Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2022 – 11:35 am BST

PDB ID	:	7QE2
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:

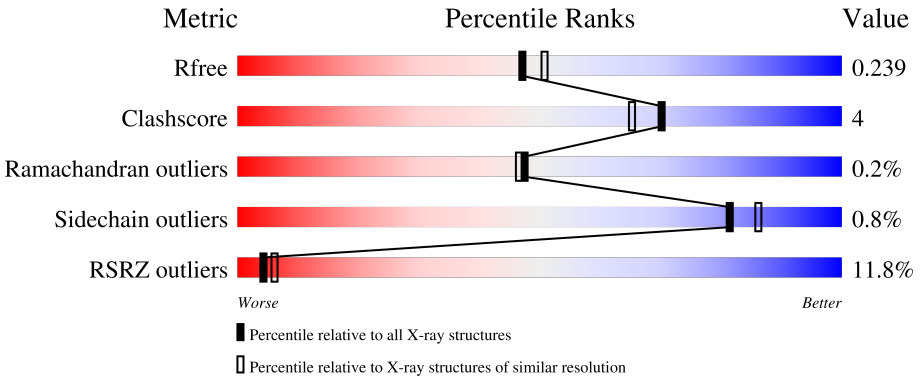
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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 <=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	11% 89% 7%
1	B	759	12% 86% 10%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	802	-	X	-	-

2 Entry composition

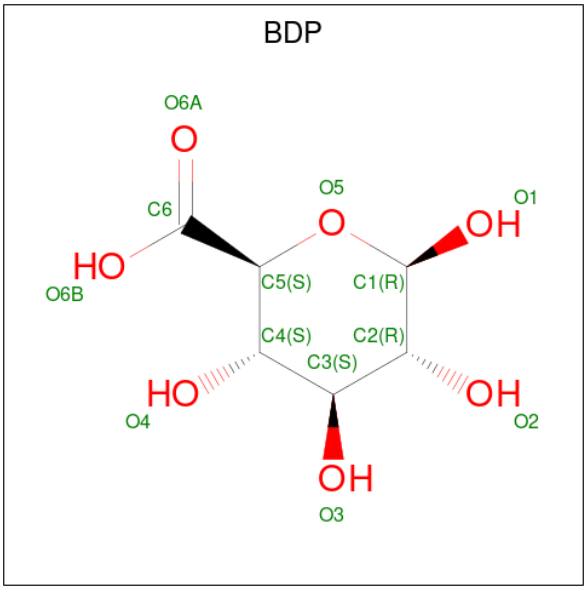
There are 6 unique types of molecules in this entry. The entry contains 11709 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

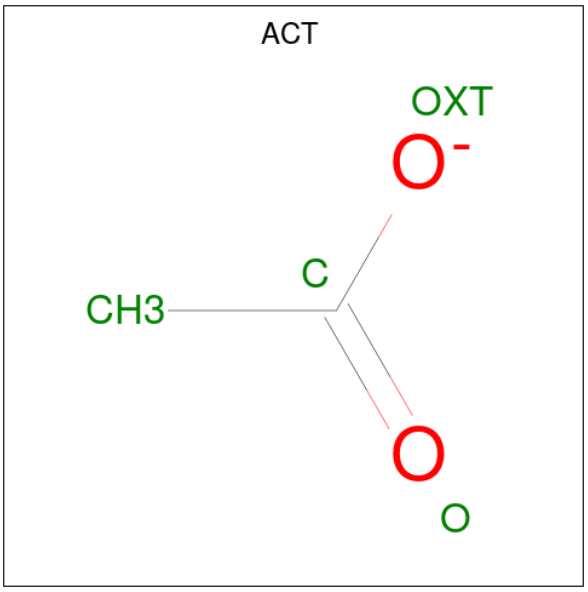
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	737	Total	C	N	O	S	0	2	0
			5626	3526	923	1157	20			
1	B	739	Total	C	N	O	S	0	1	0
			5630	3528	923	1159	20			

- Molecule 2 is beta-D-glucopyranuronic acid (three-letter code: 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 (three-letter code: ACT) (formula: $C_2H_3O_2$).

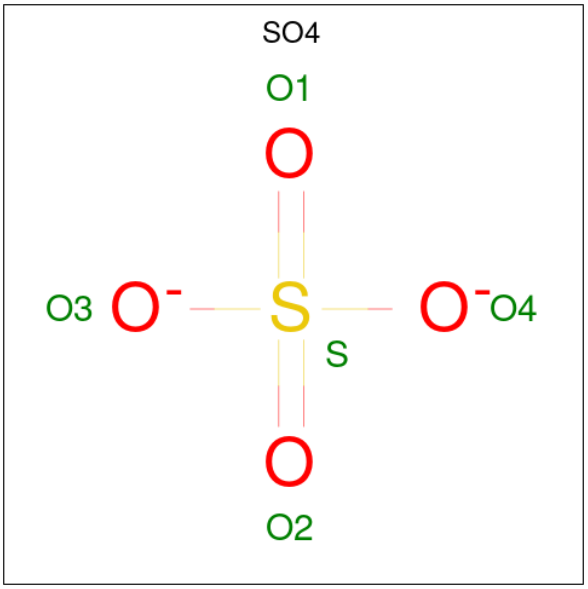


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is water.

