



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:21 AM UTC

PDB ID : 8RGK / pdb_00008rgk
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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

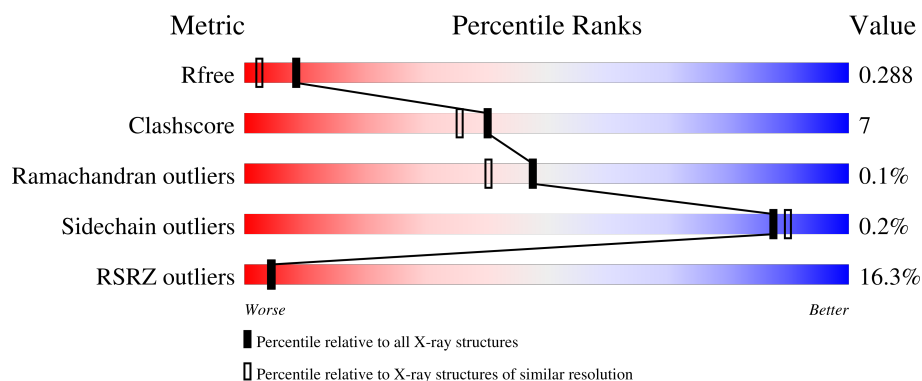
1 Overall quality at a glance

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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	25% 79% 16% .
1	B	609	7% 86% 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
1	A	582	Total	C	H	N	O	S	0	5	0
			9001	2887	4430	779	864	41			
1	B	582	Total	C	H	N	O	S	0	4	0
			9084	2903	4486	783	871	41			

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



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	A	1	Total	C	H	O	0	0
			43	14	27	2		

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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 (CCD ID: EDO) (formula: C₂H₆O₂).



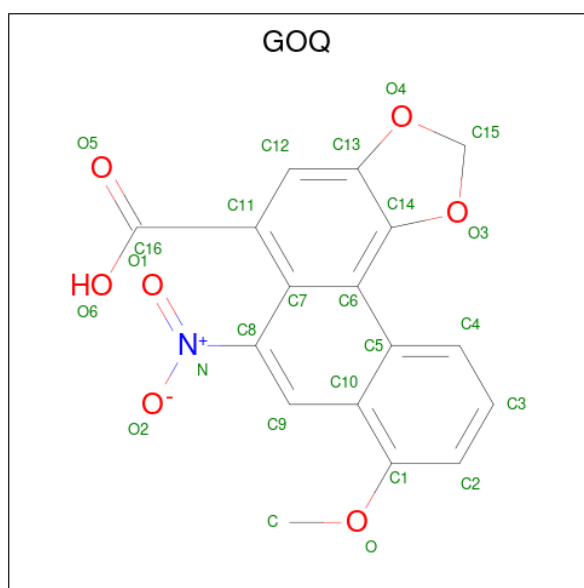
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

