



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 11:52 PM UTC

PDB ID : 7XQ1 / pdb_00007xq1
EMDB ID : EMD-33388
Title : Structure of hSLC19A1+2'3'-CDAS
Authors : Zhang, Q.X.; Zhang, X.Y.; Zhu, Y.L.; Sun, P.P.; Gao, A.; Zhang, L.G.; Gao, P.
Deposited on : 2022-05-06
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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A user guide is available at

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

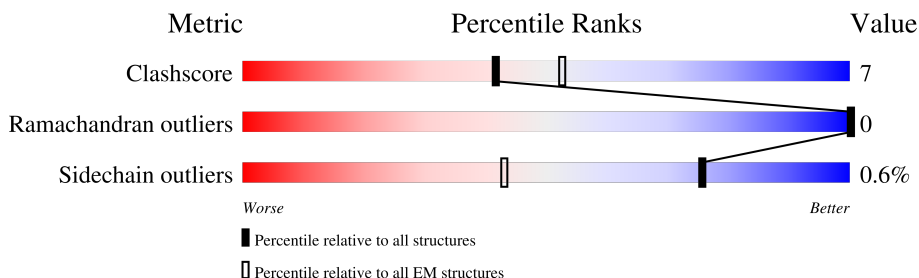
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	544	 63% 10% • 26%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3302 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Reduced folate transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	400	Total	C	N	O	S	0	0
			3214	2138	528	538	10		

There are 38 discrepancies between the modelled and reference sequences:

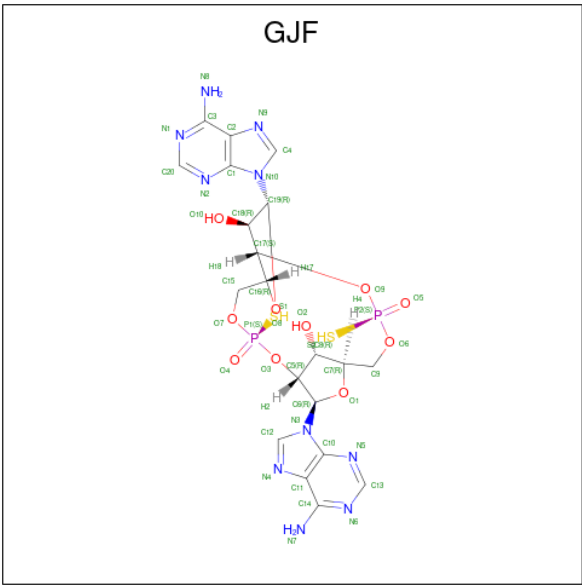
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP P41440
A	-1	GLY	-	expression tag	UNP P41440
A	0	SER	-	expression tag	UNP P41440
A	507	LYS	-	expression tag	UNP P41440
A	508	LEU	-	expression tag	UNP P41440
A	509	GLY	-	expression tag	UNP P41440
A	510	SER	-	expression tag	UNP P41440
A	511	GLU	-	expression tag	UNP P41440
A	512	ASN	-	expression tag	UNP P41440
A	513	LEU	-	expression tag	UNP P41440
A	514	TYR	-	expression tag	UNP P41440
A	515	LEU	-	expression tag	UNP P41440
A	516	GLU	-	expression tag	UNP P41440
A	517	VAL	-	expression tag	UNP P41440
A	518	LEU	-	expression tag	UNP P41440
A	519	PHE	-	expression tag	UNP P41440
A	520	GLN	-	expression tag	UNP P41440
A	521	GLY	-	expression tag	UNP P41440
A	522	PRO	-	expression tag	UNP P41440
A	523	PHE	-	expression tag	UNP P41440
A	524	GLN	-	expression tag	UNP P41440
A	525	GLY	-	expression tag	UNP P41440
A	526	GLY	-	expression tag	UNP P41440
A	527	SER	-	expression tag	UNP P41440
A	528	GLY	-	expression tag	UNP P41440
A	529	GLY	-	expression tag	UNP P41440
A	530	SER	-	expression tag	UNP P41440
A	531	GLY	-	expression tag	UNP P41440

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Chain	Residue	Modelled	Actual	Comment	Reference
A	532	HIS	-	expression tag	UNP P41440
A	533	HIS	-	expression tag	UNP P41440
A	534	HIS	-	expression tag	UNP P41440
A	535	HIS	-	expression tag	UNP P41440
A	536	HIS	-	expression tag	UNP P41440
A	537	HIS	-	expression tag	UNP P41440
A	538	HIS	-	expression tag	UNP P41440
A	539	HIS	-	expression tag	UNP P41440
A	540	HIS	-	expression tag	UNP P41440
A	541	HIS	-	expression tag	UNP P41440

