



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:41 AM UTC

PDB ID : 7QE2 / pdb_00007qe2
Title : Crystal structure of D-glucuronic acid bound to SN243
Authors : Neun, S.; Brear, P.; Campbell, E.; Omari, K.; Wagner, O.; Hyvonen, M.;
Hollfelder, F.
Deposited on : 2021-12-01
Resolution : 2.15 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

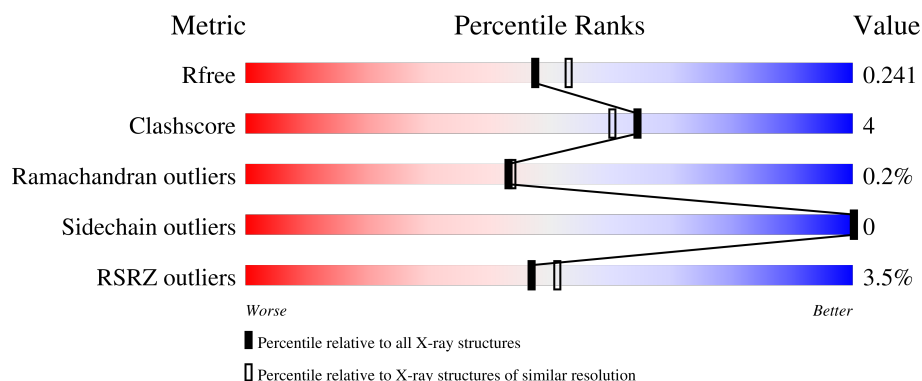
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	759	2% 88% 8% .
1	B	759	4% 86% 11% ..

2 Entry composition [i](#)

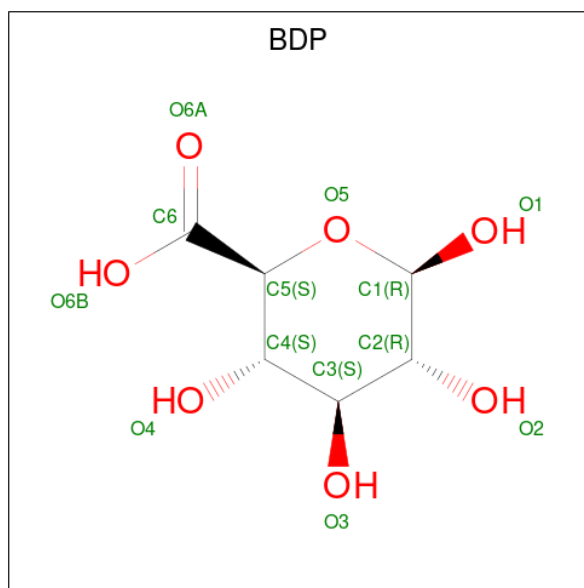
There are 6 unique types of molecules in this entry. The entry contains 11709 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SN243.

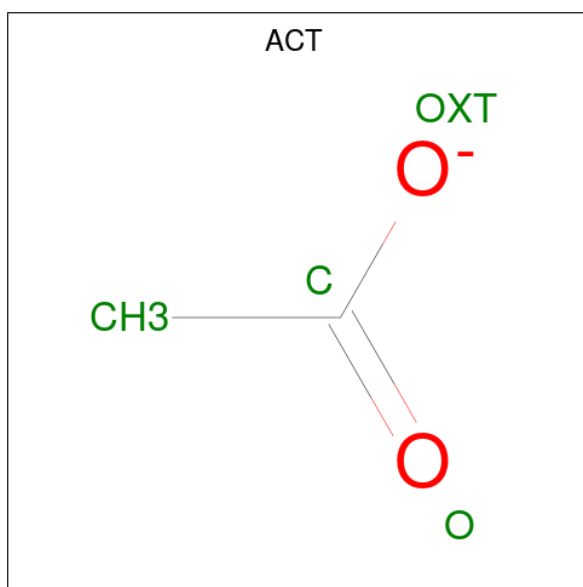
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	737	Total	C	N	O	S	0	2	0
			5626	3526	923	1157	20			
1	B	739	Total	C	N	O	S	0	1	0
			5630	3528	923	1159	20			

- Molecule 2 is beta-D-glucopyranuronic acid (CCD ID: BDP) (formula: $C_6H_{10}O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).

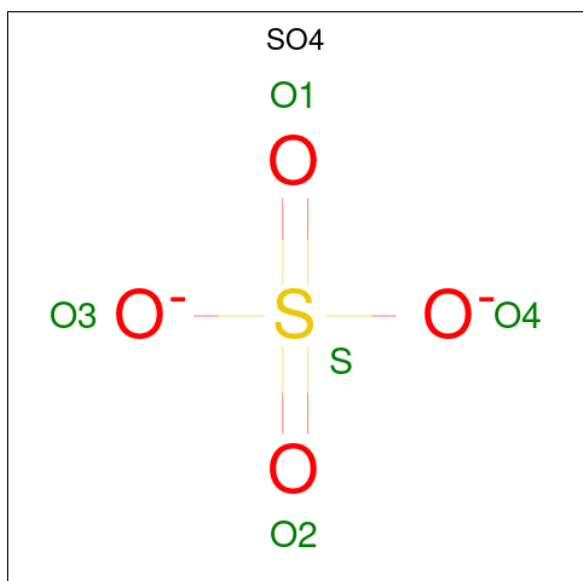


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	Zn	0	0
			19	19		
4	B	14	Total	Zn	0	0
			14	14		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

