223	HIS
1	K	225	LYS
1	K	230	VAL
1	K	233	LEU
1	K	238	GLU
1	K	240	VAL
1	K	242	LYS
1	K	250	VAL
1	K	253	GLU
1	K	265	ASN
1	K	284	ARG
1	K	299	THR
1	K	300	VAL
1	K	307	LEU
1	K	309	LEU
1	K	311	LYS
1	K	314	ILE
1	K	325	VAL
1	K	352	GLN
1	K	354	GLU
1	K	355	ASP
1	K	386	GLU
1	K	400	LEU
1	K	404	ARG
1	K	420	VAL

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Mol	Chain	Res	Type
1	K	429	LEU
1	K	437	THR
1	K	442	ILE
1	K	451	LEU
1	K	453	GLU
1	K	461	GLU
1	K	482	ASN
1	K	489	VAL
1	K	490	GLU
1	K	494	LEU
1	K	509	SER
1	K	510	ILE
1	L	5	ASP
1	L	6	ILE
1	L	11	ASP
1	L	28	LYS
1	L	58	LYS
1	L	62	LEU
1	L	74	VAL
1	L	77	VAL
1	L	79	SER
1	L	83	ASP
1	L	91	THR
1	L	139	THR
1	L	164	GLU
1	L	171	LYS
1	L	179	GLU
1	L	184	GLU
1	L	223	HIS
1	L	225	LYS
1	L	226	LYS
1	L	229	ASN
1	L	236	VAL
1	L	255	GLU
1	L	262	LEU
1	L	267	ILE
1	L	268	ARG
1	L	272	LYS
1	L	288	MET
1	L	289	LEU
1	L	291	ASP
1	L	299	THR

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Mol	Chain	Res	Type
1	L	303	GLU
1	L	307	LEU
1	L	309	LEU
1	L	310	GLU
1	L	313	THR
1	L	325	VAL
1	L	326	SER
1	L	331	THR
1	L	339	SER
1	L	344	SER
1	L	368	ARG
1	L	404	ARG
1	L	412	VAL
1	L	417	VAL
1	L	424	VAL
1	L	464	VAL
1	L	466	LEU
1	L	468	LYS
1	L	473	THR
1	L	487	ASP
1	L	509	SER
1	L	526	LYS
1	M	6	ILE
1	M	34	LYS
1	M	36	ARG
1	M	43	SER
1	M	48	THR
1	M	74	VAL
1	M	79	SER
1	M	81	THR
1	M	90	THR
1	M	139	THR
1	M	140	ASP
1	M	167	LYS
1	M	171	LYS
1	M	176	THR
1	M	183	LEU
1	M	214	ASP
1	M	215	LEU
1	M	217	ASP
1	M	223	HIS
1	M	227	ILE

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Mol	Chain	Res	Type
1	M	237	LEU
1	M	238	GLU
1	M	247	LEU
1	M	259	LEU
1	M	261	THR
1	M	262	LEU
1	M	267	ILE
1	M	270	ILE
1	M	273	VAL
1	M	310	GLU
1	M	325	VAL
1	M	331	THR
1	M	334	ASP
1	M	338	ASP
1	M	355	ASP
1	M	359	ASP
1	M	366	GLN
1	M	388	GLU
1	M	404	ARG
1	M	426	VAL
1	M	430	THR
1	M	434	GLU
1	M	442	ILE
1	M	463	SER
1	M	466	LEU
1	M	494	LEU
1	M	502	SER
1	M	518	GLU
1	N	6	ILE
1	N	11	ASP
1	N	41	GLU
1	N	42	LYS
1	N	74	VAL
1	N	80	LYS
1	N	81	THR
1	N	82	ASN
1	N	89	THR
1	N	101	ARG
1	N	136	LYS
1	N	141	ASP
1	N	158	ILE
1	N	161	ILE

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Mol	Chain	Res	Type
1	N	172	GLU
1	N	176	THR
1	N	177	VAL
1	N	183	LEU
1	N	199	TYR
1	N	200	LEU
1	N	201	SER
1	N	214	ASP
1	N	216	ASP
1	N	226	LYS
1	N	227	ILE
1	N	229	ASN
1	N	230	VAL
1	N	233	LEU
1	N	237	LEU
1	N	240	VAL
1	N	261	THR
1	N	266	THR
1	N	268	ARG
1	N	272	LYS
1	N	283	ASP
1	N	289	LEU
1	N	291	ASP
1	N	305	VAL
1	N	309	LEU
1	N	313	THR
1	N	316	ASP
1	N	325	VAL
1	N	334	ASP
1	N	345	ARG
1	N	346	VAL
1	N	354	GLU
1	N	356	THR
1	N	359	ASP
1	N	361	ASP
1	N	404	ARG
1	N	412	VAL
1	N	420	VAL
1	N	423	LEU
1	N	473	THR
1	N	484	GLU
1	N	487	ASP

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Mol	Chain	Res	Type
1	N	489	VAL
1	N	494	LEU
1	N	518	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	84	ASN
1	A	207	ASN
1	A	209	GLN
1	A	223	HIS
1	A	265	ASN
1	A	329	ASN
1	A	438	HIS
1	A	475	ASN
1	B	37	ASN
1	B	265	ASN
1	B	329	ASN
1	B	506	ASN
1	C	37	ASN
1	C	97	GLN
1	C	133	ASN
1	C	324	GLN
1	C	352	GLN
1	D	84	ASN
1	D	207	ASN
1	D	229	ASN
1	D	366	GLN
1	D	441	GLN
1	D	475	ASN
1	D	506	ASN
1	E	37	ASN
1	E	146	GLN
1	E	206	ASN
1	E	207	ASN
1	E	265	ASN
1	E	324	GLN
1	E	329	ASN
1	E	366	GLN
1	E	475	ASN
1	F	37	ASN

