



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 01:17 pm BST

PDB ID : 8RGL
Title : Structure of Human Serum Albumin in complex with Aristolochic Acid I at
1.9 Å resolution - Optimized
Authors : Pomyalov, S.; Sidorenko, V.S.; Grollman, A.P.; Shoham, G.
Deposited on : 2023-12-13
Resolution : 1.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

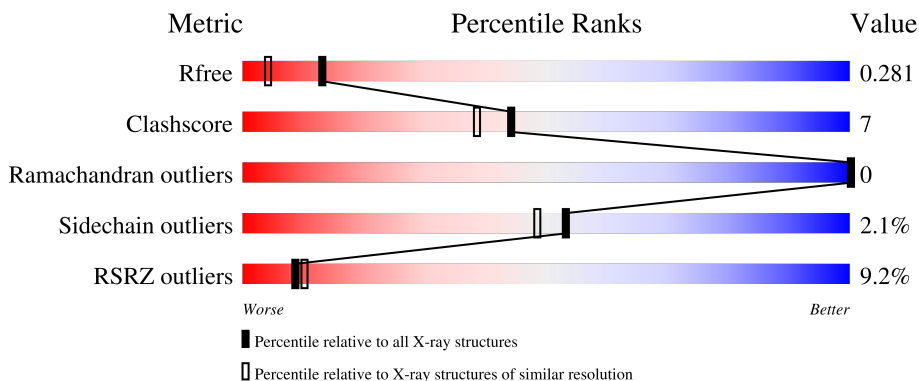
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	609	
1	B	609	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MYR	A	603	-	-	X	-

2 Entry composition [i](#)

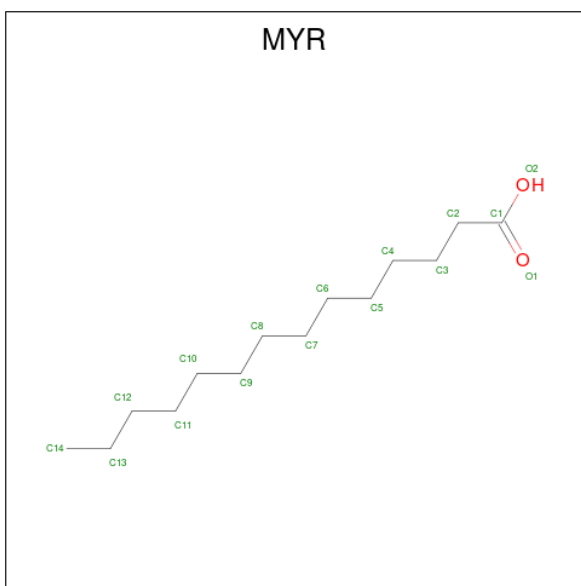
There are 5 unique types of molecules in this entry. The entry contains 19284 atoms, of which 9312 are hydrogens and 0 are deuteriums.

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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	582	Total	C	H	N	O	S	0	4	0
			9066	2900	4474	778	873	41			
1	B	582	Total	C	H	N	O	S	0	2	0
			9064	2898	4474	781	870	41			

- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



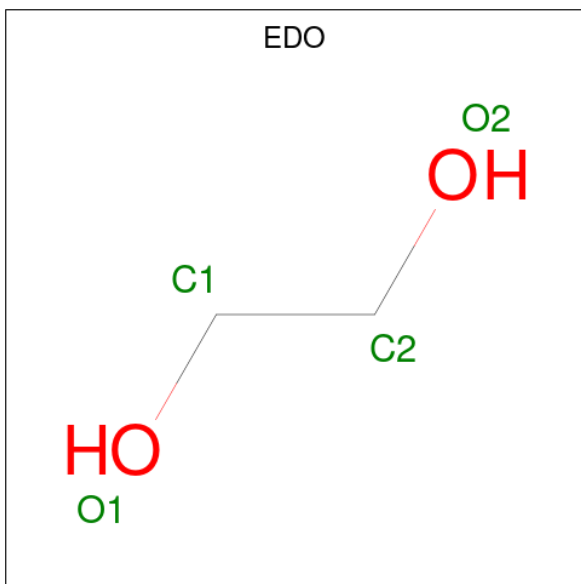
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	Total	C	H	O	0	0
			44	14	28	2		
2	A	1	Total	C	H	O	0	0
			44	14	28	2		
2	A	1	Total	C	H	O	0	0
			44	14	28	2		
2	A	1	Total	C	H	O	0	0
			44	14	28	2		

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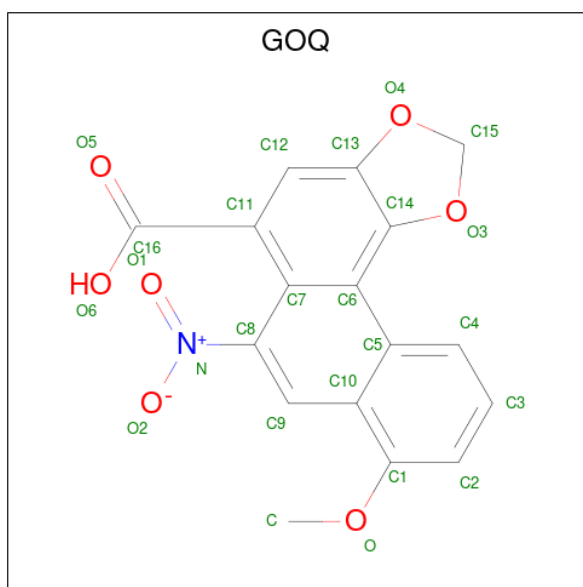
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			44	14	28	2		
2	A	1	Total	C	H	O	0	0
			44	14	28	2		
2	B	1	Total	C	H	O	0	0
			44	14	28	2		
2	B	1	Total	C	H	O	0	0
			44	14	28	2		
2	B	1	Total	C	H	O	0	0
			44	14	28	2		
2	B	1	Total	C	H	O	0	0
			44	14	28	2		
2	B	1	Total	C	H	O	0	0
			44	14	28	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is 8-methoxy-6-nitro-naphtho[1,2-e][1,3]benzodioxole-5-carboxylic acid (three-letter code: GOQ) (formula: C₁₇H₁₁NO₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
4	A	1	36	17	11	1	7	0	0
4	B	1	36	17	11	1	7	0	0