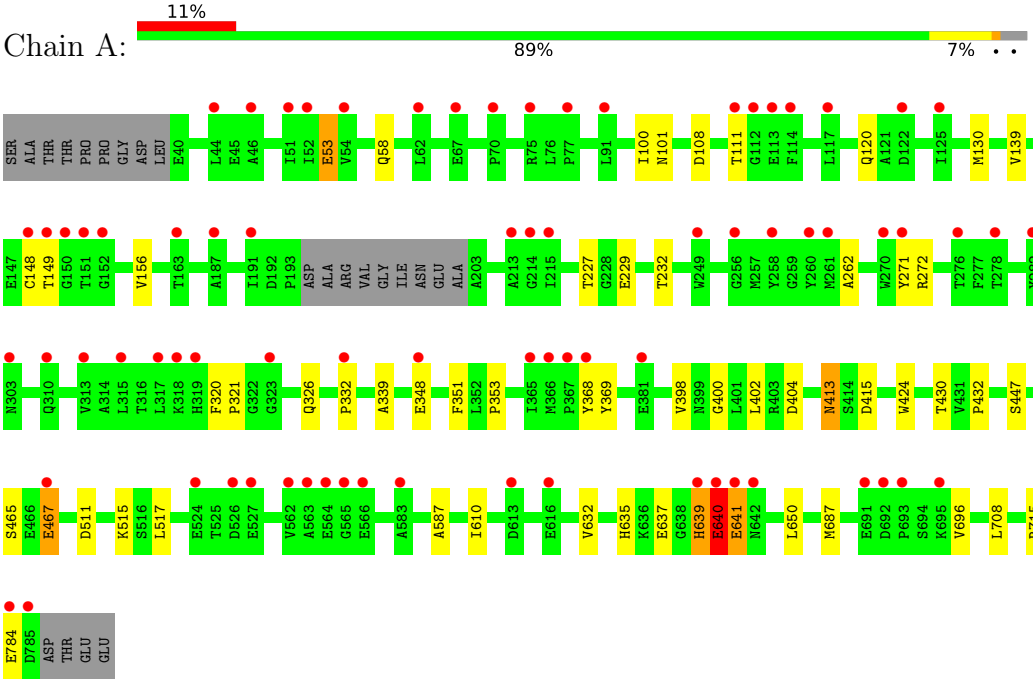
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	212	Total O 212 212	0	0
6	B	157	Total O 158 158	0	1

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

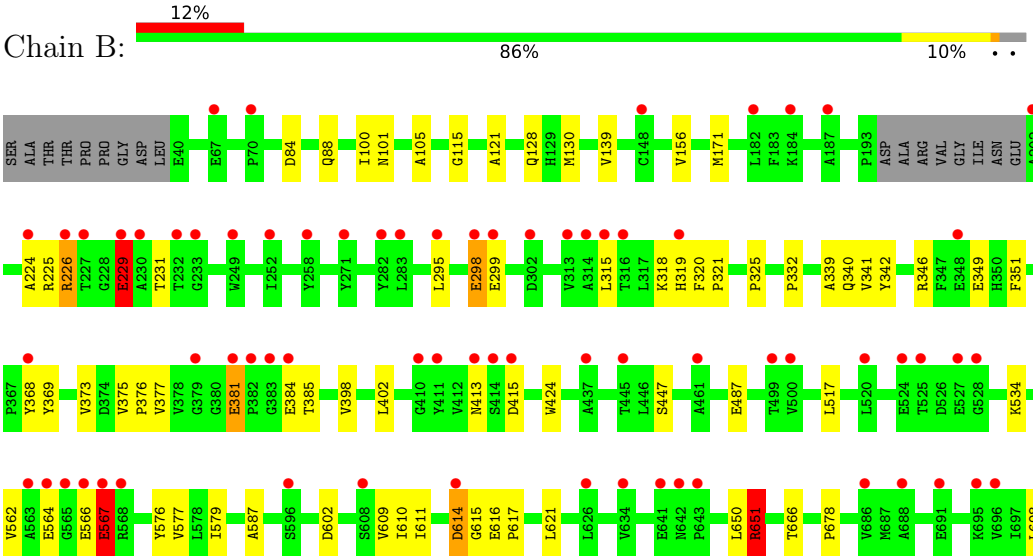
• Molecule 1: SN243

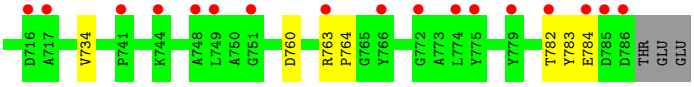
Chain A:



• Molecule 1: SN243

Chain B:




D716
A717
V734
P741
K744
A748
L749
A750
G751
D760
R763
P764
G765
Y766
G772
A773
L774
Y775
Y779
T782
Y783
E784
D785
D786
THR
GLU
GLU