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Mol	Chain	Res	Type
1	F	223	HIS
1	F	348	GLN
1	F	352	GLN
1	F	441	GLN
1	F	467	ASN
1	F	475	ASN
1	G	207	ASN
1	G	211	GLN
1	G	324	GLN
1	G	506	ASN
1	H	97	GLN
1	H	146	GLN
1	H	207	ASN
1	H	265	ASN
1	H	329	ASN
1	H	436	GLN
1	H	441	GLN
1	H	475	ASN
1	H	482	ASN
1	I	146	GLN
1	I	185	ASN
1	I	207	ASN
1	I	208	GLN
1	I	209	GLN
1	I	265	ASN
1	I	436	GLN
1	I	441	GLN
1	J	84	ASN
1	J	207	ASN
1	J	208	GLN
1	J	348	GLN
1	J	467	ASN
1	J	479	ASN
1	J	505	GLN
1	K	37	ASN
1	K	84	ASN
1	K	206	ASN
1	K	207	ASN
1	K	324	GLN
1	K	366	GLN
1	K	475	ASN
1	L	37	ASN

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Mol	Chain	Res	Type
1	L	133	ASN
1	L	153	ASN
1	L	207	ASN
1	L	352	GLN
1	L	482	ASN
1	L	506	ASN
1	M	112	ASN
1	M	146	GLN
1	M	265	ASN
1	M	348	GLN
1	M	366	GLN
1	N	37	ASN
1	N	84	ASN
1	N	229	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	GOL	F	602	-	5,5,5	0.09	0	5,5,5	0.33	0
3	SO4	K	601	-	4,4,4	0.38	0	6,6,6	0.05	0
2	GOL	F	601	-	5,5,5	0.14	0	5,5,5	0.33	0
2	GOL	B	601	-	5,5,5	0.16	0	5,5,5	0.48	0
3	SO4	I	601	-	4,4,4	0.36	0	6,6,6	0.06	0

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
2	GOL	B	601	-	-	4/4/4/4	-
2	GOL	F	602	-	-	2/4/4/4	-
2	GOL	F	601	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	601	GOL	O1-C1-C2-C3
2	F	602	GOL	O1-C1-C2-O2
2	F	602	GOL	O1-C1-C2-C3
2	B	601	GOL	O1-C1-C2-C3
2	B	601	GOL	C1-C2-C3-O3
2	B	601	GOL	O2-C2-C3-O3
2	F	601	GOL	O1-C1-C2-O2
2	B	601	GOL	O1-C1-C2-O2

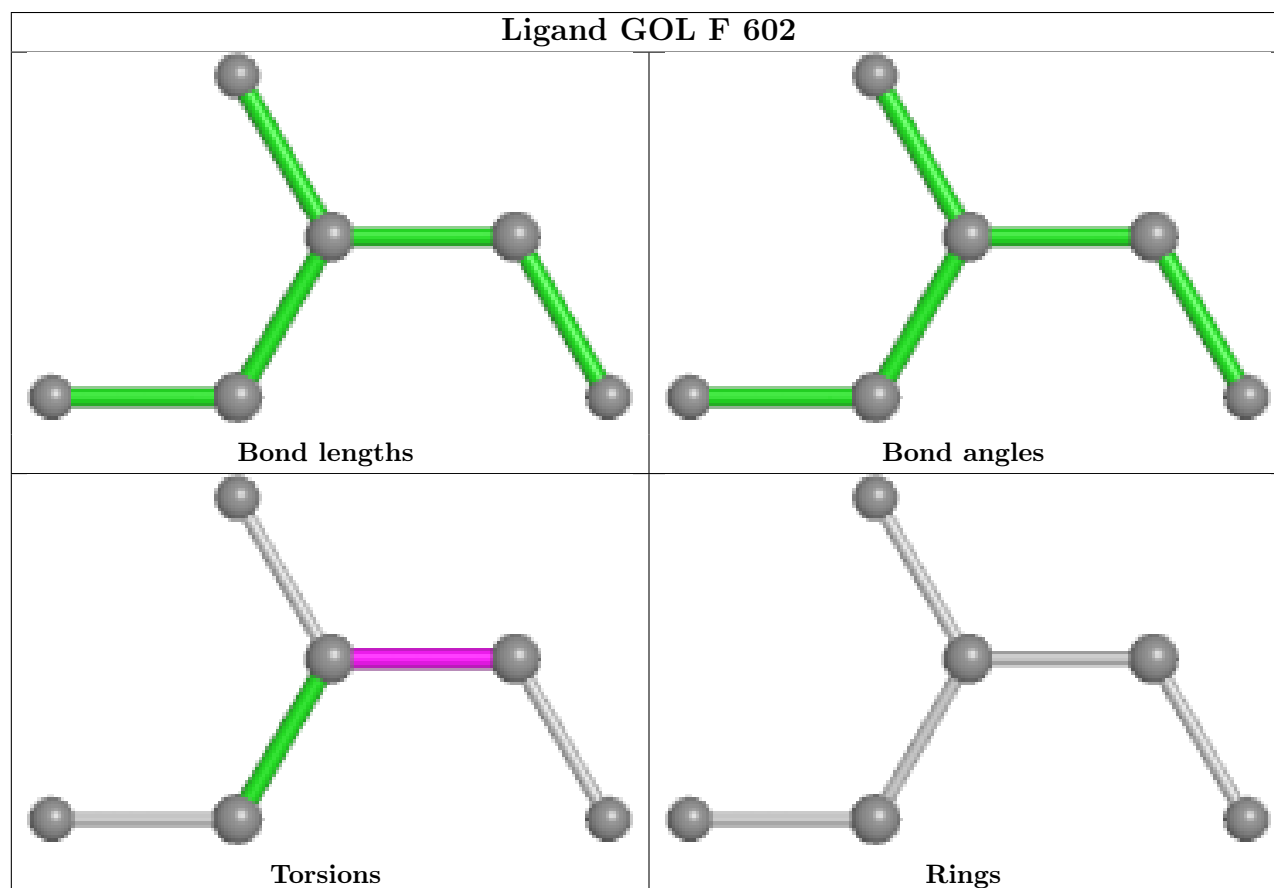
There are no ring outliers.