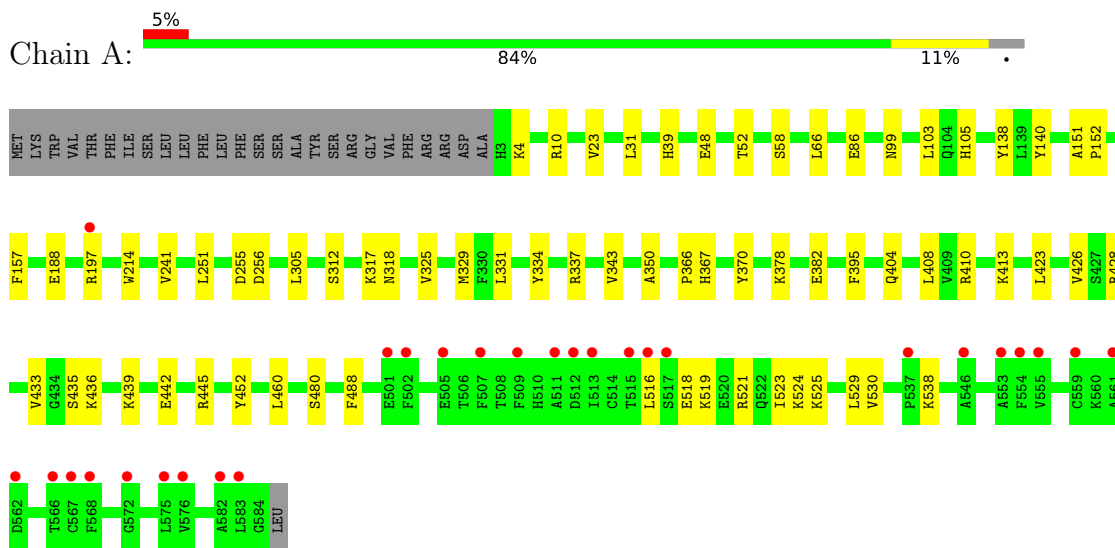
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	377	380	380	0	3
5	B	163	164	164	0	1

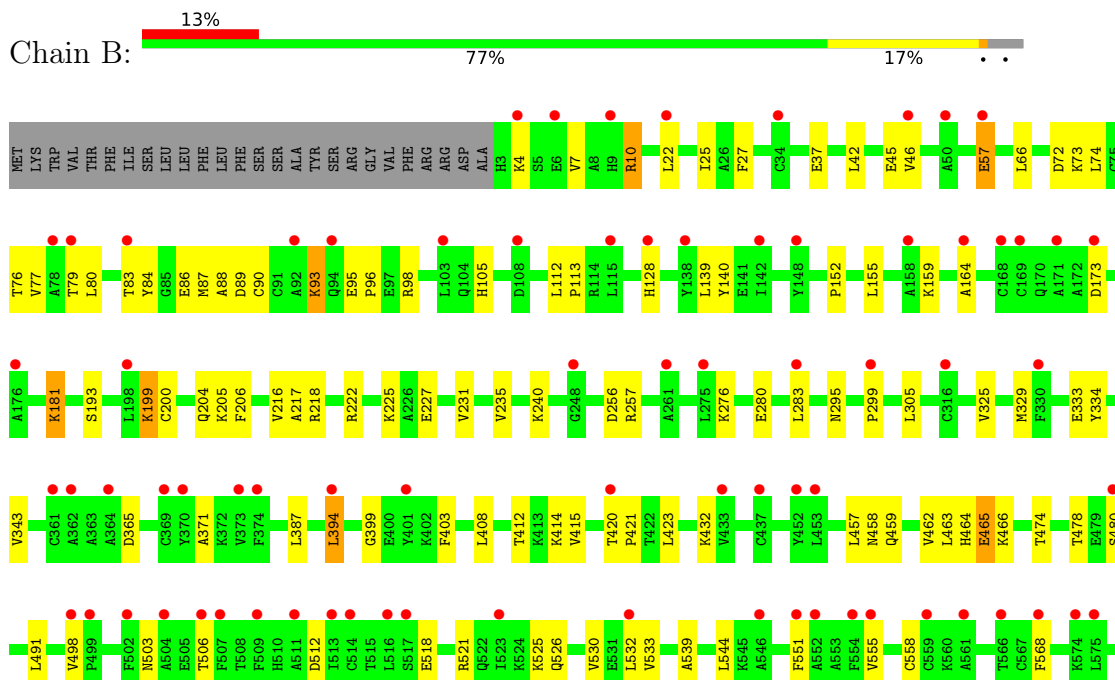
3 Residue-property plots [i](#)

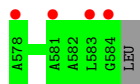
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Serum albumin



- Molecule 1: Serum albumin





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.25Å 38.19Å 181.92Å 90.00° 105.10° 90.00°	Depositor
Resolution (Å)	45.98 – 1.90 45.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (45.98-1.90) 98.3 (45.98-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.89Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.230 , 0.281 0.229 , 0.281	Depositor DCC
R_{free} test set	5016 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtrriage
Anisotropy	0.396	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.037 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19284	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.6773e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MYR, GOQ, EDO

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	0.50	0/4701	0.60	0/6351
1	B	0.32	0/4688	0.49	0/6333
All	All	0.42	0/9389	0.55	0/12684

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	4592	4474	4451	50	0
1	B	4590	4474	4462	73	2
2	A	96	168	162	18	0
2	B	96	168	162	6	0
3	A	4	6	6	0	0
4	A	25	11	0	0	0
4	B	25	11	0	0	0
5	A	380	0	0	6	0
5	B	164	0	0	4	0
All	All	9972	9312	9243	124	2

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 7.

