



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 14, 2021 – 11:15 am BST

PDB ID : 6ZRJ
Title : Crystal structure of class D Beta-lactamase OXA-48 in complex with er-tapenem
Authors : Tassone, G.; Di Pisa, F.; Benvenuti, M.; De Luca, F.; Pozzi, C.; Docquier, J.D.; Mangani, S.
Deposited on : 2020-07-13
Resolution : 1.94 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 : 2.22
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) : 2.22

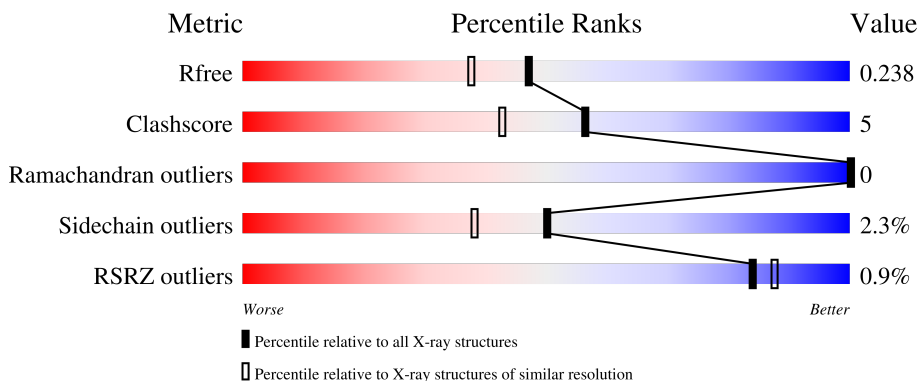
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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

Mol	Chain	Length	Quality of chain
1	A	265	 77% 14% 8% 2%
1	C	265	 83% 9% 8%
1	D	265	 82% 9% 9% 2%
1	E	265	 80% 12% 9% 2%
1	F	265	 81% 10% 9% 2%

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Mol	Chain	Length	Quality of chain
1	G	265	 <p>% 80% 10% 9%</p>
1	H	265	 <p>% 81% 10% 9%</p>
2	B	265	 <p>83% 9% 8%</p>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17792 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.

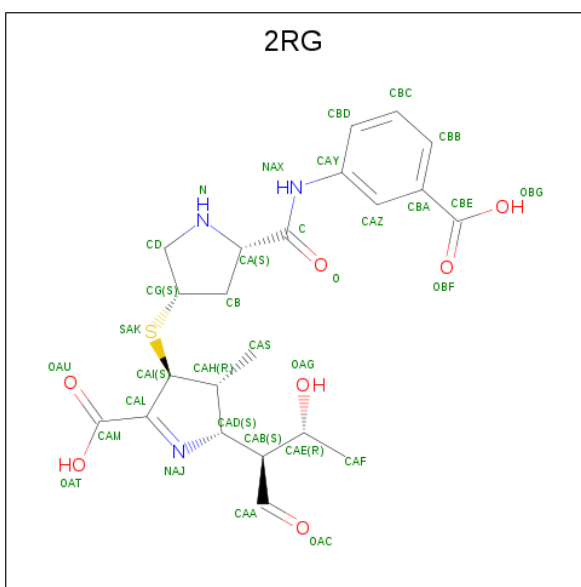
- Molecule 1 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	Total 2016	C 1286	N 350	O 370	S 10	0	11	0
1	C	243	Total 1997	C 1274	N 346	O 367	S 10	0	6	0
1	D	242	Total 1997	C 1273	N 347	O 369	S 8	0	7	0
1	E	242	Total 1967	C 1255	N 342	O 362	S 8	0	1	0
1	F	242	Total 1970	C 1258	N 345	O 360	S 7	0	3	0
1	G	242	Total 1971	C 1258	N 341	O 364	S 8	0	2	0
1	H	242	Total 1982	C 1261	N 348	O 366	S 7	0	4	0

- Molecule 2 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	243	Total 1985	C 1267	N 347	O 363	S 8	0	7	0

- Molecule 3 is (2S,3R,4S)-4-((3S,5S)-5-[(3-carboxyphenyl)carbamoyl]pyrrolidin-3-yl)sulfanyl)-2-[(1S,2R)-1-formyl-2-hydroxypropyl]-3-methyl-3,4-dihydro-2H-pyrrole-5-carboxylic acid (three-letter code: 2RG) (formula: C₂₂H₂₇N₃O₇S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	Total	C	N	O	S	0	0
			24	15	3	5	1		
3	B	1	Total	C	N	O	S	0	0
			24	15	3	5	1		
3	C	1	Total	C	N	O	S	0	0
			24	15	3	5	1		
3	D	1	Total	C	N	O	S	0	0
			24	15	3	5	1		
3	E	1	Total	C	N	O	S	0	0
			24	15	3	5	1		
3	F	1	Total	C	N	O	S	0	0
			24	15	3	5	1		
3	G	1	Total	C	N	O	S	0	0
			24	15	3	5	1		
3	H	1	Total	C	N	O	S	0	0
			24	15	3	5	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

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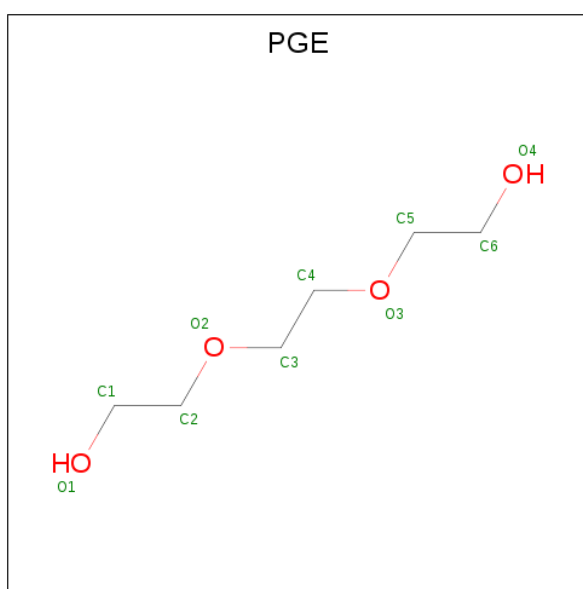
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	215	Total	O	0	7
			218	218		
7	B	221	Total	O	0	1
			222	222		
7	C	210	Total	O	0	1
			210	210		
7	D	245	Total	O	0	3
			246	246		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	160	Total 162	O 162	0	2
7	F	217	Total 222	O 222	0	5
7	G	172	Total 172	O 172	0	0
7	H	192	Total 192	O 192	0	0

3 Residue-property plots [i](#)


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.

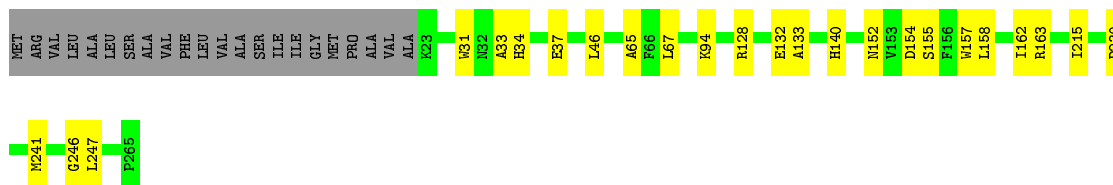
- Molecule 1: Beta-lactamase

Chain A: 




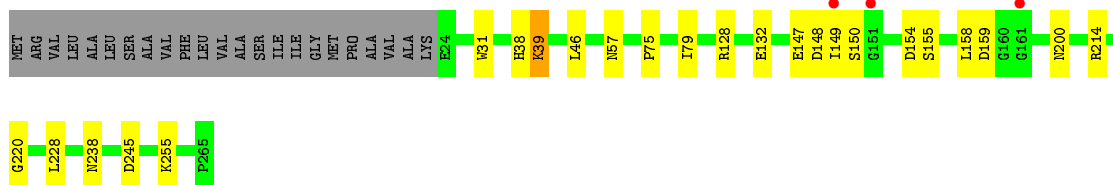
- Molecule 1: Beta-lactamase

Chain C: 




- Molecule 1: Beta-lactamase

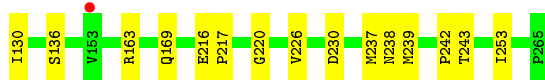
Chain D: 



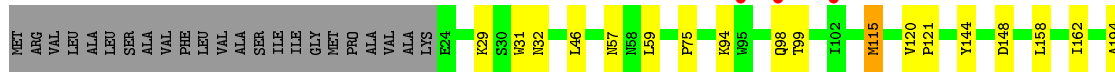
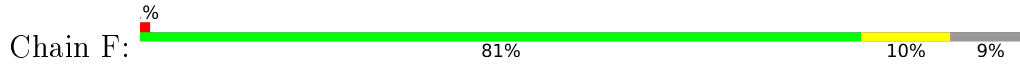
- Molecule 1: Beta-lactamase

Chain E: 