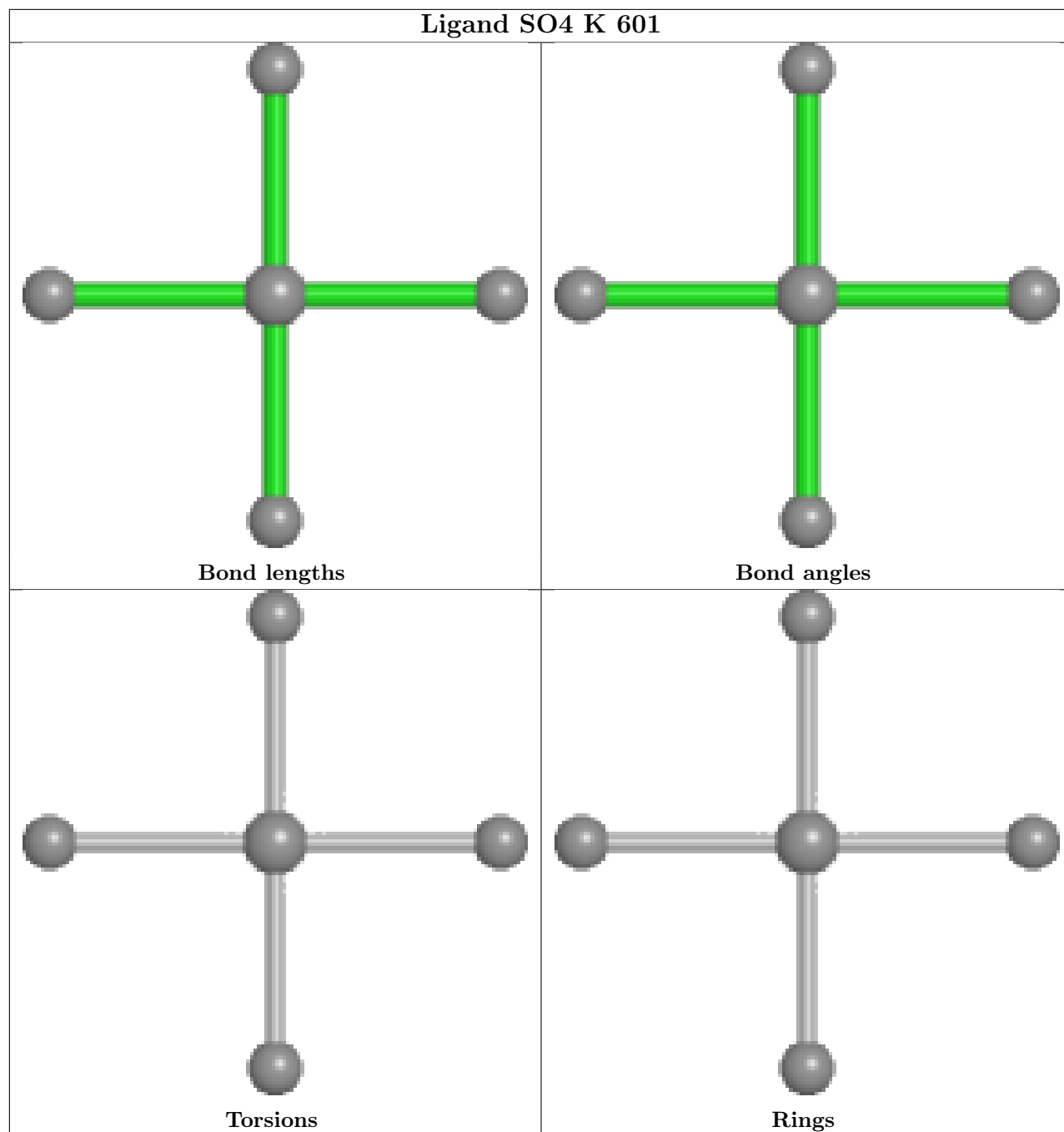
1 monomer is involved in 3 short contacts:

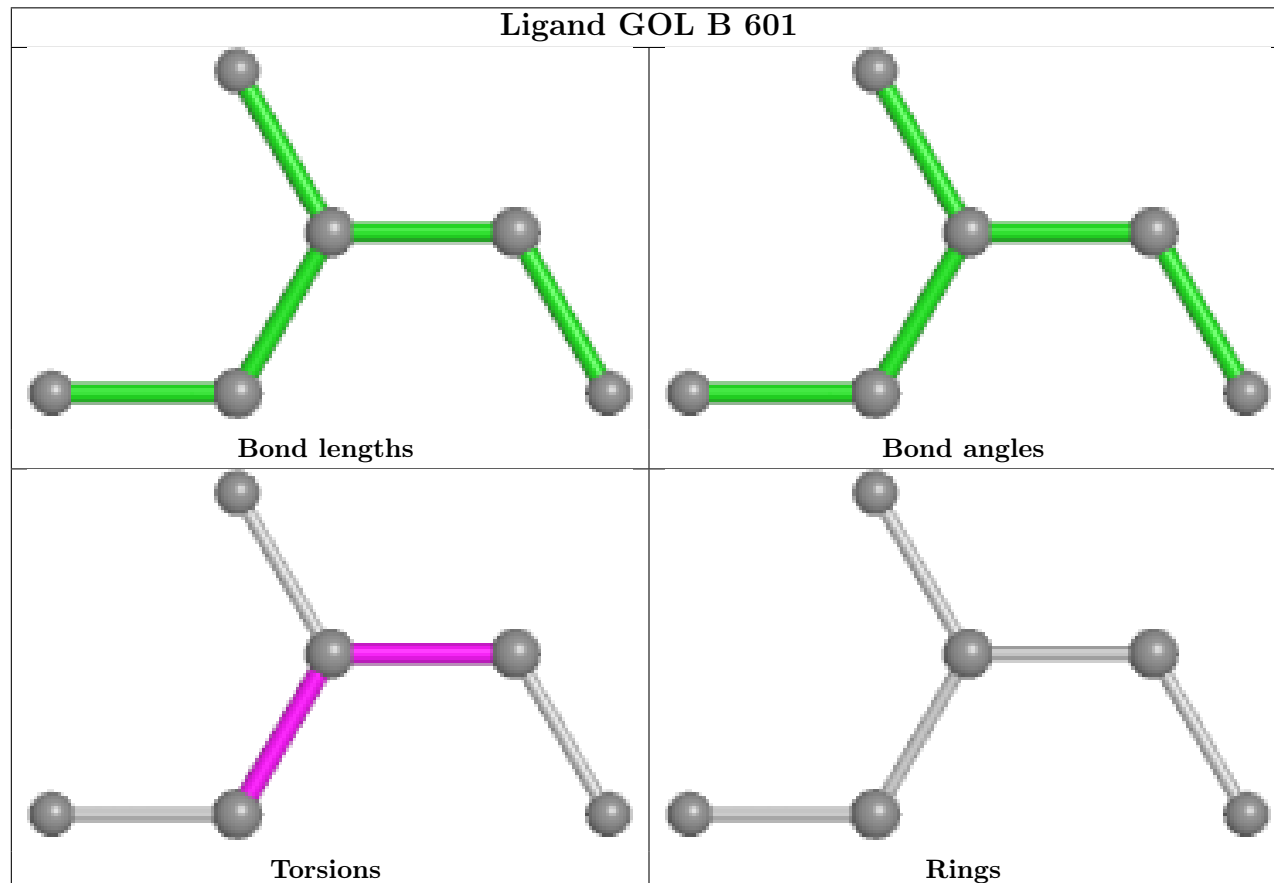
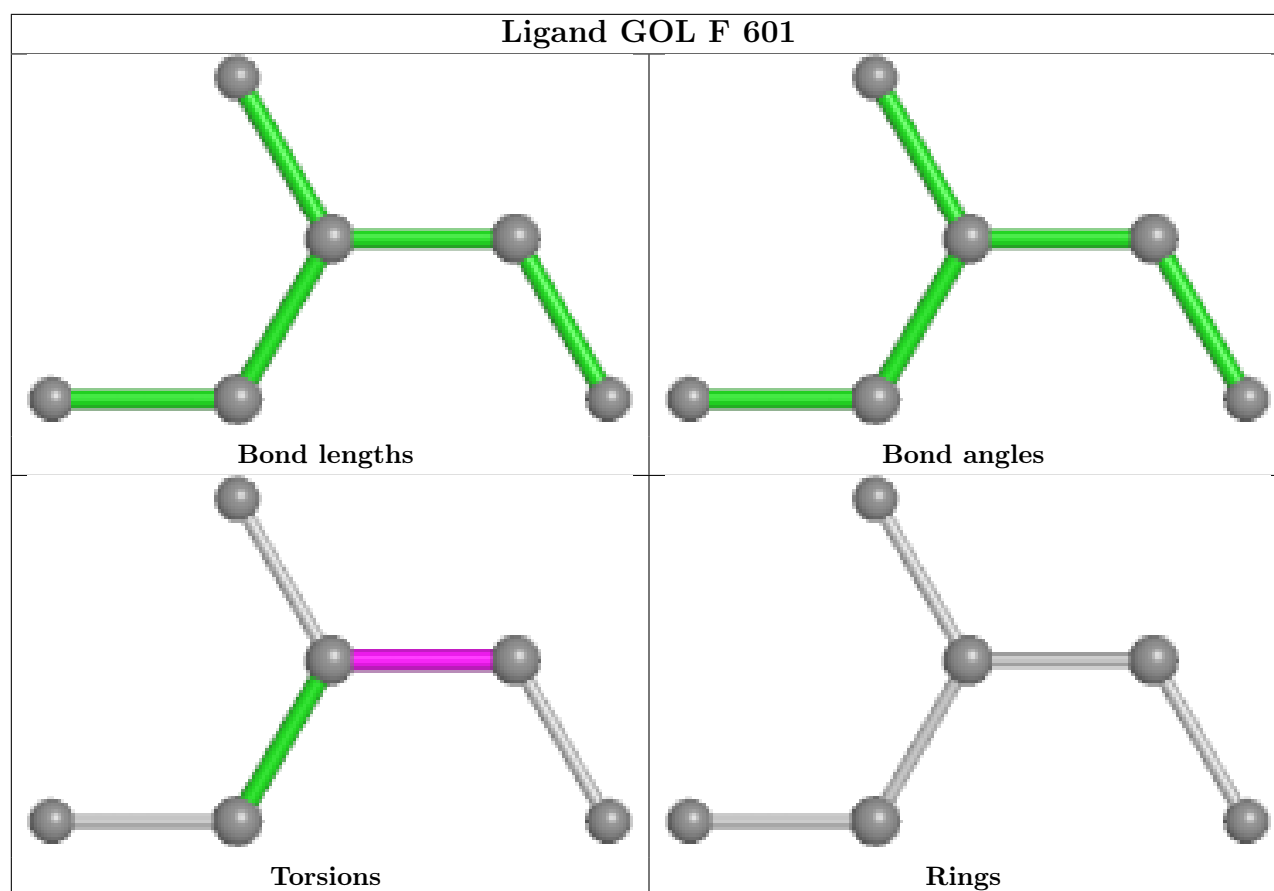
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	GOL	3	0

