



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2020 – 11:14 AM EDT

PDB ID : 6ULA
Title : Crystal structure of human GAC in complex with inhibitor UPGL00012
Authors : Huang, Q.; Cerione, R.A.
Deposited on : 2019-10-07
Resolution : 2.95 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:

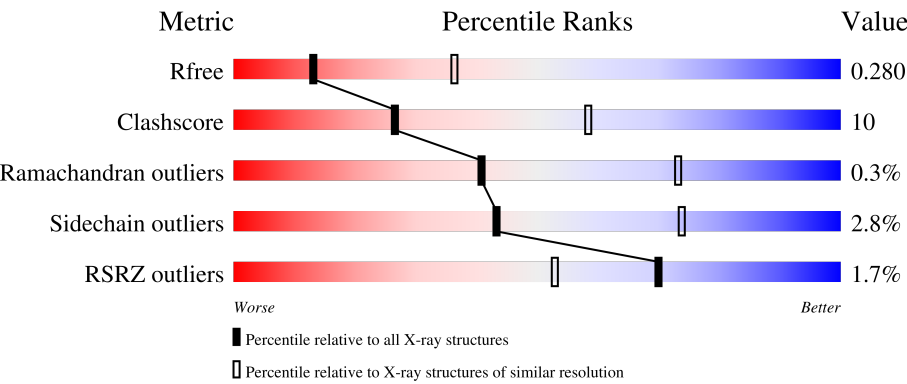
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

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 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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

Mol	Chain	Length	Quality of chain
1	A	527	
1	B	527	
1	C	527	
1	D	527	
1	E	527	

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Mol	Chain	Length	Quality of chain
1	F	527	<p>2% 59% 17% 22%</p>
1	G	527	<p>1% 60% 16% 22%</p>
1	H	527	<p>2% 61% 15% 22%</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25668 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.

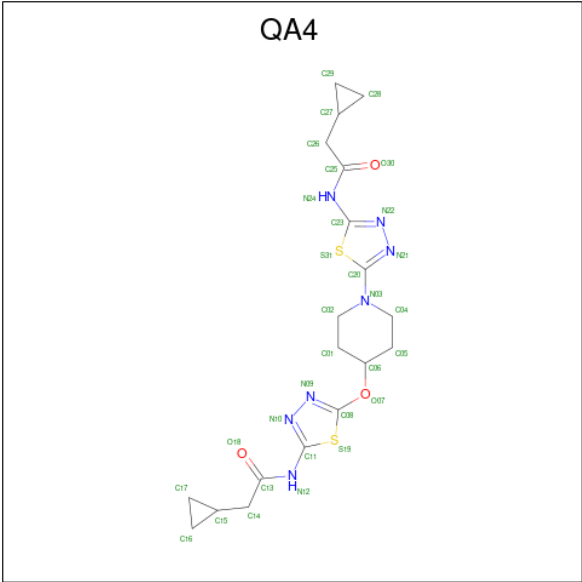
- Molecule 1 is a protein called Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	1	0	0
			3190	2034	539	589	28			
1	B	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			
1	C	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			
1	D	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			
1	E	409	Total	C	N	O	S	1	0	0
			3190	2034	539	589	28			
1	G	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			
1	F	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			
1	H	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	268	ALA	VAL	conflict	UNP O94925
B	268	ALA	VAL	conflict	UNP O94925
C	268	ALA	VAL	conflict	UNP O94925
D	268	ALA	VAL	conflict	UNP O94925
E	268	ALA	VAL	conflict	UNP O94925
G	268	ALA	VAL	conflict	UNP O94925
F	268	ALA	VAL	conflict	UNP O94925
H	268	ALA	VAL	conflict	UNP O94925

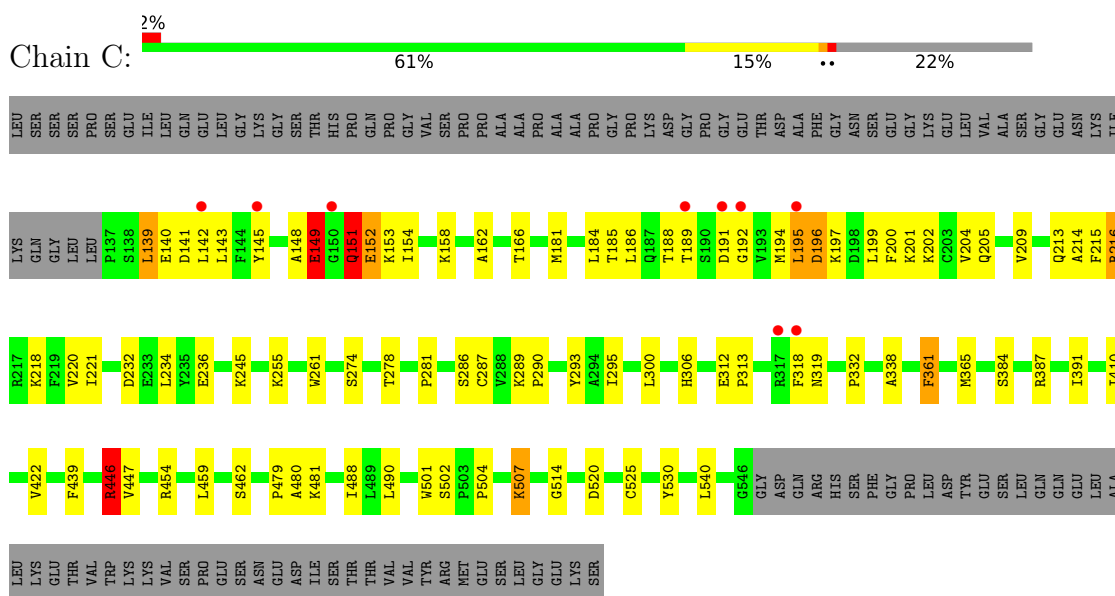
- Molecule 2 is 2-cyclopropyl-N-{5-[4-({5-[(cyclopropylacetyl)amino]-1,3,4-thiadiazol-2-yl}oxy)piperidin-1-yl]-1,3,4-thiadiazol-2-yl}acetamide (three-letter code: QA4) (formula: C₁₉H₂₅N₇O₃S₂) (labeled as "Ligand of Interest" by author).



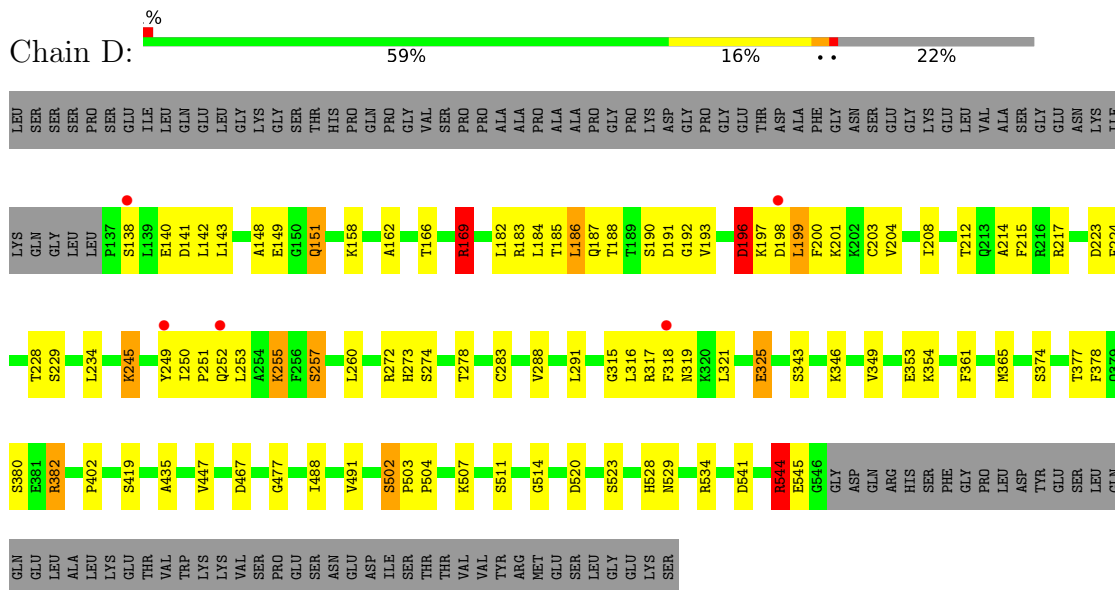
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	19	7	3	2		
2	C	1	Total	C	N	O	S	0	0
			31	19	7	3	2		
2	E	1	Total	C	N	O	S	0	0
			31	19	7	3	2		
2	E	1	Total	C	N	O	S	0	0
			31	19	7	3	2		

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

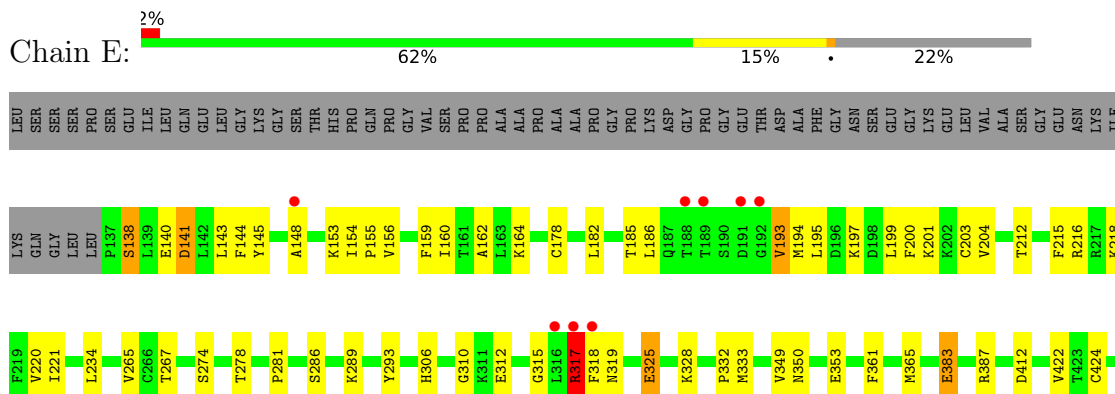
- Molecule 1: Glutaminase kidney isoform, mitochondrial

