



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 01:17 pm BST

PDB ID : 8RGK  
Title : Structure of Human Serum Albumin in complex with Aristolochic Acid at 1.9 Å resolution  
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](mailto: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>.

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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)  
Xtriage (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

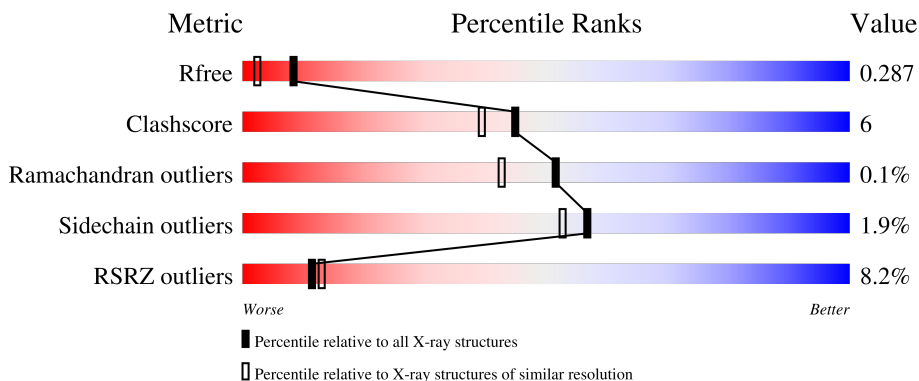
# 1 Overall quality at a glance

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  $\geq 3$ , 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	 11% 78% 17% . .
1	B	609	 5% 85% 10% .

## 2 Entry composition [i](#)

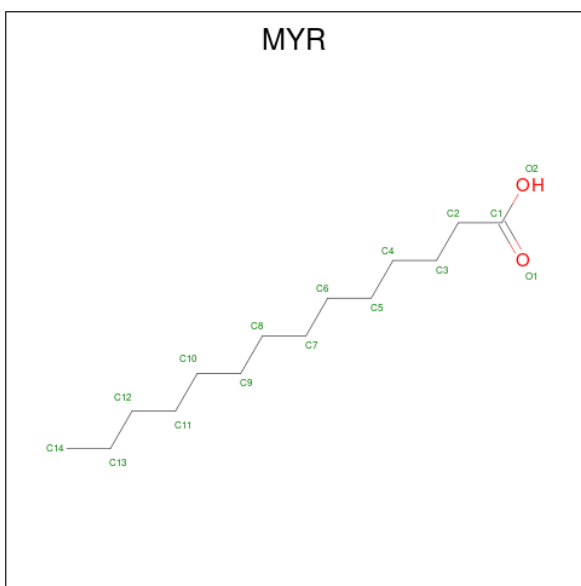
There are 5 unique types of molecules in this entry. The entry contains 19299 atoms, of which 9332 are hydrogens and 0 are deuteriums.

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	9001	2887	4430	779	864	41	0	5	0
1	B	582	9084	2903	4486	783	871	41	0	4	0

- 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	43	14	27	2	0	0
2	A	1	43	14	27	2	0	0
2	A	1	43	14	27	2	0	0
2	A	1	43	14	27	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			43	14	27	2		
2	A	1	Total	C	H	O	0	0
			43	14	27	2		
2	A	1	Total	C	H	O	0	0
			43	14	27	2		
2	B	1	Total	C	H	O	0	0
			43	14	27	2		
2	B	1	Total	C	H	O	0	0
			43	14	27	2		
2	B	1	Total	C	H	O	0	0
			43	14	27	2		
2	B	1	Total	C	H	O	0	0
			43	14	27	2		
2	B	1	Total	C	H	O	0	0
			43	14	27	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



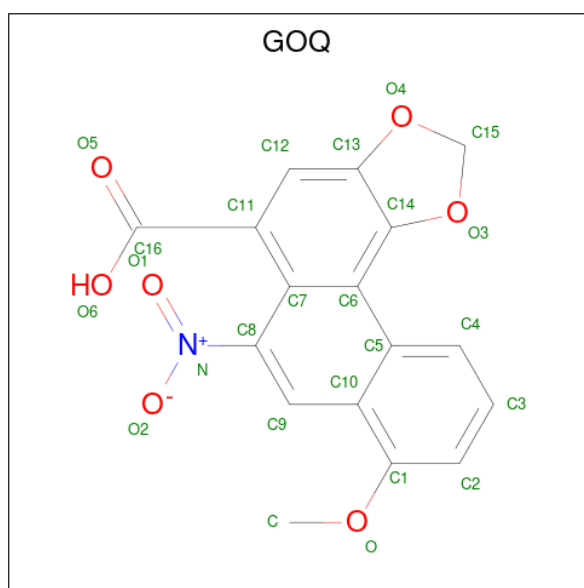
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	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: C<sub>17</sub>H<sub>11</sub>NO<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	181	Total	O	0	0
			181	181		