All (124) 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:B:72:ASP:O	1:B:76:THR:HG23	1.84	0.77
1:B:45:GLU:OE1	1:B:73:LYS:NZ	2.18	0.76
1:B:256:ASP:OD1	5:B:701:HOH:O	2.10	0.68
1:B:412:THR:HG22	1:B:423:LEU:HD13	1.75	0.68
1:A:23:VAL:HG22	2:A:601:MYR:H131	1.76	0.68
1:B:394:LEU:HD23	1:B:403:PHE:HD1	1.58	0.66
1:B:465:GLU:OE2	1:B:474:THR:HG22	1.96	0.66
1:A:524:LYS:HD2	5:A:915:HOH:O	1.95	0.65
1:A:312:SER:O	5:A:701:HOH:O	2.14	0.64
1:B:394:LEU:HD23	1:B:403:PHE:CD1	2.33	0.64
1:B:408:LEU:O	1:B:412:THR:HG23	1.99	0.63
1:B:37:GLU:OE1	1:B:37:GLU:N	2.30	0.63
1:B:503:ASN:OD1	1:B:506:THR:N	2.31	0.63
1:B:387:LEU:HD22	2:B:603:MYR:H22	1.82	0.61
1:B:459:GLN:O	1:B:463:LEU:HD13	2.01	0.60
1:A:442:GLU:HA	1:A:445:ARG:HD2	1.84	0.59
1:A:538:LYS:NZ	5:A:712:HOH:O	2.36	0.59
1:A:325:VAL:O	1:A:329:MET:HG3	2.04	0.58
1:B:227:GLU:O	1:B:231:VAL:HG23	2.03	0.58
1:A:488:PHE:HB3	2:A:603:MYR:H71	1.86	0.58
1:B:7:VAL:HA	1:B:66:LEU:HD21	1.86	0.57
1:A:423:LEU:HD23	2:A:603:MYR:H131	1.84	0.57
1:B:95:GLU:OE2	1:B:98:ARG:NE	2.34	0.57
1:B:42:LEU:O	1:B:46:VAL:HG23	2.05	0.56
1:A:460:LEU:HD13	2:A:603:MYR:H143	1.87	0.56
1:A:241:VAL:CG1	2:A:606:MYR:H143	2.36	0.56
1:B:86:GLU:HG2	1:B:105:HIS:NE2	2.20	0.56
1:B:551:PHE:O	1:B:555:VAL:HG23	2.06	0.56
1:A:331:LEU:HD13	1:A:350:ALA:HB2	1.88	0.56
1:B:205:LYS:NZ	1:B:478:THR:O	2.39	0.55
1:A:460:LEU:HD22	2:A:603:MYR:H142	1.90	0.54
1:B:408:LEU:HD21	1:B:526:GLN:HB3	1.89	0.54
1:A:241:VAL:HG22	1:A:256:ASP:HB3	1.89	0.54
1:A:408:LEU:HD21	1:A:530:VAL:HG23	1.89	0.53
1:B:415:VAL:HG23	1:B:415:VAL:O	2.08	0.53
2:A:602:MYR:H132	2:A:602:MYR:H92	1.91	0.53
1:B:457:LEU:HD21	2:B:603:MYR:H81	1.91	0.53
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:PHE:HD1	1:B:74:LEU:HD21	1.74	0.52
1:A:521:ARG:HG2	1:A:525:LYS:HE2	1.92	0.52
1:B:206:PHE:CZ	1:B:480:SER:HA	2.45	0.52
1:A:435:SER:O	1:A:439:LYS:HE2	2.09	0.51
1:A:66:LEU:HD11	2:A:601:MYR:C14	2.40	0.51
1:A:10:ARG:NH2	1:A:255:ASP:OD1	2.44	0.51
1:A:516:LEU:O	1:A:521:ARG:NH1	2.42	0.50
1:B:371:ALA:O	5:B:702:HOH:O	2.19	0.50
1:B:276:LYS:O	1:B:280:GLU:HG3	2.12	0.49
1:B:152:PRO:O	1:B:155:LEU:N	2.45	0.49
1:A:408:LEU:HD23	1:A:529:LEU:HD23	1.95	0.49
1:A:66:LEU:HD11	2:A:601:MYR:H142	1.93	0.49
1:B:408:LEU:HG	1:B:530:VAL:HG22	1.94	0.49
1:A:436:LYS:HE2	1:A:452:TYR:OH	2.13	0.48
1:B:325:VAL:O	1:B:329:MET:HG3	2.14	0.48
1:B:95:GLU:HA	1:B:95:GLU:OE1	2.13	0.48
1:B:458:ASN:O	1:B:462:VAL:HG23	2.13	0.48
1:B:25:ILE:HD11	1:B:139:LEU:HD11	1.96	0.48
1:A:241:VAL:HG11	2:A:606:MYR:H143	1.95	0.47
1:A:251:LEU:HD21	2:A:601:MYR:H102	1.96	0.47
1:B:164:ALA:HB2	1:B:181:LYS:HG2	1.96	0.47
1:B:199:LYS:N	1:B:199:LYS:HD3	2.29	0.47
1:B:257:ARG:NH1	5:B:711:HOH:O	2.38	0.47
1:B:464:HIS:CE1	1:B:474:THR:HG23	2.50	0.47
1:B:4:LYS:HB2	1:B:57:GLU:OE2	2.15	0.47
1:B:173:ASP:OD1	1:B:173:ASP:C	2.53	0.46
