Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:26 pm BST

PDB ID	:	6DHL
Title	:	Bovine glutamate dehydrogenase complexed with epicatechin-3-gallate (ECG)
Authors	:	Smith, T.J.
Deposited on	:	2018-05-20
Resolution	:	3.62 Å(reported)

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

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

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

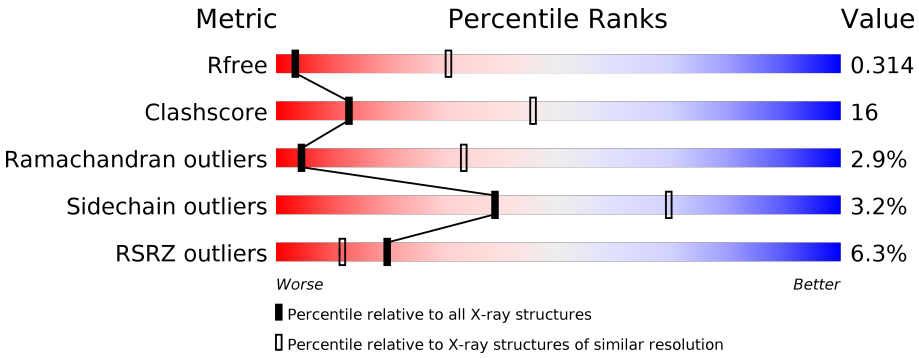
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.62 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	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	496	8% 64% 33% ·
1	B	496	6% 65% 33% ·
1	C	496	7% 66% 30% ·
1	D	496	6% 65% 32% ·
1	E	496	11% 60% 36% ·
1	F	496	9% 65% 32% ·

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Mol	Chain	Length	Quality of chain
1	G	496	6% 60% 38%
1	H	496	2% 64% 34%
1	I	496	6% 64% 34%
1	J	496	2% 65% 33%
1	K	496	5% 62% 35%
1	L	496	6% 66% 30%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	XEG	C	601	-	-	-	X
2	XEG	I	601	-	-	-	X
2	XEG	L	601	-	-	-	X

2 Entry composition

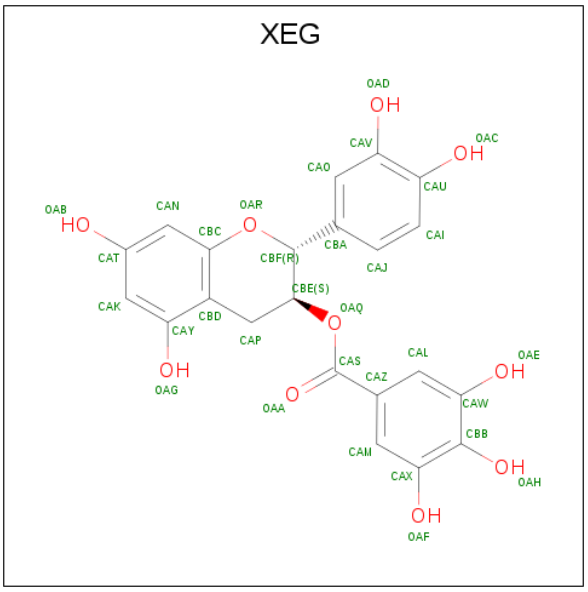
There are 2 unique types of molecules in this entry. The entry contains 46872 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate dehydrogenase 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3874	2451	679	725	19			
1	B	496	Total	C	N	O	S	0	0	0
			3874	2451	679	725	19			
1	C	496	Total	C	N	O	S	0	0	0
			3874	2451	679	725	19			
1	D	496	Total	C	N	O	S	0	0	0
			3874	2451	679	725	19			
1	E	496	Total	C	N	O	S	0	0	0
			3874	2451	679	725	19			
1	F	496	Total	C	N	O	S	0	0	0
			3874	2451	679	725	19			
1	G	496	Total	C	N	O	S	0	0	0
			3874	2451	679	725	19			
1	H	496	Total	C	N	O	S	0	0	0
			3874	2451	679	725	19			
1	I	496	Total	C	N	O	S	0	0	0
			3874	2451	679	725	19			
1	J	496	Total	C	N	O	S	0	0	0
			3874	2451	679	725	19			
1	K	496	Total	C	N	O	S	0	0	0
			3874	2451	679	725	19			
1	L	496	Total	C	N	O	S	0	0	0
			3874	2451	679	725	19			

- Molecule 2 is (2R,3S)-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3,4-dihydro-2H-chromen-3-yl 3,4,5-trihydroxybenzoate (three-letter code: XEG) (formula: $C_{22}H_{18}O_{10}$).



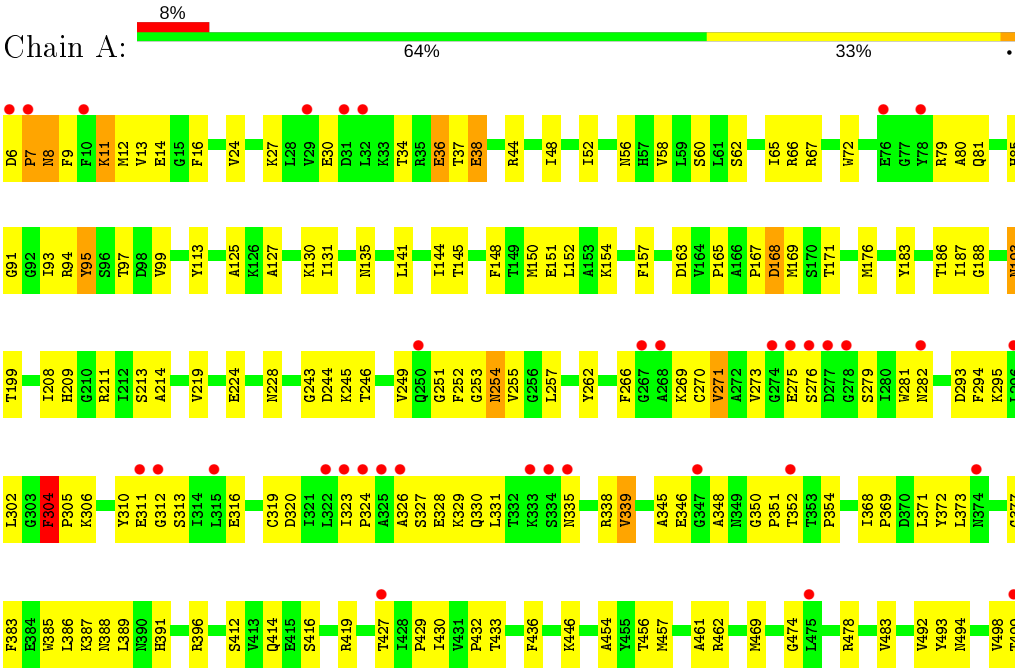
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 32 22 10	0	0
2	B	1	Total C O 32 22 10	0	0
2	C	1	Total C O 32 22 10	0	0
2	D	1	Total C O 32 22 10	0	0
2	E	1	Total C O 32 22 10	0	0
2	F	1	Total C O 32 22 10	0	0
2	G	1	Total C O 32 22 10	0	0
2	H	1	Total C O 32 22 10	0	0
2	I	1	Total C O 32 22 10	0	0
2	J	1	Total C O 32 22 10	0	0
2	K	1	Total C O 32 22 10	0	0
2	L	1	Total C O 32 22 10	0	0

3 Residue-property plots (i)

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

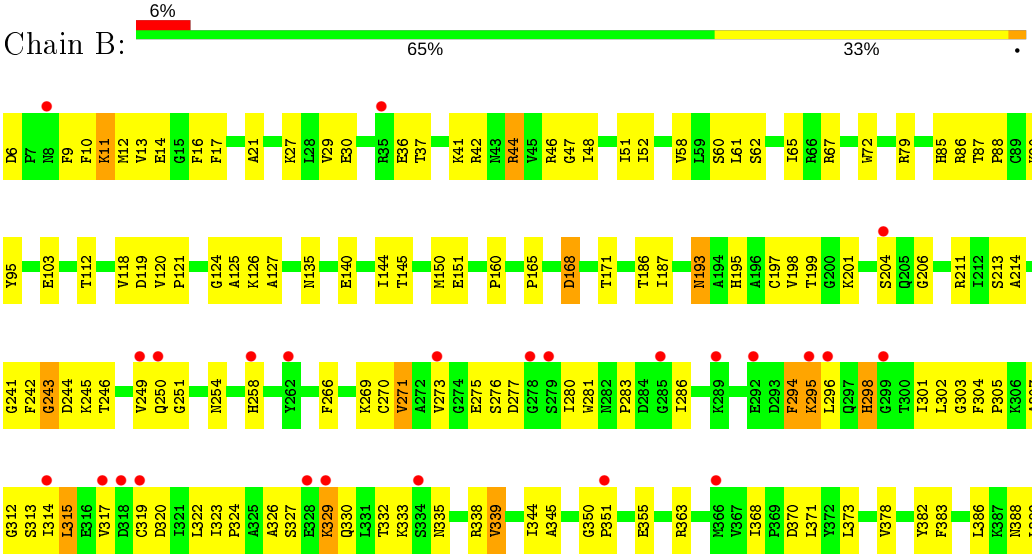
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

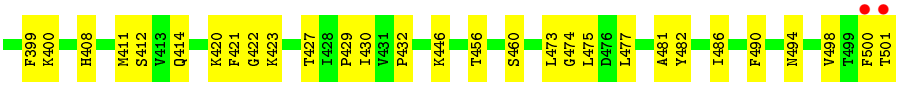
Chain A:



- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

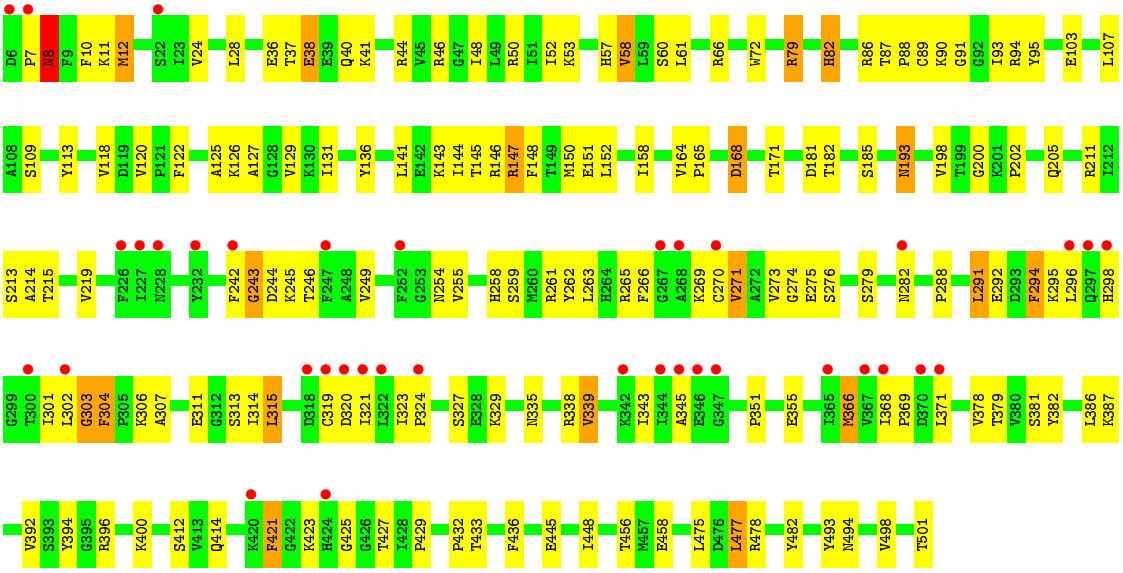
Chain B:





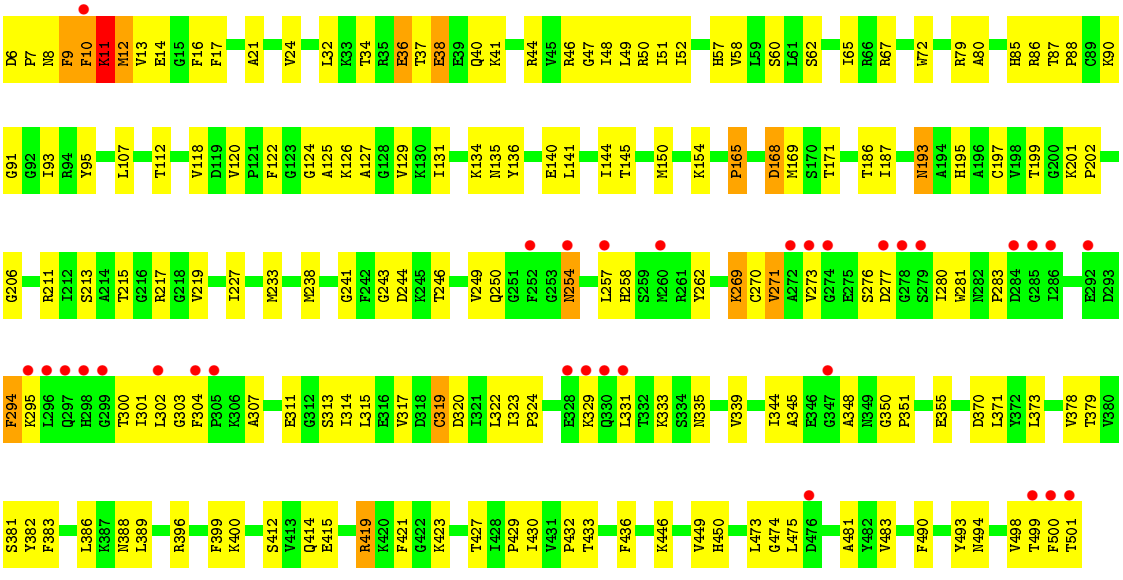
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain C:



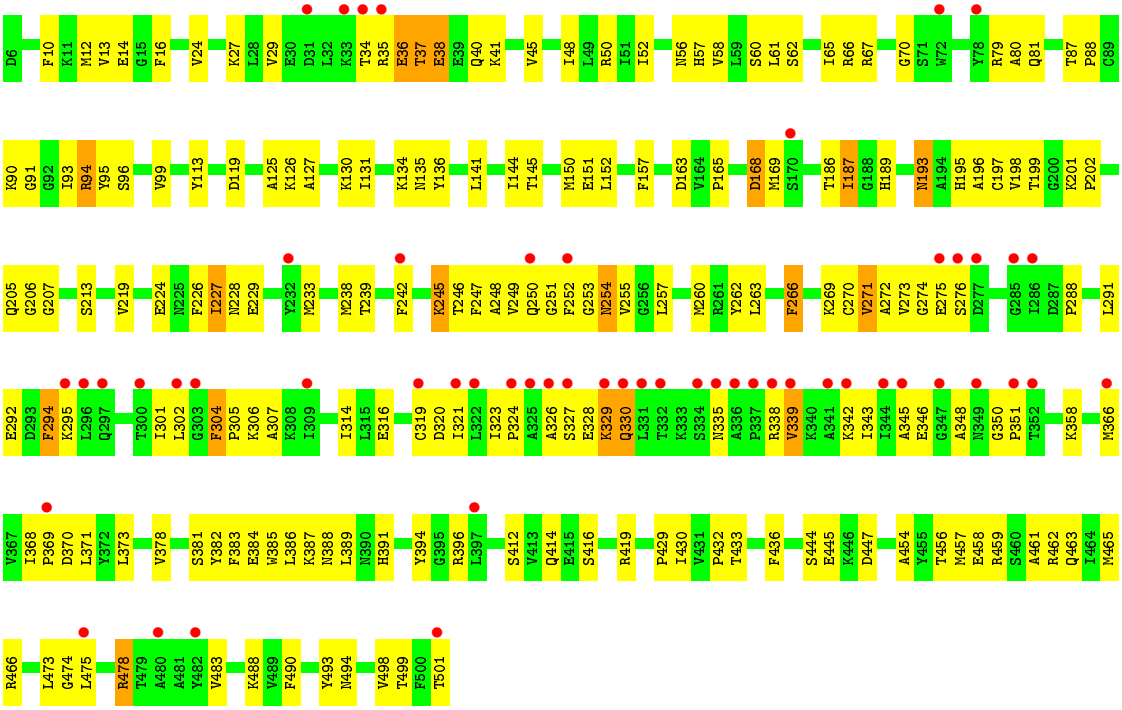
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain D:



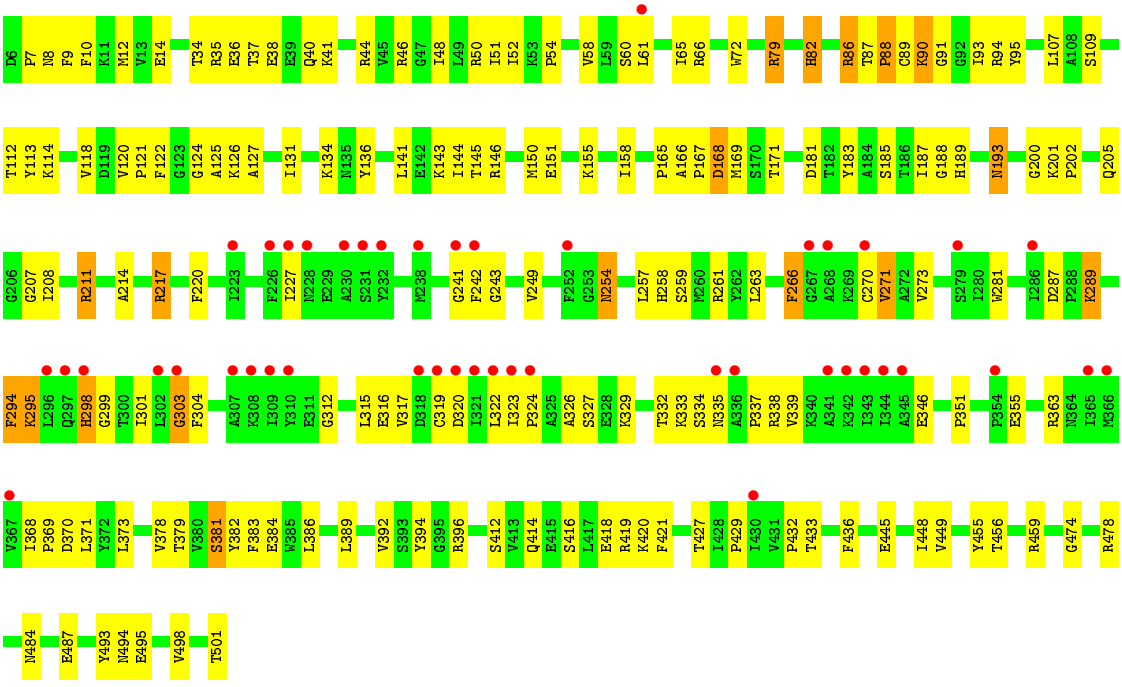
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain E:



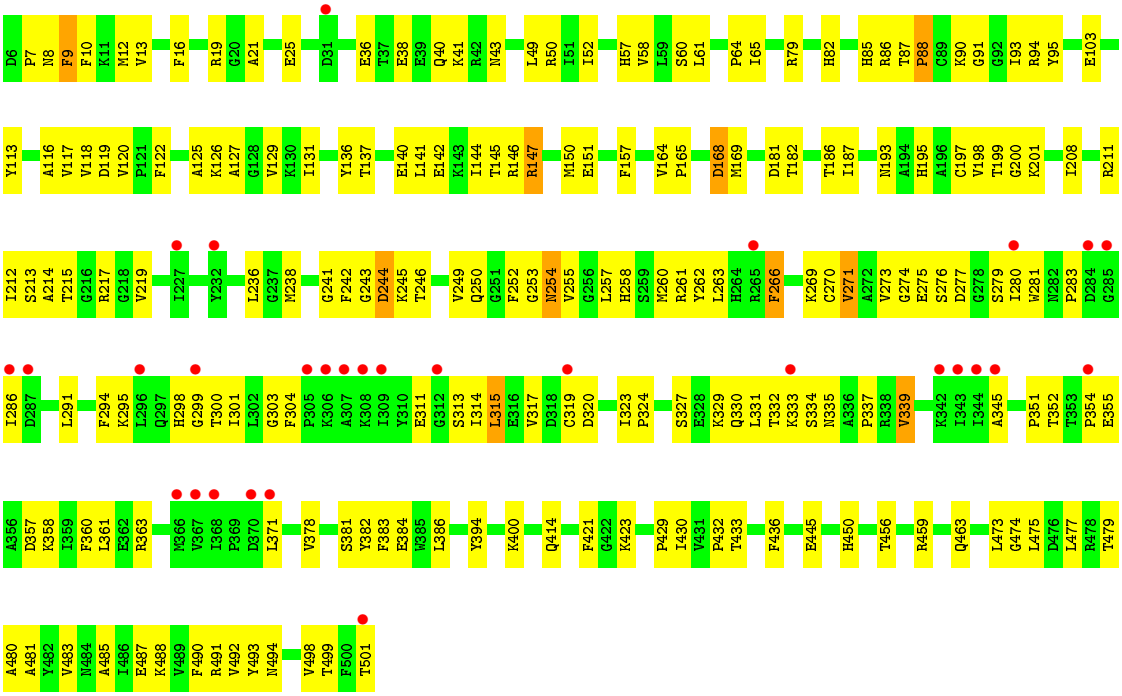
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain F:



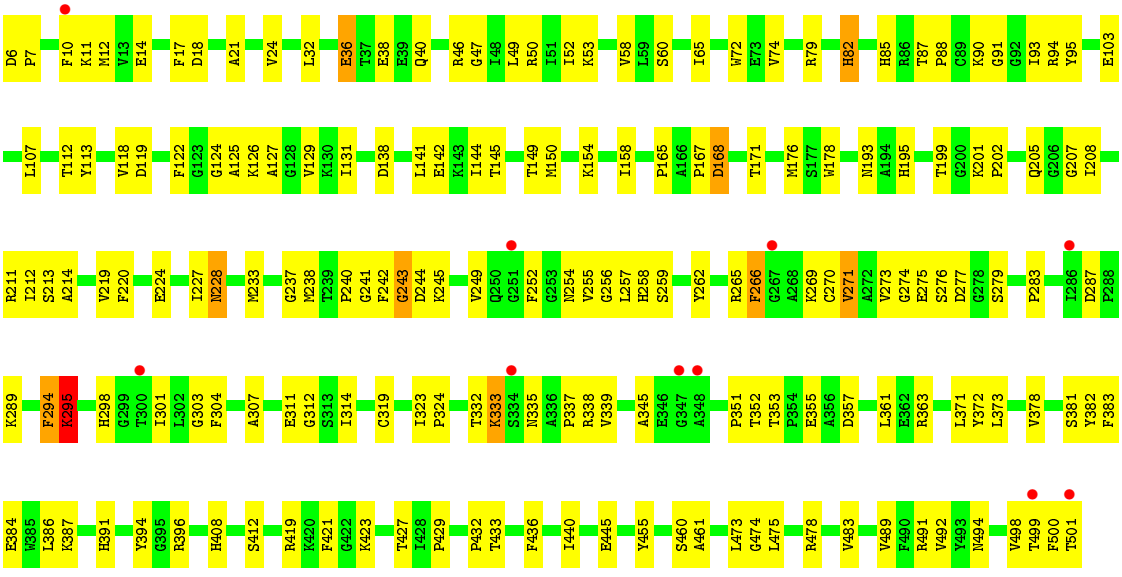
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain G:



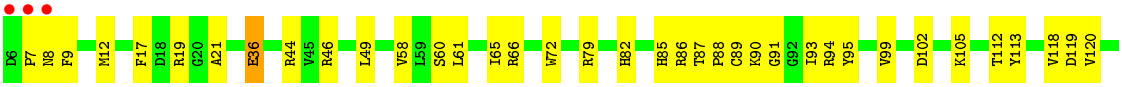
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

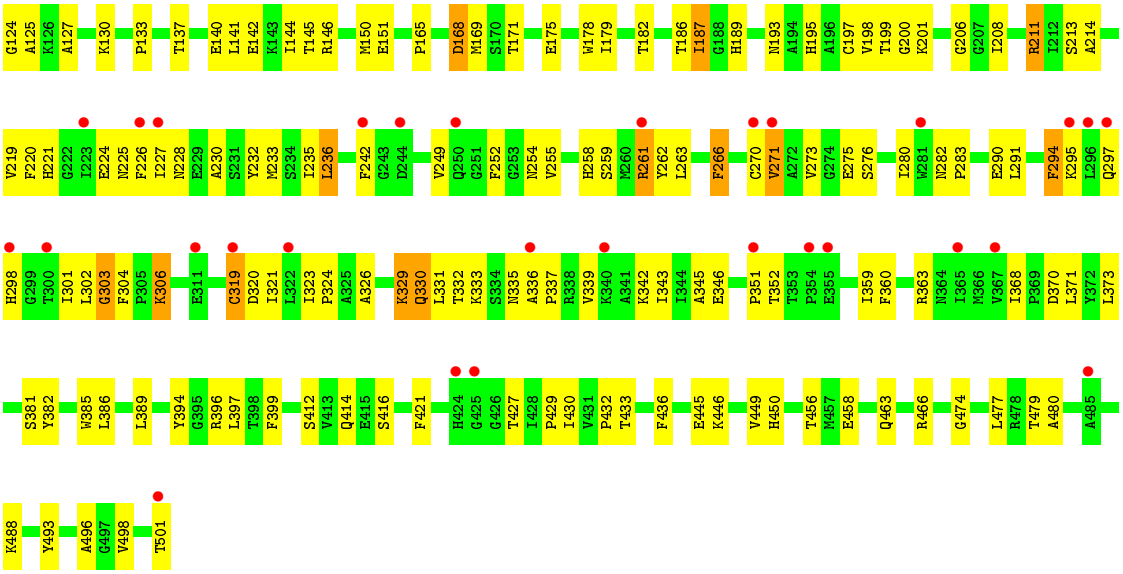
Chain H:



• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

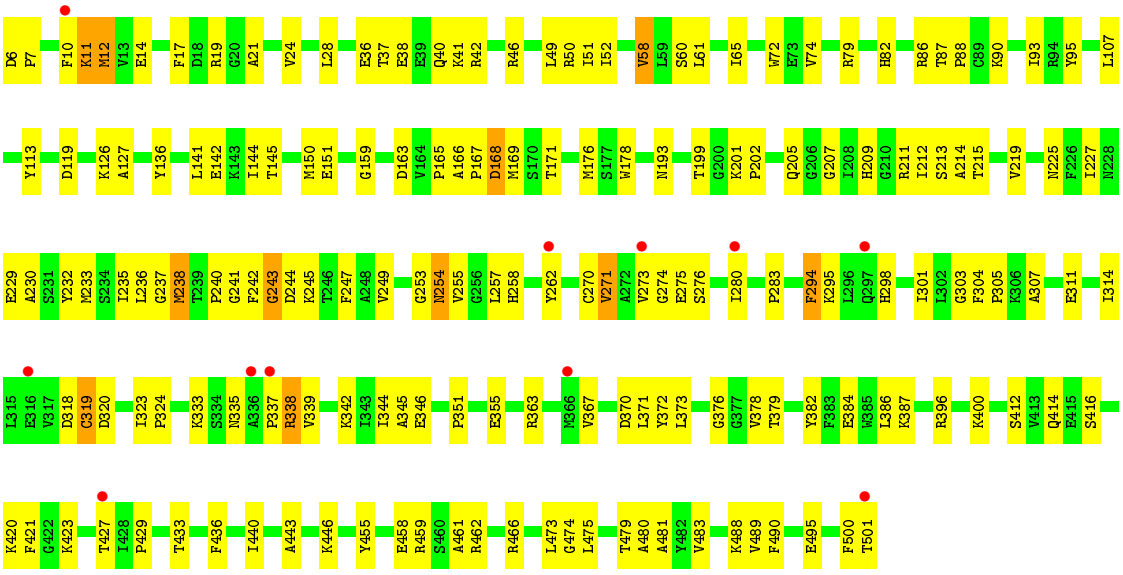
Chain I:





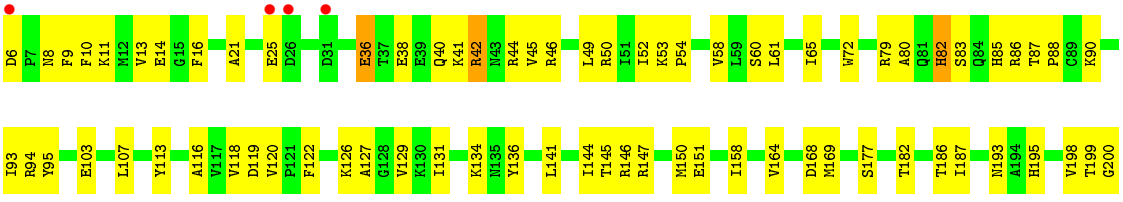
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

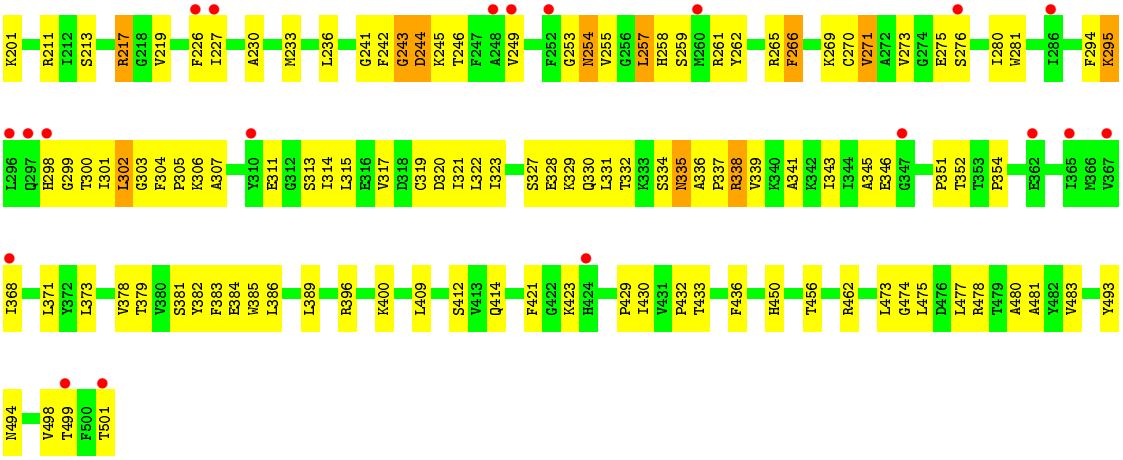
Chain J:



• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

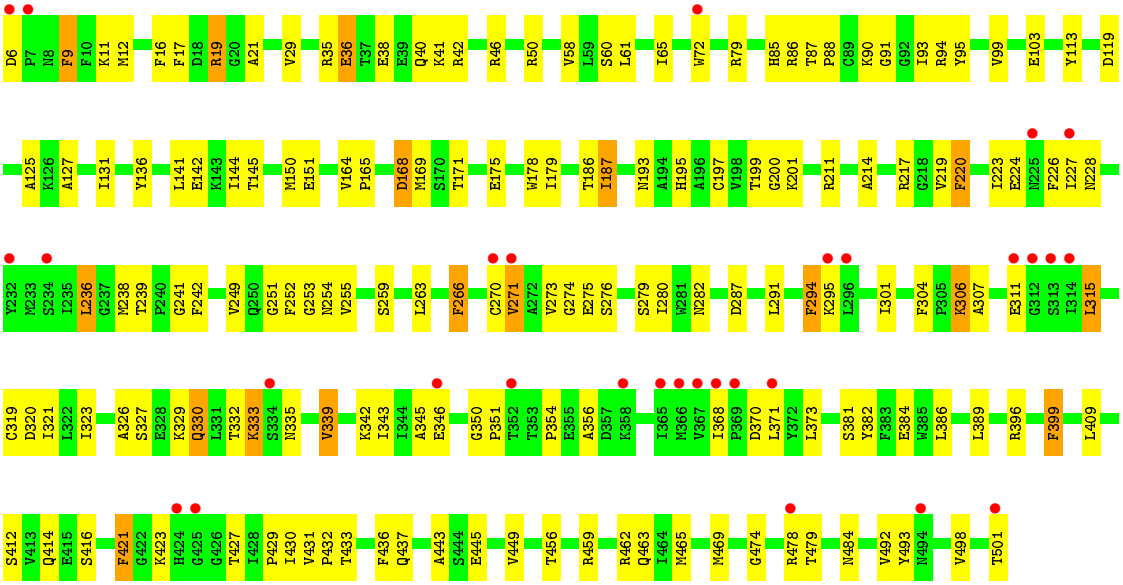
Chain K:





• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.12Å 433.18Å 95.17Å 90.00° 118.74° 90.00°	Depositor
Resolution (Å)	49.71 – 3.62 49.71 – 3.62	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.71-3.62) 98.5 (49.71-3.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.246 , 0.314 0.246 , 0.314	Depositor DCC
R_{free} test set	3751 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	106.8	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 60.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.033 for -h-l,k,h 0.033 for l,k,-h-l 0.038 for h,-k,-h-l 0.039 for -h-l,-k,l 0.420 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	46872	wwPDB-VP
Average B, all atoms (Å^2)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.28	6/3957 (0.2%)	1.12	10/5341 (0.2%)
1	B	0.27	0/3957	0.47	0/5341
1	C	0.31	1/3957 (0.0%)	0.48	2/5341 (0.0%)
1	D	0.27	0/3957	0.47	0/5341
1	E	0.27	0/3957	0.44	0/5341
1	F	0.29	0/3957	0.48	1/5341 (0.0%)
1	G	0.27	0/3957	0.46	0/5341
1	H	0.28	0/3957	0.45	0/5341
1	I	0.28	0/3957	0.47	1/5341 (0.0%)
1	J	0.29	0/3957	0.46	0/5341
1	K	0.31	1/3957 (0.0%)	0.49	1/5341 (0.0%)
1	L	0.29	0/3957	0.46	0/5341
All	All	0.46	8/47484 (0.0%)	0.55	15/64092 (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	A	0	2
1	C	0	2
1	F	0	1
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	TYR	CD1-CE1	49.08	2.12	1.39
1	A	95	TYR	CD2-CE2	48.91	2.12	1.39
1	A	95	TYR	CE1-CZ	-20.18	1.12	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	TYR	CE2-CZ	-20.09	1.12	1.38
1	A	95	TYR	CG-CD1	-17.48	1.16	1.39
1	A	95	TYR	CG-CD2	-17.35	1.16	1.39
1	K	217	ARG	CZ-NH2	-6.67	1.24	1.33
1	C	304	PHE	CE2-CZ	5.07	1.47	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	95	TYR	CE1-CZ-CE2	-35.50	63.01	119.80
1	A	95	TYR	CD1-CG-CD2	-31.30	83.48	117.90
1	A	95	TYR	CG-CD2-CE2	-29.16	97.97	121.30
1	A	95	TYR	CG-CD1-CE1	-28.81	98.25	121.30
1	A	95	TYR	CB-CG-CD2	24.87	135.92	121.00
1	A	95	TYR	CB-CG-CD1	24.42	135.65	121.00
1	A	95	TYR	CD1-CE1-CZ	-12.46	108.58	119.80
1	A	95	TYR	CZ-CE2-CD2	-12.06	108.95	119.80
1	A	95	TYR	CE1-CZ-OH	10.60	148.72	120.10
1	A	95	TYR	OH-CZ-CE2	10.42	148.24	120.10
1	C	303	GLY	C-N-CA	8.75	143.59	121.70
1	F	303	GLY	C-N-CA	8.67	143.37	121.70
1	K	302	LEU	CA-CB-CG	5.60	128.18	115.30
1	I	303	GLY	C-N-CA	5.01	134.23	121.70
1	C	477	LEU	CB-CG-CD1	-5.00	102.50	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	38	GLU	Peptide
1	A	95	TYR	Sidechain
1	C	38	GLU	Peptide
1	C	8	ASN	Peptide
1	F	312	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3874	0	3845	136	0
1	B	3874	0	3845	130	0
1	C	3874	0	3845	131	0
1	D	3874	0	3845	131	0
1	E	3874	0	3845	157	0
1	F	3874	0	3845	138	0
1	G	3874	0	3845	148	0
1	H	3874	0	3845	128	0
1	I	3874	0	3845	135	0
1	J	3874	0	3845	134	0
1	K	3874	0	3843	139	0
1	L	3874	0	3845	131	0
2	A	32	0	18	1	0
2	B	32	0	18	1	0
2	C	32	0	18	4	0
2	D	32	0	18	2	0
2	E	32	0	18	3	0
2	F	32	0	18	4	0
2	G	32	0	18	4	0
2	H	32	0	18	2	0
2	I	32	0	18	3	0
2	J	32	0	18	6	0
2	K	32	0	18	3	0
2	L	32	0	18	3	0
All	All	46872	0	46354	1537	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 16.