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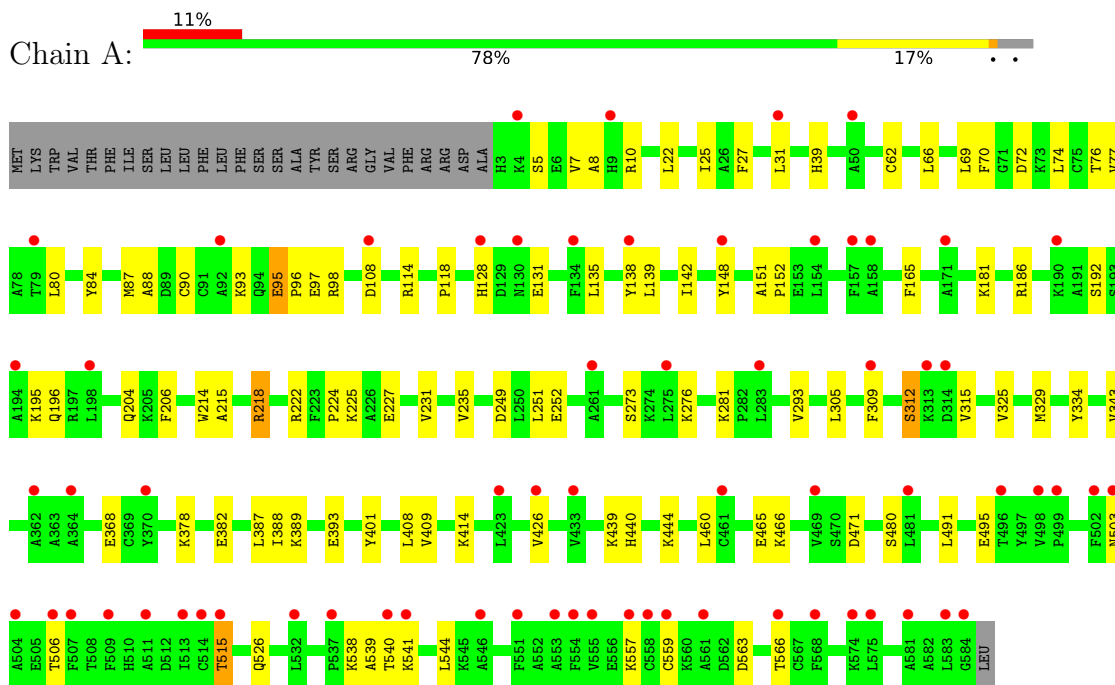
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	B	348	Total 348	O 348	0	0

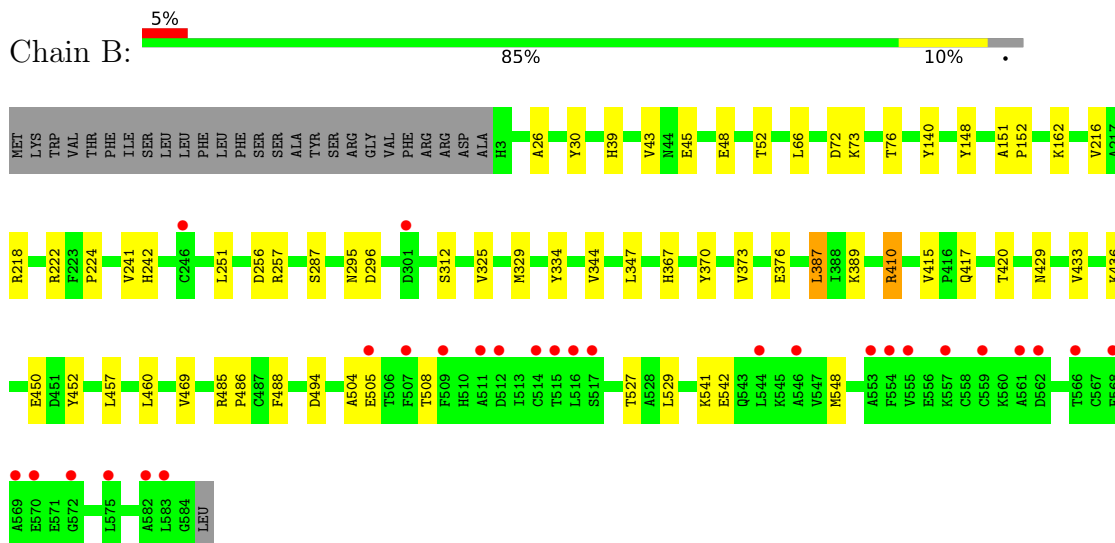
### 3 Residue-property plots [i](#)

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: 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, $\alpha$ , $\beta$ , $\gamma$	94.40Å 37.87Å 180.25Å 90.00° 105.12° 90.00°	Depositor
Resolution (Å)	47.20 – 1.90 47.20 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.20-1.90) 98.8 (47.20-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.240 , 0.289 0.239 , 0.287	Depositor DCC
$R_{free}$ test set	4931 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtrriage
Anisotropy	0.377	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	19299	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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 37.58 % 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 4.2001e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOQ, EDO, MYR

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	0.28	0/4683	0.47	0/6331
1	B	0.29	0/4704	0.48	0/6354
All	All	0.28	0/9387	0.47	0/12685

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	410	ARG	Sidechain

### 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	4571	4430	4413	69	0
1	B	4598	4486	4462	48	0
2	A	112	189	189	11	0
2	B	96	162	162	19	0
3	A	8	12	12	0	0
3	B	28	42	42	1	0
4	B	25	11	0	1	0
5	A	181	0	0	4	0
5	B	348	0	0	4	0
All	All	9967	9332	9280	121	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 6.

