



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 04:26 am BST

PDB ID : 1NJJ
Title : Crystal structure determination of T. brucei ornithine decarboxylase bound to D-ornithine and to G418
Authors : Jackson, L.K.; Goldsmith, E.J.; Phillips, M.A.
Deposited on : 2002-12-31
Resolution : 2.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

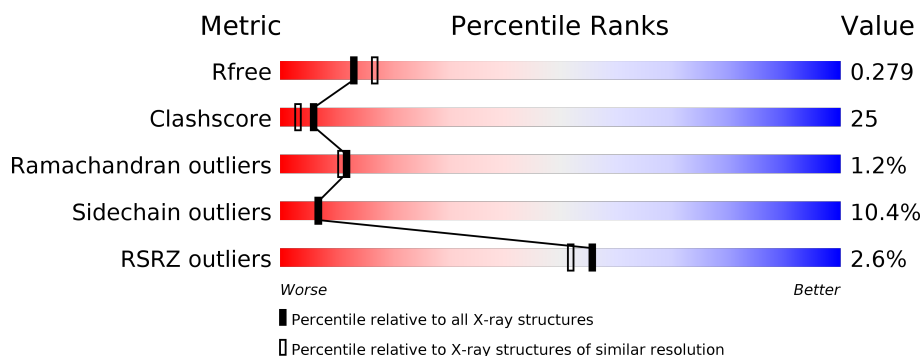
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	425	<div> <div>2%</div> <div> <div></div> <div>46%</div> <div>31%</div> <div>5%</div> <div>18%</div> </div> </div>
1	B	425	<div> <div>2%</div> <div> <div></div> <div>46%</div> <div>31%</div> <div>• •</div> <div>18%</div> </div> </div>
1	C	425	<div> <div>3%</div> <div> <div></div> <div>51%</div> <div>28%</div> <div>•</div> <div>17%</div> </div> </div>
1	D	425	<div> <div>2%</div> <div> <div></div> <div>48%</div> <div>31%</div> <div>• •</div> <div>17%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GET	A	601	X	-	-	-
2	GET	B	602	X	-	-	-
2	GET	C	603	X	-	-	-
3	ORX	C	604	-	X	-	-
3	ORX	D	426	X	-	-	-

2 Entry composition [i](#)

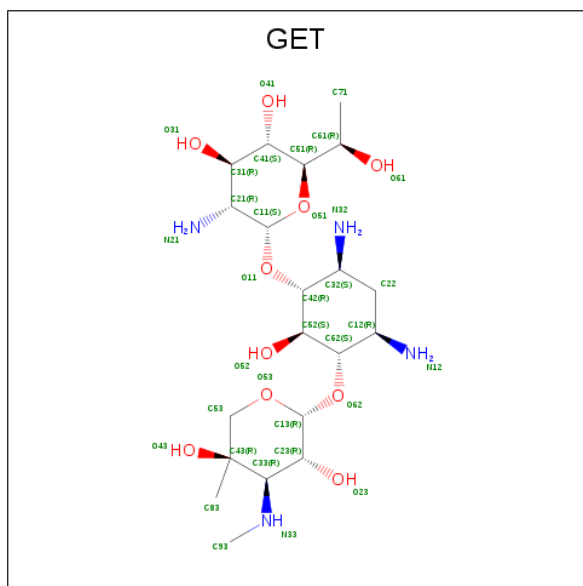
There are 4 unique types of molecules in this entry. The entry contains 11424 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ornithine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2734	1756	456	506	16			
1	B	349	Total	C	N	O	S	0	0	0
			2738	1760	457	505	16			
1	C	352	Total	C	N	O	S	0	0	0
			2770	1784	462	508	16			
1	D	354	Total	C	N	O	S	12	0	0
			2777	1784	464	513	16			

- Molecule 2 is GENETICIN (three-letter code: GET) (formula: $C_{20}H_{40}N_4O_{10}$).



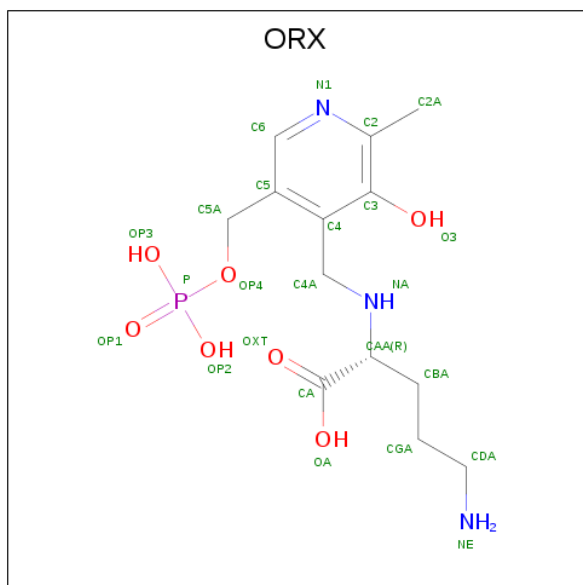
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	20	4	10		
2	B	1	Total	C	N	O	0	0
			34	20	4	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			34	20	4	10		

- Molecule 3 is N 2 -({3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL}METHYL)-D-ORNITHINE (three-letter code: ORX) (formula: C₁₃H₂₂N₃O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			24	13	3	7	1		
3	B	1	Total	C	N	O	P	0	0
			24	13	3	7	1		
3	C	1	Total	C	N	O	P	0	0
			24	13	3	7	1		
3	D	1	Total	C	N	O	P	0	0
			24	13	3	7	1		

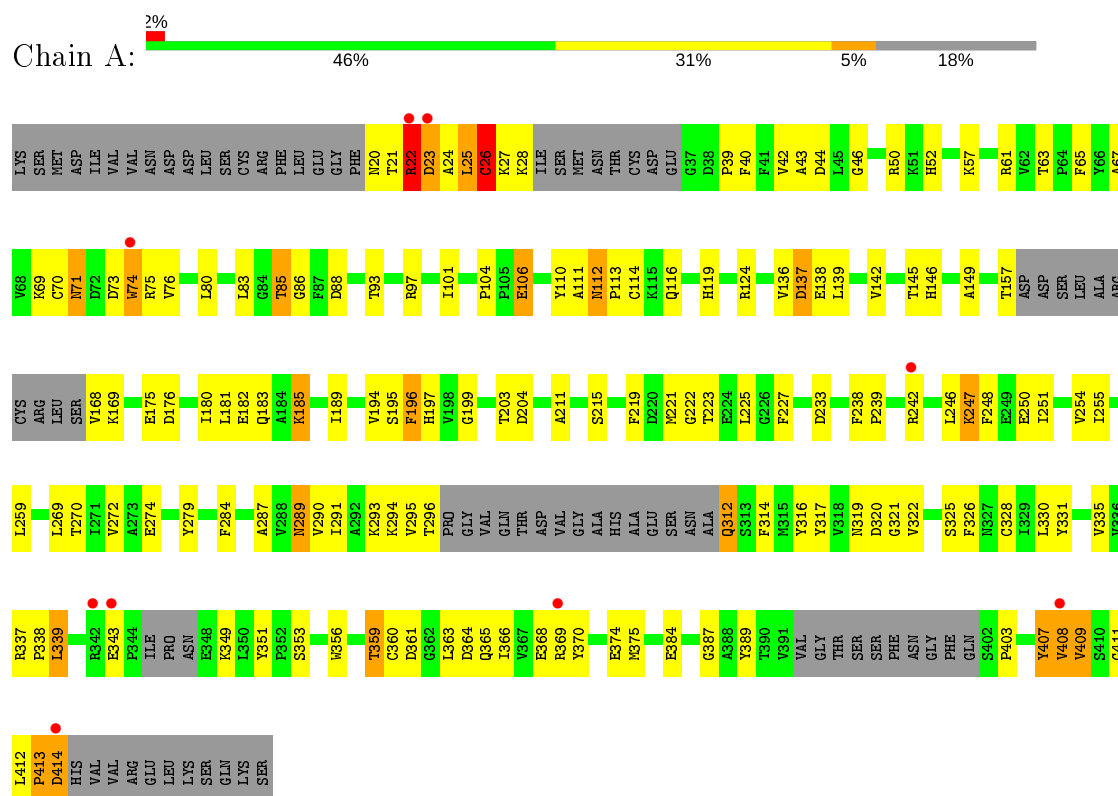
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	48	Total	O	0	0
			48	48		
4	C	59	Total	O	0	0
			59	59		
4	D	49	Total	O	0	0
			49	49		

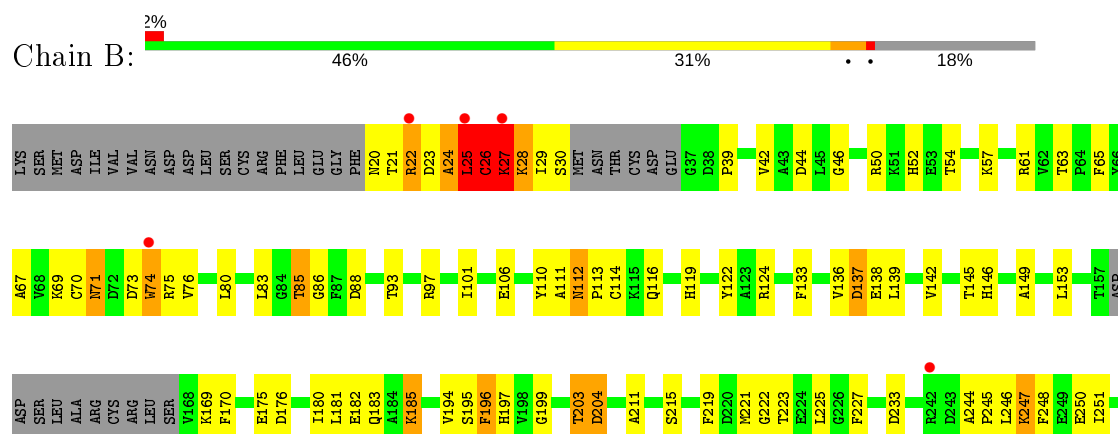
3 Residue-property plots

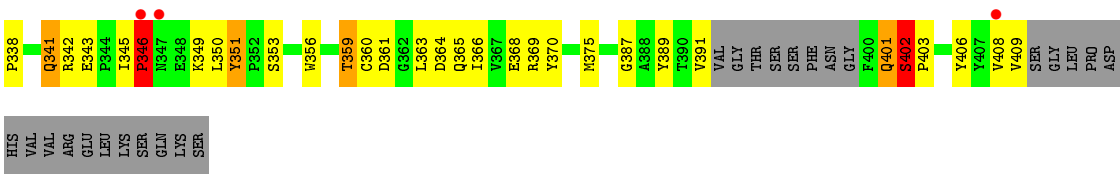
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: ornithine decarboxylase