All (1537) 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:D:249:VAL:HG12	1:D:323:ILE:HD11	1.24	1.12
1:E:245:LYS:HE3	1:E:320:ASP:CG	1.70	1.10
1:E:245:LYS:HE3	1:E:320:ASP:OD2	1.61	1.01
1:F:249:VAL:HG12	1:F:323:ILE:HD11	1.45	0.98
1:F:87:THR:HG23	1:F:88:PRO:HD3	1.45	0.97
1:L:282:ASN:HD21	1:L:306:LYS:HG3	1.32	0.94
1:E:245:LYS:CE	1:E:320:ASP:OD2	2.16	0.93
1:E:87:THR:HG23	1:E:88:PRO:HD3	1.50	0.93
1:B:249:VAL:HG12	1:B:323:ILE:HD11	1.50	0.92
1:J:87:THR:HG23	1:J:88:PRO:HD3	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:193:ASN:HD22	1:L:389:LEU:HD22	1.34	0.90
1:L:282:ASN:ND2	1:L:306:LYS:O	2.04	0.90
1:G:64:PRO:HD2	1:G:147:ARG:HH12	1.38	0.89
1:A:36:GLU:HG3	1:A:38:GLU:HG2	1.55	0.89
1:E:245:LYS:NZ	1:E:320:ASP:OD2	2.06	0.88
1:E:304:PHE:HD1	1:E:305:PRO:HD2	1.40	0.87
1:B:93:ILE:HG22	1:B:127:ALA:HB3	1.55	0.86
1:C:158:ILE:HD12	1:C:165:PRO:HD3	1.58	0.86
1:A:249:VAL:HG22	1:A:273:VAL:HG22	1.58	0.86
1:I:85:HIS:HB3	1:I:493:TYR:HE1	1.41	0.86
1:K:249:VAL:HG12	1:K:323:ILE:HD11	1.58	0.83
1:G:87:THR:HG23	1:G:88:PRO:HD3	1.60	0.83
1:D:249:VAL:HG12	1:D:323:ILE:CD1	2.06	0.82
1:G:275:GLU:HG2	1:G:276:SER:H	1.44	0.82
1:C:150:MET:HG3	1:F:501:THR:HB	1.62	0.82
1:L:249:VAL:HG12	1:L:323:ILE:HD11	1.61	0.82
1:F:249:VAL:HG12	1:F:323:ILE:CD1	2.10	0.82
1:K:254:ASN:H	1:K:257:LEU:HD12	1.45	0.81
1:A:249:VAL:HG12	1:A:323:ILE:HD11	1.60	0.81
1:L:193:ASN:HD22	1:L:389:LEU:CD2	1.92	0.81
1:D:193:ASN:HD22	1:D:389:LEU:HD22	1.43	0.81
1:I:282:ASN:ND2	1:I:306:LYS:O	2.14	0.81
1:B:294:PHE:CD1	1:B:298:HIS:HE1	1.99	0.81
1:D:93:ILE:HG22	1:D:127:ALA:HB3	1.63	0.80
1:E:245:LYS:HE3	1:E:320:ASP:CB	2.12	0.80
1:G:212:ILE:HG13	1:G:258:HIS:HE1	1.46	0.80
1:J:87:THR:CG2	1:J:88:PRO:HD3	2.11	0.79
1:D:249:VAL:CG1	1:D:323:ILE:HD11	2.09	0.79
1:E:213:SER:HB3	1:E:262:TYR:HE2	1.48	0.79
1:K:93:ILE:HG22	1:K:127:ALA:HB3	1.66	0.78
1:E:93:ILE:HG22	1:E:127:ALA:HB3	1.64	0.78
1:I:85:HIS:HB3	1:I:493:TYR:CE1	2.17	0.78
1:K:257:LEU:HD11	1:K:295:LYS:HE3	1.66	0.78
1:A:93:ILE:HG22	1:A:127:ALA:HB3	1.63	0.78
1:I:150:MET:HG3	1:L:501:THR:HB	1.65	0.78
1:I:330:GLN:O	1:I:335:ASN:ND2	2.17	0.78
1:C:249:VAL:HG12	1:C:323:ILE:HD11	1.64	0.78
1:G:249:VAL:HG12	1:G:323:ILE:HD11	1.66	0.77
1:A:346:GLU:OE1	1:A:478:ARG:NH1	2.17	0.77
1:C:200:GLY:HA2	1:C:211:ARG:HD2	1.65	0.77
1:A:219:VAL:HG13	1:A:373:LEU:HD21	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:9:PHE:HB3	1:I:12:MET:HG2	1.66	0.77
1:B:501:THR:HB	1:E:150:MET:HG3	1.66	0.77
1:E:249:VAL:HG12	1:E:323:ILE:HD11	1.66	0.77
1:G:93:ILE:HG22	1:G:127:ALA:HB3	1.67	0.76
1:L:93:ILE:HG22	1:L:127:ALA:HB3	1.67	0.76
1:G:501:THR:HB	1:J:150:MET:HG3	1.67	0.76
1:H:150:MET:HG3	1:K:501:THR:HB	1.66	0.76
1:A:11:LYS:HG3	1:A:14:GLU:HB2	1.68	0.76
1:I:319:CYS:SG	1:I:320:ASP:N	2.59	0.76
1:J:427:THR:HG22	1:J:429:PRO:HD3	1.68	0.76
1:C:93:ILE:HG22	1:C:127:ALA:HB3	1.68	0.76
1:B:275:GLU:O	1:B:277:ASP:N	2.19	0.75
1:K:38:GLU:HB2	1:K:40:GLN:H	1.50	0.75
1:F:158:ILE:HD12	1:F:165:PRO:HD3	1.67	0.75
1:C:38:GLU:HB2	1:C:40:GLN:H	1.51	0.75
1:F:211:ARG:HA	1:F:214:ALA:HB2	1.66	0.75
1:I:93:ILE:HG22	1:I:127:ALA:HB3	1.67	0.75
1:H:93:ILE:HG22	1:H:127:ALA:HB3	1.69	0.75
1:E:90:LYS:NZ	1:E:199:THR:OG1	2.19	0.75
1:H:201:LYS:O	1:H:211:ARG:NH2	2.20	0.75
1:J:38:GLU:HB2	1:J:40:GLN:H	1.52	0.75
1:E:249:VAL:HG22	1:E:273:VAL:HG22	1.66	0.74
1:I:61:LEU:HD21	1:I:151:GLU:HB3	1.68	0.74
1:K:298:HIS:CE1	1:K:304:PHE:HZ	2.04	0.74
1:J:93:ILE:HG22	1:J:127:ALA:HB3	1.69	0.74
1:J:17:PHE:O	1:J:21:ALA:N	2.17	0.74
1:G:113:TYR:HB2	1:G:371:LEU:HD11	1.68	0.74
1:A:254:ASN:N	1:A:257:LEU:HD12	2.02	0.74
1:G:291:LEU:HD21	1:G:304:PHE:HB2	1.69	0.74
1:K:298:HIS:HE1	1:K:304:PHE:HZ	1.34	0.74
1:I:249:VAL:HG12	1:I:323:ILE:HD11	1.70	0.73
1:J:249:VAL:HG12	1:J:323:ILE:HD11	1.70	0.73
1:B:294:PHE:HD1	1:B:298:HIS:HE1	1.35	0.73
1:E:245:LYS:CE	1:E:320:ASP:CG	2.53	0.73
1:K:319:CYS:SG	1:K:320:ASP:N	2.62	0.73
1:A:36:GLU:HG3	1:A:38:GLU:CG	2.19	0.73
1:D:8:ASN:O	1:D:9:PHE:HD1	1.71	0.73
1:L:327:SER:HB3	1:L:330:GLN:HE22	1.53	0.73
1:K:200:GLY:HA2	1:K:211:ARG:HD2	1.70	0.73
1:K:294:PHE:CE2	1:K:301:ILE:HA	2.24	0.73
1:C:427:THR:HG22	1:C:429:PRO:HD3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:LEU:HD21	1:F:151:GLU:HB3	1.71	0.72
1:A:67:ARG:NH2	1:A:135:ASN:O	2.22	0.72
1:B:90:LYS:NZ	1:B:199:THR:OG1	2.21	0.72
1:I:498:VAL:HB	1:L:72:TRP:HH2	1.54	0.72
1:B:193:ASN:HD22	1:B:389:LEU:HD22	1.53	0.72
1:H:427:THR:HG22	1:H:429:PRO:HD3	1.69	0.72
1:K:327:SER:HB3	1:K:330:GLN:HE22	1.55	0.72
1:K:332:THR:HG23	1:K:334:SER:H	1.53	0.72
1:H:17:PHE:O	1:H:21:ALA:N	2.19	0.71
1:H:287:ASP:OD2	1:H:289:LYS:NZ	2.21	0.71
1:J:319:CYS:SG	1:J:320:ASP:N	2.62	0.71
1:A:65:ILE:HD13	1:A:144:ILE:HG12	1.72	0.71
1:E:219:VAL:HG13	1:E:373:LEU:HD21	1.70	0.71
1:F:242:PHE:HE2	1:F:266:PHE:HB3	1.56	0.71
1:E:328:GLU:OE1	1:E:329:LYS:NZ	2.23	0.71
1:F:378:VAL:HA	1:F:381:SER:HB2	1.72	0.71
1:G:315:LEU:H	1:G:315:LEU:HD23	1.56	0.71
1:B:327:SER:HB3	1:B:330:GLN:HE22	1.55	0.70
1:C:249:VAL:HG22	1:C:273:VAL:HG22	1.74	0.70
1:J:212:ILE:HG13	1:J:258:HIS:HE1	1.55	0.70
1:H:90:LYS:NZ	1:H:199:THR:OG1	2.24	0.70
1:A:270:CYS:SG	1:A:271:VAL:N	2.64	0.70
1:F:141:LEU:HD12	1:F:144:ILE:HD12	1.74	0.70
1:J:249:VAL:HG22	1:J:273:VAL:HG22	1.74	0.70
1:D:271:VAL:HG23	1:D:283:PRO:HA	1.74	0.70
1:F:201:LYS:O	1:F:211:ARG:NH1	2.24	0.69
1:H:58:VAL:HG13	1:K:60:SER:HB2	1.72	0.69
1:I:219:VAL:HG13	1:I:373:LEU:HD21	1.72	0.69
1:I:394:TYR:HB2	1:I:445:GLU:HG3	1.73	0.69
1:K:90:LYS:NZ	1:K:199:THR:OG1	2.22	0.69
1:A:195:HIS:CE1	1:B:87:THR:HG22	2.26	0.69
1:L:432:PRO:HG2	1:L:437:GLN:HG2	1.73	0.69
1:A:304:PHE:CD1	1:A:305:PRO:HD3	2.28	0.69
1:F:168:ASP:N	1:F:171:THR:OG1	2.26	0.69
1:C:366:MET:CE	1:C:477:LEU:HD11	2.22	0.69
1:A:56:ASN:HA	1:D:62:SER:HB3	1.74	0.69
1:G:150:MET:HG3	1:J:501:THR:HB	1.75	0.69
1:K:270:CYS:SG	1:K:271:VAL:N	2.66	0.68
1:E:119:ASP:HA	2:E:601:XEG:HAI	1.76	0.68
1:C:60:SER:HB2	1:F:58:VAL:HG13	1.75	0.68
1:L:85:HIS:HB3	1:L:493:TYR:HE1	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:THR:HG22	1:E:195:HIS:CE1	2.29	0.68
1:C:262:TYR:HD1	1:C:265:ARG:HD2	1.59	0.68
1:A:329:LYS:H	1:A:351:PRO:HA	1.57	0.68
1:D:319:CYS:SG	1:D:320:ASP:N	2.67	0.68
1:F:7:PRO:HD2	1:F:329:LYS:HD2	1.75	0.68
1:J:219:VAL:HG13	1:J:373:LEU:HD21	1.74	0.68
1:J:459:ARG:NH2	2:J:601:XEG:OAH	2.27	0.68
1:I:72:TRP:HH2	1:L:498:VAL:HB	1.58	0.68
1:E:246:THR:HG22	1:E:269:LYS:HB3	1.76	0.68
1:K:280:ILE:HD11	1:K:301:ILE:HD11	1.76	0.68
1:K:294:PHE:CE1	1:K:304:PHE:CE1	2.82	0.68
1:F:90:LYS:HD3	1:F:378:VAL:HG23	1.75	0.67
1:E:304:PHE:CD1	1:E:305:PRO:HD2	2.26	0.67
1:H:212:ILE:HG13	1:H:258:HIS:HE1	1.57	0.67
1:K:249:VAL:HG22	1:K:273:VAL:HG22	1.75	0.67
1:D:90:LYS:NZ	1:D:199:THR:OG1	2.27	0.67
1:J:202:PRO:HG2	1:J:205:GLN:HG3	1.75	0.67
1:H:219:VAL:HG13	1:H:373:LEU:HD21	1.76	0.67
1:I:414:GLN:OE1	1:I:430:ILE:HG12	1.94	0.67
1:E:65:ILE:HD13	1:E:144:ILE:HG12	1.75	0.67
1:H:500:PHE:HB3	1:J:500:PHE:HB3	1.76	0.67
1:H:275:GLU:HG2	1:H:276:SER:H	1.59	0.67
1:H:207:GLY:O	1:H:387:LYS:NZ	2.22	0.67
1:I:280:ILE:HD11	1:I:301:ILE:HD11	1.77	0.66
1:I:19:ARG:NE	1:I:479:THR:HG21	2.09	0.66
1:I:396:ARG:NH1	1:K:456:THR:OG1	2.28	0.66
1:B:315:LEU:H	1:B:315:LEU:HD23	1.60	0.66
1:A:36:GLU:OE1	1:A:44:ARG:NH2	2.27	0.66
1:J:119:ASP:HA	2:J:601:XEG:HAI	1.77	0.66
1:F:94:ARG:HG3	1:F:169:MET:HB2	1.77	0.66
1:K:275:GLU:HG2	1:K:276:SER:H	1.59	0.66
1:B:29:VAL:HB	1:B:41:LYS:HE3	1.77	0.66
1:H:213:SER:HB3	1:H:262:TYR:HE2	1.60	0.66
1:K:383:PHE:HA	1:K:386:LEU:HD12	1.78	0.66
1:L:427:THR:HG22	1:L:429:PRO:HD3	1.78	0.66
1:C:181:ASP:OD1	1:E:499:THR:OG1	2.12	0.66
1:F:294:PHE:CD2	1:F:301:ILE:HD12	2.30	0.66
1:F:79:ARG:HH11	1:F:127:ALA:HB2	1.61	0.66
1:K:65:ILE:HD13	1:K:144:ILE:HG12	1.77	0.66
1:L:90:LYS:NZ	1:L:199:THR:OG1	2.29	0.66
1:A:501:THR:HB	1:D:150:MET:HG3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:MET:HG3	1:E:501:THR:HB	1.76	0.66
1:K:113:TYR:HB2	1:K:371:LEU:HD11	1.78	0.66
1:D:323:ILE:HG22	1:D:345:ALA:HB3	1.76	0.66
1:H:294:PHE:CD2	1:H:301:ILE:HD12	2.31	0.66
1:B:271:VAL:HG23	1:B:283:PRO:HA	1.76	0.66
1:B:383:PHE:HA	1:B:386:LEU:HD12	1.78	0.66
1:J:337:PRO:O	1:J:363:ARG:NH2	2.29	0.65
1:B:72:TRP:CH2	1:E:498:VAL:HB	2.32	0.65
1:H:304:PHE:H	1:H:307:ALA:HB3	1.59	0.65
1:I:90:LYS:NZ	1:I:199:THR:OG1	2.30	0.65
1:J:275:GLU:HG2	1:J:276:SER:H	1.60	0.65
1:L:249:VAL:HG22	1:L:273:VAL:HG22	1.77	0.65
1:A:254:ASN:H	1:A:257:LEU:HD12	1.62	0.65
1:C:8:ASN:ND2	1:C:355:GLU:OE1	2.30	0.65
1:G:90:LYS:NZ	1:G:199:THR:OG1	2.24	0.65
1:C:113:TYR:HB2	1:C:371:LEU:HD11	1.79	0.65
1:C:58:VAL:HG13	1:F:60:SER:HB2	1.78	0.65
1:E:291:LEU:HD11	1:E:307:ALA:HB2	1.77	0.65
1:I:8:ASN:O	1:I:329:LYS:NZ	2.27	0.65
1:L:319:CYS:SG	1:L:320:ASP:N	2.69	0.65
1:E:196:ALA:HB2	1:E:388:ASN:HB2	1.79	0.65
1:F:90:LYS:NZ	1:F:381:SER:HB3	2.12	0.65
1:E:61:LEU:HD21	1:E:151:GLU:HB3	1.79	0.64
1:I:211:ARG:HA	1:I:214:ALA:HB2	1.78	0.64
1:E:291:LEU:HD21	1:E:304:PHE:HB2	1.78	0.64
1:C:24:VAL:HG12	1:C:28:LEU:HG	1.78	0.64
1:B:61:LEU:HD21	1:B:151:GLU:HB3	1.80	0.64
1:L:113:TYR:HB2	1:L:371:LEU:HD11	1.78	0.64
1:I:498:VAL:HB	1:L:72:TRP:CH2	2.32	0.64
1:F:258:HIS:HA	1:F:261:ARG:HB3	1.80	0.64
1:F:249:VAL:HG22	1:F:273:VAL:HG22	1.80	0.64
1:L:9:PHE:CZ	1:L:354:PRO:HD2	2.33	0.64
1:A:90:LYS:NZ	1:A:199:THR:OG1	2.29	0.64
1:B:168:ASP:N	1:B:171:THR:OG1	2.31	0.64
1:B:323:ILE:HG22	1:B:345:ALA:HB3	1.78	0.64
1:J:323:ILE:HG22	1:J:345:ALA:HB3	1.80	0.64
1:I:456:THR:OG1	1:J:396:ARG:NH1	2.29	0.64
1:J:274:GLY:HA3	1:J:314:ILE:HD13	1.80	0.64
1:F:394:TYR:HB3	1:F:448:ILE:HD12	1.80	0.64
1:K:315:LEU:HD22	1:K:322:LEU:HD21	1.78	0.63
1:C:456:THR:OG1	1:D:396:ARG:NH1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:275:GLU:HG2	1:I:276:SER:H	1.63	0.63
1:I:427:THR:HG22	1:I:429:PRO:HD3	1.81	0.63
1:J:61:LEU:HD21	1:J:151:GLU:HB3	1.80	0.63
1:J:207:GLY:O	1:J:387:LYS:NZ	2.25	0.63
1:E:328:GLU:HG2	1:E:329:LYS:HG3	1.81	0.63
1:H:412:SER:HB3	1:L:432:PRO:HA	1.81	0.63
1:L:193:ASN:ND2	1:L:389:LEU:HD22	2.10	0.63
1:J:168:ASP:N	1:J:171:THR:OG1	2.29	0.63
1:G:60:SER:HB2	1:J:58:VAL:HG13	1.80	0.63
1:B:126:LYS:NZ	1:B:168:ASP:OD2	2.29	0.63
1:B:204:SER:OG	1:F:495:GLU:OE1	2.17	0.63
1:G:65:ILE:HD13	1:G:144:ILE:HG12	1.79	0.63
1:K:79:ARG:HH11	1:K:127:ALA:HB2	1.63	0.63
1:A:113:TYR:HB2	1:A:371:LEU:HD11	1.79	0.63
1:B:11:LYS:HB2	1:B:14:GLU:HB2	1.80	0.63
1:D:11:LYS:HB2	1:D:14:GLU:HB2	1.81	0.63
1:F:211:ARG:NE	1:F:384:GLU:OE2	2.32	0.63
1:F:79:ARG:HD2	1:F:127:ALA:HB2	1.79	0.63
1:A:499:THR:HG22	1:A:501:THR:HG23	1.80	0.63
1:C:107:LEU:HD23	1:C:126:LYS:HE2	1.80	0.63
1:E:245:LYS:HE3	1:E:320:ASP:HB3	1.80	0.63
1:F:158:ILE:HD12	1:F:165:PRO:CD	2.29	0.63
1:G:249:VAL:HG22	1:G:273:VAL:HG22	1.81	0.62
1:G:319:CYS:SG	1:G:320:ASP:N	2.72	0.62
1:A:150:MET:HG3	1:D:501:THR:HB	1.81	0.62
1:A:383:PHE:HA	1:A:386:LEU:HD12	1.81	0.62
1:J:107:LEU:HD23	1:J:126:LYS:HE2	1.81	0.62
1:L:315:LEU:H	1:L:315:LEU:HD23	1.64	0.62
1:L:85:HIS:HB3	1:L:493:TYR:CE1	2.33	0.62
1:L:294:PHE:CE2	1:L:301:ILE:HA	2.34	0.62
1:I:94:ARG:HG3	1:I:169:MET:HB2	1.81	0.62
1:L:19:ARG:NE	1:L:479:THR:HG21	2.15	0.62
1:D:378:VAL:O	1:D:382:TYR:N	2.32	0.62
1:I:19:ARG:HE	1:I:479:THR:HG21	1.64	0.62
1:J:294:PHE:CE2	1:J:301:ILE:HG13	2.33	0.62
1:L:275:GLU:HG2	1:L:276:SER:H	1.64	0.62
1:E:346:GLU:OE1	1:E:478:ARG:NH1	2.32	0.62
1:G:327:SER:HB3	1:G:330:GLN:HE22	1.63	0.62
1:H:337:PRO:O	1:H:363:ARG:NH2	2.32	0.62
1:J:90:LYS:HZ1	1:J:166:ALA:HB2	1.65	0.62
1:E:48:ILE:O	1:E:52:ILE:HG13	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:38:GLU:HB2	1:L:40:GLN:H	1.64	0.62
1:J:24:VAL:HG13	1:J:483:VAL:HG23	1.82	0.62
1:A:433:THR:HG23	1:A:436:PHE:H	1.64	0.62
1:A:58:VAL:HG13	1:D:60:SER:OG	2.00	0.62
1:E:304:PHE:H	1:E:307:ALA:HB3	1.65	0.62
1:E:29:VAL:HB	1:E:41:LYS:HD3	1.81	0.62
1:F:200:GLY:HA2	1:F:211:ARG:HD2	1.82	0.62
1:G:300:THR:HG22	1:G:301:ILE:N	2.15	0.62
1:A:498:VAL:HB	1:D:72:TRP:CH2	2.35	0.61
1:G:400:LYS:HB2	1:H:455:TYR:HB2	1.81	0.61
1:H:240:PRO:O	1:H:242:PHE:N	2.32	0.61
1:H:501:THR:HB	1:K:150:MET:HG3	1.80	0.61
1:G:201:LYS:O	1:G:211:ARG:NH2	2.33	0.61
1:D:249:VAL:CG2	1:D:273:VAL:HG22	2.29	0.61
1:E:250:GLN:HE22	1:E:330:GLN:HE21	1.47	0.61
1:G:456:THR:OG1	1:L:396:ARG:NH1	2.28	0.61
1:J:213:SER:HB3	1:J:262:TYR:HE2	1.64	0.61
1:J:480:ALA:HA	1:J:483:VAL:CG1	2.29	0.61
1:H:396:ARG:NH2	1:L:119:ASP:O	2.33	0.61
1:K:298:HIS:HE1	1:K:304:PHE:CZ	2.18	0.61
1:A:81:GLN:NE2	1:A:163:ASP:OD1	2.33	0.61
1:C:303:GLY:O	1:C:304:PHE:HD1	1.83	0.61
1:G:181:ASP:OD1	1:H:499:THR:OG1	2.19	0.61
1:G:94:ARG:HG3	1:G:169:MET:HB2	1.83	0.61
1:B:79:ARG:HH11	1:B:127:ALA:HB2	1.64	0.61
1:C:57:HIS:CD2	1:F:155:LYS:HE3	2.36	0.61
1:I:17:PHE:O	1:I:21:ALA:N	2.32	0.61
1:I:433:THR:HG23	1:I:436:PHE:H	1.65	0.61
1:C:378:VAL:HA	1:C:381:SER:HB2	1.82	0.61
1:E:81:GLN:NE2	1:E:163:ASP:OD1	2.33	0.61
1:F:319:CYS:SG	1:F:320:ASP:N	2.74	0.61
1:G:270:CYS:SG	1:G:271:VAL:N	2.73	0.61
1:H:323:ILE:HG22	1:H:345:ALA:HB3	1.83	0.61
1:J:119:ASP:O	1:K:396:ARG:NH2	2.30	0.61
1:A:48:ILE:O	1:A:52:ILE:HG13	2.00	0.61
1:F:298:HIS:CE1	1:F:304:PHE:HZ	2.19	0.61
1:H:421:PHE:CZ	1:H:423:LYS:HB2	2.36	0.61
1:H:87:THR:OG1	1:H:88:PRO:HD3	2.01	0.61
1:L:433:THR:HG23	1:L:436:PHE:H	1.65	0.61
1:A:432:PRO:HA	1:F:412:SER:HB3	1.81	0.60
1:C:79:ARG:HH11	1:C:127:ALA:HB2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:219:VAL:HG13	1:L:373:LEU:HD21	1.83	0.60
1:C:394:TYR:HB2	1:C:445:GLU:HG3	1.82	0.60
1:D:36:GLU:OE1	1:D:41:LYS:HG2	2.02	0.60
1:F:113:TYR:HB2	1:F:371:LEU:HD11	1.82	0.60
1:G:303:GLY:O	1:G:304:PHE:HD1	1.83	0.60
1:C:366:MET:CE	1:C:475:LEU:HD23	2.30	0.60
1:F:427:THR:HG22	1:F:429:PRO:HD3	1.83	0.60
1:E:87:THR:CG2	1:E:88:PRO:HD3	2.27	0.60
1:K:131:ILE:HB	1:K:136:TYR:CE2	2.37	0.60
1:A:196:ALA:HB2	1:A:388:ASN:HB2	1.82	0.60
1:I:294:PHE:CE2	1:I:301:ILE:HA	2.35	0.60
1:J:225:ASN:ND2	1:J:458:GLU:HA	2.17	0.60
1:F:87:THR:CG2	1:F:88:PRO:HD3	2.26	0.60
1:H:274:GLY:HA3	1:H:314:ILE:HD13	1.82	0.60
1:E:67:ARG:NH2	1:E:135:ASN:O	2.35	0.60
1:H:433:THR:HG23	1:H:436:PHE:H	1.67	0.60
1:I:113:TYR:HB2	1:I:371:LEU:HD11	1.83	0.60
1:C:72:TRP:HH2	1:F:498:VAL:HB	1.66	0.60
1:H:21:ALA:HB1	1:H:49:LEU:HD23	1.83	0.60
1:D:168:ASP:N	1:D:171:THR:OG1	2.34	0.59
1:G:38:GLU:HB2	1:G:40:GLN:H	1.66	0.59
1:G:490:PHE:HE2	1:G:494:ASN:HD22	1.50	0.59
1:J:136:TYR:HB2	1:J:141:LEU:CD1	2.33	0.59
1:I:249:VAL:HG22	1:I:273:VAL:HG22	1.83	0.59
1:L:315:LEU:HD12	1:L:339:VAL:HG22	1.84	0.59
1:A:282:ASN:ND2	1:A:306:LYS:O	2.34	0.59
1:D:219:VAL:HG13	1:D:373:LEU:HD21	1.82	0.59
1:C:72:TRP:CH2	1:F:498:VAL:HB	2.36	0.59
1:J:79:ARG:HH11	1:J:127:ALA:HB2	1.67	0.59
1:K:254:ASN:N	1:K:257:LEU:HD12	2.17	0.59
1:B:58:VAL:HG13	1:E:60:SER:OG	2.03	0.59
1:H:249:VAL:HG12	1:H:323:ILE:HD11	1.83	0.59
1:E:12:MET:HG2	1:E:329:LYS:HD3	1.84	0.59
1:K:303:GLY:O	1:K:304:PHE:HD1	1.85	0.59
1:G:300:THR:HG22	1:G:301:ILE:H	1.65	0.59
1:J:10:PHE:O	1:J:12:MET:N	2.35	0.59
1:G:79:ARG:HD3	1:G:157:PHE:HB3	1.85	0.59
1:J:240:PRO:O	1:J:242:PHE:N	2.36	0.59
1:J:280:ILE:HD11	1:J:301:ILE:HD11	1.84	0.59
1:G:498:VAL:HB	1:J:72:TRP:HH2	1.68	0.59
1:J:11:LYS:HB2	1:J:14:GLU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:118:VAL:HG23	1:K:120:VAL:HG23	1.83	0.59
1:K:249:VAL:HA	1:K:323:ILE:HG13	1.85	0.59
1:D:213:SER:HA	1:D:258:HIS:ND1	2.18	0.58
1:G:323:ILE:HG22	1:G:345:ALA:HB3	1.85	0.58
1:G:332:THR:HG23	1:G:334:SER:H	1.68	0.58
1:K:6:ASP:HB3	1:K:332:THR:HG21	1.85	0.58
1:L:142:GLU:HG3	1:L:178:TRP:CD2	2.38	0.58
1:L:270:CYS:SG	1:L:271:VAL:N	2.76	0.58
1:H:6:ASP:N	1:H:332:THR:HG1	2.00	0.58
1:B:304:PHE:H	1:B:307:ALA:HB3	1.68	0.58
1:C:90:LYS:HG3	1:C:122:PHE:CD1	2.38	0.58
1:C:294:PHE:CD2	1:C:301:ILE:HD12	2.38	0.58
1:G:211:ARG:HA	1:G:214:ALA:HB2	1.85	0.58
1:J:142:GLU:HG3	1:J:178:TRP:CE2	2.39	0.58
1:D:249:VAL:HG22	1:D:273:VAL:HG22	1.86	0.58
1:A:456:THR:OG1	1:F:396:ARG:NH1	2.37	0.58
1:H:113:TYR:HB2	1:H:371:LEU:HD11	1.85	0.58
1:L:414:GLN:OE1	1:L:430:ILE:HG12	2.04	0.58
1:G:429:PRO:HA	1:L:416:SER:HB3	1.85	0.58
1:G:58:VAL:HG13	1:J:60:SER:HB2	1.85	0.58
1:H:212:ILE:HG13	1:H:258:HIS:CE1	2.39	0.58
1:I:58:VAL:HG13	1:L:60:SER:HB2	1.86	0.58
1:B:94:ARG:NH1	1:B:103:GLU:OE2	2.37	0.58
1:H:233:MET:O	1:H:237:GLY:N	2.36	0.58
1:D:46:ARG:HG2	1:D:50:ARG:HH11	1.69	0.58
1:D:473:LEU:O	1:D:475:LEU:N	2.36	0.58
1:I:208:ILE:HG22	1:I:211:ARG:HD3	1.86	0.58
1:L:321:ILE:HA	1:L:343:ILE:O	2.04	0.58
1:D:350:GLY:N	1:D:370:ASP:OD2	2.37	0.58
1:I:501:THR:HB	1:L:150:MET:HG3	1.86	0.58
1:J:480:ALA:HA	1:J:483:VAL:HG12	1.84	0.58
1:E:385:TRP:O	1:E:389:LEU:HG	2.04	0.57
1:F:270:CYS:SG	1:F:271:VAL:N	2.77	0.57
1:F:414:GLN:HB2	1:F:429:PRO:HD2	1.87	0.57
1:I:72:TRP:CH2	1:L:498:VAL:HB	2.39	0.57
1:L:323:ILE:HG22	1:L:345:ALA:HB3	1.84	0.57
1:C:141:LEU:HD12	1:C:144:ILE:HD12	1.87	0.57
1:G:146:ARG:HG2	1:G:182:THR:OG1	2.04	0.57
1:K:146:ARG:HG2	1:K:182:THR:OG1	2.04	0.57
1:A:498:VAL:HB	1:D:72:TRP:HH2	1.69	0.57
1:F:394:TYR:HB2	1:F:445:GLU:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:432:PRO:HA	1:J:412:SER:HB3	1.86	0.57
1:J:433:THR:HG23	1:J:436:PHE:H	1.69	0.57
1:K:21:ALA:HB1	1:K:49:LEU:HD23	1.87	0.57
1:A:396:ARG:NE	2:B:601:XEG:OAF	2.34	0.57
1:A:87:THR:HB	1:A:88:PRO:HD3	1.87	0.57
1:H:294:PHE:CE2	1:H:301:ILE:HA	2.39	0.57
1:C:400:LYS:NZ	1:E:458:GLU:OE1	2.36	0.57
1:G:79:ARG:HH11	1:G:127:ALA:HB2	1.69	0.57
1:A:12:MET:SD	1:A:329:LYS:HD2	2.44	0.57
1:B:270:CYS:SG	1:B:271:VAL:N	2.77	0.57
1:B:91:GLY:HA3	1:B:125:ALA:O	2.04	0.57
1:C:118:VAL:HG23	1:C:120:VAL:HG23	1.87	0.57
1:D:79:ARG:HH11	1:D:127:ALA:HB2	1.69	0.57
1:I:291:LEU:CD1	1:I:304:PHE:HD2	2.17	0.57
1:B:60:SER:OG	1:E:58:VAL:HG13	2.05	0.57
1:D:10:PHE:O	1:D:12:MET:N	2.36	0.57
1:G:212:ILE:HG13	1:G:258:HIS:CE1	2.34	0.57
1:G:195:HIS:CD2	1:H:87:THR:CG2	2.88	0.57
1:H:72:TRP:HH2	1:K:498:VAL:HB	1.70	0.57
1:E:242:PHE:CE2	1:E:266:PHE:HB3	2.39	0.57
1:C:258:HIS:HA	1:C:261:ARG:HB3	1.85	0.57
1:I:294:PHE:CD2	1:I:301:ILE:HD12	2.40	0.57
1:I:323:ILE:HG22	1:I:345:ALA:HB3	1.87	0.57
1:A:429:PRO:HA	1:F:416:SER:HB3	1.86	0.57
1:B:303:GLY:O	1:B:304:PHE:HD1	1.87	0.57
1:E:29:VAL:HG12	1:E:41:LYS:HB2	1.87	0.57
1:H:168:ASP:N	1:H:171:THR:OG1	2.37	0.57
1:L:242:PHE:HE2	1:L:266:PHE:HB3	1.69	0.57
1:I:332:THR:OG1	1:I:333:LYS:N	2.37	0.56
1:F:334:SER:O	1:F:338:ARG:NH2	2.38	0.56
1:F:36:GLU:HG3	1:F:37:THR:N	2.20	0.56
1:G:337:PRO:O	1:G:363:ARG:NH2	2.38	0.56
1:B:65:ILE:HD13	1:B:144:ILE:HG12	1.85	0.56
1:K:88:PRO:HG2	1:K:122:PHE:CE2	2.41	0.56
1:L:9:PHE:HZ	1:L:354:PRO:HD2	1.69	0.56
1:B:378:VAL:O	1:B:382:TYR:N	2.38	0.56
1:C:37:THR:HA	1:C:41:LYS:HD2	1.87	0.56
1:E:254:ASN:H	1:E:257:LEU:HD12	1.70	0.56
1:H:60:SER:HB2	1:K:58:VAL:HG13	1.88	0.56
1:L:186:THR:OG1	1:L:187:ILE:N	2.38	0.56
1:L:274:GLY:HA2	1:L:279:SER:HA	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:323:ILE:HG22	1:K:345:ALA:HB3	1.87	0.56
1:L:165:PRO:HD2	1:L:197:CYS:O	2.05	0.56
1:A:213:SER:HB3	1:A:262:TYR:HE2	1.71	0.56
1:A:348:ALA:HB3	1:A:351:PRO:HG3	1.87	0.56
1:B:151:GLU:HG3	1:E:57:HIS:HE2	1.71	0.56
1:D:6:ASP:O	1:D:8:ASN:N	2.39	0.56
1:B:211:ARG:HA	1:B:214:ALA:HB2	1.88	0.56
1:C:498:VAL:HB	1:F:72:TRP:CH2	2.40	0.56
1:E:13:VAL:HA	1:E:16:PHE:CD2	2.40	0.56
1:G:432:PRO:HA	1:L:412:SER:HB3	1.88	0.56
1:I:85:HIS:CD2	1:I:86:ARG:HG2	2.41	0.56
1:D:65:ILE:HD13	1:D:144:ILE:HG12	1.88	0.56
1:D:331:LEU:HA	1:D:335:ASN:HD21	1.70	0.56
1:I:458:GLU:OE1	1:J:400:LYS:NZ	2.37	0.56
1:L:61:LEU:HD21	1:L:151:GLU:HB2	1.88	0.56
1:L:200:GLY:HA2	1:L:211:ARG:HD2	1.88	0.56
1:C:181:ASP:O	1:C:185:SER:OG	2.18	0.56
1:A:60:SER:HB2	1:D:58:VAL:CG1	2.36	0.56
1:I:36:GLU:HG3	1:I:44:ARG:HH21	1.69	0.56
1:K:255:VAL:O	1:K:259:SER:OG	2.16	0.56
1:L:329:LYS:H	1:L:351:PRO:HA	1.71	0.56
1:A:94:ARG:HE	1:A:169:MET:HG3	1.70	0.56
1:F:249:VAL:CG2	1:F:273:VAL:HG22	2.36	0.56
1:I:321:ILE:HA	1:I:343:ILE:O	2.05	0.56
1:J:90:LYS:NZ	1:J:199:THR:OG1	2.35	0.56
1:J:243:GLY:O	1:J:245:LYS:N	2.39	0.56
1:C:213:SER:HB3	1:C:262:TYR:HE2	1.70	0.56
1:C:296:LEU:HD21	1:E:35:ARG:HG3	1.87	0.56
1:E:113:TYR:HB2	1:E:371:LEU:HD11	1.87	0.56
1:J:270:CYS:SG	1:J:271:VAL:N	2.77	0.56
1:L:94:ARG:NH2	1:L:169:MET:SD	2.79	0.56
1:L:282:ASN:ND2	1:L:306:LYS:HG3	2.13	0.56
1:L:94:ARG:HD3	1:L:169:MET:HB2	1.88	0.56
1:C:158:ILE:CD1	1:C:165:PRO:HD3	2.34	0.55
1:J:382:TYR:CZ	1:J:386:LEU:HD11	2.40	0.55
1:D:421:PHE:CZ	1:D:423:LYS:HB2	2.42	0.55
1:H:141:LEU:HD12	1:H:144:ILE:HD12	1.88	0.55
1:H:213:SER:HB3	1:H:262:TYR:CE2	2.41	0.55
1:K:95:TYR:OH	1:K:145:THR:HG22	2.06	0.55
1:L:332:THR:OG1	1:L:333:LYS:N	2.39	0.55
1:I:165:PRO:HD2	1:I:197:CYS:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:217:ARG:CZ	1:K:450:HIS:CE1	2.78	0.55
1:D:87:THR:OG1	1:D:88:PRO:HD3	2.07	0.55
1:F:107:LEU:HD23	1:F:126:LYS:HE2	1.88	0.55
1:G:254:ASN:H	1:G:257:LEU:HD12	1.69	0.55
1:G:358:LYS:HA	1:G:361:LEU:HD22	1.86	0.55
1:K:195:HIS:O	1:K:201:LYS:HE3	2.06	0.55
1:B:400:LYS:HB2	1:F:455:TYR:HB2	1.88	0.55
1:E:238:MET:HE3	1:E:342:LYS:HB2	1.87	0.55
1:G:280:ILE:HD11	1:G:301:ILE:HD11	1.88	0.55
1:J:21:ALA:HB1	1:J:49:LEU:HD23	1.88	0.55
1:C:61:LEU:HD21	1:C:151:GLU:HB2	1.88	0.55
1:H:271:VAL:HG23	1:H:283:PRO:HA	1.88	0.55
1:H:249:VAL:HG22	1:H:273:VAL:HG22	1.89	0.55
1:K:331:LEU:HB2	1:K:352:THR:HA	1.89	0.55
1:C:211:ARG:HA	1:C:214:ALA:HB2	1.87	0.55
1:K:217:ARG:NE	1:K:450:HIS:ND1	2.55	0.55
1:A:79:ARG:NH2	1:A:163:ASP:OD2	2.39	0.55
1:B:249:VAL:HA	1:B:323:ILE:HG13	1.89	0.55
1:A:154:LYS:HE3	1:E:189:HIS:CD2	2.41	0.55
1:B:58:VAL:HG13	1:E:60:SER:HG	1.72	0.55
1:C:46:ARG:O	1:C:50:ARG:HG3	2.07	0.55
1:B:280:ILE:HD11	1:B:301:ILE:HD11	1.90	0.54
1:D:383:PHE:HD1	1:D:449:VAL:HG13	1.72	0.54
1:D:154:LYS:HB3	1:F:189:HIS:HE2	1.72	0.54
1:I:65:ILE:HD13	1:I:144:ILE:HG12	1.90	0.54
1:J:46:ARG:O	1:J:50:ARG:HG3	2.07	0.54
1:A:246:THR:HA	1:A:269:LYS:O	2.07	0.54
1:C:291:LEU:HD21	1:C:304:PHE:HB2	1.88	0.54
1:C:315:LEU:HD23	1:C:315:LEU:H	1.72	0.54
1:H:107:LEU:HD23	1:H:126:LYS:HE2	1.87	0.54
1:K:94:ARG:NH1	1:K:103:GLU:OE2	2.40	0.54
1:B:118:VAL:HG23	1:B:120:VAL:HG23	1.90	0.54
1:B:193:ASN:HD22	1:B:389:LEU:CD2	2.20	0.54
1:C:242:PHE:HE2	1:C:266:PHE:HB3	1.71	0.54
1:F:303:GLY:O	1:F:304:PHE:HD1	1.90	0.54
1:H:255:VAL:O	1:H:259:SER:OG	2.21	0.54
1:D:303:GLY:O	1:D:304:PHE:HD1	1.90	0.54
1:F:66:ARG:HD3	1:F:72:TRP:CE2	2.41	0.54
1:H:396:ARG:NH1	1:L:456:THR:OG1	2.40	0.54
1:A:386:LEU:HD22	1:F:392:VAL:HG13	1.89	0.54
1:A:36:GLU:CG	1:A:38:GLU:HG2	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ASP:OD1	1:A:6:ASP:N	2.41	0.54
1:B:421:PHE:CZ	1:B:423:LYS:HB3	2.43	0.54
1:B:6:ASP:N	1:B:6:ASP:OD1	2.41	0.54
1:D:195:HIS:O	1:D:201:LYS:HE3	2.07	0.54
1:D:44:ARG:O	1:D:48:ILE:HG12	2.08	0.54
1:F:65:ILE:HD13	1:F:144:ILE:HG12	1.89	0.54
1:F:89:CYS:HB3	1:F:125:ALA:HB2	1.88	0.54
1:I:332:THR:N	1:I:335:ASN:OD1	2.31	0.54
1:L:168:ASP:N	1:L:171:THR:OG1	2.33	0.54
1:A:91:GLY:HA3	1:A:125:ALA:O	2.08	0.54
1:A:311:GLU:HG3	1:A:312:GLY:H	1.73	0.54
1:C:89:CYS:HB3	1:C:125:ALA:HB2	1.90	0.54
1:C:242:PHE:CE2	1:C:266:PHE:HB3	2.43	0.54
1:C:294:PHE:CE2	1:C:301:ILE:HA	2.43	0.54
1:G:195:HIS:CD2	1:H:87:THR:HG21	2.43	0.54
1:K:230:ALA:HA	1:K:233:MET:HB2	1.89	0.54
1:A:186:THR:OG1	1:A:187:ILE:N	2.41	0.54
1:B:198:VAL:O	1:B:201:LYS:NZ	2.35	0.54
1:C:366:MET:HE1	1:C:477:LEU:HD11	1.88	0.54
1:C:414:GLN:HB2	1:C:429:PRO:HD2	1.89	0.54
1:K:242:PHE:HE2	1:K:266:PHE:HB3	1.73	0.54
1:A:319:CYS:SG	1:A:320:ASP:N	2.81	0.54
1:B:311:GLU:HG3	1:B:312:GLY:H	1.73	0.54
1:I:259:SER:O	1:I:263:LEU:HB2	2.08	0.54
1:I:324:PRO:HG2	1:I:351:PRO:HG2	1.90	0.54
1:K:298:HIS:CE1	1:K:304:PHE:CZ	2.92	0.54
1:C:158:ILE:CD1	1:C:165:PRO:CD	2.86	0.54
1:D:165:PRO:HD2	1:D:197:CYS:O	2.08	0.54
1:G:195:HIS:O	1:G:201:LYS:HE3	2.07	0.54
1:G:394:TYR:HB2	1:G:445:GLU:HG3	1.88	0.54
1:C:394:TYR:HB3	1:C:448:ILE:HD12	1.89	0.53
1:E:238:MET:CE	1:E:245:LYS:HE2	2.38	0.53
1:E:294:PHE:CE2	1:E:301:ILE:HG13	2.43	0.53
1:I:165:PRO:HG2	1:I:198:VAL:HG23	1.90	0.53
1:B:338:ARG:O	1:B:363:ARG:NH1	2.41	0.53
1:J:225:ASN:HD21	1:J:458:GLU:HA	1.73	0.53
1:B:427:THR:HG22	1:B:429:PRO:HD3	1.90	0.53
1:C:158:ILE:HD12	1:C:165:PRO:CD	2.32	0.53
1:D:17:PHE:O	1:D:21:ALA:N	2.38	0.53
1:H:79:ARG:HH11	1:H:127:ALA:HB2	1.73	0.53
1:C:288:PRO:O	1:C:292:GLU:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ARG:O	1:C:48:ILE:HG12	2.07	0.53
1:F:107:LEU:HB3	1:F:126:LYS:HG2	1.88	0.53
1:D:414:GLN:HB2	1:D:429:PRO:HD2	1.90	0.53
1:D:498:VAL:HG13	1:D:498:VAL:O	2.09	0.53
1:F:333:LYS:HE2	1:F:355:GLU:HG2	1.89	0.53
1:G:246:THR:HA	1:G:269:LYS:O	2.09	0.53
1:H:243:GLY:O	1:H:245:LYS:N	2.41	0.53
1:J:480:ALA:C	1:J:483:VAL:HG12	2.28	0.53
1:K:61:LEU:HD21	1:K:151:GLU:HB3	1.88	0.53
1:I:412:SER:HB3	1:K:432:PRO:HA	1.90	0.53
1:K:25:GLU:OE2	1:K:46:ARG:NH2	2.42	0.53
1:L:399:PHE:CE1	1:L:443:ALA:HB1	2.43	0.53
1:C:38:GLU:HB2	1:C:40:GLN:N	2.22	0.53
1:D:38:GLU:HB3	1:D:40:GLN:H	1.74	0.53
1:B:396:ARG:NH1	1:F:456:THR:OG1	2.37	0.53
1:J:90:LYS:NZ	1:J:166:ALA:HB2	2.24	0.53
1:C:498:VAL:HB	1:F:72:TRP:HH2	1.72	0.53
1:F:93:ILE:HG22	1:F:127:ALA:HB3	1.89	0.53
1:H:352:THR:HG21	1:H:357:ASP:OD1	2.08	0.53
1:I:91:GLY:HA3	1:I:125:ALA:O	2.09	0.53
1:K:414:GLN:OE1	1:K:429:PRO:HD2	2.09	0.53
1:E:348:ALA:HB3	1:E:351:PRO:HG3	1.89	0.53
1:E:52:ILE:HG12	1:E:493:TYR:HE2	1.73	0.53
1:G:298:HIS:CE1	1:G:304:PHE:HZ	2.26	0.53
1:L:91:GLY:HA3	1:L:125:ALA:O	2.09	0.53
1:A:385:TRP:O	1:A:389:LEU:HG	2.09	0.53
1:G:8:ASN:O	1:G:329:LYS:NZ	2.38	0.53
1:K:433:THR:HG23	1:K:436:PHE:H	1.71	0.53
1:J:238:MET:HE3	1:J:342:LYS:HD2	1.90	0.53
1:J:455:TYR:HB2	1:K:400:LYS:HB2	1.91	0.53
1:A:345:ALA:HB1	1:A:373:LEU:HD22	1.91	0.52
1:G:200:GLY:H	1:G:384:GLU:CD	2.13	0.52
1:K:141:LEU:O	1:K:145:THR:HG23	2.09	0.52
1:L:141:LEU:O	1:L:145:THR:HG23	2.08	0.52
1:A:13:VAL:HA	1:A:16:PHE:CD2	2.44	0.52
1:G:141:LEU:O	1:G:145:THR:HG23	2.09	0.52
1:I:94:ARG:NE	1:I:169:MET:HG3	2.24	0.52
1:I:321:ILE:HG12	1:I:343:ILE:HG23	1.91	0.52
1:K:246:THR:HA	1:K:269:LYS:O	2.08	0.52
1:L:321:ILE:HG12	1:L:343:ILE:HG23	1.91	0.52
1:B:60:SER:HG	1:E:58:VAL:HG13	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:382:TYR:O	1:G:386:LEU:HG	2.09	0.52
1:K:131:ILE:HB	1:K:136:TYR:HE2	1.73	0.52
1:C:87:THR:OG1	1:C:88:PRO:HD3	2.10	0.52
1:E:219:VAL:HA	1:E:373:LEU:HG	1.91	0.52
1:E:316:GLU:HA	1:E:339:VAL:HA	1.92	0.52
1:I:282:ASN:HD21	1:I:306:LYS:HB2	1.74	0.52
1:K:16:PHE:CZ	1:K:354:PRO:HD3	2.45	0.52
1:E:224:GLU:O	1:E:228:ASN:HB2	2.10	0.52
1:K:87:THR:OG1	1:K:88:PRO:HD3	2.09	0.52
1:B:294:PHE:CD1	1:B:298:HIS:CE1	2.90	0.52
1:E:335:ASN:OD1	1:E:335:ASN:N	2.43	0.52
1:E:52:ILE:HG12	1:E:493:TYR:CE2	2.45	0.52
1:I:343:ILE:HD11	1:I:368:ILE:HD11	1.92	0.52
1:D:270:CYS:SG	1:D:271:VAL:N	2.83	0.52
1:E:186:THR:OG1	1:E:187:ILE:N	2.37	0.52
1:G:95:TYR:OH	1:G:145:THR:HG22	2.09	0.52
1:F:459:ARG:NH2	2:F:601:XEG:OAH	2.37	0.52
1:I:230:ALA:HA	1:I:233:MET:HB2	1.92	0.52
1:J:141:LEU:O	1:J:145:THR:HG23	2.10	0.52
1:J:420:LYS:HG3	1:J:421:PHE:N	2.25	0.52
1:C:259:SER:O	1:C:263:LEU:HB2	2.10	0.52
1:C:52:ILE:O	1:C:82:HIS:NE2	2.42	0.52
1:D:67:ARG:NH2	1:D:135:ASN:O	2.43	0.52
1:F:131:ILE:HB	1:F:136:TYR:HE2	1.74	0.52
1:H:324:PRO:HG2	1:H:351:PRO:HG2	1.92	0.52
1:I:58:VAL:CG1	1:L:60:SER:HB2	2.40	0.52
1:K:83:SER:OG	1:K:85:HIS:ND1	2.33	0.52
1:E:126:LYS:NZ	1:E:168:ASP:OD2	2.24	0.51
1:H:142:GLU:HG3	1:H:178:TRP:CE2	2.45	0.51
1:K:246:THR:OG1	1:K:271:VAL:HB	2.10	0.51
1:A:34:THR:HG23	1:A:36:GLU:HB3	1.93	0.51
1:B:112:THR:OG1	1:B:124:GLY:HA3	2.11	0.51
1:E:152:LEU:HB3	1:E:157:PHE:HB2	1.92	0.51
1:I:255:VAL:O	1:I:259:SER:OG	2.14	0.51
1:A:281:TRP:CD1	1:A:310:TYR:CD1	2.98	0.51
1:A:412:SER:HB3	1:B:432:PRO:HA	1.91	0.51
1:F:158:ILE:CD1	1:F:165:PRO:CD	2.88	0.51
1:F:169:MET:HE3	1:F:327:SER:HA	1.92	0.51
1:F:51:ILE:O	1:F:54:PRO:HD2	2.10	0.51
1:G:357:ASP:O	1:G:361:LEU:HD22	2.10	0.51
1:I:242:PHE:HE2	1:I:266:PHE:HB3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:294:PHE:HE2	1:I:302:LEU:H	1.57	0.51
1:J:421:PHE:HZ	1:J:423:LYS:HE3	1.75	0.51
1:B:165:PRO:HD2	1:B:197:CYS:O	2.10	0.51
1:B:414:GLN:OE1	1:B:430:ILE:HG12	2.10	0.51
1:C:275:GLU:HG2	1:C:276:SER:H	1.75	0.51
1:G:433:THR:HG23	1:G:436:PHE:H	1.75	0.51
1:I:119:ASP:O	1:J:396:ARG:NH2	2.40	0.51
1:K:8:ASN:HA	1:K:329:LYS:HE3	1.92	0.51
1:C:366:MET:HE2	1:C:475:LEU:HD23	1.92	0.51
1:D:280:ILE:HD13	1:D:307:ALA:HB1	1.92	0.51
1:E:462:ARG:O	1:E:466:ARG:HG2	2.10	0.51
1:G:19:ARG:HH11	1:G:479:THR:HG21	1.74	0.51
1:G:275:GLU:HG2	1:G:276:SER:N	2.21	0.51
1:I:142:GLU:HG3	1:I:178:TRP:CE2	2.46	0.51
1:A:279:SER:HB3	1:A:310:TYR:HB3	1.93	0.51
1:A:16:PHE:CE1	1:A:354:PRO:HD3	2.46	0.51
1:C:303:GLY:O	1:C:304:PHE:CD1	2.62	0.51
1:D:281:TRP:CZ3	1:D:317:VAL:HG13	2.46	0.51
1:H:394:TYR:HB2	1:H:445:GLU:HG3	1.92	0.51
1:A:141:LEU:O	1:A:145:THR:HG23	2.11	0.51
1:A:165:PRO:HG2	1:A:198:VAL:HG23	1.91	0.51
1:B:382:TYR:CE1	1:B:386:LEU:HD11	2.46	0.51
1:E:238:MET:HE2	1:E:245:LYS:HE2	1.91	0.51
1:J:298:HIS:CE1	1:J:304:PHE:HZ	2.29	0.51
1:L:304:PHE:H	1:L:307:ALA:HB3	1.75	0.51
1:E:288:PRO:O	1:E:292:GLU:HB3	2.10	0.51
1:G:186:THR:OG1	1:G:187:ILE:N	2.43	0.51
1:J:254:ASN:H	1:J:257:LEU:HD12	1.76	0.51
1:G:118:VAL:HG23	1:G:120:VAL:HG23	1.92	0.51
1:I:175:GLU:O	1:I:179:ILE:HG13	2.11	0.51
1:K:116:ALA:HA	2:K:601:XEG:OAC	2.11	0.51
1:C:291:LEU:HD11	1:C:307:ALA:HB2	1.93	0.51
1:D:118:VAL:HG23	1:D:120:VAL:HG23	1.93	0.51
1:F:259:SER:O	1:F:263:LEU:HB2	2.10	0.51
1:F:281:TRP:CZ3	1:F:317:VAL:HG13	2.46	0.51
1:I:221:HIS:O	1:I:225:ASN:ND2	2.44	0.51
1:I:337:PRO:O	1:I:363:ARG:NH2	2.43	0.51
1:I:477:LEU:HA	1:I:480:ALA:HB3	1.91	0.51
1:B:319:CYS:SG	1:B:320:ASP:N	2.84	0.50
1:B:44:ARG:O	1:B:48:ILE:HG12	2.11	0.50
1:C:335:ASN:N	1:C:335:ASN:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:277:ASP:OD2	1:G:300:THR:HG21	2.11	0.50
1:B:498:VAL:HG13	1:B:498:VAL:O	2.11	0.50
1:D:433:THR:HG23	1:D:436:PHE:H	1.76	0.50
1:G:242:PHE:HE2	1:G:266:PHE:HB3	1.76	0.50
1:C:131:ILE:HB	1:C:136:TYR:HE2	1.75	0.50
1:C:164:VAL:HG13	1:C:198:VAL:HA	1.93	0.50
1:D:303:GLY:O	1:D:304:PHE:CD1	2.64	0.50
1:E:165:PRO:HD2	1:E:197:CYS:O	2.12	0.50
1:E:168:ASP:OD1	1:E:169:MET:N	2.44	0.50
1:G:213:SER:HB3	1:G:262:TYR:HE2	1.77	0.50
1:J:480:ALA:CA	1:J:483:VAL:HG12	2.42	0.50
1:K:119:ASP:HA	2:K:601:XEG:HAI	1.91	0.50
1:A:313:SER:OG	1:A:316:GLU:HG2	2.11	0.50
1:C:274:GLY:HA2	1:C:279:SER:HA	1.93	0.50
1:F:141:LEU:O	1:F:145:THR:HG23	2.11	0.50
1:B:186:THR:OG1	1:B:187:ILE:N	2.45	0.50
1:C:270:CYS:SG	1:C:271:VAL:N	2.84	0.50
1:C:315:LEU:HD12	1:C:339:VAL:HG22	1.93	0.50
1:D:21:ALA:HB1	1:D:49:LEU:HD23	1.94	0.50
1:E:250:GLN:NE2	1:E:330:GLN:HE21	2.09	0.50
1:F:335:ASN:OD1	1:F:335:ASN:N	2.44	0.50
1:F:484:ASN:O	1:F:487:GLU:HG2	2.11	0.50
1:I:219:VAL:HA	1:I:373:LEU:HG	1.93	0.50
1:I:294:PHE:HD2	1:I:301:ILE:HD12	1.76	0.50
1:I:463:GLN:OE1	1:I:488:LYS:NZ	2.38	0.50
1:A:281:TRP:HD1	1:A:310:TYR:CD1	2.30	0.50
1:D:36:GLU:O	1:D:37:THR:OG1	2.25	0.50
1:F:281:TRP:HZ3	1:F:317:VAL:HG13	1.77	0.50
1:F:337:PRO:O	1:F:363:ARG:NH2	2.45	0.50
1:G:383:PHE:HA	1:G:386:LEU:HD12	1.93	0.50
1:H:473:LEU:O	1:H:475:LEU:N	2.44	0.50
1:H:6:ASP:N	1:H:7:PRO:HD3	2.27	0.50
1:A:151:GLU:OE1	1:D:57:HIS:NE2	2.39	0.50
1:B:213:SER:HA	1:B:258:HIS:ND1	2.27	0.50
1:C:396:ARG:NH1	1:E:456:THR:OG1	2.38	0.50
1:G:13:VAL:O	1:G:16:PHE:N	2.43	0.50
1:G:378:VAL:HA	1:G:381:SER:HB2	1.94	0.50
1:I:291:LEU:CD1	1:I:304:PHE:CD2	2.95	0.50
1:G:57:HIS:NE2	1:J:151:GLU:HG3	2.27	0.50
1:J:271:VAL:HG23	1:J:283:PRO:HA	1.94	0.50
1:K:421:PHE:HZ	1:K:423:LYS:HE3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:332:THR:OG1	1:F:355:GLU:OE1	2.21	0.50
1:I:186:THR:OG1	1:I:187:ILE:N	2.45	0.50
1:J:495:GLU:O	1:K:177:SER:OG	2.19	0.50
1:A:11:LYS:HG3	1:A:14:GLU:CB	2.41	0.50
1:A:99:VAL:O	1:A:130:LYS:HE2	2.12	0.50
1:A:9:PHE:CD2	1:A:329:LYS:NZ	2.76	0.50
1:B:327:SER:HB3	1:B:330:GLN:NE2	2.25	0.50
1:A:60:SER:HB2	1:D:58:VAL:HG13	1.94	0.50
1:K:323:ILE:HA	1:K:345:ALA:O	2.12	0.50
1:B:303:GLY:O	1:B:304:PHE:CD1	2.64	0.49
1:B:315:LEU:HD13	1:B:335:ASN:HD22	1.77	0.49
1:D:294:PHE:CD2	1:D:301:ILE:HD12	2.47	0.49
1:E:343:ILE:HA	1:E:366:MET:HB3	1.93	0.49
1:G:499:THR:HG22	1:G:501:THR:HG23	1.94	0.49
1:J:213:SER:HB3	1:J:262:TYR:CE2	2.47	0.49
1:L:61:LEU:HD21	1:L:151:GLU:CB	2.42	0.49
1:D:333:LYS:HG3	1:D:355:GLU:HG2	1.94	0.49
1:D:91:GLY:HA3	1:D:125:ALA:O	2.12	0.49
1:E:91:GLY:HA3	1:E:125:ALA:O	2.12	0.49
1:E:141:LEU:O	1:E:145:THR:HG23	2.12	0.49
1:E:94:ARG:HD3	1:E:169:MET:HB3	1.93	0.49
1:E:251:GLY:O	1:E:253:GLY:N	2.45	0.49
1:E:274:GLY:HA3	1:E:314:ILE:HD13	1.94	0.49
1:L:6:ASP:HB2	1:L:332:THR:HG21	1.95	0.49
1:L:85:HIS:CD2	1:L:86:ARG:HG2	2.46	0.49
1:B:47:GLY:O	1:B:51:ILE:HG13	2.12	0.49
1:C:366:MET:HE3	1:C:475:LEU:HD23	1.93	0.49
1:C:412:SER:HB3	1:E:432:PRO:HA	1.94	0.49
1:D:277:ASP:OD2	1:D:300:THR:OG1	2.26	0.49
1:C:66:ARG:HH11	1:F:498:VAL:HG11	1.76	0.49
1:F:66:ARG:HD3	1:F:72:TRP:CZ2	2.47	0.49
1:H:208:ILE:H	1:H:211:ARG:HE	1.59	0.49
1:J:227:ILE:HD12	1:J:242:PHE:HD1	1.76	0.49
1:J:335:ASN:OD1	1:J:335:ASN:N	2.45	0.49
1:A:66:ARG:HD3	1:A:72:TRP:CE2	2.47	0.49
1:C:382:TYR:O	1:C:386:LEU:HG	2.13	0.49
1:D:304:PHE:H	1:D:307:ALA:HB3	1.77	0.49
1:F:82:HIS:CG	1:F:109:SER:HA	2.47	0.49
1:J:338:ARG:O	1:J:363:ARG:NH1	2.45	0.49
1:J:372:TYR:OH	1:J:461:ALA:HB2	2.12	0.49
1:K:329:LYS:H	1:K:351:PRO:HA	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:SER:HB3	1:F:432:PRO:HA	1.94	0.49
1:E:378:VAL:HA	1:E:381:SER:HB2	1.95	0.49
1:F:38:GLU:HB2	1:F:40:GLN:H	1.75	0.49
1:H:224:GLU:O	1:H:228:ASN:HB2	2.11	0.49
1:H:311:GLU:HG3	1:H:312:GLY:H	1.78	0.49
1:L:16:PHE:CZ	1:L:354:PRO:HD3	2.48	0.49
1:A:209:HIS:HB3	1:A:446:LYS:HB3	1.95	0.49
1:A:251:GLY:O	1:A:253:GLY:N	2.46	0.49
1:A:327:SER:OG	1:A:328:GLU:N	2.45	0.49
1:C:421:PHE:CE1	1:C:423:LYS:HB2	2.47	0.49
1:E:275:GLU:HG2	1:E:276:SER:H	1.77	0.49
1:F:208:ILE:H	1:F:211:ARG:HH11	1.60	0.49
1:G:208:ILE:O	1:G:211:ARG:NH1	2.45	0.49
1:J:473:LEU:O	1:J:475:LEU:N	2.46	0.49
1:H:303:GLY:O	1:H:304:PHE:HD1	1.94	0.49
1:K:499:THR:HG22	1:K:501:THR:HG23	1.94	0.49
1:B:249:VAL:CG1	1:B:323:ILE:HD11	2.34	0.49
1:B:6:ASP:N	1:B:355:GLU:OE1	2.45	0.49
1:E:382:TYR:CZ	1:E:386:LEU:HD11	2.48	0.49
1:B:62:SER:HB3	1:E:56:ASN:HA	1.93	0.49
1:G:213:SER:HB3	1:G:262:TYR:CE2	2.48	0.49
1:A:168:ASP:H	1:A:171:THR:HG1	1.58	0.49
1:A:224:GLU:O	1:A:228:ASN:HB2	2.12	0.49
1:B:87:THR:OG1	1:B:88:PRO:HD3	2.11	0.49
1:C:94:ARG:NH1	1:C:103:GLU:OE2	2.46	0.49
1:J:113:TYR:HB2	1:J:371:LEU:HD11	1.94	0.49