- Molecule 2 is (1 {R},3 {S},6 {R},8 {R},9 {R},10 {S},12 {S},15 {R},17 {R},18 {R})-8,17-bis(6-aminopurin-9-yl)-3,12-bis(oxidanylidene)-3,12-bis(sulfanyl)-2,4,7,11,13,16-hexaoxa-3 λ ^5,12 λ ^5-diphosphatricyclo[13.2.1.0^6,10]octadecane-9,18-diol (CCD ID: GJF) (formula: C₂₀H₂₄N₁₀O₁₀P₂S₂) (labeled as "Ligand of Interest" by depositor).

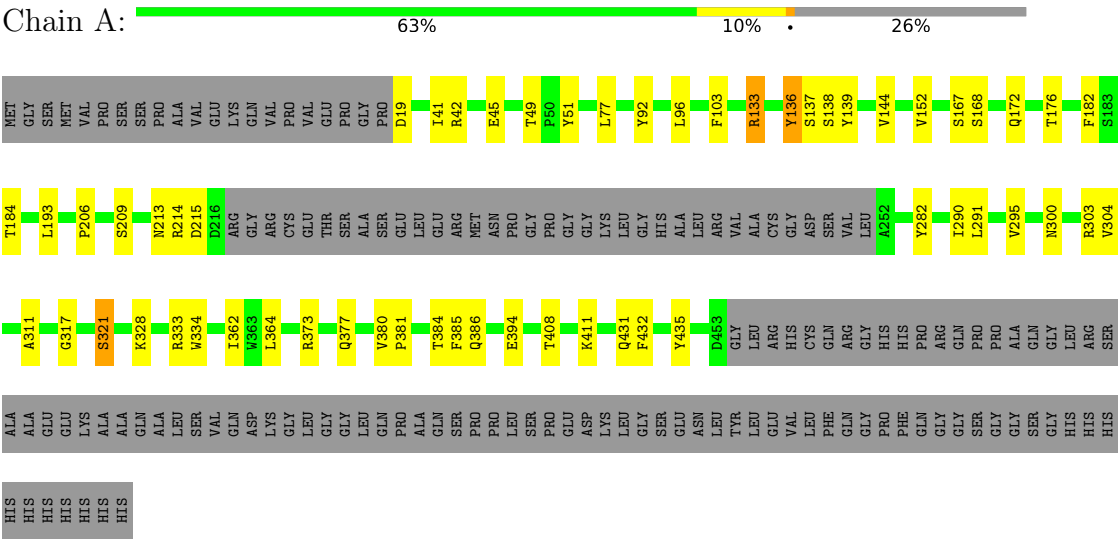


Mol	Chain	Residues	Atoms					AltConf	
2	A	1	Total	C	N	O	P	S	0
			44	20	10	10	2	2	
2	A	1	Total	C	N	O	P	S	0
			44	20	10	10	2	2	

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. 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. 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: Reduced folate transporter



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	169536	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

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: GJF

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	0.22	0/3303	0.50	3/4502 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	SER	N-CA-C	-5.44	105.43	111.36
1	A	133	ARG	N-CA-C	-5.09	105.43	111.69
1	A	136	TYR	N-CA-C	5.07	117.21	111.02