• Molecule 1: ornithine decarboxylase





HIS
VAL
VAL
ARG
GLU
LEU
LYS
SER
GLN
LYS
SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.82Å 88.54Å 150.44Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	35.00 – 2.45 33.91 – 2.45	Depositor EDS
% Data completeness (in resolution range)	87.6 (35.00-2.45) 87.5 (33.91-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.45Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.260 , 0.283 0.259 , 0.279	Depositor DCC
R_{free} test set	6399 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 19.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.138 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11424	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.43	1/2797 (0.0%)	0.90	11/3790 (0.3%)
1	B	0.51	2/2802 (0.1%)	0.89	14/3799 (0.4%)
1	C	0.39	0/2834	0.76	5/3838 (0.1%)
1	D	0.43	0/2842	0.81	13/3853 (0.3%)
All	All	0.44	3/11275 (0.0%)	0.84	43/15280 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	204	ASP	CG-OD2	-5.89	1.11	1.25
1	A	204	ASP	CG-OD2	-5.51	1.12	1.25
1	B	27	LYS	CA-C	5.07	1.66	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ARG	NE-CZ-NH2	-16.88	111.86	120.30
1	A	61	ARG	NE-CZ-NH1	15.88	128.24	120.30
1	D	337	ARG	NE-CZ-NH2	-14.63	112.98	120.30
1	B	337	ARG	NE-CZ-NH2	-14.24	113.18	120.30
1	D	337	ARG	NE-CZ-NH1	14.16	127.38	120.30
1	C	337	ARG	NE-CZ-NH2	14.01	127.30	120.30
1	A	337	ARG	NE-CZ-NH1	-13.91	113.35	120.30
1	C	337	ARG	NE-CZ-NH1	-13.89	113.35	120.30
1	A	337	ARG	NE-CZ-NH2	13.76	127.18	120.30
1	B	337	ARG	NE-CZ-NH1	13.61	127.10	120.30
1	B	204	ASP	CB-CG-OD1	13.27	130.24	118.30
1	A	204	ASP	CB-CG-OD1	12.61	129.65	118.30
1	B	61	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	C	337	ARG	CD-NE-CZ	7.24	133.74	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ARG	CD-NE-CZ	7.23	133.73	123.60
1	A	137	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	B	137	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	B	337	ARG	CD-NE-CZ	7.22	133.70	123.60
1	D	337	ARG	CD-NE-CZ	7.17	133.64	123.60
1	A	337	ARG	CD-NE-CZ	7.16	133.63	123.60
1	B	25	LEU	CB-CA-C	-7.07	96.78	110.20
1	D	312	GLN	N-CA-C	-6.84	92.53	111.00
1	D	137	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	B	61	ARG	NE-CZ-NH2	6.55	123.57	120.30
1	D	391	VAL	N-CA-C	6.33	128.10	111.00
1	B	403	PRO	N-CA-C	-6.20	95.99	112.10
1	D	137	ASP	CB-CA-C	6.13	122.66	110.40
1	B	26	CYS	C-N-CA	6.02	136.76	121.70
1	D	137	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	24	ALA	CA-C-N	-5.90	104.23	117.20
1	A	24	ALA	N-CA-C	-5.88	95.13	111.00
1	D	402	SER	N-CA-C	-5.79	95.38	111.00
1	B	204	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	A	349	LYS	N-CA-C	-5.73	95.53	111.00
1	D	401	GLN	N-CA-C	5.71	126.41	111.00
1	D	20	ASN	N-CA-C	-5.71	95.60	111.00
1	B	24	ALA	C-N-CA	5.55	135.56	121.70
1	D	204	ASP	CB-CG-OD1	5.44	123.20	118.30
1	C	204	ASP	CB-CG-OD1	5.38	123.14	118.30
1	D	61	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	B	402	SER	N-CA-C	5.23	125.13	111.00
1	B	341	GLN	CA-C-N	-5.13	105.91	117.20
1	C	61	ARG	NE-CZ-NH1	-5.07	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2734	0	2701	144	0
1	B	2738	0	2712	162	0
1	C	2770	0	2742	132	0
1	D	2777	0	2745	139	0
2	A	34	0	40	5	0
2	B	34	0	40	13	0
2	C	34	0	40	10	0
3	A	24	0	19	2	0
3	B	24	0	18	3	0
3	C	24	0	19	1	0
3	D	24	0	19	2	0
4	A	51	0	0	8	0
4	B	48	0	0	2	0
4	C	59	0	0	3	0
4	D	49	0	0	4	0
All	All	11424	0	11095	555	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (555) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:HIS:ND1	1:A:149:ALA:HB2	1.63	1.13
1:C:146:HIS:ND1	1:C:149:ALA:HB2	1.63	1.12
1:B:146:HIS:ND1	1:B:149:ALA:HB2	1.63	1.11
1:D:146:HIS:ND1	1:D:149:ALA:HB2	1.64	1.10
1:C:124:ARG:HB2	1:C:146:HIS:HD2	1.26	1.00
1:A:124:ARG:HB2	1:A:146:HIS:HD2	1.26	1.00
1:B:124:ARG:HB2	1:B:146:HIS:HD2	1.26	1.00
1:B:24:ALA:HA	1:B:27:LYS:HD3	1.40	0.99
1:D:124:ARG:HB2	1:D:146:HIS:HD2	1.26	0.99
1:B:345:ILE:CG1	1:B:346:PRO:HD2	1.98	0.93
1:B:246:LEU:HD23	1:B:251:ILE:HD11	1.53	0.90
1:B:345:ILE:HG13	1:B:346:PRO:HD2	1.55	0.87
1:C:16:LEU:HD11	1:C:406:TYR:CD2	2.11	0.85
1:C:16:LEU:HD11	1:C:406:TYR:HD2	1.39	0.84
1:B:22:ARG:HB3	2:B:602:GET:H311	1.58	0.84
1:A:124:ARG:CB	1:A:146:HIS:HD2	1.91	0.83
1:D:124:ARG:CB	1:D:146:HIS:HD2	1.91	0.83
1:B:124:ARG:CB	1:B:146:HIS:HD2	1.91	0.83
1:B:345:ILE:HG13	1:B:348:GLU:HG3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ARG:CB	1:C:146:HIS:HD2	1.91	0.81
1:C:392:VAL:HG21	4:C:648:HOH:O	1.80	0.80
1:B:21:THR:O	1:B:25:LEU:HD12	1.81	0.79
1:C:22:ARG:HB3	2:C:603:GET:O41	1.83	0.79
1:B:222:GLY:O	1:B:227:PHE:HB2	1.83	0.78
1:B:25:LEU:O	1:B:29:ILE:HG13	1.84	0.78
1:A:222:GLY:O	1:A:227:PHE:HB2	1.84	0.77
1:A:316:TYR:CE2	1:A:375:MET:HB2	2.19	0.77
1:C:222:GLY:O	1:C:227:PHE:HB2	1.85	0.77
1:D:222:GLY:O	1:D:227:PHE:HB2	1.85	0.77
1:C:22:ARG:HG3	1:C:23:ASP:N	2.00	0.76
1:D:310:ASN:ND2	1:D:311:ALA:H	1.83	0.76
1:D:44:ASP:HA	1:D:408:VAL:HG13	1.67	0.75
1:B:341:GLN:HG2	1:B:380:TRP:HB2	1.69	0.74
1:D:39:PRO:HD3	1:D:319:ASN:ND2	2.02	0.73
1:B:39:PRO:HD3	1:B:319:ASN:ND2	2.03	0.73
1:D:20:ASN:HD21	1:D:22:ARG:HD2	1.54	0.73
1:B:71:ASN:HD22	1:B:73:ASP:H	1.37	0.73
1:C:71:ASN:HD22	1:C:73:ASP:H	1.36	0.73
1:D:124:ARG:HB2	1:D:146:HIS:CD2	2.19	0.72
1:B:21:THR:O	1:B:25:LEU:CD1	2.37	0.72
1:B:345:ILE:CG1	1:B:348:GLU:HG3	2.19	0.72
1:B:116:GLN:HB3	1:B:119:HIS:CD2	2.24	0.72
1:A:116:GLN:HB3	1:A:119:HIS:CD2	2.25	0.72
1:D:116:GLN:HB3	1:D:119:HIS:CD2	2.25	0.72
1:D:71:ASN:HD22	1:D:73:ASP:H	1.36	0.71
1:D:28:LYS:HE2	1:D:406:TYR:CZ	2.26	0.71
1:A:39:PRO:HD3	1:A:319:ASN:ND2	2.04	0.71
1:A:71:ASN:HD22	1:A:73:ASP:H	1.36	0.71
1:C:359:THR:CG2	1:C:361:ASP:H	2.04	0.71
1:A:359:THR:CG2	1:A:361:ASP:H	2.03	0.71
1:D:359:THR:CG2	1:D:361:ASP:H	2.04	0.71
1:C:116:GLN:HB3	1:C:119:HIS:CD2	2.25	0.70
1:D:310:ASN:ND2	1:D:311:ALA:N	2.39	0.70
1:C:39:PRO:HD3	1:C:319:ASN:ND2	2.07	0.70
1:B:295:VAL:HG12	1:B:296:THR:H	1.57	0.70
1:B:359:THR:CG2	1:B:361:ASP:H	2.05	0.70
1:C:16:LEU:HD13	1:C:406:TYR:HB3	1.73	0.70
1:B:124:ARG:HB2	1:B:146:HIS:CD2	2.18	0.69
1:B:29:ILE:HD12	1:B:341:GLN:OE1	1.92	0.69
1:B:345:ILE:CB	1:B:346:PRO:CD	2.70	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:O	1:A:27:LYS:N	2.26	0.69
1:C:69:LYS:HE2	4:C:657:HOH:O	1.93	0.69
1:C:359:THR:HG23	1:C:361:ASP:H	1.57	0.69
1:B:312:GLN:HE21	1:B:312:GLN:HA	1.57	0.69
1:B:345:ILE:HB	1:B:346:PRO:CD	2.23	0.69
1:A:359:THR:HG23	1:A:361:ASP:H	1.58	0.68
1:C:124:ARG:HB2	1:C:146:HIS:CD2	2.19	0.68
1:B:52:HIS:CD2	1:B:83:LEU:HB3	2.29	0.68
1:A:21:THR:HG23	1:A:42:VAL:HG11	1.75	0.68
1:A:124:ARG:CB	1:A:146:HIS:CD2	2.77	0.68
1:C:52:HIS:CD2	1:C:83:LEU:HB3	2.28	0.68
1:A:331:TYR:CE2	1:B:330:LEU:HD12	2.29	0.67
1:B:50:ARG:HG3	1:B:50:ARG:HH11	1.60	0.67
1:B:70:CYS:HA	1:B:389:TYR:CE2	2.28	0.67
1:D:310:ASN:HB2	1:D:349:LYS:HE2	1.76	0.67
1:D:52:HIS:CD2	1:D:83:LEU:HB3	2.29	0.67
1:A:70:CYS:HA	1:A:389:TYR:CE2	2.29	0.67
1:C:70:CYS:HA	1:C:389:TYR:CE2	2.28	0.67
1:B:359:THR:HG23	1:B:361:ASP:H	1.59	0.67
1:A:195:SER:HB2	1:A:233:ASP:HB3	1.76	0.67
1:C:22:ARG:HG3	1:C:23:ASP:H	1.59	0.67
1:C:80:LEU:HB3	1:C:85:THR:HG21	1.77	0.67
1:D:359:THR:HG23	1:D:361:ASP:H	1.58	0.67
1:A:52:HIS:CD2	1:A:83:LEU:HB3	2.28	0.67
1:C:50:ARG:HH11	1:C:50:ARG:HG3	1.60	0.67
1:D:124:ARG:CB	1:D:146:HIS:CD2	2.77	0.67
1:C:124:ARG:CB	1:C:146:HIS:CD2	2.77	0.66
1:C:331:TYR:CE2	1:D:330:LEU:HD12	2.30	0.66
1:D:70:CYS:HA	1:D:389:TYR:CE2	2.30	0.66
1:C:195:SER:HB2	1:C:233:ASP:HB3	1.78	0.66
1:A:50:ARG:HH11	1:A:50:ARG:HG3	1.61	0.66
1:D:50:ARG:HG3	1:D:50:ARG:HH11	1.60	0.66
1:A:312:GLN:HE21	1:A:312:GLN:HA	1.61	0.65
1:A:80:LEU:HB3	1:A:85:THR:HG21	1.78	0.65
1:B:195:SER:HB2	1:B:233:ASP:HB3	1.76	0.65
1:C:16:LEU:CD1	1:C:406:TYR:HB3	2.27	0.65
1:A:124:ARG:HB2	1:A:146:HIS:CD2	2.19	0.65
1:B:71:ASN:ND2	1:B:73:ASP:H	1.95	0.65
1:B:124:ARG:CB	1:B:146:HIS:CD2	2.76	0.64
1:C:289:ASN:HD22	1:C:290:VAL:N	1.95	0.64
1:D:195:SER:HB2	1:D:233:ASP:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:ASN:ND2	1:D:73:ASP:H	1.94	0.64
1:D:289:ASN:HD22	1:D:290:VAL:N	1.96	0.64
1:D:310:ASN:CG	1:D:311:ALA:H	2.00	0.64
1:B:203:THR:O	1:B:246:LEU:HD13	1.97	0.64
1:D:80:LEU:HB3	1:D:85:THR:HG21	1.79	0.64
1:C:71:ASN:ND2	1:C:73:ASP:H	1.96	0.64
1:A:339:LEU:HD11	2:A:601:GET:H421	1.79	0.63
1:B:80:LEU:HB3	1:B:85:THR:HG21	1.79	0.63
1:A:25:LEU:HD21	1:A:287:ALA:HB2	1.79	0.63
1:A:293:LYS:HD3	1:A:314:PHE:CD2	2.33	0.63
1:C:157:THR:HG21	1:C:197:HIS:C	2.18	0.63
1:B:295:VAL:HG12	1:B:296:THR:N	2.14	0.62
1:D:242:ARG:HH11	1:D:242:ARG:HG2	1.64	0.62
1:A:71:ASN:ND2	1:A:73:ASP:H	1.96	0.62
1:A:168:VAL:HG13	1:A:169:LYS:N	2.15	0.61
1:A:23:ASP:HB2	4:A:653:HOH:O	2.00	0.61
1:B:289:ASN:HD22	1:B:290:VAL:N	1.97	0.61
1:C:289:ASN:HD22	1:C:289:ASN:C	2.03	0.61
1:A:289:ASN:HD22	1:A:290:VAL:N	1.98	0.61
1:B:345:ILE:HG13	1:B:346:PRO:CD	2.29	0.61
1:C:293:LYS:HE2	1:C:314:PHE:CD2	2.35	0.61
1:B:345:ILE:CB	1:B:346:PRO:HD2	2.30	0.61
1:C:284:PHE:HB2	1:C:387:GLY:CA	2.30	0.61
1:A:22:ARG:HB2	2:A:601:GET:O41	2.01	0.61
1:A:136:VAL:O	1:A:139:LEU:HB2	2.01	0.61
1:A:289:ASN:HD22	1:A:289:ASN:C	2.04	0.61
1:B:341:GLN:C	2:B:602:GET:H711	2.21	0.61
1:D:289:ASN:C	1:D:289:ASN:HD22	2.03	0.60
1:B:136:VAL:O	1:B:139:LEU:HB2	2.01	0.60
1:B:195:SER:CB	1:B:233:ASP:HB3	2.31	0.60
1:B:284:PHE:HB2	1:B:387:GLY:CA	2.31	0.60