1:K:382:TYR:O	1:K:386:LEU:HG	2.12	0.49
1:E:370:ASP:OD1	1:E:478:ARG:NH1	2.45	0.49
1:E:38:GLU:HG3	1:E:40:GLN:H	1.77	0.49
1:G:253:GLY:O	1:G:255:VAL:N	2.45	0.49
1:G:329:LYS:H	1:G:351:PRO:HA	1.78	0.49
1:G:36:GLU:OE1	1:G:41:LYS:HG2	2.13	0.49
1:H:378:VAL:HA	1:H:381:SER:HB2	1.93	0.49
1:A:382:TYR:CE1	1:A:386:LEU:HD11	2.47	0.48
1:B:140:GLU:O	1:B:144:ILE:HG13	2.13	0.48
1:D:315:LEU:HB3	1:D:322:LEU:HD21	1.95	0.48
1:F:220:PHE:CZ	1:F:266:PHE:HE2	2.31	0.48
1:G:88:PRO:HG2	1:G:122:PHE:CE2	2.48	0.48
1:I:193:ASN:HD22	1:I:389:LEU:HA	1.78	0.48
1:J:232:TYR:HD1	1:J:235:ILE:HD12	1.77	0.48
1:D:281:TRP:HZ3	1:D:317:VAL:HG13	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:VAL:HA	1:D:323:ILE:HG13	1.95	0.48
1:H:72:TRP:CH2	1:K:498:VAL:HB	2.47	0.48
1:K:53:LYS:HG3	1:K:54:PRO:HD3	1.95	0.48
1:I:60:SER:HB2	1:L:58:VAL:CG1	2.43	0.48
1:H:205:GLN:NE2	1:L:492:VAL:O	2.47	0.48
1:H:382:TYR:CZ	1:H:386:LEU:HD11	2.48	0.48
1:A:282:ASN:ND2	1:A:306:LYS:HB3	2.28	0.48
1:D:490:PHE:HE2	1:D:494:ASN:HD22	1.61	0.48
1:E:270:CYS:SG	1:E:271:VAL:N	2.86	0.48
1:H:195:HIS:O	1:H:201:LYS:HE3	2.12	0.48
1:J:52:ILE:HD13	1:J:489:VAL:HG12	1.95	0.48
1:K:300:THR:HG22	1:K:301:ILE:H	1.79	0.48
1:L:280:ILE:HD13	1:L:307:ALA:HB1	1.95	0.48
1:B:27:LYS:HA	1:B:30:GLU:HB2	1.96	0.48
1:C:282:ASN:ND2	1:C:306:LYS:O	2.43	0.48
1:K:321:ILE:HA	1:K:343:ILE:O	2.13	0.48
1:A:335:ASN:OD1	1:A:335:ASN:N	2.46	0.48
1:G:87:THR:CG2	1:G:88:PRO:HD3	2.39	0.48
1:H:202:PRO:HA	1:H:211:ARG:HH22	1.78	0.48
1:H:335:ASN:OD1	1:H:335:ASN:N	2.47	0.48
1:I:85:HIS:CB	1:I:493:TYR:HE1	2.19	0.48
1:K:379:THR:O	1:K:382:TYR:HB3	2.14	0.48
1:L:445:GLU:O	1:L:449:VAL:HG23	2.13	0.48
1:A:427:THR:HG22	1:A:429:PRO:HD3	1.95	0.48
1:G:91:GLY:HA3	1:G:125:ALA:O	2.14	0.48
1:J:294:PHE:CE2	1:J:301:ILE:HA	2.48	0.48
1:K:8:ASN:OD1	1:K:9:PHE:N	2.47	0.48
1:L:220:PHE:O	1:L:224:GLU:N	2.45	0.48
1:B:335:ASN:OD1	1:B:335:ASN:N	2.47	0.48
1:C:202:PRO:HG2	1:C:205:GLN:HG3	1.96	0.48
1:H:202:PRO:HG2	1:H:205:GLN:HG3	1.96	0.48
1:I:291:LEU:HD11	1:I:304:PHE:CD2	2.49	0.48
1:I:496:ALA:HB2	1:J:205:GLN:HE22	1.78	0.48
1:L:459:ARG:NH2	2:L:601:XEG:OAH	2.42	0.48
1:I:303:GLY:O	1:I:304:PHE:CD1	2.67	0.48
1:K:305:PRO:C	1:K:307:ALA:H	2.17	0.48
1:A:244:ASP:OD1	1:A:244:ASP:N	2.45	0.48
1:B:10:PHE:O	1:B:12:MET:N	2.45	0.48
1:B:315:LEU:CD1	1:B:335:ASN:HD22	2.26	0.48
1:B:315:LEU:HD12	1:B:339:VAL:HG22	1.95	0.48
1:C:263:LEU:HA	1:C:263:LEU:HD12	1.69	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:319:CYS:SG	1:E:320:ASP:N	2.84	0.48
1:E:45:VAL:HG22	1:E:490:PHE:CZ	2.49	0.48
1:H:279:SER:HB3	1:H:314:ILE:HG12	1.95	0.48
1:J:421:PHE:CZ	1:J:423:LYS:HE3	2.49	0.48
1:L:350:GLY:N	1:L:370:ASP:OD2	2.45	0.48
1:B:280:ILE:HD13	1:B:307:ALA:HB1	1.95	0.47
1:C:421:PHE:CZ	1:C:423:LYS:HB2	2.49	0.47
1:D:95:TYR:OH	1:D:145:THR:HG22	2.13	0.47
1:H:94:ARG:NH1	1:H:103:GLU:OE2	2.46	0.47
2:C:601:XEG:OAF	1:D:396:ARG:NE	2.35	0.47
1:E:444:SER:N	1:E:447:ASP:OD2	2.43	0.47
1:K:303:GLY:O	1:K:304:PHE:CD1	2.65	0.47
1:L:368:ILE:HG21	1:L:373:LEU:HD13	1.96	0.47
1:B:13:VAL:O	1:B:16:PHE:N	2.47	0.47
1:B:249:VAL:HG12	1:B:323:ILE:CD1	2.32	0.47
1:C:319:CYS:SG	1:C:320:ASP:N	2.87	0.47
1:C:433:THR:HG23	1:C:436:PHE:H	1.78	0.47
1:D:246:THR:HA	1:D:269:LYS:O	2.14	0.47
1:D:329:LYS:H	1:D:351:PRO:HA	1.79	0.47
1:E:248:ALA:HB1	1:E:272:ALA:HB3	1.95	0.47
1:E:459:ARG:NH1	2:E:601:XEG:OAH	2.38	0.47
1:H:372:TYR:OH	1:H:461:ALA:HB2	2.12	0.47
1:I:213:SER:HB3	1:I:262:TYR:HE2	1.79	0.47
1:I:242:PHE:CE2	1:I:266:PHE:HB3	2.50	0.47
1:J:87:THR:HG23	1:J:88:PRO:CD	2.32	0.47
1:B:250:GLN:HG3	1:B:314:ILE:HD12	1.95	0.47
1:D:140:GLU:O	1:D:144:ILE:HG13	2.15	0.47
1:D:85:HIS:CD2	1:D:86:ARG:HG2	2.49	0.47
1:F:303:GLY:O	1:F:304:PHE:CD1	2.67	0.47
1:F:44:ARG:O	1:F:48:ILE:HG12	2.14	0.47
1:G:217:ARG:NE	1:G:450:HIS:CD2	2.82	0.47
2:I:601:XEG:OAF	1:J:396:ARG:NE	2.40	0.47
1:L:291:LEU:HD11	1:L:304:PHE:HB2	1.96	0.47
1:A:304:PHE:CG	1:A:305:PRO:HD3	2.48	0.47
1:E:473:LEU:O	1:E:475:LEU:N	2.48	0.47
1:G:303:GLY:O	1:G:304:PHE:CD1	2.67	0.47
1:G:52:ILE:HG12	1:G:493:TYR:CE2	2.48	0.47
1:G:9:PHE:HD1	1:G:10:PHE:N	2.12	0.47
1:H:361:LEU:HD12	1:H:361:LEU:O	2.15	0.47
1:J:211:ARG:HA	1:J:214:ALA:HB2	1.95	0.47
1:J:213:SER:HA	1:J:258:HIS:ND1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ASN:HD22	1:A:389:LEU:HA	1.79	0.47
1:F:369:PRO:HB3	1:F:478:ARG:HG3	1.97	0.47
1:B:195:HIS:O	1:B:201:LYS:HE3	2.14	0.47
1:C:91:GLY:HA3	1:C:125:ALA:O	2.14	0.47
1:E:246:THR:HA	1:E:269:LYS:O	2.14	0.47
1:H:91:GLY:HA3	1:H:125:ALA:O	2.14	0.47
2:K:601:XEG:HAJ	2:K:601:XEG:HBE	1.44	0.47
1:L:219:VAL:HA	1:L:373:LEU:HG	1.95	0.47
1:L:251:GLY:HA3	1:L:326:ALA:HB2	1.97	0.47
1:B:151:GLU:HG3	1:E:57:HIS:NE2	2.30	0.47
1:B:311:GLU:HG3	1:B:312:GLY:N	2.30	0.47
1:C:129:VAL:HG12	1:C:131:ILE:HG12	1.94	0.47
2:F:601:XEG:HBE	2:F:601:XEG:HAJ	1.49	0.47
1:L:251:GLY:O	1:L:253:GLY:N	2.48	0.47
1:A:372:TYR:OH	1:A:461:ALA:HB2	2.14	0.47
1:A:58:VAL:HG13	1:D:60:SER:HG	1.80	0.47
1:G:131:ILE:HB	1:G:136:TYR:CE2	2.49	0.47
1:I:236:LEU:HD21	1:I:342:LYS:HG3	1.97	0.47
1:L:259:SER:O	1:L:263:LEU:HB2	2.15	0.47
1:H:138:ASP:OD2	1:L:35:ARG:NH1	2.48	0.47
1:A:219:VAL:HA	1:A:373:LEU:HG	1.97	0.47
1:A:382:TYR:CZ	1:A:386:LEU:HD11	2.49	0.47
1:B:322:LEU:O	1:B:344:ILE:HA	2.15	0.47
1:E:37:THR:HA	1:E:41:LYS:HE3	1.97	0.47
1:F:169:MET:CE	1:F:327:SER:HA	2.44	0.47
1:I:220:PHE:O	1:I:224:GLU:N	2.42	0.47
1:I:297:GLN:O	1:I:298:HIS:ND1	2.44	0.47
1:K:346:GLU:OE1	1:K:478:ARG:NH1	2.48	0.47
1:H:419:ARG:HH12	1:L:431:VAL:HG11	1.80	0.47
1:H:419:ARG:NH1	1:L:431:VAL:HG11	2.30	0.47
1:A:8:ASN:HB3	1:A:9:PHE:CD2	2.50	0.47
1:B:304:PHE:N	1:B:307:ALA:HB3	2.29	0.47
1:B:329:LYS:HA	1:B:351:PRO:HA	1.96	0.47
1:D:432:PRO:HA	1:E:412:SER:HB3	1.97	0.47
1:G:315:LEU:HD12	1:G:339:VAL:CG2	2.45	0.47
1:G:94:ARG:NH1	1:G:103:GLU:OE2	2.46	0.47
1:I:208:ILE:O	1:I:211:ARG:NH1	2.47	0.47
1:I:385:TRP:O	1:I:389:LEU:HG	2.15	0.47
1:J:95:TYR:OH	1:J:145:THR:HG22	2.15	0.47
1:K:335:ASN:OD1	1:K:335:ASN:N	2.47	0.47
1:A:387:LYS:O	1:A:391:HIS:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:VAL:HG13	1:B:373:LEU:HD21	1.97	0.46
1:C:315:LEU:HD11	1:C:335:ASN:HD22	1.79	0.46
1:G:117:VAL:HG23	1:G:485:ALA:HB2	1.97	0.46
1:G:331:LEU:HB2	1:G:352:THR:HA	1.97	0.46
1:G:378:VAL:O	1:G:382:TYR:N	2.39	0.46
1:G:40:GLN:HG2	1:G:43:ASN:HD21	1.78	0.46
1:G:85:HIS:CD2	1:G:86:ARG:HG2	2.49	0.46
1:H:332:THR:OG1	1:H:333:LYS:N	2.47	0.46
1:I:226:PHE:HE2	1:I:477:LEU:HD13	1.80	0.46
1:K:321:ILE:HG12	1:K:343:ILE:HG23	1.96	0.46
1:L:287:ASP:OD1	1:L:287:ASP:N	2.48	0.46
1:C:321:ILE:HA	1:C:343:ILE:O	2.15	0.46
1:G:116:ALA:HA	2:G:601:XEG:OAC	2.15	0.46
1:H:119:ASP:HA	2:H:601:XEG:HAI	1.96	0.46
1:C:343:ILE:HD11	1:C:368:ILE:HD11	1.96	0.46
1:E:96:SER:O	1:E:130:LYS:HA	2.15	0.46
1:E:79:ARG:NH2	1:E:163:ASP:OD2	2.36	0.46
1:H:36:GLU:OE2	1:H:40:GLN:HB3	2.16	0.46
1:B:95:TYR:OH	1:B:145:THR:HG22	2.16	0.46
1:C:10:PHE:O	1:C:12:MET:N	2.49	0.46
1:D:335:ASN:N	1:D:335:ASN:OD1	2.48	0.46
1:D:446:LYS:HB3	1:D:450:HIS:HE1	1.80	0.46
1:J:323:ILE:HA	1:J:345:ALA:O	2.16	0.46
1:C:477:LEU:HD12	1:C:477:LEU:H	1.81	0.46
1:C:82:HIS:CG	1:C:109:SER:HA	2.51	0.46
1:C:458:GLU:OE1	1:D:400:LYS:NZ	2.49	0.46
1:E:99:VAL:O	1:E:130:LYS:HE2	2.16	0.46
1:I:382:TYR:O	1:I:386:LEU:HG	2.15	0.46
1:L:65:ILE:HD13	1:L:144:ILE:HG12	1.97	0.46
1:L:238:MET:HG3	1:L:239:THR:H	1.79	0.46
1:B:246:THR:HA	1:B:269:LYS:O	2.16	0.46
1:D:79:ARG:HA	1:D:127:ALA:HA	1.97	0.46
1:F:249:VAL:CG1	1:F:323:ILE:HD11	2.30	0.46
1:J:229:GLU:OE2	1:J:462:ARG:NH2	2.46	0.46
1:K:242:PHE:CE2	1:K:266:PHE:HB3	2.50	0.46
1:A:245:LYS:HG2	1:A:320:ASP:OD2	2.15	0.46
1:A:86:ARG:HH21	2:A:601:XEG:HBF	1.81	0.46
1:B:150:MET:HG3	1:E:501:THR:CB	2.46	0.46
1:B:17:PHE:O	1:B:21:ALA:N	2.32	0.46
1:B:294:PHE:CD2	1:B:301:ILE:HD12	2.51	0.46
1:B:456:THR:O	1:B:460:SER:OG	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:GLN:OE1	1:D:430:ILE:HG13	2.16	0.46
1:F:36:GLU:HG3	1:F:37:THR:H	1.81	0.46
1:H:126:LYS:NZ	1:H:168:ASP:OD2	2.45	0.46
1:I:118:VAL:HG23	1:I:120:VAL:HG23	1.98	0.46
1:J:488:LYS:HE3	2:J:601:XEG:CAT	2.45	0.46
1:L:17:PHE:O	1:L:21:ALA:N	2.44	0.46
1:I:60:SER:HB2	1:L:58:VAL:HG13	1.97	0.46
1:A:152:LEU:O	1:A:157:PHE:N	2.46	0.46
1:E:383:PHE:HA	1:E:386:LEU:HD12	1.97	0.46
1:H:436:PHE:O	1:H:440:ILE:HG12	2.15	0.46
1:G:195:HIS:HD2	1:H:87:THR:HG21	1.80	0.46
1:I:236:LEU:HD11	1:I:342:LYS:O	2.16	0.46
1:J:42:ARG:HD3	1:J:46:ARG:HH21	1.81	0.46
1:L:87:THR:OG1	1:L:88:PRO:HD3	2.16	0.46
1:D:126:LYS:NZ	1:D:168:ASP:OD2	2.46	0.46
1:D:206:GLY:O	1:D:388:ASN:ND2	2.41	0.46
1:F:112:THR:OG1	1:F:124:GLY:HA3	2.15	0.46
1:F:242:PHE:CE2	1:F:266:PHE:HB3	2.44	0.46
1:H:294:PHE:HD2	1:H:301:ILE:HD12	1.80	0.46
1:H:311:GLU:HG3	1:H:312:GLY:N	2.31	0.46
1:I:270:CYS:SG	1:I:271:VAL:N	2.87	0.46
2:I:601:XEG:HBE	2:I:601:XEG:HAJ	1.43	0.46
1:J:36:GLU:OE1	1:J:37:THR:N	2.49	0.46
2:J:601:XEG:CAL	2:J:601:XEG:HAP	2.46	0.46
1:K:13:VAL:HG13	1:K:14:GLU:OE1	2.16	0.46
1:A:253:GLY:O	1:A:255:VAL:N	2.49	0.46
1:B:206:GLY:O	1:B:388:ASN:ND2	2.39	0.46
1:B:315:LEU:HD12	1:B:339:VAL:CG2	2.46	0.46
1:D:324:PRO:HD2	1:D:345:ALA:O	2.16	0.46
1:D:382:TYR:CE1	1:D:386:LEU:HD11	2.51	0.46
2:D:601:XEG:HBE	2:D:601:XEG:HAJ	1.43	0.46
1:G:480:ALA:O	1:G:483:VAL:HG12	2.15	0.46
1:H:213:SER:HA	1:H:258:HIS:ND1	2.31	0.46
1:I:346:GLU:HB3	1:I:370:ASP:HB3	1.98	0.46
1:I:193:ASN:ND2	1:I:389:LEU:HA	2.30	0.46
1:K:136:TYR:HB2	1:K:141:LEU:CD1	2.46	0.46
1:K:432:PRO:HB2	1:K:436:PHE:HD1	1.80	0.46
1:K:226:PHE:HE2	1:K:477:LEU:CD1	2.29	0.46
1:A:330:GLN:O	1:A:335:ASN:ND2	2.46	0.45
1:D:499:THR:HG22	1:D:501:THR:HG23	1.98	0.45
1:G:333:LYS:HG2	1:G:355:GLU:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:168:ASP:N	1:I:171:THR:OG1	2.40	0.45
1:A:324:PRO:HD2	1:A:345:ALA:O	2.17	0.45
1:B:421:PHE:O	1:B:423:LYS:N	2.49	0.45
1:E:13:VAL:HA	1:E:16:PHE:HD2	1.80	0.45
1:E:202:PRO:HG2	1:E:205:GLN:CG	2.46	0.45
1:E:323:ILE:HA	1:E:345:ALA:O	2.16	0.45
1:E:58:VAL:HG23	1:E:80:ALA:HB2	1.98	0.45
1:F:193:ASN:OD1	1:F:193:ASN:N	2.49	0.45
1:G:473:LEU:O	1:G:475:LEU:N	2.50	0.45
1:H:112:THR:OG1	1:H:124:GLY:HA3	2.17	0.45
1:J:462:ARG:HD2	1:J:466:ARG:HH21	1.81	0.45
1:L:236:LEU:HD11	1:L:342:LYS:O	2.17	0.45
1:B:273:VAL:HG21	1:B:286:ILE:HD11	1.99	0.45
1:C:255:VAL:O	1:C:259:SER:OG	2.23	0.45
1:F:52:ILE:O	1:F:82:HIS:NE2	2.50	0.45
1:G:315:LEU:HD12	1:G:339:VAL:HG22	1.96	0.45
1:J:294:PHE:CD2	1:J:301:ILE:HG13	2.51	0.45
1:K:186:THR:OG1	1:K:187:ILE:N	2.50	0.45
1:L:346:GLU:CD	1:L:478:ARG:HH12	2.20	0.45
1:L:42:ARG:HD3	1:L:46:ARG:HH21	1.81	0.45
1:B:490:PHE:HE2	1:B:494:ASN:HD22	1.65	0.45
1:C:323:ILE:HG22	1:C:345:ALA:HB3	1.97	0.45
1:D:254:ASN:H	1:D:257:LEU:HD12	1.81	0.45
1:E:499:THR:CG2	1:E:501:THR:HG23	2.46	0.45
1:C:501:THR:CG2	1:F:150:MET:HG3	2.47	0.45
1:D:154:LYS:HB3	1:F:189:HIS:NE2	2.32	0.45
1:G:9:PHE:HD1	1:G:10:PHE:H	1.63	0.45
1:G:243:GLY:O	1:G:245:LYS:N	2.46	0.45
1:I:112:THR:OG1	1:I:124:GLY:HA3	2.16	0.45
1:I:169:MET:HE1	1:I:326:ALA:O	2.17	0.45
1:J:346:GLU:OE1	1:J:370:ASP:N	2.44	0.45
1:K:281:TRP:CZ3	1:K:317:VAL:HG13	2.51	0.45
1:C:338:ARG:HG2	1:C:339:VAL:H	1.81	0.45
1:D:301:ILE:HG13	1:D:302:LEU:N	2.31	0.45
1:K:126:LYS:HD2	1:K:126:LYS:HA	1.84	0.45
1:A:208:ILE:H	1:A:211:ARG:NH1	2.13	0.45
1:A:329:LYS:HB2	1:A:329:LYS:HE2	1.52	0.45
1:B:396:ARG:NE	2:F:601:XEG:OAF	2.47	0.45
1:I:87:THR:OG1	1:I:88:PRO:HD3	2.15	0.45
1:J:421:PHE:CZ	1:J:423:LYS:HB3	2.51	0.45
1:C:141:LEU:O	1:C:145:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:ASP:N	1:C:171:THR:OG1	2.41	0.45
1:C:38:GLU:O	1:C:41:LYS:HD3	2.17	0.45
1:E:251:GLY:HA3	1:E:326:ALA:HB2	1.97	0.45
1:E:345:ALA:HB1	1:E:373:LEU:HD22	1.98	0.45
1:F:315:LEU:CD1	1:F:335:ASN:HD22	2.30	0.45
1:G:274:GLY:HA2	1:G:279:SER:HA	1.97	0.45
1:I:141:LEU:O	1:I:145:THR:HG23	2.16	0.45
1:K:79:ARG:HA	1:K:127:ALA:HA	1.97	0.45
1:L:90:LYS:O	1:L:125:ALA:N	2.49	0.45
1:A:338:ARG:HG2	1:A:339:VAL:H	1.81	0.45
1:D:227:ILE:HA	1:D:233:MET:HE2	1.99	0.45
1:E:95:TYR:OH	1:E:145:THR:HG22	2.17	0.45
1:G:249:VAL:HA	1:G:323:ILE:HG13	1.99	0.45
1:H:24:VAL:HG13	1:H:483:VAL:CG2	2.46	0.45
1:I:416:SER:HB3	1:K:429:PRO:HA	1.99	0.45
1:J:480:ALA:HA	1:J:483:VAL:HG11	1.98	0.45
1:L:211:ARG:HA	1:L:214:ALA:HB2	1.98	0.45
1:L:46:ARG:HG2	1:L:50:ARG:HH11	1.82	0.45
1:D:249:VAL:HG12	1:D:323:ILE:CG1	2.47	0.45
1:F:118:VAL:HG23	1:F:120:VAL:HG23	1.97	0.45
1:F:202:PRO:HG2	1:F:205:GLN:HG3	1.99	0.45
1:F:86:ARG:HD2	1:F:86:ARG:HA	1.84	0.45
1:G:90:LYS:HD2	1:G:164:VAL:O	2.17	0.45
1:H:95:TYR:OH	1:H:145:THR:HG22	2.16	0.45
1:I:200:GLY:HA2	1:I:211:ARG:HE	1.81	0.45
1:J:249:VAL:CG2	1:J:273:VAL:HG22	2.46	0.45
1:B:330:GLN:O	1:B:335:ASN:ND2	2.49	0.45
1:D:131:ILE:HB	1:D:136:TYR:HE2	1.82	0.45
1:D:193:ASN:HD22	1:D:389:LEU:CD2	2.21	0.45
1:C:501:THR:HG22	1:F:150:MET:HG3	1.99	0.45
1:G:197:CYS:SG	1:G:198:VAL:HG12	2.57	0.45
1:I:95:TYR:HB3	1:I:133:PRO:HG3	1.98	0.45
1:I:79:ARG:HH11	1:I:127:ALA:HB2	1.81	0.45
1:J:167:PRO:HD3	1:J:176:MET:HG3	1.98	0.45
1:J:230:ALA:HA	1:J:233:MET:HG2	1.98	0.45
1:J:304:PHE:H	1:J:307:ALA:HB3	1.82	0.45
1:L:382:TYR:O	1:L:386:LEU:HG	2.17	0.45
1:A:244:ASP:O	1:A:245:LYS:HG3	2.17	0.44
1:B:391:HIS:O	1:F:382:TYR:OH	2.34	0.44
1:E:247:PHE:HE1	1:E:260:MET:HG3	1.83	0.44
1:F:379:THR:O	1:F:382:TYR:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:TYR:HB2	1:G:141:LEU:CD1	2.47	0.44
1:A:94:ARG:HE	1:A:169:MET:CG	2.31	0.44
1:B:86:ARG:HG3	1:B:121:PRO:HA	1.98	0.44
1:B:193:ASN:OD1	1:B:193:ASN:N	2.50	0.44
1:B:473:LEU:O	1:B:475:LEU:N	2.47	0.44
1:C:274:GLY:HA3	1:C:314:ILE:HD13	1.99	0.44
1:B:72:TRP:HH2	1:E:498:VAL:HB	1.81	0.44
1:F:217:ARG:HA	1:F:220:PHE:HB3	2.00	0.44
1:I:9:PHE:HB3	1:I:12:MET:CG	2.43	0.44
1:F:315:LEU:HD22	1:F:322:LEU:HD21	1.98	0.44
2:H:601:XEG:HAP	2:H:601:XEG:CAZ	2.47	0.44
1:J:414:GLN:OE1	1:J:429:PRO:HD2	2.18	0.44
1:L:195:HIS:O	1:L:201:LYS:HE3	2.18	0.44
1:C:324:PRO:HG2	1:C:351:PRO:HG2	1.99	0.44
1:G:250:GLN:HB2	1:G:324:PRO:HA	2.00	0.44
1:G:21:ALA:HB1	1:G:49:LEU:HD23	1.99	0.44
2:J:601:XEG:CAZ	2:J:601:XEG:HAP	2.48	0.44
1:K:213:SER:HB3	1:K:262:TYR:HE2	1.83	0.44
1:K:253:GLY:O	1:K:255:VAL:N	2.51	0.44
1:K:473:LEU:O	1:K:475:LEU:N	2.50	0.44
1:L:175:GLU:O	1:L:179:ILE:HG13	2.17	0.44
1:D:244:ASP:N	1:D:244:ASP:OD1	2.46	0.44
1:F:249:VAL:HA	1:F:323:ILE:HG13	1.99	0.44
1:F:324:PRO:HG2	1:F:351:PRO:HG2	2.00	0.44
1:G:331:LEU:HD22	1:G:360:PHE:HZ	1.82	0.44
2:G:601:XEG:HBE	2:G:601:XEG:HAJ	1.45	0.44
1:H:65:ILE:HD13	1:H:144:ILE:HG12	1.99	0.44
1:I:66:ARG:HD3	1:I:72:TRP:CE2	2.53	0.44
1:J:344:ILE:O	1:J:367:VAL:HA	2.18	0.44
1:K:168:ASP:OD1	1:K:169:MET:N	2.51	0.44
1:K:42:ARG:O	1:K:46:ARG:HG2	2.17	0.44
1:D:322:LEU:O	1:D:344:ILE:HA	2.18	0.44
1:G:137:THR:H	1:G:140:GLU:HB2	1.80	0.44
1:G:168:ASP:OD1	1:G:169:MET:HG2	2.17	0.44
1:G:358:LYS:HA	1:G:361:LEU:CD2	2.48	0.44
1:I:323:ILE:HA	1:I:345:ALA:O	2.18	0.44
1:I:331:LEU:HB2	1:I:352:THR:HA	1.99	0.44
1:K:244:ASP:N	1:K:244:ASP:OD1	2.51	0.44
1:B:242:PHE:HE2	1:B:266:PHE:HB3	1.81	0.44
1:C:53:LYS:O	1:C:82:HIS:HE1	2.00	0.44
2:E:601:XEG:HAJ	2:E:601:XEG:HBE	1.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:263:LEU:HA	1:G:263:LEU:HD12	1.86	0.44
1:G:64:PRO:HB3	1:J:51:ILE:HG12	1.99	0.44
1:K:14:GLU:OE1	1:K:14:GLU:N	2.51	0.44
1:L:421:PHE:CZ	1:L:423:LYS:HB3	2.52	0.44
1:C:36:GLU:OE1	1:C:37:THR:N	2.51	0.44
1:D:47:GLY:O	1:D:51:ILE:HG13	2.18	0.44
1:E:165:PRO:HG2	1:E:198:VAL:HG23	1.99	0.44
1:I:336:ALA:HB3	1:I:359:ILE:HD12	2.00	0.44
1:J:79:ARG:NH2	1:J:163:ASP:OD2	2.37	0.44
1:B:36:GLU:HG3	1:B:37:THR:N	2.32	0.44
1:C:432:PRO:HA	1:D:412:SER:HB3	1.99	0.44
1:D:415:GLU:O	1:D:419:ARG:HD2	2.18	0.44
1:E:387:LYS:O	1:E:391:HIS:N	2.51	0.44
1:F:445:GLU:O	1:F:449:VAL:HG23	2.18	0.44
1:H:167:PRO:HD3	1:H:176:MET:HG3	2.00	0.44
1:J:209:HIS:HB3	1:J:446:LYS:HB3	2.00	0.44
1:K:11:LYS:HB2	1:K:14:GLU:HG2	2.00	0.44
1:L:255:VAL:O	1:L:259:SER:OG	2.18	0.44
1:L:382:TYR:CZ	1:L:386:LEU:HD11	2.53	0.44
1:A:499:THR:HG23	1:F:146:ARG:NH1	2.32	0.43
1:B:243:GLY:O	1:B:245:LYS:N	2.51	0.43
1:B:251:GLY:HA3	1:B:326:ALA:HB2	2.00	0.43
1:D:141:LEU:O	1:D:145:THR:HG23	2.18	0.43
1:E:226:PHE:C	1:E:228:ASN:H	2.22	0.43
1:F:368:ILE:HG21	1:F:373:LEU:HD13	2.00	0.43
1:G:281:TRP:CZ3	1:G:317:VAL:HG13	2.53	0.43
1:H:383:PHE:HA	1:H:386:LEU:HD12	2.00	0.43
1:I:142:GLU:HG3	1:I:178:TRP:CD2	2.53	0.43
2:J:601:XEG:HBE	2:J:601:XEG:HAJ	1.48	0.43
1:K:11:LYS:HB2	1:K:14:GLU:CG	2.48	0.43
1:K:294:PHE:HE2	1:K:302:LEU:H	1.65	0.43
1:A:24:VAL:HG13	1:A:483:VAL:HG23	1.99	0.43
1:B:281:TRP:CZ3	1:B:317:VAL:HG13	2.53	0.43
1:C:387:LYS:HD2	1:C:445:GLU:OE2	2.17	0.43
1:C:61:LEU:HD21	1:C:151:GLU:CB	2.48	0.43
1:D:36:GLU:HG2	1:D:38:GLU:OE2	2.18	0.43
1:F:169:MET:HE1	1:F:326:ALA:O	2.17	0.43
1:I:89:CYS:HB3	1:I:125:ALA:HB2	2.00	0.43
1:I:137:THR:H	1:I:140:GLU:HB2	1.83	0.43
1:A:454:ALA:O	1:A:457:MET:N	2.51	0.43
1:B:332:THR:OG1	1:B:333:LYS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:601:XEG:OAF	1:E:396:ARG:NE	2.50	0.43
1:F:193:ASN:HD22	1:F:389:LEU:HA	1.83	0.43
1:H:24:VAL:HG13	1:H:483:VAL:HG22	2.00	0.43
1:I:102:ASP:HA	1:I:105:LYS:HB3	2.00	0.43
1:I:99:VAL:O	1:I:130:LYS:HE2	2.18	0.43
1:L:236:LEU:HD21	1:L:342:LYS:HB3	2.00	0.43
1:L:238:MET:HG3	1:L:239:THR:N	2.32	0.43
1:L:370:ASP:OD1	1:L:370:ASP:N	2.52	0.43
1:C:36:GLU:OE1	1:C:41:LYS:HG3	2.18	0.43
1:E:304:PHE:N	1:E:307:ALA:HB3	2.32	0.43
1:F:14:GLU:OE1	1:F:14:GLU:N	2.45	0.43
1:F:207:GLY:HA3	1:F:211:ARG:NH1	2.33	0.43
1:H:88:PRO:HG2	1:H:122:PHE:CD2	2.54	0.43
1:I:258:HIS:HA	1:I:261:ARG:HB3	1.99	0.43
1:J:253:GLY:O	1:J:255:VAL:N	2.51	0.43
1:J:324:PRO:HD2	1:J:345:ALA:O	2.17	0.43
1:J:90:LYS:HE3	1:J:378:VAL:HG23	2.00	0.43
1:A:148:PHE:CZ	1:A:152:LEU:HD11	2.54	0.43
1:B:301:ILE:HG13	1:B:302:LEU:N	2.34	0.43
1:A:416:SER:HB3	1:B:429:PRO:HA	2.01	0.43
1:D:193:ASN:OD1	1:D:193:ASN:N	2.52	0.43
1:D:427:THR:HG22	1:D:429:PRO:HD3	2.01	0.43
1:E:414:GLN:OE1	1:E:429:PRO:HD2	2.17	0.43
1:H:211:ARG:HA	1:H:214:ALA:HB2	1.99	0.43
1:H:432:PRO:HB2	1:H:436:PHE:HD1	1.84	0.43
1:K:257:LEU:HB3	1:K:258:HIS:HD2	1.83	0.43
1:K:480:ALA:O	1:K:483:VAL:HG12	2.18	0.43
1:A:52:ILE:HG12	1:A:493:TYR:HE2	1.84	0.43
1:C:478:ARG:HD2	1:C:482:TYR:HE2	1.84	0.43
1:E:254:ASN:N	1:E:257:LEU:HD12	2.33	0.43
1:E:207:GLY:HA2	1:E:384:GLU:OE1	2.18	0.43
1:E:462:ARG:HD3	1:E:465:MET:HE2	1.99	0.43
1:F:257:LEU:HD11	1:F:295:LYS:CE	2.49	0.43
1:F:91:GLY:O	1:F:165:PRO:HA	2.18	0.43
1:I:352:THR:HG23	1:I:360:PHE:HE2	1.84	0.43
1:L:263:LEU:HD12	1:L:263:LEU:HA	1.80	0.43
1:B:295:LYS:HB3	1:B:296:LEU:H	1.53	0.43
1:B:477:LEU:O	1:B:481:ALA:N	2.52	0.43
1:F:263:LEU:HD12	1:F:263:LEU:HA	1.70	0.43
1:G:477:LEU:H	1:G:477:LEU:HD12	1.82	0.43
1:I:446:LYS:HG2	1:I:450:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:215:THR:O	1:J:219:VAL:HG23	2.18	0.43
1:K:52:ILE:O	1:K:82:HIS:NE2	2.51	0.43
1:K:90:LYS:HD2	1:K:164:VAL:O	2.19	0.43
1:L:90:LYS:NZ	1:L:381:SER:HB3	2.34	0.43
1:A:414:GLN:OE1	1:A:430:ILE:HG23	2.18	0.43
1:D:446:LYS:HB3	1:D:450:HIS:CE1	2.53	0.43
1:D:48:ILE:O	1:D:52:ILE:HG13	2.18	0.43
1:E:193:ASN:HD22	1:E:389:LEU:HA	1.82	0.43
1:J:86:ARG:HA	1:J:86:ARG:HD3	1.83	0.43
1:A:152:LEU:HB3	1:A:157:PHE:HB2	2.00	0.43
2:C:601:XEG:HBE	2:C:601:XEG:HAJ	1.44	0.43
1:D:215:THR:O	1:D:219:VAL:HG23	2.18	0.43
1:D:348:ALA:HB3	1:D:351:PRO:HG3	2.01	0.43
1:E:368:ILE:HA	1:E:369:PRO:HD3	1.89	0.43
1:G:12:MET:SD	1:G:329:LYS:HE2	2.59	0.43
1:G:19:ARG:HD3	1:G:479:THR:HG21	2.01	0.43
1:I:321:ILE:HG12	1:I:343:ILE:CG2	2.49	0.43
1:J:305:PRO:C	1:J:307:ALA:H	2.22	0.43
1:J:247:PHE:HA	1:J:319:CYS:SG	2.59	0.43
1:J:207:GLY:HA2	1:J:384:GLU:OE1	2.19	0.43
1:J:436:PHE:O	1:J:440:ILE:HG12	2.18	0.43
1:L:282:ASN:HD21	1:L:306:LYS:CG	2.18	0.43
1:L:280:ILE:HD11	1:L:301:ILE:HD11	2.01	0.43
1:A:36:GLU:CG	1:A:38:GLU:CG	2.94	0.43
1:C:249:VAL:HG12	1:C:323:ILE:CD1	2.43	0.43
1:C:392:VAL:HG13	1:E:386:LEU:HD22	2.01	0.43
1:F:95:TYR:OH	1:F:145:THR:HG22	2.19	0.43
1:H:10:PHE:O	1:H:12:MET:N	2.42	0.43
1:K:219:VAL:HG13	1:K:373:LEU:HD21	2.01	0.43
1:K:414:GLN:OE1	1:K:430:ILE:HG23	2.19	0.43
1:L:19:ARG:HE	1:L:479:THR:HG21	1.82	0.43
1:A:246:THR:HB	1:A:271:VAL:HB	2.00	0.42
1:A:6:ASP:HA	1:A:7:PRO:HD3	1.93	0.42
1:C:120:VAL:O	1:C:122:PHE:N	2.46	0.42
1:C:131:ILE:HB	1:C:136:TYR:CE2	2.52	0.42
1:C:246:THR:HA	1:C:269:LYS:O	2.19	0.42
1:C:423:LYS:HB3	1:C:423:LYS:HE3	1.73	0.42
1:D:202:PRO:HA	1:D:211:ARG:HH22	1.84	0.42
1:E:24:VAL:HG13	1:E:483:VAL:HG22	2.00	0.42
1:F:46:ARG:HB3	1:F:50:ARG:HH11	1.83	0.42
1:G:61:LEU:HD21	1:G:151:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:313:SER:OG	1:G:314:ILE:N	2.49	0.42
1:G:414:GLN:OE1	1:G:429:PRO:HD2	2.19	0.42
1:H:255:VAL:HG13	1:H:256:GLY:H	1.84	0.42
1:L:131:ILE:HB	1:L:136:TYR:HE2	1.84	0.42
2:L:601:XEG:CAL	2:L:601:XEG:HAP	2.49	0.42
1:A:168:ASP:OD1	1:A:169:MET:N	2.52	0.42
1:A:27:LYS:HB2	1:A:27:LYS:HE3	1.74	0.42
1:A:331:LEU:HB2	1:A:352:THR:HA	2.01	0.42
1:B:67:ARG:NH2	1:B:135:ASN:O	2.52	0.42
1:B:345:ALA:HA	1:B:368:ILE:HB	2.01	0.42
1:C:294:PHE:HD2	1:C:301:ILE:HD12	1.80	0.42
1:E:36:GLU:HB3	1:E:37:THR:H	1.68	0.42
1:E:416:SER:O	1:E:419:ARG:HB2	2.19	0.42
1:F:166:ALA:HB1	1:F:167:PRO:HD2	2.00	0.42
1:J:159:GLY:N	1:J:163:ASP:O	2.47	0.42
1:J:6:ASP:HA	1:J:7:PRO:HD3	1.90	0.42
1:L:321:ILE:HG12	1:L:343:ILE:CG2	2.49	0.42
1:B:482:TYR:O	1:B:486:ILE:HG13	2.19	0.42
1:D:217:ARG:HD3	1:D:262:TYR:CE2	2.54	0.42
1:D:371:LEU:HD23	1:D:481:ALA:HB1	2.01	0.42
1:G:217:ARG:NE	1:G:450:HIS:HD2	2.16	0.42
1:G:488:LYS:O	1:G:492:VAL:HG23	2.18	0.42
1:I:232:TYR:HD1	1:I:235:ILE:HD12	1.84	0.42
1:K:107:LEU:HB3	1:K:126:LYS:HG2	2.00	0.42
1:K:421:PHE:CZ	1:K:423:LYS:HE3	2.53	0.42
1:A:251:GLY:HA3	1:A:326:ALA:HB2	2.02	0.42
1:A:432:PRO:HB2	1:A:436:PHE:HD1	1.84	0.42
1:E:27:LYS:HB2	1:E:27:LYS:HE2	1.81	0.42
1:E:329:LYS:HA	1:E:351:PRO:O	2.19	0.42
1:F:382:TYR:CZ	1:F:386:LEU:HD11	2.54	0.42
1:G:126:LYS:HD2	1:G:126:LYS:HA	1.87	0.42
1:H:227:ILE:HA	1:H:233:MET:CE	2.48	0.42
1:H:378:VAL:O	1:H:382:TYR:N	2.48	0.42
1:H:118:VAL:HA	1:H:460:SER:OG	2.19	0.42
1:H:498:VAL:HG13	1:H:498:VAL:O	2.19	0.42
1:A:275:GLU:HB3	1:A:276:SER:H	1.55	0.42
1:B:350:GLY:N	1:B:370:ASP:OD2	2.50	0.42
2:C:601:XEG:HAP	2:C:601:XEG:CAZ	2.50	0.42
1:D:32:LEU:HG	1:D:34:THR:HG22	2.00	0.42
1:G:491:ARG:HG2	1:G:491:ARG:H	1.50	0.42
1:H:52:ILE:HD13	1:H:489:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:271:VAL:HG23	1:I:283:PRO:HA	2.02	0.42
1:L:91:GLY:O	1:L:165:PRO:HA	2.20	0.42
1:A:97:THR:N	1:A:131:ILE:O	2.53	0.42
1:C:193:ASN:OD1	1:C:193:ASN:N	2.52	0.42
1:C:86:ARG:HA	1:C:86:ARG:HD3	1.92	0.42
1:E:201:LYS:HE2	1:E:206:GLY:O	2.20	0.42
1:E:263:LEU:HD12	1:E:263:LEU:HA	1.78	0.42
1:E:382:TYR:CE1	1:E:386:LEU:HD11	2.55	0.42
1:E:394:TYR:N	1:E:445:GLU:HG3	2.34	0.42
1:F:90:LYS:HZ1	1:F:381:SER:HB3	1.83	0.42
2:F:601:XEG:CAL	2:F:601:XEG:HAP	2.49	0.42
1:H:141:LEU:O	1:H:145:THR:HG23	2.18	0.42
1:J:168:ASP:OD1	1:J:169:MET:N	2.52	0.42
1:J:333:LYS:NZ	1:J:355:GLU:HG2	2.34	0.42
1:L:315:LEU:HD11	1:L:335:ASN:HB2	2.01	0.42
1:A:90:LYS:HE2	1:A:378:VAL:HG23	2.01	0.42
1:D:331:LEU:HA	1:D:335:ASN:ND2	2.33	0.42
1:F:287:ASP:OD1	1:F:289:LYS:HD3	2.19	0.42
1:F:433:THR:HG23	1:F:436:PHE:H	1.85	0.42
1:G:488:LYS:HG2	2:G:601:XEG:CAN	2.50	0.42
1:H:208:ILE:HG22	1:H:211:ARG:HD3	2.00	0.42
1:I:90:LYS:NZ	1:I:381:SER:HB3	2.35	0.42
1:K:52:ILE:HG12	1:K:493:TYR:CE2	2.55	0.42
1:L:90:LYS:HD2	1:L:164:VAL:O	2.20	0.42
1:L:223:ILE:O	1:L:227:ILE:HG12	2.19	0.42
2:L:601:XEG:HBE	2:L:601:XEG:HAJ	1.46	0.42
1:A:316:GLU:HA	1:A:339:VAL:HA	2.01	0.42
1:D:304:PHE:N	1:D:307:ALA:HB3	2.34	0.42
1:D:80:ALA:O	1:D:125:ALA:HA	2.20	0.42
1:E:14:GLU:N	1:E:14:GLU:OE1	2.44	0.42
1:K:129:VAL:HG12	1:K:131:ILE:HG12	2.00	0.42
1:K:85:HIS:CD2	1:K:86:ARG:HG2	2.54	0.42
1:L:9:PHE:CD2	1:L:12:MET:HG2	2.54	0.42
1:L:95:TYR:OH	1:L:145:THR:HG22	2.20	0.42
1:C:143:LYS:O	1:C:147:ARG:HB2	2.20	0.42
1:C:146:ARG:HG2	1:C:182:THR:OG1	2.19	0.42
1:E:227:ILE:HA	1:E:233:MET:HE2	2.02	0.42
1:F:200:GLY:H	1:F:384:GLU:CD	2.23	0.42
1:F:414:GLN:OE1	1:F:429:PRO:HD2	2.20	0.42
1:H:257:LEU:HD11	1:H:295:LYS:NZ	2.35	0.42
1:I:145:THR:OG1	1:I:146:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:201:LYS:HE2	1:I:206:GLY:O	2.20	0.42
1:K:200:GLY:H	1:K:384:GLU:CD	2.23	0.42
1:L:465:MET:O	1:L:469:MET:HG3	2.20	0.42
1:A:350:GLY:N	1:A:351:PRO:HD3	2.35	0.42
1:D:129:VAL:HG12	1:D:131:ILE:HG12	2.01	0.42
1:F:41:LYS:H	1:F:41:LYS:HG3	1.58	0.42
1:G:165:PRO:HD2	1:G:197:CYS:O	2.19	0.42
1:H:10:PHE:O	1:H:12:MET:HG3	2.19	0.42
1:J:324:PRO:HG2	1:J:351:PRO:HG2	2.01	0.42
1:J:382:TYR:CE2	1:J:386:LEU:HD11	2.55	0.42
1:J:65:ILE:HD13	1:J:144:ILE:HG12	2.01	0.42
1:K:243:GLY:O	1:K:245:LYS:N	2.44	0.42
1:A:167:PRO:HD3	1:A:176:MET:HG3	2.02	0.41
1:A:7:PRO:HB2	1:A:8:ASN:H	1.69	0.41
1:A:94:ARG:HG2	1:A:169:MET:HB2	2.02	0.41
1:B:160:PRO:HG3	1:B:193:ASN:O	2.19	0.41
1:C:213:SER:CB	1:C:262:TYR:HE2	2.33	0.41
1:C:379:THR:O	1:C:382:TYR:HB3	2.20	0.41
1:E:201:LYS:HD2	1:E:205:GLN:O	2.20	0.41
1:G:16:PHE:CZ	1:G:354:PRO:HD3	2.55	0.41
1:G:271:VAL:HG23	1:G:283:PRO:HA	2.02	0.41
1:H:158:ILE:HD12	1:H:165:PRO:CD	2.50	0.41
1:H:491:ARG:H	1:H:491:ARG:HG2	1.62	0.41
1:J:371:LEU:HD23	1:J:481:ALA:HB1	2.02	0.41
1:K:217:ARG:HH11	1:K:217:ARG:HD3	1.68	0.41
1:L:242:PHE:CE2	1:L:266:PHE:HB3	2.53	0.41
1:A:368:ILE:HA	1:A:369:PRO:HD3	1.95	0.41
1:A:37:THR:OG1	1:A:37:THR:O	2.32	0.41
1:C:148:PHE:O	1:C:152:LEU:HG	2.19	0.41
1:C:215:THR:O	1:C:219:VAL:HG23	2.20	0.41
2:C:601:XEG:CAL	2:C:601:XEG:HAP	2.50	0.41
1:D:107:LEU:HD23	1:D:126:LYS:HE2	2.02	0.41
1:D:112:THR:OG1	1:D:124:GLY:HA3	2.20	0.41
1:E:433:THR:HG23	1:E:436:PHE:H	1.84	0.41
1:E:66:ARG:HD2	1:E:70:GLY:HA2	2.01	0.41
1:F:346:GLU:HG2	1:F:351:PRO:HD2	2.02	0.41
1:G:164:VAL:HG13	1:G:198:VAL:HA	2.02	0.41
1:G:215:THR:O	1:G:219:VAL:HG23	2.21	0.41
1:G:244:ASP:O	1:G:245:LYS:HD2	2.20	0.41
1:H:145:THR:O	1:H:149:THR:OG1	2.36	0.41
1:I:429:PRO:HA	1:J:416:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:378:VAL:HA	1:K:381:SER:HB2	2.01	0.41
1:K:58:VAL:HA	1:K:80:ALA:HA	2.02	0.41
1:B:315:LEU:HD11	1:B:335:ASN:HB2	2.02	0.41
1:B:324:PRO:HD2	1:B:345:ALA:O	2.20	0.41
1:D:131:ILE:HB	1:D:136:TYR:CE2	2.55	0.41
1:D:250:GLN:HB2	1:D:314:ILE:HG21	2.02	0.41
1:D:88:PRO:HG2	1:D:122:PHE:CE2	2.55	0.41
1:E:248:ALA:CB	1:E:272:ALA:HB3	2.50	0.41
1:E:454:ALA:O	1:E:457:MET:N	2.53	0.41
1:G:129:VAL:HG12	1:G:131:ILE:HG12	2.02	0.41
1:H:46:ARG:HG2	1:H:50:ARG:HH11	1.84	0.41
1:I:195:HIS:CE1	1:K:87:THR:HG22	2.54	0.41
1:I:445:GLU:O	1:I:449:VAL:HG23	2.20	0.41
1:J:19:ARG:HG2	1:J:479:THR:HG22	2.02	0.41
1:K:164:VAL:HG13	1:K:198:VAL:HA	2.01	0.41
1:K:327:SER:OG	1:K:328:GLU:N	2.53	0.41
1:K:336:ALA:N	1:K:337:PRO:HD2	2.35	0.41
1:A:214:ALA:HB1	1:A:377:GLY:HA2	2.03	0.41
1:E:131:ILE:HB	1:E:136:TYR:HE2	1.85	0.41
1:E:324:PRO:HD2	1:E:345:ALA:O	2.19	0.41
1:E:432:PRO:HB2	1:E:436:PHE:HD1	1.85	0.41
1:G:300:THR:CG2	1:G:301:ILE:H	2.33	0.41
1:H:14:GLU:HG2	1:H:14:GLU:H	1.66	0.41
1:K:409:LEU:O	1:K:412:SER:N	2.54	0.41
1:K:371:LEU:HD23	1:K:481:ALA:HB1	2.01	0.41
1:L:323:ILE:HA	1:L:345:ALA:O	2.20	0.41
1:B:193:ASN:ND2	1:B:389:LEU:HD22	2.29	0.41
1:B:371:LEU:HD23	1:B:481:ALA:HB1	2.02	0.41
1:C:294:PHE:HE2	1:C:302:LEU:H	1.67	0.41
1:D:9:PHE:HE1	1:D:329:LYS:NZ	2.18	0.41
1:E:34:THR:OG1	1:E:35:ARG:N	2.53	0.41
1:E:24:VAL:HG13	1:E:483:VAL:CG2	2.50	0.41
1:F:91:GLY:HA3	1:F:125:ALA:O	2.21	0.41
1:G:244:ASP:OD1	1:G:244:ASP:N	2.51	0.41
1:H:270:CYS:SG	1:H:271:VAL:N	2.94	0.41
1:I:263:LEU:HA	1:I:263:LEU:HD12	1.89	0.41
1:K:294:PHE:CZ	1:K:304:PHE:CE1	3.09	0.41
1:L:332:THR:HA	1:L:356:ALA:HB2	2.01	0.41
1:A:86:ARG:HA	1:A:86:ARG:HD3	1.91	0.41
1:B:42:ARG:HD3	1:B:46:ARG:HH21	1.86	0.41
1:C:136:TYR:HB2	1:C:141:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:GLY:O	1:E:255:VAL:N	2.54	0.41
1:E:463:GLN:OE1	1:E:488:LYS:NZ	2.37	0.41
1:F:134:LYS:HG2	1:F:134:LYS:H	1.57	0.41
1:G:421:PHE:HZ	1:G:423:LYS:HE2	1.86	0.41
1:G:432:PRO:HB2	1:G:436:PHE:HD1	1.86	0.41
1:H:207:GLY:HA2	1:H:384:GLU:OE1	2.20	0.41
1:J:36:GLU:OE1	1:J:41:LYS:HG2	2.21	0.41
1:G:50:ARG:O	1:J:74:VAL:HG11	2.21	0.41
1:L:42:ARG:O	1:L:46:ARG:N	2.35	0.41
1:B:79:ARG:HA	1:B:127:ALA:HA	2.02	0.41
1:B:500:PHE:HB3	1:D:500:PHE:HB3	2.03	0.41
1:C:321:ILE:HG12	1:C:343:ILE:HG23	2.03	0.41
1:E:461:ALA:O	1:E:465:MET:HG3	2.20	0.41
1:F:383:PHE:HA	1:F:386:LEU:HD12	2.03	0.41
1:G:238:MET:HE2	1:G:320:ASP:HB3	2.03	0.41
1:H:345:ALA:HB1	1:H:373:LEU:HD22	2.02	0.41
1:H:47:GLY:HA3	1:K:72:TRP:HB2	2.03	0.41
1:H:32:LEU:HD13	1:H:494:ASN:HD21	1.85	0.41
1:J:212:ILE:HG13	1:J:258:HIS:CE1	2.45	0.41
1:J:376:GLY:HA2	1:J:379:THR:HB	2.03	0.41
1:J:28:LEU:HD22	1:J:490:PHE:CD2	2.56	0.41
1:J:61:LEU:HD12	1:J:61:LEU:HA	1.87	0.41
1:L:459:ARG:O	1:L:463:GLN:HG3	2.20	0.41
1:B:305:PRO:C	1:B:307:ALA:H	2.24	0.41
1:B:48:ILE:O	1:B:52:ILE:HG13	2.20	0.41
1:C:249:VAL:HA	1:C:323:ILE:HG13	2.02	0.41
1:D:134:LYS:H	1:D:134:LYS:HG2	1.47	0.41
1:D:227:ILE:HA	1:D:233:MET:CE	2.51	0.41
1:E:229:GLU:OE2	1:E:462:ARG:NH2	2.54	0.41
1:E:327:SER:OG	1:E:328:GLU:N	2.54	0.41
1:E:350:GLY:N	1:E:351:PRO:HD3	2.35	0.41
1:J:227:ILE:HD12	1:J:242:PHE:CD1	2.53	0.41
1:L:201:LYS:HG2	1:L:384:GLU:OE1	2.21	0.41
1:L:29:VAL:O	1:L:41:LYS:NZ	2.53	0.41
1:H:408:HIS:HB3	1:L:436:PHE:CD2	2.56	0.41
1:L:79:ARG:HH11	1:L:127:ALA:HB2	1.85	0.41
1:A:323:ILE:HA	1:A:345:ALA:O	2.21	0.41
1:A:211:ARG:HA	1:A:380:VAL:HG11	2.02	0.41
1:B:219:VAL:HA	1:B:373:LEU:HG	2.02	0.41
1:G:257:LEU:HB3	1:G:258:HIS:HD2	1.85	0.41
1:G:315:LEU:HD11	1:G:335:ASN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:432:PRO:CB	1:H:436:PHE:HD1	2.33	0.41
1:I:146:ARG:HG2	1:I:182:THR:OG1	2.21	0.41
1:L:350:GLY:N	1:L:351:PRO:HD3	2.36	0.41
1:A:12:MET:HG3	1:A:13:VAL:H	1.86	0.41
1:A:183:TYR:CE2	1:A:188:GLY:HA3	2.56	0.41
1:A:193:ASN:OD1	1:A:193:ASN:N	2.54	0.41
1:D:186:THR:OG1	1:D:187:ILE:N	2.52	0.41
1:D:414:GLN:OE1	1:D:429:PRO:HD2	2.21	0.41
1:E:227:ILE:HD11	1:E:343:ILE:HD13	2.02	0.41
1:E:193:ASN:HD22	1:E:389:LEU:HD22	1.86	0.41
1:F:12:MET:HG2	1:F:12:MET:H	1.63	0.41
1:F:346:GLU:HB3	1:F:370:ASP:HB3	2.02	0.41
1:F:34:THR:OG1	1:F:35:ARG:N	2.53	0.41
1:F:414:GLN:O	1:F:418:GLU:HG3	2.21	0.41
1:G:119:ASP:HA	2:G:601:XEG:HAI	2.03	0.41
1:I:21:ALA:HB1	1:I:49:LEU:HD23	2.03	0.41
1:J:303:GLY:O	1:J:304:PHE:CD1	2.74	0.41
1:K:41:LYS:O	1:K:45:VAL:HG23	2.21	0.41
1:A:282:ASN:HD21	1:A:306:LYS:HB3	1.84	0.41
1:A:85:HIS:HB2	1:A:492:VAL:HG11	2.03	0.41
1:B:408:HIS:O	1:B:412:SER:OG	2.20	0.41
1:B:85:HIS:CD2	1:B:86:ARG:HG2	2.56	0.41
1:C:323:ILE:HG22	1:C:345:ALA:O	2.21	0.41
1:D:315:LEU:HD22	1:D:322:LEU:HD21	2.03	0.41
1:E:321:ILE:HG12	1:E:343:ILE:HG23	2.02	0.41
1:F:8:ASN:O	1:F:10:PHE:N	2.52	0.41
1:G:459:ARG:O	1:G:463:GLN:HG2	2.21	0.41
1:H:18:ASP:OD1	1:H:53:LYS:HD3	2.21	0.41
1:H:353:THR:OG1	1:H:355:GLU:HG2	2.21	0.41
1:J:233:MET:O	1:J:237:GLY:N	2.54	0.41
1:K:335:ASN:O	1:K:338:ARG:HG2	2.22	0.41
1:L:409:LEU:HA	1:L:409:LEU:HD12	1.91	0.41
1:A:58:VAL:HA	1:A:80:ALA:HA	2.03	0.40
1:C:369:PRO:HB3	1:C:478:ARG:HD3	2.02	0.40
1:D:13:VAL:HG23	1:D:16:PHE:HD2	1.86	0.40
1:D:378:VAL:HA	1:D:381:SER:HB2	2.03	0.40
1:F:181:ASP:O	1:F:185:SER:OG	2.19	0.40
1:G:249:VAL:HG12	1:G:323:ILE:CD1	2.45	0.40
1:G:358:LYS:HD2	1:G:358:LYS:HA	1.92	0.40
1:H:129:VAL:HG12	1:H:131:ILE:HG12	2.03	0.40
1:K:385:TRP:O	1:K:389:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:THR:O	1:D:382:TYR:HB3	2.21	0.40
1:G:201:LYS:HG2	1:G:201:LYS:H	1.65	0.40
1:G:357:ASP:HA	1:G:360:PHE:HB2	2.03	0.40
1:G:371:LEU:HD23	1:G:481:ALA:HB1	2.03	0.40
1:G:487:GLU:O	1:G:491:ARG:HG2	2.20	0.40
1:H:220:PHE:CZ	1:H:266:PHE:HE2	2.39	0.40
1:H:88:PRO:HG2	1:H:122:PHE:CE2	2.56	0.40
1:I:226:PHE:C	1:I:228:ASN:H	2.24	0.40
1:I:368:ILE:HG21	1:I:373:LEU:HD13	2.03	0.40
1:J:440:ILE:HA	1:J:443:ALA:HB2	2.02	0.40
1:K:432:PRO:CB	1:K:436:PHE:HD1	2.34	0.40
1:L:211:ARG:HD3	1:L:384:GLU:OE2	2.20	0.40
1:L:226:PHE:C	1:L:228:ASN:H	2.25	0.40
1:A:368:ILE:HG21	1:A:373:LEU:HD13	2.03	0.40
1:D:10:PHE:HB3	1:D:11:LYS:H	1.67	0.40
1:D:24:VAL:HG13	1:D:483:VAL:CG2	2.52	0.40
1:E:193:ASN:N	1:E:193:ASN:OD1	2.54	0.40
1:E:36:GLU:HG2	1:E:38:GLU:OE2	2.21	0.40
1:F:114:LYS:HG2	1:F:371:LEU:O	2.22	0.40
1:F:183:TYR:CE2	1:F:188:GLY:HA3	2.56	0.40
1:G:260:MET:HE1	1:G:286:ILE:HD11	2.02	0.40
1:G:300:THR:CG2	1:G:301:ILE:N	2.83	0.40
1:G:414:GLN:OE1	1:G:430:ILE:HG23	2.22	0.40
1:G:79:ARG:HA	1:G:127:ALA:HA	2.03	0.40
1:H:82:HIS:N	1:H:124:GLY:O	2.53	0.40
1:H:387:LYS:O	1:H:391:HIS:N	2.55	0.40
1:H:36:GLU:OE1	1:H:38:GLU:N	2.54	0.40
1:H:74:VAL:HG11	1:K:50:ARG:O	2.20	0.40
1:K:319:CYS:O	1:K:341:ALA:HA	2.21	0.40
1:K:368:ILE:HG21	1:K:373:LEU:HD13	2.03	0.40
1:C:95:TYR:OH	1:C:145:THR:HG22	2.21	0.40
1:F:90:LYS:HD2	1:F:122:PHE:CD1	2.56	0.40
1:F:315:LEU:CD2	1:F:322:LEU:HD21	2.52	0.40
1:F:86:ARG:HG2	1:F:121:PRO:C	2.42	0.40
1:I:291:LEU:HD12	1:I:291:LEU:HA	1.62	0.40
2:I:601:XEG:CAL	2:I:601:XEG:HAPA	2.52	0.40
1:K:343:ILE:HD11	1:K:368:ILE:HD11	2.04	0.40
1:L:99:VAL:HA	1:L:103:GLU:OE1	2.21	0.40
1:C:243:GLY:O	1:C:245:LYS:N	2.45	0.40
1:D:280:ILE:HD11	1:D:301:ILE:HD11	2.03	0.40
1:E:430:ILE:H	1:E:430:ILE:HG13	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:254:ASN:H	1:F:257:LEU:HD12	1.87	0.40
1:H:154:LYS:HE3	1:I:189:HIS:NE2	2.36	0.40
1:H:85:HIS:HB2	1:H:492:VAL:HG11	2.02	0.40
1:I:141:LEU:HD12	1:I:144:ILE:HD12	2.04	0.40
1:I:282:ASN:ND2	1:I:306:LYS:HB2	2.37	0.40
1:I:396:ARG:HB3	1:I:397:LEU:HD12	2.04	0.40
1:J:201:LYS:O	1:J:211:ARG:NH2	2.55	0.40
1:K:88:PRO:HG2	1:K:122:PHE:CD2	2.57	0.40
1:K:313:SER:OG	1:K:314:ILE:N	2.53	0.40
1:K:38:GLU:O	1:K:41:LYS:HD3	2.21	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	494/496 (100%)	428 (87%)	52 (10%)	14 (3%)	5 34
1	B	494/496 (100%)	421 (85%)	58 (12%)	15 (3%)	4 32
1	C	494/496 (100%)	418 (85%)	60 (12%)	16 (3%)	4 31
1	D	494/496 (100%)	423 (86%)	55 (11%)	16 (3%)	4 31
1	E	494/496 (100%)	426 (86%)	53 (11%)	15 (3%)	4 32
1	F	494/496 (100%)	420 (85%)	59 (12%)	15 (3%)	4 32
1	G	494/496 (100%)	421 (85%)	60 (12%)	13 (3%)	5 35
1	H	494/496 (100%)	420 (85%)	61 (12%)	13 (3%)	5 35
1	I	494/496 (100%)	411 (83%)	69 (14%)	14 (3%)	5 34
1	J	494/496 (100%)	420 (85%)	58 (12%)	16 (3%)	4 31
1	K	494/496 (100%)	422 (85%)	55 (11%)	17 (3%)	3 30
1	L	494/496 (100%)	418 (85%)	66 (13%)	10 (2%)	7 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5928/5952 (100%)	5048 (85%)	706 (12%)	174 (3%)	4 33