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.31 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.196 , 0.239 0.196 , 0.239	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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BDP, SO4, ACT, 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	0.56	11/5751 (0.2%)	0.67	11/7841 (0.1%)
1	B	0.56	8/5755 (0.1%)	0.80	21/7847 (0.3%)
All	All	0.56	19/11506 (0.2%)	0.74	32/15688 (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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	298	GLU	CD-OE1	10.84	1.37	1.25
1	B	564	GLU	CD-OE1	9.69	1.36	1.25
1	B	615	GLY	C-N	8.73	1.54	1.34
1	B	229	GLU	CB-CG	-8.67	1.35	1.52
1	A	640	GLU	CA-CB	8.45	1.72	1.53
1	A	144	GLU	CG-CD	8.34	1.64	1.51
1	A	450	SER	CB-OG	8.11	1.52	1.42
1	A	467	GLU	CD-OE1	8.04	1.34	1.25
1	A	144	GLU	CD-OE1	7.47	1.33	1.25
1	A	640	GLU	CD-OE1	6.83	1.33	1.25
1	A	641	GLU	CG-CD	-6.77	1.41	1.51
1	B	381	GLU	CB-CG	6.66	1.64	1.52
1	A	641	GLU	CD-OE2	6.66	1.32	1.25
1	B	381	GLU	CD-OE1	6.42	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	640	GLU	CD-OE2	6.28	1.32	1.25
1	B	298	GLU	CD-OE2	5.80	1.32	1.25
1	A	640	GLU	CB-CG	5.28	1.62	1.52
1	A	144	GLU	CD-OE2	5.26	1.31	1.25
1	B	229	GLU	CG-CD	-5.02	1.44	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	567	GLU	CA-CB-CG	20.41	158.30	113.40
1	B	614	ASP	CB-CG-OD1	-15.76	104.11	118.30
1	B	226	ARG	NE-CZ-NH1	11.88	126.24	120.30
1	B	567	GLU	CB-CA-C	-11.60	87.19	110.40
1	B	226	ARG	CG-CD-NE	10.38	133.61	111.80
1	A	144	GLU	CG-CD-OE2	-10.01	98.28	118.30
1	B	614	ASP	CB-CA-C	-9.98	90.43	110.40
1	B	229	GLU	CB-CA-C	-9.86	90.67	110.40
1	B	564	GLU	CA-CB-CG	9.71	134.77	113.40
1	B	226	ARG	CB-CG-CD	9.61	136.59	111.60
1	B	567	GLU	N-CA-CB	8.59	126.07	110.60
1	A	144	GLU	CG-CD-OE1	7.96	134.23	118.30
1	A	784	GLU	CA-CB-CG	7.44	129.76	113.40
1	B	299	GLU	CB-CA-C	7.15	124.70	110.40
1	B	226	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	B	381	GLU	CA-CB-CG	6.85	128.46	113.40
1	B	567	GLU	CG-CD-OE2	-6.65	105.01	118.30
1	A	641	GLU	C-N-CA	-6.40	105.70	121.70
1	B	614	ASP	CB-CG-OD2	6.25	123.92	118.30
1	B	229	GLU	CA-CB-CG	6.24	127.14	113.40
1	B	651	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	226	ARG	CA-CB-CG	-6.07	100.05	113.40
1	B	298	GLU	CG-CD-OE2	-5.67	106.95	118.30
1	A	640	GLU	CA-CB-CG	5.63	125.78	113.40
1	A	53	GLU	CG-CD-OE1	5.44	129.19	118.30
1	A	784	GLU	N-CA-CB	5.44	120.38	110.60
1	A	640	GLU	CB-CA-C	5.33	121.05	110.40
1	A	783	TYR	C-N-CA	-5.30	108.46	121.70
1	A	640	GLU	CG-CD-OE2	-5.24	107.83	118.30
1	B	567	GLU	CB-CG-CD	5.23	128.31	114.20
1	B	229	GLU	CG-CD-OE2	-5.10	108.10	118.30
1	A	640	GLU	N-CA-CB	-5.03	101.55	110.60

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
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 (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	5626	0	5291	30	0
1	B	5630	0	5293	50	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	80	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 (80) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:381:GLU:CD	1:B:384:GLU:HG3	2.19	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:B:121:ALA:HB1	1:B:171:MET:HE1	1.90	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:A:637:GLU:O	6:A:901:HOH:O	2.18	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:B:229:GLU:OE2	1:B:231:THR:OG1	2.11	0.49
1:B:666:THR:OG1	1:B:709:ASP:OD1	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:398:VAL:O	1:B:402:LEU:HB3	2.16	0.46
1:A:632:VAL:HG23	1:A:635:HIS:CE1	2.52	0.45
1:B:346:ARG:HD2	1:B:349:GLU:CD	2.37	0.45
1:B:101:ASN:HB2	1:B:130:MET:HE1	1.98	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: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:A:101:ASN:HB2	1:A:130:MET:HE1	2.00	0.42
1:A:413:ASN:HD22	1:A:413:ASN:C	2.23	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: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: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:566:GLU:O	1:B:567:GLU:C	2.58	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%)	41 37
1	B	736/759 (97%)	713 (97%)	22 (3%)	1 (0%)	51 53
All	All	1471/1518 (97%)	1428 (97%)	40 (3%)	3 (0%)	47 46