2:A:601:GET:H21	2:A:601:GET:O52	2.00	0.60
1:B:21:THR:C	1:B:23:ASP:H	2.03	0.60
1:B:338:PRO:HG2	1:B:370:TYR:CD2	2.36	0.60
1:A:195:SER:CB	1:A:233:ASP:HB3	2.31	0.60
1:D:284:PHE:HB2	1:D:387:GLY:CA	2.32	0.60
1:A:284:PHE:HB2	1:A:387:GLY:CA	2.31	0.60
1:B:345:ILE:CG1	1:B:346:PRO:CD	2.79	0.60
1:A:338:PRO:HG2	1:A:370:TYR:CD2	2.36	0.60
1:A:361:ASP:OD1	1:A:363:LEU:HB3	2.02	0.60
1:B:246:LEU:HD23	1:B:251:ILE:CD1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ASN:C	1:B:289:ASN:HD22	2.05	0.60
1:C:237:GLY:HA2	3:C:604:ORX:OP1	2.02	0.60
1:C:215:SER:O	1:C:219:PHE:HB2	2.02	0.59
1:C:338:PRO:HG2	1:C:370:TYR:CD2	2.37	0.59
1:C:361:ASP:OD1	1:C:363:LEU:HB3	2.02	0.59
1:D:176:ASP:O	1:D:180:ILE:HG13	2.03	0.59
1:D:409:VAL:HG22	1:D:409:VAL:O	2.02	0.59
1:A:21:THR:O	1:A:23:ASP:N	2.35	0.59
1:A:21:THR:C	1:A:23:ASP:H	2.06	0.59
1:D:293:LYS:HG2	1:D:294:LYS:H	1.67	0.59
1:C:195:SER:CB	1:C:233:ASP:HB3	2.32	0.59
1:C:22:ARG:HB3	2:C:603:GET:C41	2.32	0.59
1:A:409:VAL:O	1:A:409:VAL:HG23	2.01	0.59
1:B:345:ILE:HB	1:B:346:PRO:HD3	1.84	0.59
1:D:215:SER:O	1:D:219:PHE:HB2	2.03	0.59
1:D:361:ASP:OD1	1:D:363:LEU:HB3	2.02	0.59
1:D:20:ASN:ND2	1:D:22:ARG:HD2	2.17	0.59
1:A:359:THR:HB	1:A:364:ASP:OD2	2.03	0.59
1:D:338:PRO:HG2	1:D:370:TYR:CD2	2.38	0.59
1:D:195:SER:CB	1:D:233:ASP:HB3	2.33	0.58
1:B:20:ASN:ND2	1:B:22:ARG:HG3	2.18	0.58
1:B:21:THR:C	1:B:23:ASP:N	2.53	0.58
1:D:185:LYS:HD3	4:D:451:HOH:O	2.02	0.58
1:B:359:THR:HB	1:B:364:ASP:OD2	2.03	0.58
1:D:359:THR:HB	1:D:364:ASP:OD2	2.03	0.58
1:B:361:ASP:OD1	1:B:363:LEU:HB3	2.03	0.58
1:D:316:TYR:CE2	1:D:375:MET:HB2	2.39	0.58
1:B:138:GLU:O	1:B:142:VAL:HG23	2.04	0.58
1:D:293:LYS:HG2	1:D:294:LYS:N	2.18	0.58
1:B:215:SER:O	1:B:219:PHE:HB2	2.04	0.58
1:B:25:LEU:CD2	1:B:382:LEU:HD21	2.34	0.58
1:B:345:ILE:HG12	1:B:348:GLU:OE2	2.04	0.58
1:A:197:HIS:HE1	1:A:199:GLY:HA2	1.69	0.58
1:A:409:VAL:O	1:A:409:VAL:CG2	2.51	0.58
1:B:384:GLU:OE1	2:B:602:GET:H131	2.03	0.58
1:D:409:VAL:CG2	1:D:409:VAL:O	2.52	0.58
1:C:16:LEU:HD12	1:C:16:LEU:N	2.19	0.57
1:C:359:THR:HB	1:C:364:ASP:OD2	2.04	0.57
1:D:20:ASN:HD21	1:D:22:ARG:CD	2.17	0.57
1:A:215:SER:O	1:A:219:PHE:HB2	2.04	0.57
1:D:312:GLN:O	1:D:351:TYR:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ARG:NH1	1:B:50:ARG:HG3	2.20	0.57
1:C:197:HIS:HE1	1:C:199:GLY:HA2	1.70	0.57
1:C:293:LYS:HE2	1:C:314:PHE:CE2	2.40	0.57
1:A:124:ARG:HG3	1:A:146:HIS:CD2	2.40	0.57
1:D:97:ARG:HG3	1:D:97:ARG:HH11	1.70	0.56
1:A:328:CYS:HA	4:A:651:HOH:O	2.03	0.56
1:A:25:LEU:HD23	1:A:40:PHE:CZ	2.40	0.56
1:C:176:ASP:O	1:C:180:ILE:HG13	2.05	0.56
1:C:360:CYS:HA	1:D:170:PHE:HE1	1.71	0.56
1:B:44:ASP:HA	1:B:408:VAL:HG22	1.88	0.56
1:B:124:ARG:HG3	1:B:146:HIS:CD2	2.40	0.56
1:C:384:GLU:OE2	2:C:603:GET:H21	2.06	0.56
1:B:339:LEU:HD21	2:B:602:GET:H421	1.86	0.56
1:B:176:ASP:O	1:B:180:ILE:HG13	2.06	0.56
1:B:197:HIS:HE1	1:B:199:GLY:HA2	1.71	0.56
1:D:124:ARG:HG3	1:D:146:HIS:CD2	2.40	0.56
1:C:124:ARG:HG3	1:C:146:HIS:CD2	2.41	0.56
1:A:22:ARG:HG2	4:A:653:HOH:O	2.06	0.55
1:B:22:ARG:CB	2:B:602:GET:H311	2.34	0.55
1:A:138:GLU:O	1:A:142:VAL:HG23	2.07	0.55
1:A:168:VAL:HG13	1:A:169:LYS:H	1.72	0.55
1:C:88:ASP:OD1	1:C:111:ALA:HB3	2.07	0.55
1:D:88:ASP:OD1	1:D:111:ALA:HB3	2.06	0.55
1:D:138:GLU:O	1:D:142:VAL:HG23	2.05	0.55
1:B:312:GLN:HA	1:B:312:GLN:NE2	2.21	0.55
1:A:176:ASP:O	1:A:180:ILE:HG13	2.07	0.55
1:A:197:HIS:CE1	1:A:199:GLY:HA2	2.42	0.55
1:B:341:GLN:HA	2:B:602:GET:C71	2.37	0.55
1:B:341:GLN:HA	2:B:602:GET:H711	1.89	0.55
1:C:331:TYR:HE2	1:D:330:LEU:HD12	1.72	0.55
1:C:26:CYS:O	1:C:28:LYS:N	2.39	0.54
1:A:50:ARG:HG3	1:A:50:ARG:NH1	2.22	0.54
1:A:114:CYS:HB3	1:B:292:ALA:CB	2.37	0.54
1:C:136:VAL:O	1:C:139:LEU:HB2	2.08	0.54
1:C:348:GLU:O	1:C:348:GLU:HG2	2.07	0.54
1:D:197:HIS:HE1	1:D:199:GLY:HA2	1.71	0.54
1:C:330:LEU:HD12	1:D:331:TYR:CE2	2.42	0.54
1:B:69:LYS:HE2	4:B:620:HOH:O	2.06	0.54
1:B:97:ARG:HG3	1:B:97:ARG:HH11	1.72	0.54
1:C:50:ARG:HG3	1:C:50:ARG:NH1	2.21	0.54
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ARG:CG	1:A:22:ARG:O	2.55	0.54
1:A:25:LEU:HD23	1:A:40:PHE:HZ	1.72	0.54
1:C:67:ALA:HB1	1:C:69:LYS:HE3	1.90	0.54
1:D:136:VAL:O	1:D:139:LEU:HB2	2.07	0.54
1:B:345:ILE:CD1	1:B:346:PRO:HD2	2.37	0.53
1:C:138:GLU:O	1:C:142:VAL:HG23	2.08	0.53
1:B:71:ASN:HD22	1:B:71:ASN:C	2.10	0.53
1:D:242:ARG:NH1	1:D:242:ARG:HG2	2.23	0.53
1:C:197:HIS:CE1	1:C:199:GLY:HA2	2.43	0.53
1:D:71:ASN:HD22	1:D:71:ASN:C	2.12	0.53
1:C:196:PHE:C	1:C:196:PHE:CD1	2.81	0.53
1:D:50:ARG:HG3	1:D:50:ARG:NH1	2.20	0.53
1:A:331:TYR:HE2	1:B:330:LEU:HD12	1.72	0.53
1:B:67:ALA:HB1	1:B:69:LYS:HE3	1.91	0.53
1:B:88:ASP:OD1	1:B:111:ALA:HB3	2.09	0.53
1:A:293:LYS:HG2	1:A:294:LYS:N	2.24	0.53
1:C:255:ILE:O	1:C:259:LEU:HB2	2.09	0.53
1:D:67:ALA:HB1	1:D:69:LYS:HE3	1.91	0.53
1:A:360:CYS:HA	1:B:170:PHE:HE1	1.73	0.53
1:B:133:PHE:CE1	1:B:153:LEU:HD13	2.44	0.52
1:B:197:HIS:CE1	1:B:199:GLY:HA2	2.44	0.52
1:B:316:TYR:CE2	1:B:375:MET:HB2	2.44	0.52
1:B:75:ARG:HD2	1:B:75:ARG:N	2.23	0.52
1:A:196:PHE:CD1	1:A:196:PHE:C	2.82	0.52
1:C:97:ARG:HG3	1:C:97:ARG:HH11	1.72	0.52
1:B:341:GLN:CA	2:B:602:GET:H711	2.40	0.52
1:B:70:CYS:HA	1:B:389:TYR:CD2	2.45	0.52
1:C:22:ARG:HA	1:C:25:LEU:HB2	1.92	0.52
1:D:196:PHE:CD1	1:D:196:PHE:C	2.82	0.52
1:A:75:ARG:N	1:A:75:ARG:HD2	2.24	0.52
1:D:197:HIS:CE1	1:D:199:GLY:HA2	2.44	0.52
1:A:338:PRO:HG2	1:A:370:TYR:HD2	1.74	0.52
1:C:71:ASN:HD22	1:C:71:ASN:C	2.13	0.52
1:C:353:SER:O	1:C:369:ARG:HA	2.10	0.52
1:B:196:PHE:C	1:B:196:PHE:CD1	2.82	0.52
1:A:330:LEU:HD12	1:B:331:TYR:CE2	2.45	0.52
1:D:353:SER:O	1:D:369:ARG:HA	2.10	0.52
1:C:136:VAL:HG23	4:C:624:HOH:O	2.10	0.51
1:C:75:ARG:HD2	1:C:75:ARG:N	2.24	0.51
1:A:181:LEU:HD12	1:A:221:MET:HE3	1.92	0.51
1:B:338:PRO:HG2	1:B:370:TYR:HD2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:THR:HG23	1:A:42:VAL:CG1	2.40	0.51
1:D:75:ARG:N	1:D:75:ARG:HD2	2.24	0.51
1:A:44:ASP:HA	1:A:408:VAL:O	2.11	0.51
1:A:71:ASN:C	1:A:71:ASN:HD22	2.13	0.51
1:C:22:ARG:NH1	2:C:603:GET:H511	2.25	0.51
1:C:320:ASP:OD1	1:C:403:PRO:HG2	2.11	0.51
1:A:70:CYS:HA	1:A:389:TYR:CD2	2.45	0.51
1:B:345:ILE:CG1	1:B:348:GLU:CG	2.89	0.51
1:C:70:CYS:HA	1:C:389:TYR:CD2	2.44	0.51
1:A:73:ASP:HB3	1:A:76:VAL:CG2	2.41	0.51
1:D:338:PRO:HG2	1:D:370:TYR:HD2	1.76	0.51
1:A:365:GLN:HE21	1:A:368:GLU:HA	1.75	0.51
1:C:243:ASP:OD1	2:C:603:GET:H832	2.11	0.51
1:D:69:LYS:HE2	4:D:454:HOH:O	2.11	0.51
1:B:345:ILE:HG12	1:B:348:GLU:CD	2.31	0.50
1:B:365:GLN:HE21	1:B:368:GLU:HA	1.77	0.50
1:D:21:THR:HG21	1:D:44:ASP:HB2	1.93	0.50
1:A:88:ASP:OD1	1:A:111:ALA:HB3	2.11	0.50
1:A:169:LYS:HD2	1:B:356:TRP:CE3	2.46	0.50
1:C:221:MET:O	1:C:225:LEU:HD23	2.11	0.50
1:C:338:PRO:HG2	1:C:370:TYR:HD2	1.76	0.50
1:D:183:GLN:HA	1:D:183:GLN:HE21	1.77	0.50
1:D:255:ILE:O	1:D:259:LEU:HB2	2.11	0.50
1:A:255:ILE:O	1:A:259:LEU:HB2	2.11	0.50
1:A:67:ALA:HB1	1:A:69:LYS:HE3	1.93	0.50
1:B:23:ASP:O	1:B:26:CYS:C	2.49	0.50
1:C:65:PHE:HA	1:C:86:GLY:O	2.12	0.50
1:B:44:ASP:HA	1:B:408:VAL:CG2	2.41	0.50
1:D:274:GLU:O	3:D:426:ORX:H6	2.11	0.50
1:B:25:LEU:O	1:B:29:ILE:CG1	2.58	0.50
1:C:196:PHE:CD2	1:C:211:ALA:HB1	2.47	0.50
1:C:73:ASP:HB3	1:C:76:VAL:CG2	2.42	0.50
1:A:221:MET:O	1:A:225:LEU:HD23	2.11	0.49
1:A:25:LEU:O	1:A:28:LYS:N	2.45	0.49
1:D:221:MET:O	1:D:225:LEU:HD23	2.11	0.49
1:A:196:PHE:CD2	1:A:211:ALA:HB1	2.47	0.49
1:B:353:SER:O	1:B:369:ARG:HA	2.12	0.49
1:D:181:LEU:HD12	1:D:221:MET:HE3	1.94	0.49
1:B:124:ARG:CG	1:B:146:HIS:CD2	2.95	0.49
1:B:255:ILE:O	1:B:259:LEU:HB2	2.12	0.49
1:A:124:ARG:CG	1:A:146:HIS:CD2	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ALA:O	1:A:407:TYR:HA	2.12	0.49
1:B:65:PHE:HA	1:B:86:GLY:O	2.12	0.49
1:D:124:ARG:CG	1:D:146:HIS:CD2	2.96	0.49
1:A:293:LYS:HD3	1:A:314:PHE:HD2	1.75	0.49
1:A:65:PHE:HA	1:A:86:GLY:O	2.13	0.49
1:B:221:MET:O	1:B:225:LEU:HD23	2.12	0.49
1:B:54:THR:HG23	4:B:638:HOH:O	2.11	0.49
1:D:196:PHE:C	1:D:196:PHE:HD1	2.16	0.49
1:D:365:GLN:NE2	1:D:368:GLU:HA	2.27	0.49
1:A:353:SER:O	1:A:369:ARG:HA	2.11	0.49
1:C:365:GLN:NE2	1:C:368:GLU:HA	2.27	0.49
1:D:25:LEU:HD23	1:D:40:PHE:HE1	1.78	0.49
1:B:114:CYS:HA	1:B:138:GLU:OE1	2.12	0.49
1:C:181:LEU:HD12	1:C:221:MET:HE3	1.95	0.49
1:C:22:ARG:HH12	2:C:603:GET:H511	1.77	0.49
1:D:320:ASP:O	1:D:366:ILE:HD11	2.13	0.49
1:A:196:PHE:HD1	1:A:196:PHE:C	2.16	0.49
1:B:181:LEU:HD12	1:B:221:MET:HE3	1.94	0.49
1:B:196:PHE:CD2	1:B:211:ALA:HB1	2.48	0.49
1:C:157:THR:HG22	1:C:196:PHE:HB2	1.93	0.49
1:C:203:THR:O	1:C:246:LEU:HD13	2.13	0.49
1:D:196:PHE:CD2	1:D:211:ALA:HB1	2.48	0.49
1:D:43:ALA:O	1:D:408:VAL:HG12	2.13	0.49
1:A:21:THR:C	1:A:23:ASP:N	2.66	0.49
1:C:16:LEU:N	1:C:16:LEU:CD1	2.76	0.49
1:A:293:LYS:HD3	1:A:314:PHE:CE2	2.47	0.49
1:B:25:LEU:CD2	1:B:382:LEU:CD2	2.91	0.49
1:B:73:ASP:HB3	1:B:76:VAL:CG2	2.42	0.49
1:C:196:PHE:C	1:C:196:PHE:HD1	2.15	0.49
1:D:70:CYS:HA	1:D:389:TYR:CD2	2.48	0.49
1:D:73:ASP:HB3	1:D:76:VAL:CG2	2.42	0.49
1:A:183:GLN:HA	1:A:183:GLN:HE21	1.78	0.48
1:A:169:LYS:HB2	1:B:356:TRP:CZ3	2.47	0.48
1:C:112:ASN:HD22	1:C:113:PRO:CD	2.26	0.48
1:C:22:ARG:HB3	2:C:603:GET:H41	1.78	0.48
1:D:21:THR:CG2	1:D:44:ASP:HB2	2.43	0.48
1:C:183:GLN:HA	1:C:183:GLN:HE21	1.78	0.48
1:A:331:TYR:CE2	1:B:330:LEU:CD1	2.96	0.48
1:D:112:ASN:HD22	1:D:113:PRO:CD	2.26	0.48
1:D:365:GLN:HE21	1:D:368:GLU:HA	1.78	0.48
1:A:359:THR:HG22	1:A:361:ASP:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:HG3	1:A:97:ARG:NH1	2.28	0.48