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	3214	0	3292	43	0
2	A	88	0	0	6	0
All	All	3302	0	3292	45	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 (45) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:GJF:N8	2:A:602:GJF:S2	2.53	0.80
1:A:384:THR:OG1	2:A:601:GJF:S1	2.44	0.74
2:A:601:GJF:S2	2:A:602:GJF:N8	2.61	0.73
1:A:386:GLN:HA	1:A:386:GLN:OE1	2.02	0.59
1:A:373:ARG:O	1:A:377:GLN:HG3	2.03	0.58
1:A:136:TYR:O	1:A:139:TYR:HB3	2.04	0.56
1:A:300:ASN:HD22	1:A:303:ARG:HG2	1.70	0.56
1:A:182:PHE:HZ	1:A:304:VAL:HG11	1.70	0.56
1:A:144:VAL:HG11	1:A:152:VAL:HG11	1.88	0.55
1:A:328:LYS:HE3	1:A:381:PRO:O	2.07	0.55
1:A:317:GLY:HA3	1:A:377:GLN:OE1	2.07	0.54
1:A:77:LEU:HD13	1:A:408:THR:HG22	1.90	0.54
1:A:291:LEU:HD13	1:A:432:PHE:CD2	2.42	0.53
1:A:49:THR:HG21	1:A:290:ILE:HG12	1.92	0.52
1:A:19:ASP:N	1:A:19:ASP:OD1	2.43	0.52
1:A:317:GLY:HA3	1:A:377:GLN:CD	2.35	0.52
1:A:41:ILE:HA	1:A:167:SER:HB2	1.93	0.51
1:A:377:GLN:O	1:A:381:PRO:HD3	2.11	0.50
1:A:295:VAL:HB	1:A:362:ILE:HD13	1.93	0.49
1:A:384:THR:CB	2:A:601:GJF:S1	3.00	0.49
1:A:214:ARG:NH1	1:A:394:GLU:OE2	2.44	0.49
1:A:282:TYR:HD1	1:A:411:LYS:HD2	1.78	0.49
1:A:380:VAL:N	1:A:381:PRO:CD	2.75	0.48
1:A:42:ARG:HB2	1:A:45:GLU:HB2	1.94	0.48
1:A:377:GLN:O	1:A:381:PRO:CD	2.62	0.47
1:A:431:GLN:NE2	1:A:435:TYR:OH	2.47	0.46
1:A:172:GLN:NE2	1:A:176:THR:OG1	2.47	0.46
1:A:51:TYR:HD1	1:A:182:PHE:HB3	1.81	0.46
1:A:77:LEU:HA	1:A:408:THR:HG21	1.98	0.45
1:A:328:LYS:HE2	1:A:385:PHE:HB2	1.99	0.44
1:A:215:ASP:OD1	1:A:215:ASP:N	2.40	0.44
1:A:137:SER:C	1:A:139:TYR:H	2.24	0.44
1:A:182:PHE:CZ	1:A:304:VAL:HG11	2.53	0.43
1:A:364:LEU:HD23	1:A:364:LEU:O	2.18	0.43
1:A:384:THR:HB	2:A:601:GJF:S1	2.59	0.42
1:A:139:TYR:HE1	1:A:206:PRO:HD3	1.85	0.42
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.87	0.41
1:A:92:TYR:CE1	1:A:138:SER:OG	2.66	0.41
1:A:168:SER:HB2	1:A:311:ALA:HB2	2.03	0.41
1:A:184:THR:O	1:A:184:THR:HG22	2.21	0.41
1:A:96:LEU:HD11	1:A:136:TYR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:SER:N	1:A:213:ASN:O	2.53	0.41
1:A:333:ARG:HH11	1:A:334:TRP:HE1	1.67	0.41
1:A:42:ARG:NH1	1:A:103:PHE:CZ	2.89	0.40
1:A:377:GLN:NE2	2:A:602:GJF:O2	2.54	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 PDB entries followed by that with respect to all EM entries.

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	396/544 (73%)	385 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	345/457 (76%)	343 (99%)	2 (1%)	78	80

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

Mol	Chain	Res	Type
1	A	133	ARG
1	A	321	SER

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	63	GLN
1	A	277	ASN
1	A	289	HIS
1	A	293	ASN
1	A	300	ASN
1	A	355	HIS
1	A	377	GLN

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](#)

2 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	GJF	A	602	-	44,50,50	1.78	14 (31%)	64,78,78	2.16	19 (29%)
2	GJF	A	601	-	44,50,50	1.77	14 (31%)	64,78,78	2.32	21 (32%)

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	GJF	A	602	-	-	5/26/62/62	0/6/7/7
2	GJF	A	601	-	-	6/26/62/62	0/6/7/7