All (121) 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:312:SER:O	5:B:701:HOH:O	2.07	0.71
1:B:45:GLU:OE1	1:B:73:LYS:NZ	2.25	0.70
1:B:460:LEU:HD13	2:B:606:MYR:H142	1.78	0.66
1:A:84:TYR:CB	1:A:87:MET:HE2	2.28	0.64
1:A:222:ARG:HD2	1:A:293:VAL:HG13	1.81	0.63
1:A:84:TYR:HB2	1:A:87:MET:HE2	1.82	0.62
1:B:415:VAL:HG23	1:B:415:VAL:O	2.01	0.60
1:A:325:VAL:HG22	2:A:605:MYR:H101	1.84	0.59
1:B:148:TYR:OH	5:B:702:HOH:O	2.17	0.59
1:A:563:ASP:OD1	1:A:566:THR:HG22	2.03	0.58
1:A:222:ARG:HH11	1:A:222:ARG:HG2	1.69	0.58
1:B:387:LEU:HD13	2:B:605:MYR:H92	1.86	0.57
1:A:408:LEU:HD21	1:A:526:GLN:HB3	1.86	0.57
1:B:417:GLN:NE2	1:B:494:ASP:OD2	2.33	0.57
1:A:312:SER:O	5:A:701:HOH:O	2.17	0.57
1:B:152:PRO:HG3	2:B:603:MYR:H51	1.86	0.57
2:B:605:MYR:H91	2:B:606:MYR:H21	1.86	0.57
1:B:429:ASN:ND2	5:B:716:HOH:O	2.39	0.55
1:B:242:HIS:CE1	2:B:607:MYR:H141	2.42	0.54
1:A:414:LYS:NZ	1:A:491:LEU:O	2.28	0.54
1:B:241:VAL:HG22	1:B:256:ASP:HB3	1.90	0.53
1:A:495:GLU:OE1	1:A:538:LYS:NZ	2.40	0.53
2:A:606:MYR:H92	2:A:606:MYR:H21	1.91	0.52
1:A:77:VAL:HB	1:A:80:LEU:HD13	1.91	0.52
1:B:387:LEU:HB3	2:B:605:MYR:H92	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:LEU:HD11	1:B:548:MET:SD	2.50	0.52
1:A:401:TYR:OH	2:A:604:MYR:O1	2.21	0.51
1:A:72:ASP:O	1:A:76:THR:HG23	2.11	0.51
1:A:218:ARG:HH12	1:A:222:ARG:HH21	1.58	0.51
1:A:7:VAL:HG22	1:A:66:LEU:HD23	1.92	0.51
1:A:387:LEU:HD22	2:A:602:MYR:H22	1.92	0.50
1:A:10:ARG:HE	1:A:66:LEU:CD1	2.23	0.50
1:A:80:LEU:HD23	1:A:88:ALA:HA	1.93	0.50
1:A:539:ALA:HB3	1:A:544:LEU:HD21	1.93	0.50
1:B:66:LEU:HD21	2:B:603:MYR:H132	1.93	0.50
1:A:90:CYS:HA	1:A:93:LYS:HD2	1.94	0.49
1:A:325:VAL:O	1:A:329:MET:HG3	2.12	0.49
1:B:457:LEU:HD12	3:B:608:EDO:H22	1.95	0.49
1:B:389:LYS:NZ	5:B:709:HOH:O	2.37	0.48
1:A:142:ILE:HG13	2:A:606:MYR:H112	1.96	0.48
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.95	0.48
1:B:218[B]:ARG:NH1	1:B:222:ARG:HE	2.11	0.48
1:A:368:GLU:OE2	1:B:410:ARG:NH1	2.41	0.48
1:A:181:LYS:NZ	5:A:722:HOH:O	2.44	0.47
1:A:27:PHE:HB3	1:A:39:HIS:CD2	2.49	0.47
1:B:410:ARG:NH1	1:B:410:ARG:HG3	2.29	0.47
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.96	0.47
1:B:417:GLN:O	1:B:469:VAL:HG11	2.15	0.47
1:B:436:LYS:HG2	1:B:452:TYR:CE2	2.49	0.47
1:B:344:VAL:CG2	2:B:605:MYR:H22	2.44	0.47
1:A:22:LEU:HD13	2:A:603:MYR:H81	1.97	0.47
1:A:165:PHE:CE2	2:A:606:MYR:H62	2.49	0.47
1:B:450:GLU:HA	2:B:605:MYR:H31	1.96	0.47
1:A:305:LEU:HB3	1:A:309:PHE:HD2	1.79	0.46
1:A:389:LYS:HD2	1:A:393:GLU:HG3	1.97	0.46
1:A:206:PHE:CZ	1:A:480:SER:HA	2.50	0.46
1:A:312:SER:O	1:A:315:VAL:HG23	2.15	0.46
1:A:252:GLU:OE1	1:A:252:GLU:HA	2.15	0.46
1:B:72:ASP:O	1:B:76:THR:HG23	2.16	0.46
1:B:417:GLN:HB3	1:B:469:VAL:HG12	1.98	0.46
1:B:542:GLU:OE1	1:B:542:GLU:N	2.48	0.46
1:A:251:LEU:HD21	2:A:603:MYR:H132	1.98	0.46
1:A:388:ILE:HG13	2:A:601:MYR:H72	1.98	0.46
