



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:29 AM UTC

PDB ID : 6QCN / pdb_00006qcn
Title : Human Sirt2 in complex with ADP-ribose and the inhibitor quercetin
Authors : Riemer, S.; You, W.; Steegborn, C.
Deposited on : 2018-12-29
Resolution : 2.23 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

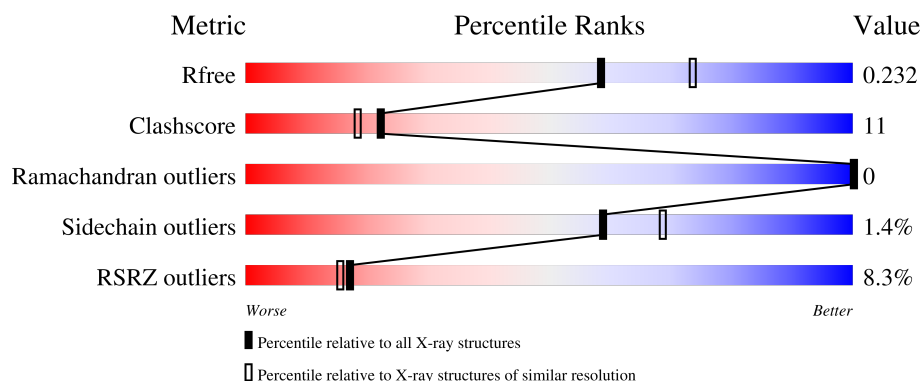
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	304	7% 73% 23% ..
1	B	304	10% 70% 27% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4859 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 NAD-dependent protein deacetylase sirtuin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2374	1524	394	437	19			
1	B	300	Total	C	N	O	S	0	0	0
			2361	1515	389	438	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	HIS	-	expression tag	UNP Q8IXJ6
A	54	MET	-	expression tag	UNP Q8IXJ6
B	53	HIS	-	expression tag	UNP Q8IXJ6
B	54	MET	-	expression tag	UNP Q8IXJ6

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

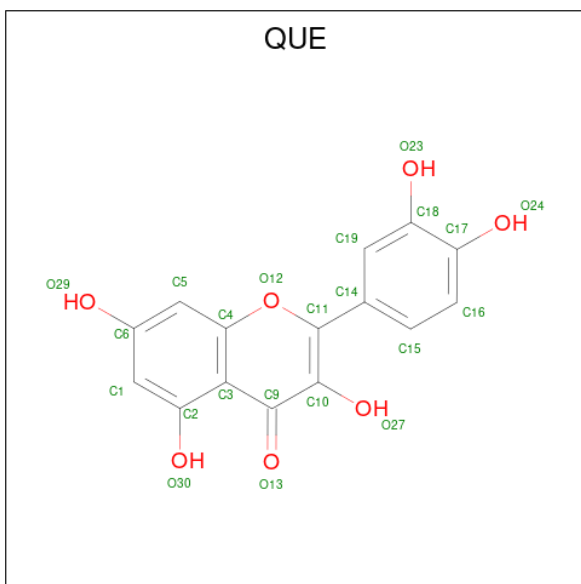
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL [HYDROXY-[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (CCD ID: AR6) (formula: C₁₅H₂₃N₅O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 36	C 15	N 5	O 14	P 2	0	0
3	B	1	Total 36	C 15	N 5	O 14	P 2	0	0

- Molecule 4 is 3,5,7,3',4'-PENTAHYDROXYFLAVONE (CCD ID: QUE) (formula: $C_{15}H_{10}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			22	15	7		

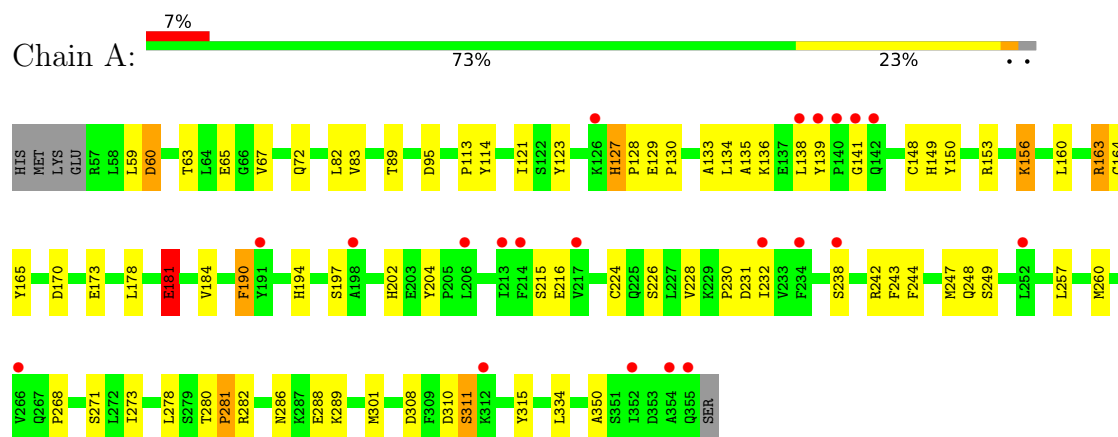
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total 11	O 11	0	0
5	B	17	Total 17	O 17	0	0