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	GJF	C20-N2	3.77	1.40	1.33
2	A	602	GJF	C20-N2	3.61	1.40	1.33
2	A	601	GJF	C13-N5	3.51	1.40	1.33
2	A	601	GJF	C13-N6	3.46	1.40	1.33
2	A	602	GJF	C13-N5	3.46	1.40	1.33
2	A	602	GJF	C13-N6	3.38	1.39	1.33
2	A	602	GJF	C20-N1	3.28	1.39	1.33
2	A	601	GJF	C2-C1	-3.25	1.33	1.39
2	A	602	GJF	C2-C1	-3.22	1.33	1.39
2	A	601	GJF	C2-N9	-3.21	1.33	1.39
2	A	601	GJF	C11-N4	-3.21	1.33	1.39
2	A	602	GJF	C11-N4	-3.15	1.33	1.39
2	A	601	GJF	C11-C10	-3.14	1.33	1.39
2	A	601	GJF	C20-N1	3.13	1.39	1.33
2	A	602	GJF	C2-N9	-3.12	1.33	1.39
2	A	602	GJF	C11-C10	-3.08	1.33	1.39
2	A	602	GJF	C11-C14	-2.88	1.33	1.41
2	A	602	GJF	C2-C3	-2.79	1.33	1.41
2	A	601	GJF	C4-N10	-2.77	1.32	1.37
2	A	601	GJF	C11-C14	-2.72	1.33	1.41
2	A	601	GJF	C2-C3	-2.67	1.33	1.41
2	A	602	GJF	C12-N3	-2.67	1.33	1.37
2	A	601	GJF	C12-N3	-2.47	1.33	1.37
2	A	602	GJF	C4-N10	-2.46	1.33	1.37
2	A	602	GJF	C10-N3	-2.36	1.32	1.37
2	A	601	GJF	C10-N3	-2.29	1.32	1.37
2	A	602	GJF	C1-N10	-2.26	1.33	1.37
2	A	601	GJF	C1-N10	-2.00	1.33	1.37

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	GJF	N6-C13-N5	-7.04	117.93	128.58
2	A	601	GJF	N6-C13-N5	-6.97	118.03	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	GJF	N2-C20-N1	-6.91	118.13	128.58
2	A	601	GJF	N2-C20-N1	-6.51	118.73	128.58
2	A	601	GJF	C2-C1-N2	-4.82	120.08	126.72
2	A	601	GJF	N10-C4-N9	-4.66	107.32	113.94
2	A	601	GJF	N3-C12-N4	-4.56	107.46	113.94
2	A	601	GJF	C11-C10-N5	-4.25	120.86	126.72
2	A	602	GJF	C11-C10-N5	-4.22	120.90	126.72
2	A	602	GJF	N10-C4-N9	-4.20	107.98	113.94
2	A	602	GJF	N3-C12-N4	-4.16	108.04	113.94
2	A	602	GJF	C2-C1-N2	-4.03	121.17	126.72
2	A	601	GJF	O1-C6-C5	-3.53	100.50	106.59
2	A	602	GJF	C13-N5-C10	3.24	119.75	111.83
2	A	601	GJF	C3-C2-C1	3.23	121.59	117.18
2	A	601	GJF	C13-N5-C10	3.21	119.67	111.83
2	A	601	GJF	C2-N9-C4	3.21	108.49	103.45
2	A	601	GJF	C11-N4-C12	3.18	108.44	103.45
2	A	601	GJF	N2-C1-N10	3.16	132.55	127.17
2	A	601	GJF	C20-N2-C1	3.12	119.45	111.83
2	A	602	GJF	C20-N2-C1	3.08	119.36	111.83
2	A	601	GJF	C1-N10-C4	2.95	108.83	105.74
2	A	602	GJF	C2-C3-N8	-2.90	116.12	123.29
2	A	601	GJF	C2-C3-N8	-2.87	116.19	123.29
2	A	602	GJF	C11-C14-N7	-2.86	116.19	123.29
2	A	601	GJF	C11-C14-N7	-2.86	116.21	123.29
2	A	602	GJF	C2-N9-C4	2.77	107.81	103.45
2	A	602	GJF	C11-N4-C12	2.68	107.66	103.45
2	A	601	GJF	C14-C11-C10	2.66	120.81	117.18
2	A	602	GJF	C10-N3-C12	2.65	108.52	105.74
2	A	602	GJF	N5-C10-N3	2.63	131.63	127.17
2	A	601	GJF	C10-N3-C12	2.56	108.42	105.74
2	A	601	GJF	C10-C11-N4	-2.52	107.70	110.58
2	A	602	GJF	C14-C11-C10	2.51	120.60	117.18
2	A	601	GJF	N5-C10-N3	2.37	131.19	127.17
2	A	602	GJF	C1-N10-C4	2.36	108.22	105.74
2	A	602	GJF	C3-C2-C1	2.33	120.36	117.18
2	A	602	GJF	N2-C1-N10	2.28	131.04	127.17
2	A	601	GJF	C1-C2-N9	-2.27	107.99	110.58
2	A	602	GJF	C1-C2-N9	-2.08	108.20	110.58

There are no chirality outliers.