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%)	589 (100%)	3 (0%)	88 92
1	B	592/607 (98%)	586 (99%)	6 (1%)	76 81
All	All	1184/1214 (98%)	1175 (99%)	9 (1%)	81 86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	TYR
1	A	413	ASN
1	A	424	TRP
1	B	351	PHE
1	B	368	TYR
1	B	413	ASN
1	B	424	TRP
1	B	487	GLU
1	B	651	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	310	GLN
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 monosaccharides 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	$\#\|Z\|>2$
2	BDP	A	801	-	13,13,13	0.79	1 (7%)	18,19,19	0.91	0
2	BDP	B	801	-	13,13,13	0.90	1 (7%)	18,19,19	0.92	0
5	SO4	A	824	-	4,4,4	0.25	0	6,6,6	0.10	0
5	SO4	A	825	-	4,4,4	0.17	0	6,6,6	0.18	0
5	SO4	A	826	-	4,4,4	0.14	0	6,6,6	0.26	0
3	ACT	A	802	-	3,3,3	1.70	1 (33%)	3,3,3	1.67	2 (66%)
5	SO4	B	817	-	4,4,4	0.12	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	A	801	-	-	2/4/24/24	0/1/1/1
2	BDP	B	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	-3.05	1.20	1.30
2	A	801	BDP	O6B-C6	-2.58	1.22	1.30
3	A	802	ACT	CH3-C	2.52	1.59	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	802	ACT	O-C-CH3	-2.05	114.36	122.33
3	A	802	ACT	OXT-C-O	2.03	129.54	122.05

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

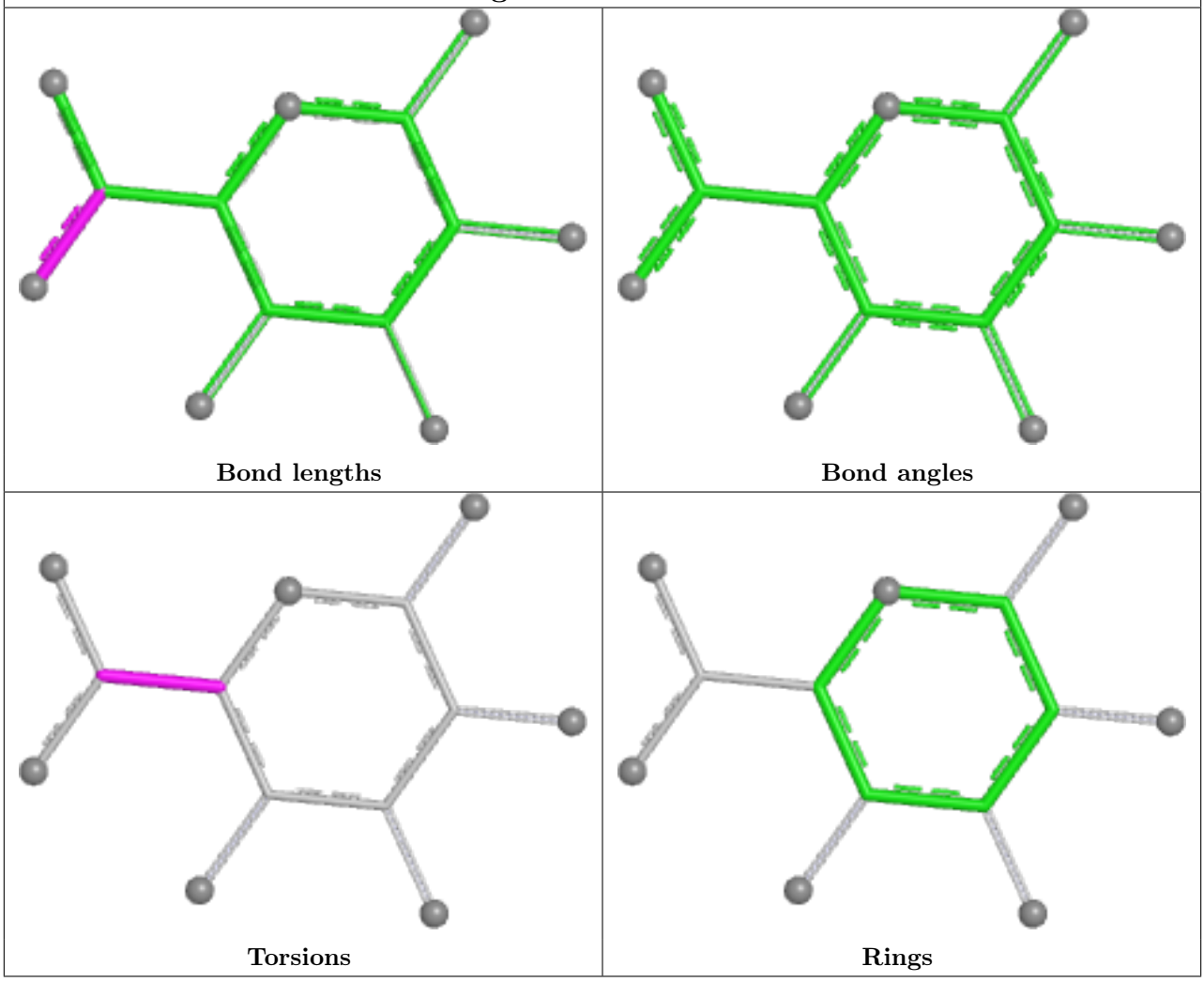
There are no ring outliers.