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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 (CCD ID: GOQ) (formula: C₁₇H₁₁NO₇) (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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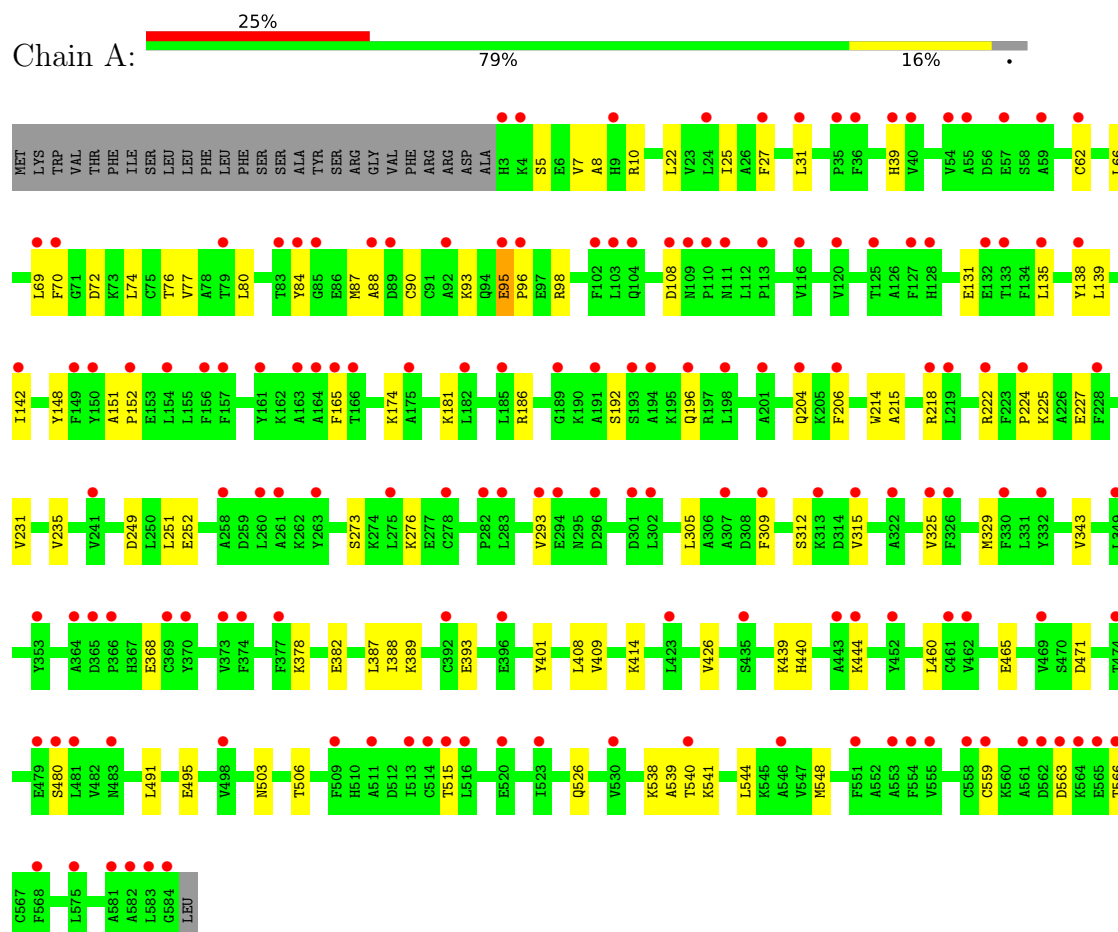
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	348	Total	O	0	0
			348	348		

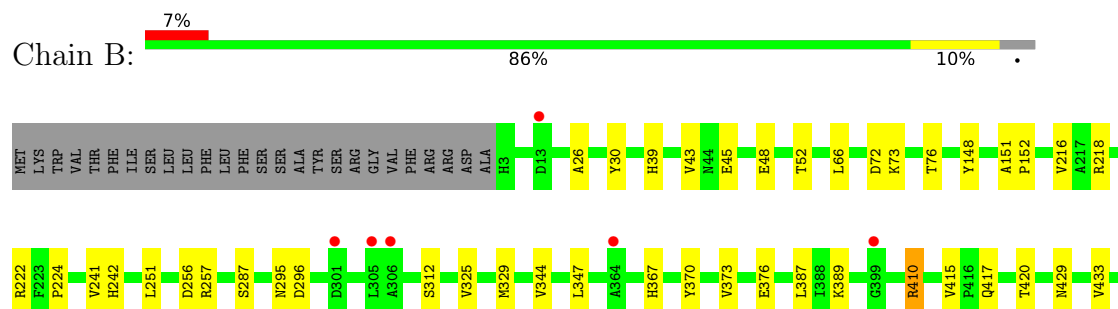
3 Residue-property plots

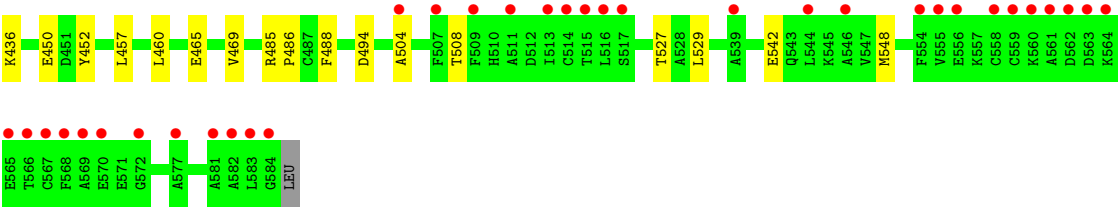
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	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
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.240 , 0.289 0.240 , 0.288	Depositor DCC
R_{free} test set	4934 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19299	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 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.*