1:B:325:VAL:O	1:B:329:MET:HG3	2.14	0.46
1:A:409:VAL:HG11	1:A:541:LYS:HE2	1.98	0.45
1:B:488:PHE:HB3	2:B:606:MYR:H71	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLN:OE1	1:A:204:GLN:HA	2.16	0.45
1:A:186:ARG:HA	1:A:186:ARG:HD3	1.84	0.45
1:A:224:PRO:HD2	1:A:225:LYS:H	1.82	0.45
1:A:378:LYS:O	1:A:382:GLU:HG3	2.16	0.45
1:A:515:THR:O	1:A:515:THR:OG1	2.34	0.45
1:A:5:SER:HB3	1:A:8:ALA:HB3	1.99	0.45
1:A:539:ALA:CB	1:A:544:LEU:HD21	2.46	0.45
1:B:222:ARG:HD3	1:B:295:ASN:OD1	2.16	0.45
1:B:410:ARG:HG3	1:B:410:ARG:HH11	1.80	0.45
1:A:25:ILE:HD11	1:A:139:LEU:HD11	1.99	0.45
1:A:426:VAL:HG21	1:A:460:LEU:HD13	1.98	0.44
1:B:39:HIS:O	1:B:43:VAL:HG23	2.16	0.44
1:A:227[B]:GLU:O	1:A:231:VAL:HG23	2.18	0.44
1:B:287:SER:OG	2:B:603:MYR:O1	2.25	0.44
1:A:439:LYS:HE3	1:A:439:LYS:HA	2.00	0.43
1:A:281:LYS:NZ	5:A:736:HOH:O	2.51	0.43
1:A:84:TYR:CB	1:A:87:MET:CE	2.96	0.43
2:A:603:MYR:H82	2:A:603:MYR:H51	1.80	0.43
1:B:216:VAL:HG21	2:B:604:MYR:H122	2.00	0.43
1:B:251:LEU:HD21	2:B:603:MYR:H102	2.00	0.43
1:A:70:PHE:CZ	1:A:74:LEU:HD11	2.54	0.43
1:B:347:LEU:HD22	2:B:604:MYR:H31	2.00	0.43
1:A:138:TYR:CG	2:A:606:MYR:H71	2.53	0.43
1:B:504:ALA:O	1:B:508:THR:HG23	2.19	0.43
1:B:257:ARG:HG2	2:B:607:MYR:H122	2.00	0.42
1:A:31:LEU:CD1	1:A:77:VAL:HG21	2.49	0.42
1:A:95[B]:GLU:HB2	1:A:96[B]:PRO:HD3	2.01	0.42
1:A:503:ASN:OD1	1:A:506:THR:N	2.51	0.42
1:A:540:THR:O	1:A:544:LEU:HG	2.19	0.42
1:B:433:VAL:HG12	2:B:605:MYR:H141	2.02	0.42
1:A:95[A]:GLU:OE2	1:A:98:ARG:NE	2.43	0.42
2:B:605:MYR:H52	2:B:605:MYR:C1	2.50	0.42
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.54	0.41
1:A:273:SER:O	1:A:276:LYS:CE	2.68	0.41
1:A:440:HIS:HB3	1:A:444:LYS:HB2	2.01	0.41
1:B:218[A]:ARG:NH1	2:B:607:MYR:H22	2.35	0.41
1:B:367:HIS:HA	1:B:370:TYR:CE1	2.55	0.41
1:A:87:MET:O	1:A:87:MET:HG2	2.21	0.41
1:A:249:ASP:OD2	1:A:252:GLU:HG2	2.20	0.41
1:A:471:ASP:OD1	5:A:702:HOH:O	2.22	0.41
1:A:131:GLU:O	1:A:135:LEU:HD22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:SER:O	1:A:196:GLN:HG2	2.21	0.41
4:B:601:GOQ:N	4:B:601:GOQ:C16	2.84	0.41
1:A:27:PHE:HE1	1:A:74:LEU:HD12	1.85	0.41
1:B:26:ALA:O	1:B:30:TYR:HD1	2.04	0.41
1:B:48:GLU:O	1:B:52:THR:HG23	2.21	0.41
1:B:485:ARG:HB3	1:B:486:PRO:HD3	2.02	0.41
1:B:529:LEU:CD1	2:B:602:MYR:H52	2.50	0.41
1:A:7:VAL:HG21	1:A:69:LEU:HD13	2.03	0.41
1:B:373:VAL:O	1:B:376:GLU:HB2	2.21	0.40
1:A:5:SER:OG	1:A:62:CYS:O	2.36	0.40
1:A:215:ALA:HB3	1:A:235:VAL:HG13	2.03	0.40
1:A:151:ALA:HB3	1:A:152:PRO:HD3	2.04	0.40
1:A:108:ASP:HB2	1:A:148:TYR:HE2	1.87	0.40
1:B:420:THR:HG21	1:B:527:THR:HG23	2.02	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	585/609 (96%)	566 (97%)	17 (3%)	2 (0%)	41	31
1	B	584/609 (96%)	570 (98%)	14 (2%)	0	100	100
All	All	1169/1218 (96%)	1136 (97%)	31 (3%)	2 (0%)	51	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95[A]	GLU
1	A	95[B]	GLU