2 monomers are involved in 2 short contacts:

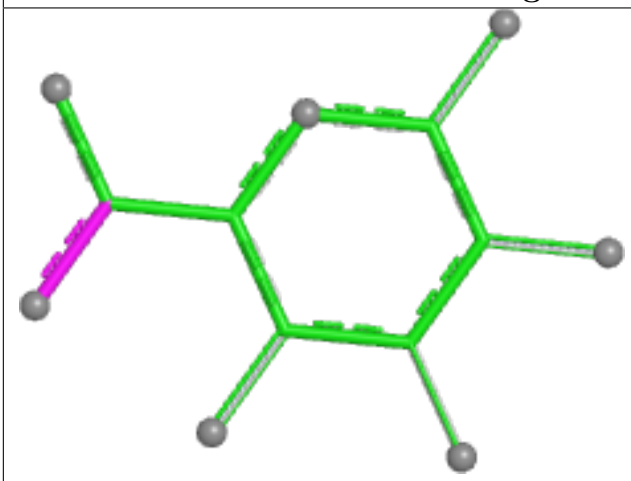
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	BDP	1	0
2	B	801	BDP	1	0

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 then 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.

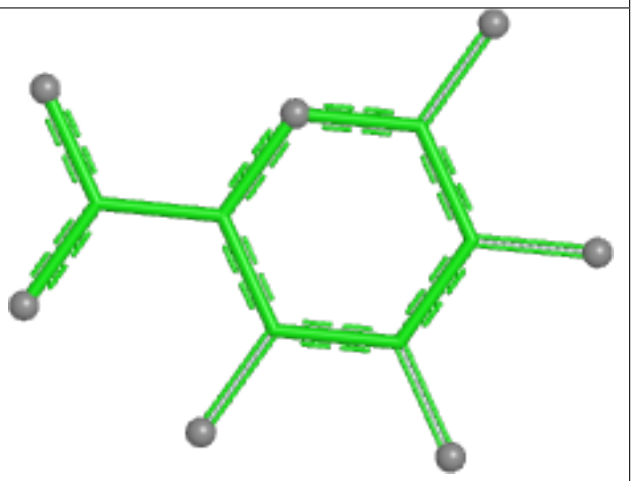
Ligand BDP A 801



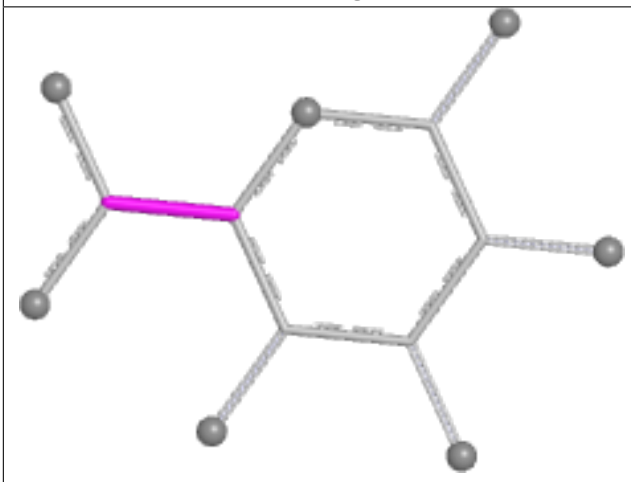
Ligand BDP B 801



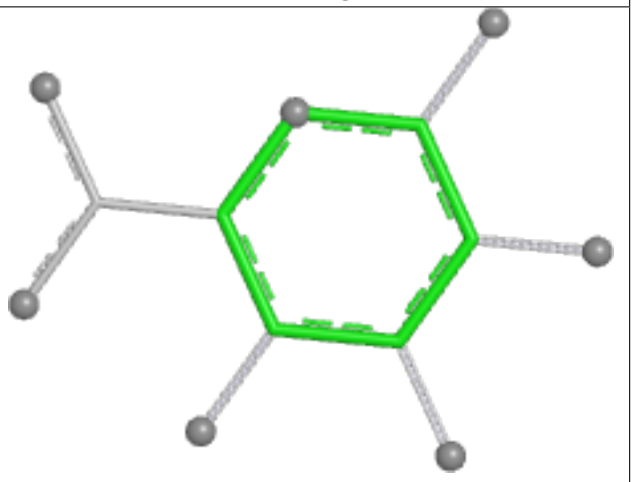
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	0.86	81 (10%)	5 8	40, 51, 77, 112	0
1	B	739/759 (97%)	0.98	93 (12%)	3 5	42, 58, 84, 122	0
All	All	1476/1518 (97%)	0.92	174 (11%)	4 6	40, 55, 81, 122	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	565	GLY	12.0
1	A	565	GLY	10.1
1	A	151	THR	8.8
1	A	148	CYS	6.0
1	B	227	THR	5.9
1	A	564	GLU	5.7
1	A	150	GLY	5.6
1	B	786	ASP	5.6
1	B	784	GLU	5.4
1	A	641	GLU	5.2
1	B	567	GLU	5.1
1	B	232	THR	5.0
1	B	381	GLU	5.0
1	B	785	ASP	5.0
1	B	596	SER	4.8
1	A	114	PHE	4.8
1	A	563	ALA	4.7
1	B	766	TYR	4.6
1	B	564	GLU	4.6
1	A	149	THR	4.6
1	B	382	PRO	4.6
1	B	282	TYR	4.6
1	B	626	LEU	4.4
1	A	639	HIS	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	152	GLY	4.4
1	A	642	ASN	4.3
1	A	381	GLU	4.3
1	B	642	ASN	4.3
1	B	229	GLU	4.2
1	A	640	GLU	4.2
1	B	779	TYR	4.2
1	A	144	GLU	4.2
1	B	202	ALA	4.1
1	B	230	ALA	4.1
1	A	310	GLN	4.0
1	B	566	GLU	4.0
1	A	52	ILE	3.9
1	A	111	THR	3.9
1	A	785	ASP	3.8
1	B	695	LYS	3.8
1	A	187	ALA	3.8
1	A	67	GLU	3.7
1	A	691	GLU	3.7
1	A	146	VAL	3.7
1	A	526	ASP	3.6
1	A	527	GLU	3.5
1	A	51	ILE	3.5
1	B	365	ILE	3.4
1	A	62	LEU	3.4
1	B	524	GLU	3.4
1	A	91	LEU	3.4
1	A	260	TYR	3.4
1	A	271	TYR	3.3
1	A	566	GLU	3.3
1	B	187	ALA	3.3
1	B	528	GLY	3.3
1	B	226	ARG	3.3
1	B	716	ASP	3.3
1	B	355[A]	GLN	3.2
1	B	608	SER	3.2
1	A	613	ASP	3.2
1	B	384	GLU	3.2
1	B	283	LEU	3.2
1	B	751	GLY	3.2
1	A	213	ALA	3.1
1	A	125	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	741	PRO	3.1
1	B	271	TYR	3.1