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	0.16	0/4683	0.31	0/6331
1	B	0.17	0/4704	0.33	0/6354
All	All	0.16	0/9387	0.32	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	71	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	123	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 7.

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TYR:CB	1:A:87:MET:HE2	2.19	0.72
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:A:84:TYR:HB2	1:A:87:MET:HE2	1.76	0.68
1:B:460:LEU:HD13	2:B:606:MYR:H142	1.78	0.66
1:A:222:ARG:HD2	1:A:293:VAL:HG13	1.81	0.63
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: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:389:LYS:NZ	5:B:709:HOH:O	2.37	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:287:SER:OG	2:B:603:MYR:O1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:LEU:HB3	2:B:605:MYR:H92	1.92	0.52
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:174:LYS:NZ	5:A:717:HOH:O	2.40	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:148:TYR:OH	5:B:702:HOH:O	2.17	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:A:544:LEU:HB3	1:A:548:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:MET:HE2	1:A:87:MET:HB3	1.88	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
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:A:439:LYS:HE3	1:A:439:LYS:HA	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLU:O	1:A:135:LEU:HD22	2.21	0.41
1:A:192:SER:O	1:A:196:GLN:HG2	2.21	0.41
1:A:465:GLU:CD	1:A:465:GLU:C	2.89	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	585/609 (96%)	566 (97%)	17 (3%)	2 (0%)	36	29
1	B	584/609 (96%)	570 (98%)	14 (2%)	0	100	100
All	All	1169/1218 (96%)	1136 (97%)	31 (3%)	2 (0%)	48	36

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%)	491 (100%)	1 (0%)	87	90
1	B	500/533 (94%)	499 (100%)	1 (0%)	87	90
All	All	992/1066 (93%)	990 (100%)	2 (0%)	87	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	559	CYS
1	B	465	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	A	288	HIS
1	B	267	ASN
1	B	288	HIS
1	B	338	HIS
1	B	390	GLN
1	B	483	ASN

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 oligosaccharides 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	A	606	-	15,15,15	0.64	0	15,15,15	1.01	0
2	MYR	B	605	-	15,15,15	0.62	0	15,15,15	1.03	0
4	GOQ	B	601	-	28,28,28	0.54	0	30,42,42	0.87	2 (6%)
3	EDO	A	608	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	B	614	-	3,3,3	0.43	0	2,2,2	0.34	0
2	MYR	A	602	-	15,15,15	0.81	1 (6%)	15,15,15	1.60	2 (13%)
2	MYR	B	602	-	15,15,15	0.63	0	15,15,15	1.07	0
2	MYR	B	606	-	15,15,15	0.61	0	15,15,15	1.15	1 (6%)
2	MYR	A	605	-	15,15,15	0.62	0	15,15,15	1.10	0
3	EDO	B	608	-	3,3,3	0.46	0	2,2,2	0.28	0
3	EDO	B	612	-	3,3,3	0.42	0	2,2,2	0.39	0
2	MYR	A	607	-	15,15,15	0.62	0	15,15,15	1.14	1 (6%)
3	EDO	B	609	-	3,3,3	0.43	0	2,2,2	0.41	0
3	EDO	B	610	-	3,3,3	0.41	0	2,2,2	0.40	0
3	EDO	B	611	-	3,3,3	0.41	0	2,2,2	0.38	0
2	MYR	A	601	-	15,15,15	0.63	0	15,15,15	0.98	0
2	MYR	A	604	-	15,15,15	0.62	0	15,15,15	1.10	0
3	EDO	A	609	-	3,3,3	0.44	0	2,2,2	0.35	0
3	EDO	B	613	-	3,3,3	0.47	0	2,2,2	0.33	0
2	MYR	B	603	-	15,15,15	0.61	0	15,15,15	1.20	2 (13%)
2	MYR	B	607	-	15,15,15	0.63	0	15,15,15	1.04	1 (6%)
2	MYR	A	603	-	15,15,15	0.59	0	15,15,15	1.15	1 (6%)
2	MYR	B	604	-	15,15,15	0.62	0	15,15,15	1.15	1 (6%)