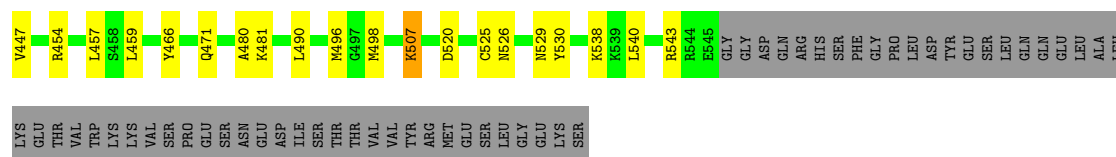


- Molecule 1: Glutaminase kidney isoform, mitochondrial

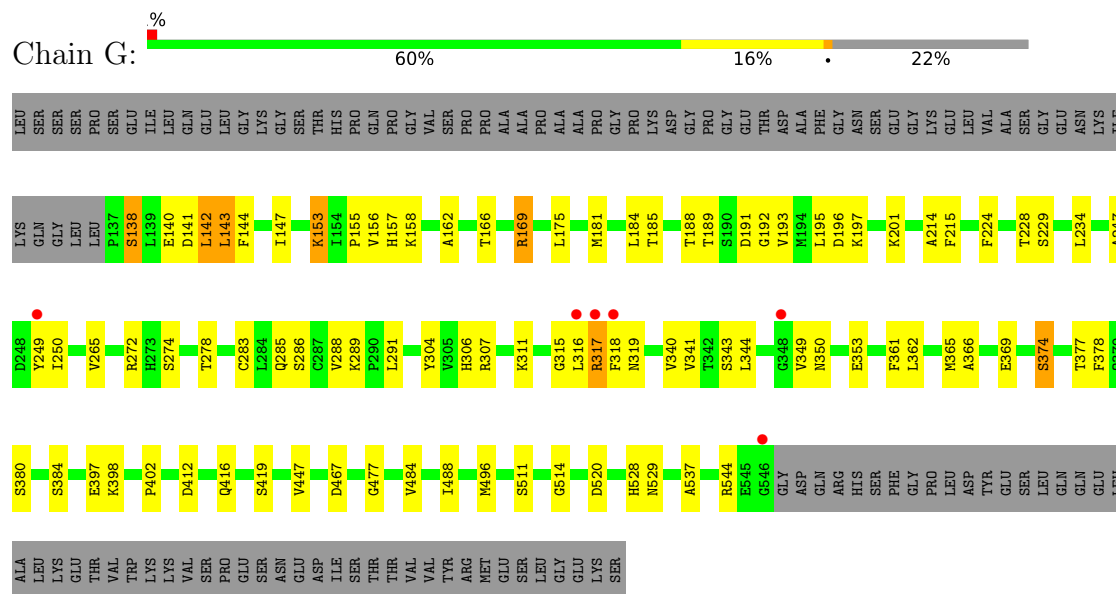


- Molecule 1: Glutaminase kidney isoform, mitochondrial

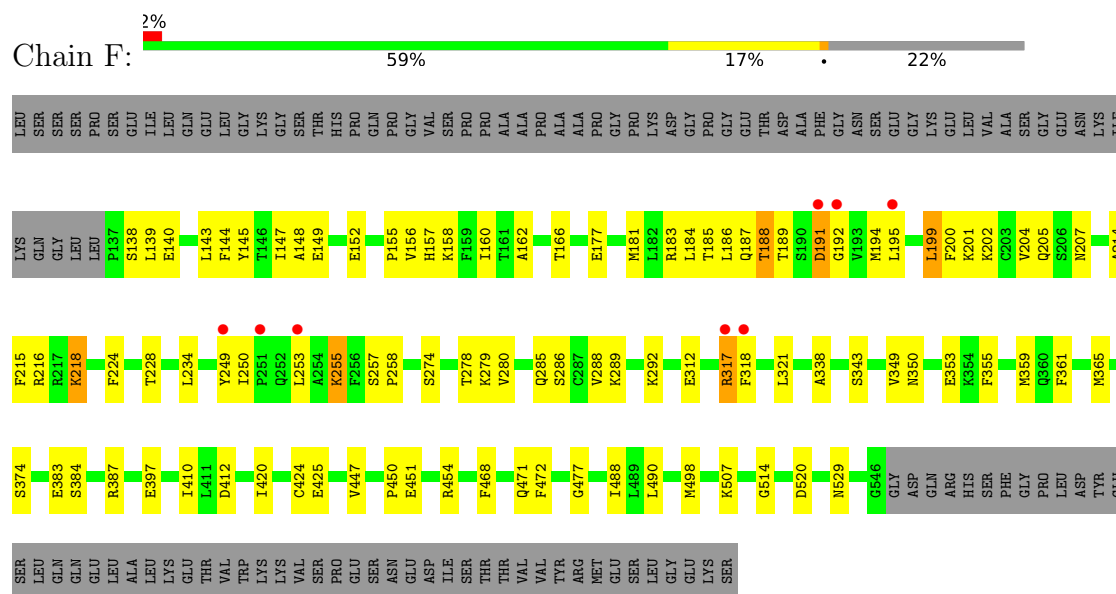




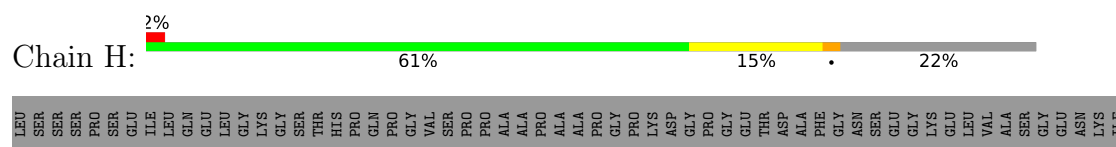
• Molecule 1: Glutaminase kidney isoform, mitochondrial

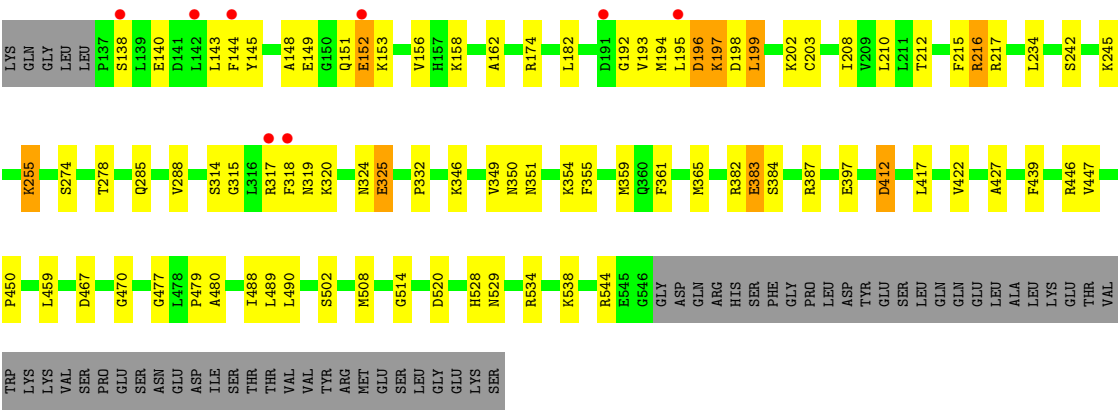


• Molecule 1: Glutaminase kidney isoform, mitochondrial



• Molecule 1: Glutaminase kidney isoform, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.72Å 138.89Å 177.15Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	37.89 – 2.95 38.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.1 (37.89-2.95) 94.5 (38.80-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.217 , 0.279 0.217 , 0.280	Depositor DCC
R_{free} test set	1992 reflections (1.61%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 14.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.438 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25668	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3974e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QA4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.53	0/3262	0.74	5/4403 (0.1%)
1	B	0.55	1/3266 (0.0%)	0.85	10/4408 (0.2%)
1	C	0.56	2/3266 (0.1%)	0.87	14/4408 (0.3%)
1	D	0.58	3/3266 (0.1%)	0.80	10/4408 (0.2%)
1	E	0.60	3/3262 (0.1%)	0.81	11/4403 (0.2%)
1	F	0.62	3/3266 (0.1%)	0.79	10/4408 (0.2%)
1	G	0.54	0/3266	0.87	16/4408 (0.4%)
1	H	0.58	4/3266 (0.1%)	0.82	11/4408 (0.2%)
All	All	0.57	16/26120 (0.1%)	0.82	87/35254 (0.2%)

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	B	0	1
1	C	0	1
1	D	0	2
1	E	0	3
1	F	0	1
All	All	0	8

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	255	LYS	CD-CE	13.03	1.83	1.51
1	E	317	ARG	CZ-NH2	12.27	1.49	1.33
1	E	317	ARG	CZ-NH1	-8.47	1.22	1.33
1	F	255	LYS	CE-NZ	7.72	1.68	1.49
1	B	317	ARG	CA-CB	7.70	1.70	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	255	LYS	CD-CE	7.12	1.69	1.51
1	H	152	GLU	CB-CG	6.78	1.65	1.52
1	E	325	GLU	CD-OE2	6.63	1.32	1.25
1	D	255	LYS	CD-CE	6.32	1.67	1.51
1	D	325	GLU	CB-CG	5.67	1.62	1.52
1	H	538	LYS	CD-CE	5.58	1.65	1.51
1	D	245	LYS	CE-NZ	5.54	1.62	1.49
1	H	325	GLU	CB-CG	5.31	1.62	1.52
1	C	446	ARG	CD-NE	-5.27	1.37	1.46
1	F	280	VAL	C-N	-5.21	1.24	1.34
1	H	538	LYS	CE-NZ	5.01	1.61	1.49

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	139	LEU	CB-CG-CD1	-15.32	84.95	111.00
1	B	139	LEU	CA-CB-CG	14.91	149.58	115.30
1	G	143	LEU	CB-CG-CD2	-14.21	86.84	111.00
1	B	317	ARG	NE-CZ-NH2	-14.00	113.30	120.30
1	G	317	ARG	NE-CZ-NH1	12.13	126.37	120.30
1	E	538	LYS	CD-CE-NZ	-12.03	84.04	111.70
1	A	139	LEU	CB-CG-CD1	-11.37	91.68	111.00
1	B	316	LEU	CB-CG-CD2	-11.22	91.92	111.00
1	G	317	ARG	CA-CB-CG	-10.27	90.80	113.40
1	C	446	ARG	NE-CZ-NH2	-10.01	115.29	120.30
1	H	325	GLU	CA-CB-CG	9.90	135.19	113.40
1	F	317	ARG	CB-CG-CD	-9.83	86.05	111.60
1	C	139	LEU	CB-CG-CD2	9.82	127.70	111.00
1	G	317	ARG	CG-CD-NE	9.57	131.90	111.80
1	D	196	ASP	CB-CG-OD1	-9.42	109.82	118.30
1	C	446	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	B	147	ILE	CG1-CB-CG2	-9.00	91.60	111.40
1	E	317	ARG	NE-CZ-NH1	-8.84	115.88	120.30
1	E	538	LYS	CA-CB-CG	-8.70	94.26	113.40
1	G	317	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	B	198	ASP	CB-CG-OD2	-8.56	110.59	118.30
1	H	152	GLU	CA-CB-CG	8.42	131.92	113.40
1	C	216	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	G	143	LEU	CB-CG-CD1	8.20	124.94	111.00
1	E	325	GLU	CA-CB-CG	8.08	131.18	113.40
1	G	317	ARG	CD-NE-CZ	-8.00	112.39	123.60
1	H	199	LEU	CA-CB-CG	7.96	133.60	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	LEU	CA-CB-CG	-7.95	97.02	115.30
1	F	191	ASP	CB-CG-OD2	-7.84	111.25	118.30
1	G	143	LEU	CA-CB-CG	7.57	132.70	115.30
1	G	317	ARG	CB-CA-C	7.24	124.88	110.40
1	G	169	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	B	317	ARG	CG-CD-NE	-7.22	96.64	111.80
1	H	192	GLY	N-CA-C	-7.21	95.09	113.10
1	C	196	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	E	538	LYS	CB-CG-CD	7.15	130.19	111.60
1	H	151	GLN	CA-CB-CG	-7.08	97.83	113.40
1	C	191	ASP	CB-CG-OD2	-7.07	111.93	118.30
1	D	199	LEU	CA-CB-CG	7.01	131.43	115.30
1	C	191	ASP	CB-CG-OD1	7.00	124.60	118.30
1	B	198	ASP	CB-CG-OD1	7.00	124.60	118.30
1	D	186	LEU	CB-CG-CD2	-6.85	99.35	111.00
1	D	255	LYS	CD-CE-NZ	-6.83	96.00	111.70
1	A	255	LYS	CD-CE-NZ	-6.73	96.22	111.70
1	D	196	ASP	CB-CA-C	-6.72	96.96	110.40
1	D	169	ARG	NE-CZ-NH1	-6.67	116.97	120.30
1	G	315	GLY	N-CA-C	-6.59	96.62	113.10
1	C	446	ARG	CG-CD-NE	6.42	125.28	111.80
1	G	169	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	D	186	LEU	CB-CG-CD1	6.36	121.81	111.00
1	B	316	LEU	CB-CG-CD1	6.22	121.58	111.00
1	C	446	ARG	CB-CG-CD	-6.22	95.42	111.60
1	F	255	LYS	CB-CG-CD	-6.20	95.48	111.60
1	F	152	GLU	CA-CB-CG	6.19	127.03	113.40
1	E	317	ARG	CG-CD-NE	-6.18	98.83	111.80
1	F	139	LEU	CA-CB-CG	6.15	129.44	115.30
1	F	255	LYS	CB-CA-C	-6.10	98.19	110.40
1	D	544	ARG	CG-CD-NE	6.06	124.53	111.80
1	C	216	ARG	CB-CG-CD	-6.04	95.90	111.60
1	H	151	GLN	C-N-CA	-5.93	106.88	121.70
1	E	141	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	A	191	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	B	544	ARG	CG-CD-NE	5.62	123.61	111.80
1	E	383	GLU	CA-CB-CG	5.61	125.75	113.40
1	A	187	GLN	CA-CB-CG	-5.59	101.10	113.40
1	G	398	LYS	CB-CG-CD	5.56	126.07	111.60
1	G	142	LEU	CA-CB-CG	5.52	128.00	115.30
1	H	489	LEU	CA-CB-CG	5.49	127.93	115.30
1	C	151	GLN	CA-CB-CG	5.45	125.38	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	141	ASP	CB-CA-C	-5.43	99.54	110.40
1	G	143	LEU	CD1-CG-CD2	-5.39	94.34	110.50
1	H	538	LYS	CD-CE-NZ	5.38	124.08	111.70
1	F	191	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	190	SER	C-N-CA	-5.35	108.33	121.70
1	H	245	LYS	CD-CE-NZ	-5.33	99.44	111.70
1	D	186	LEU	CA-CB-CG	5.32	127.54	115.30
1	C	152	GLU	CA-CB-CG	5.22	124.88	113.40
1	F	255	LYS	CA-CB-CG	5.20	124.84	113.40
1	H	152	GLU	CB-CA-C	5.20	120.80	110.40
1	H	325	GLU	CB-CA-C	-5.20	100.00	110.40
1	E	471	GLN	CA-CB-CG	-5.18	102.00	113.40
1	C	152	GLU	N-CA-CB	-5.13	101.37	110.60
1	F	199	LEU	CA-CB-CG	5.06	126.94	115.30
1	E	317	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	D	325	GLU	CA-CB-CG	-5.04	102.31	113.40
1	F	383	GLU	CA-CB-CG	5.03	124.46	113.40
1	G	317	ARG	N-CA-CB	-5.01	101.58	110.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	317	ARG	Sidechain
1	C	151	GLN	Peptide
1	D	151	GLN	Peptide
1	D	190	SER	Peptide
1	E	317	ARG	Sidechain
1	E	325	GLU	Sidechain
1	E	383	GLU	Peptide
1	F	191	ASP	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3190	0	3167	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3194	0	3170	65	0
1	C	3194	0	3170	66	0
1	D	3194	0	3170	76	0
1	E	3190	0	3165	69	0
1	F	3194	0	3170	70	0
1	G	3194	0	3170	66	0
1	H	3194	0	3170	73	0
2	A	31	0	0	1	0
2	C	31	0	0	0	0
2	E	62	0	0	2	0
All	All	25668	0	25352	525	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 10.