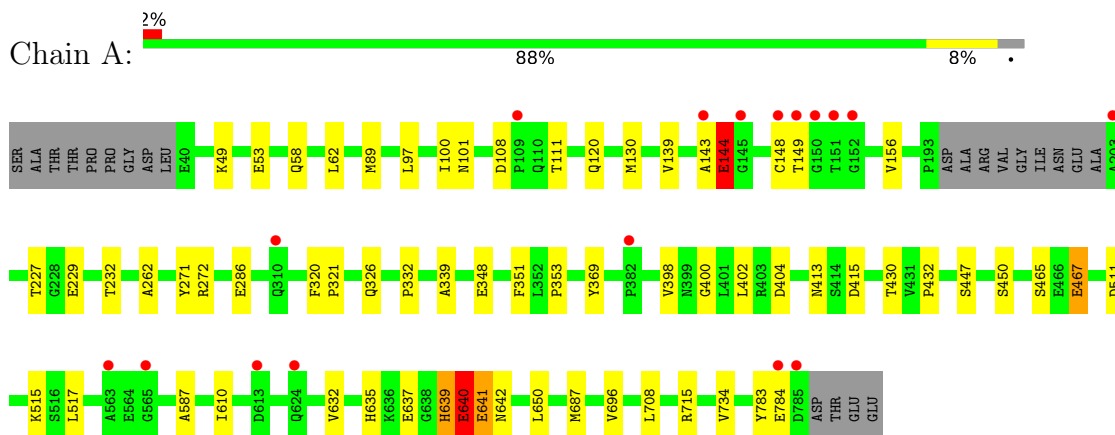
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	212	Total	O	0	0
			212	212		
6	B	157	Total	O	0	1
			158	158		

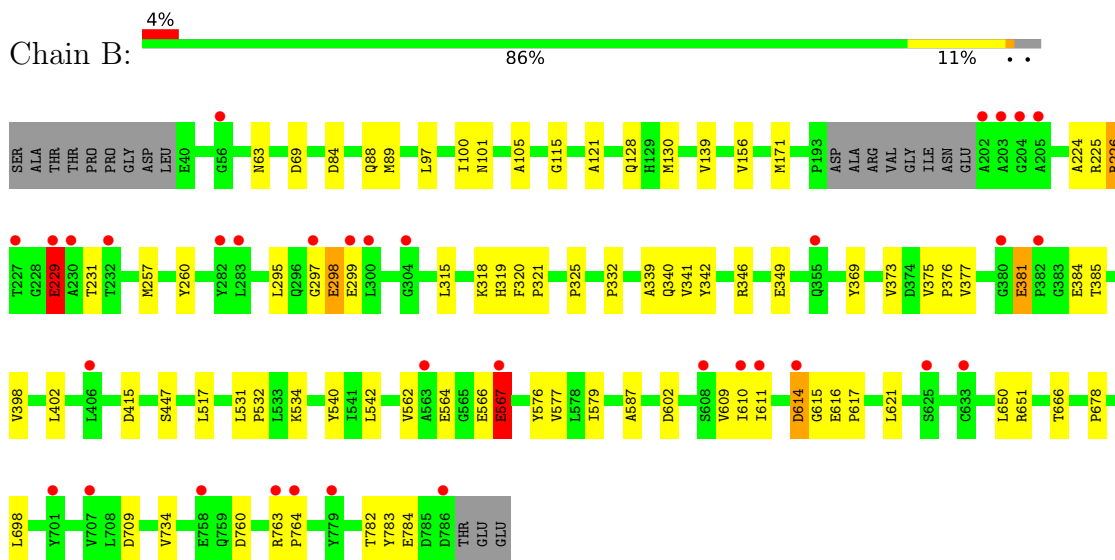
3 Residue-property plots

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: SN243



• Molecule 1: SN243



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.23Å 82.18Å 93.18Å 66.74° 89.26° 89.34°	Depositor
Resolution (Å)	48.31 – 2.15 48.31 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.31-2.15) 97.3 (48.31-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.196 , 0.239 0.198 , 0.241	Depositor DCC
R_{free} test set	4764 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-l 0.000 for -h,k,k-l 0.000 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11709	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ACT, BDP, ZN

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	0.47	2/5751 (0.0%)	0.70	17/7841 (0.2%)
1	B	0.46	4/5755 (0.1%)	0.79	19/7847 (0.2%)
All	All	0.46	6/11506 (0.1%)	0.75	36/15688 (0.2%)

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	A	0	5
1	B	0	3
All	All	0	8

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	640	GLU	CA-CB	11.28	1.72	1.53
1	B	615	GLY	C-N	7.45	1.54	1.33
1	B	298	GLU	CD-OE1	6.44	1.37	1.25
1	B	564	GLU	CD-OE1	5.77	1.36	1.25
1	B	229	GLU	CB-CG	-5.59	1.35	1.52
1	A	450	SER	CB-OG	5.32	1.52	1.42