All (11) torsion outliers are listed below:

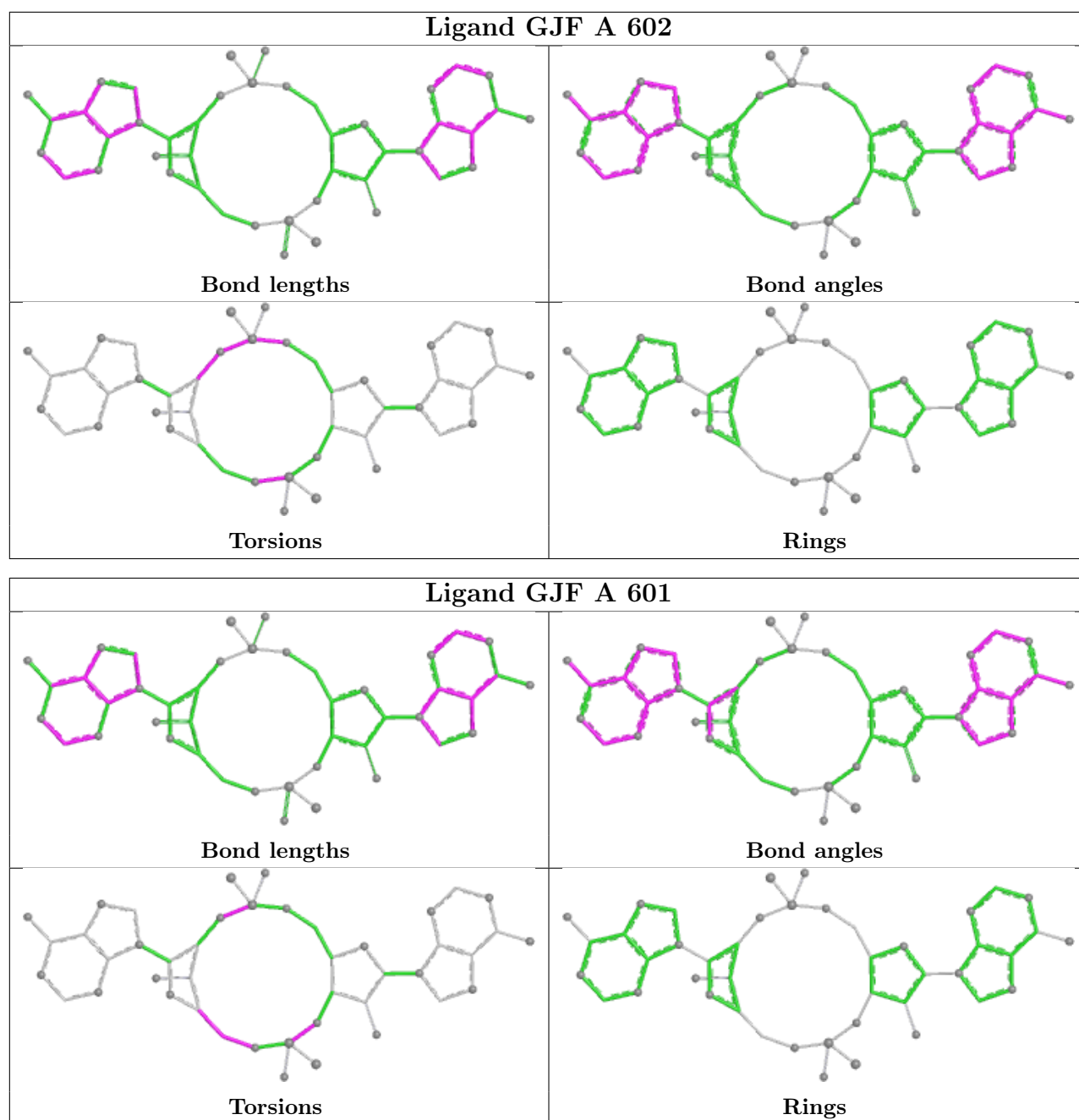
Mol	Chain	Res	Type	Atoms
2	A	601	GJF	C5-O3-P1-O7
2	A	601	GJF	C17-O9-P2-O5
2	A	601	GJF	C5-O3-P1-O4
2	A	601	GJF	O1-C7-C9-O6
2	A	601	GJF	C8-C7-C9-O6
2	A	602	GJF	C5-O3-P1-O4
2	A	602	GJF	C5-O3-P1-O7
2	A	602	GJF	C6-C5-O3-P1
2	A	602	GJF	C9-O6-P2-O9
2	A	602	GJF	C15-O7-P1-O3
2	A	601	GJF	C7-C9-O6-P2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	GJF	3	0
2	A	601	GJF	5	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 Map visualisation

This section contains visualisations of the EMDB entry EMD-33388. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.