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	-	-	11/13/13/13	-
2	MYR	B	605	-	-	6/13/13/13	-
4	GOQ	B	601	-	-	2/8/16/16	0/4/4/4
3	EDO	A	608	-	-	0/1/1/1	-
3	EDO	B	614	-	-	1/1/1/1	-
2	MYR	A	602	-	-	8/13/13/13	-
2	MYR	B	602	-	-	8/13/13/13	-
2	MYR	B	606	-	-	7/13/13/13	-
2	MYR	A	605	-	-	7/13/13/13	-
3	EDO	B	608	-	-	0/1/1/1	-
3	EDO	B	612	-	-	0/1/1/1	-
2	MYR	A	607	-	-	9/13/13/13	-
3	EDO	B	609	-	-	1/1/1/1	-
3	EDO	B	610	-	-	1/1/1/1	-
3	EDO	B	611	-	-	1/1/1/1	-
2	MYR	A	601	-	-	7/13/13/13	-
2	MYR	A	604	-	-	7/13/13/13	-
3	EDO	A	609	-	-	0/1/1/1	-
3	EDO	B	613	-	-	1/1/1/1	-
2	MYR	B	603	-	-	4/13/13/13	-
2	MYR	B	607	-	-	9/13/13/13	-
2	MYR	A	603	-	-	8/13/13/13	-
2	MYR	B	604	-	-	9/13/13/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	MYR	C2-C1	2.07	1.55	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	GOQ	C8-C7-C6	-3.30	116.44	118.69
2	A	602	MYR	O2-C1-C2	3.19	124.09	114.00
2	A	602	MYR	O2-C1-O1	-2.78	116.18	123.33
4	B	601	GOQ	C12-C11-C16	-2.38	113.65	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	607	MYR	C3-C2-C1	-2.24	108.66	114.51
2	B	603	MYR	C3-C2-C1	-2.22	108.71	114.51
2	B	604	MYR	C3-C2-C1	-2.14	108.92	114.51
2	B	603	MYR	O2-C1-C2	2.09	120.59	114.00
2	B	606	MYR	O2-C1-C2	2.06	120.52	114.00
2	A	603	MYR	C3-C2-C1	-2.06	109.13	114.51
2	B	607	MYR	O2-C1-C2	2.04	120.44	114.00

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

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

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

There are no ring outliers.

14 monomers are involved in 32 short contacts:

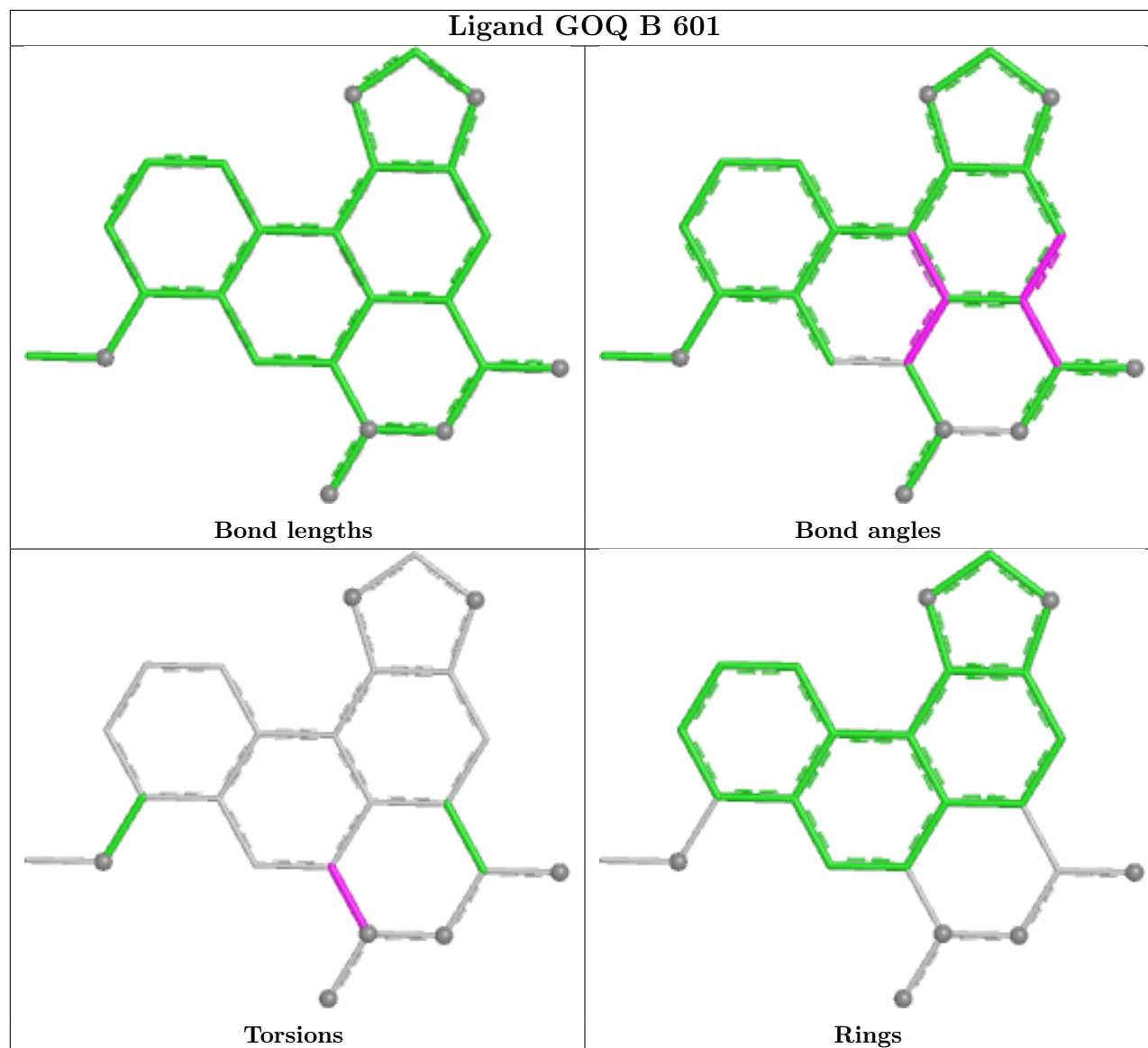
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	606	MYR	4	0
2	B	605	MYR	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	GOQ	1	0
2	A	602	MYR	1	0
2	B	602	MYR	1	0
2	B	606	MYR	3	0
2	A	605	MYR	1	0
3	B	608	EDO	1	0
2	A	601	MYR	1	0
2	A	604	MYR	1	0
2	B	603	MYR	4	0
2	B	607	MYR	3	0
2	A	603	MYR	3	0
2	B	604	MYR	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	582/609 (95%)	1.58	150 (25%) 1 1	25, 58, 73, 91	3 (0%)
1	B	582/609 (95%)	0.42	40 (6%) 23 24	10, 30, 62, 81	2 (0%)
All	All	1164/1218 (95%)	1.00	190 (16%) 4 4	10, 49, 70, 91	5 (0%)