1:B:412:THR:CG2	1:B:530:VAL:HG13	2.45	0.46
1:B:420:THR:N	1:B:421:PRO:HD2	2.31	0.46
1:B:399:GLY:O	1:B:403:PHE:CB	2.64	0.46
1:B:532:LEU:HD13	2:B:604:MYR:H102	1.98	0.46
1:A:99:ASN:O	1:A:103:LEU:HD23	2.16	0.46
1:A:305:LEU:HD21	1:A:337:ARG:HD2	1.98	0.45
1:B:412:THR:HG21	1:B:530:VAL:HG13	1.98	0.45
1:A:317:LYS:HE3	1:A:318:ASN:OD1	2.16	0.45
1:A:157:PHE:HE1	1:A:188:GLU:HB3	1.81	0.45
1:A:428:ARG:CZ	1:A:523:ILE:HD11	2.46	0.45
1:B:216:VAL:HG22	1:B:235:VAL:HG21	1.98	0.45
1:B:399:GLY:O	1:B:403:PHE:HB2	2.17	0.45
1:B:7:VAL:HG12	5:B:710:HOH:O	2.17	0.45
1:B:532:LEU:HD22	2:B:604:MYR:H82	2.00	0.45
1:A:31:LEU:HB2	1:A:39:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:LYS:NZ	1:B:491:LEU:O	2.41	0.44
1:A:367:HIS:HA	1:A:370:TYR:CE1	2.52	0.44
1:B:42:LEU:HD23	1:B:42:LEU:N	2.33	0.44
1:B:225:LYS:HG2	1:B:299:PRO:HD3	2.00	0.44
1:B:283:LEU:C	1:B:283:LEU:HD23	2.38	0.44
1:B:200:CYS:O	1:B:204:GLN:HG2	2.17	0.44
1:B:77:VAL:HB	1:B:80:LEU:HD13	1.99	0.44
1:A:426:VAL:HG11	2:A:603:MYR:H141	1.99	0.43
1:A:4:LYS:HZ3	1:A:58:SER:HG	1.65	0.43
1:A:197:ARG:HG2	5:A:1018:HOH:O	2.17	0.43
1:B:80:LEU:HD23	1:B:88:ALA:HA	2.01	0.43
1:B:10:ARG:HG3	1:B:66:LEU:HD11	2.00	0.43
1:B:22:LEU:HD13	2:B:601:MYR:H72	2.01	0.43
1:B:112:LEU:HB3	1:B:113:PRO:HD2	2.00	0.43
1:B:412:THR:OG1	1:B:533:VAL:HG11	2.19	0.43
1:A:413:LYS:NZ	1:B:365:ASP:OD2	2.48	0.43
1:B:558:CYS:HB3	1:B:568:PHE:CD2	2.54	0.43
1:A:426:VAL:CB	2:A:603:MYR:H141	2.49	0.43
1:B:387:LEU:HD22	2:B:603:MYR:C2	2.49	0.42
2:A:603:MYR:H21	5:A:899:HOH:O	2.19	0.42
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.54	0.42
1:B:305:LEU:HD21	1:B:333:GLU:HB3	2.00	0.42
1:A:433:VAL:HG22	1:A:452:TYR:HB3	2.00	0.42
1:B:539:ALA:HB3	1:B:544:LEU:HD21	2.02	0.42
1:A:395:PHE:CZ	1:A:435:SER:HA	2.55	0.42
1:B:521:ARG:HG2	1:B:525:LYS:HE2	2.01	0.42
1:A:86:GLU:HG3	1:A:105:HIS:NE2	2.34	0.41
1:A:404:GLN:HG2	1:A:428:ARG:HA	2.01	0.41
1:A:410:ARG:NH1	2:A:603:MYR:O1	2.53	0.41
1:A:423:LEU:HD23	2:A:603:MYR:C13	2.50	0.41
1:B:84:TYR:HB3	1:B:87:MET:HB3	2.02	0.41
1:A:378:LYS:O	1:A:382:GLU:HG3	2.20	0.41
1:B:79:THR:HG22	1:B:83:THR:OG1	2.21	0.41
1:A:426:VAL:HG11	2:A:603:MYR:C14	2.49	0.41
1:A:366:PRO:HD2	5:A:880:HOH:O	2.21	0.41
1:B:222:ARG:HA	1:B:295:ASN:OD1	2.20	0.41
1:B:518:GLU:OE1	1:B:521:ARG:NH2	2.53	0.41
1:A:48:GLU:O	1:A:52:THR:HG23	2.21	0.41
1:A:518:GLU:HG3	1:A:519:LYS:N	2.35	0.41
1:B:498:VAL:O	1:B:498:VAL:CG1	2.69	0.41
1:B:218[B]:ARG:HD2	1:B:218[B]:ARG:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ALA:HB3	1:B:343:VAL:HG13	2.03	0.40
1:B:84:TYR:CB	1:B:87:MET:HE2	2.51	0.40
1:A:66:LEU:HD21	2:A:601:MYR:H132	2.04	0.40
1:B:90:CYS:HA	1:B:93:LYS:HD2	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:GLU:OE1	1:B:159:LYS:NZ[1_565]	2.04	0.16
1:B:86:GLU:OE1	1:B:159:LYS:HZ1[1_565]	1.55	0.05