1	B	313	VAL	3.0
1	A	270	TRP	3.0
1	B	527	GLU	3.0
1	A	215	ILE	2.9
1	B	748	ALA	2.9
1	A	317	LEU	2.9
1	B	461	ALA	2.9
1	A	75	ARG	2.8
1	B	249	TRP	2.8
1	B	691	GLU	2.8
1	A	163	THR	2.8
1	A	366	MET	2.8
1	A	214	GLY	2.8
1	B	686	VAL	2.7
1	B	368	TYR	2.7
1	A	313	VAL	2.7
1	B	772	GLY	2.7
1	B	437	ALA	2.7
1	B	563	ALA	2.7
1	B	316	THR	2.7
1	B	525	THR	2.7
1	B	366	MET	2.7
1	A	348	GLU	2.7
1	B	148	CYS	2.6
1	A	302	ASP	2.6
1	B	782	THR	2.6
1	B	445	THR	2.6
1	A	323	GLY	2.6
1	B	774	LEU	2.6
1	A	258	TYR	2.6
1	A	282	TYR	2.6
1	B	383	GLY	2.6
1	A	315	LEU	2.6
1	B	707	VAL	2.5
1	B	775	TYR	2.5
1	B	717	ALA	2.5
1	A	524	GLU	2.5
1	A	145	GLY	2.5
1	B	749	LEU	2.5
1	B	224	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	643	PRO	2.5
1	A	616	GLU	2.5
1	A	70	PRO	2.4
1	A	278	THR	2.4
1	A	54	VAL	2.4
1	B	763	ARG	2.4
1	B	688	ALA	2.4
1	B	67	GLU	2.4
1	B	70	PRO	2.4
1	A	191	ILE	2.4
1	B	258	TYR	2.4
1	B	314	ALA	2.4
1	A	112	GLY	2.4
1	B	410	GLY	2.4
1	B	696	VAL	2.4
1	B	413	ASN	2.3
1	B	500	VAL	2.3
1	B	302	ASP	2.3
1	B	299	GLU	2.3
1	A	249	TRP	2.3
1	B	641	GLU	2.3
1	B	568	ARG	2.3
1	A	467	GLU	2.3
1	A	784	GLU	2.3
1	A	693	PRO	2.3
1	A	367	PRO	2.3
1	B	379	GLY	2.3
1	A	318	LYS	2.2
1	A	562	VAL	2.2
1	A	319	HIS	2.2
1	A	113	GLU	2.2
1	A	117	LEU	2.2
1	B	315	LEU	2.2
1	B	319	HIS	2.2
1	B	184	LYS	2.2
1	B	744	LYS	2.2
1	A	256	GLY	2.2
1	B	233	GLY	2.2
1	A	122	ASP	2.2
1	B	614	ASP	2.2
1	A	276	THR	2.2
1	B	298	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	295	LEU	2.2
1	A	303	ASN	2.2
1	A	583	ALA	2.2
1	B	414	SER	2.2
1	A	332	PRO	2.2
1	A	692	ASP	2.1
1	A	695	LYS	2.1
1	B	182	LEU	2.1
1	A	368	TYR	2.1
1	A	44	LEU	2.1
1	B	499	THR	2.1
1	B	220	LEU	2.1
1	A	46	ALA	2.1
1	B	411	TYR	2.1
1	B	252	ILE	2.1
1	B	520	LEU	2.1
1	A	365	ILE	2.0
1	A	77	PRO	2.0
1	A	261	MET	2.0
1	A	452	VAL	2.0
1	B	204	GLY	2.0
1	B	415	ASP	2.0
1	B	348	GLU	2.0
1	B	634	VAL	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^{th} 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.