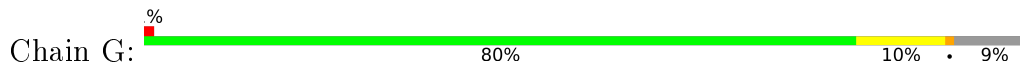




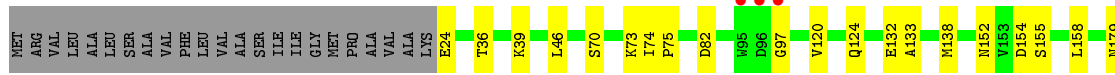
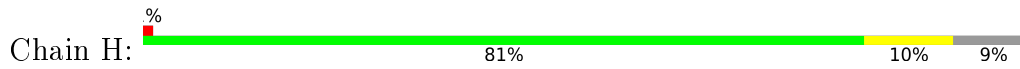
● Molecule 1: Beta-lactamase



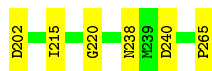
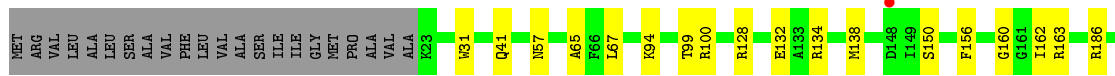
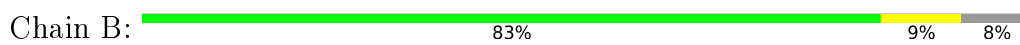
● Molecule 1: Beta-lactamase



● Molecule 1: Beta-lactamase



● Molecule 2: Beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.83Å 162.84Å 108.16Å 90.00° 90.59° 90.00°	Depositor
Resolution (Å)	48.51 – 1.94 48.51 – 1.94	Depositor EDS
% Data completeness (in resolution range)	97.1 (48.51-1.94) 97.1 (48.51-1.94)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.94Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.188 , 0.237 0.188 , 0.238	Depositor DCC
R_{free} test set	8005 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtrriage
Anisotropy	0.003	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.099 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17792	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.88% 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: 2RG, EDO, KCX, PGE, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/2070	0.75	0/2801
1	C	0.40	0/2048	0.76	0/2772
1	D	0.44	0/2042	0.80	0/2761
1	E	0.35	0/2006	0.72	0/2717
1	F	0.38	0/2015	0.73	0/2728
1	G	0.36	0/2013	0.72	0/2726
1	H	0.38	0/2028	0.72	0/2748
2	B	0.44	0/2046	0.77	0/2770
All	All	0.39	0/16268	0.75	0/22023

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2016	0	1948	22	0
1	C	1997	0	1931	19	0
1	D	1997	0	1929	16	0
1	E	1967	0	1886	21	0
1	F	1970	0	1910	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1971	0	1895	22	0
1	H	1982	0	1900	19	0
2	B	1985	0	1915	16	0
3	A	24	0	19	2	0
3	B	24	0	19	0	0
3	C	24	0	19	2	0
3	D	24	0	19	0	0
3	E	24	0	19	1	0
3	F	24	0	19	3	0
3	G	24	0	19	1	0
3	H	24	0	19	3	0
4	A	8	0	12	0	0
4	B	24	0	36	2	0
4	C	8	0	12	0	0
4	D	4	0	6	0	0
4	F	4	0	6	0	0
4	G	4	0	6	0	0
4	H	8	0	12	0	0
5	A	1	0	0	1	0
6	D	10	0	14	2	0
7	A	218	0	0	3	0
7	B	222	0	0	6	0
7	C	210	0	0	4	0
7	D	246	0	0	5	0
7	E	162	0	0	3	0
7	F	222	0	0	1	0
7	G	172	0	0	4	0
7	H	192	0	0	3	0
All	All	17792	0	15570	158	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 5.