### 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	492/533 (92%)	478 (97%)	14 (3%)	43	36
1	B	500/533 (94%)	494 (99%)	6 (1%)	71	70
All	All	992/1066 (93%)	972 (98%)	20 (2%)	57	51

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97[A]	GLU
1	A	97[B]	GLU
1	A	114	ARG
1	A	118	PRO
1	A	128	HIS
1	A	195	LYS
1	A	218	ARG
1	A	312	SER
1	A	334	TYR
1	A	465	GLU
1	A	466	LYS
1	A	515	THR
1	A	557	LYS
1	A	559	CYS
1	B	140	TYR
1	B	162	LYS
1	B	334	TYR
1	B	387	LEU
1	B	505	GLU
1	B	541	LYS

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](#)

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](#)

23 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	B	604	-	15,15,15	0.61	0	15,15,15	1.15	1 (6%)
2	MYR	A	602	-	15,15,15	0.79	1 (6%)	15,15,15	1.60	2 (13%)
2	MYR	B	606	-	15,15,15	0.60	0	15,15,15	1.16	1 (6%)
3	EDO	B	609	-	3,3,3	0.46	0	2,2,2	0.37	0
3	EDO	B	612	-	3,3,3	0.45	0	2,2,2	0.35	0
3	EDO	B	610	-	3,3,3	0.44	0	2,2,2	0.35	0
4	GOQ	B	601	-	27,28,28	0.47	0	34,42,42	1.02	2 (5%)
2	MYR	A	606	-	15,15,15	0.63	0	15,15,15	1.01	0
2	MYR	A	603	-	15,15,15	0.58	0	15,15,15	1.15	1 (6%)
2	MYR	A	607	-	15,15,15	0.61	0	15,15,15	1.15	1 (6%)
3	EDO	A	609	-	3,3,3	0.47	0	2,2,2	0.30	0
2	MYR	A	601	-	15,15,15	0.62	0	15,15,15	0.98	0
3	EDO	B	608	-	3,3,3	0.49	0	2,2,2	0.24	0
3	EDO	B	613	-	3,3,3	0.50	0	2,2,2	0.28	0
2	MYR	A	604	-	15,15,15	0.60	0	15,15,15	1.10	0
2	MYR	B	605	-	15,15,15	0.60	0	15,15,15	1.03	0
3	EDO	B	614	-	3,3,3	0.46	0	2,2,2	0.30	0
2	MYR	B	603	-	15,15,15	0.60	0	15,15,15	1.21	2 (13%)
2	MYR	B	607	-	15,15,15	0.62	0	15,15,15	1.04	0
3	EDO	A	608	-	3,3,3	0.47	0	2,2,2	0.29	0
3	EDO	B	611	-	3,3,3	0.44	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MYR	A	605	-	15,15,15	0.61	0	15,15,15	1.11	0
2	MYR	B	602	-	15,15,15	0.61	0	15,15,15	1.07	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	B	604	-	-	9/13/13/13	-
2	MYR	A	602	-	-	8/13/13/13	-
2	MYR	B	606	-	-	7/13/13/13	-
3	EDO	B	609	-	-	1/1/1/1	-
3	EDO	B	612	-	-	0/1/1/1	-
3	EDO	B	610	-	-	1/1/1/1	-
4	GOQ	B	601	-	-	2/8/16/16	0/4/4/4
2	MYR	A	606	-	-	11/13/13/13	-
2	MYR	A	603	-	-	8/13/13/13	-
2	MYR	A	607	-	-	9/13/13/13	-
3	EDO	A	609	-	-	0/1/1/1	-
2	MYR	A	601	-	-	7/13/13/13	-
3	EDO	B	608	-	-	0/1/1/1	-
3	EDO	B	613	-	-	1/1/1/1	-
2	MYR	A	604	-	-	7/13/13/13	-
2	MYR	B	605	-	-	6/13/13/13	-
3	EDO	B	614	-	-	1/1/1/1	-
2	MYR	B	603	-	-	4/13/13/13	-
2	MYR	B	607	-	-	9/13/13/13	-
3	EDO	A	608	-	-	0/1/1/1	-
3	EDO	B	611	-	-	1/1/1/1	-
2	MYR	A	605	-	-	7/13/13/13	-
2	MYR	B	602	-	-	8/13/13/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	MYR	C2-C1	2.06	1.55	1.50

All (10) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	GOQ	C12-C11-C16	-4.10	113.65	118.27
4	B	601	GOQ	C8-C7-C6	-3.30	116.44	118.69
2	A	602	MYR	O2-C1-C2	3.13	124.09	114.03
2	A	602	MYR	O2-C1-O1	-2.85	116.18	123.30
2	A	607	MYR	C3-C2-C1	-2.31	108.66	114.47
2	B	603	MYR	C3-C2-C1	-2.29	108.71	114.47
2	B	604	MYR	C3-C2-C1	-2.20	108.92	114.47
2	A	603	MYR	C3-C2-C1	-2.12	109.13	114.47
2	B	603	MYR	O2-C1-C2	2.04	120.59	114.03
2	B	606	MYR	O2-C1-C2	2.02	120.52	114.03

There are no chirality outliers.

All (107) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	A	601	MYR	C9-C10-C11-C12
2	B	606	MYR	C2-C3-C4-C5
3	B	610	EDO	O1-C1-C2-O2
3	B	613	EDO	O1-C1-C2-O2
2	A	602	MYR	C9-C10-C11-C12
2	B	602	MYR	C5-C6-C7-C8
2	B	604	MYR	C5-C6-C7-C8
2	A	605	MYR	C1-C2-C3-C4
2	A	602	MYR	C2-C3-C4-C5
2	A	602	MYR	C7-C8-C9-C10
2	B	607	MYR	C10-C11-C12-C13
2	B	604	MYR	C2-C3-C4-C5
2	A	607	MYR	C11-C10-C9-C8
2	B	605	MYR	C3-C4-C5-C6
2	A	603	MYR	C11-C12-C13-C14
2	A	607	MYR	C3-C4-C5-C6
2	A	606	MYR	C11-C12-C13-C14
2	B	606	MYR	C11-C12-C13-C14
2	A	603	MYR	C7-C8-C9-C10
2	B	602	MYR	C4-C5-C6-C7
2	A	607	MYR	C11-C12-C13-C14
2	A	602	MYR	C1-C2-C3-C4
2	B	607	MYR	C5-C6-C7-C8
2	A	602	MYR	C10-C11-C12-C13
2	A	605	MYR	C5-C6-C7-C8
2	A	607	MYR	C10-C11-C12-C13
2	B	607	MYR	C9-C10-C11-C12
2	A	605	MYR	C6-C7-C8-C9
2	A	604	MYR	C6-C7-C8-C9
2	B	607	MYR	C2-C3-C4-C5
2	B	602	MYR	C6-C7-C8-C9
2	A	605	MYR	C4-C5-C6-C7
2	A	606	MYR	C4-C5-C6-C7
2	A	605	MYR	C11-C12-C13-C14
2	B	603	MYR	C6-C7-C8-C9
2	A	604	MYR	C9-C10-C11-C12
2	A	601	MYR	C11-C10-C9-C8
2	B	605	MYR	C2-C3-C4-C5
2	B	607	MYR	C4-C5-C6-C7
2	B	605	MYR	C11-C12-C13-C14
2	B	604	MYR	C3-C4-C5-C6
2	B	605	MYR	C1-C2-C3-C4