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	584/609 (96%)	574 (98%)	10 (2%)	0	100	100
1	B	582/609 (96%)	569 (98%)	13 (2%)	0	100	100
All	All	1166/1218 (96%)	1143 (98%)	23 (2%)	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	500/533 (94%)	496 (99%)	4 (1%)	81	82
1	B	498/533 (93%)	481 (97%)	17 (3%)	37	28
All	All	998/1066 (94%)	977 (98%)	21 (2%)	53	48

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	TYR
1	A	140	TYR
1	A	334	TYR
1	A	480	SER
1	B	10	ARG
1	B	57	GLU
1	B	89	ASP
1	B	93	LYS
1	B	96	PRO
1	B	128	HIS
1	B	140	TYR
1	B	181	LYS
1	B	193	SER
1	B	199	LYS
1	B	240	LYS
1	B	334	TYR
1	B	394	LEU
1	B	432	LYS
1	B	465	GLU
1	B	466	LYS
1	B	512	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	B	464	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 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	MYR	A	606	-	15,15,15	0.21	0	15,15,15	0.20	0
2	MYR	A	603	-	15,15,15	0.16	0	15,15,15	0.20	0
2	MYR	B	603	-	15,15,15	0.19	0	15,15,15	0.18	0
3	EDO	A	607	-	3,3,3	0.62	0	2,2,2	0.12	0
2	MYR	A	604	-	15,15,15	0.19	0	15,15,15	0.19	0
2	MYR	B	602	-	15,15,15	0.16	0	15,15,15	0.24	0
2	MYR	B	606	-	15,15,15	0.17	0	15,15,15	0.17	0
2	MYR	B	605	-	15,15,15	0.18	0	15,15,15	0.17	0
2	MYR	B	604	-	15,15,15	0.15	0	15,15,15	0.22	0
2	MYR	B	601	-	15,15,15	0.19	0	15,15,15	0.22	0
2	MYR	A	601	-	15,15,15	0.19	0	15,15,15	0.38	0
2	MYR	A	605	-	15,15,15	0.22	0	15,15,15	0.16	0
4	GOQ	B	607	-	27,28,28	0.50	0	34,42,42	1.03	2 (5%)
4	GOQ	A	608	-	27,28,28	0.62	0	34,42,42	1.22	2 (5%)
2	MYR	A	602	-	15,15,15	0.30	0	15,15,15	0.17	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYR	A	606	-	-	4/13/13/13	-
2	MYR	A	603	-	-	8/13/13/13	-
2	MYR	B	603	-	-	4/13/13/13	-
3	EDO	A	607	-	-	0/1/1/1	-
2	MYR	A	604	-	-	3/13/13/13	-
2	MYR	B	602	-	-	3/13/13/13	-
2	MYR	B	606	-	-	4/13/13/13	-
2	MYR	B	605	-	-	2/13/13/13	-
2	MYR	B	604	-	-	3/13/13/13	-
2	MYR	B	601	-	-	2/13/13/13	-
2	MYR	A	601	-	-	1/13/13/13	-
2	MYR	A	605	-	-	3/13/13/13	-
4	GOQ	B	607	-	-	2/8/16/16	0/4/4/4
4	GOQ	A	608	-	-	2/8/16/16	0/4/4/4
2	MYR	A	602	-	-	7/13/13/13	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	608	GOQ	C8-C7-C6	-4.59	115.55	118.69
4	A	608	GOQ	C12-C11-C16	-4.53	113.16	118.27
4	B	607	GOQ	C12-C11-C16	-4.39	113.31	118.27
4	B	607	GOQ	C8-C7-C6	-3.30	116.43	118.69

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	608	GOQ	C7-C8-N-O1
4	A	608	GOQ	C9-C8-N-O1
2	B	601	MYR	C7-C8-C9-C10
2	A	602	MYR	C9-C10-C11-C12
2	B	606	MYR	C6-C7-C8-C9
2	B	606	MYR	C3-C4-C5-C6
2	B	603	MYR	C3-C4-C5-C6
2	A	606	MYR	C4-C5-C6-C7
2	A	603	MYR	C7-C8-C9-C10
2	A	602	MYR	C4-C5-C6-C7

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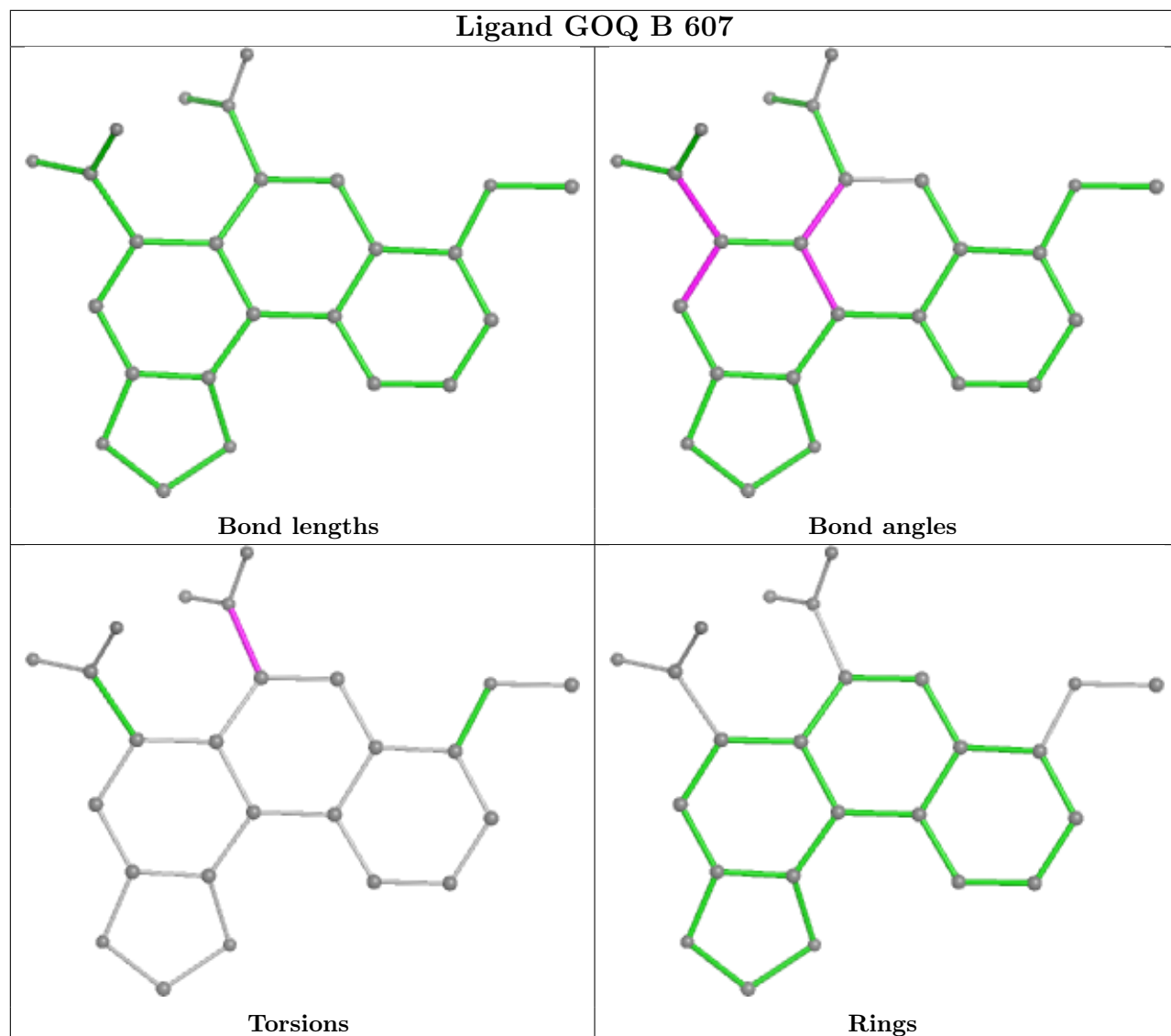
Mol	Chain	Res	Type	Atoms
2	A	606	MYR	C5-C6-C7-C8
4	B	607	GOQ	C9-C8-N-O1
2	A	602	MYR	C10-C11-C12-C13
2	B	602	MYR	C10-C11-C12-C13
2	A	602	MYR	C3-C4-C5-C6
2	B	606	MYR	C9-C10-C11-C12
2	A	603	MYR	C5-C6-C7-C8
2	A	602	MYR	C1-C2-C3-C4
2	A	601	MYR	C2-C3-C4-C5
2	B	605	MYR	C5-C6-C7-C8
2	A	603	MYR	C11-C12-C13-C14
4	B	607	GOQ	C7-C8-N-O1
2	B	601	MYR	C4-C5-C6-C7
2	A	604	MYR	O2-C1-C2-C3
2	A	603	MYR	C10-C11-C12-C13
2	B	603	MYR	C7-C8-C9-C10
2	B	604	MYR	O1-C1-C2-C3
2	B	606	MYR	C4-C5-C6-C7
2	A	603	MYR	C2-C3-C4-C5
2	A	605	MYR	O2-C1-C2-C3
2	B	603	MYR	O1-C1-C2-C3
2	B	604	MYR	O2-C1-C2-C3
2	A	604	MYR	O1-C1-C2-C3
2	A	605	MYR	O1-C1-C2-C3
2	A	602	MYR	O2-C1-C2-C3
2	A	603	MYR	C11-C10-C9-C8
2	A	602	MYR	O1-C1-C2-C3
2	A	606	MYR	O1-C1-C2-C3
2	B	605	MYR	C6-C7-C8-C9
2	B	603	MYR	O2-C1-C2-C3
2	A	606	MYR	O2-C1-C2-C3
2	A	604	MYR	C2-C3-C4-C5
2	B	602	MYR	C1-C2-C3-C4
2	B	604	MYR	C10-C11-C12-C13
2	A	605	MYR	C6-C7-C8-C9
2	B	602	MYR	C3-C4-C5-C6
2	A	603	MYR	C3-C4-C5-C6
2	A	603	MYR	O2-C1-C2-C3