All (158) 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)
2:B:67:LEU:HD21	2:B:160:GLY:HA2	1.36	1.05
1:D:38:HIS:HE1	7:D:678:HOH:O	1.46	0.98
1:G:135:MET:CG	1:G:149:ILE:HD11	2.03	0.88
5:A:504:CL:CL	7:B:771:HOH:O	2.29	0.87
1:E:237:MET:CE	1:E:239:MET:HE3	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:PRO:HD2	7:E:661:HOH:O	1.76	0.83
2:B:67:LEU:HD22	7:B:626:HOH:O	1.78	0.83
1:C:33:ALA:O	1:C:37:GLU:HB2	1.83	0.79
1:A:237[A]:MET:CE	1:A:250:ARG:HA	2.15	0.77
1:G:135:MET:HG2	1:G:149:ILE:HD11	1.66	0.77
1:A:152[B]:ASN:HB2	1:A:155:SER:OG	1.87	0.75
1:D:39:LYS:HE2	7:D:696:HOH:O	1.87	0.74
1:E:216:GLU:OE2	1:E:217:PRO:HA	1.88	0.73
1:H:70:SER:HB3	1:H:73:KCX:HE3	1.70	0.72
1:E:237:MET:HE1	1:E:239:MET:HE3	1.73	0.70
1:G:218:LYS:HE3	7:G:615:HOH:O	1.92	0.68
1:G:135:MET:HG3	1:G:149:ILE:HD11	1.73	0.67
1:E:237:MET:HE3	1:E:239:MET:HE3	1.77	0.65
1:H:97:GLY:HA3	7:H:747:HOH:O	1.95	0.65
2:B:41:GLN:HB2	2:B:240:ASP:OD2	1.97	0.64
1:C:241[B]:MET:HE1	1:C:247:LEU:N	2.12	0.64
1:A:258[A]:LEU:HB3	1:A:264:ILE:HG12	1.80	0.64
1:C:128:ARG:NH1	1:C:154:ASP:OD2	2.31	0.63
1:F:115:MET:HE2	1:F:194:ALA:O	2.00	0.61
1:E:239:MET:HE2	1:E:253:ILE:HD12	1.83	0.61
1:E:87:LYS:HB3	7:E:751:HOH:O	2.00	0.61
1:G:152:ASN:HB2	1:G:155:SER:OG	1.99	0.61
1:C:241[B]:MET:HE3	1:C:246:GLY:H	1.66	0.60
3:A:501:2RG:HA	7:A:757:HOH:O	2.01	0.60
1:D:228:LEU:O	6:D:401:PGE:H2	2.03	0.59
1:A:237[A]:MET:HE2	1:A:250:ARG:HA	1.85	0.59
1:E:239:MET:CE	1:E:253:ILE:HD12	2.32	0.59
1:D:132:GLU:HG2	1:D:149:ILE:HD13	1.85	0.58
2:B:67:LEU:CD2	2:B:160:GLY:HA2	2.23	0.57
1:C:155:SER:HA	1:C:158:LEU:CD1	2.34	0.57
3:A:501:2RG:HDA	3:A:501:2RG:OAU	2.04	0.57
1:G:138:MET:CE	1:G:138:MET:HA	2.34	0.57
1:A:255:LYS:HA	1:A:258[B]:LEU:HD12	1.87	0.56
1:H:246:GLY:O	1:H:249:LEU:HB2	2.06	0.56
1:D:38:HIS:O	1:D:39:LYS:HB2	2.04	0.56
1:C:132:GLU:HG3	7:C:693:HOH:O	2.05	0.56
2:B:31:TRP:HB2	2:B:57:ASN:HB3	1.87	0.55
3:E:501:2RG:HDA	3:E:501:2RG:OAU	2.06	0.55
1:H:152:ASN:HB2	1:H:155:SER:OG	2.06	0.55
1:D:147:GLU:HB3	7:D:547:HOH:O	2.07	0.55
1:F:212:SER:O	1:F:218:LYS:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:GLU:HA	7:G:691:HOH:O	2.06	0.55
1:G:170:ILE:O	1:G:174:ARG:HG3	2.06	0.54
1:F:158:LEU:HD21	3:F:501:2RG:CAF	2.38	0.54
1:G:157:TRP:CD1	1:G:158:LEU:HD13	2.42	0.54
1:C:94:LYS:HG2	7:C:625:HOH:O	2.08	0.53
1:G:200:ASN:HB2	7:G:649:HOH:O	2.09	0.53
3:H:501:2RG:OAU	3:H:501:2RG:HDA	2.09	0.53
1:C:157:TRP:NE1	1:C:158:LEU:HD11	2.24	0.53
1:C:155:SER:HA	1:C:158:LEU:HD13	1.92	0.52
1:A:246:GLY:O	1:A:249:LEU:HB2	2.10	0.52
1:E:42:GLY:HA2	1:E:61:ARG:NH2	2.24	0.52
1:C:67:LEU:HD11	1:C:215:ILE:HD12	1.92	0.52
1:D:200:ASN:O	6:D:401:PGE:H52	2.09	0.51
2:B:202:ASP:OD2	2:B:265:PRO:HG3	2.10	0.51
1:A:67:LEU:HD11	1:A:215:ILE:HD12	1.91	0.51
1:H:124:GLN:HG2	1:H:154:ASP:O	2.11	0.51
1:F:148:ASP:O	1:F:162:ILE:HB	2.11	0.51
1:C:140:HIS:HB2	7:C:766:HOH:O	2.10	0.51
1:A:237[A]:MET:HE3	1:A:250:ARG:HG2	1.93	0.51
1:A:128:ARG:NH1	1:A:154:ASP:OD2	2.44	0.50
1:A:115[A]:MET:HG3	1:A:194:ALA:HB1	1.92	0.50
1:A:237[A]:MET:HE1	1:A:250:ARG:HA	1.90	0.50
2:B:134:ARG:O	2:B:138:MET:HG2	2.12	0.50
1:A:43:VAL:HG22	1:A:44:VAL:N	2.27	0.49
2:B:100:ARG:HD2	7:B:643:HOH:O	2.12	0.49
1:C:152[A]:ASN:HB2	1:C:155:SER:OG	2.11	0.49
1:C:241[B]:MET:HE1	1:C:247:LEU:CA	2.41	0.49
1:A:170:ILE:O	1:A:174:ARG:HG3	2.12	0.49
1:C:157:TRP:HA	1:C:162:ILE:CG2	2.42	0.49
1:F:220:GLY:O	1:F:238:ASN:HA	2.12	0.49
1:H:243:THR:HA	7:H:604:HOH:O	2.12	0.49
1:H:73:KCX:CX	1:H:120:VAL:HG22	2.42	0.49
1:F:115:MET:HE1	1:F:195:MET:HA	1.95	0.49
3:C:501:2RG:HG	3:C:501:2RG:CAM	2.42	0.48
1:F:158:LEU:HD21	3:F:501:2RG:HAF	1.95	0.48
1:F:205:ILE:HG12	1:F:226:VAL:HG22	1.96	0.48
1:E:26:GLN:HB2	7:E:743:HOH:O	2.13	0.47
1:C:157:TRP:CE2	1:C:158:LEU:HD11	2.50	0.47
2:B:150:SER:O	2:B:156:PHE:HB2	2.14	0.47
4:B:504:EDO:H11	7:B:794:HOH:O	2.13	0.47
2:B:220:GLY:O	2:B:238:ASN:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LYS:HE3	7:A:672:HOH:O	2.14	0.47
1:D:155:SER:HA	1:D:158:LEU:HD12	1.97	0.46
1:E:73:KCX:HE2	1:E:118:SER:C	2.36	0.46
1:A:65:ALA:HB1	1:A:163:ARG:HB3	1.97	0.46
1:D:159:ASP:HB3	1:D:214:ARG:HD3	1.97	0.46
1:H:138:MET:HA	1:H:138:MET:CE	2.46	0.45
1:A:220:GLY:O	1:A:238:ASN:HA	2.17	0.45
1:H:120:VAL:CG2	3:H:501:2RG:HAE	2.45	0.45
2:B:163:ARG:HD2	7:B:608:HOH:O	2.16	0.45
3:C:501:2RG:HASB	3:C:501:2RG:OAG	2.15	0.45
1:G:179:ASN:HA	1:G:188:GLN:OE1	2.16	0.45
1:A:165:SER:OG	1:A:168:GLU:HG3	2.17	0.45
1:G:138:MET:HA	1:G:138:MET:HE2	1.98	0.44
1:D:128:ARG:HD3	1:D:154[B]:ASP:OD2	2.17	0.44
1:G:120:VAL:N	1:G:121:PRO:CD	2.81	0.44
1:G:155:SER:O	1:G:158:LEU:HB2	2.18	0.44
2:B:67:LEU:HD11	2:B:215:ILE:HG13	2.00	0.44
1:E:163:ARG:HG2	1:E:163:ARG:HH11	1.82	0.44
1:H:70:SER:CB	1:H:73:KCX:HE3	2.44	0.44
1:H:24:GLU:HA	7:H:735:HOH:O	2.17	0.44
1:E:237:MET:HE3	1:E:239:MET:CE	2.47	0.43
1:F:29:LYS:O	1:F:32:ASN:HB2	2.18	0.43
1:E:116:LYS:HD3	1:E:117:TYR:CE2	2.53	0.43
2:B:65:ALA:HB1	2:B:163:ARG:HB3	2.00	0.43
1:C:31:TRP:O	1:C:34:HIS:N	2.46	0.43
1:G:94:LYS:HA	1:G:108:ASP:OD1	2.18	0.43
1:F:94:LYS:HB3	1:F:94:LYS:HE3	1.75	0.43
1:E:126:PHE:O	1:E:130:ILE:HG13	2.19	0.43
2:B:128:ARG:NH2	7:B:616:HOH:O	2.49	0.43
1:E:27:GLU:HA	1:E:56:THR:O	2.19	0.43
1:G:261:GLU:O	1:G:262:LYS:HB2	2.19	0.43
1:C:65:ALA:HB1	1:C:163:ARG:HB3	2.01	0.43
1:E:70:SER:HA	1:E:73:KCX:OQ2	2.19	0.43
1:F:75:PRO:HG3	1:F:144:TYR:CE2	2.53	0.43
1:F:265:PRO:HD3	7:F:753:HOH:O	2.18	0.43
1:G:48:ASN:HB2	1:G:233:TRP:CH2	2.53	0.43
1:G:65:ALA:HB1	1:G:163:ARG:HB3	2.01	0.42
1:H:179:ASN:HA	1:H:188:GLN:OE1	2.19	0.42
1:E:85:VAL:HG13	1:E:129:GLN:OE1	2.19	0.42
1:G:24:GLU:HG2	7:G:691:HOH:O	2.19	0.42
1:G:158:LEU:HD11	3:G:501:2RG:CAF	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:TYR:CZ	1:A:232[B]:VAL:HG21	2.54	0.42
1:F:120:VAL:N	1:F:121:PRO:HD2	2.34	0.42
1:H:70:SER:HA	1:H:73:KCX:OQ2	2.20	0.42
1:A:43:VAL:CG1	1:A:61:ARG:HG2	2.50	0.42
1:C:241[B]:MET:HE3	1:C:246:GLY:N	2.34	0.42
1:H:73:KCX:HD3	1:H:208:LYS:HE3	2.02	0.42
1:D:220:GLY:O	1:D:238:ASN:HA	2.20	0.41
1:G:135:MET:HG3	1:G:149:ILE:CD1	2.47	0.41
1:H:74:ILE:HB	1:H:75:PRO:CD	2.50	0.41
1:A:178:HIS:HB3	1:A:180:LYS:HE2	2.01	0.41
1:D:31:TRP:HB2	1:D:57:ASN:HB3	2.01	0.41
1:E:120:VAL:N	1:E:121:PRO:CD	2.83	0.41
3:F:501:2RG:HASB	3:F:501:2RG:OAG	2.20	0.41
1:G:177:TYR:CZ	1:G:232:VAL:HG21	2.55	0.41
1:F:31:TRP:HB2	1:F:57:ASN:HB3	2.02	0.41
1:H:132:GLU:HG3	1:H:133:ALA:N	2.35	0.41
1:H:158:LEU:HD21	3:H:501:2RG:CAF	2.50	0.41
1:A:41:GLN:HG2	7:A:667:HOH:O	2.19	0.41
1:E:220:GLY:O	1:E:238:ASN:HA	2.20	0.41
1:C:133:ALA:HB3	7:C:621:HOH:O	2.20	0.41
2:B:67:LEU:HD23	2:B:162:ILE:O	2.21	0.40
2:B:186:ARG:HD3	4:B:504:EDO:C1	2.52	0.40
1:D:75:PRO:O	1:D:79:ILE:HG13	2.21	0.40
1:D:255:LYS:HE3	7:D:614:HOH:O	2.21	0.40
1:D:132:GLU:HB2	7:D:699:HOH:O	2.21	0.40
1:D:148:ASP:HB3	1:D:150:SER:OG	2.22	0.40
1:E:163:ARG:HG2	1:E:163:ARG:NH1	2.36	0.40
1:H:36:THR:O	1:H:39:LYS:N	2.42	0.40
1:H:261:GLU:HB2	1:H:263:ILE:HD12	2.03	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	249/265 (94%)	239 (96%)	10 (4%)	0	100	100
1	C	245/265 (92%)	236 (96%)	9 (4%)	0	100	100
1	D	243/265 (92%)	237 (98%)	6 (2%)	0	100	100
1	E	240/265 (91%)	232 (97%)	8 (3%)	0	100	100
1	F	242/265 (91%)	236 (98%)	6 (2%)	0	100	100
1	G	241/265 (91%)	231 (96%)	10 (4%)	0	100	100
1	H	243/265 (92%)	232 (96%)	11 (4%)	0	100	100
2	B	246/265 (93%)	241 (98%)	5 (2%)	0	100	100
All	All	1949/2120 (92%)	1884 (97%)	65 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	213/227 (94%)	200 (94%)	13 (6%)	18	6
1	C	210/227 (92%)	208 (99%)	2 (1%)	76	71
1	D	211/227 (93%)	208 (99%)	3 (1%)	67	58
1	E	203/227 (89%)	198 (98%)	5 (2%)	47	35
1	F	206/227 (91%)	200 (97%)	6 (3%)	42	28
1	G	205/227 (90%)	199 (97%)	6 (3%)	42	28
1	H	207/227 (91%)	205 (99%)	2 (1%)	76	71
2	B	209/228 (92%)	206 (99%)	3 (1%)	67	58
All	All	1664/1817 (92%)	1624 (98%)	40 (2%)	50	36