All (174) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	PHE
1	A	254	ASN
1	B	168	ASP
1	B	276	SER
1	C	12	MET
1	D	10	PHE
1	D	168	ASP
1	E	252	PHE
1	F	316	GLU
1	G	7	PRO
1	G	295	LYS
1	H	238	MET
1	H	241	GLY
1	J	241	GLY
1	J	244	ASP
1	L	252	PHE
1	A	7	PRO
1	A	36	GLU
1	A	302	LEU
1	B	241	GLY
1	B	243	GLY
1	B	244	ASP
1	B	295	LYS
1	B	329	LYS
1	B	422	GLY
1	B	474	GLY
1	C	271	VAL
1	D	295	LYS
1	D	474	GLY
1	E	36	GLU
1	E	254	ASN
1	E	295	LYS
1	E	474	GLY
1	F	168	ASP
1	F	271	VAL
1	G	254	ASN
1	G	271	VAL

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Mol	Chain	Res	Type
1	G	474	GLY
1	H	168	ASP
1	H	243	GLY
1	H	244	ASP
1	H	252	PHE
1	H	254	ASN
1	H	271	VAL
1	H	295	LYS
1	H	474	GLY
1	I	7	PRO
1	I	168	ASP
1	I	271	VAL
1	I	306	LYS
1	I	329	LYS
1	I	474	GLY
1	J	11	LYS
1	J	168	ASP
1	J	243	GLY
1	J	254	ASN
1	J	271	VAL
1	J	295	LYS
1	J	474	GLY
1	K	241	GLY
1	K	254	ASN
1	K	271	VAL
1	K	306	LYS
1	K	474	GLY
1	L	241	GLY
1	L	474	GLY
1	A	62	SER
1	A	304	PHE
1	B	238	MET
1	B	254	ASN
1	B	271	VAL
1	B	313	SER
1	C	254	ASN
1	C	291	LEU
1	C	295	LYS
1	C	327	SER
1	D	11	LYS
1	D	36	GLU
1	D	238	MET