All (525) 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:F:255:LYS:CE	1:F:255:LYS:CD	1.83	1.55
1:F:255:LYS:CE	1:F:255:LYS:NZ	1.68	1.51
1:F:250:ILE:HD11	1:F:253:LEU:HG	1.22	1.17
1:H:467:ASP:CB	1:H:508:MET:CE	2.27	1.12
1:H:467:ASP:HB2	1:H:508:MET:CE	1.79	1.11
1:A:378:PHE:CE2	1:A:382:ARG:NH2	2.20	1.10
1:H:467:ASP:HB3	1:H:508:MET:HE1	1.24	1.09
1:C:145:TYR:OH	1:C:197:LYS:NZ	1.86	1.09
1:E:195:LEU:HD23	1:E:199:LEU:CD2	1.83	1.09
1:H:467:ASP:HB2	1:H:508:MET:HE2	1.07	1.05
1:H:467:ASP:CB	1:H:508:MET:HE2	1.86	1.00
1:D:196:ASP:OD1	1:D:198:ASP:N	1.95	0.98
1:E:195:LEU:HD23	1:E:199:LEU:HD22	1.01	0.98
1:E:317:ARG:HH12	1:H:325:GLU:N	1.65	0.94
1:H:467:ASP:HB3	1:H:508:MET:CE	1.95	0.94
1:G:316:LEU:HD11	1:G:467:ASP:HA	1.50	0.92
1:E:195:LEU:CD2	1:E:199:LEU:HD22	1.96	0.91
1:B:195:LEU:HD23	1:B:199:LEU:HD23	1.52	0.91
1:C:151:GLN:HG3	1:C:152:GLU:HB3	1.51	0.91
1:A:250:ILE:HD11	1:A:253:LEU:HG	1.50	0.91
1:D:196:ASP:OD1	1:D:199:LEU:N	2.04	0.90
1:E:317:ARG:HH12	1:H:325:GLU:H	1.03	0.90
1:A:378:PHE:HE2	1:A:382:ARG:NH2	1.63	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:196:ASP:OD1	1:H:199:LEU:N	2.04	0.90
1:D:252:GLN:HE22	1:D:380:SER:CB	1.84	0.89
1:G:316:LEU:C	1:G:317:ARG:HG3	1.85	0.89
1:F:255:LYS:CB	1:F:255:LYS:CE	2.50	0.88
1:C:149:GLU:OE2	1:C:158:LYS:NZ	2.08	0.87
1:H:319:ASN:ND2	1:H:467:ASP:OD1	2.09	0.85
1:H:467:ASP:CB	1:H:508:MET:HE1	1.93	0.85
1:F:255:LYS:HB3	1:F:255:LYS:HE3	1.56	0.85
1:D:252:GLN:HE22	1:D:380:SER:HB3	1.42	0.83
1:A:378:PHE:CZ	1:A:382:ARG:NH2	2.43	0.82
1:F:255:LYS:HB3	1:F:255:LYS:CE	2.07	0.82
1:D:252:GLN:NE2	1:D:380:SER:OG	2.12	0.82
1:E:234:LEU:HD22	1:E:520:ASP:HB3	1.63	0.81
1:C:289:LYS:HD3	1:C:338:ALA:HB2	1.61	0.81
1:C:166:THR:HG21	1:C:214:ALA:HB1	1.63	0.80
1:E:317:ARG:NH1	1:H:325:GLU:H	1.77	0.80
1:A:319:ASN:ND2	1:A:467:ASP:OD1	2.14	0.80
1:G:529:ASN:ND2	1:F:529:ASN:OD1	2.14	0.80
1:A:143:LEU:HD13	1:A:212:THR:HG22	1.62	0.80
1:H:480:ALA:HB2	1:H:490:LEU:HD12	1.67	0.77
1:G:377:THR:HG23	1:G:419:SER:HB3	1.66	0.77
1:G:319:ASN:ND2	1:G:467:ASP:OD1	2.19	0.76
1:H:197:LYS:HD3	1:H:197:LYS:H	1.51	0.76
1:C:234:LEU:HD22	1:C:520:ASP:HB3	1.68	0.75
1:A:250:ILE:HD12	1:A:252:GLN:HB2	1.69	0.74
1:G:234:LEU:HD22	1:G:520:ASP:HB3	1.69	0.74
1:H:196:ASP:CG	1:H:199:LEU:H	1.91	0.74
1:B:259:ASP:OD1	1:G:307:ARG:NH2	2.21	0.74
1:D:377:THR:HG23	1:D:419:SER:HB3	1.69	0.74
1:F:216:ARG:O	1:F:218:LYS:HD2	1.87	0.74
1:A:151:GLN:HG3	1:A:152:GLU:H	1.53	0.73
1:E:387:ARG:HB2	1:G:397:GLU:HG3	1.70	0.73
1:F:183:ARG:O	1:F:187:GLN:HG3	1.88	0.73
1:H:274:SER:HB3	1:H:278:THR:HG21	1.72	0.72
1:G:374:SER:OG	1:G:377:THR:HG22	1.89	0.72
1:F:274:SER:HB3	1:F:278:THR:HG21	1.72	0.72
1:E:138:SER:OG	1:E:141:ASP:OD1	2.06	0.72
1:D:234:LEU:HD22	1:D:520:ASP:HB3	1.71	0.72
1:C:154:ILE:O	1:C:195:LEU:HD12	1.91	0.71
1:E:480:ALA:HB2	1:E:490:LEU:HD12	1.72	0.71
1:G:143:LEU:HD22	1:G:143:LEU:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:156:VAL:HG12	1:H:195:LEU:HD11	1.73	0.71
1:G:162:ALA:HB1	1:G:215:PHE:HE1	1.56	0.70
1:A:274:SER:HB3	1:A:278:THR:HG21	1.74	0.70
1:E:529:ASN:OD1	1:H:529:ASN:ND2	2.25	0.70
1:H:196:ASP:OD1	1:H:198:ASP:N	2.25	0.69
1:B:143:LEU:HG	1:B:212:THR:HG22	1.73	0.69
1:H:143:LEU:HD13	1:H:143:LEU:O	1.92	0.69
1:B:317:ARG:HH21	1:B:317:ARG:HA	1.59	0.68
1:D:274:SER:HB3	1:D:278:THR:HG21	1.76	0.68
1:F:145:TYR:HA	1:F:148:ALA:HB3	1.76	0.68
1:G:274:SER:HB3	1:G:278:THR:HG21	1.74	0.68
1:H:234:LEU:HD22	1:H:520:ASP:HB3	1.74	0.68
1:H:439:PHE:CE2	1:H:446:ARG:HB2	2.29	0.68
1:C:332:PRO:HD2	1:C:459:LEU:HD13	1.76	0.68
1:B:480:ALA:HB2	1:B:490:LEU:HD12	1.76	0.68
1:C:439:PHE:HE1	1:C:446:ARG:NH1	1.91	0.68
1:C:148:ALA:O	1:C:151:GLN:HB3	1.93	0.67
1:G:349:VAL:CG1	1:G:353:GLU:HB2	2.25	0.67
1:D:374:SER:OG	1:D:377:THR:HG22	1.94	0.67
1:D:283:CYS:SG	1:D:377:THR:HG21	2.35	0.67
1:C:181:MET:HE1	1:C:202:LYS:HE2	1.76	0.67
1:A:160:ILE:HD12	1:A:164:LYS:HE3	1.76	0.66
1:E:178:CYS:O	1:E:182:LEU:HD13	1.96	0.66
1:H:383:GLU:OE2	1:H:384:SER:OG	2.11	0.66
1:A:180:ASP:OD1	1:A:183:ARG:NH1	2.22	0.66
1:A:251:PRO:O	1:A:255:LYS:HG3	1.95	0.66
1:B:234:LEU:HD22	1:B:520:ASP:HB3	1.76	0.66
1:G:283:CYS:SG	1:G:377:THR:HG21	2.35	0.66
1:H:149:GLU:HG3	1:H:158:LYS:NZ	2.10	0.66
1:F:250:ILE:HG13	1:F:253:LEU:H	1.59	0.66
1:F:285:GLN:O	1:F:288:VAL:HG12	1.96	0.66
1:C:480:ALA:HB2	1:C:490:LEU:HD12	1.76	0.66
1:F:255:LYS:HB2	1:F:255:LYS:CE	2.25	0.66
1:D:217:ARG:HH12	1:D:223:ASP:HA	1.60	0.65
1:D:349:VAL:CG1	1:D:353:GLU:HB2	2.27	0.65
1:F:147:ILE:O	1:F:158:LYS:NZ	2.30	0.65
1:G:189:THR:OG1	1:G:191:ASP:OD1	2.15	0.65
1:A:507:LYS:HE2	1:A:507:LYS:H	1.63	0.64
1:D:200:PHE:O	1:D:204:VAL:HG22	1.97	0.64
1:C:148:ALA:O	1:C:149:GLU:HB2	1.97	0.64
1:D:208:ILE:O	1:D:212:THR:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:332:PRO:HD2	1:H:459:LEU:HD13	1.80	0.64
1:D:250:ILE:HG12	1:D:253:LEU:HD12	1.80	0.64
1:H:162:ALA:HB1	1:H:215:PHE:HE1	1.63	0.64
1:B:317:ARG:HH22	1:B:319:ASN:H	1.44	0.64
1:B:439:PHE:CE2	1:B:446:ARG:HB2	2.32	0.64
1:C:192:GLY:C	1:C:194:MET:H	2.01	0.64
1:D:507:LYS:H	1:D:507:LYS:HE2	1.63	0.64
1:D:140:GLU:HG3	1:D:208:ILE:HG12	1.80	0.63
1:E:317:ARG:NH1	1:H:325:GLU:N	2.40	0.63
1:G:316:LEU:HD22	1:F:312:GLU:OE1	1.98	0.63
1:E:195:LEU:CD2	1:E:199:LEU:CD2	2.68	0.63
1:E:265:VAL:HG22	1:E:498:MET:HE2	1.80	0.63
1:A:265:VAL:HG22	1:A:498:MET:HE2	1.79	0.62
1:F:387:ARG:HB2	1:H:397:GLU:HG3	1.80	0.62
1:E:145:TYR:HA	1:E:148:ALA:HB3	1.80	0.62
1:A:252:GLN:HB3	1:A:377:THR:HG22	1.81	0.62
1:F:488:ILE:HD12	1:F:514:GLY:HA3	1.81	0.62
1:E:286:SER:OG	1:E:466:TYR:OH	2.16	0.62
1:F:155:PRO:HB2	1:F:157:HIS:CE1	2.35	0.62
1:C:439:PHE:CE1	1:C:446:ARG:NH1	2.68	0.61
1:B:332:PRO:HD2	1:B:459:LEU:HD13	1.82	0.61
1:D:325:GLU:CD	1:D:325:GLU:H	2.01	0.61
1:D:196:ASP:CG	1:D:199:LEU:H	2.03	0.61
1:A:321:LEU:HD13	2:A:601:QA4:N12	2.17	0.60
1:F:181:MET:O	1:F:185:THR:HG23	2.00	0.60
1:G:138:SER:O	1:G:142:LEU:HG	2.02	0.60
1:G:147:ILE:O	1:G:158:LYS:NZ	2.34	0.60
1:B:153:LYS:HB2	1:B:194:MET:CE	2.31	0.60
1:A:196:ASP:N	1:A:196:ASP:OD1	2.28	0.60
1:D:185:THR:HA	1:D:188:THR:OG1	2.02	0.59
1:F:216:ARG:O	1:F:218:LYS:NZ	2.29	0.59
1:E:153:LYS:C	1:E:194:MET:HE3	2.22	0.59
1:C:152:GLU:CD	1:C:153:LYS:H	2.05	0.59
1:A:378:PHE:HZ	1:A:382:ARG:HH21	1.39	0.59
1:E:333:MET:HG3	1:E:481:LYS:HE2	1.83	0.59
1:E:141:ASP:OD2	1:E:197:LYS:HD3	2.02	0.59
1:A:374:SER:O	1:A:374:SER:OG	2.21	0.59
1:E:274:SER:HB3	1:E:278:THR:HG21	1.84	0.59
1:B:198:ASP:O	1:B:201:LYS:HB3	2.03	0.58
1:D:252:GLN:OE1	1:D:252:GLN:N	2.36	0.58
2:E:601:QA4:C11	1:F:321:LEU:HD22	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:545:GLU:OE1	1:D:545:GLU:N	2.36	0.58
1:H:148:ALA:O	1:H:149:GLU:HB2	2.04	0.58
1:H:346:LYS:HB3	1:H:354:LYS:HG2	1.85	0.58
1:B:317:ARG:HH22	1:B:319:ASN:N	2.01	0.58
1:A:181:MET:O	1:A:185:THR:HG23	2.03	0.58
1:A:349:VAL:CG1	1:A:353:GLU:HB2	2.34	0.58
1:C:188:THR:OG1	1:C:189:THR:HG23	2.04	0.58
1:A:387:ARG:HB2	1:B:397:GLU:HG3	1.86	0.58
1:E:185:THR:HG21	1:E:199:LEU:HD21	1.85	0.58
1:B:154:ILE:HG23	1:B:158:LYS:HE3	1.85	0.57
1:G:488:ILE:HD12	1:G:514:GLY:HA3	1.85	0.57
1:D:343:SER:OG	1:D:402:PRO:HD2	2.04	0.57
1:G:249:TYR:CD1	1:G:250:ILE:HG23	2.39	0.57
1:A:488:ILE:HD12	1:A:514:GLY:HA3	1.86	0.57
1:E:507:LYS:H	1:E:507:LYS:HE2	1.68	0.57
1:D:502:SER:OG	1:D:504:PRO:HD2	2.04	0.57
1:F:216:ARG:O	1:F:218:LYS:CD	2.53	0.57
1:B:365:MET:HG3	1:B:447:VAL:HG11	1.86	0.57
1:H:149:GLU:HG3	1:H:158:LYS:HZ1	1.68	0.57
1:H:156:VAL:HG13	1:H:193:VAL:O	2.04	0.57
1:E:315:GLY:C	1:E:317:ARG:H	2.06	0.57
1:H:365:MET:HG3	1:H:447:VAL:HG11	1.86	0.57
1:C:293:TYR:OH	1:C:306:HIS:NE2	2.30	0.56
1:E:286:SER:HG	1:E:466:TYR:HH	1.49	0.56
1:F:234:LEU:HD22	1:F:520:ASP:HB3	1.87	0.56
1:A:315:GLY:O	1:A:318:PHE:N	2.38	0.56
1:B:479:PRO:HG3	1:C:530:TYR:CE1	2.40	0.56
1:D:162:ALA:HB1	1:D:215:PHE:HE1	1.68	0.56
1:G:185:THR:HA	1:G:188:THR:OG1	2.06	0.56
1:H:143:LEU:HD23	1:H:212:THR:HG22	1.87	0.56
1:A:374:SER:OG	1:A:377:THR:HG23	2.05	0.56
1:D:224:PHE:O	1:D:228:THR:HG23	2.05	0.56