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	28	ASN

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Mol	Chain	Res	Type
1	A	40	SER
1	A	41	GLN
1	A	52	GLN
1	A	70	SER
1	A	101	ASP
1	A	162	ILE
1	A	169	GLN
1	A	237[A]	MET
1	A	237[B]	MET
1	A	258[A]	LEU
1	A	258[B]	LEU
2	B	94	LYS
2	B	99	THR
2	B	132	GLU
1	C	46	LEU
1	C	230	ASP
1	D	39	LYS
1	D	46	LEU
1	D	245	ASP
1	E	136	SER
1	E	169	GLN
1	E	226	VAL
1	E	230	ASP
1	E	243	THR
1	F	46	LEU
1	F	59	LEU
1	F	98	GLN
1	F	99	THR
1	F	115	MET
1	F	243	THR
1	G	24	GLU
1	G	52	GLN
1	G	101	ASP
1	G	149	ILE
1	G	158	LEU
1	G	243	THR
1	H	46	LEU
1	H	82	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues 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
1	KCX	F	73	1	7,11,12	0.41	0	4,12,14	0.45	0
1	KCX	G	73	1	7,11,12	0.63	0	4,12,14	1.25	0
1	KCX	A	73	1	7,11,12	0.41	0	4,12,14	0.52	0
1	KCX	D	73	1	7,11,12	0.54	0	4,12,14	0.56	0
1	KCX	E	73	1	7,11,12	0.47	0	4,12,14	0.38	0
1	KCX	H	73	1	7,11,12	0.42	0	4,12,14	0.41	0
1	KCX	C	73	1	7,11,12	0.50	0	4,12,14	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	F	73	1	-	1/7/10/12	-
1	KCX	G	73	1	-	1/7/10/12	-
1	KCX	A	73	1	-	0/7/10/12	-
1	KCX	D	73	1	-	0/7/10/12	-
1	KCX	E	73	1	-	1/7/10/12	-
1	KCX	H	73	1	-	1/7/10/12	-
1	KCX	C	73	1	-	1/7/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	G	73	KCX	O-C-CA-CB
1	F	73	KCX	CG-CD-CE-NZ
1	C	73	KCX	CG-CD-CE-NZ
1	E	73	KCX	CG-CD-CE-NZ
1	H	73	KCX	CE-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	73	KCX	2	0
1	H	73	KCX	5	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 1 is monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	B	503	-	3,3,3	0.26	0	2,2,2	0.46	0
4	EDO	C	503	-	3,3,3	0.48	0	2,2,2	1.32	0
3	2RG	E	501	1	20,25,35	0.95	1 (5%)	10,36,50	0.82	0
4	EDO	B	506	-	3,3,3	0.27	0	2,2,2	0.20	0
4	EDO	A	503	-	3,3,3	0.12	0	2,2,2	0.03	0
3	2RG	H	501	1	20,25,35	0.66	0	10,36,50	0.66	0
4	EDO	H	502	-	3,3,3	0.20	0	2,2,2	0.17	0
4	EDO	B	505	-	3,3,3	0.18	0	2,2,2	0.27	0
4	EDO	A	502	-	3,3,3	0.07	0	2,2,2	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	2RG	B	501	2	20,25,35	0.89	2 (10%)	10,36,50	0.74	0
3	2RG	C	501	1	20,25,35	0.68	0	10,36,50	0.84	0
3	2RG	D	402	1	20,25,35	1.04	1 (5%)	10,36,50	0.96	1 (10%)
4	EDO	H	503	-	3,3,3	0.14	0	2,2,2	0.54	0
4	EDO	G	502	-	3,3,3	0.17	0	2,2,2	0.30	0
4	EDO	B	504	-	3,3,3	0.13	0	2,2,2	0.72	0
4	EDO	B	507	-	3,3,3	0.29	0	2,2,2	0.29	0
4	EDO	C	502	-	3,3,3	0.26	0	2,2,2	0.63	0
3	2RG	F	501	1	20,25,35	0.66	0	10,36,50	0.72	0
3	2RG	A	501	1	20,25,35	0.83	1 (5%)	10,36,50	1.47	2 (20%)
6	PGE	D	401	-	9,9,9	0.41	0	8,8,8	0.36	0
4	EDO	D	403	-	3,3,3	0.22	0	2,2,2	0.30	0
4	EDO	B	502	-	3,3,3	0.16	0	2,2,2	0.60	0
3	2RG	G	501	1	20,25,35	0.89	2 (10%)	10,36,50	0.94	1 (10%)
4	EDO	F	502	-	3,3,3	0.08	0	2,2,2	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	C	503	-	-	0/1/1/1	-
3	2RG	E	501	1	-	1/14/47/55	0/2/2/3
4	EDO	B	506	-	-	1/1/1/1	-
4	EDO	A	503	-	-	1/1/1/1	-
3	2RG	H	501	1	-	2/14/47/55	0/2/2/3
4	EDO	H	502	-	-	0/1/1/1	-
4	EDO	B	505	-	-	0/1/1/1	-
4	EDO	A	502	-	-	0/1/1/1	-
3	2RG	B	501	2	-	4/14/47/55	0/2/2/3
3	2RG	C	501	1	-	4/14/47/55	0/2/2/3
3	2RG	D	402	1	-	4/14/47/55	0/2/2/3
4	EDO	H	503	-	-	1/1/1/1	-
4	EDO	G	502	-	-	0/1/1/1	-
4	EDO	B	504	-	-	1/1/1/1	-
4	EDO	B	507	-	-	0/1/1/1	-
4	EDO	C	502	-	-	0/1/1/1	-
3	2RG	F	501	1	-	4/14/47/55	0/2/2/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2RG	A	501	1	-	4/14/47/55	0/2/2/3
6	PGE	D	401	-	-	7/7/7/7	-
4	EDO	D	403	-	-	0/1/1/1	-
4	EDO	B	502	-	-	1/1/1/1	-
3	2RG	G	501	1	-	0/14/47/55	0/2/2/3
4	EDO	F	502	-	-	1/1/1/1	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	2RG	CG-SAK	3.36	1.88	1.82
3	E	501	2RG	CG-SAK	2.77	1.87	1.82
3	B	501	2RG	CG-SAK	2.58	1.87	1.82
3	B	501	2RG	CAM-CAL	-2.41	1.48	1.52
3	G	501	2RG	CAM-CAL	-2.33	1.48	1.52
3	A	501	2RG	CG-SAK	2.32	1.87	1.82
3	G	501	2RG	CG-SAK	2.02	1.86	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	2RG	CAB-CAD-NAJ	-2.84	106.41	111.94
3	A	501	2RG	C-CA-N	2.84	117.19	111.88
3	G	501	2RG	CAB-CAD-NAJ	-2.33	107.42	111.94
3	D	402	2RG	C-CA-N	2.19	115.97	111.88

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	2RG	O-C-CA-N
3	A	501	2RG	NAX-C-CA-N
3	B	501	2RG	O-C-CA-N
3	B	501	2RG	NAX-C-CA-N
3	C	501	2RG	O-C-CA-N
3	C	501	2RG	NAX-C-CA-N
3	D	402	2RG	O-C-CA-N
3	D	402	2RG	NAX-C-CA-N
3	E	501	2RG	NAX-C-CA-N
3	F	501	2RG	NAX-C-CA-N
3	H	501	2RG	NAX-C-CA-N

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Mol	Chain	Res	Type	Atoms
6	D	401	PGE	O1-C1-C2-O2
6	D	401	PGE	O2-C3-C4-O3
6	D	401	PGE	O3-C5-C6-O4
6	D	401	PGE	C3-C4-O3-C5
4	F	502	EDO	O1-C1-C2-O2
6	D	401	PGE	C4-C3-O2-C2
6	D	401	PGE	C6-C5-O3-C4
4	B	506	EDO	O1-C1-C2-O2
3	A	501	2RG	O-C-CA-CB
3	B	501	2RG	O-C-CA-CB
3	C	501	2RG	O-C-CA-CB
3	D	402	2RG	O-C-CA-CB
3	H	501	2RG	NAX-C-CA-CB
6	D	401	PGE	C1-C2-O2-C3
4	B	502	EDO	O1-C1-C2-O2
4	H	503	EDO	O1-C1-C2-O2
3	F	501	2RG	O-C-CA-N
4	A	503	EDO	O1-C1-C2-O2
4	B	504	EDO	O1-C1-C2-O2
3	A	501	2RG	NAX-C-CA-CB
3	B	501	2RG	NAX-C-CA-CB
3	C	501	2RG	NAX-C-CA-CB
3	D	402	2RG	NAX-C-CA-CB
3	F	501	2RG	O-C-CA-CB
3	F	501	2RG	NAX-C-CA-CB