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	568	PHE	5.2
1	A	564	LYS	4.3
1	B	569	ALA	4.2
1	A	154	LEU	4.0
1	B	516	LEU	4.0
1	B	511	ALA	4.0
1	A	558	CYS	3.8
1	A	198	LEU	3.8
1	A	584	GLY	3.7
1	A	31	LEU	3.7
1	A	283	LEU	3.7
1	B	555	VAL	3.7
1	A	509	PHE	3.7
1	A	514	CYS	3.7
1	A	138	TYR	3.6
1	B	554	PHE	3.6
1	B	561	ALA	3.5
1	B	568	PHE	3.5
1	A	275	LEU	3.5
1	A	108	ASP	3.5
1	A	566	THR	3.4
1	A	315	VAL	3.4
1	A	511	ALA	3.4
1	A	258	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	261	ALA	3.3
1	B	517	SER	3.3
1	A	562	ASP	3.3
1	B	509	PHE	3.3
1	A	57	GLU	3.2
1	A	575	LEU	3.2
1	A	102	PHE	3.2
1	A	175	ALA	3.2
1	B	564	LYS	3.2
1	A	204	GLN	3.2
1	B	507	PHE	3.2
1	A	103	LEU	3.1
1	B	584	GLY	3.1
1	A	111	ASN	3.1
1	A	322	ALA	3.1
1	A	513	ILE	3.1
1	A	370	TYR	3.1
1	A	516	LEU	3.1
1	A	326	PHE	3.1
1	A	559	CYS	3.1
1	A	555	VAL	3.1
1	A	166	THR	3.1
1	B	566	THR	3.1
1	A	201	ALA	3.0
1	A	224	PRO	3.0
1	B	504	ALA	3.0
1	A	373	VAL	2.9
1	A	4	LYS	2.9
1	B	565	GLU	2.9
1	A	540	THR	2.9
1	A	282	PRO	2.9
1	A	89	ASP	2.9
1	A	128	HIS	2.8
1	B	582	ALA	2.8
1	A	561	ALA	2.8
1	A	85	GLY	2.8
1	A	135	LEU	2.8
1	A	125	THR	2.8
1	A	157	PHE	2.8
1	B	514	CYS	2.8
1	B	559	CYS	2.8
1	B	556	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	563	ASP	2.8
1	A	241	VAL	2.8
1	A	309	PHE	2.7
1	A	189	GLY	2.7
1	B	515	THR	2.7
1	A	554	PHE	2.7
1	A	366	PRO	2.7
1	A	565	GLU	2.7
1	B	570	GLU	2.7
1	A	165	PHE	2.7
1	B	567	CYS	2.7
1	A	296	ASP	2.7
1	A	95[A]	GLU	2.7
1	A	520	GLU	2.7
1	B	513	ILE	2.7
1	A	222	ARG	2.6
1	B	399	GLY	2.6
1	A	70	PHE	2.6
1	B	13[A]	ASP	2.6
1	A	443	ALA	2.6
1	B	546	ALA	2.6
1	A	110	PRO	2.5
1	A	278	CYS	2.5
1	A	452	TYR	2.5
1	A	149	PHE	2.5
1	B	560	LYS	2.5
1	A	59	ALA	2.5
1	A	483	ASN	2.5
1	A	474	THR	2.5