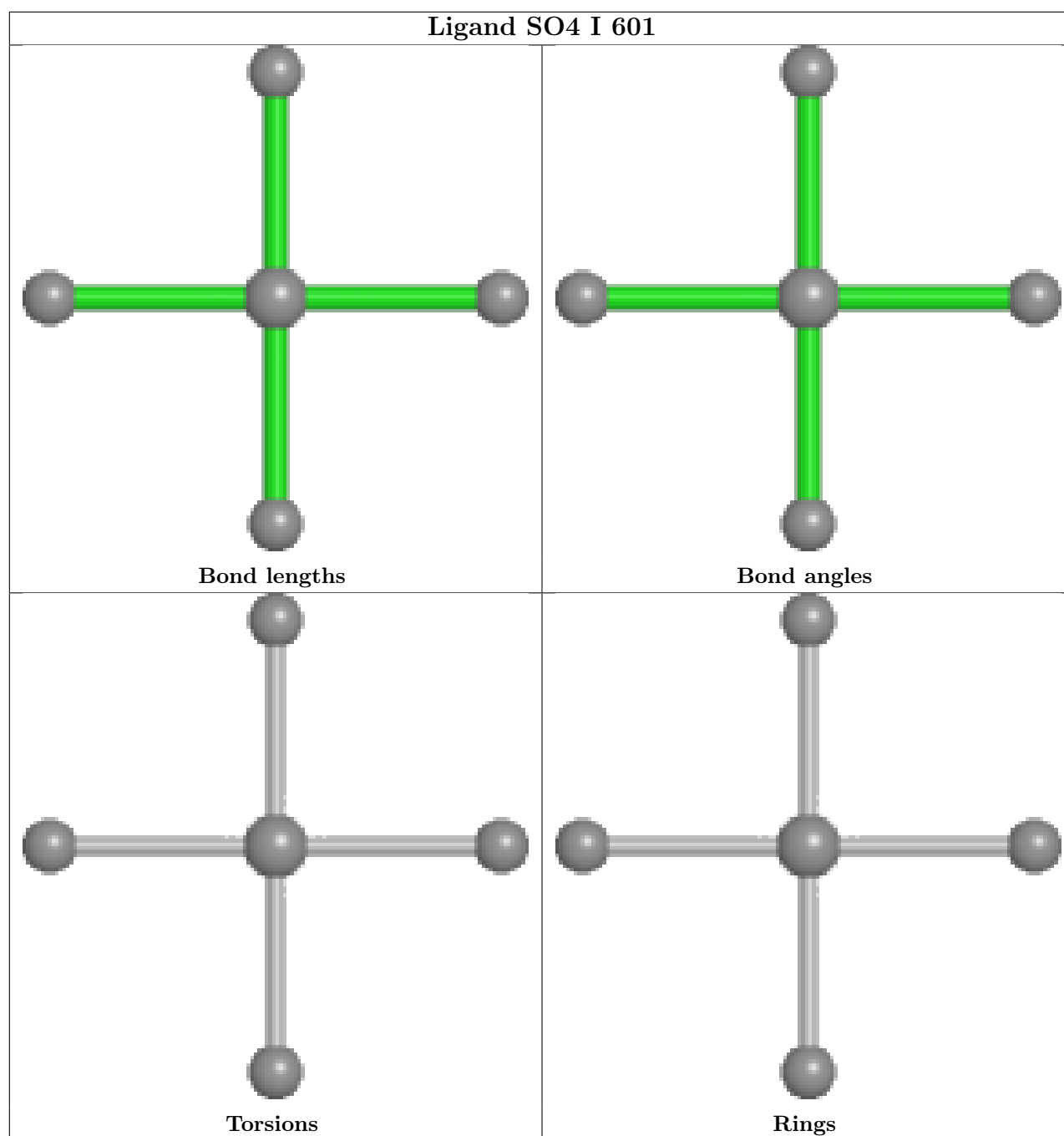
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.









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 ⓘ

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	525/525 (100%)	-0.31	2 (0%) 92 89	37, 68, 104, 128	0
1	B	525/525 (100%)	-0.22	3 (0%) 89 84	36, 68, 104, 124	0
1	C	525/525 (100%)	-0.20	3 (0%) 89 84	34, 73, 128, 168	0
1	D	525/525 (100%)	-0.20	7 (1%) 77 66	29, 78, 146, 173	0
1	E	525/525 (100%)	-0.12	3 (0%) 89 84	34, 79, 136, 183	0
1	F	525/525 (100%)	-0.21	3 (0%) 89 84	30, 73, 113, 137	0
1	G	525/525 (100%)	-0.26	2 (0%) 92 89	32, 65, 98, 127	0
1	H	525/525 (100%)	-0.18	7 (1%) 77 66	39, 75, 119, 156	0
1	I	525/525 (100%)	-0.25	1 (0%) 95 94	39, 74, 117, 162	0
1	J	525/525 (100%)	-0.07	8 (1%) 73 62	37, 90, 140, 165	0
1	K	518/525 (98%)	-0.04	8 (1%) 73 62	43, 84, 140, 179	0
1	L	525/525 (100%)	-0.09	5 (0%) 82 73	40, 82, 129, 148	0
1	M	525/525 (100%)	0.04	16 (3%) 50 36	41, 94, 146, 174	0
1	N	524/525 (99%)	-0.08	10 (1%) 66 54	38, 91, 149, 220	0
All	All	7342/7350 (99%)	-0.16	78 (1%) 80 70	29, 76, 133, 220	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	223	HIS	5.6
1	K	263	VAL	5.4
1	L	525	PRO	5.0
1	K	203	TYR	4.2
1	A	357	SER	3.9
1	M	526	LYS	3.9
1	C	526	LYS	3.8
1	J	141	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	J	357	SER	3.5
1	L	357	SER	3.5
1	E	223	HIS	3.4
1	K	84	ASN	3.4
1	M	223	HIS	3.4
1	M	292	MET	3.4
1	M	220	ILE	3.3
1	D	526	LYS	3.3
1	B	357	SER	3.3
1	L	526	LYS	3.3
1	J	187	LEU	3.2
1	H	525	PRO	3.2
1	H	523	ASP	3.2
1	M	525	PRO	3.1
1	H	526	LYS	3.0
1	G	5	ASP	2.9
1	I	526	LYS	2.9
1	E	271	VAL	2.8
1	J	526	LYS	2.8
1	D	334	ASP	2.8
1	M	215	LEU	2.8
1	D	525	PRO	2.7
1	N	224	ASP	2.7
1	M	288	MET	2.7
1	N	357	SER	2.7
1	J	139	THR	2.6
1	A	526	LYS	2.6
1	N	526	LYS	2.6
1	N	250	VAL	2.5
1	F	526	LYS	2.5
1	L	223	HIS	2.5
1	F	228	SER	2.5
1	N	525	PRO	2.5
1	D	261	THR	2.5
1	K	264	VAL	2.5
1	G	158	ILE	2.5
1	D	357	SER	2.4
1	M	369	VAL	2.4
1	H	252	GLU	2.4
1	N	236	VAL	2.4
1	E	525	PRO	2.4
1	K	208	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	141	ASP	2.3
1	N	220	ILE	2.3
1	C	525	PRO	2.3
1	F	525	PRO	2.3
1	N	222	LEU	2.3
1	H	181	SER	2.3
1	M	193	MET	2.3
1	K	525	PRO	2.2
1	M	200	LEU	2.2
1	K	262	LEU	2.2
1	L	360	TYR	2.2
1	H	2	ALA	2.2
1	M	356	THR	2.2
1	J	525	PRO	2.2
1	J	181	SER	2.1
1	D	221	LEU	2.1
1	M	224	ASP	2.1
1	C	270	ILE	2.1
1	M	221	LEU	2.1
1	B	525	PRO	2.1
1	B	184	GLU	2.1
1	D	279	PRO	2.1
1	K	182	GLY	2.1
1	J	207	ASN	2.0
1	M	139	THR	2.0
1	M	247	LEU	2.0
1	N	251	ALA	2.0
1	M	311	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