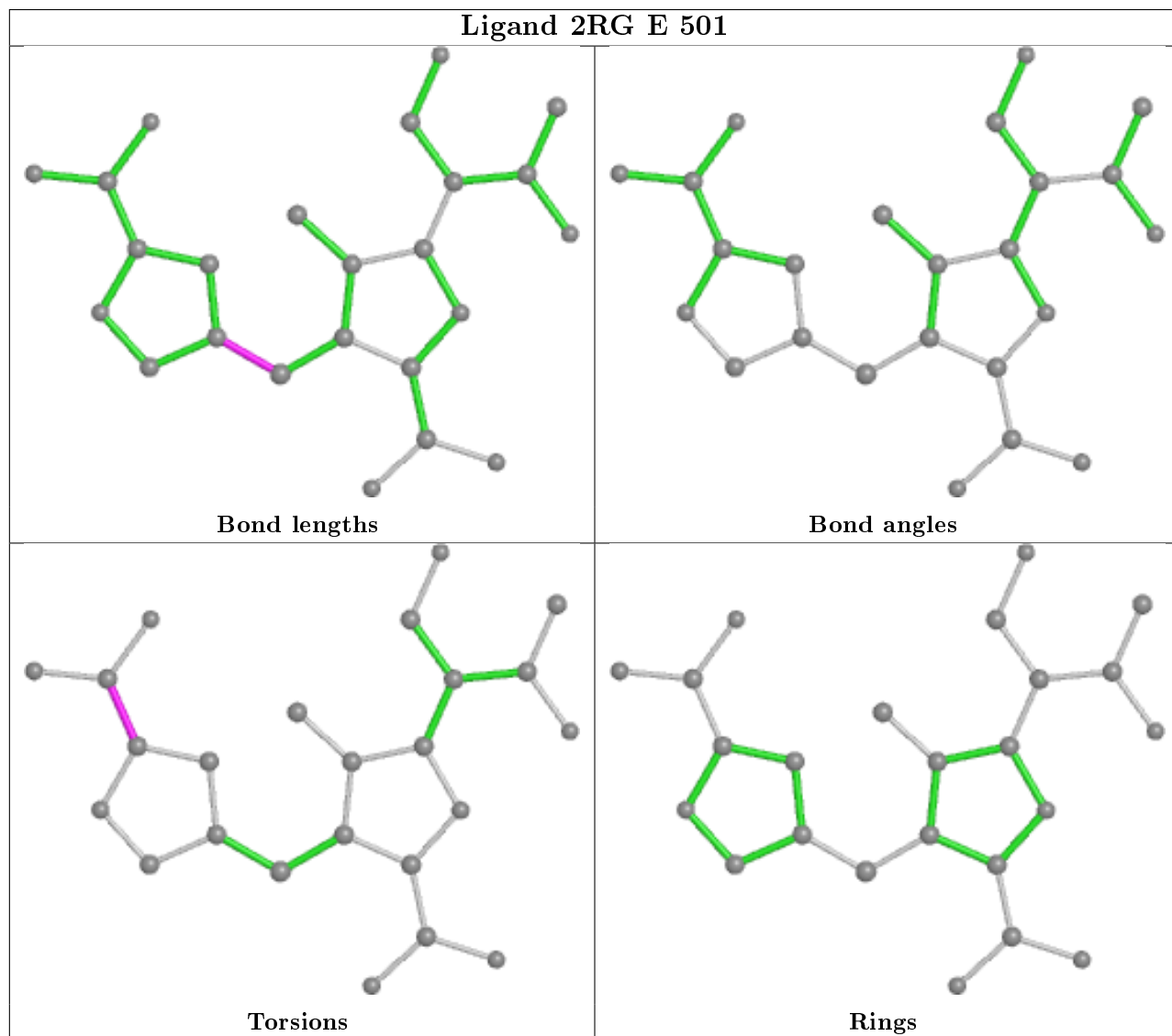
There are no ring outliers.

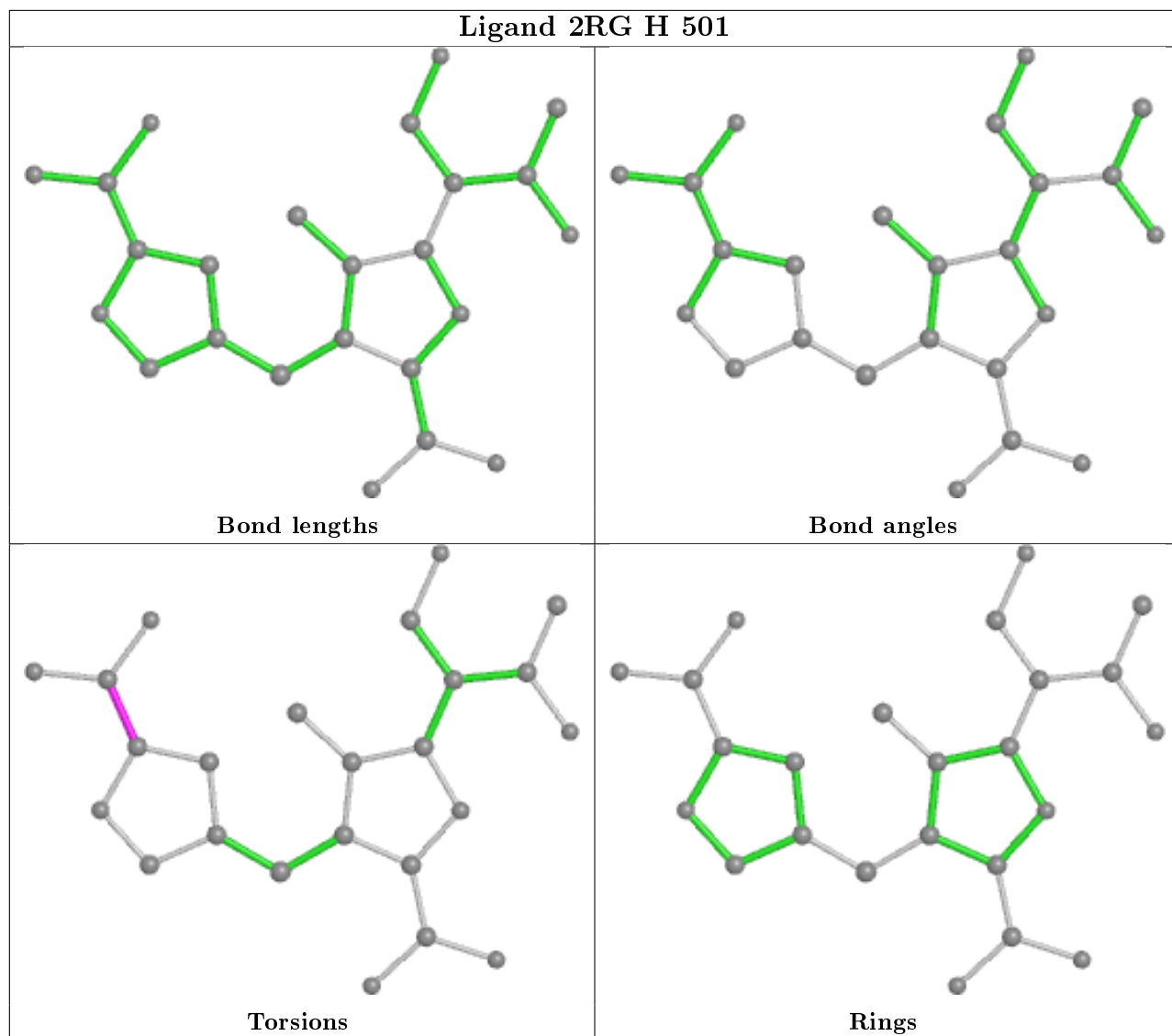
8 monomers are involved in 16 short contacts:

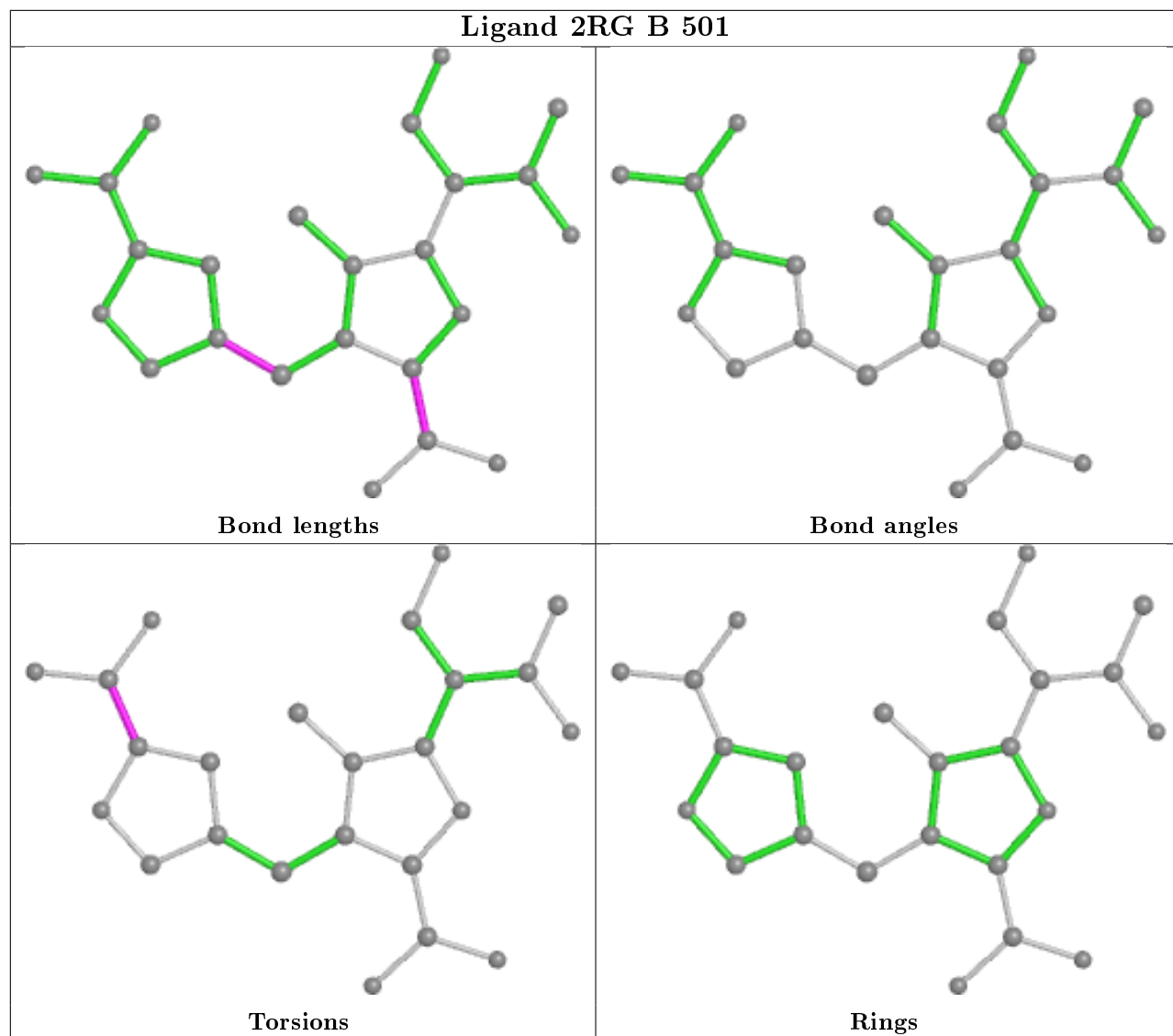
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	501	2RG	1	0
3	H	501	2RG	3	0
3	C	501	2RG	2	0
4	B	504	EDO	2	0
3	F	501	2RG	3	0
3	A	501	2RG	2	0
6	D	401	PGE	2	0
3	G	501	2RG	1	0

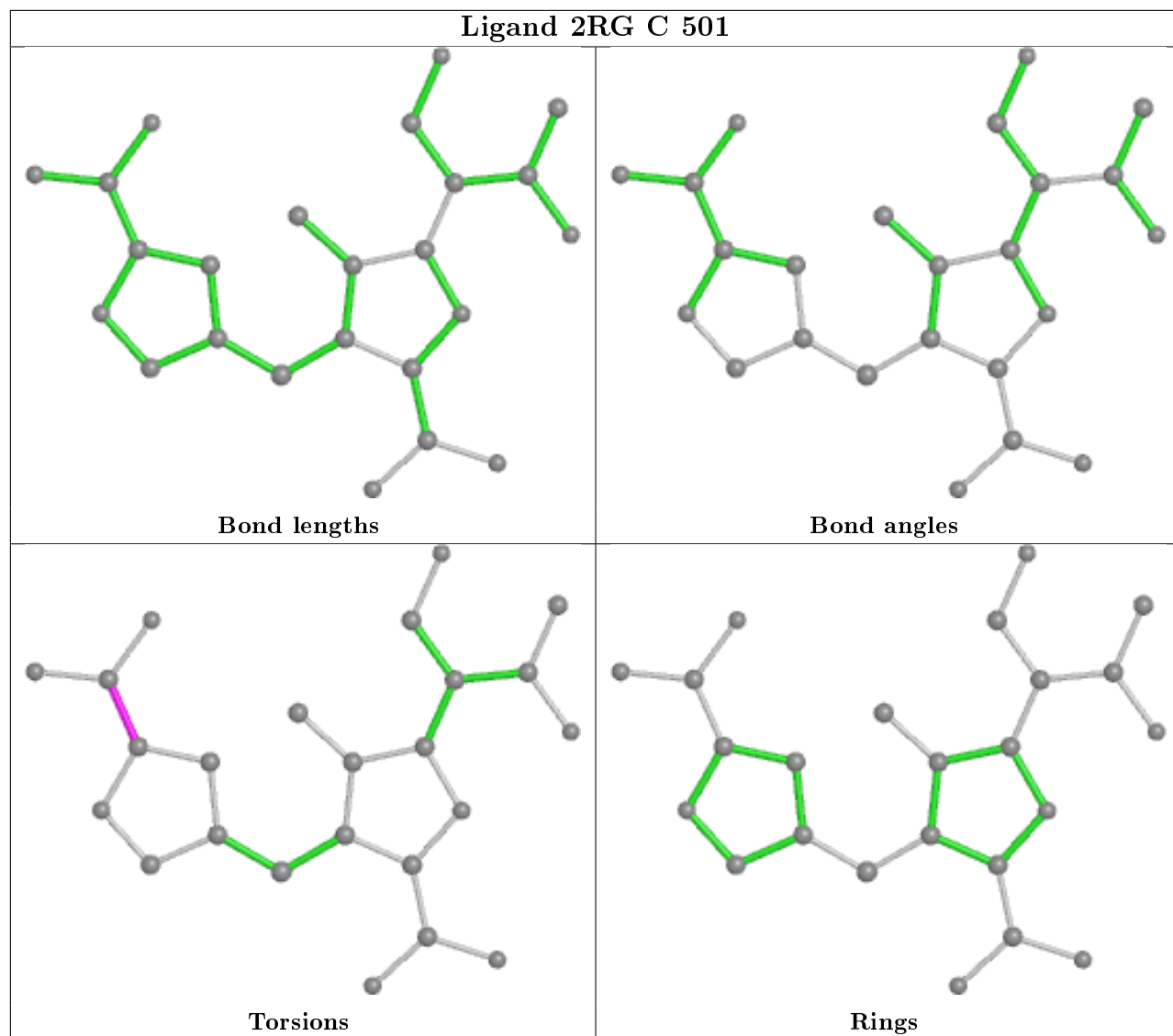
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