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	567	GLU	CA-CB-CG	22.10	158.30	114.10
1	B	567	GLU	CB-CA-C	-11.67	87.19	110.42
1	B	226	ARG	CB-CG-CD	11.00	136.59	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	GLU	CB-CA-C	-10.95	90.67	109.83
1	A	783	TYR	CA-C-N	-10.69	108.46	122.79
1	A	783	TYR	C-N-CA	-10.69	108.46	122.79
1	B	564	GLU	CA-CB-CG	10.33	134.77	114.10
1	B	226	ARG	CG-CD-NE	9.82	133.61	112.00
1	B	614	ASP	CB-CA-C	-9.43	90.43	110.32
1	A	641	GLU	CA-C-N	-9.25	105.70	122.35
1	A	641	GLU	C-N-CA	-9.25	105.70	122.35
1	B	567	GLU	CB-CG-CD	9.24	128.31	112.60
1	B	299	GLU	CB-CA-C	9.23	124.70	110.67
1	B	567	GLU	N-CA-CB	9.22	126.07	110.49
1	A	144	GLU	CG-CD-OE2	-8.75	98.28	118.40
1	A	642	ASN	CB-CA-C	7.84	118.33	110.33
1	A	784	GLU	CA-CB-CG	7.83	129.76	114.10
1	B	381	GLU	CA-CB-CG	7.18	128.46	114.10
1	B	226	ARG	CA-CB-CG	-7.03	100.05	114.10
1	A	144	GLU	CG-CD-OE1	6.88	134.23	118.40
1	A	467	GLU	CB-CG-CD	6.63	123.87	112.60
1	B	564	GLU	CB-CA-C	-6.58	100.57	109.71
1	A	784	GLU	N-CA-CB	6.54	120.38	110.11
1	B	229	GLU	CA-CB-CG	6.52	127.14	114.10
1	B	297	GLY	CA-C-N	6.27	129.84	120.31
1	B	297	GLY	C-N-CA	6.27	129.84	120.31
1	B	614	ASP	CB-CG-OD1	-6.21	104.11	118.40
1	A	784	GLU	CB-CG-CD	6.04	122.87	112.60
1	A	640	GLU	CA-CB-CG	5.84	125.78	114.10
1	B	567	GLU	CG-CD-OE2	-5.82	105.01	118.40
1	A	640	GLU	CB-CA-C	5.34	121.05	110.42
1	A	640	GLU	N-CA-CB	-5.29	101.55	110.49
1	A	641	GLU	N-CA-C	5.27	119.62	111.56
1	B	564	GLU	CB-CG-CD	5.14	121.34	112.60
1	A	642	ASN	CA-C-O	5.01	124.35	119.99
1	A	784	GLU	CB-CA-C	-5.01	104.06	111.72

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	ALA	Peptide
1	A	144	GLU	Sidechain
1	A	639	HIS	Peptide
1	A	640	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	641	GLU	Sidechain
1	B	229	GLU	Peptide
1	B	298	GLU	Sidechain
1	B	567	GLU	Peptide

5.2 Too-close contacts ⓘ

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	5626	0	5291	32	0
1	B	5630	0	5293	54	0
2	A	13	0	9	1	0
2	B	13	0	9	1	0
3	A	4	0	3	0	0
4	A	19	0	0	0	0
4	B	14	0	0	0	0
5	A	15	0	0	0	0
5	B	5	0	0	0	0
6	A	212	0	0	2	1
6	B	158	0	0	1	1
All	All	11709	0	10605	86	1

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 4.