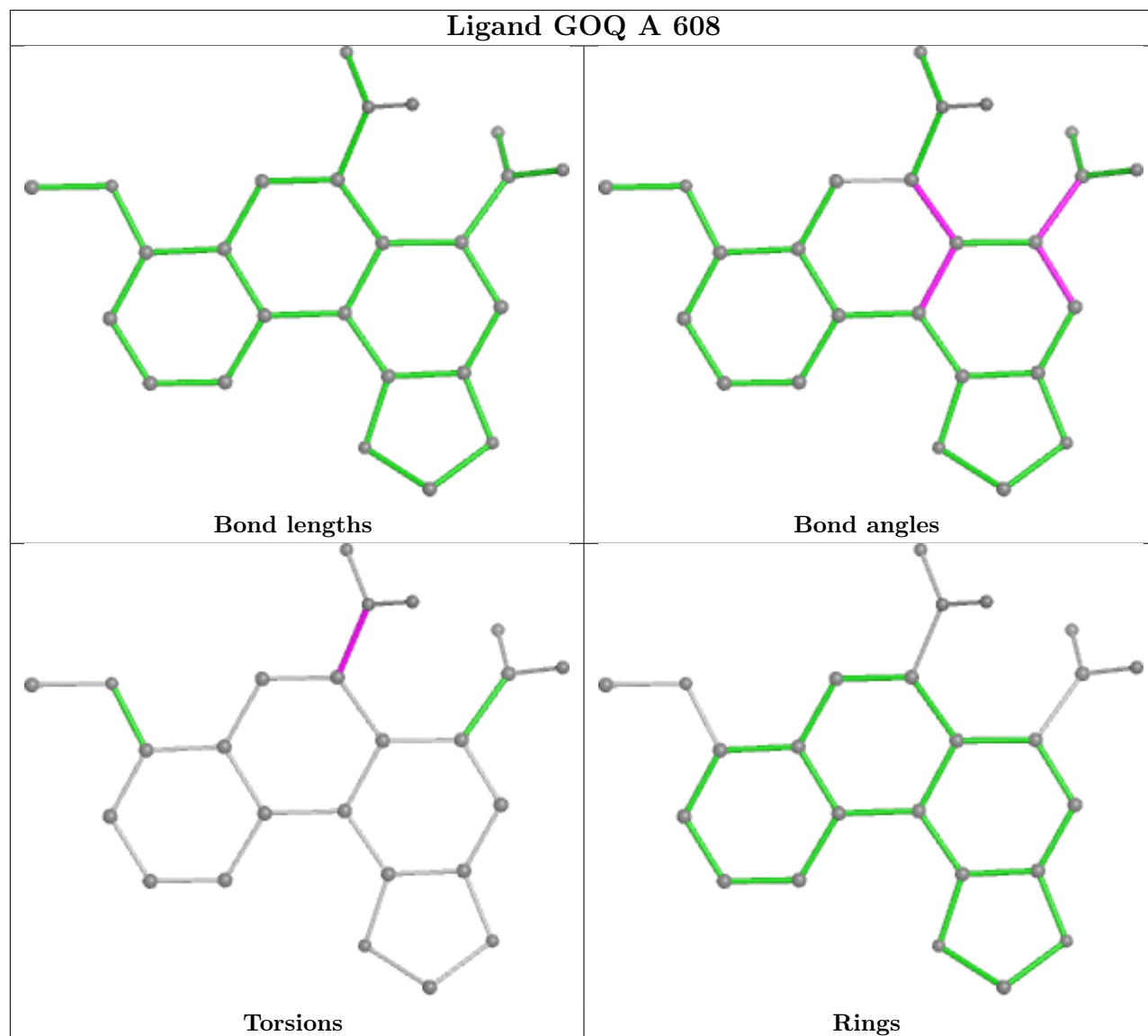
There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	606	MYR	2	0
2	A	603	MYR	10	0
2	B	603	MYR	3	0
2	B	604	MYR	2	0
2	B	601	MYR	1	0
2	A	601	MYR	5	0
2	A	602	MYR	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	582/609 (95%)	0.56	28 (4%) 30 33	7, 25, 56, 74	0
1	B	582/609 (95%)	1.06	79 (13%) 3 3	38, 54, 70, 89	0
All	All	1164/1218 (95%)	0.81	107 (9%) 9 10	7, 46, 67, 89	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	559	CYS	5.2
1	B	555	VAL	5.0
1	B	568	PHE	4.7
1	A	553	ALA	4.7
1	B	513	ILE	4.3
1	B	566	THR	4.2
1	B	507	PHE	4.1
1	B	364	ALA	4.1
1	B	433	VAL	4.0
1	A	561	ALA	4.0
1	B	516	LEU	3.8
1	A	555	VAL	3.8
1	B	559	CYS	3.8
1	B	504	ALA	3.7
1	B	498	VAL	3.7
1	B	164	ALA	3.5
1	B	551	PHE	3.4
1	B	362	ALA	3.3
1	A	566	THR	3.3
1	B	546	ALA	3.3
1	A	511	ALA	3.2
1	B	581	ALA	3.1
1	B	554	PHE	3.1
1	B	561	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	79	THR	3.1
1	A	554	PHE	3.1
1	B	480	SER	3.0
1	B	198	LEU	3.0
1	B	509	PHE	3.0
1	B	499	PRO	3.0
1	B	452	TYR	3.0
1	A	509	PHE	3.0
1	B	517	SER	3.0
1	B	261	ALA	3.0
1	A	575	LEU	3.0
1	A	502	PHE	2.9
1	A	537	PRO	2.9
1	A	583	LEU	2.9
1	B	9	HIS	2.9
1	B	437	CYS	2.9
1	B	92	ALA	2.8
1	B	552	ALA	2.8
1	A	501	GLU	2.8
1	B	78	ALA	2.7
1	B	511	ALA	2.7
1	B	370	TYR	2.7
1	B	108	ASP	2.7
1	B	374	PHE	2.7
1	A	568	PHE	2.7
1	B	373	VAL	2.7
1	B	275	LEU	2.7
1	B	283	LEU	2.7
1	B	34	CYS	2.7
1	B	83	THR	2.7
1	A	576	VAL	2.6
1	B	502	PHE	2.6
1	B	115	LEU	2.6
1	B	171	ALA	2.6
1	B	574	LYS	2.5
1	B	299	PRO	2.5
1	A	582	ALA	2.5
1	B	138	TYR	2.5
1	B	50	ALA	2.5
1	B	148	TYR	2.5
1	B	583	LEU	2.5
1	B	369	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	584	GLY	2.5
1	B	94	GLN	2.5
1	B	578	ALA	2.4
1	A	516	LEU	2.4
1	B	514	CYS	2.4
1	A	515	THR	2.4
1	B	22	LEU	2.4
1	B	4	LYS	2.4
1	A	512	ASP	2.4
1	A	507	PHE	2.4
1	A	513	ILE	2.4
1	B	46	VAL	2.4
1	B	168	CYS	2.3
1	B	158	ALA	2.3
1	A	567	CYS	2.3
1	B	506	THR	2.3
1	A	517	SER	2.3
1	B	173	ASP	2.3
1	A	546	ALA	2.2
1	B	532	LEU	2.2
1	B	57	GLU	2.2
1	B	316	CYS	2.2
1	A	505	GLU	2.2
1	A	197	ARG	2.2
1	B	394	LEU	2.2
1	B	169	CYS	2.2
1	A	572	GLY	2.2
1	B	6	GLU	2.2
1	B	103	LEU	2.2
1	B	330	PHE	2.2
1	B	361	CYS	2.2
1	B	128	HIS	2.1
1	B	248	GLY	2.1
1	B	420	THR	2.1
1	B	575	LEU	2.1
1	B	401	TYR	2.1
1	A	562	ASP	2.1
1	B	142	ILE	2.1
1	B	453	LEU	2.1
1	B	176	ALA	2.1
1	B	523	ILE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