1	A	163	ALA	2.5
1	A	164	ALA	2.5
1	A	553	ALA	2.5
1	A	582	ALA	2.5
1	B	581	ALA	2.5
1	A	116	VAL	2.5
1	A	469	VAL	2.5
1	A	515	THR	2.5
1	A	142	ILE	2.5
1	A	193	SER	2.5
1	A	307	ALA	2.5
1	B	562	ASP	2.5
1	B	563	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	577	ALA	2.4
1	A	54	VAL	2.4
1	A	182	LEU	2.4
1	A	127	PHE	2.4
1	A	228[A]	PHE	2.4
1	A	313	LYS	2.4
1	A	365	ASP	2.4
1	A	191	ALA	2.4
1	A	546	ALA	2.4
1	A	435	SER	2.4
1	A	24	LEU	2.3
1	A	69	LEU	2.3
1	A	219	LEU	2.3
1	A	423	LEU	2.3
1	A	156	PHE	2.3
1	A	132	GLU	2.3
1	A	479	GLU	2.3
1	A	194	ALA	2.3
1	A	35	PRO	2.3
1	A	583	LEU	2.3
1	A	55	ALA	2.3
1	A	88	ALA	2.3
1	A	325	VAL	2.3
1	A	104	GLN	2.3
1	A	62	CYS	2.3
1	B	558	CYS	2.3
1	A	206	PHE	2.3
1	A	581	ALA	2.3
1	B	572	GLY	2.3
1	A	369	CYS	2.3
1	B	544	LEU	2.3
1	A	152	PRO	2.2
1	A	161	TYR	2.2
1	A	263	TYR	2.2
1	A	396	GLU	2.2
1	A	523	ILE	2.2
1	A	120	VAL	2.2
1	A	9	HIS	2.2
1	A	109	ASN	2.2
1	A	92	ALA	2.2
1	A	330	PHE	2.2
1	A	40	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	462	VAL	2.2
1	A	83	THR	2.2
1	A	392	CYS	2.2
1	A	260	LEU	2.2
1	A	364	ALA	2.2
1	B	364	ALA	2.2
1	A	36	PHE	2.2
1	A	374	PHE	2.2
1	A	530	VAL	2.2
1	A	481	LEU	2.2
1	B	539	ALA	2.2
1	A	3	HIS	2.1
1	A	27	PHE	2.1
1	A	294	GLU	2.1
1	A	353	TYR	2.1
1	A	444	LYS	2.1
1	A	39	HIS	2.1
1	A	301	ASP	2.1
1	A	293	VAL	2.1
1	A	96[A]	PRO	2.1
1	A	113	PRO	2.1
1	A	461	CYS	2.1
1	B	305	LEU	2.1
1	B	301	ASP	2.1
1	A	185	LEU	2.1
1	A	349	LEU	2.1
1	B	583	LEU	2.1
1	B	306	ALA	2.1
1	A	150	TYR	2.0
1	A	79	THR	2.0
1	A	133	THR	2.0
1	A	196	GLN	2.0
1	A	498	VAL	2.0
1	A	302	LEU	2.0
1	A	218	ARG	2.0
1	A	480	SER	2.0
1	A	377	PHE	2.0
1	A	551	PHE	2.0
1	A	84	TYR	2.0
1	A	332	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