All (86) 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:377:VAL:HB	1:B:384:GLU:HB3	1.60	0.83
1:B:381:GLU:HB3	1:B:384:GLU:HB2	1.65	0.76
1:A:465:SER:HB2	1:A:467:GLU:OE1	1.88	0.73
1:A:53:GLU:HB2	1:A:58:GLN:HG2	1.71	0.72
1:B:614:ASP:HB2	1:B:616:GLU:H	1.56	0.70
1:A:120:GLN:NE2	6:A:902:HOH:O	2.25	0.69
1:B:229:GLU:OE2	1:B:231:THR:OG1	2.11	0.68
1:B:381:GLU:CD	1:B:384:GLU:HG3	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ALA:HB2	1:B:610:ILE:HD11	1.77	0.66
1:B:602:ASP:OD1	6:B:901:HOH:O	2.14	0.65
1:B:341:VAL:HG12	1:B:373:VAL:HG21	1.80	0.64
1:B:381:GLU:HB3	1:B:384:GLU:CB	2.27	0.63
1:B:763:ARG:HD2	1:B:764:PRO:HD2	1.82	0.61
1:B:534:LYS:HG2	1:B:576:TYR:OH	2.01	0.61
1:A:148:CYS:O	1:A:149:THR:HG23	2.05	0.56
1:A:232:THR:HB	1:A:286:GLU:HG3	1.87	0.56
1:B:517:LEU:HD23	1:B:734:VAL:HG11	1.88	0.56
1:B:381:GLU:HB3	1:B:384:GLU:CG	2.35	0.56
1:A:262:ALA:HB1	1:A:353:PRO:HB2	1.89	0.55
1:B:340:GLN:O	1:B:373:VAL:HG22	2.07	0.54
1:B:587:ALA:HB1	1:B:650:LEU:HD12	1.89	0.54
1:A:430:THR:HB	1:A:432:PRO:HD2	1.89	0.54
1:A:100:ILE:HG23	1:A:447:SER:HA	1.90	0.54
1:A:687:MET:HG2	1:A:696:VAL:HG21	1.91	0.53
1:B:376:PRO:HA	1:B:384:GLU:O	2.09	0.52
1:B:540:TYR:HB3	1:B:577:VAL:HG22	1.93	0.50
1:B:332:PRO:HB2	1:B:369:TYR:HB2	1.92	0.50
1:B:229:GLU:OE2	1:B:231:THR:HG23	2.11	0.50
1:B:346:ARG:HD2	1:B:349:GLU:CD	2.37	0.50
1:B:121:ALA:HB1	1:B:171:MET:HE1	1.94	0.50
1:A:637:GLU:O	6:A:901:HOH:O	2.18	0.49
1:B:666:THR:OG1	1:B:709:ASP:OD1	2.29	0.49
1:A:332:PRO:HB2	1:A:369:TYR:HB2	1.95	0.49
1:A:639:HIS:O	1:A:640:GLU:HB3	2.12	0.49
1:A:89:MET:HE1	1:A:97:LEU:HD11	1.95	0.48
1:B:415:ASP:OD1	2:B:801:BDP:H1	2.12	0.48
1:B:562:VAL:HG21	1:B:567:GLU:O	2.13	0.48
1:B:224:ALA:HB2	1:B:229:GLU:O	2.13	0.48
1:A:49:LYS:NZ	1:A:62:LEU:O	2.46	0.48
1:B:84:ASP:O	1:B:88:GLN:HG3	2.13	0.48
1:B:346:ARG:HD2	1:B:349:GLU:OE2	2.14	0.48
1:A:398:VAL:O	1:A:402:LEU:HB3	2.14	0.47
1:A:708:LEU:O	1:A:715:ARG:HD2	2.14	0.47
1:B:375:VAL:O	1:B:385:THR:HA	2.15	0.47
1:A:415:ASP:OD1	2:A:801:BDP:H1	2.15	0.47
1:A:400:GLY:O	1:A:404:ASP:HB2	2.14	0.47
1:A:413:ASN:HD22	1:A:413:ASN:C	2.23	0.47
1:A:108:ASP:HB3	1:A:111:THR:OG1	2.13	0.47
1:B:609:VAL:HA	1:B:621:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:VAL:O	1:B:402:LEU:HB3	2.16	0.46
1:B:101:ASN:HB2	1:B:130:MET:HE1	1.99	0.45
1:A:632:VAL:HG23	1:A:635:HIS:CE1	2.52	0.45
1:B:566:GLU:O	1:B:567:GLU:C	2.58	0.45
1:B:320:PHE:CD1	1:B:321:PRO:HA	2.51	0.45
1:A:320:PHE:CD1	1:A:321:PRO:HA	2.52	0.45
1:A:587:ALA:HB1	1:A:650:LEU:HD12	1.99	0.45
1:A:139:VAL:HA	1:A:156:VAL:O	2.17	0.44
1:A:326:GLN:OE1	1:A:332:PRO:HD3	2.17	0.44
1:B:100:ILE:HG23	1:B:447:SER:HA	2.00	0.44
1:B:784:GLU:N	1:B:784:GLU:OE2	2.51	0.44
1:B:128:GLN:HB2	1:B:130:MET:HG3	2.00	0.44
1:B:611:ILE:HA	1:B:617:PRO:HA	2.00	0.43
1:A:339:ALA:HB2	1:A:610:ILE:HD11	1.99	0.43
1:A:101:ASN:HB2	1:A:130:MET:HE1	2.00	0.43
1:B:105:ALA:HB1	1:B:115:GLY:HA2	2.00	0.43
1:B:760:ASP:HB2	1:B:763:ARG:HB3	2.01	0.43
1:B:651:ARG:HH21	1:B:651:ARG:HD3	1.66	0.43
1:A:348:GLU:HA	1:A:351:PHE:CE2	2.54	0.43
1:B:63:ASN:HD21	1:B:69:ASP:CG	2.27	0.42
1:B:542:LEU:HG	1:B:678:PRO:HG2	2.02	0.42
1:A:271:TYR:CE1	1:A:272:ARG:HG2	2.55	0.42
1:B:782:THR:OG1	1:B:783:TYR:N	2.53	0.42
1:B:295:LEU:HD12	1:B:315:LEU:HD11	2.02	0.42
1:B:139:VAL:HA	1:B:156:VAL:O	2.19	0.41
1:B:257:MET:HE1	1:B:260:TYR:CE1	2.55	0.41
1:B:579:ILE:HB	1:B:698:LEU:HD23	2.02	0.41
1:B:325:PRO:HG3	1:B:342:TYR:CE2	2.56	0.41
1:B:229:GLU:OE2	1:B:231:THR:CG2	2.69	0.41
1:A:511:ASP:OD1	1:A:515:LYS:HE3	2.20	0.41
1:B:89:MET:HE1	1:B:97:LEU:HD11	2.02	0.41
1:A:227:THR:OG1	1:A:229:GLU:HG2	2.20	0.40
1:A:517:LEU:HD23	1:A:734:VAL:HG11	2.04	0.40
1:B:318:LYS:HA	1:B:319:HIS:HA	1.77	0.40
1:B:531:LEU:HA	1:B:532:PRO:C	2.46	0.40
1:B:614:ASP:OD1	1:B:616:GLU:O	2.40	0.40
1:B:225:ARG:HH22	1:B:226:ARG:CZ	2.35	0.40