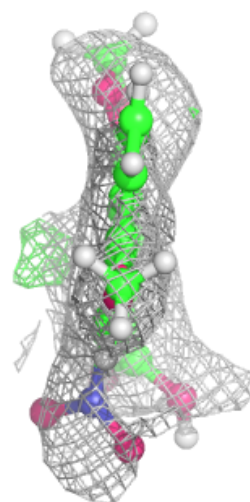
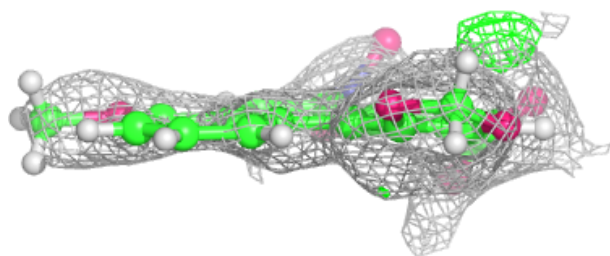
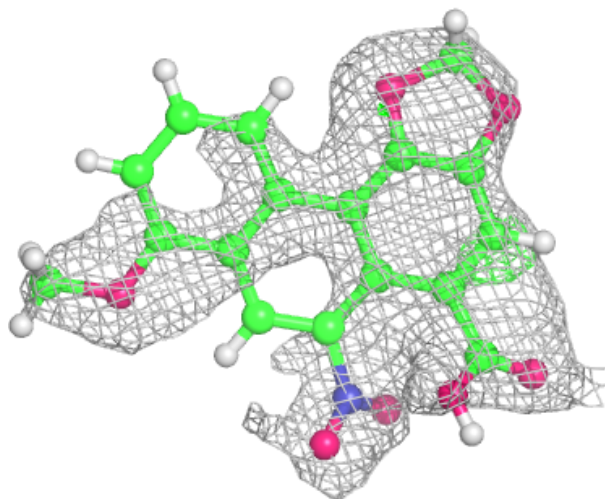
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