1:B:196:PHE:HD1	1:B:196:PHE:C	2.16	0.48
1:C:114:CYS:HA	1:C:138:GLU:OE1	2.13	0.48
1:C:124:ARG:CG	1:C:146:HIS:CD2	2.96	0.48
1:D:310:ASN:CG	1:D:311:ALA:N	2.63	0.48
1:D:97:ARG:NH1	1:D:97:ARG:HG3	2.28	0.48
1:B:183:GLN:HE21	1:B:183:GLN:HA	1.78	0.48
1:B:28:LYS:HE3	1:B:406:TYR:CE1	2.49	0.48
1:C:331:TYR:CE2	1:D:330:LEU:CD1	2.97	0.48
1:A:73:ASP:HB3	1:A:76:VAL:HG23	1.95	0.48
1:B:320:ASP:O	1:B:366:ILE:HD11	2.13	0.48
1:C:246:LEU:HD23	1:C:251:ILE:HD11	1.95	0.48
1:C:320:ASP:O	1:C:366:ILE:HD11	2.14	0.48
1:C:391:VAL:CG2	1:C:392:VAL:HG22	2.44	0.48
1:D:65:PHE:HA	1:D:86:GLY:O	2.14	0.48
1:A:320:ASP:O	1:A:366:ILE:HD11	2.13	0.48
1:B:342:ARG:O	1:B:343:GLU:C	2.52	0.48
1:B:112:ASN:HD22	1:B:113:PRO:CD	2.27	0.48
1:B:292:ALA:HB3	1:B:317:TYR:HB2	1.96	0.48
1:B:65:PHE:O	1:B:274:GLU:HA	2.14	0.48
1:C:365:GLN:HE21	1:C:368:GLU:HA	1.78	0.48
1:A:339:LEU:CD1	2:A:601:GET:H421	2.43	0.47
1:B:21:THR:HG23	1:B:42:VAL:HG11	1.96	0.47
1:D:80:LEU:HD21	1:D:279:TYR:CD2	2.49	0.47
1:A:312:GLN:NE2	1:A:312:GLN:HA	2.29	0.47
1:C:391:VAL:HG22	1:C:392:VAL:HG22	1.96	0.47
1:D:114:CYS:HA	1:D:138:GLU:OE1	2.14	0.47
1:A:114:CYS:HA	1:A:138:GLU:OE1	2.15	0.47
1:A:289:ASN:CG	4:A:641:HOH:O	2.52	0.47
1:B:73:ASP:HB3	1:B:76:VAL:HG23	1.96	0.47
1:B:97:ARG:HG3	1:B:97:ARG:NH1	2.29	0.47
1:C:157:THR:CG2	1:C:196:PHE:HB2	2.44	0.47
1:A:384:GLU:OE1	2:A:601:GET:H531	2.15	0.47
1:C:97:ARG:HG3	1:C:97:ARG:NH1	2.30	0.47
1:B:345:ILE:HG13	1:B:348:GLU:CG	2.40	0.47
1:D:202:SER:HB2	4:D:469:HOH:O	2.15	0.47
1:D:65:PHE:O	1:D:274:GLU:HA	2.13	0.47
1:D:345:ILE:HG23	1:D:346:PRO:HD2	1.97	0.47
1:C:74:TRP:HE1	1:C:101:ILE:HG22	1.80	0.47
1:D:73:ASP:HB3	1:D:76:VAL:HG23	1.96	0.47
1:A:25:LEU:O	1:A:26:CYS:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ARG:NH1	4:A:634:HOH:O	2.46	0.47
1:D:341:GLN:HG3	1:D:342:ARG:N	2.25	0.47
1:A:293:LYS:HE2	1:A:375:MET:O	2.14	0.47
1:A:80:LEU:HD21	1:A:279:TYR:CD2	2.50	0.47
1:B:112:ASN:HD22	1:B:113:PRO:HD2	1.80	0.47
1:C:63:THR:HB	1:C:272:VAL:HG12	1.97	0.47
1:C:116:GLN:NE2	1:D:319:ASN:HB3	2.30	0.47
1:A:63:THR:HB	1:A:272:VAL:HG12	1.97	0.47
1:A:295:VAL:HG12	1:A:296:THR:N	2.30	0.47
1:C:169:LYS:HB2	1:D:356:TRP:CZ3	2.50	0.47
1:C:73:ASP:HB3	1:C:76:VAL:HG23	1.96	0.47
1:C:293:LYS:O	1:D:137:ASP:OD2	2.34	0.46
1:A:247:LYS:O	1:A:251:ILE:HG13	2.14	0.46
1:B:80:LEU:HD21	1:B:279:TYR:CD2	2.49	0.46
1:C:80:LEU:HD21	1:C:279:TYR:CD2	2.50	0.46
1:D:359:THR:HG22	1:D:361:ASP:H	1.79	0.46
1:B:74:TRP:HE1	1:B:101:ILE:HG22	1.79	0.46
1:A:295:VAL:HG12	1:A:296:THR:H	1.81	0.46
1:B:247:LYS:O	1:B:251:ILE:HG13	2.15	0.46
1:D:44:ASP:HA	1:D:408:VAL:CG1	2.41	0.46
1:A:65:PHE:O	1:A:274:GLU:HA	2.16	0.46
1:A:365:GLN:NE2	1:A:368:GLU:HA	2.30	0.46
1:C:65:PHE:O	1:C:274:GLU:HA	2.15	0.46
1:D:112:ASN:HD22	1:D:113:PRO:HD2	1.81	0.46
1:A:74:TRP:HE1	1:A:101:ILE:HG22	1.80	0.46
1:A:22:ARG:HA	4:A:648:HOH:O	2.15	0.46
1:A:359:THR:O	1:B:169:LYS:NZ	2.39	0.46
1:C:137:ASP:OD2	1:D:293:LYS:O	2.34	0.46
1:A:413:PRO:O	1:A:414:ASP:C	2.54	0.46
1:A:112:ASN:HD22	1:A:113:PRO:CD	2.29	0.46
1:A:116:GLN:NE2	1:B:319:ASN:HB3	2.30	0.46
1:C:157:THR:CG2	1:C:197:HIS:H	2.29	0.46
1:D:137:ASP:HA	1:D:140:GLU:HG3	1.98	0.46
1:D:247:LYS:O	1:D:251:ILE:HG13	2.16	0.46
3:A:602:ORX:H4A1	3:A:602:ORX:OXT	2.16	0.45
1:C:247:LYS:O	1:C:251:ILE:HG13	2.17	0.45
1:D:293:LYS:HE2	1:D:375:MET:O	2.16	0.45
1:B:365:GLN:NE2	1:B:368:GLU:HA	2.32	0.45
1:D:332:ASP:O	1:D:333:HIS:HB2	2.17	0.45
1:A:69:LYS:HE2	4:A:611:HOH:O	2.17	0.45
1:B:28:LYS:C	1:B:30:SER:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:GLN:O	1:C:119:HIS:HB2	2.17	0.45
1:D:28:LYS:HE2	1:D:406:TYR:CE1	2.52	0.45
1:B:21:THR:O	1:B:25:LEU:HD13	2.16	0.45
1:C:112:ASN:HD22	1:C:113:PRO:HD2	1.80	0.45
1:A:412:LEU:HA	1:A:413:PRO:HD3	1.66	0.45
1:C:339:LEU:HD21	2:C:603:GET:H111	1.99	0.45
1:B:63:THR:HB	1:B:272:VAL:HG12	1.98	0.45
1:D:25:LEU:HD23	1:D:40:PHE:CE1	2.52	0.45
1:A:112:ASN:HD22	1:A:113:PRO:HD2	1.82	0.44
1:B:314:PHE:O	1:B:353:SER:HA	2.17	0.44
1:D:80:LEU:HB3	1:D:85:THR:CG2	2.47	0.44
1:D:74:TRP:HE1	1:D:101:ILE:HG22	1.81	0.44
1:B:22:ARG:HA	2:B:602:GET:C31	2.48	0.44
1:A:80:LEU:HB3	1:A:85:THR:CG2	2.46	0.44
1:B:21:THR:HG23	1:B:42:VAL:CG1	2.48	0.44
1:B:25:LEU:HD21	1:B:382:LEU:HD22	1.99	0.44
1:A:25:LEU:C	1:A:27:LYS:N	2.71	0.44
1:A:116:GLN:O	1:A:119:HIS:HB2	2.18	0.44
1:B:345:ILE:HD12	1:B:346:PRO:HD2	1.99	0.44
1:A:185:LYS:HD3	4:A:615:HOH:O	2.18	0.44
1:D:194:VAL:HG12	1:D:195:SER:N	2.33	0.44
1:A:157:THR:CG2	1:A:196:PHE:HB2	2.48	0.43
1:C:80:LEU:HB3	1:C:85:THR:CG2	2.46	0.43
1:D:104:PRO:HB2	1:D:106:GLU:OE1	2.18	0.43
1:C:169:LYS:HD2	1:D:356:TRP:CE3	2.53	0.43
1:A:293:LYS:HG2	1:A:294:LYS:H	1.82	0.43
1:C:293:LYS:CE	1:C:314:PHE:CE2	3.01	0.43
1:C:359:THR:HG22	1:C:361:ASP:H	1.80	0.43
1:D:63:THR:HB	1:D:272:VAL:HG12	1.99	0.43
1:A:104:PRO:HB2	1:A:106:GLU:OE1	2.18	0.43
1:B:169:LYS:HE2	1:B:170:PHE:CE1	2.53	0.43
1:D:28:LYS:HE2	1:D:406:TYR:CE2	2.53	0.43
1:C:114:CYS:HB3	1:D:292:ALA:CB	2.48	0.43
1:A:314:PHE:CE2	1:A:374:GLU:HG3	2.53	0.43
1:D:116:GLN:O	1:D:119:HIS:HB2	2.18	0.43
1:D:248:PHE:O	1:D:251:ILE:HB	2.19	0.43
1:A:269:LEU:HD12	1:A:270:THR:H	1.84	0.43
1:C:293:LYS:HE2	1:C:314:PHE:HD2	1.81	0.43
1:D:292:ALA:HB3	1:D:317:TYR:HB2	2.00	0.43
1:D:321:GLY:C	1:D:326:PHE:HB2	2.40	0.42
1:A:168:VAL:CG1	1:A:169:LYS:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:THR:O	1:B:23:ASP:N	2.52	0.42
1:C:221:MET:O	1:C:225:LEU:CD2	2.67	0.42
1:C:269:LEU:HD12	1:C:270:THR:H	1.84	0.42
1:D:310:ASN:CB	1:D:349:LYS:HE2	2.46	0.42
1:A:242:ARG:HH11	1:A:242:ARG:HG3	1.82	0.42
1:A:248:PHE:O	1:A:251:ILE:HB	2.20	0.42
1:C:339:LEU:HD11	2:C:603:GET:H421	2.02	0.42
1:D:237:GLY:HA2	3:D:426:ORX:OP1	2.20	0.42
1:C:104:PRO:HB2	1:C:106:GLU:OE1	2.19	0.42
1:D:295:VAL:HG12	1:D:296:THR:N	2.35	0.42
1:A:274:GLU:O	3:A:602:ORX:H6	2.19	0.42
1:A:356:TRP:CZ3	1:B:169:LYS:HB2	2.55	0.42
1:B:22:ARG:HB3	2:B:602:GET:C31	2.40	0.42
1:B:248:PHE:O	1:B:251:ILE:HB	2.20	0.42
1:A:294:LYS:HE3	1:B:114:CYS:SG	2.60	0.42
1:B:20:ASN:HD21	1:B:22:ARG:HG3	1.85	0.42
1:B:332:ASP:O	1:B:333:HIS:HB2	2.19	0.42
1:D:182:GLU:O	1:D:185:LYS:HB3	2.19	0.42
1:D:75:ARG:CD	1:D:75:ARG:N	2.82	0.42
1:B:194:VAL:HG12	1:B:195:SER:N	2.35	0.42
1:B:321:GLY:C	1:B:326:PHE:HB2	2.40	0.42
1:B:322:VAL:CG2	1:B:364:ASP:HA	2.49	0.42
1:B:276:GLY:HA3	3:B:603:ORX:OP2	2.19	0.42
1:C:182:GLU:O	1:C:185:LYS:HB3	2.19	0.42
1:C:241:THR:C	1:C:243:ASP:H	2.23	0.42
1:D:25:LEU:HD11	1:D:285:THR:HG21	2.02	0.42
1:B:116:GLN:O	1:B:119:HIS:HB2	2.19	0.42
1:B:259:LEU:HD21	1:B:271:ILE:HD13	2.02	0.42
1:B:22:ARG:HB3	2:B:602:GET:N21	2.35	0.42
1:B:274:GLU:O	3:B:603:ORX:H6	2.19	0.42
1:C:356:TRP:CE3	1:D:169:LYS:HD2	2.55	0.42
1:A:221:MET:O	1:A:225:LEU:CD2	2.68	0.41
1:A:246:LEU:HG	1:A:251:ILE:HD11	2.02	0.41
1:B:182:GLU:O	1:B:185:LYS:HB3	2.19	0.41
1:C:75:ARG:CD	1:C:75:ARG:N	2.83	0.41
1:A:291:ILE:HG12	1:A:317:TYR:O	2.20	0.41
1:C:113:PRO:O	1:C:138:GLU:HG2	2.20	0.41
1:C:139:LEU:HD22	1:C:189:ILE:HG13	2.02	0.41
1:C:46:GLY:O	1:C:50:ARG:HG3	2.20	0.41
1:D:22:ARG:H	1:D:22:ARG:HG3	1.48	0.41
1:A:250:GLU:O	1:A:254:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLY:C	1:A:326:PHE:HB2	2.40	0.41
1:B:359:THR:HG22	1:B:361:ASP:H	1.79	0.41
1:D:242:ARG:CG	1:D:242:ARG:HH11	2.33	0.41
1:A:194:VAL:HG12	1:A:195:SER:N	2.35	0.41
1:A:46:GLY:O	1:A:50:ARG:HG3	2.20	0.41
1:B:119:HIS:O	1:B:122:TYR:N	2.54	0.41
1:C:194:VAL:HG12	1:C:195:SER:N	2.34	0.41
2:C:603:GET:H231	2:C:603:GET:H122	1.84	0.41
1:A:139:LEU:HD22	1:A:189:ILE:HG13	2.01	0.41
1:A:238:PHE:HA	1:A:239:PRO:HD3	1.89	0.41
1:B:244:ALA:HA	1:B:245:PRO:HD3	1.88	0.41
1:C:170:PHE:HE1	1:D:360:CYS:HA	1.86	0.41
1:D:221:MET:O	1:D:225:LEU:CD2	2.68	0.41
1:B:22:ARG:HA	2:B:602:GET:H311	2.03	0.41
1:D:183:GLN:HA	1:D:183:GLN:NE2	2.35	0.41
1:D:197:HIS:HA	4:D:445:HOH:O	2.20	0.41
1:B:29:ILE:HG23	1:B:380:TRP:NE1	2.36	0.41
1:C:248:PHE:O	1:C:251:ILE:HB	2.20	0.41
1:C:343:GLU:OE1	1:C:343:GLU:HA	2.21	0.41
1:D:139:LEU:HD22	1:D:189:ILE:HG13	2.02	0.41
1:A:182:GLU:O	1:A:185:LYS:HB3	2.20	0.41
1:B:25:LEU:HD21	1:B:382:LEU:CD2	2.50	0.41
1:B:69:LYS:HD2	3:B:603:ORX:H4A2	2.03	0.41
1:C:322:VAL:CG2	1:C:364:ASP:HA	2.51	0.41
1:D:309:SER:HA	1:D:350:LEU:O	2.21	0.41
1:A:22:ARG:HB2	1:A:22:ARG:HE	1.50	0.41
1:B:269:LEU:HD12	1:B:270:THR:H	1.85	0.41
1:B:65:PHE:HA	1:B:86:GLY:C	2.42	0.41
1:B:46:GLY:O	1:B:50:ARG:HG3	2.21	0.41
1:C:321:GLY:C	1:C:326:PHE:HB2	2.41	0.41
1:A:322:VAL:CG2	1:A:364:ASP:HA	2.52	0.40
1:A:339:LEU:HA	1:A:339:LEU:HD22	1.87	0.40
1:B:250:GLU:O	1:B:254:VAL:HG23	2.21	0.40
1:C:332:ASP:O	1:C:333:HIS:HB2	2.21	0.40
1:C:183:GLN:HA	1:C:183:GLN:NE2	2.37	0.40
1:D:104:PRO:HA	1:D:105:PRO:HD3	1.99	0.40
1:A:183:GLN:HA	1:A:183:GLN:NE2	2.37	0.40
1:B:22:ARG:CD	2:B:602:GET:H212	2.34	0.40
1:D:119:HIS:O	1:D:122:TYR:N	2.54	0.40
1:D:113:PRO:O	1:D:138:GLU:HG2	2.22	0.40
1:D:20:ASN:ND2	1:D:22:ARG:CD	2.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:GLU:O	1:D:254:VAL:HG23	2.21	0.40
1:D:59:LEU:HD21	1:D:252:ALA:HA	2.03	0.40
1:D:99:ARG:HH11	1:D:99:ARG:HG3	1.86	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	337/425 (79%)	307 (91%)	23 (7%)	7 (2%)	7	5
1	B	339/425 (80%)	307 (91%)	29 (9%)	3 (1%)	17	19
1	C	340/425 (80%)	314 (92%)	23 (7%)	3 (1%)	17	19
1	D	344/425 (81%)	314 (91%)	26 (8%)	4 (1%)	13	12
All	All	1360/1700 (80%)	1242 (91%)	101 (7%)	17 (1%)	12	11