1:E:310:GLY:HA2	1:E:328:LYS:NZ	2.21	0.56
1:F:199:LEU:HA	1:F:202:LYS:HB2	1.88	0.56
1:H:199:LEU:HA	1:H:202:LYS:HB3	1.86	0.56
1:C:365:MET:HG3	1:C:447:VAL:HG11	1.87	0.56
1:D:541:ASP:HB3	1:D:544:ARG:HG3	1.86	0.56
1:B:138:SER:HB3	1:B:141:ASP:HB2	1.87	0.56
1:F:192:GLY:C	1:F:194:MET:H	2.09	0.56
1:F:477:GLY:O	1:F:529:ASN:HB2	2.05	0.56
1:A:285:GLN:HA	1:A:418:CYS:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:530:TYR:CE1	1:H:479:PRO:HG3	2.42	0.55
1:G:316:LEU:HD11	1:G:467:ASP:CA	2.32	0.55
1:H:199:LEU:HD12	1:H:202:LYS:HD2	1.88	0.55
1:A:234:LEU:HD22	1:A:520:ASP:HB3	1.88	0.55
1:F:349:VAL:CG1	1:F:353:GLU:HB2	2.37	0.55
1:A:454:ARG:HD2	1:D:528:HIS:CD2	2.43	0.54
1:A:317:ARG:HG2	1:D:318:PHE:CZ	2.43	0.54
1:B:349:VAL:HG11	1:B:353:GLU:HB2	1.89	0.54
1:B:422:VAL:HG21	1:B:427:ALA:HB2	1.88	0.54
1:C:140:GLU:HG2	1:C:201:LYS:HG3	1.88	0.54
1:A:397:GLU:HG3	1:B:387:ARG:HB2	1.90	0.54
1:B:155:PRO:HA	1:B:194:MET:HG2	1.89	0.54
1:F:166:THR:HG21	1:F:214:ALA:HB1	1.90	0.54
1:H:145:TYR:HA	1:H:148:ALA:HB3	1.88	0.54
1:F:162:ALA:HB1	1:F:215:PHE:HE1	1.73	0.54
1:G:285:GLN:O	1:G:288:VAL:HG12	2.07	0.54
1:A:318:PHE:HZ	1:D:317:ARG:HE	1.54	0.54
1:F:185:THR:HA	1:F:188:THR:HG23	1.90	0.54
1:G:265:VAL:HG13	1:G:496:MET:SD	2.48	0.54
1:E:332:PRO:HD2	1:E:459:LEU:HD13	1.89	0.54
1:D:349:VAL:HG11	1:D:353:GLU:HB2	1.91	0.53
1:F:249:TYR:CD2	1:F:250:ILE:HG23	2.43	0.53
1:C:201:LYS:O	1:C:205:GLN:HB2	2.09	0.53
1:F:490:LEU:HB3	1:F:498:MET:HB2	1.89	0.53
1:A:162:ALA:HB1	1:A:215:PHE:HE1	1.73	0.53
1:B:141:ASP:O	1:B:144:PHE:HB3	2.09	0.53
1:B:153:LYS:HB2	1:B:194:MET:HE2	1.91	0.53
1:C:145:TYR:OH	1:C:197:LYS:CE	2.57	0.53
1:E:216:ARG:O	1:E:218:LYS:HG2	2.08	0.53
1:E:525:CYS:HA	1:E:540:LEU:O	2.08	0.53
1:F:195:LEU:HD23	1:F:199:LEU:HD12	1.90	0.53
1:C:216:ARG:O	1:C:218:LYS:HG2	2.09	0.53
1:G:341:VAL:HA	1:G:344:LEU:HD12	1.89	0.53
1:C:185:THR:HG21	1:C:199:LEU:HD21	1.90	0.53
1:E:315:GLY:O	1:E:317:ARG:N	2.41	0.53
1:H:422:VAL:HG21	1:H:427:ALA:HB2	1.91	0.53
1:C:220:VAL:HG13	1:C:221:ILE:HG12	1.90	0.53
1:C:286:SER:OG	1:C:289:LYS:NZ	2.42	0.53
1:E:162:ALA:HB1	1:E:215:PHE:HE1	1.73	0.53
1:G:349:VAL:HG11	1:G:353:GLU:HB2	1.90	0.52
1:A:152:GLU:HG2	1:A:153:LYS:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:224:PHE:O	1:G:228:THR:HG23	2.10	0.52
1:A:151:GLN:HG3	1:A:152:GLU:N	2.23	0.52
1:G:286:SER:HB3	1:G:289:LYS:HD2	1.91	0.52
1:G:156:VAL:HG23	1:G:193:VAL:O	2.10	0.52
1:G:378:PHE:CE1	1:G:416:GLN:HG3	2.44	0.52
1:G:362:LEU:HD23	1:G:365:MET:HE1	1.91	0.52
1:A:387:ARG:HD2	1:B:397:GLU:OE2	2.10	0.51
1:B:200:PHE:O	1:B:204:VAL:HG22	2.09	0.51
1:H:174:ARG:NH1	1:H:210:LEU:HD13	2.25	0.51
1:F:188:THR:OG1	1:F:189:THR:N	2.43	0.51
1:H:195:LEU:HG	1:H:199:LEU:HD23	1.92	0.51
1:C:507:LYS:H	1:C:507:LYS:HE2	1.74	0.51
1:F:156:VAL:HG23	1:F:195:LEU:HD11	1.91	0.51
1:H:182:LEU:HD12	1:H:203:CYS:SG	2.51	0.51
1:H:216:ARG:HE	1:H:216:ARG:HA	1.75	0.51
1:E:312:GLU:OE2	1:H:470:GLY:HA3	2.11	0.51
1:E:143:LEU:HD13	1:E:212:THR:HG22	1.92	0.51
1:F:184:LEU:O	1:F:187:GLN:HB2	2.11	0.51
1:H:446:ARG:NH1	1:H:450:PRO:HD3	2.26	0.51
1:D:196:ASP:C	1:D:196:ASP:OD1	2.49	0.51
1:E:182:LEU:CD1	1:E:203:CYS:HB3	2.41	0.51
1:G:343:SER:OG	1:G:402:PRO:HD2	2.11	0.51
1:C:139:LEU:HA	1:C:142:LEU:HD12	1.93	0.51
1:D:169:ARG:HE	1:D:272:ARG:HB2	1.75	0.51
1:H:153:LYS:HB3	1:H:194:MET:HB3	1.93	0.51
1:H:315:GLY:O	1:H:318:PHE:HD2	1.92	0.51
1:H:140:GLU:HG3	1:H:208:ILE:HG12	1.93	0.50
1:B:528:HIS:CD2	1:C:454:ARG:HD2	2.46	0.50
1:F:200:PHE:O	1:F:204:VAL:HG22	2.11	0.50
1:G:318:PHE:HZ	1:F:317:ARG:HH21	1.58	0.50
1:G:340:VAL:O	1:G:343:SER:HB3	2.12	0.50
1:G:304:TYR:CE1	1:G:344:LEU:HD22	2.47	0.50
1:H:382:ARG:NH1	1:H:412:ASP:OD2	2.43	0.50
1:C:209:VAL:O	1:C:213:GLN:HG3	2.12	0.50
1:H:446:ARG:HH12	1:H:450:PRO:HD3	1.77	0.50
1:B:216:ARG:HE	1:B:216:ARG:HA	1.76	0.49
1:F:350:ASN:ND2	1:F:353:GLU:OE2	2.45	0.49
1:G:365:MET:HG3	1:G:447:VAL:HG11	1.94	0.49
1:B:470:GLY:HA3	1:C:312:GLU:HG2	1.93	0.49
1:E:267:THR:HA	1:E:496:MET:HA	1.93	0.49
1:F:289:LYS:HE3	1:F:338:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLN:CB	1:A:377:THR:HG22	2.41	0.49
1:E:281:PRO:HA	1:E:422:VAL:O	2.13	0.49
1:F:349:VAL:HG12	1:F:353:GLU:HB2	1.94	0.49
1:H:314:SER:HB2	1:H:318:PHE:HB2	1.94	0.49
1:A:188:THR:O	1:A:189:THR:OG1	2.26	0.49
1:A:454:ARG:HD2	1:D:528:HIS:CG	2.48	0.49
1:A:477:GLY:O	1:A:529:ASN:HB2	2.11	0.49
1:C:290:PRO:HD3	1:C:481:LYS:HG2	1.95	0.49
1:F:156:VAL:HG11	1:F:186:LEU:HD21	1.95	0.49
1:G:153:LYS:HB3	1:G:195:LEU:O	2.13	0.49
1:F:289:LYS:HA	1:F:292:LYS:HE2	1.94	0.48
1:G:288:VAL:HA	1:G:291:LEU:HD12	1.95	0.48
1:H:174:ARG:NH1	1:H:210:LEU:CD1	2.76	0.48
1:H:285:GLN:O	1:H:288:VAL:HG12	2.13	0.48
1:A:138:SER:HB3	1:A:141:ASP:HB2	1.93	0.48
1:B:153:LYS:HB2	1:B:194:MET:HE3	1.95	0.48
1:B:317:ARG:HH21	1:B:317:ARG:CA	2.25	0.48
1:E:153:LYS:HB3	1:E:194:MET:HE3	1.94	0.48
1:A:196:ASP:OD1	1:A:199:LEU:HB3	2.13	0.48
1:B:530:TYR:CZ	1:C:479:PRO:HG3	2.48	0.48
1:G:138:SER:HB3	1:G:141:ASP:OD1	2.14	0.48
1:B:235:TYR:CD1	1:B:275:THR:HG23	2.49	0.48
1:D:138:SER:HB2	1:D:141:ASP:OD1	2.14	0.48
1:D:196:ASP:CG	1:D:198:ASP:OD1	2.52	0.48
1:E:293:TYR:OH	1:E:306:HIS:NE2	2.39	0.48
1:A:142:LEU:O	1:A:146:THR:HG23	2.14	0.47
1:C:281:PRO:HA	1:C:422:VAL:O	2.13	0.47
1:F:255:LYS:CD	1:F:255:LYS:NZ	2.75	0.47
1:G:140:GLU:CB	1:G:201:LYS:HG3	2.44	0.47
1:A:412:ASP:O	1:A:416:GLN:HG3	2.14	0.47
1:B:140:GLU:HG3	1:B:208:ILE:HG12	1.95	0.47
1:C:189:THR:OG1	1:C:189:THR:O	2.33	0.47
2:E:601:QA4:O18	1:H:320:LYS:HE3	2.14	0.47
1:E:156:VAL:HG23	1:E:193:VAL:O	2.14	0.47
1:G:306:HIS:CE1	1:G:311:LYS:HB3	2.49	0.47
1:B:204:VAL:HG12	1:B:211:LEU:HD13	1.95	0.47
1:C:525:CYS:HA	1:C:540:LEU:O	2.14	0.47
1:D:378:PHE:HZ	1:D:382:ARG:HH21	1.62	0.47
1:F:355:PHE:HE1	1:F:420:ILE:HD11	1.80	0.47
1:F:177:GLU:OE2	1:F:207:ASN:ND2	2.36	0.47
1:G:477:GLY:O	1:G:529:ASN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ALA:HB1	1:B:215:PHE:HE1	1.79	0.47
1:C:145:TYR:HA	1:C:148:ALA:HB3	1.96	0.47
1:D:169:ARG:HH21	1:D:272:ARG:HB3	1.78	0.47
1:A:186:LEU:C	1:A:187:GLN:HG2	2.34	0.46
1:E:153:LYS:O	1:E:194:MET:HE3	2.14	0.46
1:F:140:GLU:HB3	1:F:201:LYS:HG3	1.96	0.46
1:F:144:PHE:O	1:F:148:ALA:HB2	2.15	0.46
1:G:143:LEU:HD22	1:G:143:LEU:C	2.24	0.46
1:E:454:ARG:HD2	1:H:528:HIS:CD2	2.51	0.46
1:A:235:TYR:CD2	1:A:236:GLU:HG2	2.50	0.46
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.58	0.46
1:B:193:VAL:HG12	1:B:193:VAL:O	2.14	0.46
1:E:153:LYS:HB3	1:E:194:MET:CE	2.45	0.46
1:G:544:ARG:HA	1:G:544:ARG:HH11	1.80	0.46
1:D:140:GLU:CB	1:D:201:LYS:HD2	2.45	0.46
1:B:180:ASP:HA	1:B:183:ARG:NH1	2.30	0.46
1:H:383:GLU:HG3	1:H:384:SER:N	2.30	0.46
1:D:217:ARG:NH1	1:D:223:ASP:HA	2.29	0.46
1:E:317:ARG:HB3	1:H:318:PHE:CE1	2.50	0.46
1:H:349:VAL:HG12	1:H:350:ASN:N	2.31	0.46
1:A:286:SER:HB3	1:A:289:LYS:HD2	1.97	0.46
1:A:303:GLU:H	1:A:303:GLU:CD	2.19	0.46
1:B:317:ARG:NH2	1:B:319:ASN:H	2.11	0.46
1:C:162:ALA:HB1	1:C:215:PHE:HE1	1.80	0.46
1:E:457:LEU:HD23	1:E:457:LEU:HA	1.82	0.46
1:H:355:PHE:CE2	1:H:359:MET:HE3	2.50	0.46
1:D:251:PRO:HG2	1:D:252:GLN:OE1	2.15	0.46
1:B:138:SER:OG	1:B:141:ASP:OD1	2.23	0.46
1:D:346:LYS:O	1:D:354:LYS:HE2	2.16	0.46
1:F:286:SER:HB3	1:F:289:LYS:HZ3	1.81	0.46
1:A:269:ASP:OD1	1:D:534:ARG:NH2	2.45	0.45
1:A:318:PHE:CE1	1:D:318:PHE:HE2	2.34	0.45
1:A:332:PRO:HD2	1:A:459:LEU:HD13	1.98	0.45
1:D:138:SER:O	1:D:142:LEU:HG	2.16	0.45
1:G:169:ARG:HE	1:G:272:ARG:HB2	1.81	0.45
1:B:316:LEU:O	1:B:316:LEU:HG	2.16	0.45
1:C:143:LEU:HD23	1:C:200:PHE:HZ	1.81	0.45
1:D:192:GLY:HA3	1:D:193:VAL:HA	1.79	0.45
1:A:318:PHE:CE1	1:D:318:PHE:CE2	3.04	0.45
1:A:162:ALA:HB1	1:A:215:PHE:CE1	2.51	0.45
1:A:140:GLU:HG3	1:A:208:ILE:HG12	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LEU:HD22	1:B:146:THR:OG1	2.17	0.45
1:C:439:PHE:CZ	1:C:446:ARG:CZ	3.00	0.45
1:C:261:TRP:HA	1:C:501:TRP:O	2.17	0.45
1:A:249:TYR:OH	1:A:381:GLU:OE1	2.25	0.45
1:D:140:GLU:HB2	1:D:201:LYS:CD	2.47	0.45
1:E:153:LYS:CB	1:E:194:MET:CE	2.95	0.45