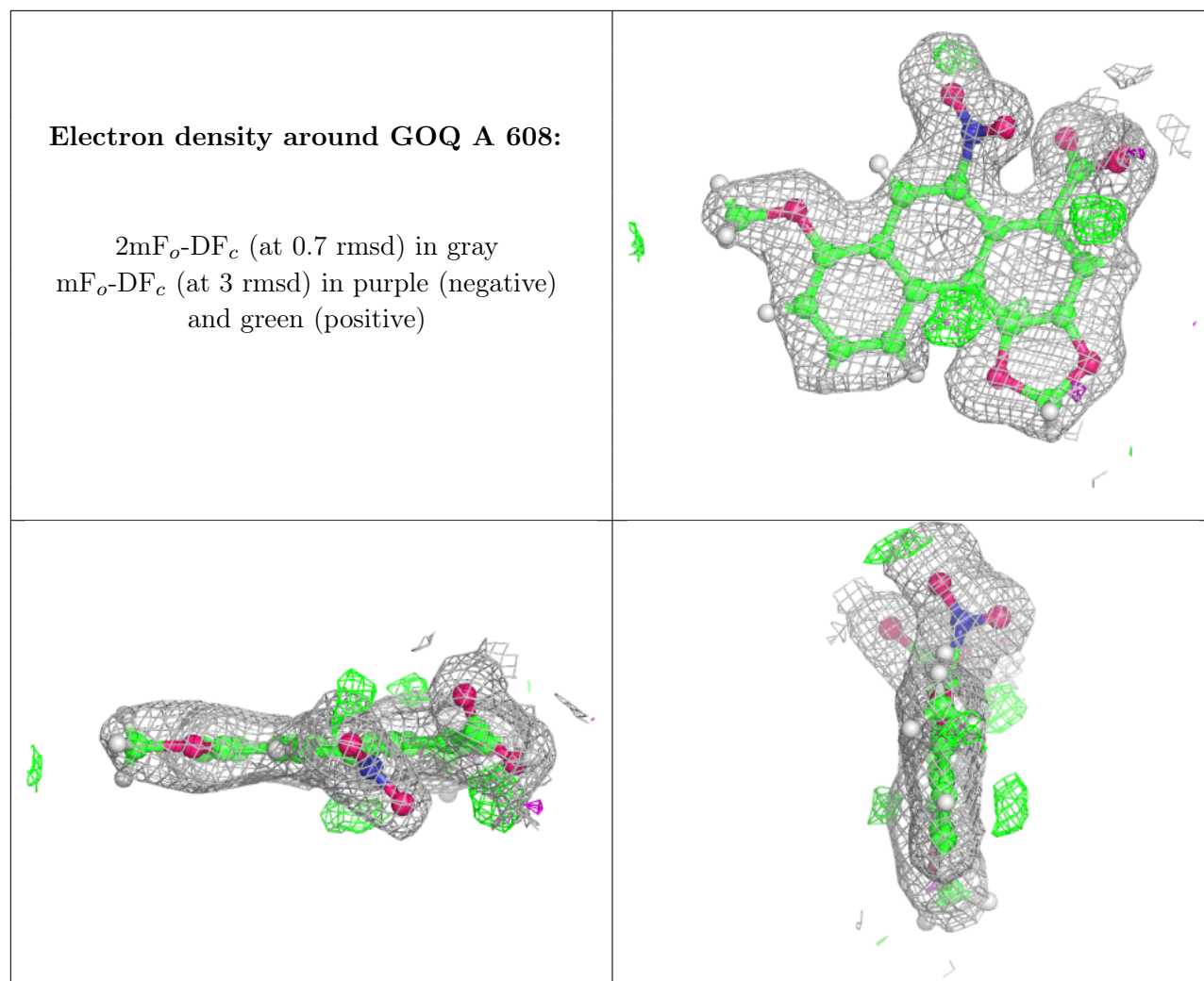
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOQ	B	607	25/25	0.72	0.26	58,65,78,78	0
2	MYR	B	604	16/16	0.73	0.29	53,71,83,86	0
2	MYR	B	606	16/16	0.75	0.22	53,67,78,80	0
2	MYR	A	603	16/16	0.80	0.24	27,39,58,59	0
2	MYR	B	605	16/16	0.80	0.26	44,60,78,81	44
2	MYR	B	601	16/16	0.81	0.20	45,62,73,75	0
2	MYR	A	604	16/16	0.82	0.17	40,52,63,68	0
2	MYR	A	606	16/16	0.84	0.22	19,37,55,59	0
2	MYR	A	605	16/16	0.86	0.17	24,32,46,49	0
2	MYR	B	603	16/16	0.86	0.18	38,52,77,82	44
4	GOQ	A	608	25/25	0.88	0.15	17,24,31,34	0
2	MYR	B	602	16/16	0.88	0.16	36,48,55,57	44
2	MYR	A	601	16/16	0.92	0.18	11,27,47,47	0
2	MYR	A	602	16/16	0.93	0.15	12,24,36,47	44
3	EDO	A	607	4/4	0.95	0.14	17,25,31,31	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 GOQ B 607:

$2mF_o-DF_c$ (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.