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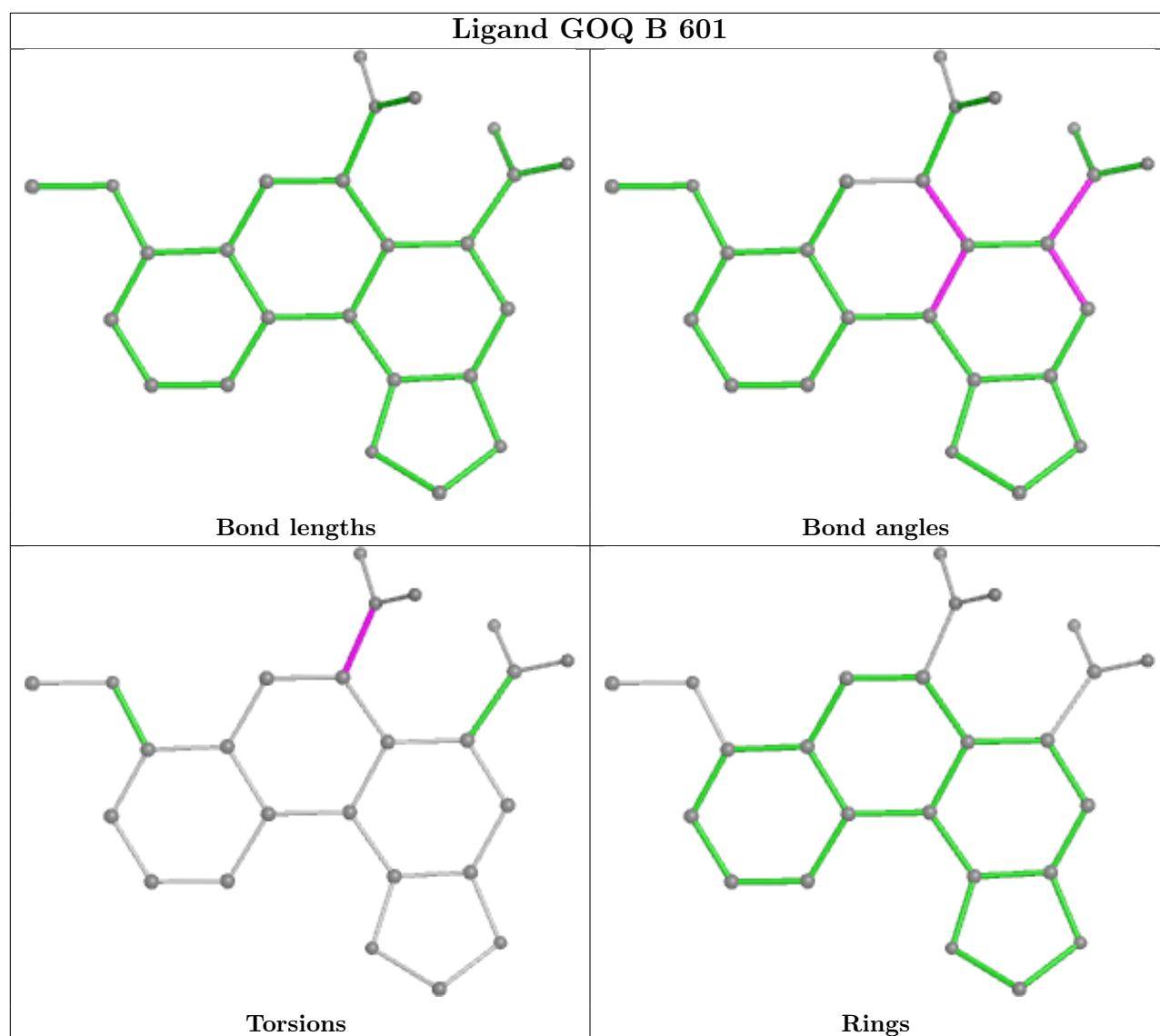
Mol	Chain	Res	Type	Atoms
2	B	603	MYR	C9-C10-C11-C12
2	A	601	MYR	C7-C8-C9-C10
2	A	604	MYR	C11-C12-C13-C14
3	B	611	EDO	O1-C1-C2-O2
2	A	604	MYR	C1-C2-C3-C4
2	B	602	MYR	O2-C1-C2-C3
2	A	606	MYR	C3-C4-C5-C6
2	B	604	MYR	C11-C12-C13-C14
2	B	607	MYR	O1-C1-C2-C3
2	A	602	MYR	O1-C1-C2-C3
2	B	607	MYR	O2-C1-C2-C3
2	A	605	MYR	O1-C1-C2-C3
2	A	602	MYR	O2-C1-C2-C3
2	A	603	MYR	C5-C6-C7-C8
2	A	607	MYR	O1-C1-C2-C3
2	A	607	MYR	O2-C1-C2-C3
2	B	606	MYR	C1-C2-C3-C4
2	A	603	MYR	O2-C1-C2-C3
2	B	602	MYR	O1-C1-C2-C3
2	A	605	MYR	O2-C1-C2-C3
3	B	614	EDO	O1-C1-C2-O2
2	A	603	MYR	O1-C1-C2-C3
2	B	604	MYR	O2-C1-C2-C3
2	A	602	MYR	C6-C7-C8-C9
2	B	604	MYR	O1-C1-C2-C3
2	A	601	MYR	O2-C1-C2-C3
2	A	606	MYR	O2-C1-C2-C3
3	B	609	EDO	O1-C1-C2-O2
2	A	601	MYR	O1-C1-C2-C3
2	A	603	MYR	C6-C7-C8-C9
2	B	607	MYR	C11-C10-C9-C8
2	A	606	MYR	O1-C1-C2-C3
2	A	607	MYR	C9-C10-C11-C12
2	B	606	MYR	O2-C1-C2-C3
2	B	606	MYR	C5-C6-C7-C8
2	B	603	MYR	C11-C12-C13-C14
2	B	602	MYR	C10-C11-C12-C13