All (1) 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)
6:A:1040:HOH:O	6:B:1048:HOH:O[1_646]	2.15	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	735/759 (97%)	715 (97%)	18 (2%)	2 (0%)	36	34
1	B	736/759 (97%)	713 (97%)	22 (3%)	1 (0%)	48	50
All	All	1471/1518 (97%)	1428 (97%)	40 (3%)	3 (0%)	43	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	GLU
1	A	640	GLU
1	B	567	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	592/607 (98%)	592 (100%)	0	100	100
1	B	592/607 (98%)	592 (100%)	0	100	100
All	All	1184/1214 (98%)	1184 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	189	ASN
1	A	310	GLN
1	B	131	HIS
1	B	293	GLN
1	B	310	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](#)

Of 40 ligands modelled in this entry, 33 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	A	826	-	4,4,4	0.26	0	6,6,6	0.22	0
3	ACT	A	802	-	3,3,3	1.81	1 (33%)	3,3,3	1.65	1 (33%)
5	SO4	A	824	-	4,4,4	0.36	0	6,6,6	0.12	0
2	BDP	B	801	-	13,13,13	0.93	1 (7%)	18,19,19	0.92	0
5	SO4	A	825	-	4,4,4	0.29	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BDP	A	801	-	13,13,13	0.82	1 (7%)	18,19,19	0.90	0
5	SO4	B	817	-	4,4,4	0.23	0	6,6,6	0.26	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	BDP	B	801	-	-	2/4/24/24	0/1/1/1
2	BDP	A	801	-	-	2/4/24/24	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	BDP	O6B-C6	-3.16	1.20	1.30
3	A	802	ACT	CH3-C	2.69	1.59	1.49
2	A	801	BDP	O6B-C6	-2.68	1.22	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	ACT	OXT-C-O	2.03	129.54	122.03

There are no chirality outliers.

All (4) torsion outliers are listed below:

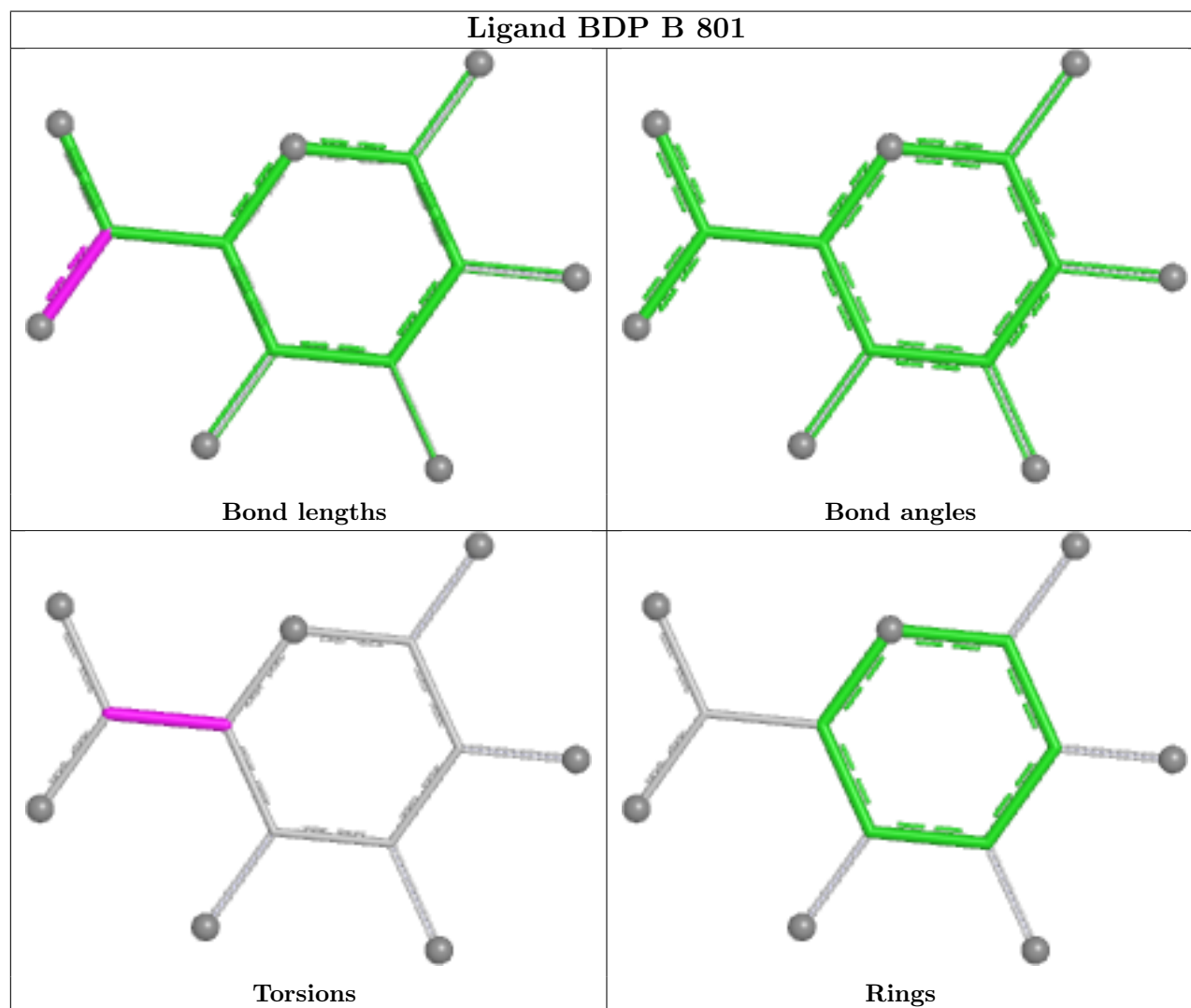
Mol	Chain	Res	Type	Atoms
2	B	801	BDP	C4-C5-C6-O6A
2	B	801	BDP	C4-C5-C6-O6B
2	A	801	BDP	O5-C5-C6-O6A
2	A	801	BDP	O5-C5-C6-O6B