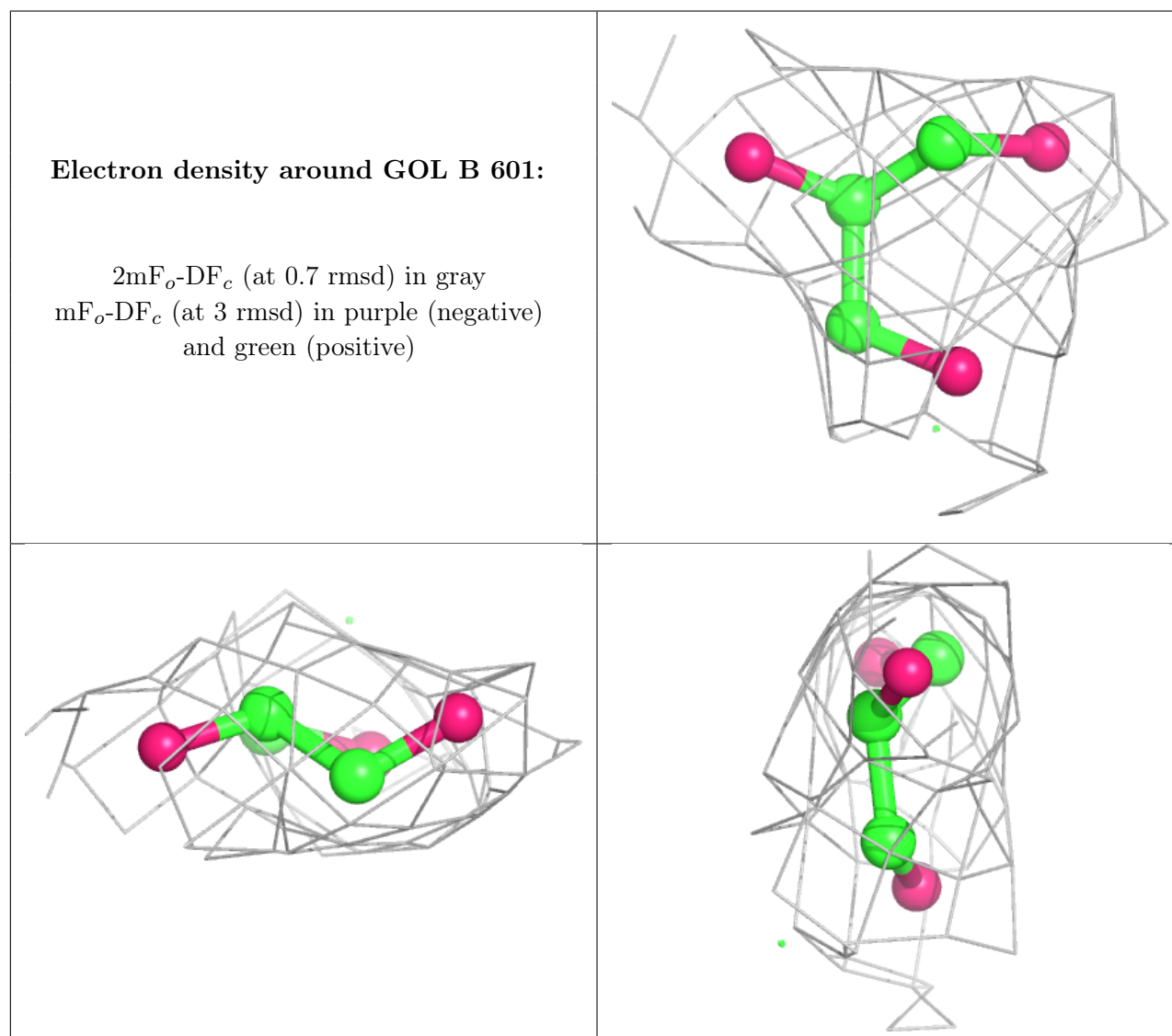
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

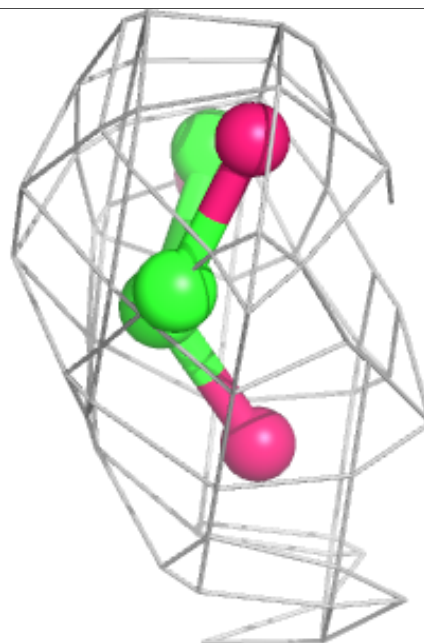
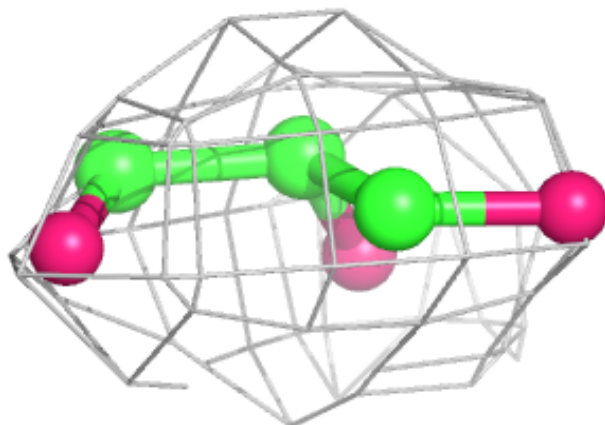
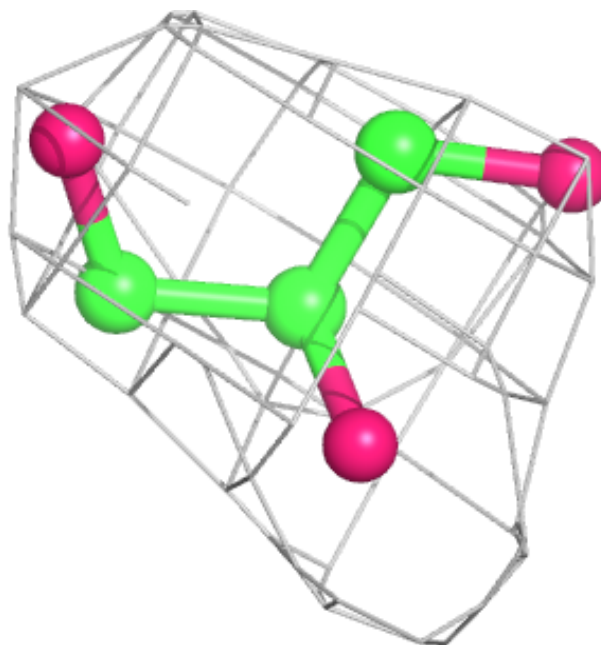
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	B	601	6/6	0.78	0.25	74,80,83,85	0
2	GOL	F	602	6/6	0.81	0.37	82,88,89,92	0
3	SO4	K	601	5/5	0.81	0.34	126,129,133,134	0
3	SO4	I	601	5/5	0.82	0.31	126,128,133,134	0
2	GOL	F	601	6/6	0.88	0.26	66,79,80,80	0