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Mol	Chain	Res	Type
1	D	241	GLY
1	D	254	ASN
1	D	313	SER
1	E	168	ASP
1	F	82	HIS
1	F	254	ASN
1	F	295	LYS
1	G	168	ASP
1	G	244	ASP
1	G	252	PHE
1	H	11	LYS
1	I	252	PHE
1	J	82	HIS
1	J	318	ASP
1	K	82	HIS
1	L	168	ASP
1	L	187	ILE
1	A	168	ASP
1	A	295	LYS
1	A	474	GLY
1	C	7	PRO
1	C	11	LYS
1	C	58	VAL
1	D	243	GLY
1	D	276	SER
1	E	37	THR
1	E	38	GLU
1	E	302	LEU
1	F	9	PHE
1	F	88	PRO
1	H	82	HIS
1	I	36	GLU
1	J	238	MET
1	J	338	ARG
1	K	10	PHE
1	K	227	ILE
1	K	243	GLY
1	K	295	LYS
1	K	335	ASN
1	L	36	GLU
1	L	295	LYS
1	A	8	ASN

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Mol	Chain	Res	Type
1	A	243	GLY
1	A	271	VAL
1	A	339	VAL
1	B	11	LYS
1	C	82	HIS
1	C	168	ASP
1	C	244	ASP
1	C	329	LYS
1	C	339	VAL
1	D	271	VAL
1	E	227	ILE
1	E	329	LYS
1	E	339	VAL
1	F	339	VAL
1	F	474	GLY
1	G	82	HIS
1	H	339	VAL
1	I	82	HIS
1	I	227	ILE
1	I	254	ASN
1	I	339	VAL
1	J	339	VAL
1	K	36	GLU
1	K	257	LEU
1	L	271	VAL
1	L	339	VAL
1	C	243	GLY
1	C	425	GLY
1	D	7	PRO
1	E	62	SER
1	G	241	GLY
1	I	295	LYS
1	J	58	VAL
1	K	244	ASP
1	L	254	ASN
1	B	339	VAL
1	E	271	VAL
1	D	339	VAL
1	F	227	ILE
1	F	241	GLY
1	F	243	GLY
1	G	339	VAL

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Mol	Chain	Res	Type
1	J	165	PRO
1	K	299	GLY
1	K	339	VAL
1	E	187	ILE
1	F	187	ILE
1	F	299	GLY
1	I	187	ILE
1	K	158	ILE
1	D	165	PRO
1	G	88	PRO
1	G	299	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	413/413 (100%)	401 (97%)	12 (3%)	42	71
1	B	413/413 (100%)	402 (97%)	11 (3%)	44	73
1	C	413/413 (100%)	400 (97%)	13 (3%)	40	70
1	D	413/413 (100%)	400 (97%)	13 (3%)	40	70
1	E	413/413 (100%)	397 (96%)	16 (4%)	32	65
1	F	413/413 (100%)	396 (96%)	17 (4%)	30	64
1	G	413/413 (100%)	402 (97%)	11 (3%)	44	73
1	H	413/413 (100%)	399 (97%)	14 (3%)	37	68
1	I	413/413 (100%)	401 (97%)	12 (3%)	42	71
1	J	413/413 (100%)	407 (98%)	6 (2%)	65	83
1	K	413/413 (100%)	399 (97%)	14 (3%)	37	68
1	L	413/413 (100%)	395 (96%)	18 (4%)	28	62
All	All	4956/4956 (100%)	4799 (97%)	157 (3%)	39	69

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	30	GLU
1	A	193	ASN
1	A	266	PHE
1	A	293	ASP
1	A	294	PHE
1	A	298	HIS
1	A	304	PHE
1	A	419	ARG
1	A	462	ARG
1	A	469	MET
1	A	494	ASN
1	B	9	PHE
1	B	44	ARG
1	B	119	ASP
1	B	193	ASN
1	B	294	PHE
1	B	298	HIS
1	B	315	LEU
1	B	399	PHE
1	B	411	MET
1	B	420	LYS
1	B	446	LYS
1	C	8	ASN
1	C	79	ARG
1	C	147	ARG
1	C	193	ASN
1	C	294	PHE
1	C	298	HIS
1	C	311	GLU
1	C	313	SER
1	C	315	LEU
1	C	366	MET
1	C	421	PHE
1	C	493	TYR
1	C	494	ASN
1	D	9	PHE
1	D	11	LYS
1	D	12	MET
1	D	38	GLU
1	D	169	MET
1	D	193	ASN
1	D	269	LYS

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Mol	Chain	Res	Type
1	D	294	PHE
1	D	311	GLU
1	D	319	CYS
1	D	399	PHE
1	D	419	ARG
1	D	493	TYR
1	E	10	PHE
1	E	50	ARG
1	E	94	ARG
1	E	134	LYS
1	E	193	ASN
1	E	239	THR
1	E	245	LYS
1	E	266	PHE
1	E	294	PHE
1	E	304	PHE
1	E	306	LYS
1	E	330	GLN
1	E	338	ARG
1	E	358	LYS
1	E	478	ARG
1	E	494	ASN
1	F	79	ARG
1	F	86	ARG
1	F	90	LYS
1	F	143	LYS
1	F	193	ASN
1	F	211	ARG
1	F	217	ARG
1	F	266	PHE
1	F	289	LYS
1	F	294	PHE
1	F	298	HIS
1	F	381	SER
1	F	419	ARG
1	F	420	LYS
1	F	421	PHE
1	F	493	TYR
1	F	494	ASN
1	G	9	PHE
1	G	25	GLU
1	G	142	GLU

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Mol	Chain	Res	Type
1	G	147	ARG
1	G	193	ASN
1	G	236	LEU
1	G	261	ARG
1	G	266	PHE
1	G	294	PHE
1	G	311	GLU
1	G	315	LEU
1	H	36	GLU
1	H	193	ASN
1	H	228	ASN
1	H	265	ARG
1	H	266	PHE
1	H	269	LYS
1	H	277	ASP
1	H	294	PHE
1	H	295	LYS
1	H	298	HIS
1	H	319	CYS
1	H	333	LYS
1	H	338	ARG
1	H	478	ARG
1	I	46	ARG
1	I	211	ARG
1	I	236	LEU
1	I	261	ARG
1	I	266	PHE
1	I	290	GLU
1	I	294	PHE
1	I	319	CYS
1	I	330	GLN
1	I	399	PHE
1	I	421	PHE
1	I	466	ARG
1	J	12	MET
1	J	193	ASN
1	J	236	LEU
1	J	294	PHE
1	J	311	GLU
1	J	319	CYS
1	K	36	GLU
1	K	42	ARG

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Mol	Chain	Res	Type
1	K	44	ARG
1	K	134	LYS
1	K	147	ARG
1	K	193	ASN
1	K	236	LEU
1	K	261	ARG
1	K	265	ARG
1	K	266	PHE
1	K	311	GLU
1	K	338	ARG
1	K	462	ARG
1	K	494	ASN
1	L	9	PHE
1	L	11	LYS
1	L	19	ARG
1	L	36	GLU
1	L	217	ARG
1	L	220	PHE
1	L	236	LEU
1	L	266	PHE
1	L	294	PHE
1	L	306	LYS
1	L	311	GLU
1	L	315	LEU
1	L	330	GLN
1	L	333	LYS
1	L	399	PHE
1	L	421	PHE
1	L	462	ARG
1	L	484	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	B	298	HIS
1	B	330	GLN
1	C	8	ASN
1	D	193	ASN
1	E	250	GLN
1	F	84	GLN
1	F	298	HIS

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Mol	Chain	Res	Type
1	G	8	ASN
1	G	195	HIS
1	G	330	GLN
1	I	82	HIS
1	I	84	GLN
1	I	193	ASN
1	I	195	HIS
1	I	225	ASN
1	J	205	GLN
1	J	225	ASN
1	K	298	HIS
1	K	330	GLN
1	L	82	HIS
1	L	84	GLN
1	L	193	ASN
1	L	330	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

12 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	XEG	C	601	-	35,35,35	2.31	12 (34%)	52,52,52	1.99	15 (28%)
2	XEG	B	601	-	35,35,35	2.25	11 (31%)	52,52,52	1.98	14 (26%)
2	XEG	D	601	-	35,35,35	2.24	12 (34%)	52,52,52	1.95	13 (25%)
2	XEG	G	601	-	35,35,35	2.27	12 (34%)	52,52,52	1.91	14 (26%)
2	XEG	F	601	-	35,35,35	2.31	12 (34%)	52,52,52	1.98	14 (26%)
2	XEG	A	601	-	35,35,35	2.24	13 (37%)	52,52,52	1.91	14 (26%)
2	XEG	H	601	-	35,35,35	2.27	12 (34%)	52,52,52	1.97	15 (28%)
2	XEG	K	601	-	35,35,35	2.25	13 (37%)	52,52,52	1.88	13 (25%)
2	XEG	J	601	-	35,35,35	2.25	11 (31%)	52,52,52	1.95	13 (25%)
2	XEG	E	601	-	35,35,35	2.22	13 (37%)	52,52,52	1.89	13 (25%)
2	XEG	L	601	-	35,35,35	2.31	11 (31%)	52,52,52	1.94	14 (26%)
2	XEG	I	601	-	35,35,35	2.32	12 (34%)	52,52,52	1.97	13 (25%)

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	XEG	C	601	-	-	8/12/24/24	0/4/4/4
2	XEG	B	601	-	-	8/12/24/24	0/4/4/4
2	XEG	D	601	-	-	8/12/24/24	0/4/4/4
2	XEG	G	601	-	-	8/12/24/24	0/4/4/4
2	XEG	F	601	-	-	8/12/24/24	0/4/4/4
2	XEG	A	601	-	-	8/12/24/24	0/4/4/4
2	XEG	H	601	-	-	8/12/24/24	0/4/4/4
2	XEG	K	601	-	-	8/12/24/24	0/4/4/4
2	XEG	J	601	-	-	8/12/24/24	0/4/4/4
2	XEG	E	601	-	-	8/12/24/24	0/4/4/4
2	XEG	L	601	-	-	8/12/24/24	0/4/4/4
2	XEG	I	601	-	-	8/12/24/24	0/4/4/4

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	601	XEG	OAR-CBC	9.13	1.50	1.38
2	C	601	XEG	OAR-CBC	9.05	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	601	XEG	OAR-CBC	9.03	1.50	1.38
2	F	601	XEG	OAR-CBC	8.92	1.50	1.38
2	B	601	XEG	OAR-CBC	8.81	1.50	1.38
2	H	601	XEG	OAR-CBC	8.79	1.50	1.38
2	J	601	XEG	OAR-CBC	8.78	1.49	1.38
2	G	601	XEG	OAR-CBC	8.72	1.49	1.38
2	D	601	XEG	OAR-CBC	8.71	1.49	1.38
2	A	601	XEG	OAR-CBC	8.70	1.49	1.38
2	K	601	XEG	OAR-CBC	8.69	1.49	1.38
2	E	601	XEG	OAR-CBC	8.55	1.49	1.38
2	L	601	XEG	OAC-CAU	4.18	1.44	1.36
2	F	601	XEG	OAC-CAU	4.16	1.44	1.36
2	J	601	XEG	OAC-CAU	4.12	1.44	1.36
2	I	601	XEG	OAC-CAU	4.09	1.44	1.36
2	B	601	XEG	OAC-CAU	4.09	1.44	1.36
2	C	601	XEG	OAC-CAU	4.08	1.44	1.36
2	H	601	XEG	OAC-CAU	4.07	1.44	1.36
2	D	601	XEG	OAC-CAU	3.99	1.44	1.36
2	G	601	XEG	OAC-CAU	3.95	1.44	1.36
2	E	601	XEG	OAC-CAU	3.91	1.44	1.36
2	A	601	XEG	OAC-CAU	3.91	1.44	1.36
2	K	601	XEG	OAC-CAU	3.82	1.44	1.36
2	B	601	XEG	OAB-CAT	3.55	1.45	1.37
2	I	601	XEG	OAB-CAT	3.55	1.45	1.37
2	D	601	XEG	OAB-CAT	3.53	1.45	1.37
2	C	601	XEG	OAB-CAT	3.52	1.45	1.37
2	F	601	XEG	OAB-CAT	3.52	1.45	1.37
2	A	601	XEG	OAB-CAT	3.51	1.45	1.37
2	E	601	XEG	OAB-CAT	3.50	1.45	1.37
2	L	601	XEG	OAB-CAT	3.50	1.45	1.37
2	G	601	XEG	OAB-CAT	3.49	1.45	1.37
2	J	601	XEG	OAB-CAT	3.46	1.45	1.37
2	H	601	XEG	OAB-CAT	3.45	1.45	1.37
2	K	601	XEG	OAB-CAT	3.44	1.45	1.37
2	G	601	XEG	OAH-CBB	3.15	1.44	1.37
2	K	601	XEG	OAH-CBB	3.13	1.44	1.37
2	I	601	XEG	OAH-CBB	3.13	1.44	1.37
2	L	601	XEG	OAH-CBB	3.12	1.44	1.37
2	A	601	XEG	OAH-CBB	3.08	1.44	1.37
2	F	601	XEG	OAH-CBB	3.08	1.44	1.37
2	E	601	XEG	OAH-CBB	3.06	1.44	1.37
2	H	601	XEG	OAH-CBB	3.05	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	XEG	OAH-CBB	3.03	1.44	1.37
2	B	601	XEG	OAH-CBB	2.99	1.43	1.37
2	J	601	XEG	OAH-CBB	2.95	1.43	1.37
2	C	601	XEG	OAH-CBB	2.95	1.43	1.37
2	F	601	XEG	CAZ-CAS	2.92	1.56	1.50
2	F	601	XEG	CAP-CBE	-2.91	1.45	1.51
2	L	601	XEG	OAD-CAV	2.90	1.42	1.36
2	H	601	XEG	OAD-CAV	2.89	1.42	1.36
2	F	601	XEG	OAD-CAV	2.89	1.42	1.36
2	C	601	XEG	CAP-CBE	-2.87	1.45	1.51
2	C	601	XEG	OAD-CAV	2.87	1.42	1.36
2	I	601	XEG	OAD-CAV	2.87	1.42	1.36
2	H	601	XEG	CAP-CBE	-2.85	1.45	1.51
2	K	601	XEG	CAP-CBE	-2.82	1.45	1.51
2	D	601	XEG	OAD-CAV	2.82	1.42	1.36
2	G	601	XEG	OAD-CAV	2.81	1.42	1.36
2	G	601	XEG	CAP-CBE	-2.80	1.45	1.51
2	B	601	XEG	OAD-CAV	2.78	1.42	1.36
2	E	601	XEG	OAD-CAV	2.78	1.42	1.36
2	A	601	XEG	OAD-CAV	2.78	1.42	1.36
2	K	601	XEG	OAD-CAV	2.77	1.42	1.36
2	J	601	XEG	OAD-CAV	2.76	1.42	1.36
2	C	601	XEG	CAZ-CAS	2.75	1.56	1.50
2	L	601	XEG	CAP-CBE	-2.72	1.46	1.51
2	L	601	XEG	OAG-CAY	2.70	1.41	1.36
2	G	601	XEG	CAZ-CAS	2.69	1.56	1.50
2	E	601	XEG	OAG-CAY	2.69	1.41	1.36
2	J	601	XEG	OAG-CAY	2.68	1.41	1.36
2	G	601	XEG	OAG-CAY	2.68	1.41	1.36
2	I	601	XEG	OAG-CAY	2.68	1.41	1.36
2	K	601	XEG	CAZ-CAS	2.67	1.56	1.50
2	C	601	XEG	OAG-CAY	2.67	1.41	1.36
2	A	601	XEG	OAG-CAY	2.67	1.41	1.36
2	F	601	XEG	OAG-CAY	2.67	1.41	1.36
2	J	601	XEG	CAP-CBE	-2.67	1.46	1.51
2	H	601	XEG	CAZ-CAS	2.66	1.56	1.50
2	K	601	XEG	OAG-CAY	2.65	1.41	1.36
2	A	601	XEG	CAP-CBE	-2.65	1.46	1.51
2	B	601	XEG	CAP-CBE	-2.65	1.46	1.51
2	H	601	XEG	OAG-CAY	2.64	1.41	1.36
2	L	601	XEG	CAZ-CAS	2.64	1.56	1.50
2	B	601	XEG	OAG-CAY	2.61	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	XEG	CAP-CBE	-2.61	1.46	1.51
2	D	601	XEG	OAG-CAY	2.60	1.41	1.36
2	I	601	XEG	CAZ-CAS	2.58	1.56	1.50
2	D	601	XEG	CAP-CBE	-2.58	1.46	1.51
2	E	601	XEG	CAZ-CAS	2.54	1.55	1.50
2	I	601	XEG	CAP-CBE	-2.53	1.46	1.51
2	J	601	XEG	CAZ-CAS	2.53	1.55	1.50
2	A	601	XEG	CAZ-CAS	2.50	1.55	1.50
2	B	601	XEG	CAZ-CAS	2.48	1.55	1.50
2	D	601	XEG	CAZ-CAS	2.47	1.55	1.50
2	L	601	XEG	CAK-CAT	2.46	1.42	1.39
2	I	601	XEG	OAQ-CAS	2.42	1.39	1.34
2	C	601	XEG	CAK-CAT	2.38	1.42	1.39
2	A	601	XEG	CBC-CBD	2.37	1.43	1.40
2	K	601	XEG	CAK-CAT	2.37	1.42	1.39
2	H	601	XEG	OAQ-CAS	2.37	1.39	1.34
2	I	601	XEG	CAK-CAT	2.36	1.42	1.39
2	G	601	XEG	CBC-CBD	2.35	1.43	1.40
2	F	601	XEG	CAK-CAT	2.34	1.42	1.39
2	E	601	XEG	CAK-CAT	2.33	1.42	1.39
2	G	601	XEG	CAK-CAT	2.31	1.42	1.39
2	A	601	XEG	CAK-CAT	2.31	1.42	1.39
2	E	601	XEG	CBC-CBD	2.31	1.43	1.40
2	J	601	XEG	CAK-CAT	2.28	1.42	1.39
2	D	601	XEG	CAK-CAT	2.27	1.42	1.39
2	K	601	XEG	CBC-CBD	2.27	1.43	1.40
2	J	601	XEG	OAQ-CAS	2.27	1.39	1.34
2	G	601	XEG	OAQ-CAS	2.26	1.39	1.34
2	B	601	XEG	OAQ-CAS	2.26	1.39	1.34
2	I	601	XEG	CBC-CBD	2.25	1.43	1.40
2	H	601	XEG	CAK-CAT	2.25	1.42	1.39
2	F	601	XEG	CBC-CBD	2.22	1.43	1.40
2	C	601	XEG	CBC-CBD	2.22	1.43	1.40
2	L	601	XEG	CBC-CBD	2.22	1.43	1.40
2	L	601	XEG	OAE-CAW	2.22	1.40	1.36
2	C	601	XEG	OAE-CAW	2.21	1.40	1.36
2	B	601	XEG	OAE-CAW	2.20	1.40	1.36
2	F	601	XEG	OAE-CAW	2.19	1.40	1.36
2	H	601	XEG	OAE-CAW	2.19	1.40	1.36
2	E	601	XEG	OAE-CAW	2.19	1.40	1.36
2	I	601	XEG	OAE-CAW	2.18	1.40	1.36
2	E	601	XEG	OAQ-CAS	2.18	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	XEG	OAE-CAW	2.18	1.40	1.36
2	G	601	XEG	OAE-CAW	2.17	1.40	1.36
2	K	601	XEG	OAQ-CAS	2.17	1.39	1.34
2	F	601	XEG	OAQ-CAS	2.16	1.39	1.34
2	D	601	XEG	OAE-CAW	2.16	1.40	1.36
2	J	601	XEG	OAE-CAW	2.15	1.40	1.36
2	K	601	XEG	OAE-CAW	2.14	1.40	1.36
2	B	601	XEG	CAK-CAT	2.14	1.42	1.39
2	D	601	XEG	OAQ-CAS	2.11	1.39	1.34
2	D	601	XEG	CBC-CBD	2.09	1.43	1.40
2	A	601	XEG	OAR-CBF	-2.09	1.42	1.45
2	C	601	XEG	OAQ-CAS	2.08	1.38	1.34
2	A	601	XEG	OAQ-CAS	2.06	1.38	1.34
2	E	601	XEG	OAR-CBF	-2.04	1.42	1.45
2	H	601	XEG	CBC-CBD	2.04	1.43	1.40
2	K	601	XEG	OAR-CBF	-2.02	1.42	1.45