There are no ring outliers.

14 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	604	MYR	2	0
2	A	602	MYR	1	0
2	B	606	MYR	3	0
4	B	601	GOQ	1	0
2	A	606	MYR	4	0
2	A	603	MYR	3	0
2	A	601	MYR	1	0
3	B	608	EDO	1	0
2	A	604	MYR	1	0
2	B	605	MYR	7	0
2	B	603	MYR	4	0
2	B	607	MYR	3	0
2	A	605	MYR	1	0
2	B	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	582/609 (95%)	1.00	67 (11%) <b>4</b> <b>5</b>	37, 53, 67, 85	0
1	B	582/609 (95%)	0.62	28 (4%) <b>30</b> <b>33</b>	9, 27, 56, 77	0
All	All	1164/1218 (95%)	0.81	95 (8%) <b>11</b> <b>13</b>	9, 45, 65, 85	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	ILE	5.6
1	A	561	ALA	5.3
1	A	568	PHE	5.1
1	B	555	VAL	5.0
1	A	555	VAL	4.6
1	B	509	PHE	4.5
1	B	511	ALA	4.2
1	A	546	ALA	4.2
1	B	559	CYS	4.1
1	A	566	THR	4.0
1	A	583	LEU	3.9
1	A	511	ALA	3.9
1	B	566	THR	3.8
1	A	509	PHE	3.8
1	A	283	LEU	3.7
1	A	559	CYS	3.7
1	A	198	LEU	3.7
1	B	561	ALA	3.7
1	B	568	PHE	3.6
1	A	499	PRO	3.5
1	A	275	LEU	3.5
1	A	575	LEU	3.5
1	A	581	ALA	3.5
1	B	507	PHE	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	554	PHE	3.5
1	B	562	ASP	3.4
1	B	516	LEU	3.4
1	A	507	PHE	3.3
1	A	362	ALA	3.3
1	A	481	LEU	3.3
1	A	502	PHE	3.2
1	B	582	ALA	3.2
1	B	553	ALA	3.1
1	A	79	THR	3.0
1	A	154	LEU	3.0
1	B	575	LEU	3.0
1	A	551	PHE	2.9
1	A	537	PRO	2.8
1	A	138	TYR	2.8
1	A	364	ALA	2.8
1	B	583	LEU	2.7
1	A	540	THR	2.7
1	B	569	ALA	2.6
1	A	498	VAL	2.6
1	A	108	ASP	2.6
1	A	496	THR	2.6
1	B	512	ASP	2.6
1	A	504	ALA	2.6
1	A	314	ASP	2.6
1	B	505	GLU	2.6
1	A	554	PHE	2.6
1	B	517	SER	2.6
1	A	50	ALA	2.5
1	B	546	ALA	2.5
1	A	574	LYS	2.5
1	A	541	LYS	2.5
1	A	426	VAL	2.5
1	A	148	TYR	2.5
1	A	92	ALA	2.4
1	A	171	ALA	2.4
1	B	572	GLY	2.4
1	A	461	CYS	2.4
1	A	506	THR	2.4
1	B	544	LEU	2.3
1	A	190	LYS	2.3
1	A	514	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	134	PHE	2.3
1	A	433	VAL	2.3
1	A	557	LYS	2.3
1	A	4	LYS	2.3
1	A	9	HIS	2.3
1	A	370	TYR	2.2
1	A	423	LEU	2.2
1	B	570	GLU	2.2
1	B	557	LYS	2.2
1	A	130	ASN	2.2
1	B	515	THR	2.2
1	A	584	GLY	2.2
1	A	157	PHE	2.2
1	A	558	CYS	2.2
1	A	503	ASN	2.2
1	B	301	ASP	2.2
1	A	158	ALA	2.1
1	A	261	ALA	2.1
1	A	553	ALA	2.1
1	A	309	PHE	2.1
1	A	515	THR	2.1
1	A	532	LEU	2.1
1	A	469	VAL	2.1
1	A	194	ALA	2.1
1	B	514	CYS	2.1
1	A	313	LYS	2.1
1	A	31	LEU	2.0
1	A	128	HIS	2.0
1	B	246	CYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