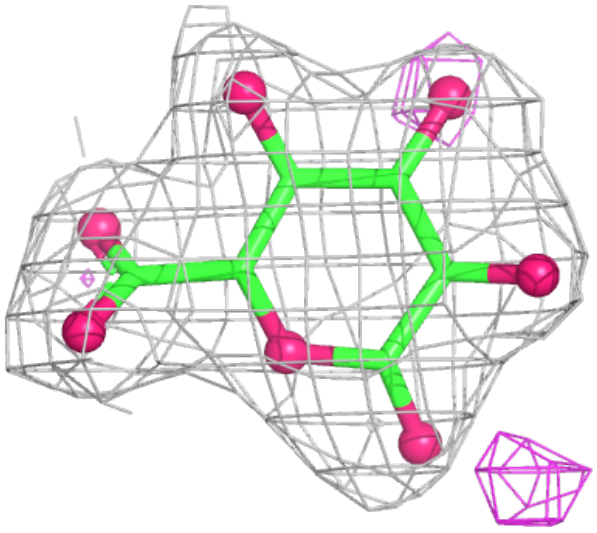
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	A	807	1/1	0.46	0.11	133,133,133,133	0
4	ZN	A	820	1/1	0.70	0.11	116,116,116,116	0
5	SO4	B	817	5/5	0.74	0.13	101,101,109,117	0
5	SO4	A	825	5/5	0.78	0.17	93,99,105,118	0
4	ZN	A	821	1/1	0.78	0.07	109,109,109,109	0
4	ZN	A	815	1/1	0.80	0.09	110,110,110,110	0
4	ZN	B	806	1/1	0.81	0.16	133,133,133,133	0
4	ZN	B	805	1/1	0.85	0.06	125,125,125,125	0
4	ZN	A	816	1/1	0.85	0.14	124,124,124,124	0
4	ZN	A	819	1/1	0.86	0.06	122,122,122,122	0
5	SO4	A	826	5/5	0.86	0.14	77,84,104,110	0
4	ZN	B	804	1/1	0.86	0.10	114,114,114,114	0
5	SO4	A	824	5/5	0.87	0.22	68,81,85,103	0
4	ZN	B	809	1/1	0.89	0.13	96,96,96,96	0
4	ZN	B	816	1/1	0.89	0.06	99,99,99,99	0
4	ZN	A	818	1/1	0.89	0.06	122,122,122,122	0
4	ZN	B	802	1/1	0.90	0.11	116,116,116,116	0
4	ZN	A	822	1/1	0.90	0.03	115,115,115,115	0
4	ZN	A	810	1/1	0.92	0.11	104,104,104,104	0
3	ACT	A	802	4/4	0.93	0.10	39,50,51,55	0
2	BDP	B	801	13/13	0.93	0.17	44,49,52,52	0
4	ZN	B	810	1/1	0.94	0.12	111,111,111,111	0
4	ZN	A	805	1/1	0.94	0.05	75,75,75,75	0
4	ZN	A	809	1/1	0.96	0.15	118,118,118,118	0
2	BDP	A	801	13/13	0.96	0.22	39,45,51,52	0
4	ZN	B	811	1/1	0.96	0.21	116,116,116,116	0
4	ZN	B	803	1/1	0.96	0.05	90,90,90,90	0
4	ZN	B	814	1/1	0.97	0.06	98,98,98,98	0
4	ZN	B	812	1/1	0.97	0.09	110,110,110,110	0
4	ZN	A	813	1/1	0.98	0.14	83,83,83,83	0
4	ZN	A	823	1/1	0.98	0.13	62,62,62,62	0
4	ZN	B	807	1/1	0.98	0.23	57,57,57,57	0
4	ZN	B	808	1/1	0.98	0.16	60,60,60,60	0
4	ZN	A	814	1/1	0.98	0.14	66,66,66,66	0
4	ZN	A	811	1/1	0.98	0.07	95,95,95,95	0
4	ZN	A	812	1/1	0.98	0.21	57,57,57,57	0
4	ZN	A	808	1/1	0.99	0.07	64,64,64,64	0
4	ZN	A	803	1/1	0.99	0.06	74,74,74,74	0
4	ZN	B	813	1/1	0.99	0.06	77,77,77,77	0
4	ZN	A	817	1/1	1.00	0.07	57,57,57,57	0