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	601	XEG	OAQ-CAS-CAZ	6.35	122.18	111.92
2	C	601	XEG	OAQ-CAS-CAZ	5.65	121.04	111.92
2	J	601	XEG	OAG-CAY-CBD	5.64	129.99	117.56
2	D	601	XEG	OAG-CAY-CBD	5.64	129.99	117.56
2	E	601	XEG	OAG-CAY-CBD	5.62	129.94	117.56
2	K	601	XEG	OAG-CAY-CBD	5.58	129.85	117.56
2	B	601	XEG	OAG-CAY-CBD	5.55	129.78	117.56
2	H	601	XEG	OAG-CAY-CBD	5.53	129.75	117.56
2	G	601	XEG	OAG-CAY-CBD	5.51	129.70	117.56
2	L	601	XEG	OAG-CAY-CBD	5.50	129.67	117.56
2	I	601	XEG	OAG-CAY-CBD	5.49	129.67	117.56
2	A	601	XEG	OAG-CAY-CBD	5.48	129.64	117.56
2	C	601	XEG	OAG-CAY-CBD	5.42	129.51	117.56
2	F	601	XEG	OAG-CAY-CBD	5.40	129.47	117.56
2	G	601	XEG	OAQ-CAS-CAZ	5.33	120.53	111.92
2	H	601	XEG	OAQ-CAS-CAZ	4.93	119.88	111.92
2	L	601	XEG	OAQ-CAS-CAZ	4.65	119.43	111.92
2	K	601	XEG	OAQ-CAS-CAZ	4.64	119.41	111.92
2	C	601	XEG	OAR-CBC-CAN	4.47	123.41	116.38
2	F	601	XEG	OAR-CBC-CAN	4.46	123.41	116.38
2	E	601	XEG	OAQ-CAS-CAZ	4.45	119.11	111.92
2	I	601	XEG	CBD-CAP-CBE	4.45	122.74	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	601	XEG	OAR-CBC-CAN	4.42	123.34	116.38
2	H	601	XEG	OAR-CBC-CAN	4.40	123.31	116.38
2	B	601	XEG	OAR-CBC-CAN	4.34	123.22	116.38
2	L	601	XEG	OAR-CBC-CAN	4.29	123.14	116.38
2	D	601	XEG	OAR-CBC-CAN	4.28	123.12	116.38
2	I	601	XEG	OAQ-CAS-CAZ	4.26	118.80	111.92
2	I	601	XEG	OAR-CBC-CAN	4.18	122.96	116.38
2	B	601	XEG	OAQ-CAS-CAZ	4.17	118.65	111.92
2	K	601	XEG	OAR-CBC-CAN	4.15	122.92	116.38
2	E	601	XEG	OAG-CAY-CAK	-4.10	108.49	119.46
2	A	601	XEG	OAG-CAY-CAK	-4.09	108.52	119.46
2	I	601	XEG	OAG-CAY-CAK	-4.06	108.58	119.46
2	D	601	XEG	OAG-CAY-CAK	-4.02	108.70	119.46
2	A	601	XEG	OAQ-CAS-CAZ	4.01	118.40	111.92
2	G	601	XEG	OAR-CBC-CAN	4.01	122.69	116.38
2	G	601	XEG	OAG-CAY-CAK	-4.00	108.76	119.46
2	E	601	XEG	OAR-CBC-CAN	4.00	122.67	116.38
2	A	601	XEG	OAR-CBC-CAN	3.99	122.66	116.38
2	J	601	XEG	OAG-CAY-CAK	-3.98	108.80	119.46
2	B	601	XEG	OAG-CAY-CAK	-3.97	108.84	119.46
2	K	601	XEG	OAG-CAY-CAK	-3.94	108.91	119.46
2	L	601	XEG	OAG-CAY-CAK	-3.93	108.93	119.46
2	H	601	XEG	OAG-CAY-CAK	-3.90	109.01	119.46
2	C	601	XEG	OAG-CAY-CAK	-3.87	109.09	119.46
2	F	601	XEG	OAG-CAY-CAK	-3.83	109.19	119.46
2	B	601	XEG	CBD-CAP-CBE	3.79	121.06	111.46
2	D	601	XEG	CAL-CAZ-CAS	-3.71	112.89	120.10
2	D	601	XEG	OAQ-CAS-CAZ	3.65	117.81	111.92
2	B	601	XEG	CAL-CAZ-CAS	-3.64	113.02	120.10
2	D	601	XEG	CBD-CAP-CBE	3.61	120.61	111.46
2	B	601	XEG	OAB-CAT-CAK	-3.59	110.50	119.84
2	H	601	XEG	OAB-CAT-CAK	-3.59	110.52	119.84
2	C	601	XEG	OAB-CAT-CAK	-3.58	110.53	119.84
2	F	601	XEG	OAB-CAT-CAK	-3.56	110.59	119.84
2	J	601	XEG	OAB-CAT-CAK	-3.55	110.62	119.84
2	G	601	XEG	OAB-CAT-CAK	-3.53	110.66	119.84
2	D	601	XEG	OAB-CAT-CAK	-3.53	110.67	119.84
2	K	601	XEG	OAB-CAT-CAK	-3.53	110.67	119.84
2	I	601	XEG	OAB-CAT-CAK	-3.49	110.76	119.84
2	A	601	XEG	CBD-CAP-CBE	3.47	120.26	111.46
2	J	601	XEG	OAQ-CAS-CAZ	3.46	117.51	111.92
2	J	601	XEG	CAL-CAZ-CAS	-3.45	113.40	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	601	XEG	OAB-CAT-CAK	-3.43	110.93	119.84
2	L	601	XEG	OAB-CAT-CAK	-3.39	111.03	119.84
2	B	601	XEG	OAB-CAT-CAN	3.39	128.65	119.84
2	J	601	XEG	CBD-CAP-CBE	3.37	120.01	111.46
2	A	601	XEG	OAB-CAT-CAK	-3.37	111.07	119.84
2	H	601	XEG	CBD-CAP-CBE	3.36	119.97	111.46
2	L	601	XEG	CBD-CAP-CBE	3.36	119.96	111.46
2	D	601	XEG	OAB-CAT-CAN	3.33	128.50	119.84
2	J	601	XEG	OAB-CAT-CAN	3.33	128.49	119.84
2	H	601	XEG	OAB-CAT-CAN	3.31	128.44	119.84
2	F	601	XEG	OAB-CAT-CAN	3.31	128.44	119.84
2	I	601	XEG	OAB-CAT-CAN	3.30	128.43	119.84
2	C	601	XEG	OAB-CAT-CAN	3.30	128.42	119.84
2	G	601	XEG	CBD-CAP-CBE	3.29	119.78	111.46
2	A	601	XEG	OAB-CAT-CAN	3.28	128.37	119.84
2	E	601	XEG	OAB-CAT-CAN	3.27	128.33	119.84
2	C	601	XEG	CBD-CAP-CBE	3.27	119.73	111.46
2	I	601	XEG	CAL-CAZ-CAS	-3.26	113.76	120.10
2	K	601	XEG	OAB-CAT-CAN	3.25	128.29	119.84
2	G	601	XEG	OAB-CAT-CAN	3.25	128.29	119.84
2	E	601	XEG	CBD-CAP-CBE	3.24	119.67	111.46
2	H	601	XEG	CAL-CAZ-CAS	-3.22	113.84	120.10
2	L	601	XEG	OAB-CAT-CAN	3.18	128.11	119.84
2	D	601	XEG	CAM-CAZ-CAS	3.12	126.17	120.10
2	B	601	XEG	CAM-CAZ-CAS	3.06	126.06	120.10
2	J	601	XEG	OAR-CBC-CBD	-3.02	116.76	122.26
2	F	601	XEG	OAR-CBC-CBD	-3.00	116.80	122.26
2	K	601	XEG	OAR-CBC-CBD	-2.95	116.89	122.26
2	H	601	XEG	OAR-CBC-CBD	-2.91	116.96	122.26
2	A	601	XEG	CAL-CAZ-CAS	-2.91	114.45	120.10
2	C	601	XEG	OAR-CBC-CBD	-2.90	116.98	122.26
2	D	601	XEG	OAR-CBC-CBD	-2.89	117.00	122.26
2	E	601	XEG	OAR-CBC-CBD	-2.86	117.05	122.26
2	L	601	XEG	CAL-CAZ-CAS	-2.85	114.57	120.10
2	E	601	XEG	CAL-CAZ-CAS	-2.83	114.61	120.10
2	A	601	XEG	OAR-CBC-CBD	-2.82	117.13	122.26
2	K	601	XEG	CBD-CAP-CBE	2.82	118.59	111.46
2	B	601	XEG	OAR-CBC-CBD	-2.81	117.14	122.26
2	I	601	XEG	CAM-CAZ-CAS	2.80	125.54	120.10
2	F	601	XEG	OAQ-CAS-OAA	-2.78	119.00	123.53
2	L	601	XEG	OAR-CBC-CBD	-2.75	117.25	122.26
2	H	601	XEG	CAM-CAZ-CAS	2.74	125.44	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	601	XEG	CAP-CBE-CBF	2.73	115.91	110.22
2	J	601	XEG	CAM-CAZ-CAS	2.71	125.36	120.10
2	G	601	XEG	CAP-CBE-CBF	2.70	115.85	110.22
2	G	601	XEG	OAR-CBC-CBD	-2.68	117.38	122.26
2	J	601	XEG	CAP-CBD-CBC	-2.67	116.32	120.98
2	A	601	XEG	CAP-CBE-CBF	2.59	115.62	110.22
2	F	601	XEG	CBD-CAP-CBE	2.59	118.03	111.46
2	L	601	XEG	CAP-CBD-CBC	-2.58	116.48	120.98
2	I	601	XEG	OAR-CBC-CBD	-2.54	117.63	122.26
2	C	601	XEG	CAP-CBE-CBF	2.53	115.49	110.22
2	B	601	XEG	OAR-CBF-CBE	2.52	115.99	109.08
2	I	601	XEG	CAP-CBE-CBF	2.51	115.46	110.22
2	F	601	XEG	CAP-CBD-CBC	-2.51	116.60	120.98
2	G	601	XEG	OAR-CBF-CBE	2.50	115.96	109.08
2	L	601	XEG	CAM-CAZ-CAS	2.49	124.95	120.10
2	A	601	XEG	OAR-CBF-CBE	2.49	115.91	109.08
2	I	601	XEG	OAR-CBF-CBE	2.48	115.88	109.08
2	E	601	XEG	CAP-CBE-CBF	2.47	115.37	110.22
2	K	601	XEG	OAR-CBF-CBE	2.44	115.78	109.08
2	G	601	XEG	CAL-CAZ-CAS	-2.44	115.37	120.10
2	C	601	XEG	CAP-CBD-CBC	-2.42	116.75	120.98
2	D	601	XEG	CAP-CBE-CBF	2.41	115.25	110.22
2	K	601	XEG	CAL-CAZ-CAS	-2.41	115.41	120.10
2	A	601	XEG	CAM-CAZ-CAS	2.40	124.77	120.10
2	C	601	XEG	CAL-CAZ-CAS	-2.40	115.43	120.10
2	C	601	XEG	OAQ-CAS-OAA	-2.40	119.61	123.53
2	H	601	XEG	OAR-CBF-CBE	2.39	115.64	109.08
2	K	601	XEG	CAP-CBE-CBF	2.37	115.16	110.22
2	E	601	XEG	OAR-CBF-CBE	2.36	115.57	109.08
2	H	601	XEG	CAP-CBE-CBF	2.35	115.12	110.22
2	C	601	XEG	OAR-CBF-CBE	2.35	115.53	109.08
2	K	601	XEG	CAP-CBD-CBC	-2.34	116.90	120.98
2	H	601	XEG	CAP-CBD-CBC	-2.34	116.90	120.98
2	D	601	XEG	CAP-CBD-CBC	-2.34	116.91	120.98
2	F	601	XEG	CAP-CBE-CBF	2.33	115.08	110.22
2	F	601	XEG	OAR-CBF-CBE	2.33	115.48	109.08
2	E	601	XEG	CAM-CAZ-CAS	2.33	124.63	120.10
2	I	601	XEG	CAN-CBC-CBD	-2.31	119.41	122.17
2	J	601	XEG	OAR-CBF-CBE	2.31	115.43	109.08
2	B	601	XEG	CAP-CBE-CBF	2.28	114.98	110.22
2	G	601	XEG	OAQ-CAS-OAA	-2.23	119.90	123.53
2	E	601	XEG	CAP-CBD-CBC	-2.23	117.10	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	601	XEG	OAR-CBF-CBE	2.20	115.13	109.08
2	A	601	XEG	CBA-CBF-CBE	-2.20	108.16	113.68
2	B	601	XEG	CAP-CBD-CBC	-2.20	117.15	120.98
2	D	601	XEG	OAR-CBF-CBE	2.17	115.05	109.08
2	G	601	XEG	CAM-CAZ-CAS	2.17	124.31	120.10
2	C	601	XEG	CAN-CBC-CBD	-2.14	119.61	122.17
2	F	601	XEG	CAL-CAZ-CAS	-2.14	115.94	120.10
2	L	601	XEG	CAN-CBC-CBD	-2.14	119.62	122.17
2	J	601	XEG	CAP-CBE-CBF	2.13	114.67	110.22
2	B	601	XEG	CAN-CBC-CBD	-2.11	119.64	122.17
2	C	601	XEG	CAM-CAZ-CAS	2.11	124.20	120.10
2	K	601	XEG	CAM-CAZ-CAS	2.07	124.14	120.10
2	H	601	XEG	OAQ-CAS-OAA	-2.07	120.16	123.53
2	H	601	XEG	CAN-CBC-CBD	-2.04	119.73	122.17
2	F	601	XEG	CAM-CAZ-CAS	2.02	124.02	120.10
2	G	601	XEG	CAP-CBD-CBC	-2.02	117.46	120.98
2	A	601	XEG	CAJ-CBA-CAO	2.00	121.07	118.76

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	XEG	OAA-CAS-OAQ-CBE
2	C	601	XEG	CAZ-CAS-OAQ-CBE
2	B	601	XEG	OAA-CAS-OAQ-CBE
2	B	601	XEG	CAZ-CAS-OAQ-CBE
2	D	601	XEG	OAA-CAS-OAQ-CBE
2	D	601	XEG	CAZ-CAS-OAQ-CBE
2	G	601	XEG	OAA-CAS-OAQ-CBE
2	G	601	XEG	CAZ-CAS-OAQ-CBE
2	F	601	XEG	OAA-CAS-OAQ-CBE
2	F	601	XEG	CAZ-CAS-OAQ-CBE
2	F	601	XEG	OAQ-CAS-CAZ-CAM
2	A	601	XEG	OAA-CAS-OAQ-CBE
2	A	601	XEG	CAZ-CAS-OAQ-CBE
2	H	601	XEG	OAA-CAS-OAQ-CBE
2	H	601	XEG	CAZ-CAS-OAQ-CBE
2	K	601	XEG	OAA-CAS-OAQ-CBE
2	K	601	XEG	CAZ-CAS-OAQ-CBE
2	J	601	XEG	OAA-CAS-OAQ-CBE
2	J	601	XEG	CAZ-CAS-OAQ-CBE
2	E	601	XEG	OAA-CAS-OAQ-CBE

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Mol	Chain	Res	Type	Atoms
2	E	601	XEG	CAZ-CAS-OAQ-CBE
2	L	601	XEG	OAA-CAS-OAQ-CBE
2	L	601	XEG	CAZ-CAS-OAQ-CBE
2	I	601	XEG	OAA-CAS-OAQ-CBE
2	I	601	XEG	CAZ-CAS-OAQ-CBE
2	C	601	XEG	OAA-CAS-CAZ-CAL
2	C	601	XEG	OAA-CAS-CAZ-CAM
2	C	601	XEG	OAQ-CAS-CAZ-CAL
2	C	601	XEG	OAQ-CAS-CAZ-CAM
2	B	601	XEG	OAQ-CAS-CAZ-CAM
2	G	601	XEG	OAA-CAS-CAZ-CAL
2	G	601	XEG	OAQ-CAS-CAZ-CAM
2	F	601	XEG	OAA-CAS-CAZ-CAL
2	F	601	XEG	OAA-CAS-CAZ-CAM
2	F	601	XEG	OAQ-CAS-CAZ-CAL
2	A	601	XEG	OAA-CAS-CAZ-CAL
2	A	601	XEG	OAA-CAS-CAZ-CAM
2	A	601	XEG	OAQ-CAS-CAZ-CAL
2	A	601	XEG	OAQ-CAS-CAZ-CAM
2	H	601	XEG	OAA-CAS-CAZ-CAL
2	H	601	XEG	OAA-CAS-CAZ-CAM
2	K	601	XEG	OAA-CAS-CAZ-CAL
2	K	601	XEG	OAA-CAS-CAZ-CAM
2	K	601	XEG	OAQ-CAS-CAZ-CAL
2	K	601	XEG	OAQ-CAS-CAZ-CAM
2	J	601	XEG	OAA-CAS-CAZ-CAL
2	J	601	XEG	OAQ-CAS-CAZ-CAM
2	E	601	XEG	OAA-CAS-CAZ-CAL
2	E	601	XEG	OAA-CAS-CAZ-CAM
2	E	601	XEG	OAQ-CAS-CAZ-CAM
2	L	601	XEG	OAA-CAS-CAZ-CAL
2	L	601	XEG	OAA-CAS-CAZ-CAM
2	L	601	XEG	OAQ-CAS-CAZ-CAL
2	L	601	XEG	OAQ-CAS-CAZ-CAM
2	I	601	XEG	OAA-CAS-CAZ-CAL
2	I	601	XEG	OAA-CAS-CAZ-CAM
2	I	601	XEG	OAQ-CAS-CAZ-CAL
2	I	601	XEG	OAQ-CAS-CAZ-CAM
2	B	601	XEG	OAA-CAS-CAZ-CAL
2	B	601	XEG	OAA-CAS-CAZ-CAM
2	B	601	XEG	OAQ-CAS-CAZ-CAL
2	D	601	XEG	OAA-CAS-CAZ-CAL

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Mol	Chain	Res	Type	Atoms
2	D	601	XEG	OAA-CAS-CAZ-CAM
2	D	601	XEG	OAQ-CAS-CAZ-CAL
2	D	601	XEG	OAQ-CAS-CAZ-CAM
2	G	601	XEG	OAA-CAS-CAZ-CAM
2	G	601	XEG	OAQ-CAS-CAZ-CAL
2	H	601	XEG	OAQ-CAS-CAZ-CAL
2	H	601	XEG	OAQ-CAS-CAZ-CAM
2	J	601	XEG	OAA-CAS-CAZ-CAM
2	J	601	XEG	OAQ-CAS-CAZ-CAL
2	E	601	XEG	OAQ-CAS-CAZ-CAL
2	C	601	XEG	CAJ-CBA-CBF-CBE
2	C	601	XEG	CAO-CBA-CBF-CBE
2	D	601	XEG	CAJ-CBA-CBF-CBE
2	G	601	XEG	CAJ-CBA-CBF-CBE
2	G	601	XEG	CAO-CBA-CBF-CBE
2	F	601	XEG	CAJ-CBA-CBF-CBE
2	F	601	XEG	CAO-CBA-CBF-CBE
2	A	601	XEG	CAJ-CBA-CBF-CBE
2	H	601	XEG	CAJ-CBA-CBF-CBE
2	K	601	XEG	CAJ-CBA-CBF-CBE
2	L	601	XEG	CAJ-CBA-CBF-CBE
2	I	601	XEG	CAJ-CBA-CBF-CBE
2	I	601	XEG	CAO-CBA-CBF-CBE
2	B	601	XEG	CAJ-CBA-CBF-CBE
2	D	601	XEG	CAO-CBA-CBF-CBE
2	E	601	XEG	CAJ-CBA-CBF-CBE
2	A	601	XEG	CAO-CBA-CBF-CBE
2	J	601	XEG	CAJ-CBA-CBF-CBE
2	L	601	XEG	CAO-CBA-CBF-CBE
2	B	601	XEG	CAO-CBA-CBF-CBE
2	H	601	XEG	CAO-CBA-CBF-CBE
2	K	601	XEG	CAO-CBA-CBF-CBE
2	J	601	XEG	CAO-CBA-CBF-CBE
2	E	601	XEG	CAO-CBA-CBF-CBE

There are no ring outliers.

12 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	XEG	4	0
2	B	601	XEG	1	0
2	D	601	XEG	2	0

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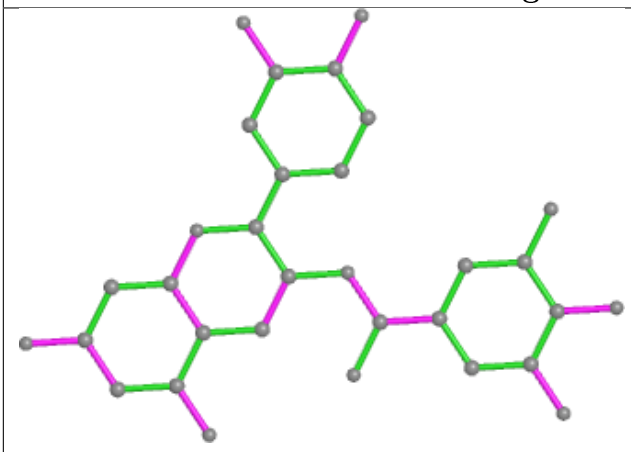
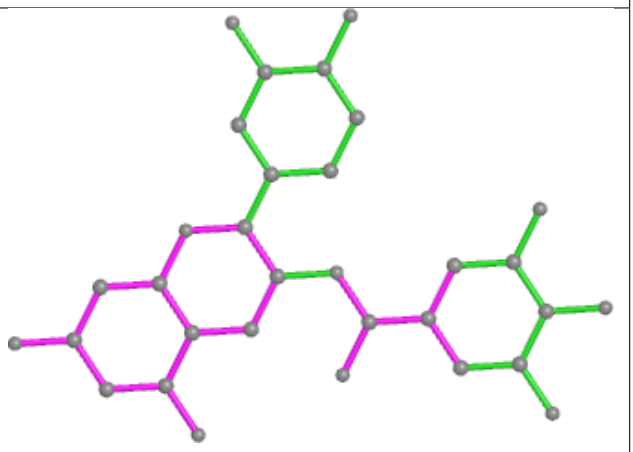
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	601	XEG	4	0
2	F	601	XEG	4	0
2	A	601	XEG	1	0
2	H	601	XEG	2	0
2	K	601	XEG	3	0
2	J	601	XEG	6	0
2	E	601	XEG	3	0
2	L	601	XEG	3	0
2	I	601	XEG	3	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

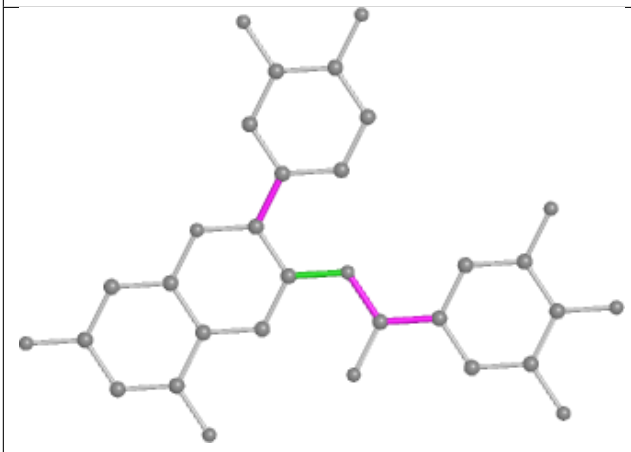
Ligand XEG C 601



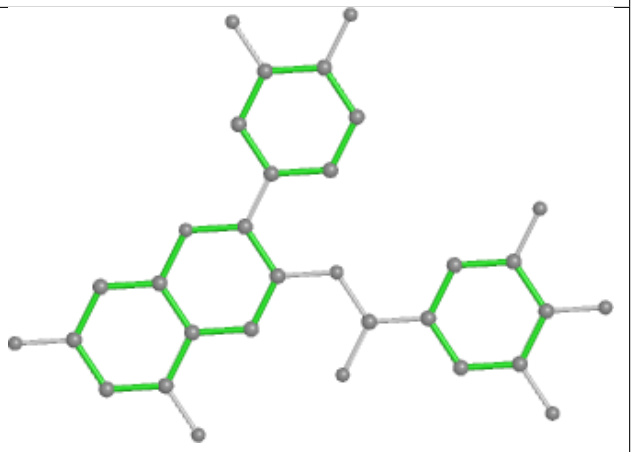
Bond lengths



Bond angles

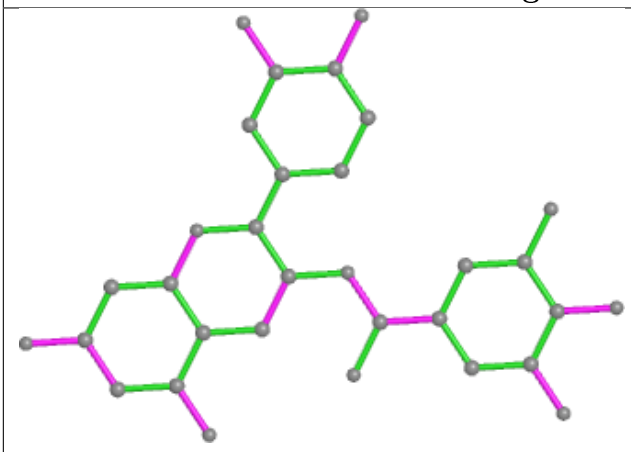


Torsions

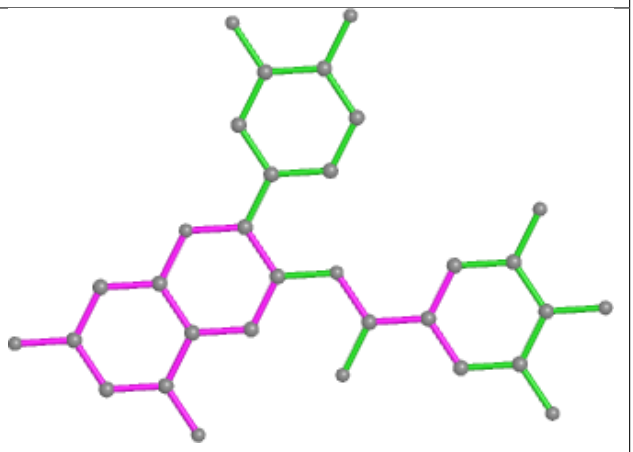


Rings

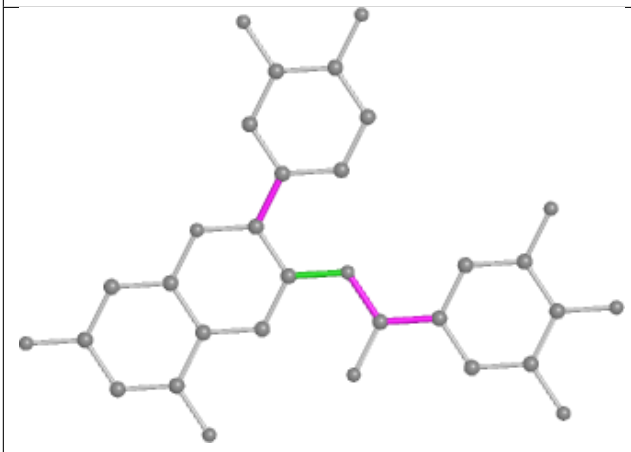
Ligand XEG B 601



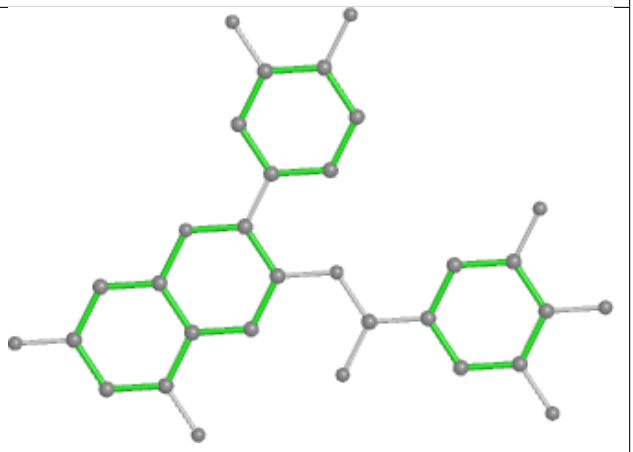
Bond lengths



Bond angles

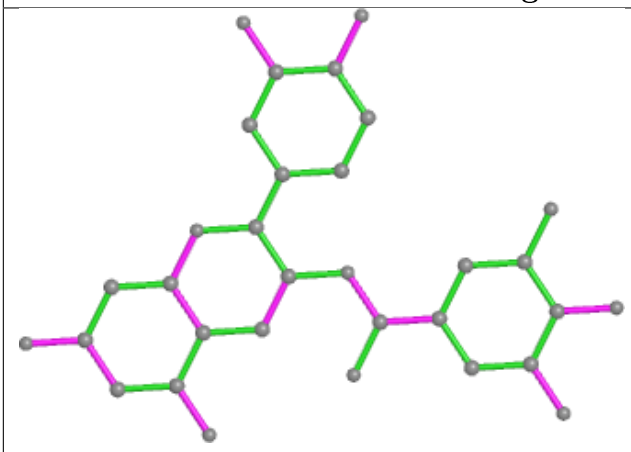


Torsions



Rings

Ligand XEG D 601



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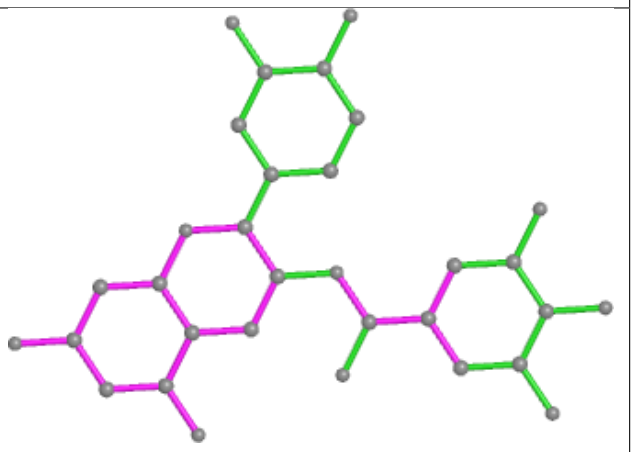
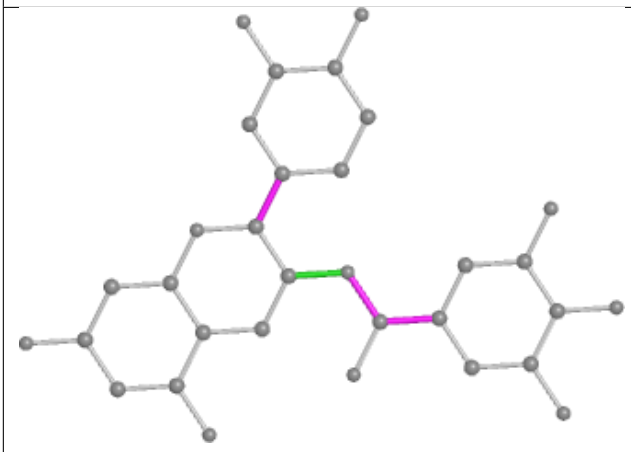
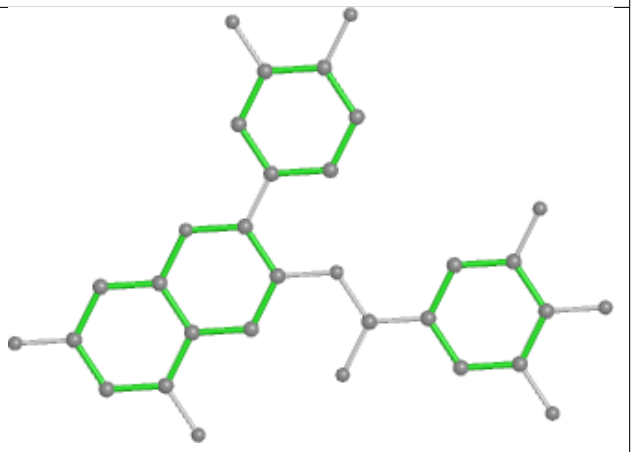


Bond angles

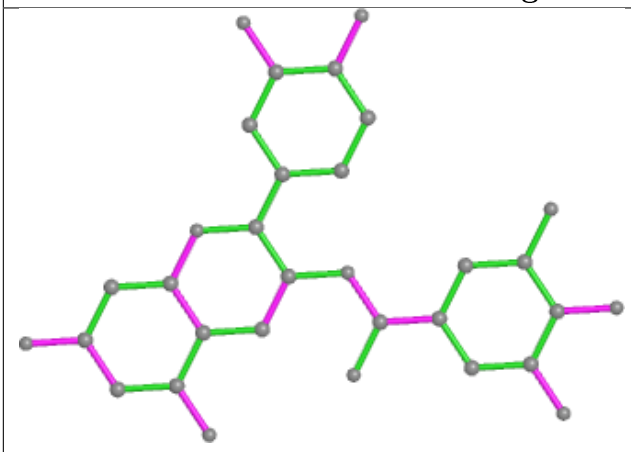


Torsions

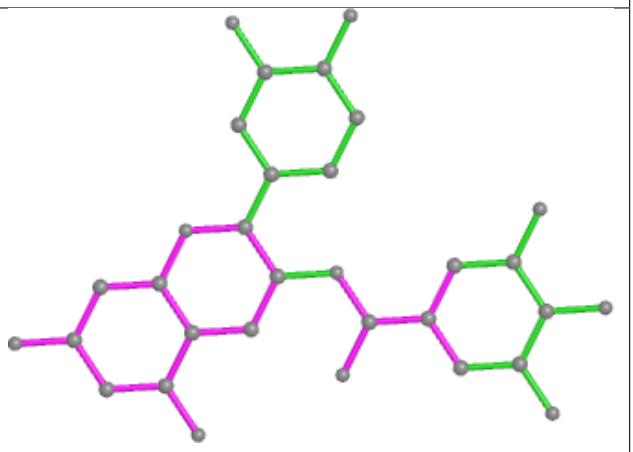


Rings

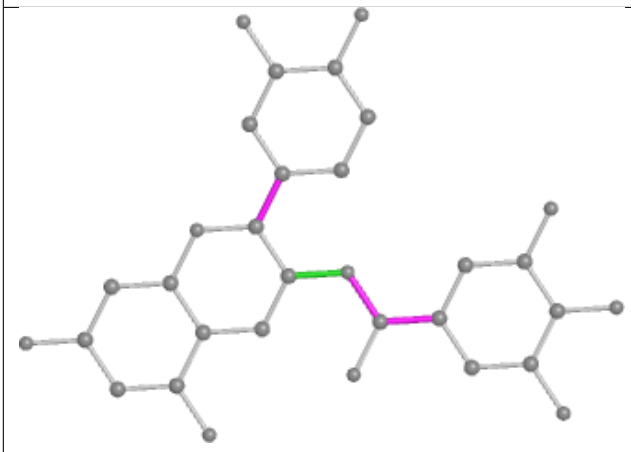
Ligand XEG G 601



Bond lengths



Bond angles



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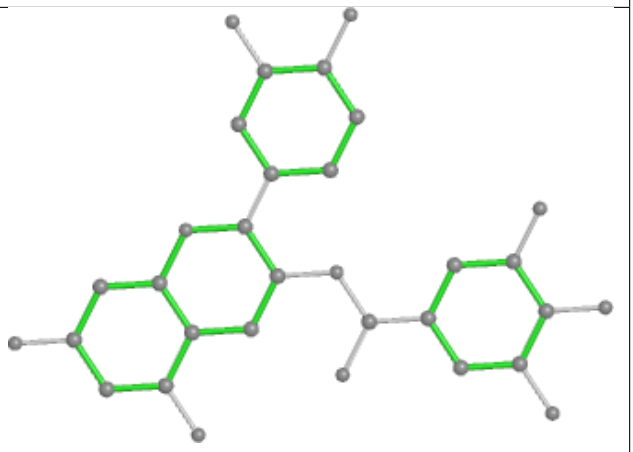
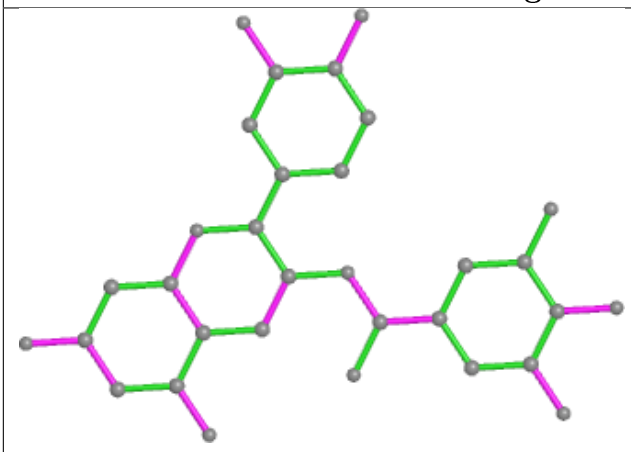
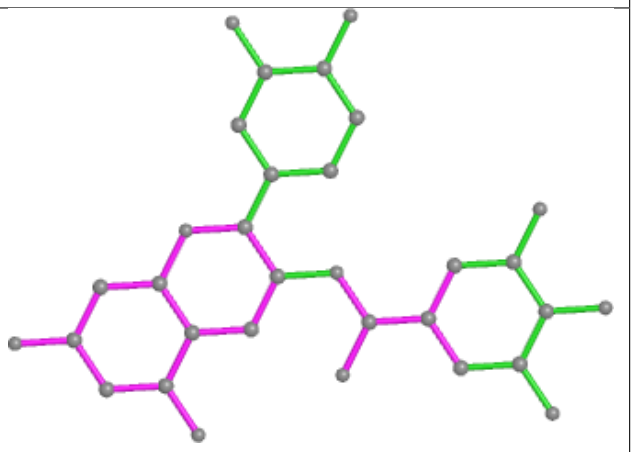


Rings

Ligand XEG F 601



Bond lengths



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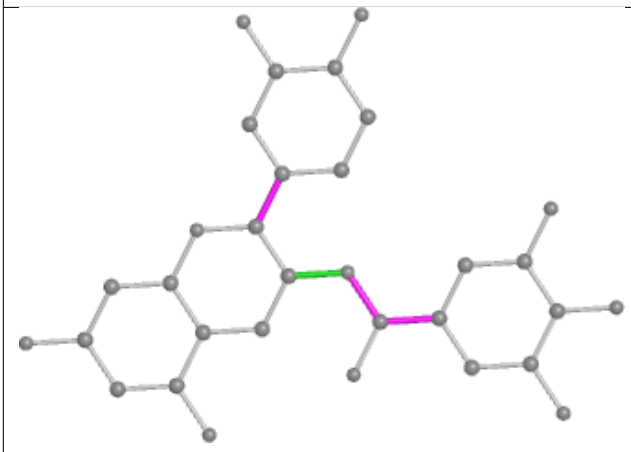

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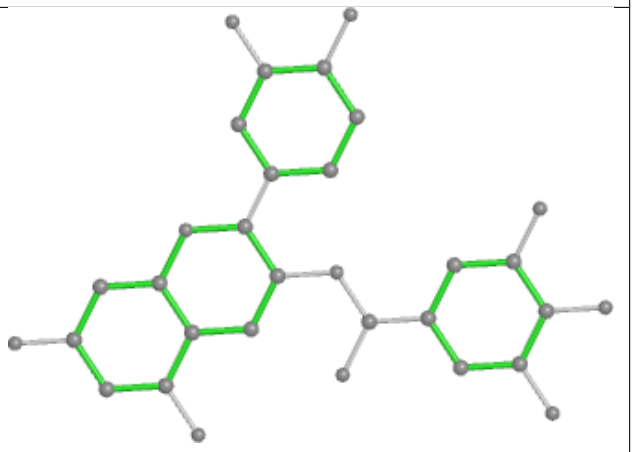
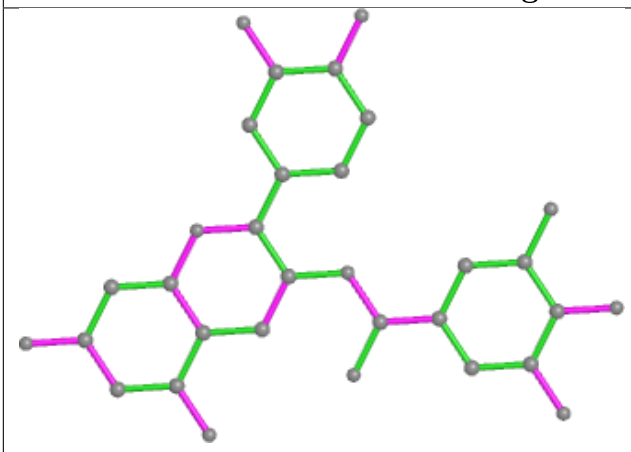