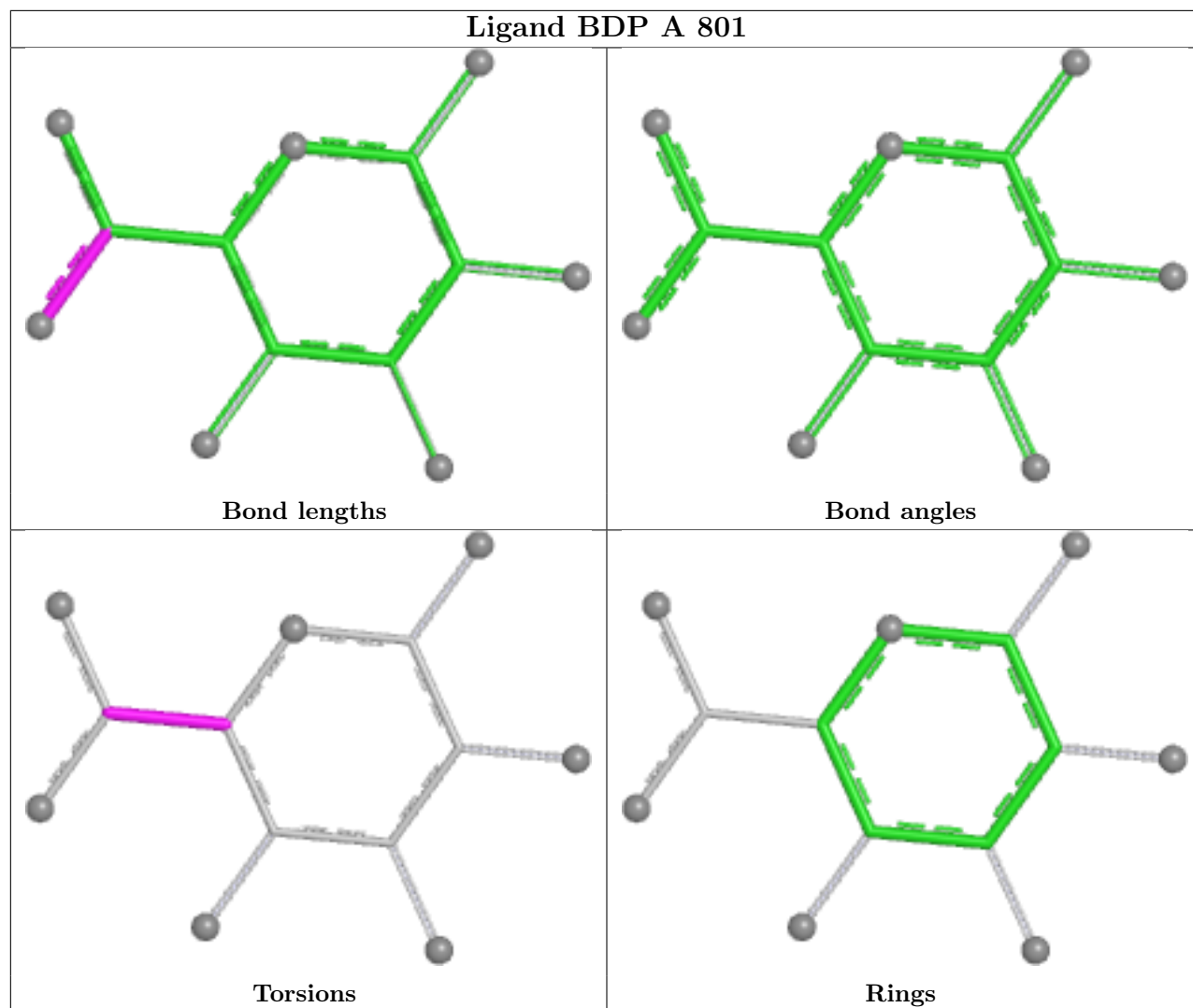
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	BDP	1	0
2	A	801	BDP	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	737/759 (97%)	0.32	17 (2%) 61 64	24, 51, 77, 112	2 (0%)
1	B	739/759 (97%)	0.64	34 (4%) 37 42	32, 58, 84, 122	1 (0%)
All	All	1476/1518 (97%)	0.48	51 (3%) 47 51	24, 55, 81, 122	3 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	GLY	6.1
1	A	565	GLY	4.3
1	B	202	ALA	4.2
1	B	608	SER	3.8
1	A	149	THR	3.5
1	B	382	PRO	3.5
1	B	227	THR	3.4
1	A	203	ALA	3.4
1	B	355[A]	GLN	3.4
1	B	229	GLU	3.3
1	A	563	ALA	3.1
1	A	148	CYS	3.1
1	B	203	ALA	3.1
1	A	151	THR	2.9
1	A	785	ASP	2.9
1	B	230	ALA	2.9
1	B	297	GLY	2.8
1	B	300	LEU	2.8
1	B	282	TYR	2.8
1	A	624[A]	GLN	2.7
1	B	758	GLU	2.7
1	A	152	GLY	2.7
1	A	143	ALA	2.7
1	B	786	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	232	THR	2.6
1	A	784	GLU	2.6
1	B	567	GLU	2.6
1	A	145	GLY	2.5
1	B	701	TYR	2.5
1	A	150	GLY	2.5
1	B	56	GLY	2.4
1	A	613	ASP	2.4
1	B	611	ILE	2.4
1	B	707	VAL	2.3
1	B	205	ALA	2.3
1	A	109	PRO	2.3
1	B	283	LEU	2.3
1	B	763	ARG	2.3
1	B	380	GLY	2.2
1	A	382	PRO	2.2
1	B	299	GLU	2.1
1	B	406	LEU	2.1
1	B	625	SER	2.1
1	B	563	ALA	2.1
1	B	614	ASP	2.1
1	A	310	GLN	2.1
1	B	633	CYS	2.0
1	B	779	TYR	2.0
1	B	610	ILE	2.0
1	B	764	PRO	2.0
1	B	304	GLY	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 oligosaccharides in this entry.