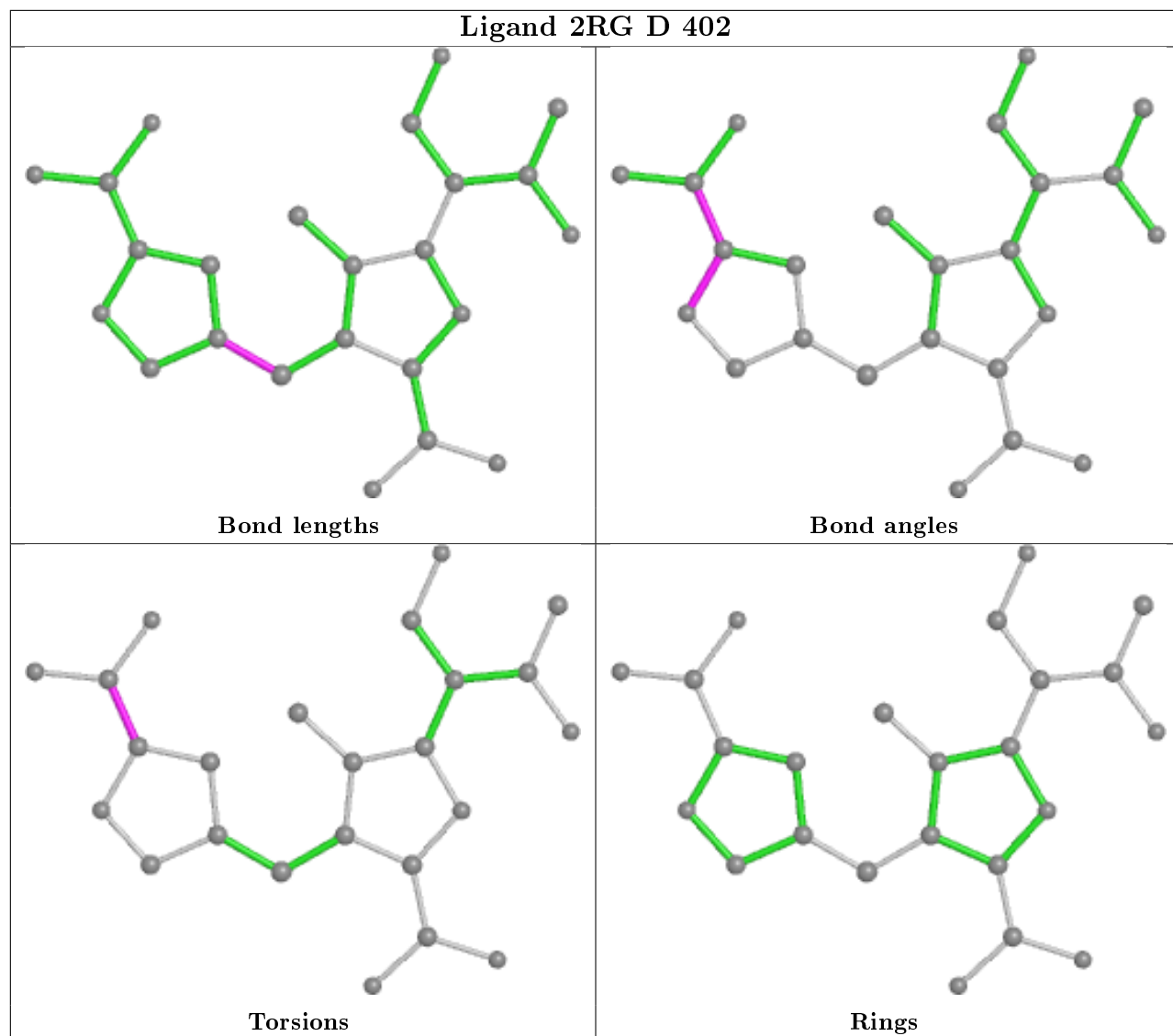
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