1:E:349:VAL:CG1	1:E:353:GLU:HB2	2.47	0.45
1:H:148:ALA:O	1:H:149:GLU:CB	2.65	0.45
1:H:196:ASP:HB2	1:H:198:ASP:H	1.82	0.45
1:A:367:GLY:HA3	1:A:442:ILE:HD11	1.99	0.45
1:B:252:GLN:NE2	1:B:376:ALA:O	2.50	0.45
1:C:196:ASP:OD1	1:C:199:LEU:HB2	2.16	0.45
1:D:196:ASP:OD2	1:D:199:LEU:HB2	2.17	0.45
1:E:265:VAL:HG22	1:E:498:MET:CE	2.44	0.45
1:B:318:PHE:HZ	1:C:318:PHE:CG	2.35	0.45
1:D:182:LEU:O	1:D:186:LEU:HB2	2.17	0.45
1:A:260:LEU:O	1:A:502:SER:HB2	2.17	0.45
1:A:380:SER:O	1:A:384:SER:HB2	2.17	0.45
1:C:145:TYR:CZ	1:C:197:LYS:CE	3.00	0.45
1:D:250:ILE:CG1	1:D:253:LEU:HD12	2.45	0.45
1:D:318:PHE:HD1	1:D:321:LEU:HG	1.81	0.45
1:F:143:LEU:HD11	1:F:215:PHE:HB2	1.98	0.45
1:F:359:MET:HB3	1:F:359:MET:HE2	1.80	0.45
1:C:140:GLU:N	1:C:140:GLU:OE1	2.50	0.44
1:D:182:LEU:HD12	1:D:203:CYS:SG	2.57	0.44
1:G:138:SER:CB	1:G:141:ASP:OD1	2.65	0.44
1:A:216:ARG:HA	1:A:216:ARG:HE	1.81	0.44
1:G:141:ASP:HA	1:G:144:PHE:CB	2.47	0.44
1:H:417:LEU:HA	1:H:417:LEU:HD23	1.67	0.44
1:A:507:LYS:H	1:A:507:LYS:CE	2.29	0.44
1:H:350:ASN:OD1	1:H:351:ASN:N	2.51	0.44
1:B:216:ARG:O	1:B:218:LYS:HG2	2.18	0.44
1:E:220:VAL:HG13	1:E:221:ILE:HG13	2.00	0.44
1:A:315:GLY:O	1:A:317:ARG:N	2.50	0.44
1:B:145:TYR:HA	1:B:148:ALA:HB3	2.00	0.44
1:B:316:LEU:HD11	1:B:467:ASP:HA	2.00	0.44
1:D:315:GLY:O	1:D:317:ARG:N	2.50	0.44
1:E:140:GLU:N	1:E:140:GLU:OE1	2.50	0.44
1:B:274:SER:HB3	1:B:278:THR:HG21	1.99	0.44
1:F:224:PHE:O	1:F:228:THR:HG23	2.18	0.44
1:G:247:ALA:HB2	1:G:484:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:PHE:CZ	1:A:542:PRO:HG2	2.53	0.44
1:C:153:LYS:HD2	1:C:194:MET:HB2	1.99	0.44
1:A:317:ARG:HG2	1:D:318:PHE:CE2	2.52	0.44
1:F:365:MET:HG3	1:F:447:VAL:HG11	2.00	0.44
1:C:439:PHE:CE2	1:C:446:ARG:HB2	2.53	0.43
1:E:153:LYS:CB	1:E:194:MET:HE3	2.47	0.43
1:G:544:ARG:HA	1:G:544:ARG:HD2	1.75	0.43
1:C:313:PRO:HG3	1:C:462:SER:HB2	2.00	0.43
1:E:144:PHE:O	1:E:148:ALA:N	2.50	0.43
1:B:412:ASP:O	1:B:416:GLN:HG3	2.18	0.43
1:D:149:GLU:HG2	1:D:158:LYS:NZ	2.32	0.43
1:F:157:HIS:HA	1:F:160:ILE:HG12	2.00	0.43
1:G:316:LEU:HB3	1:G:317:ARG:HD2	2.00	0.43
1:G:380:SER:O	1:G:384:SER:HB3	2.18	0.43
1:E:140:GLU:CB	1:E:201:LYS:HG3	2.48	0.43
1:G:318:PHE:CZ	1:F:318:PHE:CZ	3.06	0.43
1:D:162:ALA:HB1	1:D:215:PHE:CE1	2.52	0.43
1:E:159:PHE:CD2	1:E:160:ILE:HD13	2.53	0.43
1:F:143:LEU:HD23	1:F:200:PHE:HZ	1.83	0.43
1:G:537:ALA:HB2	1:F:450:PRO:HG2	2.01	0.43
1:B:143:LEU:O	1:B:143:LEU:HD13	2.19	0.43
1:E:153:LYS:HB3	1:E:194:MET:HB3	2.01	0.43
1:G:140:GLU:HB2	1:G:201:LYS:HG3	2.00	0.43
1:B:156:VAL:HB	1:B:193:VAL:HG12	2.00	0.43
1:D:166:THR:HG21	1:D:214:ALA:HB1	2.00	0.43
1:D:488:ILE:HD12	1:D:514:GLY:HA3	2.00	0.43
1:E:286:SER:HB2	1:E:289:LYS:HD2	2.01	0.43
1:F:145:TYR:HA	1:F:148:ALA:CB	2.44	0.43
1:C:166:THR:HG21	1:C:214:ALA:CB	2.41	0.43
1:D:435:ALA:HB2	1:D:491:VAL:HG13	2.01	0.43
1:A:253:LEU:HD22	1:A:485:ALA:HA	2.01	0.43
1:C:140:GLU:CB	1:C:201:LYS:HG3	2.49	0.43
1:B:196:ASP:OD1	1:B:199:LEU:CB	2.67	0.43
1:B:200:PHE:CE2	1:B:204:VAL:HG21	2.54	0.43
1:C:481:LYS:HD2	1:C:481:LYS:HA	1.90	0.43
1:D:365:MET:HG3	1:D:447:VAL:HG11	2.00	0.43
1:H:216:ARG:NH2	1:H:217:ARG:HH22	2.17	0.43
1:H:488:ILE:HD12	1:H:514:GLY:HA3	2.01	0.42
1:C:274:SER:HB3	1:C:278:THR:HG21	1.99	0.42
1:D:319:ASN:ND2	1:D:467:ASP:OD1	2.52	0.42
1:A:186:LEU:HA	1:A:186:LEU:HD23	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:TYR:CE1	1:A:261:TRP:CD1	3.07	0.42
1:D:196:ASP:OD1	1:D:198:ASP:CA	2.65	0.42
1:G:162:ALA:HB1	1:G:215:PHE:CE1	2.45	0.42
1:H:477:GLY:O	1:H:529:ASN:HB2	2.19	0.42
1:B:187:GLN:HA	1:B:190:SER:OG	2.20	0.42
1:B:196:ASP:OD1	1:B:199:LEU:HB2	2.20	0.42
1:B:349:VAL:CG1	1:B:353:GLU:HB2	2.49	0.42
1:G:141:ASP:HA	1:G:144:PHE:HB3	2.01	0.42
1:A:346:LYS:O	1:A:354:LYS:HD3	2.19	0.42
1:A:525:CYS:HA	1:A:540:LEU:O	2.19	0.42
1:B:477:GLY:O	1:B:529:ASN:HB2	2.20	0.42
1:E:318:PHE:CE2	1:H:317:ARG:HB3	2.55	0.42
1:E:349:VAL:HG11	1:E:353:GLU:HB2	2.02	0.42
1:G:155:PRO:HB2	1:G:157:HIS:CE1	2.54	0.42
1:H:255:LYS:HB3	1:H:255:LYS:HE3	1.81	0.42
1:B:219:PHE:HB3	1:B:271:GLN:OE1	2.19	0.42
1:B:379:GLN:O	1:B:382:ARG:HG2	2.18	0.42
1:E:350:ASN:ND2	1:E:353:GLU:OE2	2.52	0.42
1:F:257:SER:HA	1:F:258:PRO:HD3	1.93	0.42
1:B:166:THR:HG21	1:B:214:ALA:HB1	2.01	0.42
1:C:232:ASP:O	1:C:236:GLU:HG2	2.19	0.42
1:C:439:PHE:CE1	1:C:446:ARG:HD3	2.54	0.42
1:D:288:VAL:HA	1:D:291:LEU:HD12	2.02	0.42
1:F:278:THR:O	1:F:425:GLU:HG3	2.19	0.42
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.84	0.42
1:B:138:SER:CB	1:B:141:ASP:HB2	2.50	0.42
1:C:184:LEU:HD23	1:C:184:LEU:HA	1.88	0.42
1:E:315:GLY:C	1:E:317:ARG:N	2.71	0.42
1:A:432:ALA:HB1	1:A:441:PRO:HG2	2.02	0.41
1:F:343:SER:HA	1:F:410:ILE:HD12	2.02	0.41
1:E:278:THR:HA	1:E:424:CYS:HB2	2.01	0.41
1:F:471:GLN:HB3	1:F:471:GLN:HE21	1.75	0.41
1:A:195:LEU:HD22	1:A:200:PHE:HA	2.02	0.41
1:C:295:ILE:HG23	1:C:361:PHE:CE2	2.56	0.41
1:G:143:LEU:HD13	1:G:147:ILE:HD12	2.02	0.41
1:G:349:VAL:HG12	1:G:350:ASN:N	2.35	0.41
1:A:529:ASN:OD1	1:D:529:ASN:ND2	2.53	0.41
1:D:183:ARG:O	1:D:187:GLN:HG3	2.21	0.41
1:D:257:SER:O	1:D:260:LEU:HD12	2.20	0.41
1:D:477:GLY:O	1:D:529:ASN:HB2	2.20	0.41
1:F:192:GLY:C	1:F:194:MET:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:366:ALA:O	1:G:369:GLU:HG3	2.20	0.41
1:H:144:PHE:CE2	1:H:197:LYS:HB3	2.55	0.41
1:F:201:LYS:O	1:F:205:GLN:HB2	2.20	0.41
1:A:139:LEU:HA	1:A:142:LEU:HB2	2.03	0.41
1:B:170:THR:OG1	1:B:179:MET:SD	2.78	0.41
1:E:365:MET:HG3	1:E:447:VAL:HG11	2.03	0.41
1:G:140:GLU:N	1:G:140:GLU:OE1	2.51	0.41
1:A:366:ALA:O	1:A:369:GLU:HG3	2.21	0.41
1:C:410:ILE:HD13	1:C:410:ILE:HA	1.82	0.41
1:D:149:GLU:HA	1:D:149:GLU:OE1	2.20	0.41
1:E:200:PHE:CE2	1:E:204:VAL:HG21	2.56	0.41
1:A:349:VAL:HG11	1:A:353:GLU:HB2	2.01	0.41
1:B:240:LYS:HA	1:B:240:LYS:HD2	1.71	0.41
1:D:228:THR:HB	1:D:273:HIS:ND1	2.35	0.41
1:C:387:ARG:O	1:C:391:ILE:HG13	2.21	0.41
1:E:148:ALA:HA	1:E:154:ILE:HG12	2.03	0.41
1:E:186:LEU:HA	1:E:186:LEU:HD23	1.90	0.41
1:G:184:LEU:HD12	1:G:184:LEU:HA	1.81	0.41
1:G:362:LEU:HD23	1:G:365:MET:CE	2.51	0.41
1:H:382:ARG:HD2	1:H:412:ASP:OD1	2.19	0.41
1:A:199:LEU:O	1:A:202:LYS:HB3	2.21	0.41
1:C:200:PHE:CE1	1:C:204:VAL:HG21	2.55	0.41
1:C:502:SER:OG	1:C:504:PRO:HD2	2.21	0.41
1:D:249:TYR:N	1:D:249:TYR:CD1	2.87	0.41
1:D:316:LEU:HA	1:D:316:LEU:HD23	1.64	0.41
1:D:503:PRO:N	1:D:504:PRO:CD	2.84	0.41
1:H:196:ASP:OD2	1:H:199:LEU:CB	2.69	0.41
1:A:289:LYS:HE3	1:A:338:ALA:CB	2.50	0.41
1:D:148:ALA:O	1:D:151:GLN:HB2	2.21	0.41
1:D:184:LEU:HA	1:D:184:LEU:HD12	1.75	0.41
1:F:397:GLU:HG3	1:H:387:ARG:HB2	2.02	0.41
1:A:216:ARG:O	1:A:218:LYS:HG2	2.21	0.40
1:C:287:CYS:O	1:C:290:PRO:HD2	2.21	0.40
1:C:488:ILE:HD12	1:C:514:GLY:HA3	2.03	0.40
1:E:155:PRO:HG3	1:E:194:MET:SD	2.62	0.40
1:F:289:LYS:HE3	1:F:338:ALA:CB	2.51	0.40
1:A:490:LEU:HB3	1:A:498:MET:HB3	2.02	0.40
1:B:349:VAL:HG12	1:B:350:ASN:N	2.35	0.40
1:C:186:LEU:HA	1:C:186:LEU:HD12	1.90	0.40
1:E:526:ASN:OD1	1:E:543:ARG:NH2	2.54	0.40
1:G:175:LEU:HD23	1:G:175:LEU:HA	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:166:THR:HG21	1:G:214:ALA:HB1	2.02	0.40
1:B:261:TRP:HA	1:B:501:TRP:O	2.21	0.40
1:C:149:GLU:C	1:C:151:GLN:H	2.25	0.40
1:D:143:LEU:HD11	1:D:215:PHE:CD2	2.56	0.40
1:C:148:ALA:HA	1:C:154:ILE:HG12	2.03	0.40
1:E:162:ALA:HB1	1:E:215:PHE:CE1	2.52	0.40
1:E:317:ARG:NH1	1:H:324:ASN:HB2	2.36	0.40
1:F:278:THR:HA	1:F:424:CYS:HB2	2.03	0.40
1:G:528:HIS:CD2	1:F:454:ARG:HD2	2.56	0.40
1:F:468:PHE:CD2	1:F:472:PHE:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	407/527 (77%)	393 (97%)	11 (3%)	3 (1%)	22	56
1	B	408/527 (77%)	392 (96%)	16 (4%)	0	100	100
1	C	408/527 (77%)	397 (97%)	10 (2%)	1 (0%)	47	79
1	D	408/527 (77%)	393 (96%)	13 (3%)	2 (0%)	29	64
1	E	407/527 (77%)	397 (98%)	9 (2%)	1 (0%)	47	79
1	F	408/527 (77%)	396 (97%)	11 (3%)	1 (0%)	47	79
1	G	408/527 (77%)	394 (97%)	13 (3%)	1 (0%)	47	79
1	H	408/527 (77%)	397 (97%)	10 (2%)	1 (0%)	47	79
All	All	3262/4216 (77%)	3159 (97%)	93 (3%)	10 (0%)	41	73