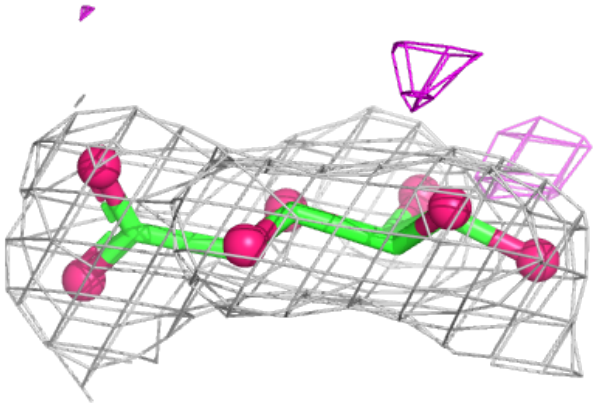
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

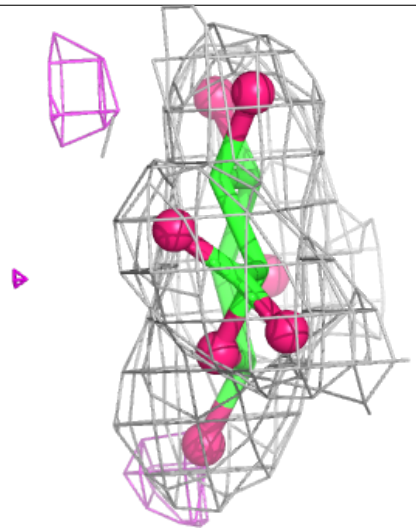
orientation to approximate a three-dimensional view.

Electron density around BDP B 801:

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

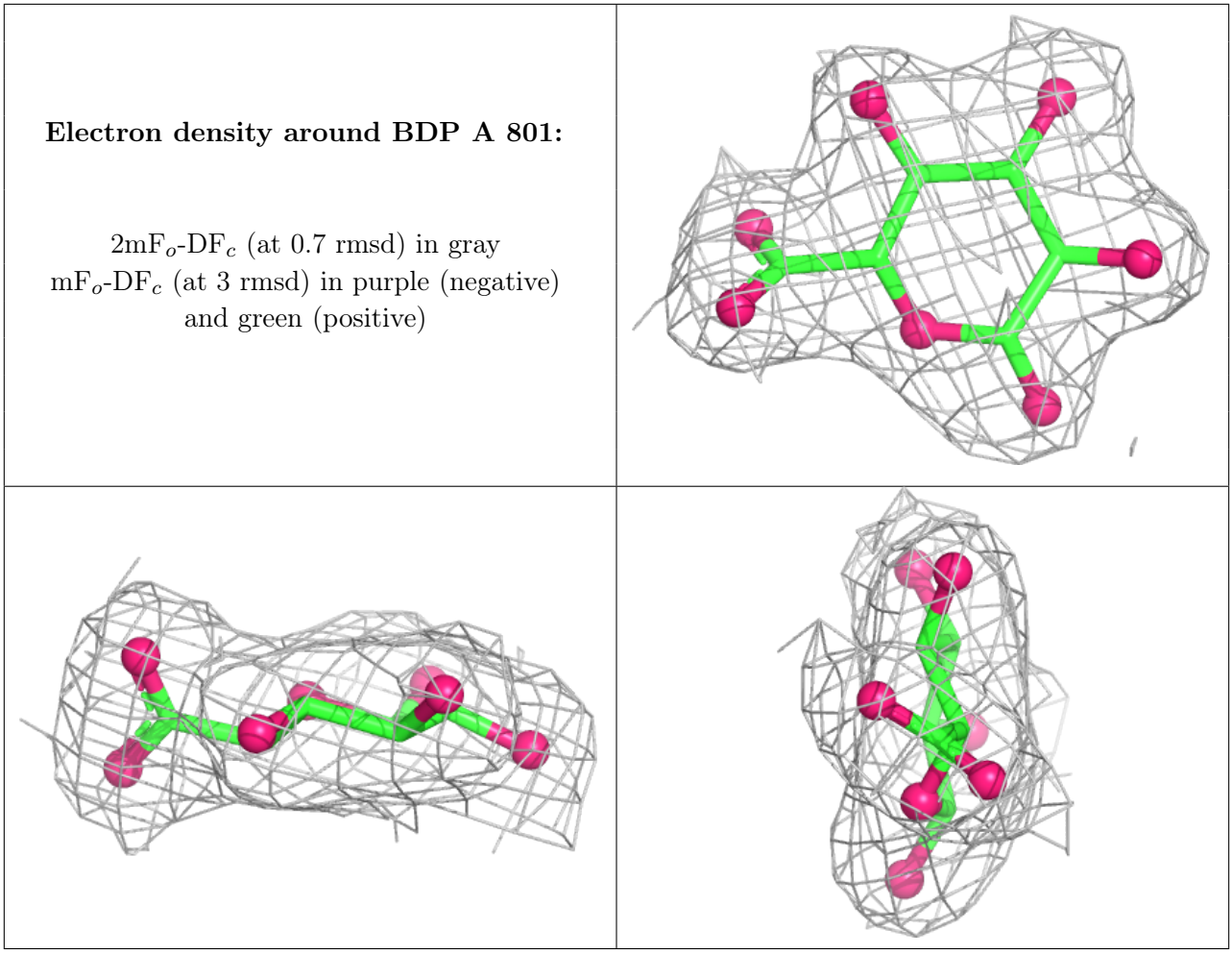






Electron density around BDP A 801:

$2mF_o$-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.