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	B	345	ILE
1	B	346	PRO
1	C	27	LYS
1	D	402	SER
1	A	411	GLY
1	C	344	PRO
1	D	312	GLN
1	A	25	LEU
1	A	26	CYS
1	D	346	PRO
1	A	403	PRO

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Mol	Chain	Res	Type
1	B	325	SER
1	C	325	SER
1	D	325	SER
1	A	325	SER
1	A	413	PRO

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	297/364 (82%)	266 (90%)	31 (10%)	7	7
1	B	298/364 (82%)	266 (89%)	32 (11%)	6	6
1	C	300/364 (82%)	269 (90%)	31 (10%)	7	7
1	D	302/364 (83%)	271 (90%)	31 (10%)	7	7
All	All	1197/1456 (82%)	1072 (90%)	125 (10%)	7	7

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	22	ARG
1	A	23	ASP
1	A	26	CYS
1	A	57	LYS
1	A	71	ASN
1	A	74	TRP
1	A	85	THR
1	A	93	THR
1	A	106	GLU
1	A	110	TYR
1	A	112	ASN
1	A	137	ASP
1	A	145	THR
1	A	175	GLU
1	A	185	LYS

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Mol	Chain	Res	Type
1	A	196	PHE
1	A	203	THR
1	A	223	THR
1	A	247	LYS
1	A	289	ASN
1	A	312	GLN
1	A	335	VAL
1	A	339	LEU
1	A	343	GLU
1	A	351	TYR
1	A	359	THR
1	A	407	TYR
1	A	408	VAL
1	A	409	VAL
1	A	414	ASP
1	B	22	ARG
1	B	25	LEU
1	B	26	CYS
1	B	27	LYS
1	B	28	LYS
1	B	57	LYS
1	B	71	ASN
1	B	74	TRP
1	B	85	THR
1	B	93	THR
1	B	106	GLU
1	B	110	TYR
1	B	112	ASN
1	B	137	ASP
1	B	145	THR
1	B	175	GLU
1	B	185	LYS
1	B	196	PHE
1	B	203	THR
1	B	204	ASP
1	B	223	THR
1	B	247	LYS
1	B	289	ASN
1	B	335	VAL
1	B	340	PRO
1	B	341	GLN
1	B	342	ARG

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Mol	Chain	Res	Type
1	B	344	PRO
1	B	351	TYR
1	B	359	THR
1	B	403	PRO
1	B	409	VAL
1	C	14	ARG
1	C	22	ARG
1	C	27	LYS
1	C	57	LYS
1	C	71	ASN
1	C	74	TRP
1	C	85	THR
1	C	93	THR
1	C	106	GLU
1	C	110	TYR
1	C	112	ASN
1	C	137	ASP
1	C	145	THR
1	C	175	GLU
1	C	185	LYS
1	C	196	PHE
1	C	203	THR
1	C	223	THR
1	C	247	LYS
1	C	289	ASN
1	C	296	THR
1	C	335	VAL
1	C	339	LEU
1	C	349	LYS
1	C	351	TYR
1	C	359	THR
1	C	391	VAL
1	C	392	VAL
1	C	403	PRO
1	C	404	THR
1	C	408	VAL
1	D	21	THR
1	D	23	ASP
1	D	57	LYS
1	D	71	ASN
1	D	74	TRP
1	D	85	THR

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Mol	Chain	Res	Type
1	D	93	THR
1	D	106	GLU
1	D	110	TYR
1	D	112	ASN
1	D	137	ASP
1	D	145	THR
1	D	175	GLU
1	D	185	LYS
1	D	196	PHE
1	D	203	THR
1	D	204	ASP
1	D	223	THR
1	D	242	ARG
1	D	247	LYS
1	D	289	ASN
1	D	296	THR
1	D	335	VAL
1	D	341	GLN
1	D	343	GLU
1	D	346	PRO
1	D	351	TYR
1	D	359	THR
1	D	401	GLN
1	D	402	SER
1	D	403	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	71	ASN
1	A	96	GLN
1	A	112	ASN
1	A	116	GLN
1	A	119	HIS
1	A	146	HIS
1	A	183	GLN
1	A	210	GLN
1	A	230	HIS
1	A	256	ASN
1	A	289	ASN
1	A	312	GLN

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Mol	Chain	Res	Type
1	A	333	HIS
1	A	365	GLN
1	B	20	ASN
1	B	71	ASN
1	B	96	GLN
1	B	112	ASN
1	B	116	GLN
1	B	119	HIS
1	B	146	HIS
1	B	183	GLN
1	B	210	GLN
1	B	256	ASN
1	B	289	ASN
1	B	312	GLN
1	B	365	GLN
1	C	71	ASN
1	C	96	GLN
1	C	112	ASN
1	C	116	GLN
1	C	119	HIS
1	C	146	HIS
1	C	183	GLN
1	C	210	GLN
1	C	256	ASN
1	C	289	ASN
1	C	312	GLN
1	C	365	GLN
1	D	20	ASN
1	D	71	ASN
1	D	96	GLN
1	D	112	ASN
1	D	116	GLN
1	D	119	HIS
1	D	146	HIS
1	D	183	GLN
1	D	210	GLN
1	D	256	ASN
1	D	289	ASN
1	D	310	ASN
1	D	365	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 ⓘ

7 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	GET	A	601	-	33,36,36	1.31	4 (12%)	43,55,55	1.65	7 (16%)
3	ORX	D	426	-	21,24,24	2.76	9 (42%)	25,33,33	4.71	15 (60%)
3	ORX	B	603	-	21,24,24	2.90	8 (38%)	25,33,33	4.77	14 (56%)
2	GET	B	602	-	33,36,36	1.12	3 (9%)	43,55,55	1.79	7 (16%)
3	ORX	A	602	-	21,24,24	3.02	8 (38%)	25,33,33	4.74	13 (52%)
3	ORX	C	604	-	21,24,24	2.57	7 (33%)	25,33,33	4.88	15 (60%)
2	GET	C	603	-	33,36,36	1.24	3 (9%)	43,55,55	1.50	5 (11%)

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	GET	A	601	-	1/1/15/16	4/13/74/74	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ORX	D	426	-	1/1/3/4	2/15/19/19	0/1/1/1
3	ORX	B	603	-	-	6/15/19/19	0/1/1/1
2	GET	B	602	-	1/1/15/16	8/13/74/74	0/3/3/3
3	ORX	A	602	-	-	4/15/19/19	0/1/1/1
3	ORX	C	604	-	-	13/15/19/19	0/1/1/1
2	GET	C	603	-	1/1/15/16	5/13/74/74	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	ORX	C3-C2	8.83	1.49	1.40
3	B	603	ORX	C3-C2	8.32	1.49	1.40
3	D	426	ORX	C3-C2	7.91	1.48	1.40
3	C	604	ORX	C3-C2	7.04	1.47	1.40
3	A	602	ORX	CAA-NA	5.67	1.57	1.47
3	B	603	ORX	CAA-NA	5.38	1.56	1.47
3	C	604	ORX	CAA-NA	5.24	1.56	1.47
3	C	604	ORX	C4A-C4	5.11	1.58	1.51
3	A	602	ORX	C4A-C4	5.06	1.58	1.51
3	B	603	ORX	C4A-C4	4.96	1.58	1.51
3	D	426	ORX	CAA-NA	4.79	1.55	1.47
3	D	426	ORX	C4A-C4	4.39	1.57	1.51
3	A	602	ORX	C5-C4	3.41	1.45	1.40
3	A	602	ORX	C2-N1	3.40	1.40	1.33
3	D	426	ORX	C3-C4	3.33	1.45	1.40
3	B	603	ORX	C2-N1	3.25	1.40	1.33
3	B	603	ORX	C3-C4	3.23	1.45	1.40
3	D	426	ORX	C2-N1	3.09	1.39	1.33
3	D	426	ORX	C5-C4	3.08	1.44	1.40
3	B	603	ORX	C5-C4	2.94	1.44	1.40
3	A	602	ORX	C3-C4	2.93	1.44	1.40
2	A	601	GET	O51-C51	2.92	1.48	1.44
2	C	603	GET	C11-C21	2.65	1.57	1.52
3	C	604	ORX	C2-N1	2.61	1.38	1.33
3	C	604	ORX	C3-C4	2.60	1.44	1.40
2	B	602	GET	O53-C13	2.55	1.47	1.41
3	D	426	ORX	C4A-NA	2.45	1.54	1.46
2	B	602	GET	O53-C53	2.45	1.47	1.43
3	B	603	ORX	C4A-NA	2.35	1.53	1.46
3	C	604	ORX	P-OP1	-2.33	1.43	1.50
3	D	426	ORX	OP4-C5A	-2.31	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	ORX	C4A-NA	2.25	1.53	1.46
3	A	602	ORX	OP4-C5A	-2.19	1.36	1.45
2	B	602	GET	O43-C43	-2.13	1.41	1.44
2	C	603	GET	C51-C61	2.12	1.55	1.52
3	B	603	ORX	P-OP1	-2.07	1.43	1.50
3	C	604	ORX	C4A-NA	2.04	1.52	1.46
3	D	426	ORX	P-OP1	-2.03	1.44	1.50
2	C	603	GET	C62-C12	2.01	1.57	1.53
2	A	601	GET	C62-C12	2.01	1.57	1.53
2	A	601	GET	C51-C61	2.01	1.55	1.52
2	A	601	GET	O53-C53	2.00	1.46	1.43

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	604	ORX	C6-C5-C4	14.72	128.53	118.12
3	A	602	ORX	C6-C5-C4	14.27	128.22	118.12
3	B	603	ORX	C6-C5-C4	13.95	127.99	118.12
3	D	426	ORX	C6-C5-C4	13.35	127.57	118.12
3	B	603	ORX	C2A-C2-C3	10.53	133.89	120.89
3	A	602	ORX	C2A-C2-C3	10.46	133.81	120.89
3	D	426	ORX	C2A-C2-C3	10.25	133.54	120.89
3	C	604	ORX	C3-C4-C5	-9.86	109.26	118.72
3	C	604	ORX	C2A-C2-C3	9.74	132.92	120.89
3	B	603	ORX	C3-C4-C5	-9.52	109.59	118.72
3	A	602	ORX	C3-C4-C5	-9.48	109.62	118.72
3	D	426	ORX	C3-C4-C5	-9.42	109.68	118.72
3	C	604	ORX	C4A-C4-C3	7.05	127.59	120.04
2	B	602	GET	O51-C51-C41	6.22	116.60	107.87
3	B	603	ORX	C4A-C4-C3	6.19	126.67	120.04
3	A	602	ORX	C4A-C4-C3	6.17	126.65	120.04
2	A	601	GET	O51-C51-C41	6.05	116.37	107.87
3	D	426	ORX	OP4-C5A-C5	5.81	120.43	109.35
3	D	426	ORX	C5A-C5-C6	-5.72	109.96	119.37
3	B	603	ORX	C5A-C5-C6	-5.51	110.31	119.37
3	C	604	ORX	C5A-C5-C6	-5.39	110.52	119.37
3	A	602	ORX	C5A-C5-C6	-5.29	110.68	119.37
3	D	426	ORX	C4A-C4-C3	5.27	125.68	120.04
2	C	603	GET	O51-C51-C41	5.01	114.91	107.87
3	A	602	ORX	C2A-C2-N1	-5.00	107.90	117.67
3	C	604	ORX	OP4-C5A-C5	4.99	118.87	109.35
3	B	603	ORX	C2A-C2-N1	-4.93	108.05	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	426	ORX	C2A-C2-N1	-4.76	108.37	117.67
3	C	604	ORX	C2A-C2-N1	-4.62	108.64	117.67
3	B	603	ORX	OP4-C5A-C5	4.48	117.89	109.35
3	D	426	ORX	C4A-C4-C5	4.43	124.64	119.71
2	B	602	GET	C71-C61-C51	-4.40	106.86	112.02
2	B	602	GET	C13-O62-C62	-4.23	107.51	117.96
3	B	603	ORX	C4A-C4-C5	3.62	123.74	119.71
3	A	602	ORX	C4A-C4-C5	3.61	123.73	119.71
2	B	602	GET	C53-O53-C13	3.50	117.18	111.53
2	C	603	GET	C13-O62-C62	-3.46	109.40	117.96
3	A	602	ORX	OP4-C5A-C5	3.37	115.77	109.35
2	A	601	GET	C13-O62-C62	-3.20	110.05	117.96
2	A	601	GET	C93-N33-C33	-3.19	109.74	114.38
2	C	603	GET	C93-N33-C33	-3.16	109.78	114.38
2	A	601	GET	C53-O53-C13	3.14	116.59	111.53
2	C	603	GET	C11-O51-C51	3.14	118.11	113.06
3	C	604	ORX	OP2-P-OP1	3.11	122.86	110.68
3	C	604	ORX	C4A-C4-C5	3.09	123.14	119.71
3	C	604	ORX	O3-C3-C2	-2.93	111.12	117.49
3	D	426	ORX	O3-C3-C2	-2.89	111.20	117.49
3	B	603	ORX	O3-C3-C2	-2.85	111.27	117.49
3	D	426	ORX	C4-C3-C2	2.80	124.35	120.06
2	A	601	GET	C11-O51-C51	2.75	117.50	113.06
3	B	603	ORX	C4-C3-C2	2.72	124.23	120.06
2	B	602	GET	C93-N33-C33	-2.58	110.63	114.38
3	A	602	ORX	C5-C6-N1	-2.56	119.56	123.82
2	A	601	GET	C13-C23-C33	2.56	113.57	109.34
3	A	602	ORX	O3-C3-C2	-2.55	111.93	117.49
3	B	603	ORX	C5-C6-N1	-2.50	119.65	123.82
3	C	604	ORX	C4-C3-C2	2.50	123.89	120.06
3	A	602	ORX	C4-C3-C2	2.48	123.86	120.06
3	A	602	ORX	OP2-P-OP1	2.47	120.37	110.68
3	B	603	ORX	OP2-P-OP1	2.47	120.35	110.68
3	D	426	ORX	C5-C6-N1	-2.44	119.76	123.82
2	B	602	GET	C41-C31-C21	2.44	115.26	111.07
3	C	604	ORX	OP4-P-OP1	2.41	113.22	106.47
3	C	604	ORX	C5-C6-N1	-2.36	119.89	123.82
3	C	604	ORX	O3-C3-C4	2.34	124.99	118.13
2	B	602	GET	C41-C51-C61	-2.29	108.67	113.15
3	D	426	ORX	OP4-P-OP1	2.20	112.66	106.47
2	A	601	GET	C62-C52-C42	2.20	113.52	108.96
3	B	603	ORX	O3-C3-C4	2.17	124.50	118.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	426	ORX	O3-C3-C4	2.15	124.45	118.13
2	C	603	GET	C53-O53-C13	2.15	114.99	111.53
3	B	603	ORX	C3-C2-N1	-2.10	118.06	120.77
3	D	426	ORX	C3-C2-N1	-2.08	118.08	120.77
3	A	602	ORX	O3-C3-C4	2.07	124.20	118.13
3	C	604	ORX	OP3-P-OP1	-2.06	102.62	110.68
3	D	426	ORX	OP2-P-OP1	2.06	118.73	110.68

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	GET	C61
3	D	426	ORX	CAA
2	B	602	GET	C61
2	C	603	GET	C61