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.



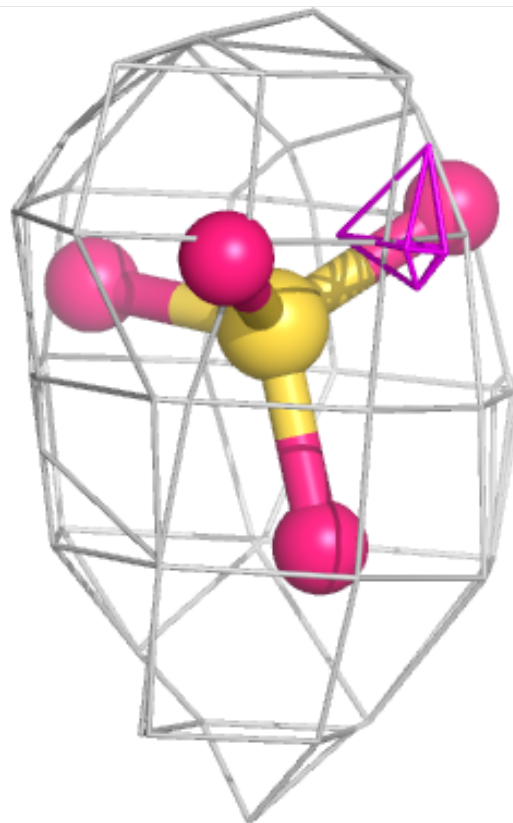
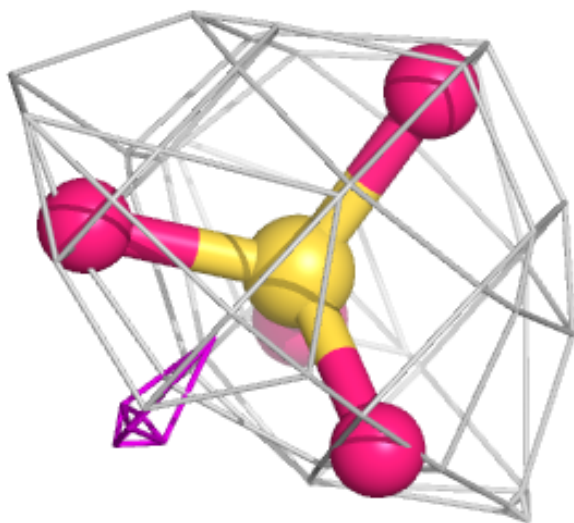
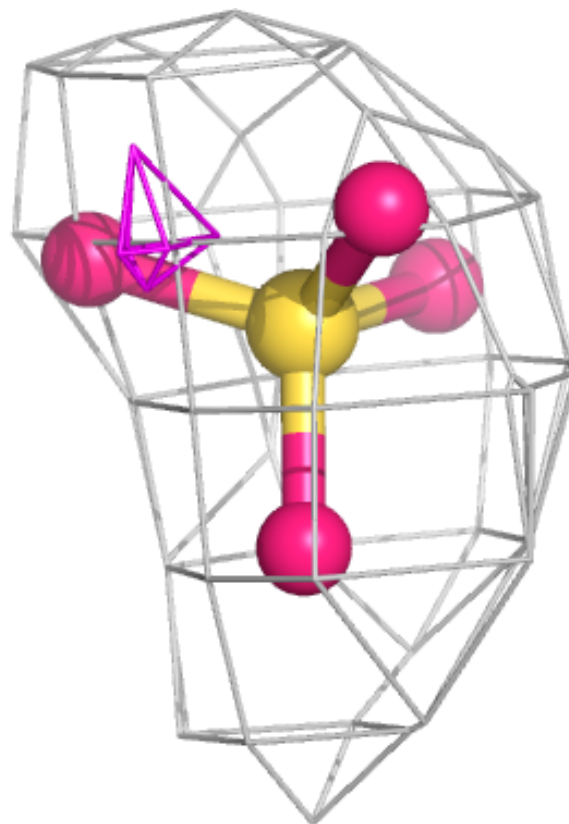
Electron density around GOL F 602:

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



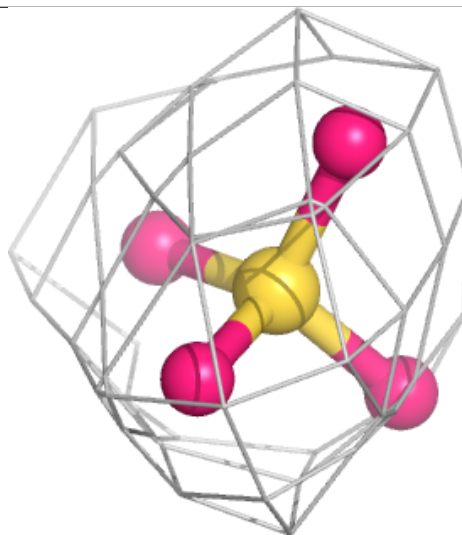
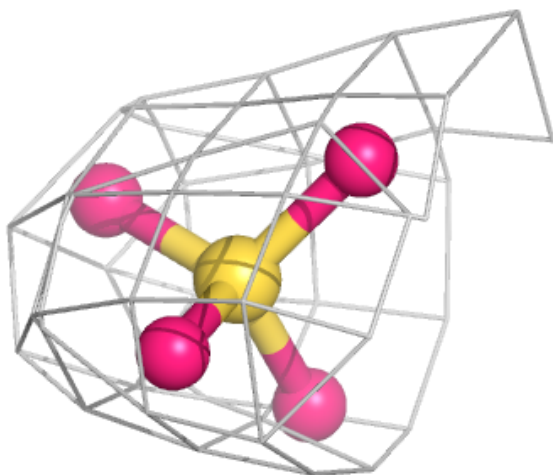
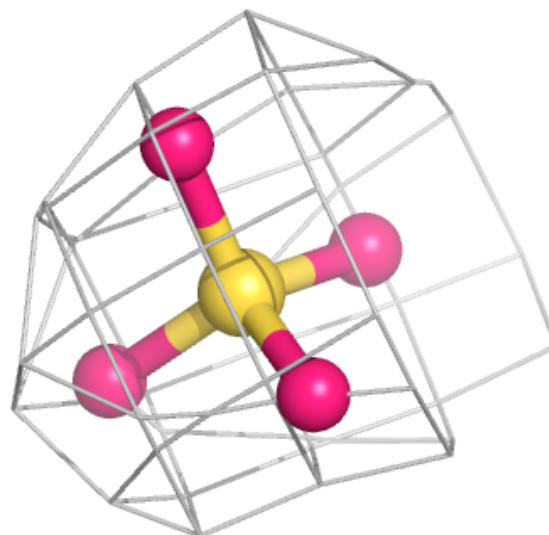
Electron density around SO4 K 601:

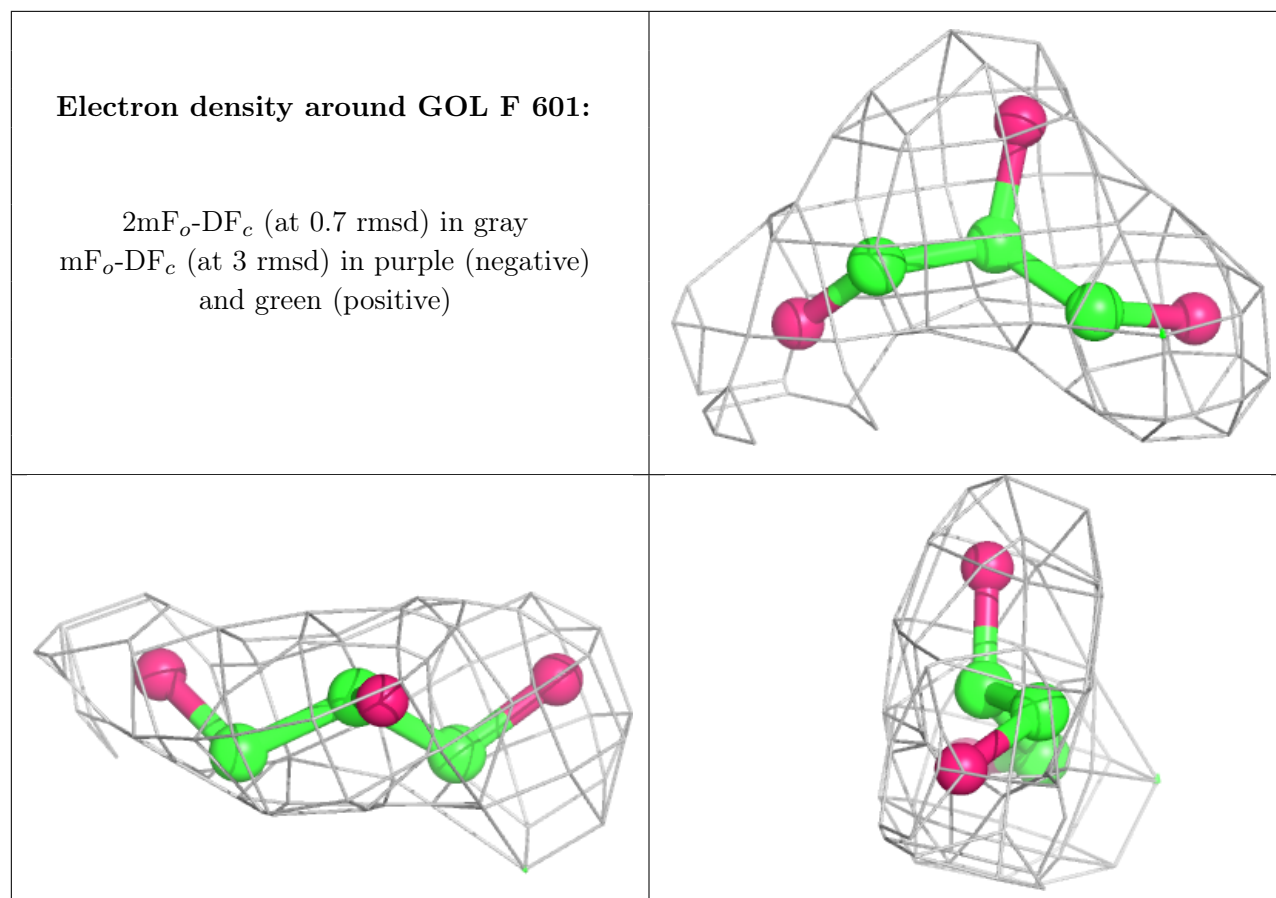
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SO4 I 601:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.