Rings

Ligand XEG A 601



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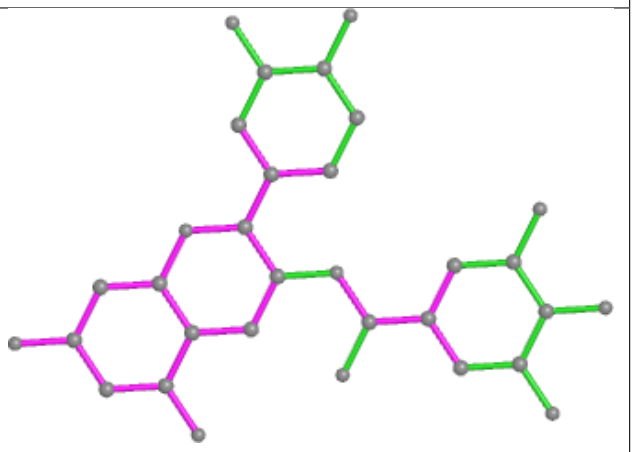
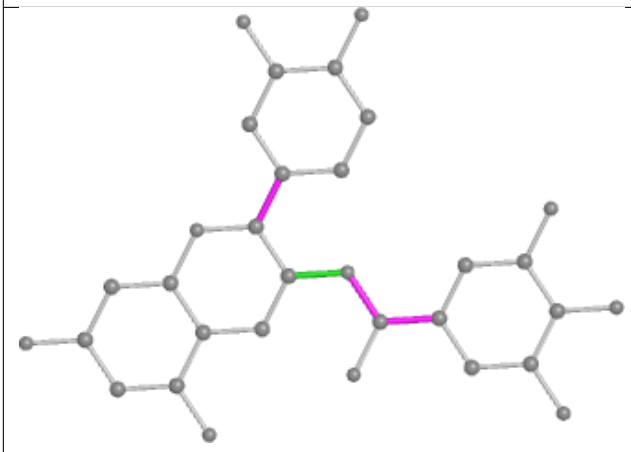


Bond angles



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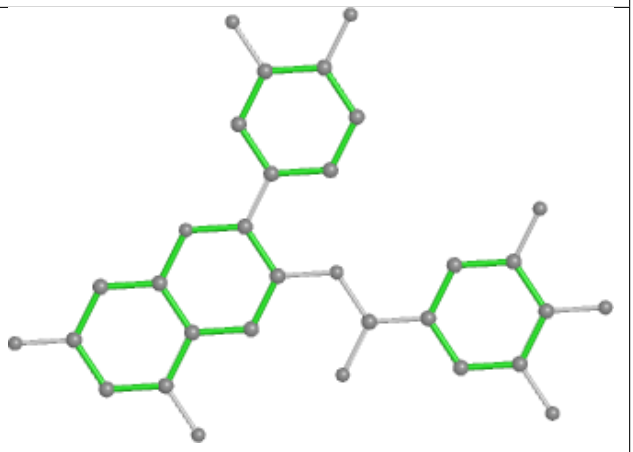
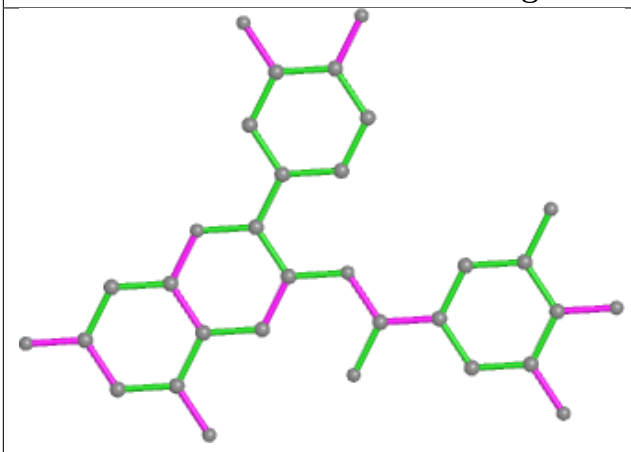


Rings

Ligand XEG H 601



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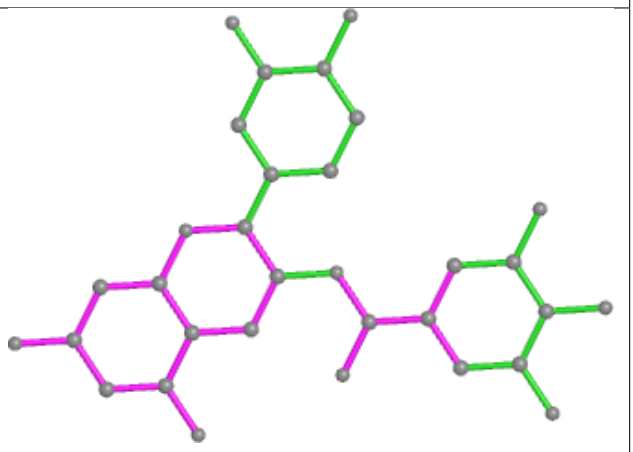

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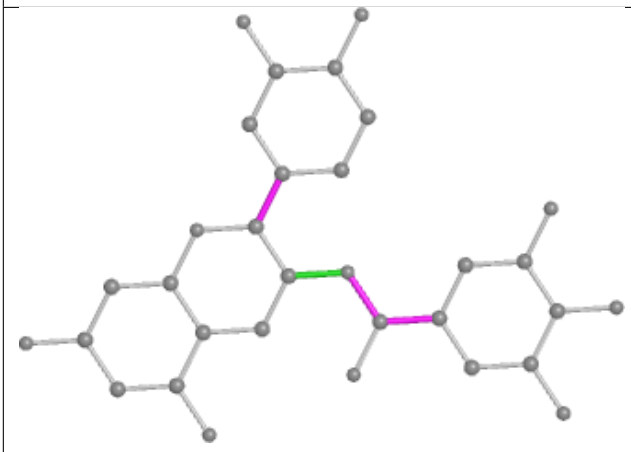

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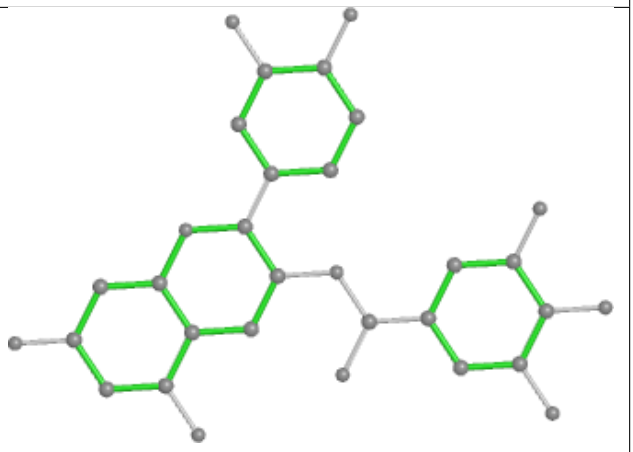
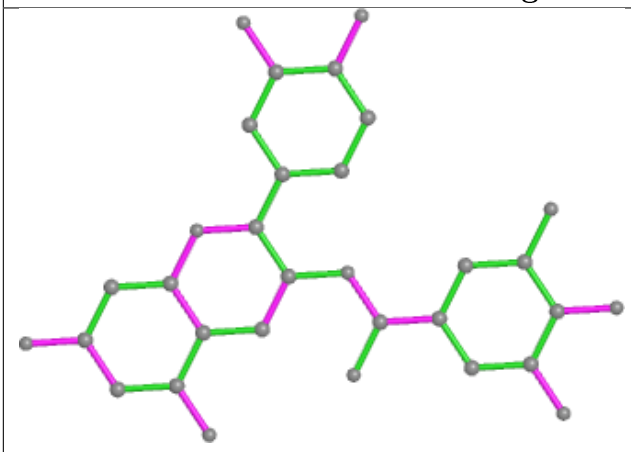


Rings

Ligand XEG K 601



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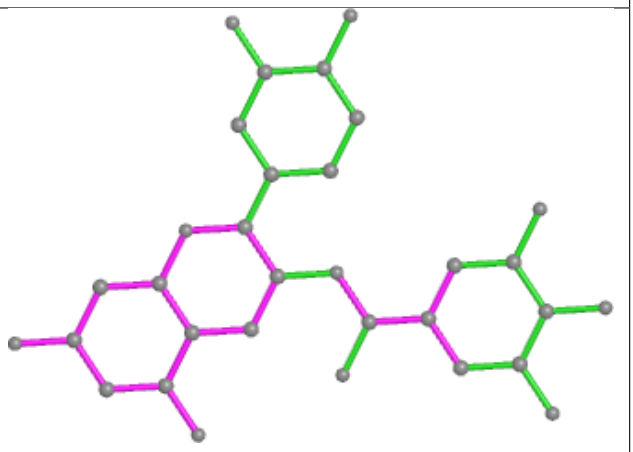

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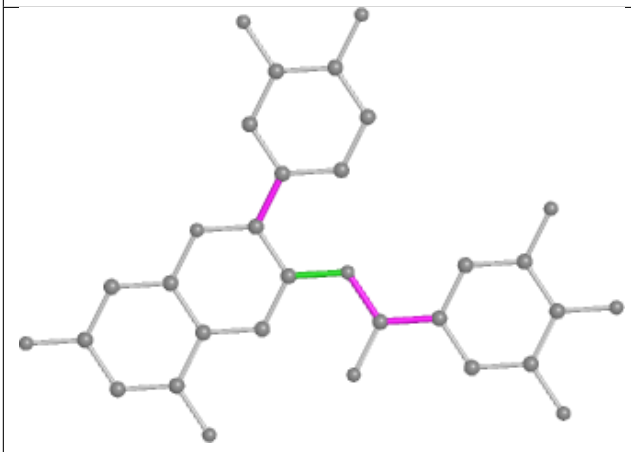

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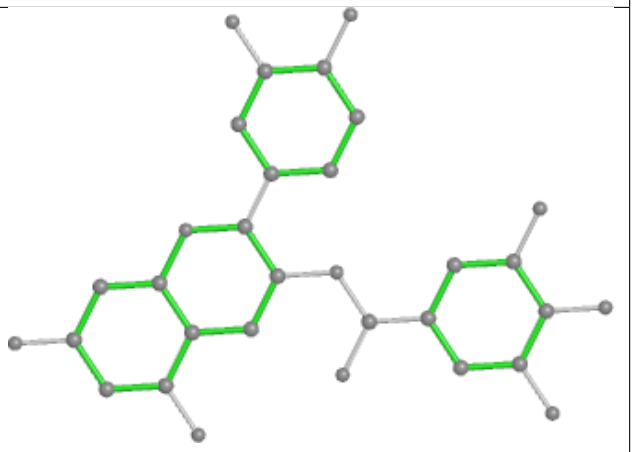
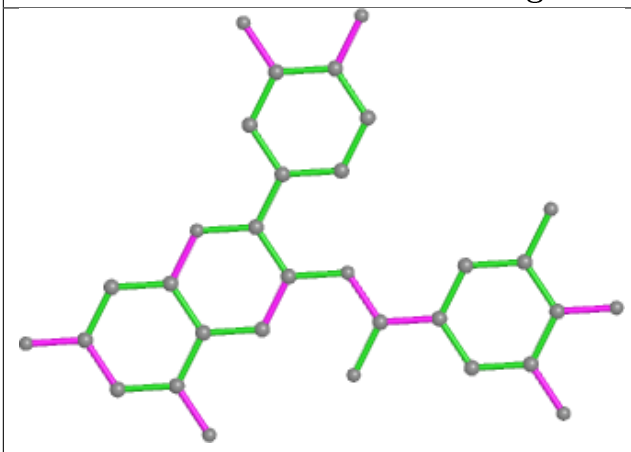


Rings

Ligand XEG J 601



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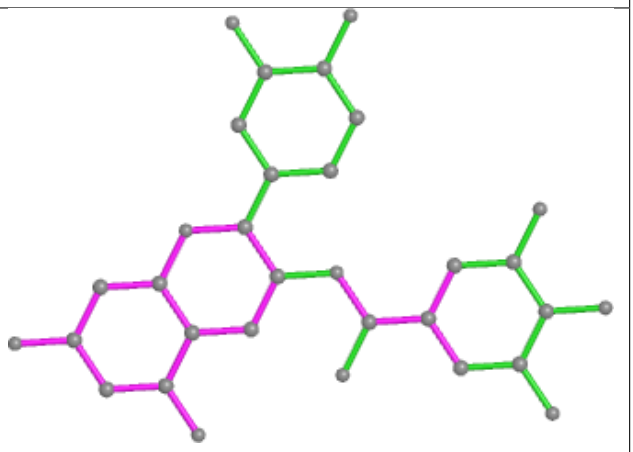
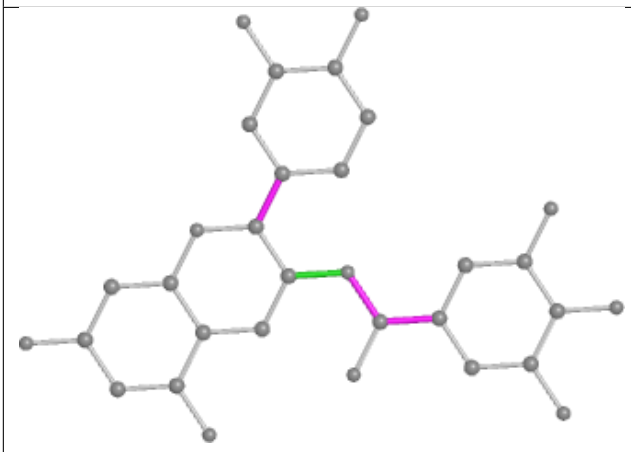


Bond angles



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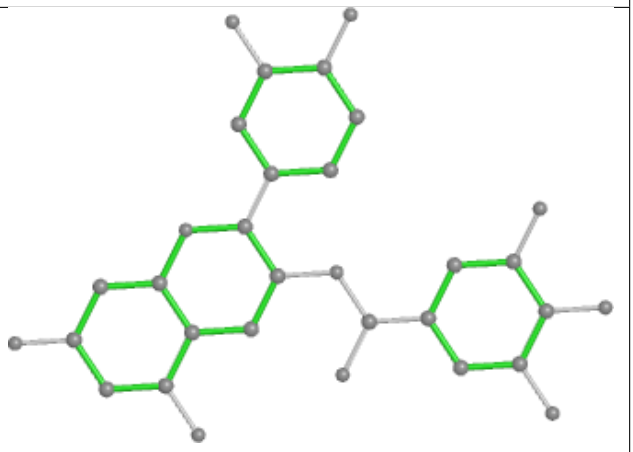
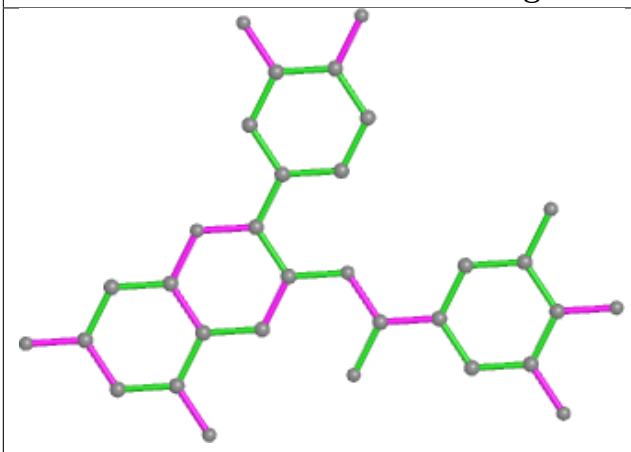
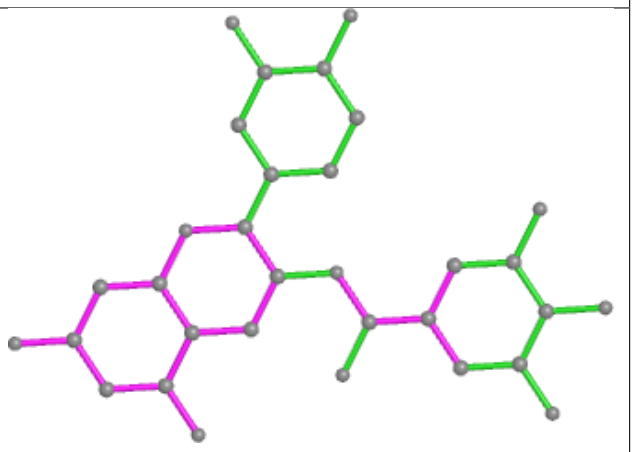


Rings

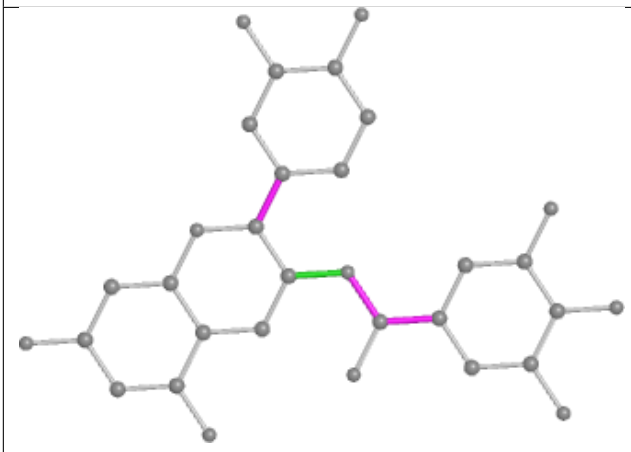
Ligand XEG E 601



Bond lengths



Bond angles



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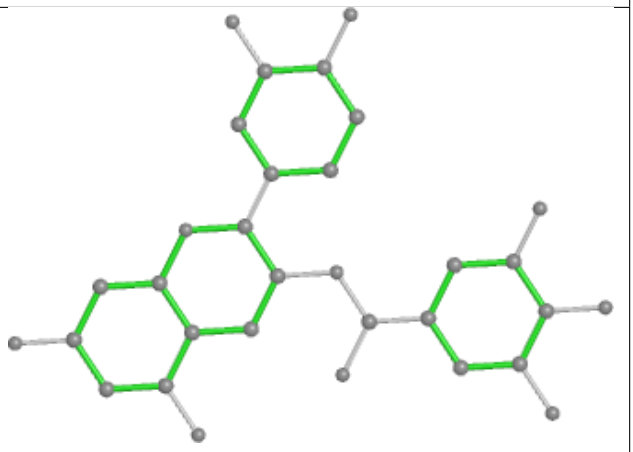
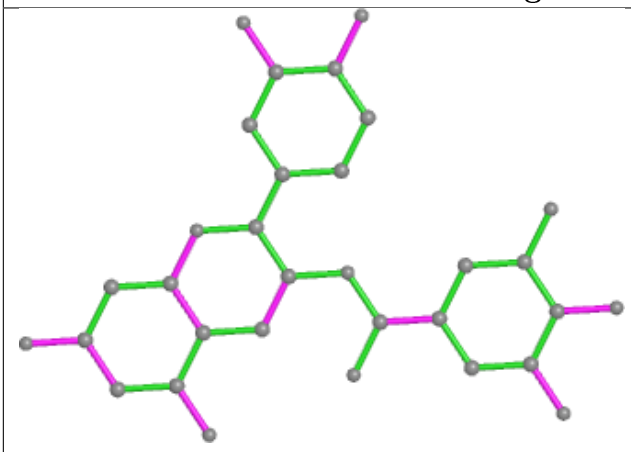
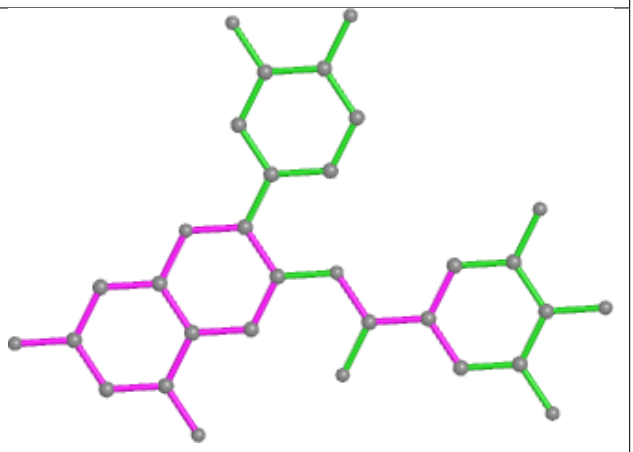


Rings

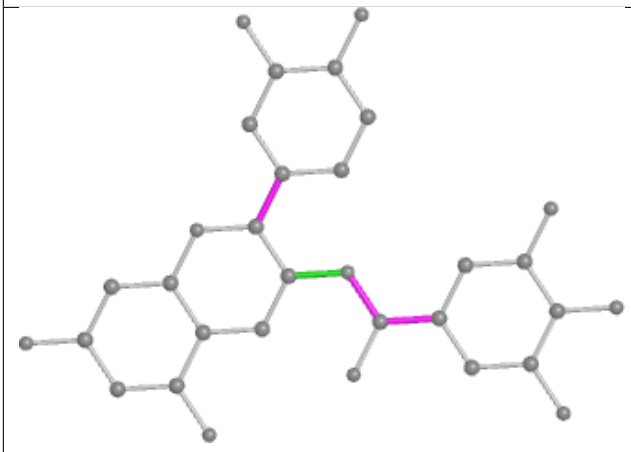
Ligand XEG L 601



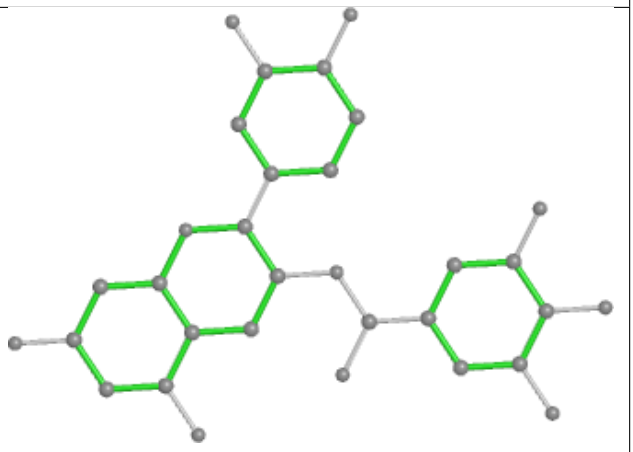
Bond lengths



Bond angles

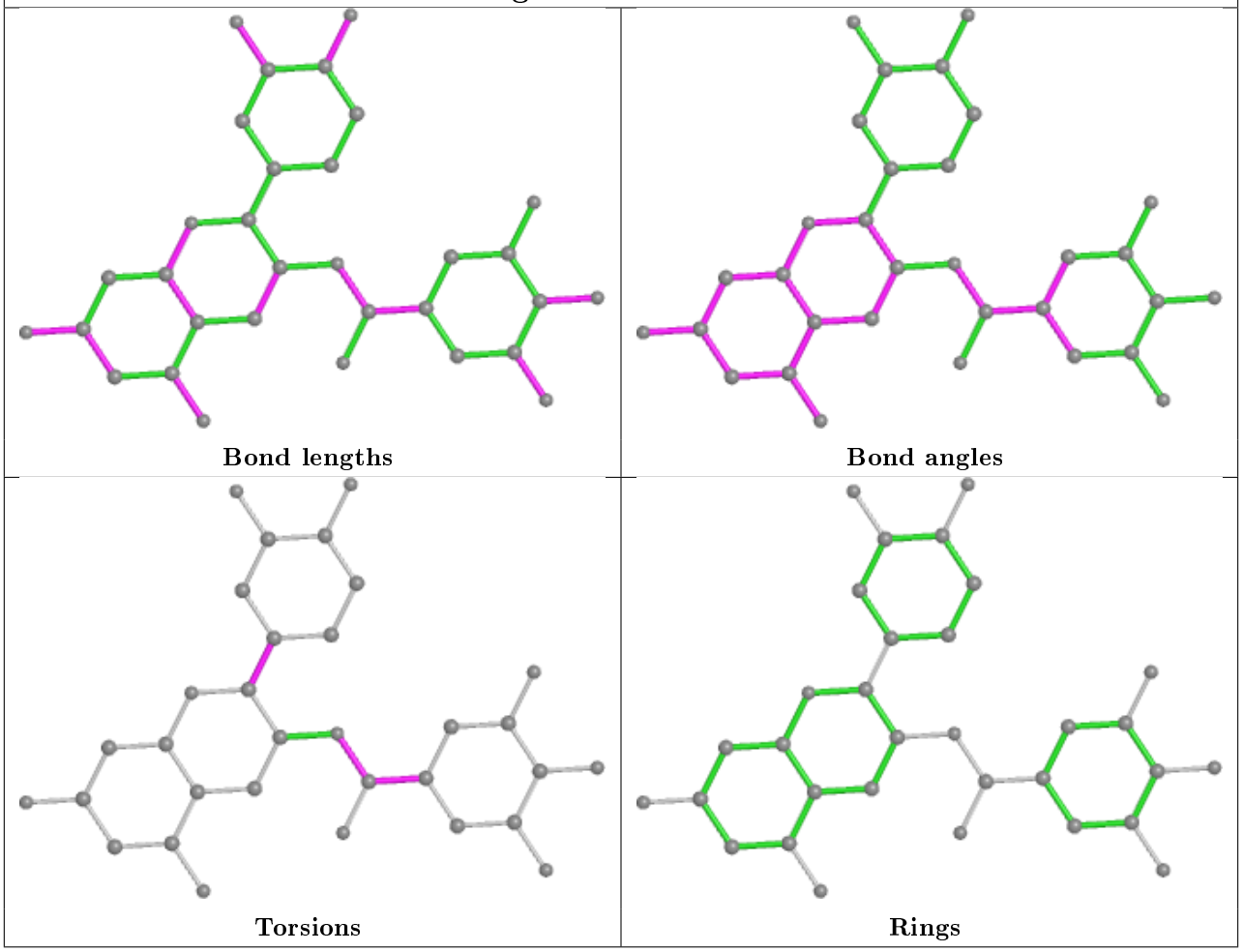


Torsions



Rings

Ligand XEG I 601



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, 95^{th} 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	496/496 (100%)	0.30	39 (7%) 12 8	66, 125, 228, 270	0
1	B	496/496 (100%)	0.14	28 (5%) 24 15	69, 119, 220, 268	0
1	C	496/496 (100%)	0.33	37 (7%) 14 8	61, 119, 224, 266	0
1	D	496/496 (100%)	0.17	32 (6%) 18 11	66, 119, 222, 275	0
1	E	496/496 (100%)	0.39	55 (11%) 5 3	66, 126, 228, 269	0
1	F	496/496 (100%)	0.33	45 (9%) 9 5	60, 120, 228, 267	0
1	G	496/496 (100%)	0.17	30 (6%) 21 12	58, 112, 219, 277	0
1	H	496/496 (100%)	-0.01	10 (2%) 65 50	60, 105, 201, 251	0
1	I	496/496 (100%)	0.20	32 (6%) 18 11	58, 112, 218, 261	0
1	J	496/496 (100%)	-0.00	11 (2%) 62 46	63, 106, 203, 251	0
1	K	496/496 (100%)	0.20	24 (4%) 30 20	61, 114, 221, 276	0
1	L	496/496 (100%)	0.17	30 (6%) 21 12	60, 114, 215, 265	0
All	All	5952/5952 (100%)	0.20	373 (6%) 20 12	58, 116, 222, 277	0

All (373) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	6	ASP	11.6
1	K	297	GLN	10.8
1	I	6	ASP	9.9
1	I	296	LEU	9.6
1	F	296	LEU	9.3
1	A	501	THR	8.9
1	F	227	ILE	8.7
1	C	227	ILE	8.2
1	F	342	LYS	8.0
1	E	501	THR	7.7
1	H	501	THR	7.7

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Mol	Chain	Res	Type	RSRZ
1	C	268	ALA	7.6
1	L	312	GLY	7.5
1	A	347	GLY	7.3
1	F	319	CYS	7.2
1	C	267	GLY	7.1
1	E	334	SER	7.0
1	K	296	LEU	7.0
1	F	318	ASP	7.0
1	E	277	ASP	6.9
1	I	424	HIS	6.8
1	D	278	GLY	6.6
1	D	501	THR	6.6
1	B	8	ASN	6.4
1	G	312	GLY	6.4
1	J	501	THR	6.4
1	B	501	THR	6.0
1	D	297	GLN	6.0
1	E	275	GLU	6.0
1	A	312	GLY	6.0
1	C	296	LEU	5.8
1	K	286	ILE	5.8
1	K	249	VAL	5.7
1	E	352	THR	5.7
1	K	248	ALA	5.6
1	F	232	TYR	5.6
1	F	297	GLN	5.5
1	B	334	SER	5.4
1	A	275	GLU	5.4
1	C	226	PHE	5.2
1	K	501	THR	5.1
1	G	286	ILE	5.1
1	F	228	ASN	5.1
1	A	298	HIS	5.1
1	D	273	VAL	4.9
1	A	324	PRO	4.8
1	K	298	HIS	4.8
1	C	228	ASN	4.8
1	C	297	GLN	4.8
1	G	227	ILE	4.7
1	C	7	PRO	4.7
1	D	305	PRO	4.7
1	G	232	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
1	K	25	GLU	4.6
1	L	296	LEU	4.6
1	D	286	ILE	4.5
1	E	322	LEU	4.5
1	K	347	GLY	4.5
1	A	352	THR	4.4
1	A	277	ASP	4.4
1	A	325	ALA	4.4
1	L	6	ASP	4.4
1	G	31	ASP	4.4
1	F	298	HIS	4.4
1	I	295	LYS	4.3
1	E	326	ALA	4.3
1	C	365	ILE	4.3
1	F	430	ILE	4.3
1	A	333	LYS	4.3
1	K	31	ASP	4.3
1	C	242	PHE	4.3
1	D	347	GLY	4.3
1	I	298	HIS	4.3
1	I	270	CYS	4.2
1	G	308	LYS	4.2
1	G	309	ILE	4.2
1	G	285	GLY	4.2
1	F	226	PHE	4.1
1	B	279	SER	4.1
1	C	344	ILE	4.1
1	G	354	PRO	4.1
1	D	302	LEU	4.1
1	A	334	SER	4.1
1	A	268	ALA	4.1
1	D	500	PHE	4.0
1	G	371	LEU	4.0
1	J	297	GLN	4.0
1	J	280	ILE	4.0
1	F	366	MET	4.0
1	E	276	SER	4.0
1	L	295	LYS	4.0
1	G	366	MET	4.0
1	E	252	PHE	4.0
1	B	258	HIS	3.9
1	E	303	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	L	7	PRO	3.9
1	E	296	LEU	3.9
1	K	252	PHE	3.8
1	F	344	ILE	3.8
1	I	226	PHE	3.8
1	L	313	SER	3.8
1	D	274	GLY	3.8
1	E	325	ALA	3.8
1	I	7	PRO	3.8
1	C	320	ASP	3.7
1	E	170	SER	3.7
1	C	322	LEU	3.7
1	B	328	GLU	3.7
1	A	475	LEU	3.7
1	F	252	PHE	3.7
1	G	343	ILE	3.7
1	B	262	TYR	3.7
1	C	270	CYS	3.7
1	B	351	PRO	3.7
1	E	34	THR	3.7
1	B	319	CYS	3.7
1	D	10	PHE	3.7
1	G	280	ILE	3.6
1	C	22	SER	3.6
1	E	349	ASN	3.6
1	B	329	LYS	3.6
1	L	311	GLU	3.6
1	E	33	LYS	3.6
1	C	282	ASN	3.6
1	C	367	VAL	3.5
1	C	321	ILE	3.5
1	K	499	THR	3.5
1	E	286	ILE	3.5
1	E	285	GLY	3.5
1	E	369	PRO	3.5
1	I	227	ILE	3.4
1	F	309	ILE	3.4
1	F	322	LEU	3.4
1	D	252	PHE	3.4
1	L	367	VAL	3.4
1	C	300	THR	3.4
1	A	296	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	499	THR	3.4
1	D	285	GLY	3.4
1	A	10	PHE	3.3
1	C	342	LYS	3.3
1	B	278	GLY	3.3
1	E	295	LYS	3.3
1	E	341	ALA	3.3
1	E	330	GLN	3.3
1	H	499	THR	3.3
1	F	302	LEU	3.3
1	F	323	ILE	3.3
1	G	342	LYS	3.3
1	A	299	GLY	3.3
1	E	327	SER	3.3
1	G	370	ASP	3.2
1	G	287	ASP	3.2
1	F	303	GLY	3.2
1	D	296	LEU	3.2
1	I	365	ILE	3.2
1	K	226	PHE	3.2
1	D	284	ASP	3.2
1	C	371	LEU	3.2
1	I	501	THR	3.2
1	B	314	ILE	3.2
1	I	319	CYS	3.2
1	E	297	GLN	3.2
1	B	295	LYS	3.2
1	C	318	ASP	3.1
1	A	32	LEU	3.1
1	C	324	PRO	3.1
1	I	300	THR	3.1
1	F	308	LYS	3.1
1	L	346	GLU	3.1
1	J	366	MET	3.1
1	G	344	ILE	3.1
1	E	347	GLY	3.1
1	J	337	PRO	3.1
1	L	352	THR	3.1
1	F	336	ALA	3.0
1	A	315	LEU	3.0
1	B	317	VAL	3.0
1	E	335	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	286	ILE	3.0
1	G	299	GLY	3.0
1	D	328	GLU	3.0
1	D	295	LYS	3.0
1	I	281	TRP	3.0
1	C	345	ALA	2.9
1	G	305	PRO	2.9
1	E	321	ILE	2.9
1	F	365	ILE	2.9
1	C	252	PHE	2.9
1	E	232	TYR	2.9
1	A	76	GLU	2.9
1	F	238	MET	2.9
1	A	78	TYR	2.9
1	L	358	LYS	2.9
1	K	260	MET	2.9
1	B	35	ARG	2.8
1	L	371	LEU	2.8
1	K	367	VAL	2.8
1	D	257	LEU	2.8
1	I	261	ARG	2.8
1	I	297	GLN	2.8
1	L	270	CYS	2.8
1	I	351	PRO	2.8
1	F	335	ASN	2.8
1	C	424	HIS	2.8
1	H	347	GLY	2.8
1	D	298	HIS	2.8
1	H	334	SER	2.7
1	E	309	ILE	2.7
1	K	365	ILE	2.7
1	A	499	THR	2.7
1	D	272	ALA	2.7
1	G	501	THR	2.7
1	A	326	ALA	2.7
1	E	336	ALA	2.7
1	E	242	PHE	2.7
1	E	300	THR	2.7
1	G	296	LEU	2.7
1	E	250	GLN	2.7
1	D	254	ASN	2.7
1	D	329	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	319	CYS	2.7
1	F	242	PHE	2.7
1	H	348	ALA	2.7
1	I	336	ALA	2.7
1	A	6	ASP	2.7
1	H	10	PHE	2.7
1	J	336	ALA	2.7
1	L	72	TRP	2.7
1	A	278	GLY	2.7
1	L	365	ILE	2.7
1	D	260	MET	2.7
1	J	273	VAL	2.6
1	L	369	PRO	2.6
1	F	267	GLY	2.6
1	B	296	LEU	2.6
1	D	292	GLU	2.6
1	C	247	PHE	2.6
1	L	478	ARG	2.6
1	B	299	GLY	2.6
1	K	310	TYR	2.6
1	I	354	PRO	2.6
1	L	271	VAL	2.6
1	A	335	ASN	2.6
1	F	320	ASP	2.6
1	K	227	ILE	2.6
1	E	482	TYR	2.6
1	E	345	ALA	2.6
1	F	367	VAL	2.6
1	I	322	LEU	2.6
1	C	232	TYR	2.5
1	B	292	GLU	2.5
1	E	331	LEU	2.5
1	H	286	ILE	2.5
1	E	324	PRO	2.5
1	I	242	PHE	2.5
1	E	397	LEU	2.5
1	G	319	CYS	2.5
1	A	267	GLY	2.5
1	I	355	GLU	2.5
1	E	319	CYS	2.5
1	E	337	PRO	2.5
1	H	251	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	289	LYS	2.5
1	K	424	HIS	2.5
1	A	7	PRO	2.5
1	A	250	GLN	2.5
1	A	374	ASN	2.4
1	D	299	GLY	2.4
1	B	250	GLN	2.4
1	F	345	ALA	2.4
1	I	250	GLN	2.4
1	L	501	THR	2.4
1	B	309	ILE	2.4
1	G	307	ALA	2.4
1	H	267	GLY	2.4
1	B	204	SER	2.4
1	F	231	SER	2.4
1	B	249	VAL	2.4
1	E	475	LEU	2.4
1	L	494	ASN	2.4
1	A	311	GLU	2.4
1	F	324	PRO	2.4
1	E	366	MET	2.4
1	I	340	LYS	2.4
1	A	322	LEU	2.4
1	C	346	GLU	2.4
1	L	314	ILE	2.4
1	A	300	THR	2.4
1	E	342	LYS	2.4
1	B	285	GLY	2.4
1	L	234	SER	2.4
1	L	366	MET	2.4
1	C	370	ASP	2.4
1	A	274	GLY	2.3
1	A	29	VAL	2.3
1	B	366	MET	2.3
1	C	302	LEU	2.3
1	H	300	THR	2.3
1	F	341	ALA	2.3
1	K	368	ILE	2.3
1	E	72	TRP	2.3
1	B	273	VAL	2.3
1	A	323	ILE	2.3
1	E	31	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	500	PHE	2.3
1	G	284	ASP	2.3
1	D	330	GLN	2.3
1	E	78	TYR	2.3
1	E	338	ARG	2.3
1	A	282	ASN	2.3
1	L	334	SER	2.3
1	F	307	ALA	2.3
1	A	427	THR	2.3
1	C	347	GLY	2.3
1	F	268	ALA	2.3
1	G	306	LYS	2.3
1	F	354	PRO	2.2
1	E	302	LEU	2.2
1	I	485	ALA	2.2
1	E	344	ILE	2.2
1	E	480	ALA	2.2
1	L	232	TYR	2.2
1	L	227	ILE	2.2
1	F	241	GLY	2.2
1	G	265	ARG	2.2
1	G	333	LYS	2.2
1	C	420	LYS	2.2
1	F	321	ILE	2.2
1	A	31	ASP	2.2
1	K	26	ASP	2.2
1	D	304	PHE	2.2
1	J	10	PHE	2.2
1	J	316	GLU	2.2
1	L	425	GLY	2.1
1	I	271	VAL	2.1
1	J	262	TYR	2.1
1	I	425	GLY	2.1
1	D	277	ASP	2.1
1	I	311	GLU	2.1
1	L	225	ASN	2.1
1	F	310	TYR	2.1
1	G	367	VAL	2.1
1	F	343	ILE	2.1
1	D	279	SER	2.1
1	F	230	ALA	2.1
1	G	345	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	223	ILE	2.1
1	K	6	ASP	2.1
1	I	367	VAL	2.1
1	F	279	SER	2.1
1	K	276	SER	2.1
1	B	318	ASP	2.1
1	L	424	HIS	2.1
1	J	427	THR	2.1
1	K	362	GLU	2.1
1	E	35	ARG	2.1
1	I	8	ASN	2.1
1	C	368	ILE	2.1
1	E	339	VAL	2.1
1	E	351	PRO	2.0
1	E	332	THR	2.0
1	D	331	LEU	2.0
1	L	368	ILE	2.0
1	I	244	ASP	2.0
1	E	329	LYS	2.0
1	F	223	ILE	2.0
1	D	476	ASP	2.0
1	G	368	ILE	2.0
1	F	61	LEU	2.0
1	C	298	HIS	2.0
1	F	270	CYS	2.0
1	A	276	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