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GET	C21-C11-O11-C42
2	A	601	GET	O51-C51-C61-O61
3	B	603	ORX	CBA-CAA-NA-C4A
3	B	603	ORX	CA-CAA-CBA-CGA
3	B	603	ORX	NA-CAA-CBA-CGA
2	B	602	GET	C21-C11-O11-C42
2	B	602	GET	C41-C51-C61-O61
2	B	602	GET	C41-C51-C61-C71
2	B	602	GET	O51-C51-C61-C71
3	C	604	ORX	CBA-CAA-NA-C4A
3	C	604	ORX	CA-CAA-CBA-CGA
3	C	604	ORX	C5-C4-C4A-NA
3	C	604	ORX	C4-C5-C5A-OP4
3	C	604	ORX	C6-C5-C5A-OP4
3	C	604	ORX	C5A-OP4-P-OP1
3	C	604	ORX	C5A-OP4-P-OP2
3	C	604	ORX	C5A-OP4-P-OP3
2	C	603	GET	C21-C11-O11-C42
2	C	603	GET	O51-C51-C61-O61
2	C	603	GET	O51-C51-C61-C71
2	C	603	GET	C23-C33-N33-C93
3	B	603	ORX	C5-C4-C4A-NA
3	C	604	ORX	NA-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
3	A	602	ORX	C5-C4-C4A-NA
3	A	602	ORX	NA-CAA-CBA-CGA
2	B	602	GET	C23-C13-O62-C62
2	B	602	GET	O51-C11-O11-C42
3	A	602	ORX	CAA-CBA-CGA-CDA
2	B	602	GET	O53-C13-O62-C62
2	A	601	GET	O51-C11-O11-C42
2	C	603	GET	O51-C11-O11-C42
3	B	603	ORX	C3-C4-C4A-NA
3	C	604	ORX	CAA-CBA-CGA-CDA
3	D	426	ORX	CBA-CAA-NA-C4A
2	A	601	GET	O51-C51-C61-C71
3	A	602	ORX	C3-C4-C4A-NA
3	D	426	ORX	CA-CAA-NA-C4A
3	B	603	ORX	CA-CAA-NA-C4A
3	C	604	ORX	C3-C4-C4A-NA
3	C	604	ORX	C4-C4A-NA-CAA
2	B	602	GET	O51-C51-C61-O61
3	C	604	ORX	CA-CAA-NA-C4A

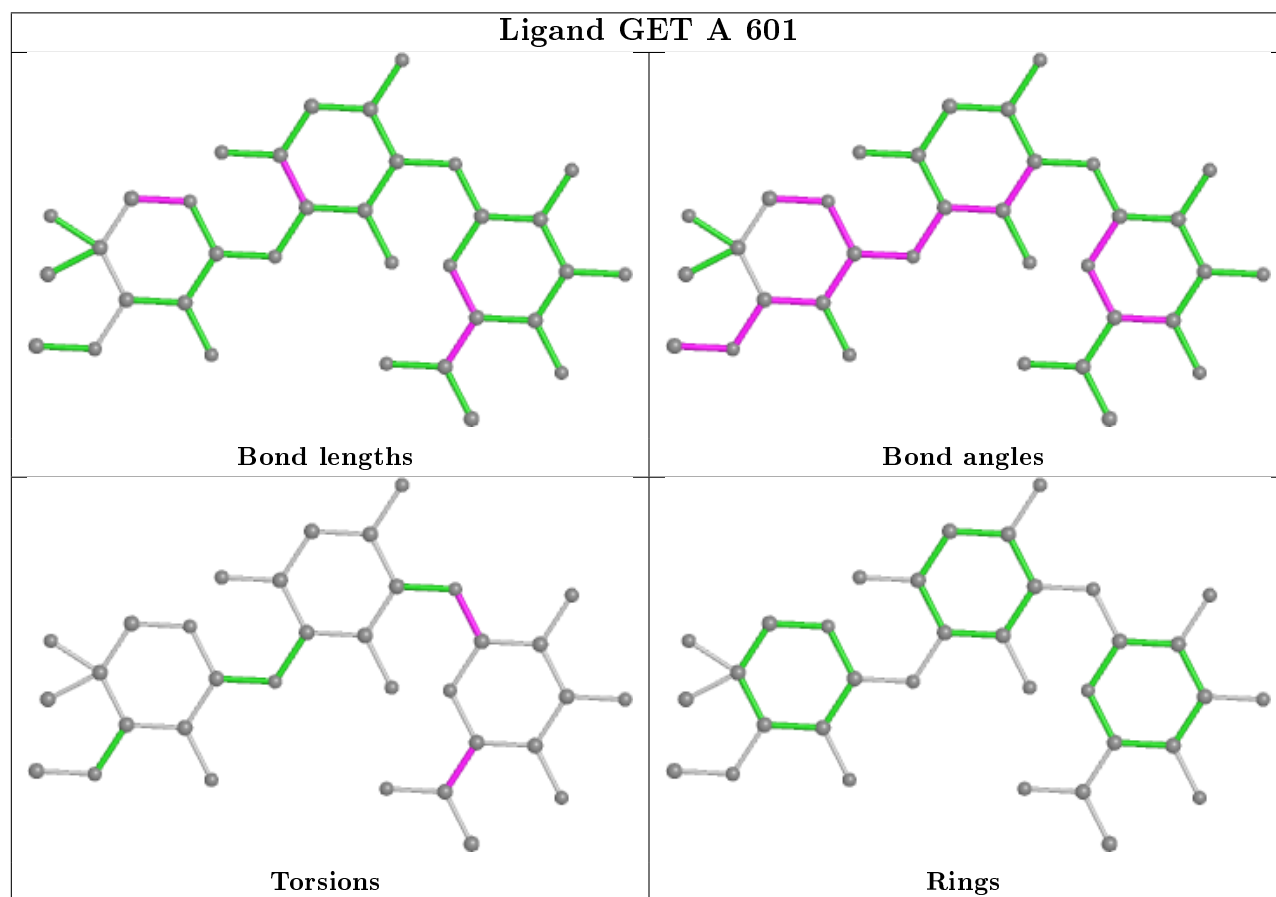
There are no ring outliers.

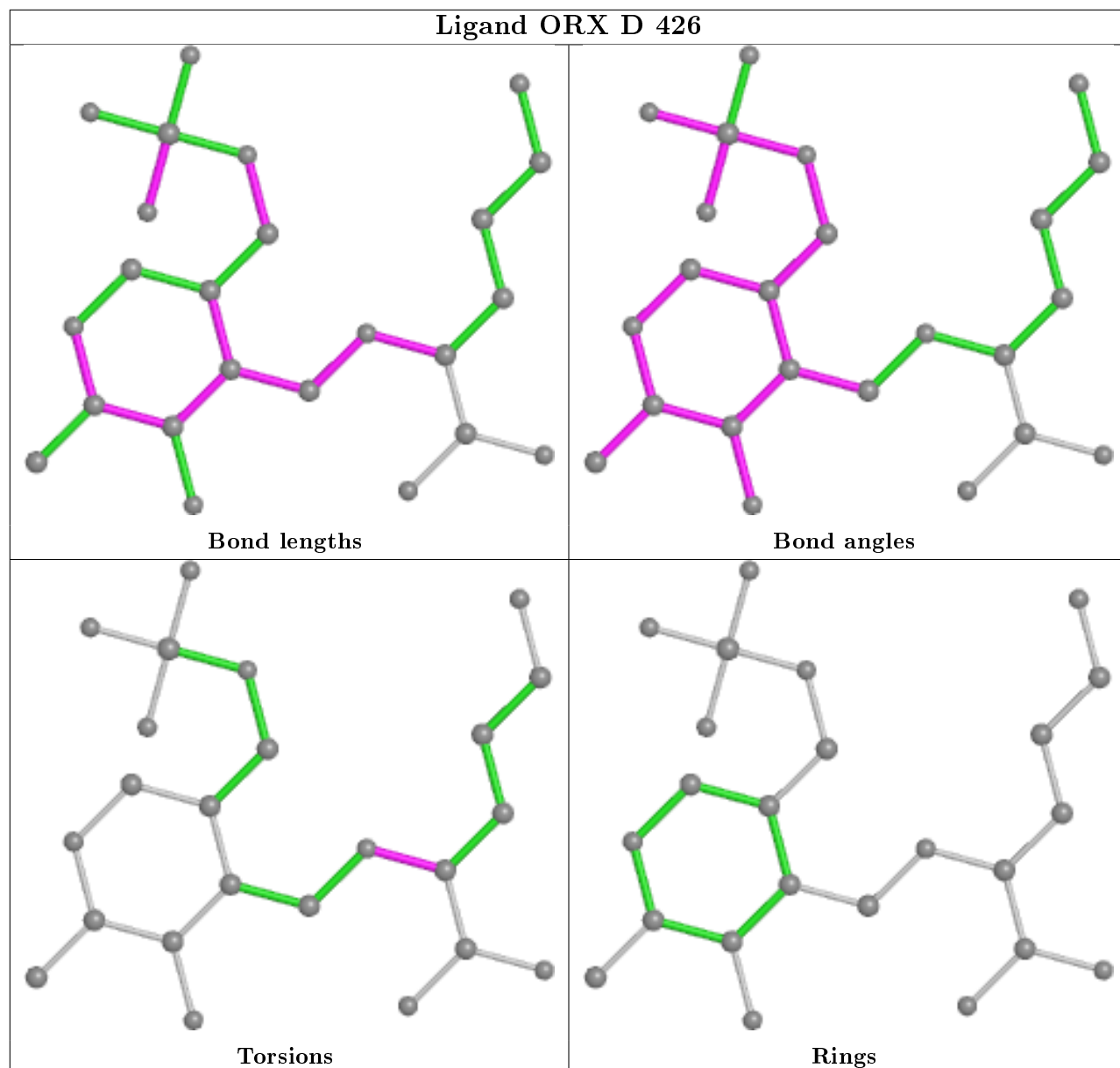
7 monomers are involved in 36 short contacts:

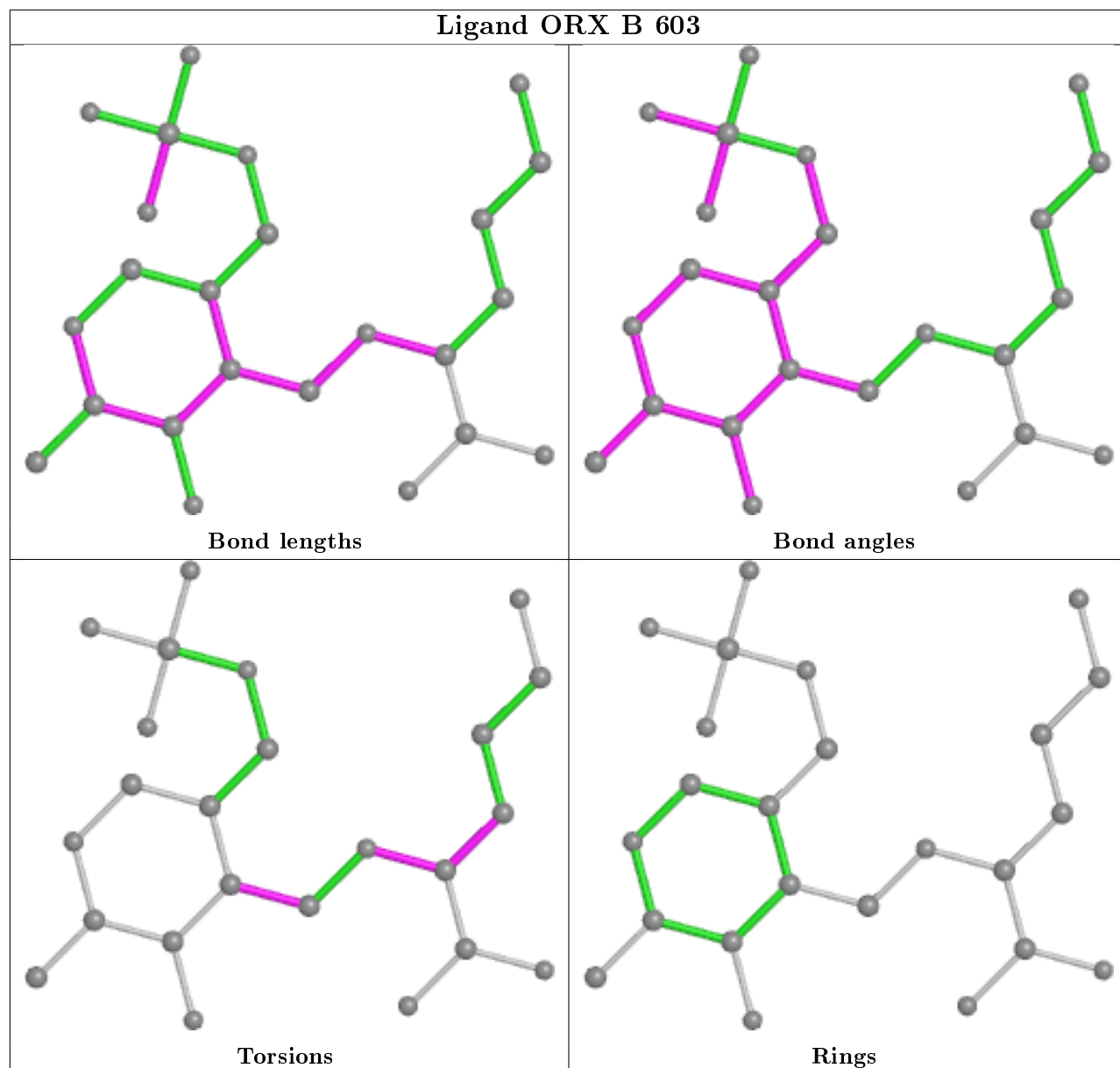
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GET	5	0
3	D	426	ORX	2	0
3	B	603	ORX	3	0
2	B	602	GET	13	0
3	A	602	ORX	2	0
3	C	604	ORX	1	0
2	C	603	GET	10	0