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	191	ASP
1	H	196	ASP
1	A	152	GLU
1	G	192	GLY
1	F	188	THR
1	A	193	VAL
1	D	196	ASP
1	A	189	THR
1	C	149	GLU
1	E	193	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/451 (78%)	344 (98%)	9 (2%)	47	76
1	B	353/451 (78%)	343 (97%)	10 (3%)	43	74
1	C	353/451 (78%)	343 (97%)	10 (3%)	43	74
1	D	353/451 (78%)	341 (97%)	12 (3%)	37	69
1	E	353/451 (78%)	347 (98%)	6 (2%)	60	83
1	F	353/451 (78%)	343 (97%)	10 (3%)	43	74
1	G	353/451 (78%)	343 (97%)	10 (3%)	43	74
1	H	353/451 (78%)	341 (97%)	12 (3%)	37	69
All	All	2824/3608 (78%)	2745 (97%)	79 (3%)	43	74

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	A	245	LYS
1	A	255	LYS
1	A	317	ARG
1	A	361	PHE
1	A	412	ASP

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Mol	Chain	Res	Type
1	A	489	LEU
1	A	502	SER
1	A	523	SER
1	B	197	LYS
1	B	216	ARG
1	B	242	SER
1	B	257	SER
1	B	319	ASN
1	B	346	LYS
1	B	361	PHE
1	B	374	SER
1	B	412	ASP
1	B	496	MET
1	C	141	ASP
1	C	149	GLU
1	C	195	LEU
1	C	245	LYS
1	C	300	LEU
1	C	319	ASN
1	C	361	PHE
1	C	384	SER
1	C	446	ARG
1	C	507	LYS
1	D	169	ARG
1	D	197	LYS
1	D	229	SER
1	D	245	LYS
1	D	255	LYS
1	D	257	SER
1	D	361	PHE
1	D	382	ARG
1	D	502	SER
1	D	511	SER
1	D	523	SER
1	D	544	ARG
1	E	138	SER
1	E	164	LYS
1	E	319	ASN
1	E	361	PHE
1	E	412	ASP
1	E	507	LYS
1	G	138	SER

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Mol	Chain	Res	Type
1	G	153	LYS
1	G	181	MET
1	G	196	ASP
1	G	197	LYS
1	G	229	SER
1	G	361	PHE
1	G	374	SER
1	G	412	ASP
1	G	511	SER
1	F	138	SER
1	F	149	GLU
1	F	218	LYS
1	F	279	LYS
1	F	361	PHE
1	F	374	SER
1	F	384	SER
1	F	412	ASP
1	F	451	GLU
1	F	507	LYS
1	H	138	SER
1	H	152	GLU
1	H	197	LYS
1	H	216	ARG
1	H	242	SER
1	H	255	LYS
1	H	361	PHE
1	H	383	GLU
1	H	412	ASP
1	H	502	SER
1	H	534	ARG
1	H	544	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	347	GLN
1	D	252	GLN
1	E	360	GLN
1	F	471	GLN
1	H	319	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	QA4	C	601	-	27,35,35	2.46	8 (29%)	28,49,49	1.96	8 (28%)
2	QA4	E	602	-	27,35,35	2.23	8 (29%)	28,49,49	1.90	5 (17%)
2	QA4	A	601	-	27,35,35	2.31	8 (29%)	28,49,49	2.42	12 (42%)
2	QA4	E	601	1	27,35,35	3.31	10 (37%)	28,49,49	3.00	10 (35%)