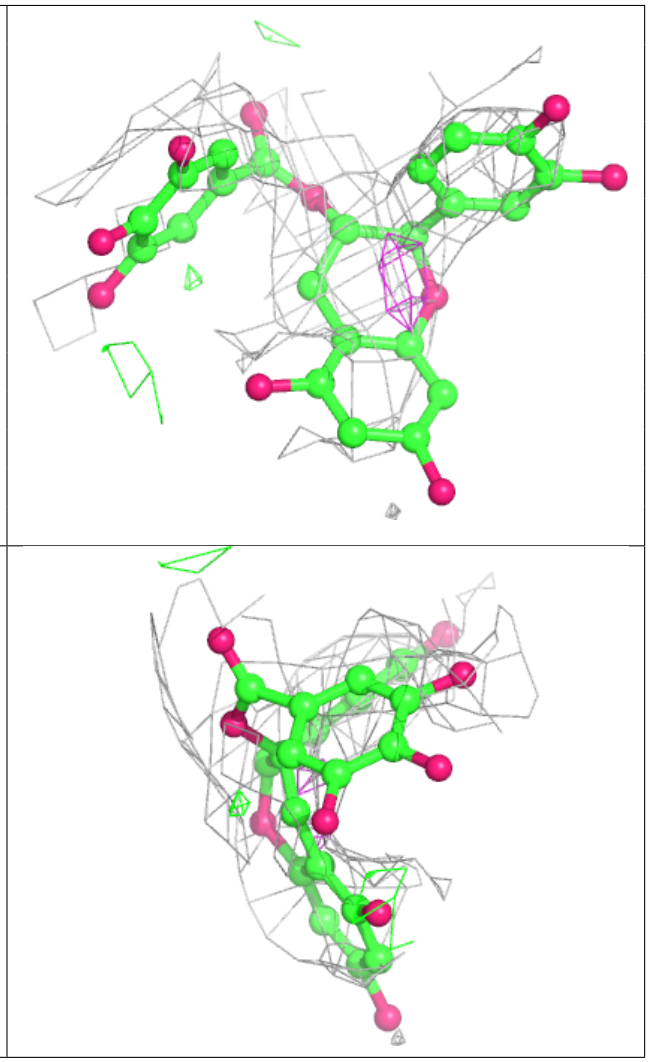
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

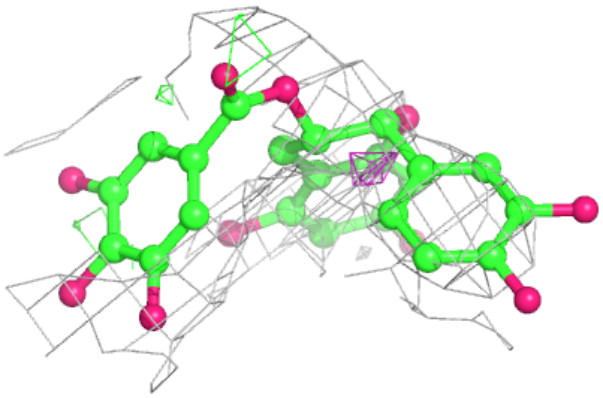
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	XEG	C	601	32/32	0.48	0.47	96,116,133,138	0
2	XEG	L	601	32/32	0.61	0.43	89,117,128,133	0
2	XEG	F	601	32/32	0.72	0.23	98,118,134,139	0
2	XEG	I	601	32/32	0.74	0.45	92,115,127,130	0
2	XEG	K	601	32/32	0.78	0.26	89,111,123,126	0
2	XEG	H	601	32/32	0.79	0.38	85,108,121,126	0
2	XEG	J	601	32/32	0.82	0.32	85,110,122,128	0
2	XEG	G	601	32/32	0.83	0.30	93,112,124,132	0
2	XEG	A	601	32/32	0.86	0.25	88,106,122,127	0
2	XEG	E	601	32/32	0.86	0.23	90,108,125,127	0
2	XEG	D	601	32/32	0.89	0.22	86,110,123,129	0
2	XEG	B	601	32/32	0.90	0.23	89,110,125,128	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 XEG C 601:

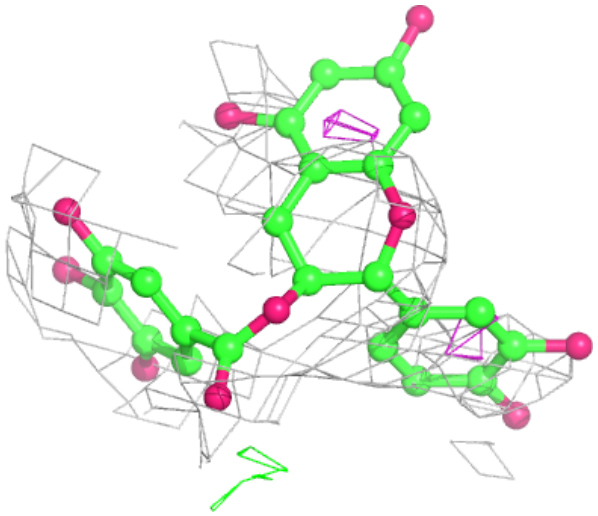
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

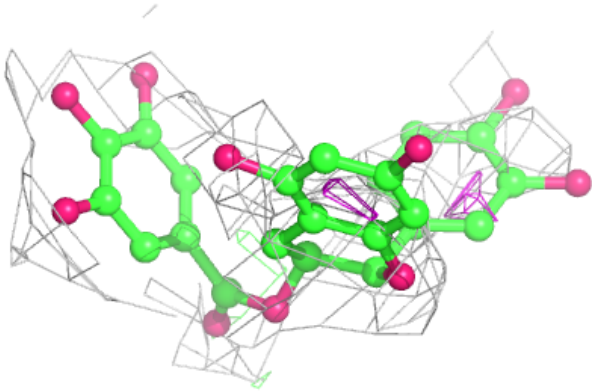


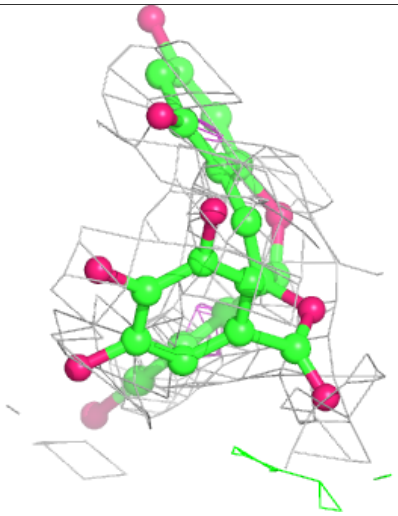


Electron density around XEG L 601:

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

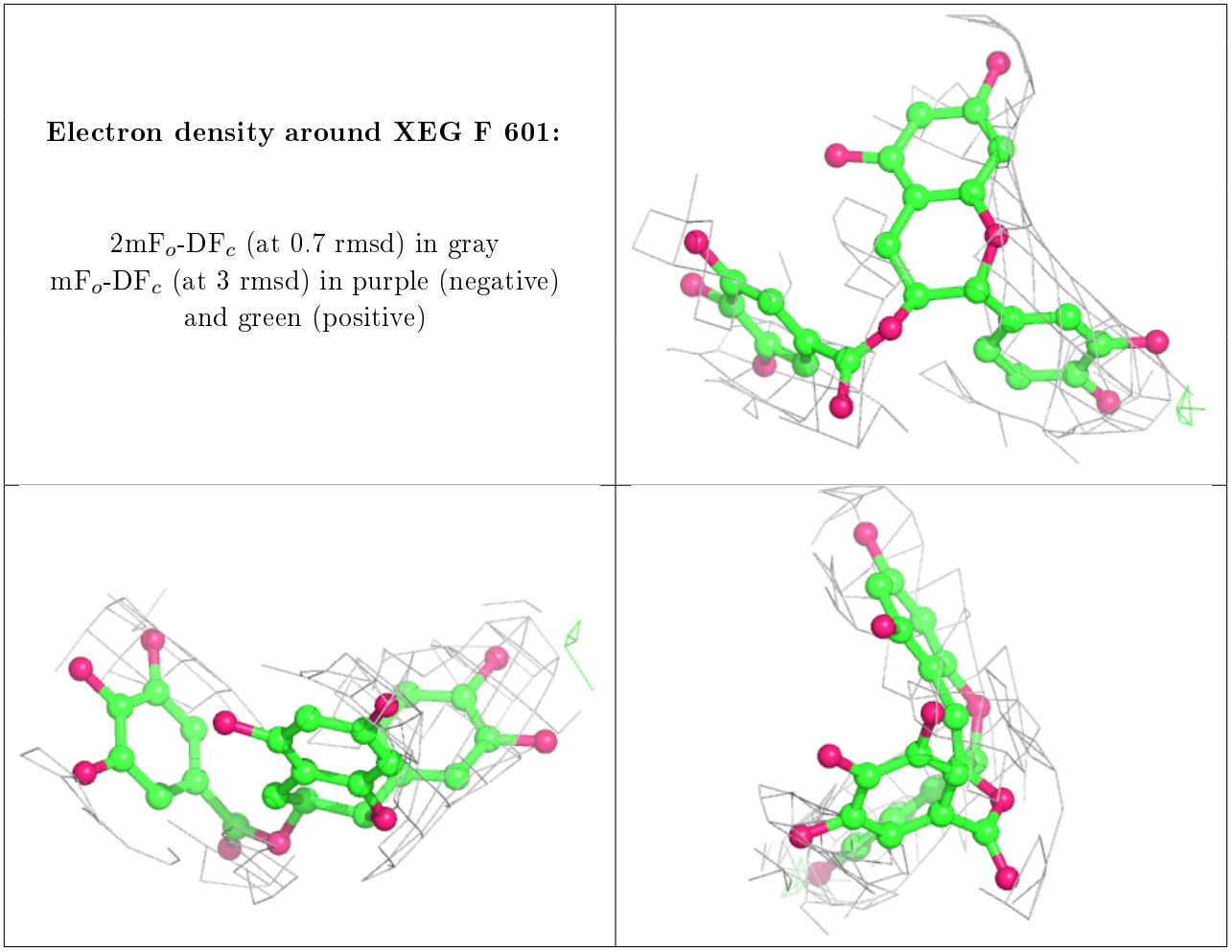






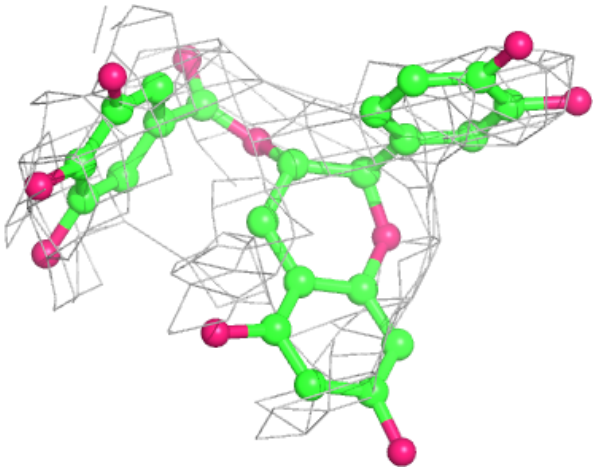
Electron density around XEG F 601:

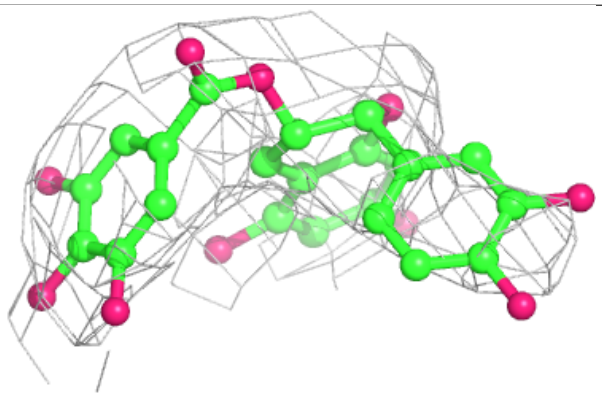
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

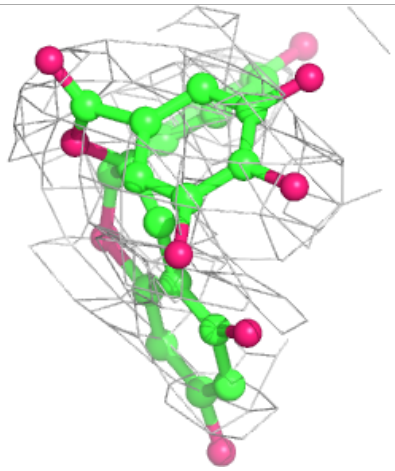


Electron density around XEG I 601:

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

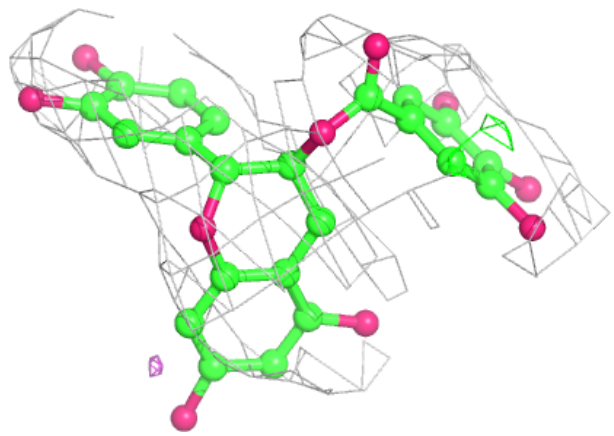


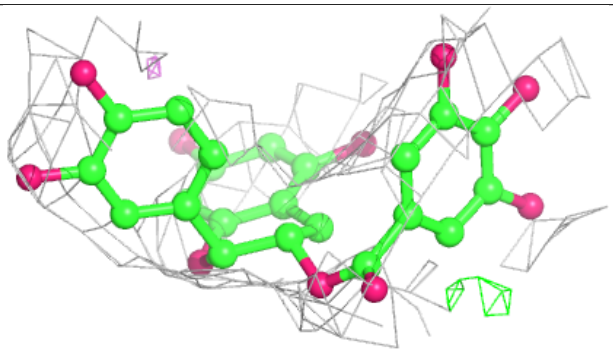




Electron density around XEG K 601:

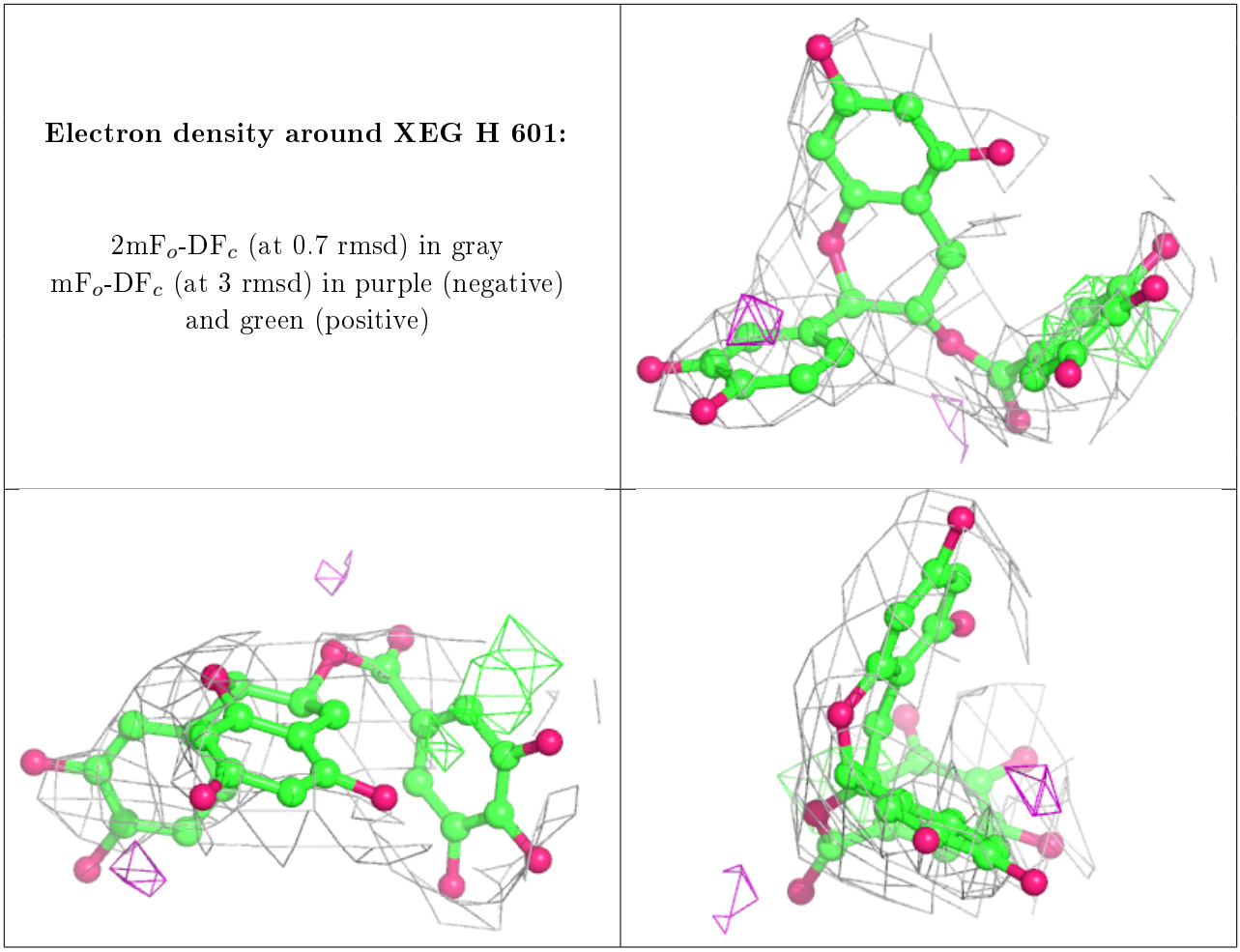
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





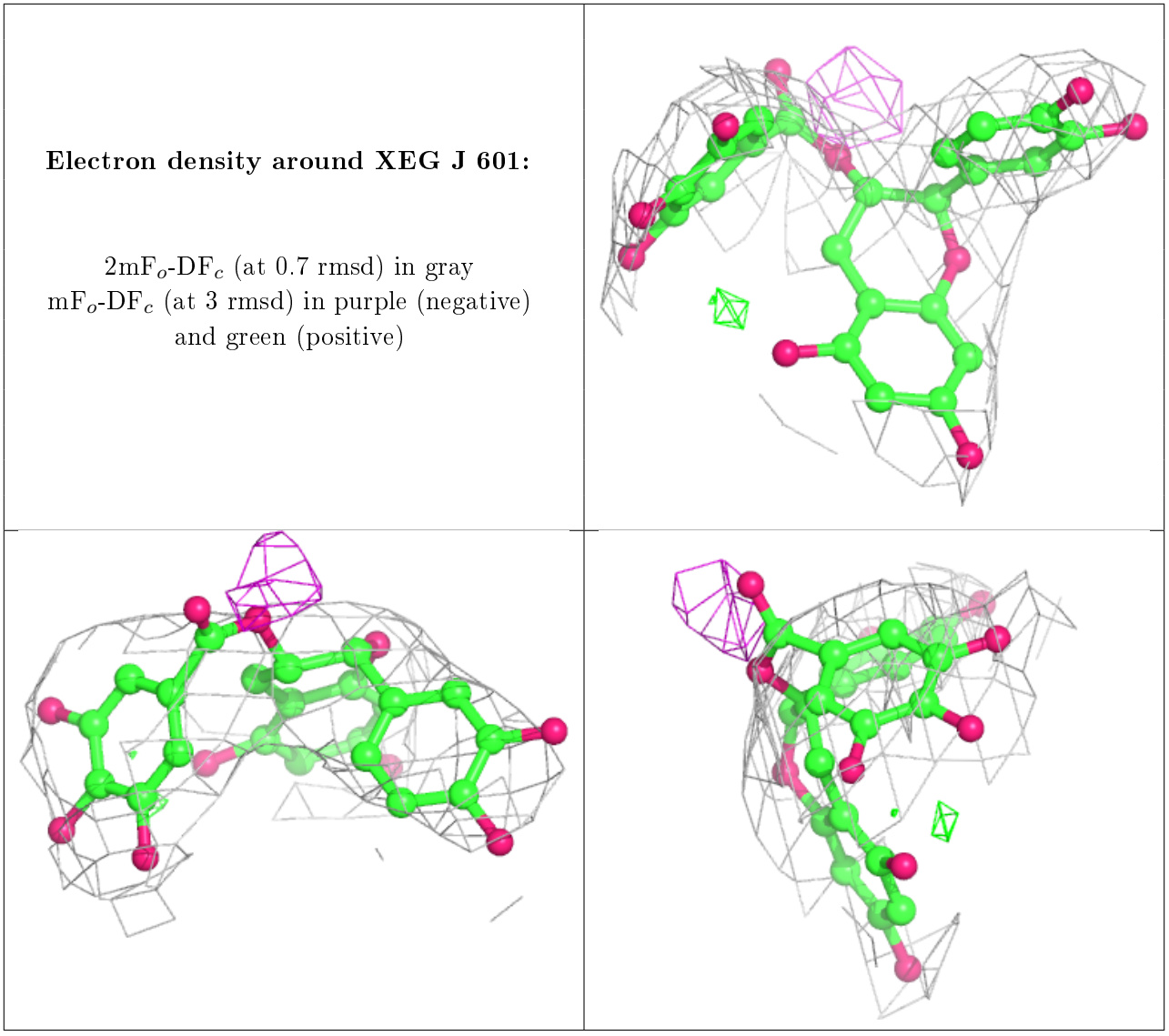
Electron density around XEG H 601:

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



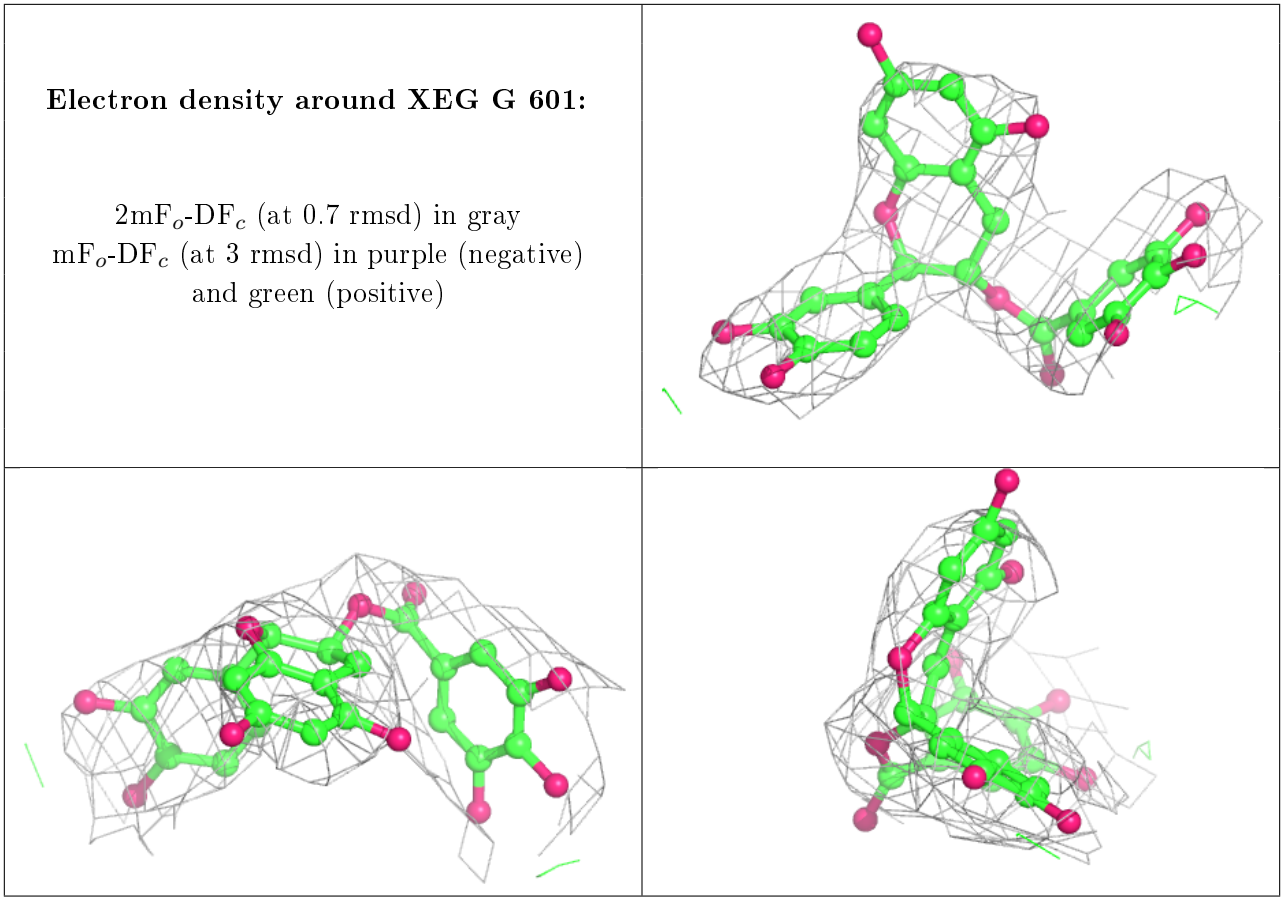
Electron density around XEG J 601:

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



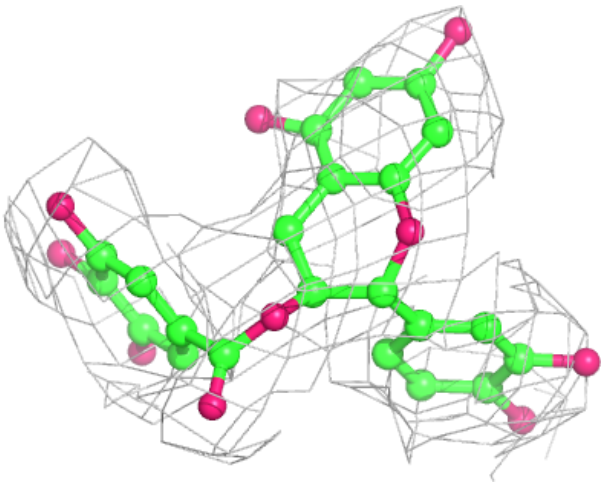
Electron density around XEG G 601:

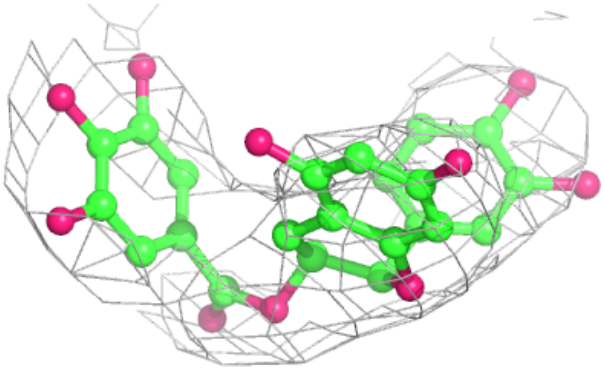
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

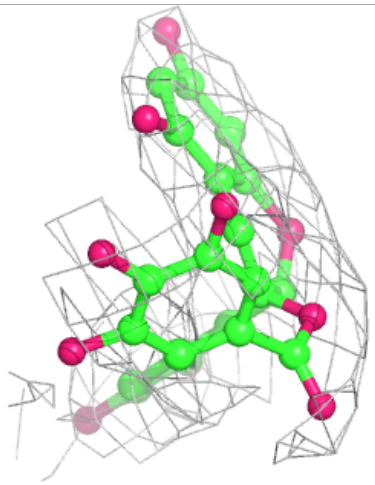


Electron density around XEG A 601:

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

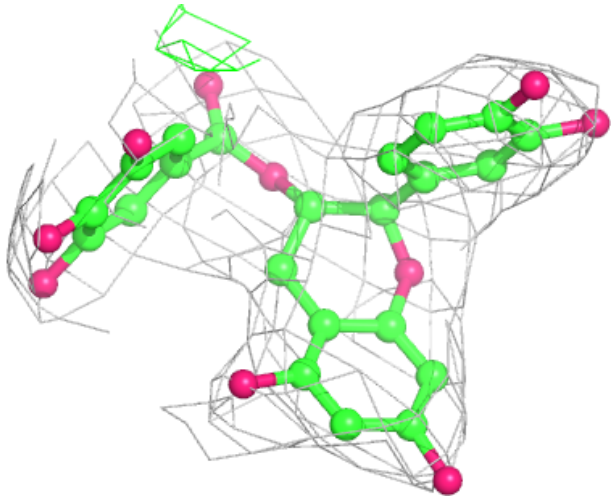


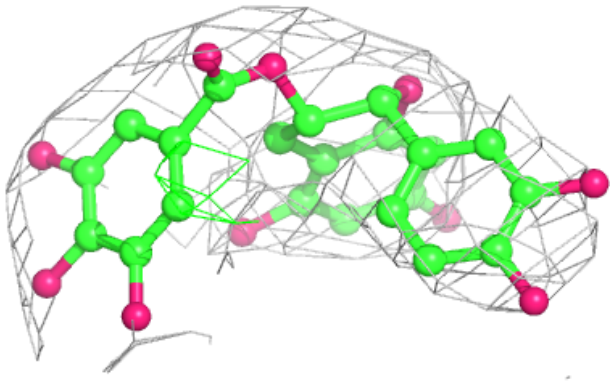


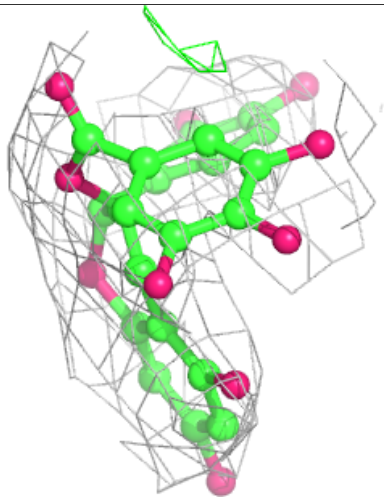


Electron density around XEG E 601:

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

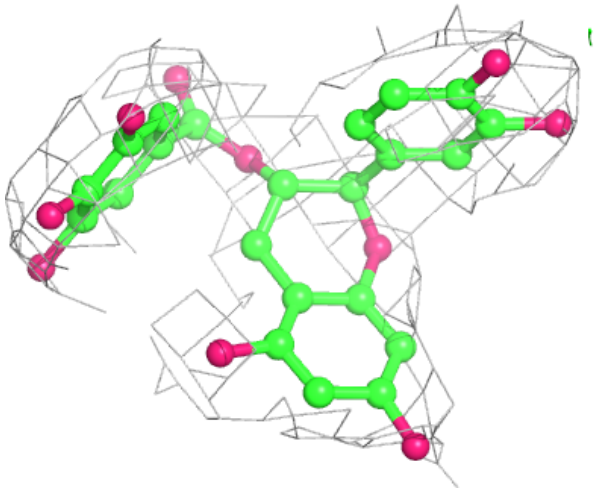


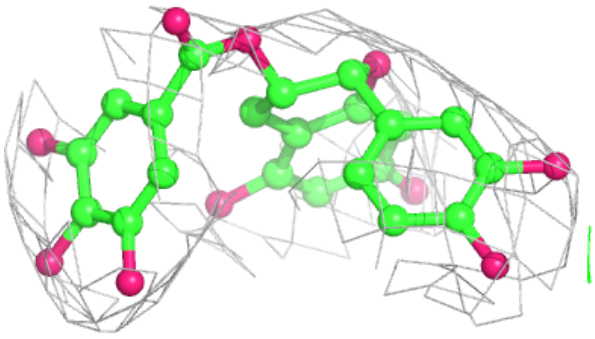


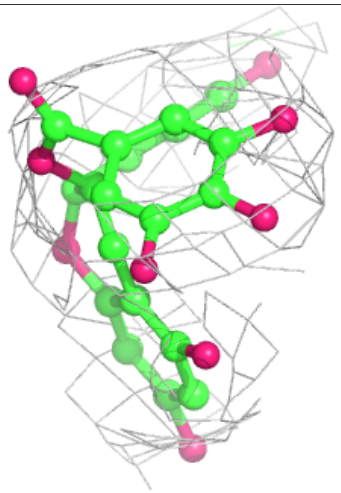


Electron density around XEG D 601:

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

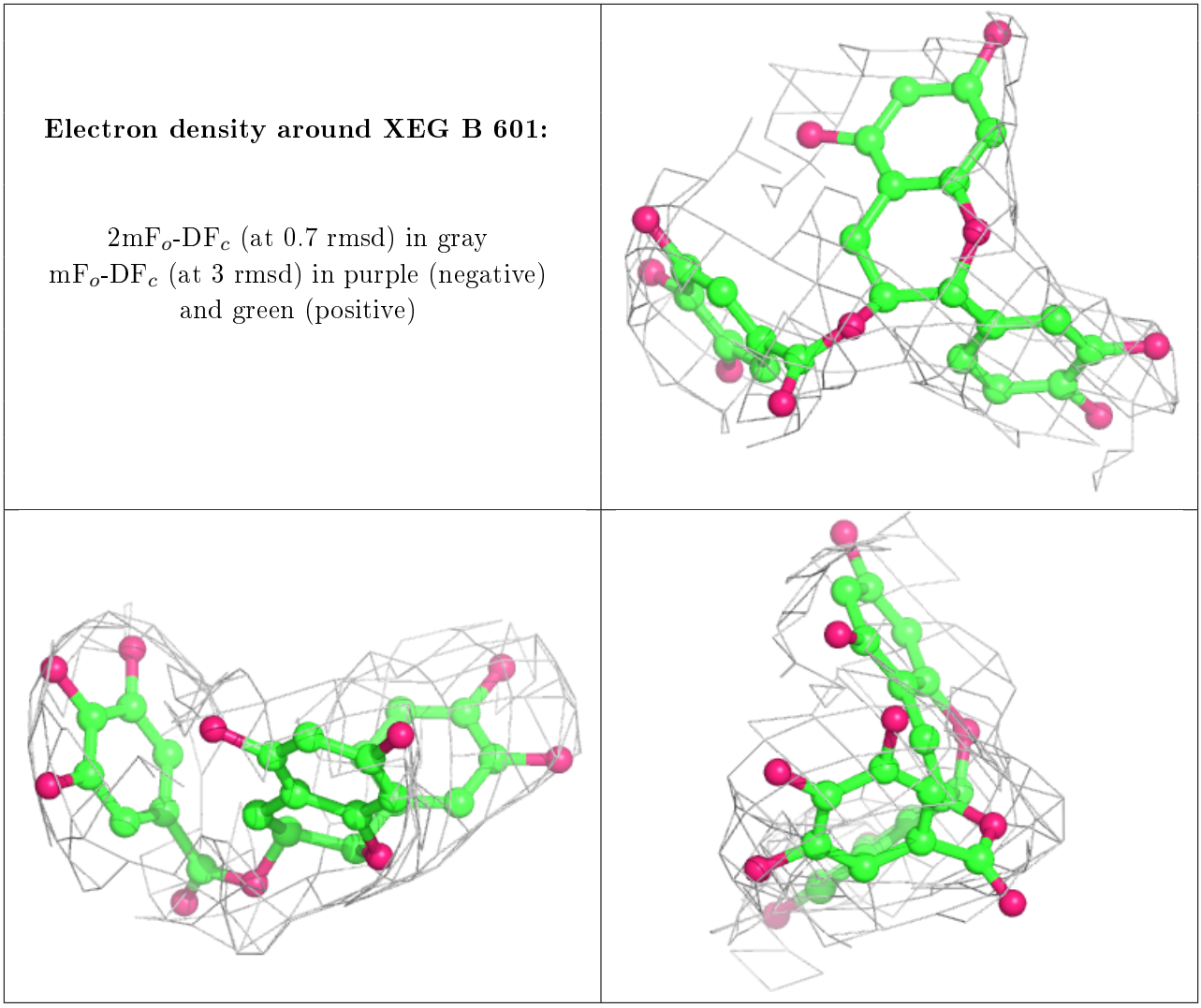






Electron density around XEG B 601:

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



6.5 Other polymers

There are no such residues in this entry.