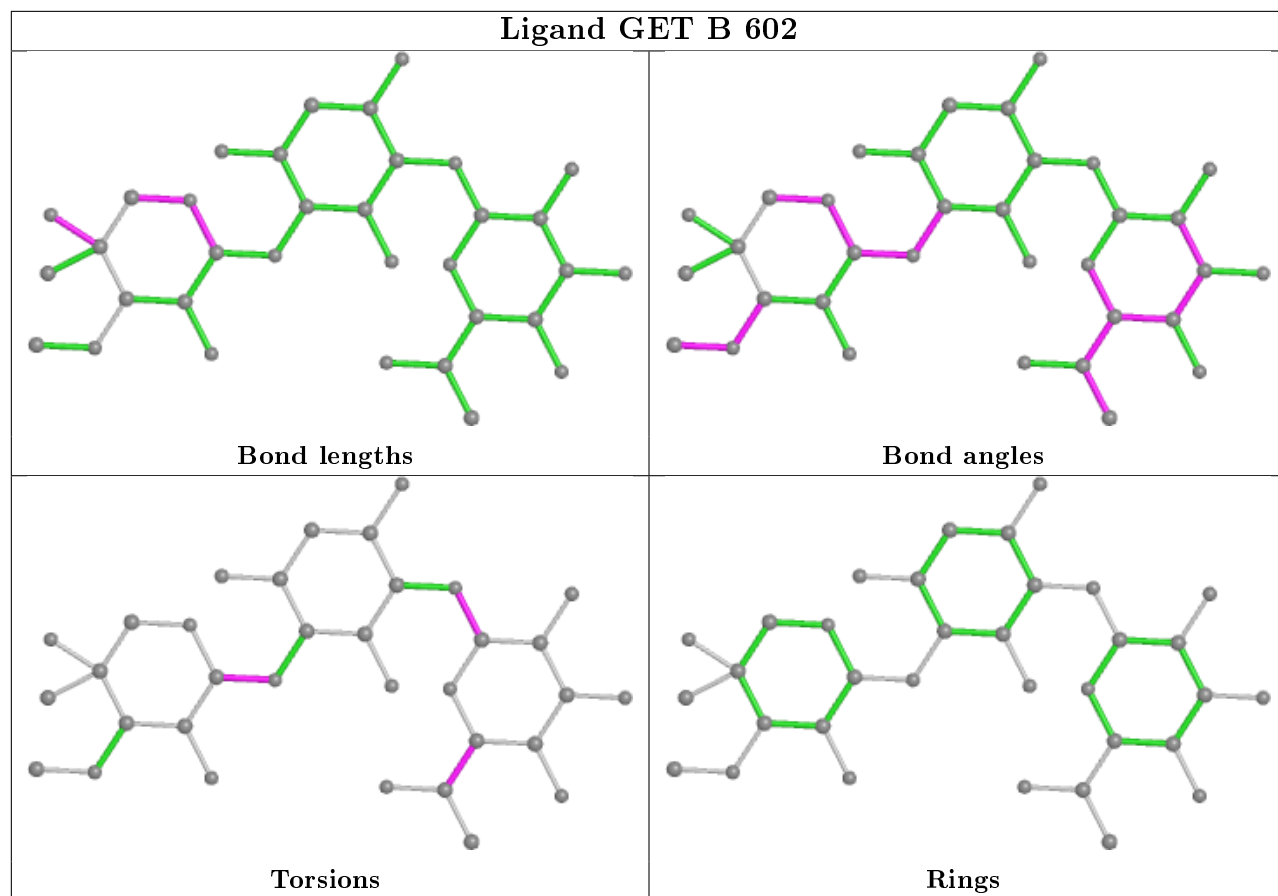
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

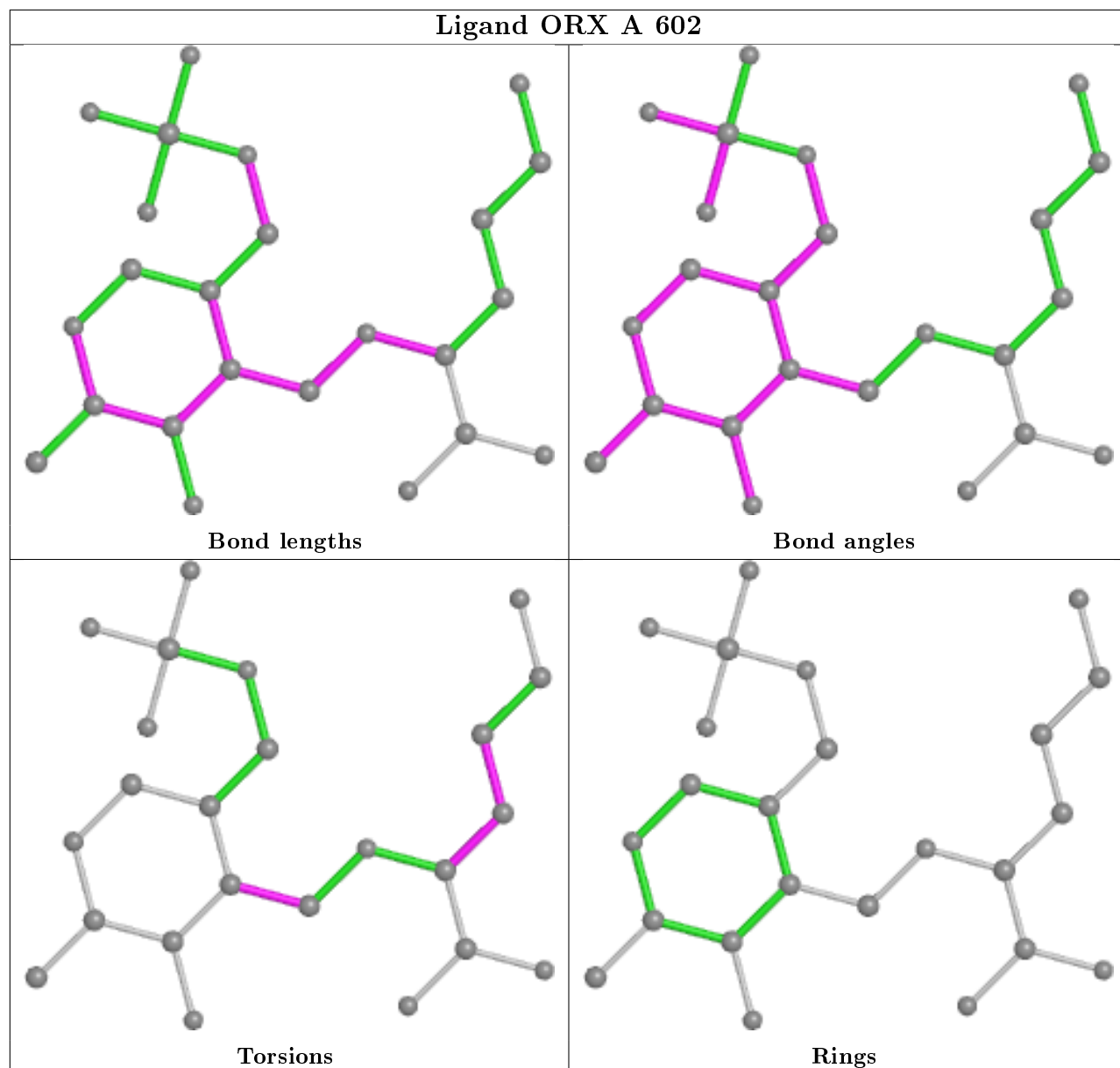
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

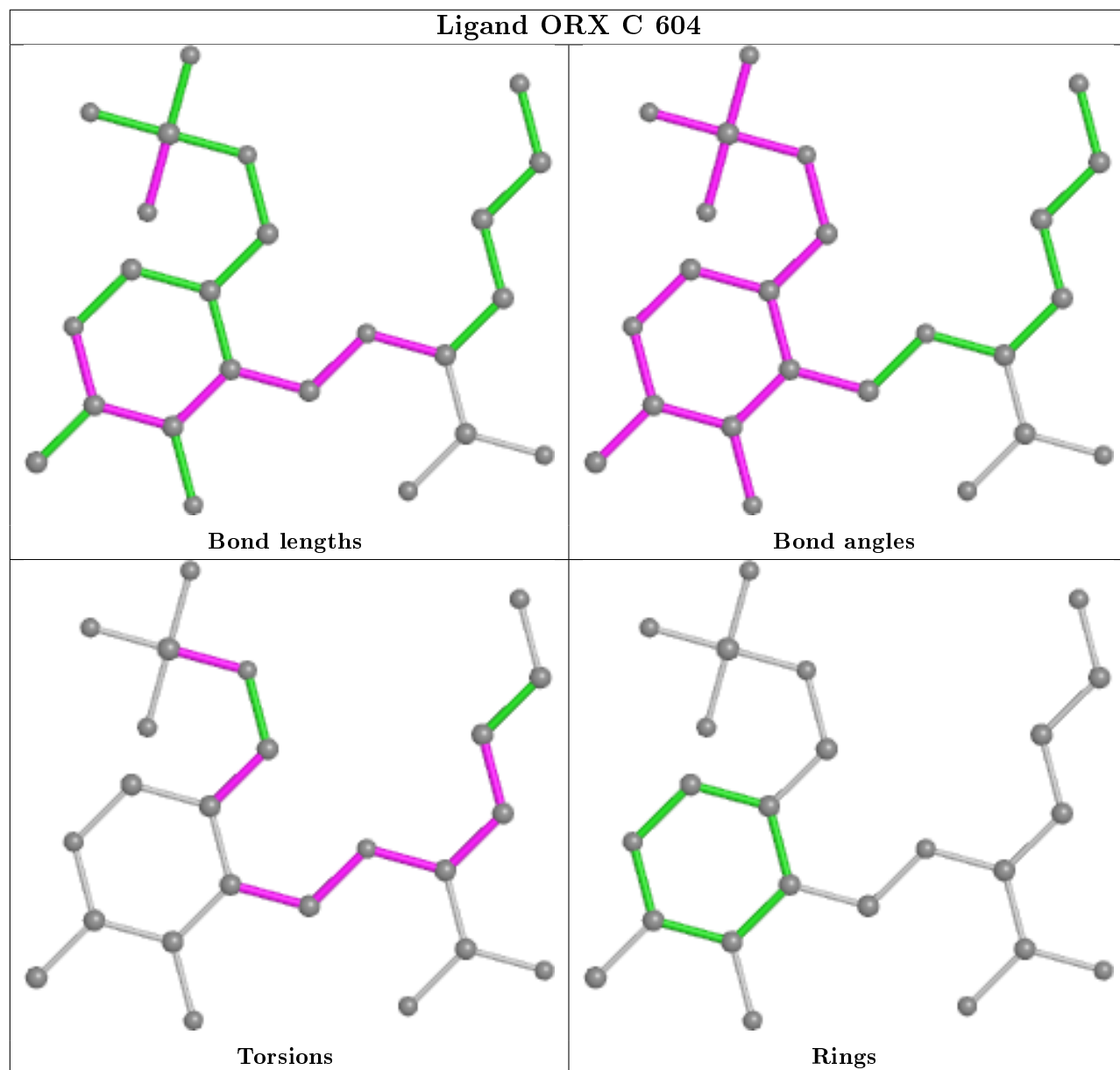


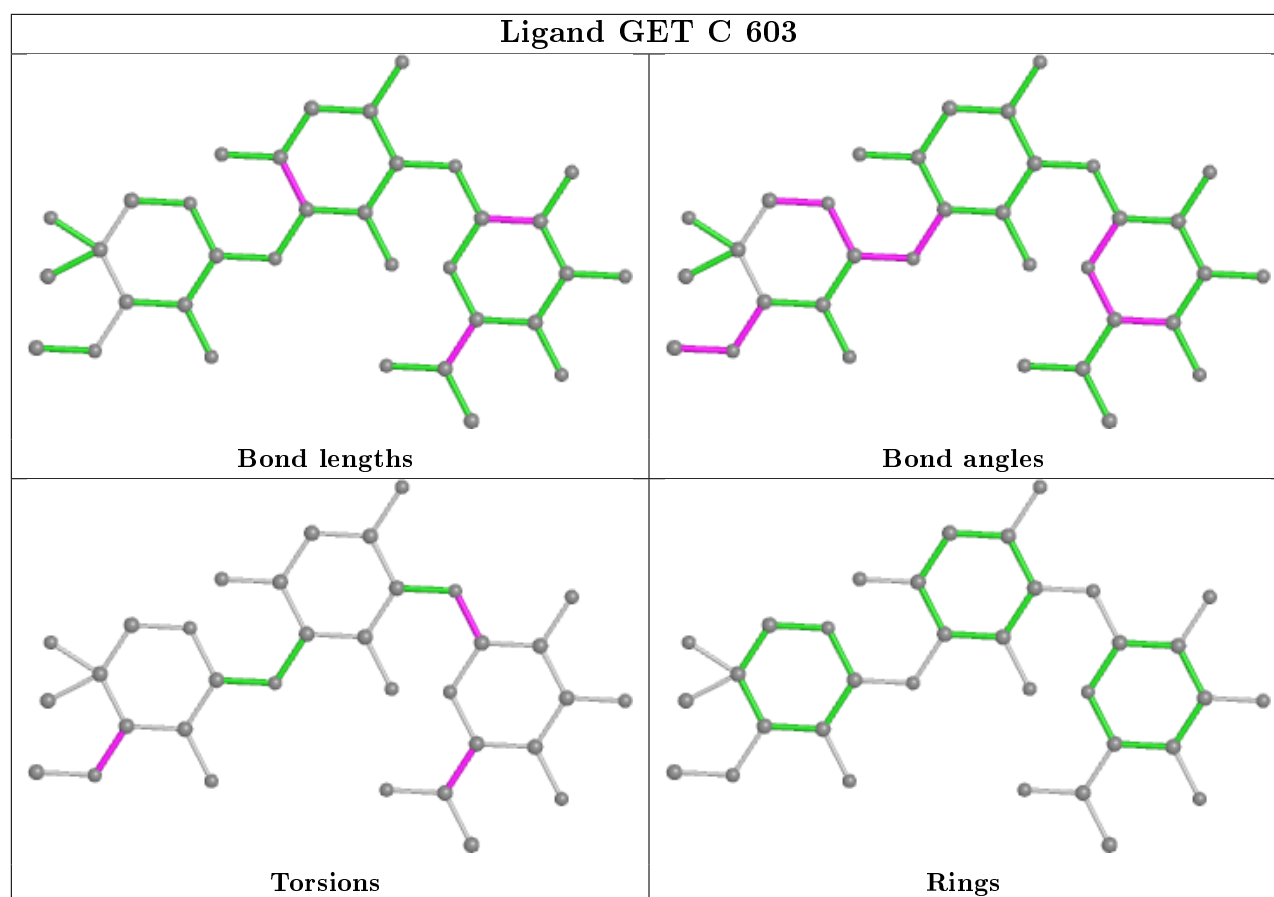












5.7 Other polymers [i](#)

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	349/425 (82%)	0.08	9 (2%) 56 52	24, 41, 74, 97	0
1	B	349/425 (82%)	0.05	8 (2%) 60 56	19, 41, 75, 97	0
1	C	352/425 (82%)	0.08	12 (3%) 45 41	22, 41, 77, 91	0
1	D	354/425 (83%)	0.08	8 (2%) 60 56	20, 40, 76, 99	2 (0%)
All	All	1404/1700 (82%)	0.07	37 (2%) 56 52	19, 41, 76, 99	2 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	74	TRP	6.1
1	A	74	TRP	4.6
1	B	27	LYS	4.5
1	D	74	TRP	4.3
1	B	22	ARG	4.2
1	B	74	TRP	3.8
1	C	19	PHE	3.5
1	D	408	VAL	3.5
1	C	15	PHE	3.4
1	A	23	ASP	3.2
1	A	414	ASP	3.0
1	D	242	ARG	2.9
1	B	347	ASN	2.8
1	C	392	VAL	2.8
1	B	242	ARG	2.8
1	A	408	VAL	2.7
1	C	27	LYS	2.6
1	D	347	ASN	2.6
1	A	22	ARG	2.6
1	C	14	ARG	2.6
1	C	312	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	28	LYS	2.4
1	B	408	VAL	2.3
1	D	309	SER	2.3
1	C	242	ARG	2.3
1	D	346	PRO	2.3
1	D	310	ASN	2.3
1	C	349	LYS	2.2
1	B	267	LEU	2.2
1	A	369	ARG	2.1
1	C	17	GLU	2.1
1	C	406	TYR	2.1
1	A	343	GLU	2.1
1	A	342	ARG	2.1
1	D	267	LEU	2.1
1	B	25	LEU	2.0
1	A	242	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