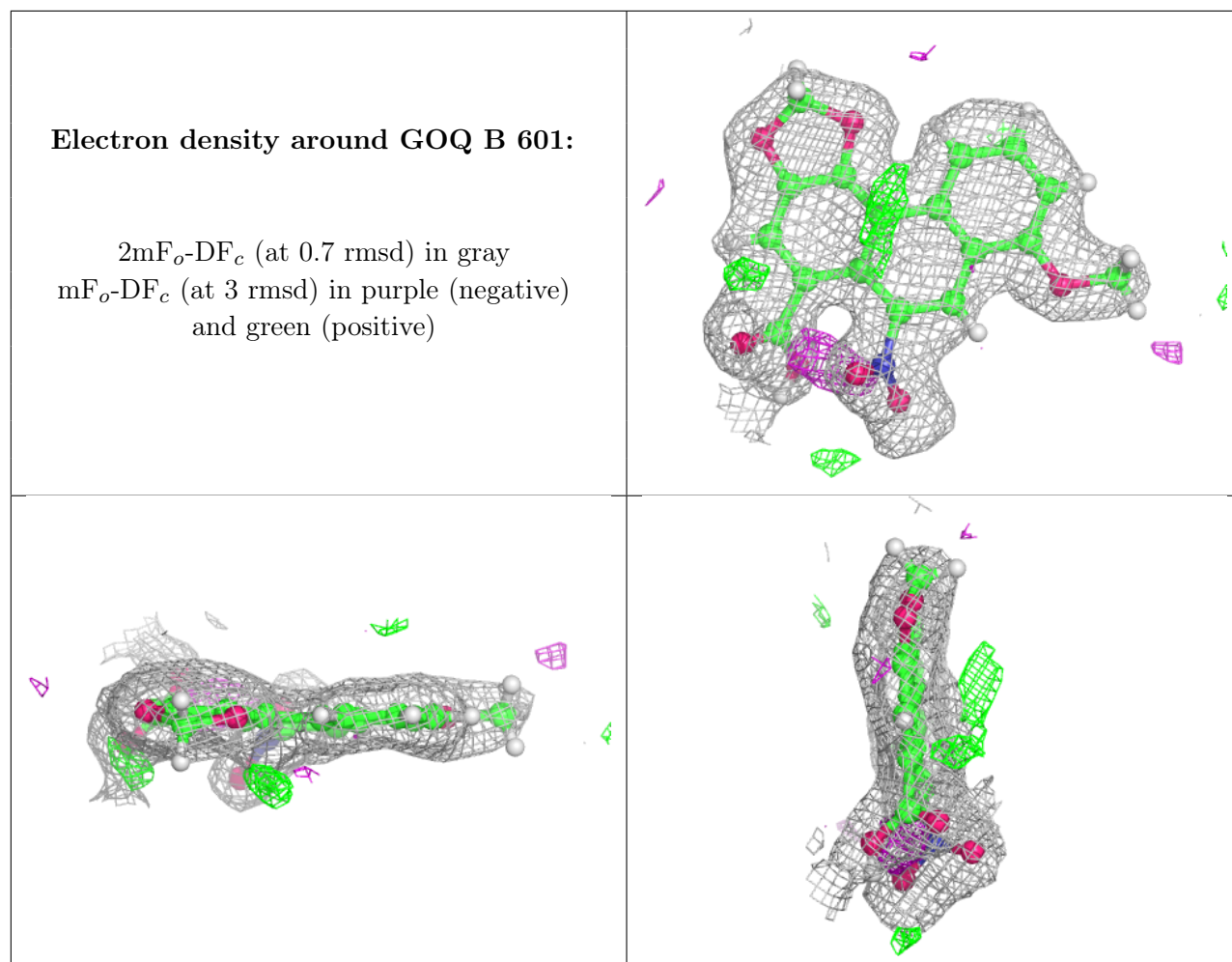


## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	EDO	A	608	4/4	0.59	0.39	55,66,72,72	0
2	MYR	A	605	16/16	0.67	0.32	44,57,63,64	43
2	MYR	A	604	16/16	0.67	0.26	49,65,76,77	0
2	MYR	A	607	16/16	0.70	0.23	47,65,73,79	0
2	MYR	A	602	16/16	0.78	0.21	34,54,65,67	43
2	MYR	A	606	16/16	0.79	0.26	48,65,76,76	0
3	EDO	B	609	4/4	0.79	0.22	39,51,60,62	0
3	EDO	A	609	4/4	0.80	0.27	51,61,68,69	0
2	MYR	B	602	16/16	0.80	0.17	38,51,62,62	0
2	MYR	B	607	16/16	0.82	0.23	24,37,55,60	0
2	MYR	B	606	16/16	0.82	0.22	23,41,57,61	0
3	EDO	B	614	4/4	0.84	0.18	39,51,61,63	0
3	EDO	B	612	4/4	0.86	0.11	31,38,50,60	0
2	MYR	B	604	16/16	0.86	0.15	22,35,47,48	0
4	GOQ	B	601	25/25	0.86	0.15	18,25,33,36	36
2	MYR	B	603	16/16	0.87	0.16	18,30,39,47	0
3	EDO	B	611	4/4	0.88	0.17	18,32,39,47	0
2	MYR	B	605	16/16	0.89	0.26	10,30,47,47	43
2	MYR	A	603	16/16	0.89	0.17	38,54,66,67	0
2	MYR	A	601	16/16	0.90	0.17	39,51,57,58	43
3	EDO	B	610	4/4	0.90	0.15	26,36,43,45	0
3	EDO	B	608	4/4	0.94	0.12	17,26,31,35	0
3	EDO	B	613	4/4	0.95	0.20	20,38,45,45	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.