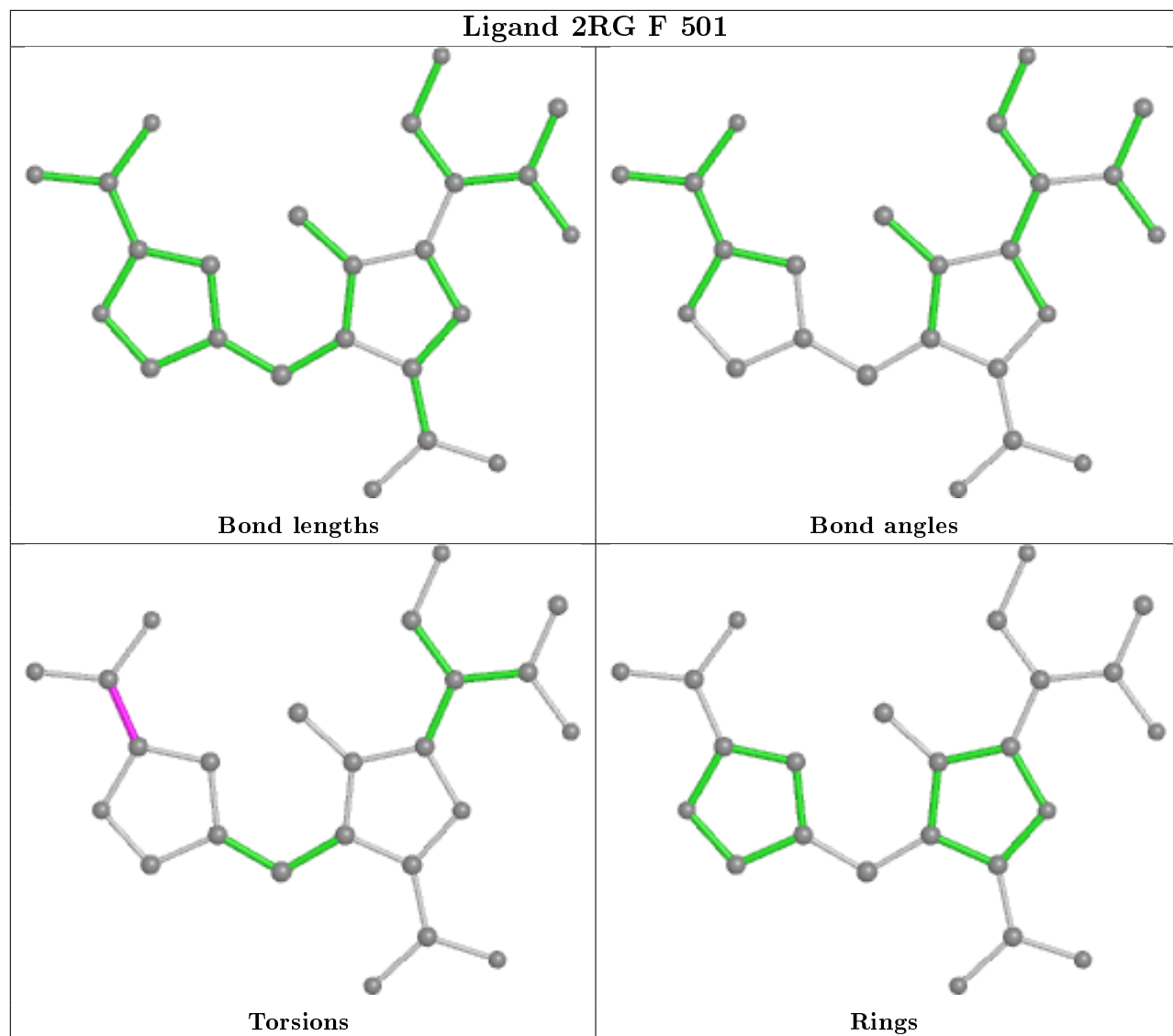


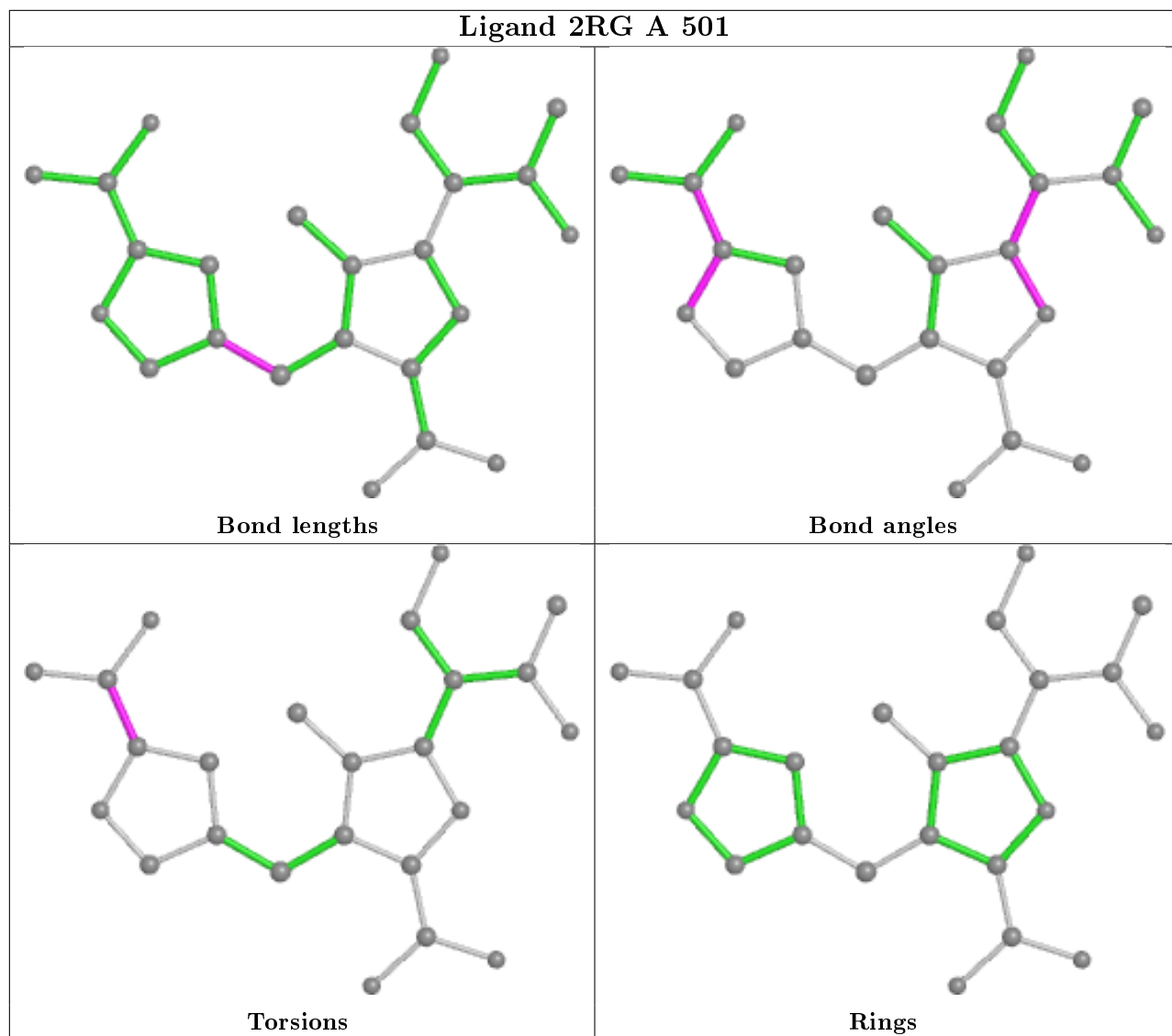


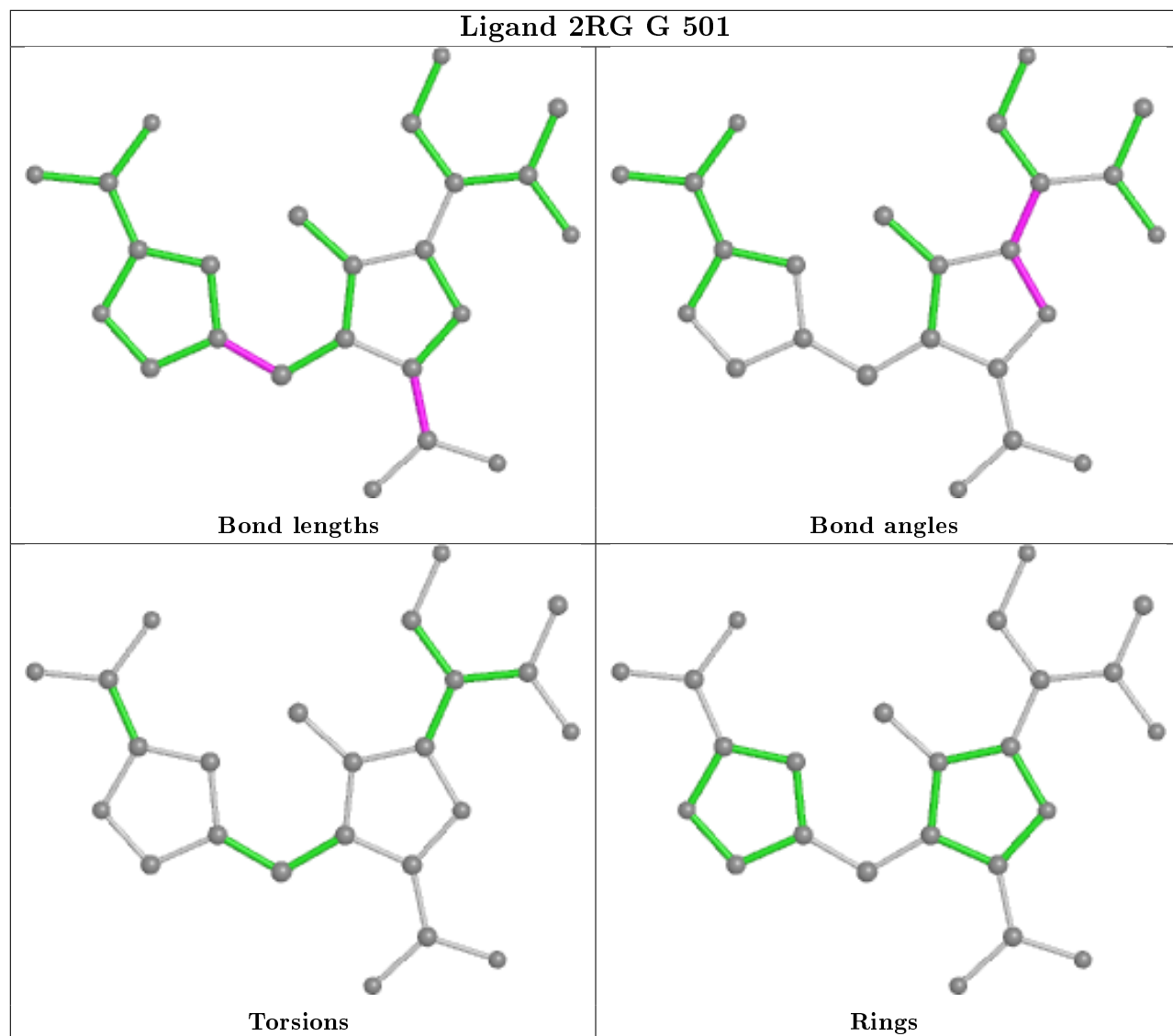












5.7 Other polymers [i](#)

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	242/265 (91%)	-0.19	0 100 100	12, 28, 50, 69	4 (1%)
1	C	242/265 (91%)	-0.27	0 100 100	9, 26, 47, 71	5 (2%)
1	D	241/265 (90%)	-0.16	3 (1%) 79 83	8, 18, 49, 88	6 (2%)
1	E	241/265 (90%)	0.04	5 (2%) 63 70	16, 32, 54, 64	5 (2%)
1	F	241/265 (90%)	-0.16	3 (1%) 79 83	12, 27, 49, 69	0
1	G	241/265 (90%)	-0.03	3 (1%) 79 83	15, 30, 52, 66	4 (1%)
1	H	241/265 (90%)	-0.04	3 (1%) 79 83	13, 29, 54, 67	5 (2%)
2	B	243/265 (91%)	-0.26	1 (0%) 92 95	10, 19, 41, 76	3 (1%)
All	All	1932/2120 (91%)	-0.13	18 (0%) 84 87	8, 26, 52, 88	32 (1%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	149	ILE	4.6
1	G	95	TRP	3.5
1	G	149	ILE	3.2
1	E	95	TRP	3.1
1	F	95	TRP	2.8
1	G	98	GLN	2.8
1	H	97	GLY	2.7
2	B	148	ASP	2.7
1	E	153	VAL	2.6
1	D	161	GLY	2.6
1	E	102	ILE	2.5
1	F	98	GLN	2.5
1	F	102	ILE	2.4
1	D	151	GLY	2.4
1	H	95	TRP	2.3
1	E	99	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	96	ASP	2.1
1	E	97	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KCX	E	73	12/13	0.92	0.14	20,27,61,66	0
1	KCX	G	73	12/13	0.92	0.13	18,23,44,48	0
1	KCX	A	73	12/13	0.93	0.13	16,18,38,43	0
1	KCX	C	73	12/13	0.94	0.13	12,15,39,46	0
1	KCX	F	73	12/13	0.95	0.10	18,24,50,56	0
1	KCX	D	73	12/13	0.95	0.14	10,13,57,59	0
1	KCX	H	73	12/13	0.95	0.14	20,24,46,47	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	2RG	F	501	24/33	0.87	0.16	35,48,61,64	0
4	EDO	C	503	4/4	0.88	0.14	33,34,41,41	0
6	PGE	D	401	10/10	0.88	0.14	39,44,49,50	0
3	2RG	A	501	24/33	0.89	0.15	27,41,68,70	0
3	2RG	G	501	24/33	0.89	0.14	37,47,69,71	0
3	2RG	D	402	24/33	0.90	0.14	19,35,59,61	0
3	2RG	H	501	24/33	0.90	0.15	38,55,76,79	0
3	2RG	E	501	24/33	0.90	0.14	35,51,73,79	0
3	2RG	C	501	24/33	0.90	0.14	27,49,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	B	504	4/4	0.91	0.14	30,33,36,39	0
3	2RG	B	501	24/33	0.91	0.14	23,33,59,60	0
4	EDO	F	502	4/4	0.91	0.13	35,40,41,44	0
4	EDO	B	503	4/4	0.91	0.16	26,28,35,37	0
4	EDO	B	502	4/4	0.92	0.13	31,36,36,42	0
4	EDO	H	503	4/4	0.93	0.12	41,41,42,45	0
4	EDO	B	506	4/4	0.94	0.14	35,35,36,40	0
4	EDO	D	403	4/4	0.95	0.15	34,36,36,41	0
4	EDO	B	505	4/4	0.95	0.13	33,35,38,47	0
4	EDO	A	503	4/4	0.95	0.12	35,35,37,42	0
4	EDO	A	502	4/4	0.95	0.10	30,34,34,39	0
4	EDO	C	502	4/4	0.96	0.12	23,25,28,30	0
4	EDO	G	502	4/4	0.96	0.09	33,34,34,36	0
4	EDO	B	507	4/4	0.97	0.09	19,26,26,28	0
4	EDO	H	502	4/4	0.97	0.07	27,28,30,32	0
5	CL	A	504	1/1	1.00	0.09	14,14,14,14	1

6.5 Other polymers [i](#)

There are no such residues in this entry.