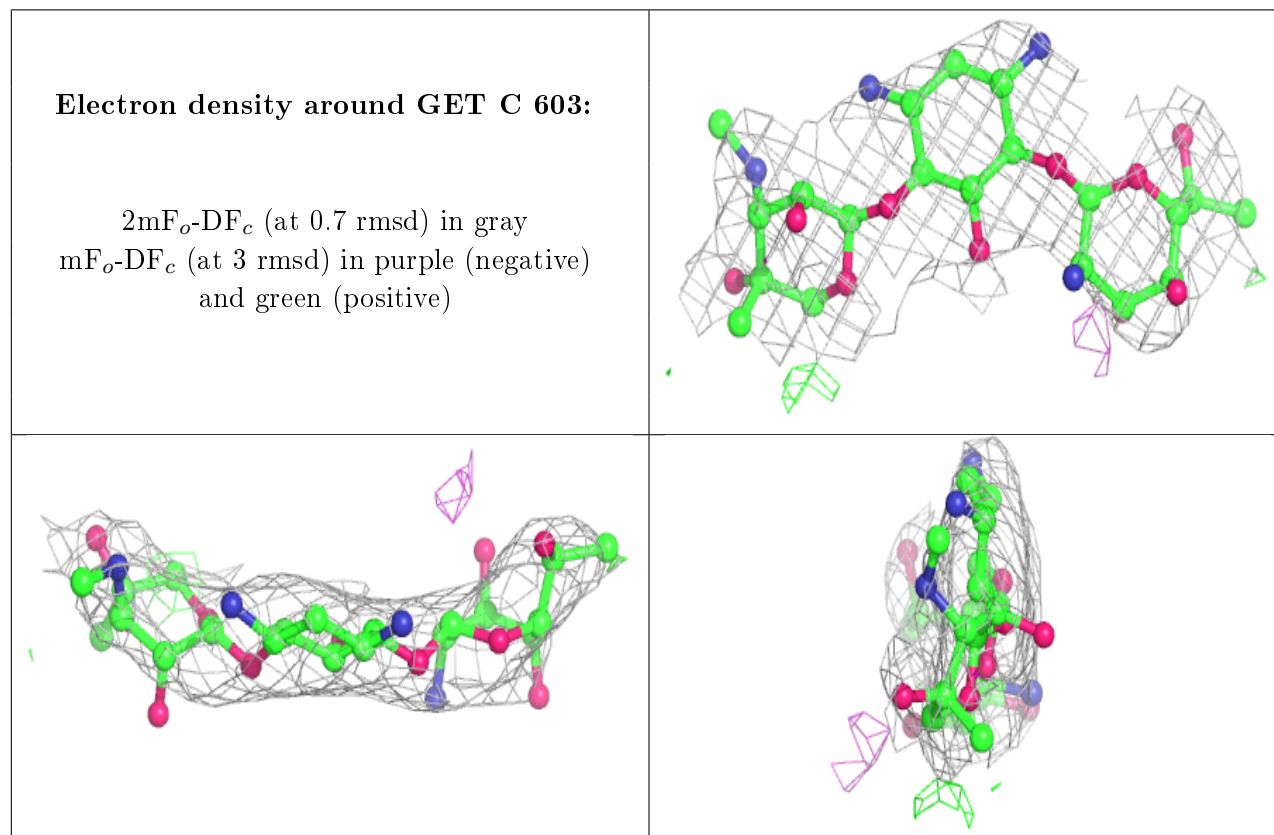
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

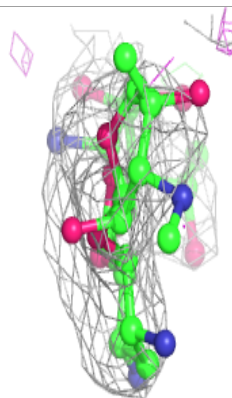
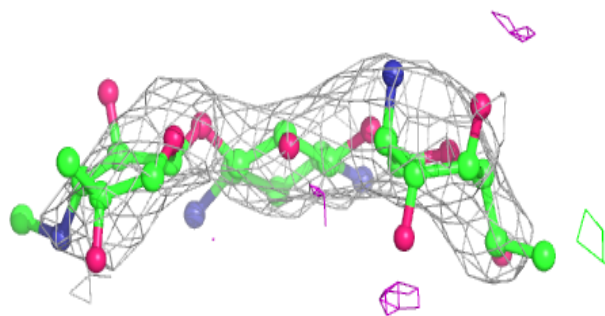
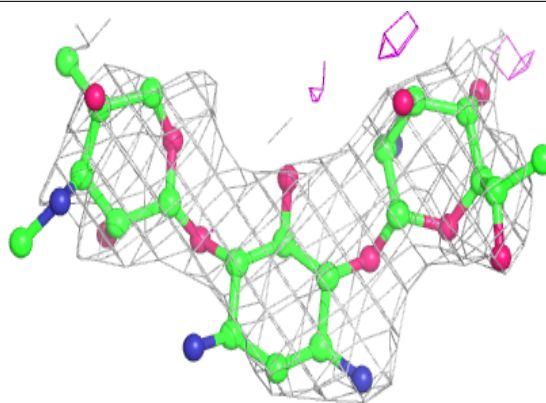
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GET	C	603	34/34	0.76	0.26	95,97,100,101	0
2	GET	A	601	34/34	0.79	0.28	99,101,106,106	0
2	GET	B	602	34/34	0.81	0.27	99,104,112,113	0
3	ORX	C	604	24/24	0.91	0.19	34,48,54,55	0
3	ORX	D	426	24/24	0.93	0.21	31,47,52,54	0
3	ORX	A	602	24/24	0.95	0.19	29,39,45,46	0
3	ORX	B	603	24/24	0.96	0.15	18,46,52,52	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.

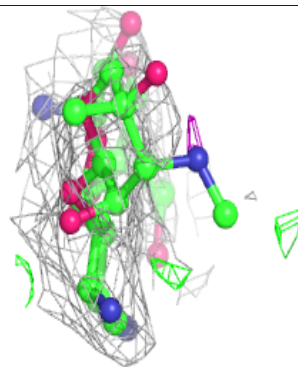
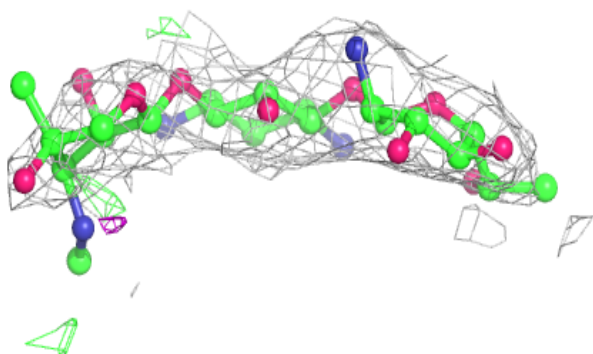
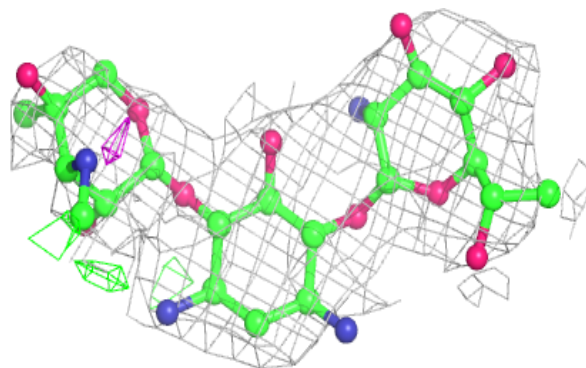


Electron density around GET A 601:

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

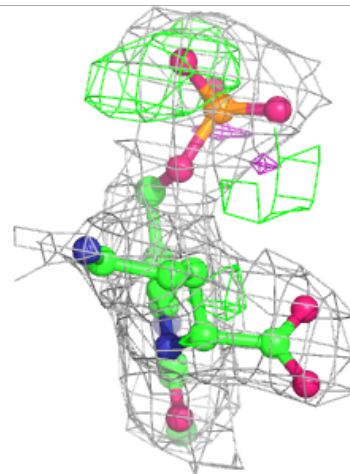
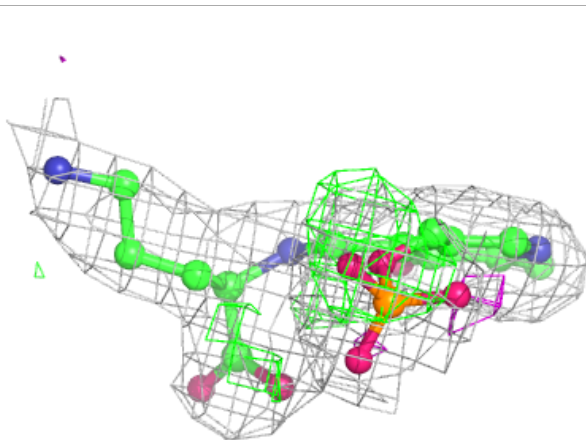
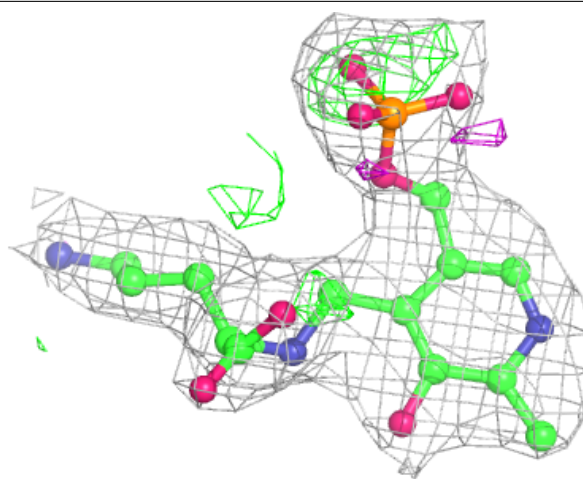
**Electron density around GET B 602:**

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



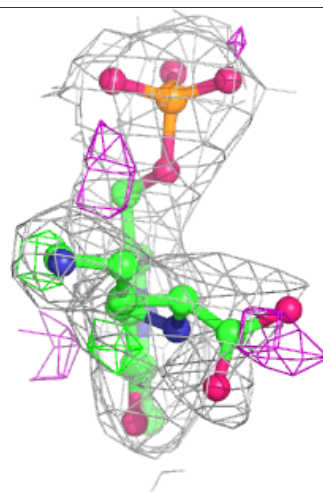
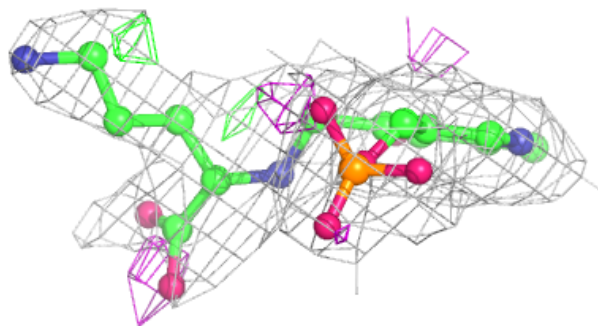
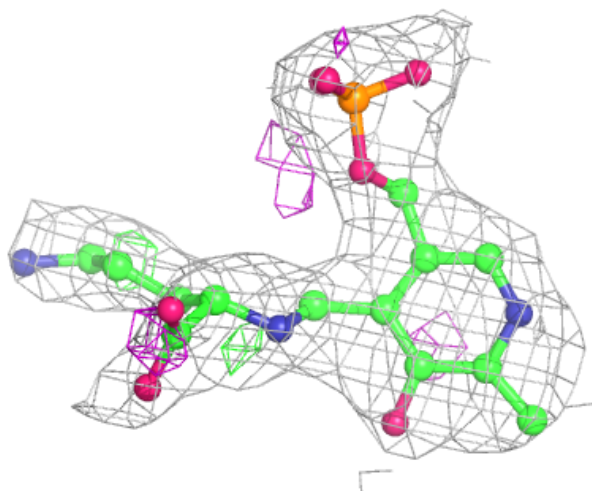
Electron density around ORX C 604:

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



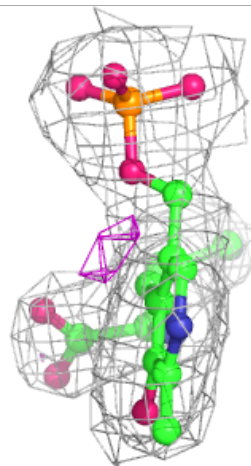
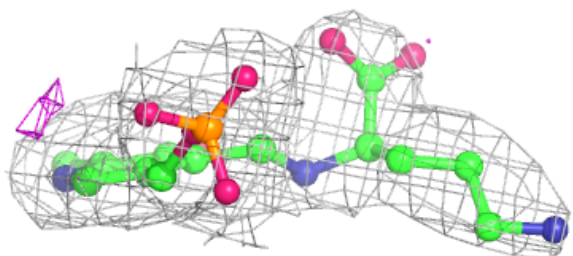
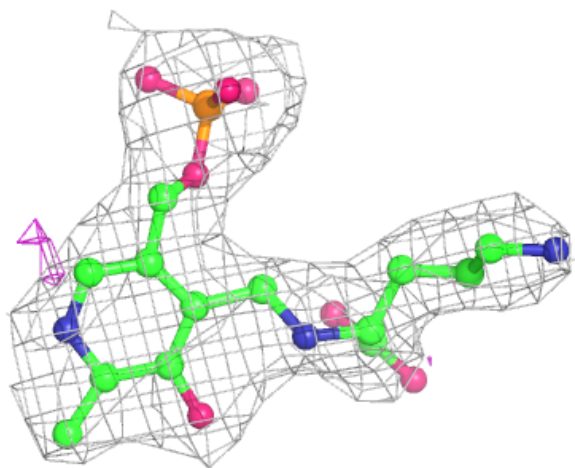
Electron density around ORX D 426:

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



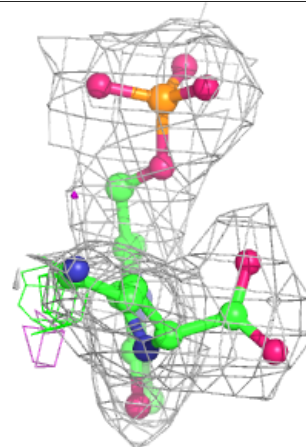
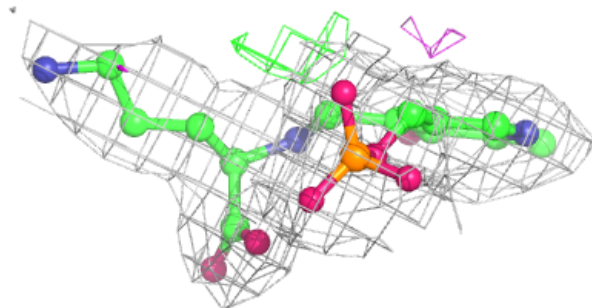
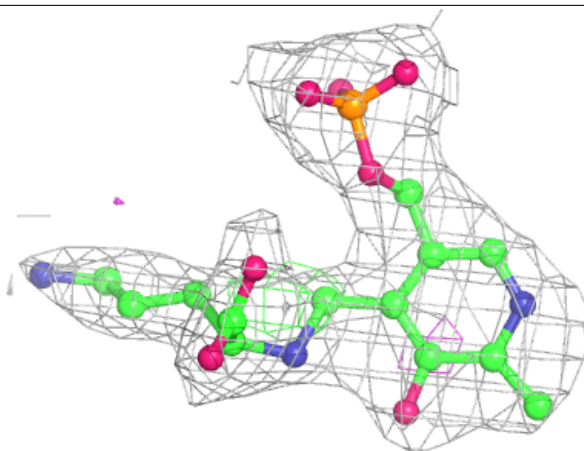
Electron density around ORX A 602:

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



Electron density around ORX B 603:

$2mF_o-DF_c$ (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.