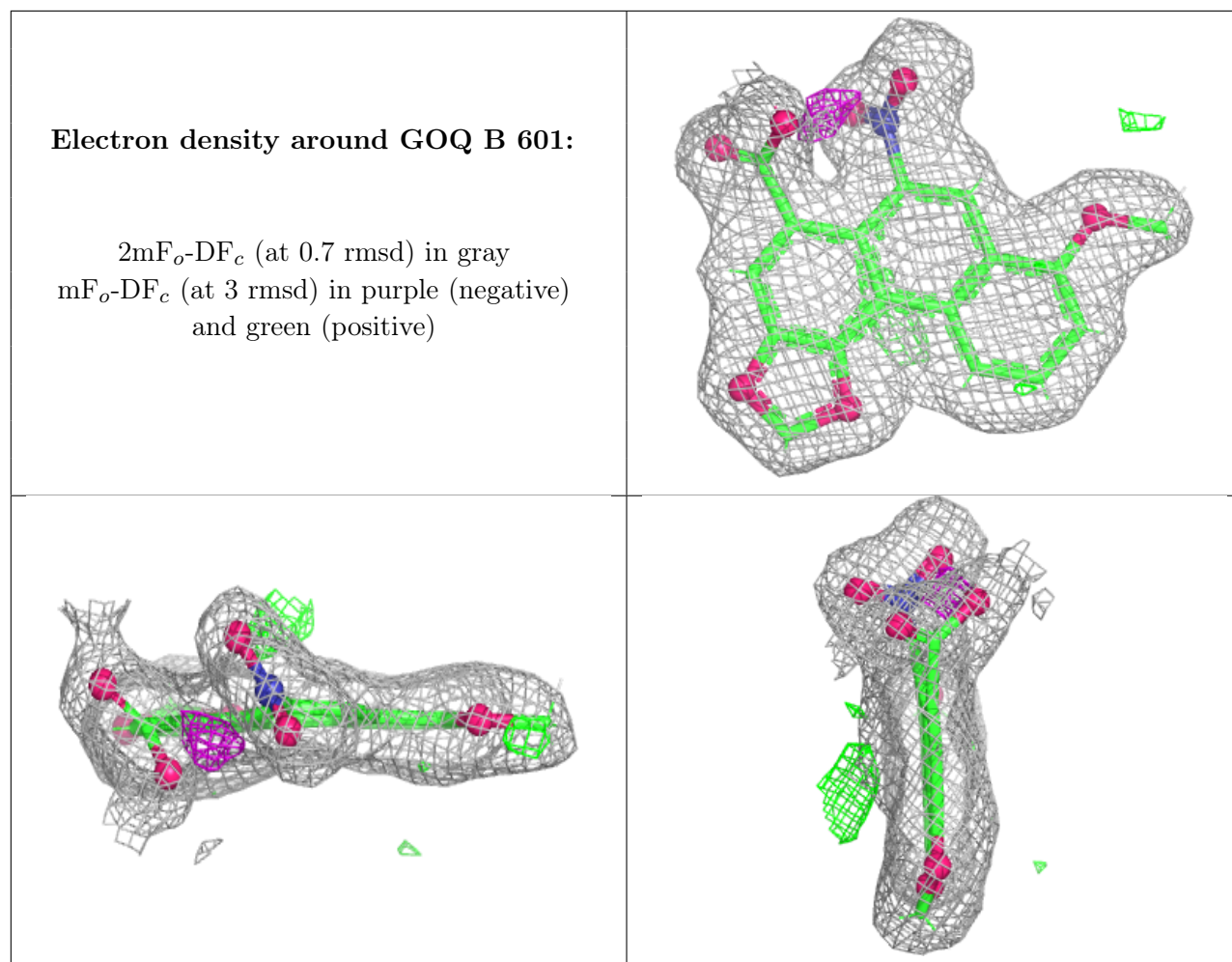
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	EDO	A	608	4/4	0.68	0.16	55,66,72,72	0
3	EDO	A	609	4/4	0.73	0.11	51,61,68,69	0
3	EDO	B	609	4/4	0.77	0.21	39,51,60,62	0
2	MYR	A	605	16/16	0.78	0.22	44,57,63,64	43
2	MYR	A	606	16/16	0.78	0.18	48,65,76,76	0
2	MYR	A	607	16/16	0.78	0.17	47,65,73,79	0
3	EDO	B	614	4/4	0.79	0.14	39,51,61,63	0
2	MYR	A	604	16/16	0.81	0.16	49,65,76,77	0
3	EDO	B	612	4/4	0.82	0.10	31,38,50,60	0
2	MYR	A	602	16/16	0.82	0.18	34,54,65,67	43
2	MYR	B	607	16/16	0.84	0.14	24,37,55,60	0
2	MYR	B	604	16/16	0.84	0.12	22,35,47,48	0
2	MYR	B	606	16/16	0.85	0.12	23,41,57,61	0
2	MYR	B	605	16/16	0.87	0.16	10,30,47,47	43
2	MYR	B	602	16/16	0.87	0.12	38,51,62,62	0
2	MYR	A	603	16/16	0.88	0.13	38,54,66,67	0
3	EDO	B	610	4/4	0.88	0.17	26,36,43,45	0
3	EDO	B	611	4/4	0.89	0.14	18,32,39,47	0
2	MYR	A	601	16/16	0.89	0.14	39,51,57,58	43
2	MYR	B	603	16/16	0.89	0.11	18,30,39,47	0
4	GOQ	B	601	25/25	0.89	0.10	18,25,33,36	36
3	EDO	B	613	4/4	0.91	0.17	20,38,45,45	0
3	EDO	B	608	4/4	0.94	0.07	17,26,31,35	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 ⓘ

There are no such residues in this entry.