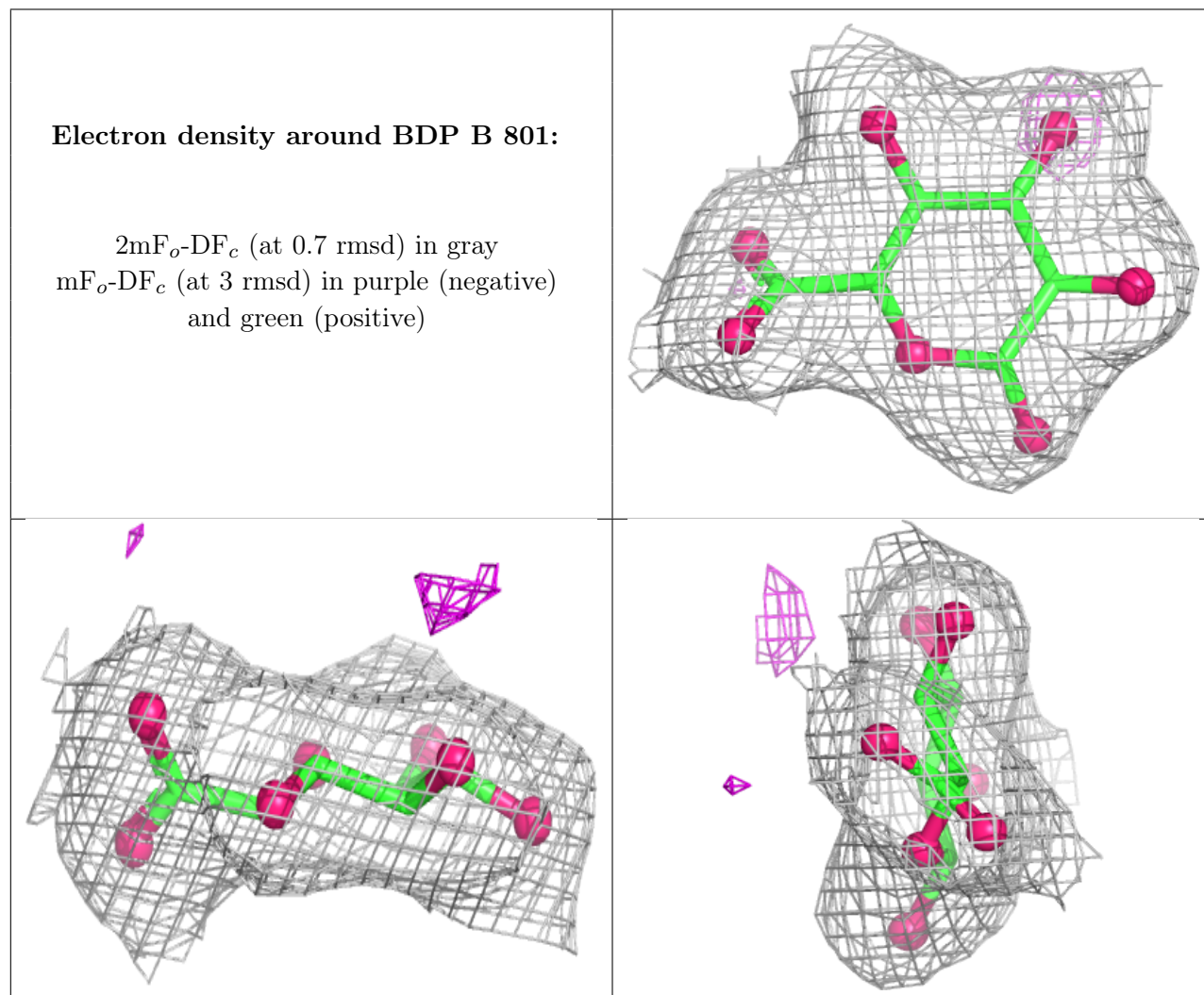
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