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	QA4	C	601	-	-	4/16/38/38	0/5/5/5
2	QA4	E	602	-	-	4/16/38/38	0/5/5/5
2	QA4	A	601	-	-	5/16/38/38	0/5/5/5
2	QA4	E	601	1	-	8/16/38/38	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	QA4	C25-N24	9.34	1.56	1.35
2	E	601	QA4	C20-N03	9.23	1.46	1.32
2	C	601	QA4	C20-N03	7.65	1.44	1.32
2	E	602	QA4	C20-N03	7.26	1.43	1.32
2	A	601	QA4	C20-N03	7.03	1.43	1.32
2	E	601	QA4	C11-N12	5.16	1.45	1.36
2	E	601	QA4	O07-C08	4.79	1.42	1.36
2	C	601	QA4	O07-C08	4.53	1.42	1.36
2	E	601	QA4	C13-N12	4.10	1.44	1.35
2	A	601	QA4	C02-N03	-4.00	1.40	1.46
2	C	601	QA4	C23-N24	3.86	1.43	1.36
2	A	601	QA4	C11-N12	3.86	1.43	1.36
2	E	601	QA4	C04-N03	-3.84	1.40	1.46
2	E	601	QA4	C23-N24	3.78	1.43	1.36
2	A	601	QA4	C13-N12	3.77	1.44	1.35
2	C	601	QA4	C11-N12	3.75	1.43	1.36
2	C	601	QA4	C04-N03	-3.66	1.41	1.46
2	C	601	QA4	C25-N24	3.62	1.43	1.35
2	C	601	QA4	C13-N12	3.60	1.43	1.35
2	A	601	QA4	C23-N24	3.54	1.42	1.36
2	E	602	QA4	C11-N12	3.49	1.42	1.36
2	E	602	QA4	C13-N12	3.46	1.43	1.35
2	E	602	QA4	C04-N03	-3.37	1.41	1.46
2	A	601	QA4	C25-N24	3.27	1.42	1.35
2	E	602	QA4	C02-N03	-3.21	1.41	1.46
2	E	602	QA4	C23-N24	3.20	1.42	1.36
2	E	602	QA4	C25-N24	3.20	1.42	1.35
2	A	601	QA4	O07-C08	3.09	1.40	1.36
2	A	601	QA4	C04-N03	-3.06	1.41	1.46
2	C	601	QA4	C02-N03	-2.79	1.42	1.46
2	E	602	QA4	O07-C08	2.75	1.39	1.36
2	E	601	QA4	C26-C25	2.67	1.57	1.51
2	E	601	QA4	C02-N03	-2.62	1.42	1.46
2	E	601	QA4	C26-C27	-2.34	1.46	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	QA4	C14-C13-N12	6.75	123.76	114.50
2	E	601	QA4	C23-N24-C25	6.41	146.85	129.54
2	E	601	QA4	C04-C05-C06	5.95	116.86	110.32
2	E	601	QA4	O30-C25-C26	-5.59	113.31	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	QA4	C23-N24-C25	-5.38	115.01	129.54
2	A	601	QA4	C04-N03-C02	5.28	123.17	111.52
2	E	601	QA4	O30-C25-N24	5.19	133.10	123.63
2	C	601	QA4	C04-N03-C02	4.80	122.11	111.52
2	E	602	QA4	C04-N03-C02	4.66	121.81	111.52
2	C	601	QA4	C02-C01-C06	-4.60	105.26	110.32
2	A	601	QA4	C14-C13-N12	4.49	120.67	114.50
2	E	602	QA4	C23-N24-C25	-4.36	117.78	129.54
2	A	601	QA4	C26-C25-N24	4.16	120.20	114.50
2	E	602	QA4	C11-N12-C13	-3.88	119.05	129.54
2	E	601	QA4	C04-N03-C02	3.56	119.38	111.52
2	E	601	QA4	C05-C06-C01	-3.51	104.96	111.74
2	E	601	QA4	O18-C13-C14	-3.32	116.63	121.50
2	A	601	QA4	O07-C06-C01	-3.31	101.00	108.31
2	C	601	QA4	C04-C05-C06	3.19	113.83	110.32
2	E	602	QA4	C14-C13-N12	3.13	118.80	114.50
2	A	601	QA4	C11-N12-C13	-3.12	121.12	129.54
2	A	601	QA4	C05-C06-C01	-3.00	105.94	111.74
2	C	601	QA4	C14-C13-N12	2.93	118.52	114.50
2	E	601	QA4	C02-C01-C06	-2.77	107.27	110.32
2	C	601	QA4	C05-C06-C01	-2.69	106.54	111.74
2	A	601	QA4	C29-C27-C26	-2.59	113.42	120.01
2	C	601	QA4	C29-C27-C26	-2.50	113.65	120.01
2	A	601	QA4	O18-C13-C14	-2.47	117.87	121.50
2	E	602	QA4	C16-C15-C14	-2.28	114.22	120.01
2	A	601	QA4	O30-C25-N24	-2.23	119.57	123.63
2	A	601	QA4	C16-C15-C14	-2.22	114.38	120.01
2	E	601	QA4	O18-C13-N12	-2.20	119.61	123.63
2	A	601	QA4	C04-C05-C06	2.17	112.70	110.32
2	C	601	QA4	C11-N12-C13	-2.11	123.84	129.54
2	C	601	QA4	C27-C26-C25	2.02	117.46	112.87

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	QA4	S31-C20-N03-C02
2	C	601	QA4	S31-C20-N03-C04
2	C	601	QA4	C05-C06-O07-C08
2	E	602	QA4	N12-C13-C14-C15
2	E	602	QA4	O18-C13-C14-C15
2	A	601	QA4	N12-C13-C14-C15

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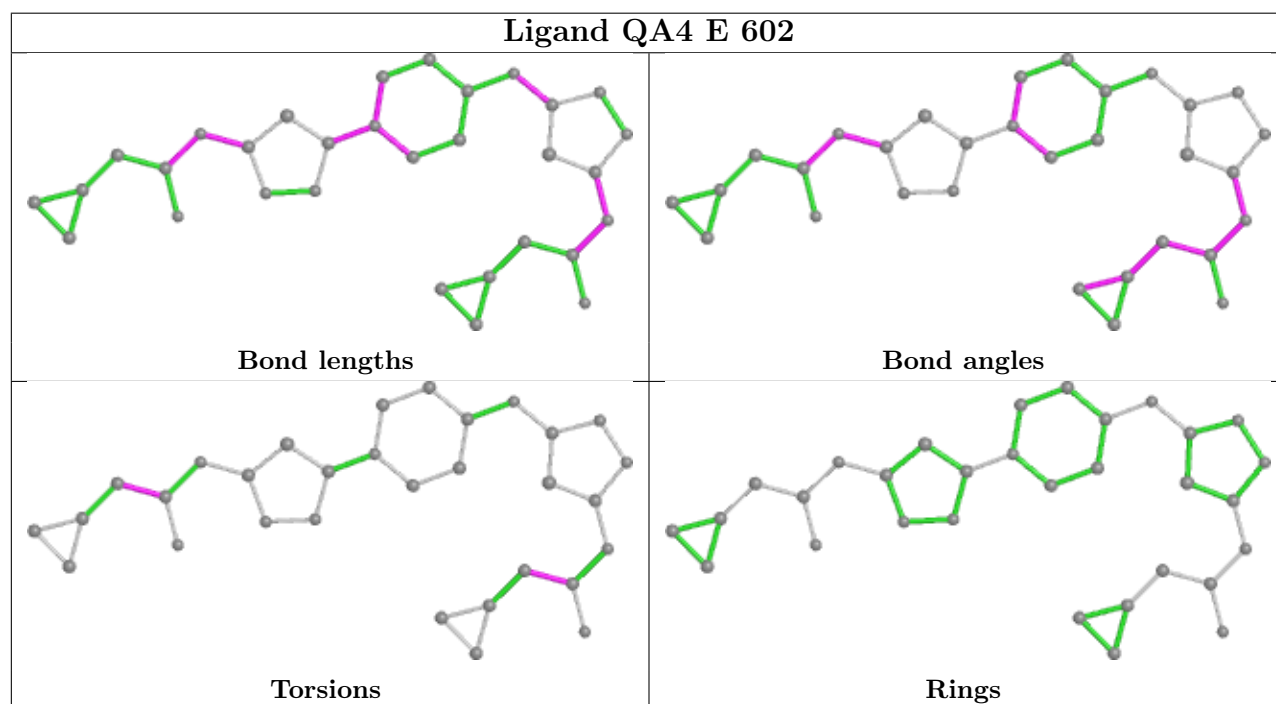
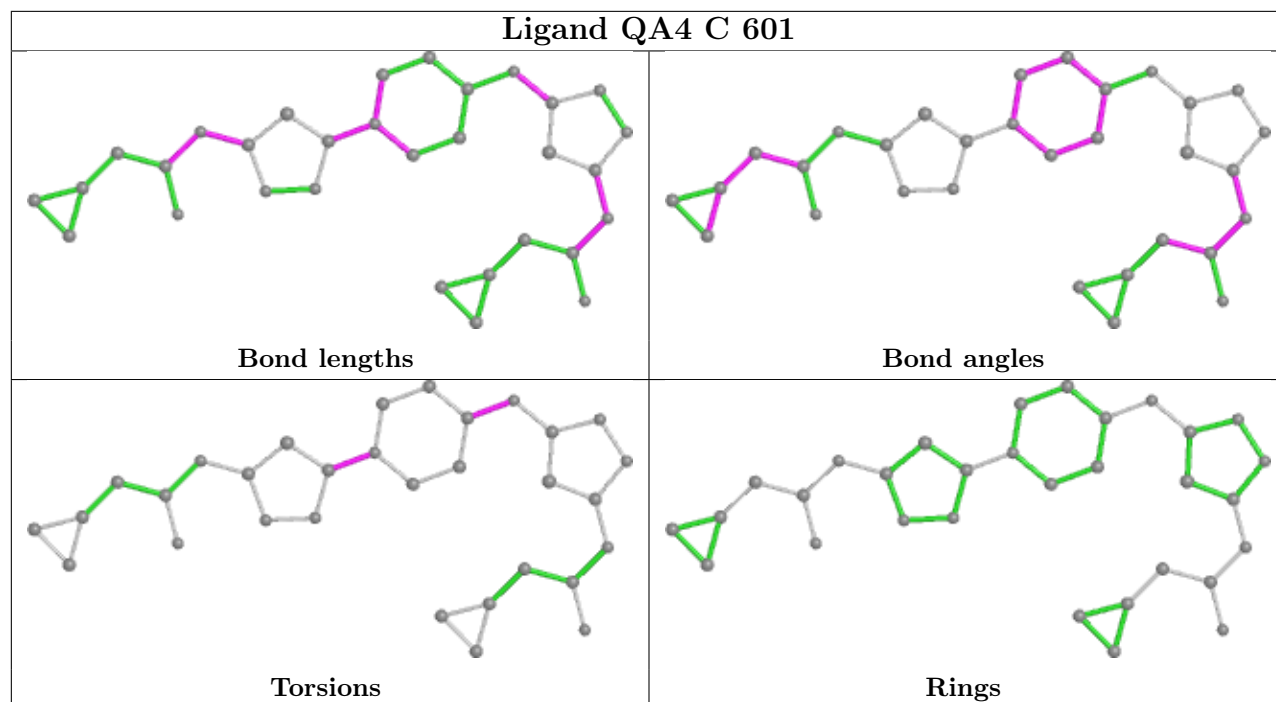
Mol	Chain	Res	Type	Atoms
2	A	601	QA4	O18-C13-C14-C15
2	A	601	QA4	N24-C25-C26-C27
2	A	601	QA4	O30-C25-C26-C27
2	E	601	QA4	S31-C20-N03-C02
2	E	601	QA4	S31-C20-N03-C04
2	E	601	QA4	N24-C25-C26-C27
2	E	601	QA4	O30-C25-C26-C27
2	E	601	QA4	C05-C06-O07-C08
2	E	601	QA4	N12-C13-C14-C15
2	E	602	QA4	O30-C25-C26-C27
2	E	601	QA4	O18-C13-C14-C15
2	C	601	QA4	C01-C06-O07-C08
2	E	602	QA4	N24-C25-C26-C27
2	E	601	QA4	O30-C25-N24-C23
2	A	601	QA4	C05-C06-O07-C08