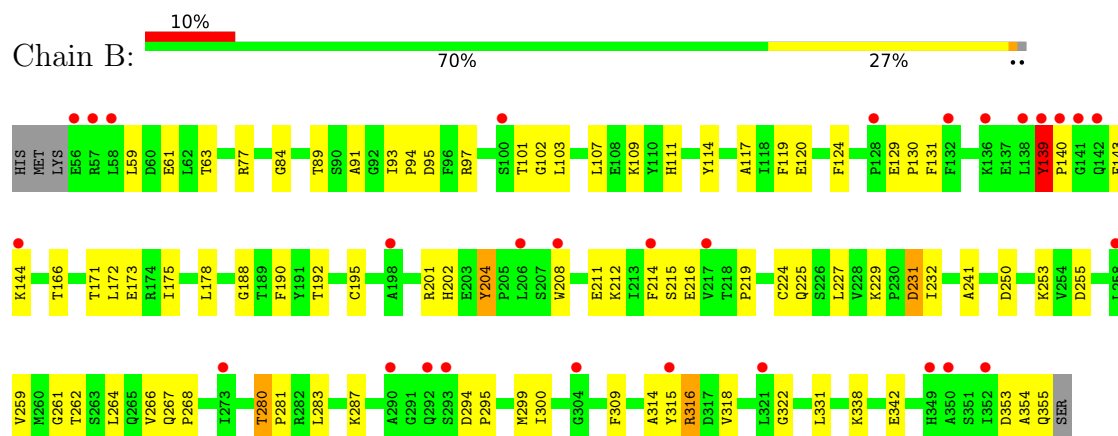
3 Residue-property plots

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: NAD-dependent protein deacetylase sirtuin-2



- Molecule 1: NAD-dependent protein deacetylase sirtuin-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.21Å 78.30Å 114.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.22 – 2.23 46.22 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.22-2.23) 99.5 (46.22-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.209 , 0.234 0.210 , 0.232	Depositor DCC
R_{free} test set	1729 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 14.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.166 for k,h,-l	Xtriage
Reported twinning fraction	0.780 for H, K, L 0.220 for -K, -H, -L	Depositor
Outliers	0 of 34573 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4859	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AR6, QUE, 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	1.23	4/2430 (0.2%)	1.65	24/3280 (0.7%)
1	B	1.20	7/2417 (0.3%)	1.67	19/3268 (0.6%)
All	All	1.22	11/4847 (0.2%)	1.66	43/6548 (0.7%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	HIS	CE1-NE2	7.30	1.39	1.32
1	B	166	THR	C-O	-6.90	1.15	1.23
1	B	93	ILE	N-CA	6.49	1.51	1.46
1	B	259	VAL	C-O	-6.29	1.17	1.24
1	B	250	ASP	C-O	6.04	1.31	1.24
1	A	127	HIS	CE1-NE2	5.68	1.38	1.32
1	B	299	MET	C-O	5.59	1.30	1.23
1	B	94	PRO	C-O	-5.44	1.17	1.23
1	A	160	LEU	C-O	5.35	1.31	1.24
1	A	238	SER	C-O	5.21	1.30	1.23
1	B	117	ALA	C-O	5.01	1.29	1.24