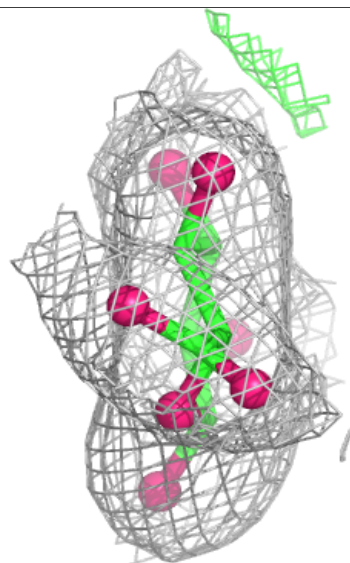
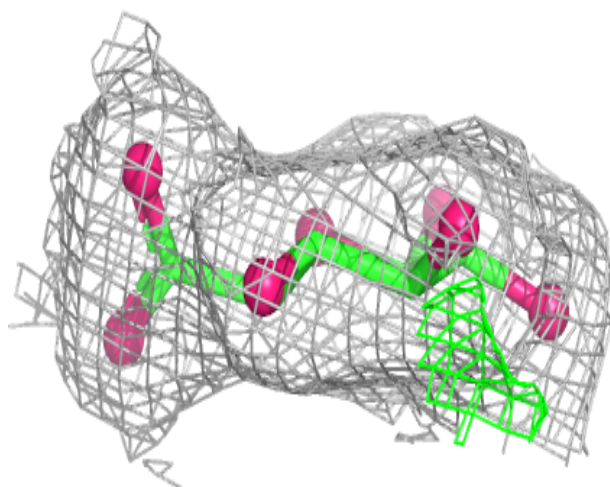
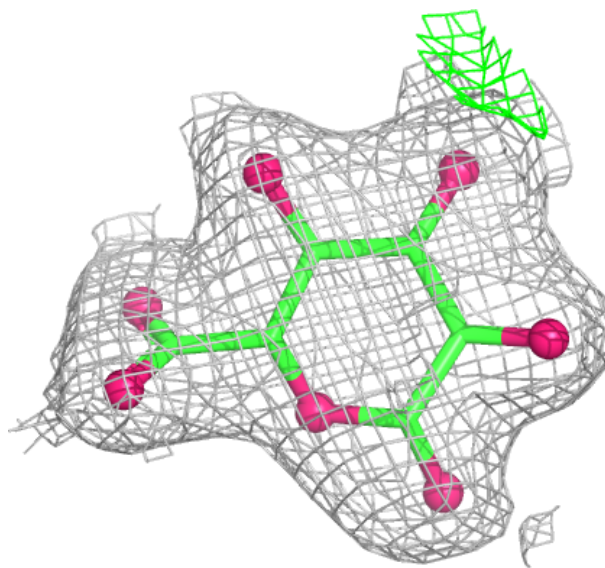
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	B	817	5/5	0.50	0.12	101,101,109,117	0
4	ZN	A	807	1/1	0.80	0.10	133,133,133,133	0
4	ZN	A	822	1/1	0.84	0.10	115,115,115,115	0
4	ZN	B	805	1/1	0.84	0.08	125,125,125,125	0
5	SO4	A	825	5/5	0.84	0.10	93,99,105,118	0
4	ZN	A	821	1/1	0.84	0.16	109,109,109,109	0
4	ZN	A	820	1/1	0.85	0.11	116,116,116,116	0
4	ZN	B	806	1/1	0.85	0.09	133,133,133,133	0
5	SO4	A	826	5/5	0.86	0.08	77,84,104,110	0
4	ZN	A	815	1/1	0.86	0.09	110,110,110,110	0
4	ZN	B	804	1/1	0.88	0.09	114,114,114,114	0
4	ZN	A	818	1/1	0.88	0.10	122,122,122,122	0
4	ZN	B	809	1/1	0.89	0.15	96,96,96,96	0
4	ZN	A	809	1/1	0.89	0.07	118,118,118,118	0
3	ACT	A	802	4/4	0.90	0.11	39,50,51,55	0
4	ZN	B	816	1/1	0.90	0.19	99,99,99,99	0
5	SO4	A	824	5/5	0.90	0.09	68,81,85,103	0
4	ZN	B	802	1/1	0.91	0.13	116,116,116,116	0
4	ZN	B	811	1/1	0.92	0.10	116,116,116,116	0
4	ZN	A	810	1/1	0.92	0.08	104,104,104,104	0
4	ZN	B	812	1/1	0.93	0.14	110,110,110,110	0
4	ZN	B	803	1/1	0.93	0.09	90,90,90,90	0
4	ZN	A	816	1/1	0.93	0.05	124,124,124,124	0
2	BDP	B	801	13/13	0.94	0.07	44,49,52,52	0
4	ZN	B	810	1/1	0.94	0.07	111,111,111,111	0
4	ZN	A	819	1/1	0.94	0.05	122,122,122,122	0
2	BDP	A	801	13/13	0.95	0.07	39,45,51,52	0
4	ZN	B	814	1/1	0.96	0.13	98,98,98,98	0
4	ZN	A	811	1/1	0.96	0.06	95,95,95,95	0
4	ZN	A	814	1/1	0.96	0.11	66,66,66,66	0
4	ZN	A	805	1/1	0.97	0.18	75,75,75,75	0
4	ZN	B	807	1/1	0.97	0.13	57,57,57,57	0
4	ZN	A	808	1/1	0.98	0.03	64,64,64,64	0
4	ZN	B	808	1/1	0.98	0.10	60,60,60,60	0
4	ZN	A	813	1/1	0.99	0.08	83,83,83,83	0
4	ZN	A	803	1/1	0.99	0.07	74,74,74,74	0
4	ZN	A	812	1/1	0.99	0.09	57,57,57,57	0
4	ZN	B	813	1/1	0.99	0.09	77,77,77,77	0
4	ZN	A	823	1/1	0.99	0.08	62,62,62,62	0
4	ZN	A	817	1/1	1.00	0.01	57,57,57,57	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 BDP A 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.