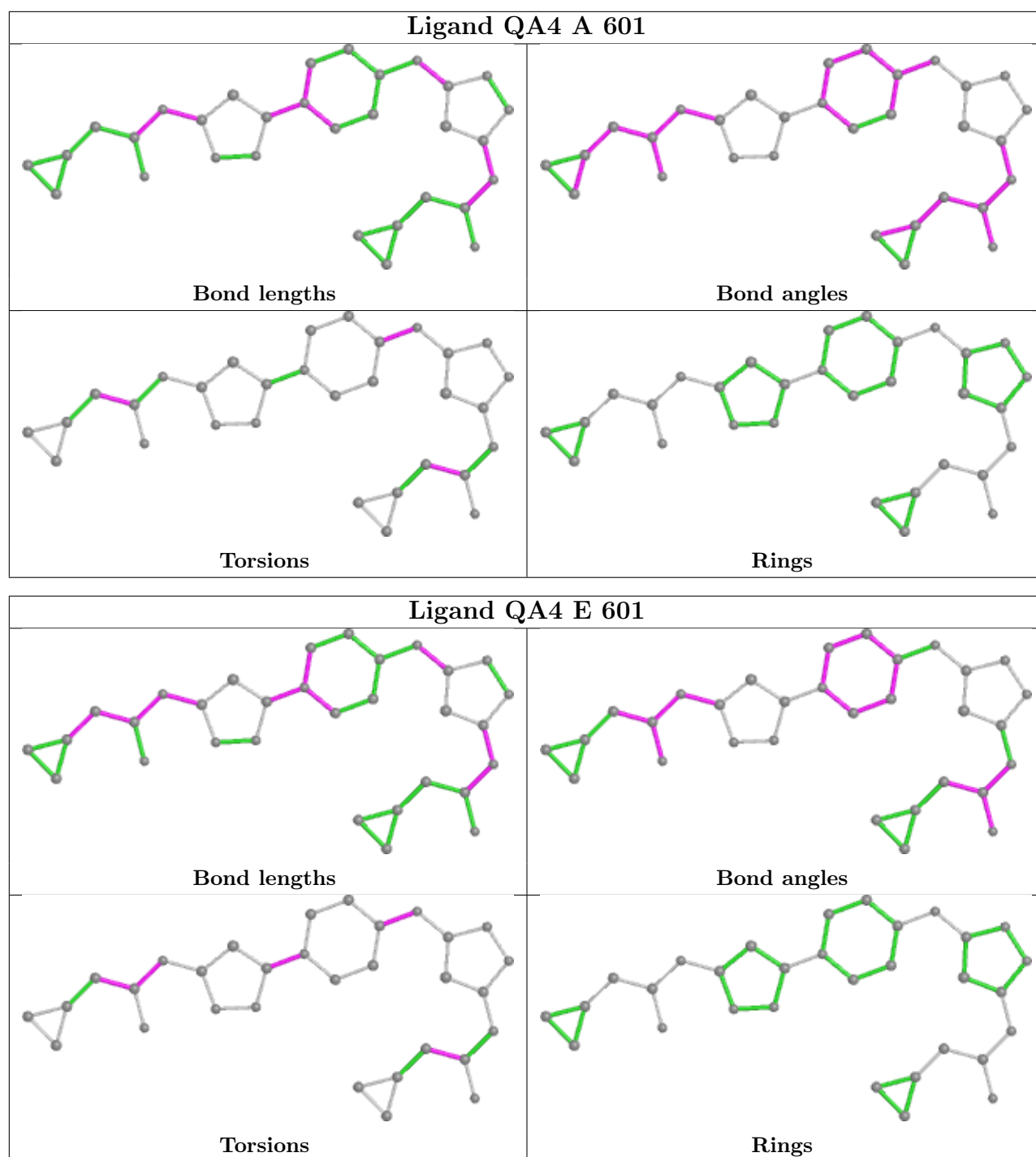
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	QA4	1	0
2	E	601	QA4	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	409/527 (77%)	-0.13	7 (1%) 70 53	25, 42, 100, 171	0
1	B	410/527 (77%)	-0.16	6 (1%) 73 57	27, 41, 91, 152	0
1	C	410/527 (77%)	-0.13	9 (2%) 62 45	27, 42, 96, 167	0
1	D	410/527 (77%)	-0.16	5 (1%) 79 63	27, 41, 95, 155	0
1	E	409/527 (77%)	-0.14	8 (1%) 65 48	26, 41, 88, 171	0
1	F	410/527 (77%)	-0.11	8 (1%) 65 48	28, 42, 101, 162	0
1	G	410/527 (77%)	-0.14	6 (1%) 73 57	28, 43, 95, 165	0
1	H	410/527 (77%)	-0.14	8 (1%) 65 48	25, 42, 97, 175	0
All	All	3278/4216 (77%)	-0.14	57 (1%) 70 53	25, 42, 97, 175	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	192	GLY	7.9
1	E	189	THR	7.7
1	C	192	GLY	7.2
1	A	191	ASP	7.1
1	A	192	GLY	6.5
1	F	317	ARG	6.4
1	C	318	PHE	6.1
1	A	318	PHE	5.8
1	H	318	PHE	5.5
1	F	192	GLY	5.2
1	E	188	THR	5.2
1	C	189	THR	5.0
1	E	318	PHE	4.9
1	F	191	ASP	4.9
1	F	318	PHE	4.5
1	B	318	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	191	ASP	4.3
1	G	318	PHE	4.1
1	E	317	ARG	3.6
1	C	150	GLY	3.6
1	D	318	PHE	3.5
1	A	189	THR	3.4
1	C	195	LEU	3.2
1	H	138	SER	3.2
1	H	191	ASP	3.1
1	H	152	GLU	3.1
1	B	190	SER	3.1
1	B	317	ARG	3.0
1	F	251	PRO	3.0
1	H	142	LEU	3.0
1	D	252	GLN	2.9
1	E	316	LEU	2.9
1	C	191	ASP	2.8
1	B	319	ASN	2.8
1	A	188	THR	2.8
1	F	195	LEU	2.7
1	C	317	ARG	2.7
1	G	317	ARG	2.7
1	C	142	LEU	2.6
1	G	348	GLY	2.6
1	A	258	PRO	2.5
1	D	198	ASP	2.5
1	B	144	PHE	2.4
1	C	145	TYR	2.4
1	G	546	GLY	2.4
1	A	152	GLU	2.3
1	E	148	ALA	2.3
1	H	144	PHE	2.3
1	H	317	ARG	2.3
1	D	138	SER	2.3
1	F	249	TYR	2.2
1	B	191	ASP	2.2
1	G	249	TYR	2.1
1	G	316	LEU	2.1
1	F	253	LEU	2.1
1	H	195	LEU	2.1
1	D	249	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

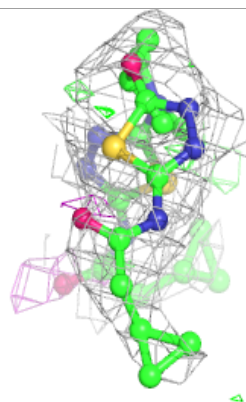
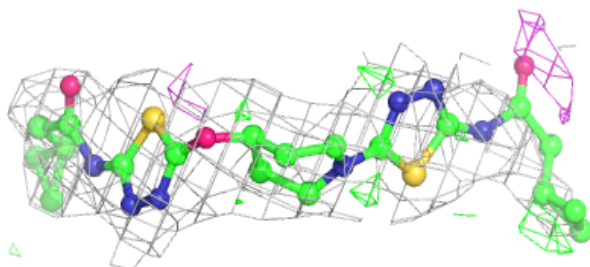
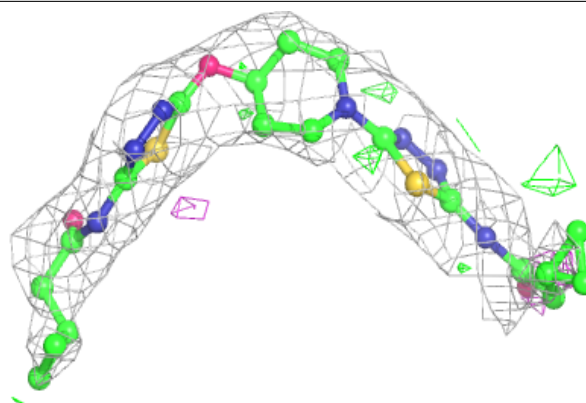
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	QA4	E	601	31/31	0.93	0.27	53,63,120,157	0
2	QA4	A	601	31/31	0.94	0.20	47,60,83,85	0
2	QA4	E	602	31/31	0.94	0.20	44,62,75,78	0
2	QA4	C	601	31/31	0.95	0.19	45,58,100,102	0

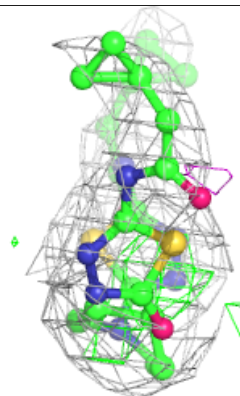
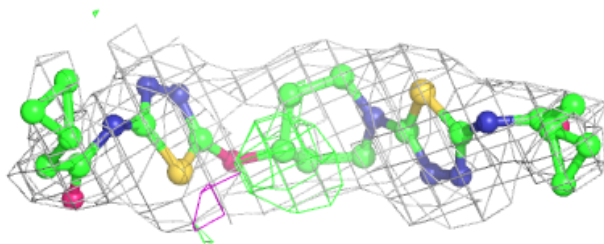
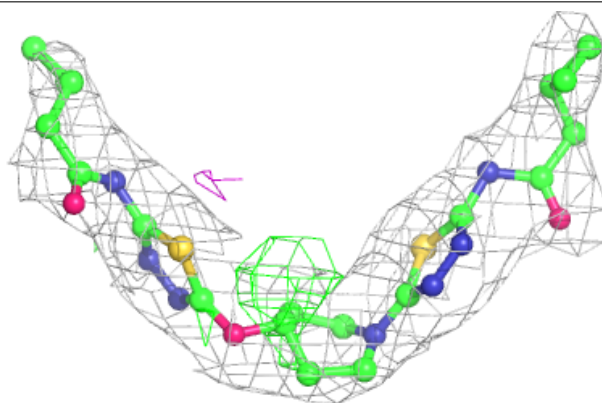
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QA4 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)

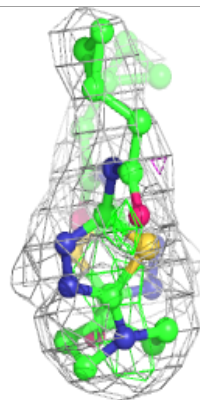
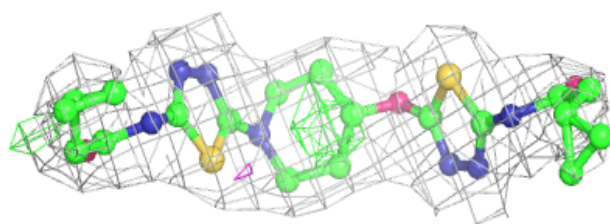
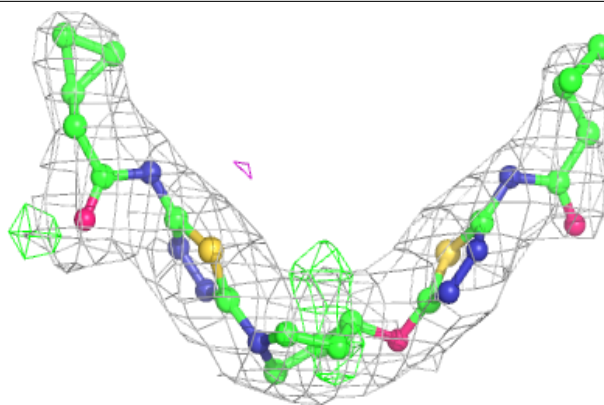
**Electron density around QA4 A 601:**

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

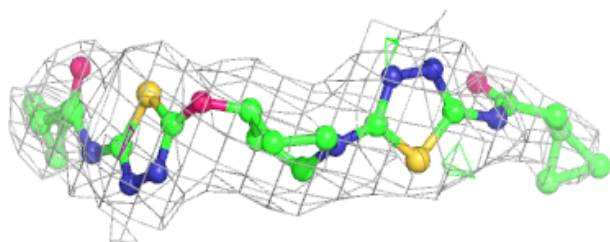
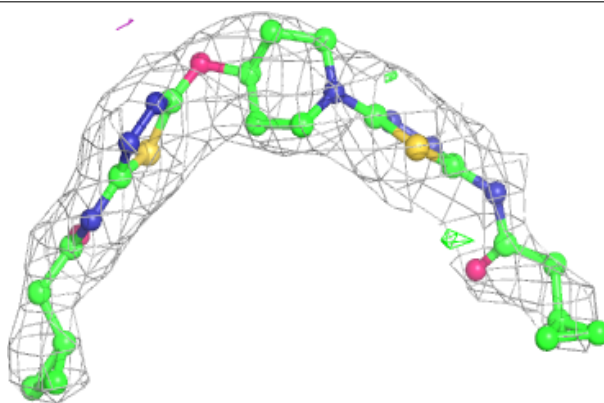


Electron density around QA4 E 602:

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

**Electron density around QA4 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.