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	PRO	CB-CA-C	7.32	120.57	110.98
1	A	231	ASP	CA-CB-CG	7.00	119.61	112.60
1	A	170	ASP	CA-C-N	6.58	133.54	123.47
1	A	170	ASP	C-N-CA	6.58	133.54	123.47
1	A	301	MET	CA-C-N	6.37	126.15	120.10
1	A	301	MET	C-N-CA	6.37	126.15	120.10
1	A	148	CYS	CA-C-N	6.37	129.34	120.29
1	A	148	CYS	C-N-CA	6.37	129.34	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	THR	CA-CB-OG1	-6.33	100.11	109.60
1	A	273	ILE	CA-C-O	-6.15	114.56	120.95
1	B	102	GLY	CA-C-N	6.10	128.73	120.38
1	B	102	GLY	C-N-CA	6.10	128.73	120.38
1	B	322	GLY	CA-C-O	-6.03	116.52	121.76
1	B	231	ASP	N-CA-C	-5.95	106.66	112.97
1	A	82	LEU	CA-C-O	-5.88	114.17	120.46
1	B	139	TYR	CB-CA-C	5.87	118.41	110.37
1	B	331	LEU	CA-C-N	5.85	128.39	120.44
1	B	331	LEU	C-N-CA	5.85	128.39	120.44
1	A	181	GLU	CB-CG-CD	5.83	122.50	112.60
1	A	281	PRO	N-CD-CG	-5.79	94.52	103.20
1	A	67	VAL	CA-C-O	-5.74	114.68	121.05
1	A	286	ASN	CA-C-O	-5.71	114.61	120.89
1	B	253	LYS	CB-CA-C	-5.70	102.28	111.18
1	B	172	LEU	N-CA-C	-5.68	106.18	113.23
1	B	119	PHE	CB-CA-C	-5.60	102.45	111.18
1	B	241	ALA	CA-C-N	5.59	127.77	120.28
1	B	241	ALA	C-N-CA	5.59	127.77	120.28
1	A	60	ASP	N-CA-C	-5.55	105.77	112.54
1	B	300	ILE	CA-C-N	5.47	128.62	120.90
1	B	300	ILE	C-N-CA	5.47	128.62	120.90
1	A	128	PRO	CA-C-N	5.43	126.52	119.78
1	A	128	PRO	C-N-CA	5.43	126.52	119.78
1	A	350	ALA	CA-C-N	5.38	128.03	120.28
1	A	350	ALA	C-N-CA	5.38	128.03	120.28
1	A	163	ARG	CB-CA-C	-5.31	101.51	110.43
1	B	77	ARG	CB-CA-C	5.30	117.62	109.03
1	B	204	TYR	CB-CA-C	5.28	117.05	108.87
1	A	156	LYS	CA-C-N	5.27	128.32	120.31
1	A	156	LYS	C-N-CA	5.27	128.32	120.31
1	B	101	THR	N-CA-C	-5.22	106.59	113.12
1	B	294	ASP	CB-CA-C	5.13	117.53	109.27
1	A	89	THR	CA-CB-OG1	5.06	117.19	109.60
1	A	63	THR	CA-C-O	-5.01	115.92	121.33

There are no chirality outliers.

There are no planarity outliers.

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	2374	0	2361	47	0
1	B	2361	0	2319	57	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	36	0	20	0	0
3	B	36	0	21	4	0
4	A	22	0	8	1	0
5	A	11	0	0	4	0
5	B	17	0	0	2	0
All	All	4859	0	4729	101	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 11.

All (101) 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:211:GLU:O	1:B:215:SER:HB2	1.66	0.95
1:B:190:PHE:CD2	1:B:232:ILE:HD11	2.07	0.88
1:B:211:GLU:O	1:B:215:SER:CB	2.35	0.75
1:A:190:PHE:CE2	1:A:232:ILE:HD11	2.21	0.74
1:A:244:PHE:CE1	1:B:295:PRO:HG3	2.22	0.73
1:B:139:TYR:CG	1:B:140:PRO:HD2	2.24	0.71
1:B:61:GLU:HG3	1:B:63:THR:OG1	1.90	0.70
1:B:202:HIS:HD2	5:B:513:HOH:O	1.77	0.66
1:B:111:HIS:CE1	5:B:503:HOH:O	2.49	0.66
1:A:65:GLU:HG3	1:A:334:LEU:HD21	1.76	0.65
1:A:129:GLU:HB2	1:A:130:PRO:HD3	1.79	0.63
1:A:244:PHE:CE1	1:B:295:PRO:CG	2.82	0.63
1:B:192:THR:OG1	1:B:231:ASP:OD2	2.12	0.63
1:A:249:SER:HB3	5:A:502:HOH:O	2.00	0.62
1:B:190:PHE:CD2	1:B:232:ILE:CD1	2.83	0.60
1:B:97:ARG:HG3	1:B:97:ARG:HH11	1.65	0.60
1:B:89:THR:OG1	3:B:402:AR6:N6	2.35	0.59
1:A:244:PHE:CZ	1:B:295:PRO:CG	2.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:GLN:OE1	1:B:268:PRO:HA	2.04	0.58
1:A:278:LEU:O	1:A:315:TYR:OH	2.15	0.56
1:B:139:TYR:C	1:B:139:TYR:CD2	2.84	0.55
1:A:224:CYS:SG	1:A:226:SER:HB2	2.47	0.55
1:A:138:LEU:C	1:A:138:LEU:HD23	2.32	0.54
1:A:163:ARG:HG3	1:A:164:CYS:N	2.22	0.54
1:B:103:LEU:O	1:B:107:LEU:HG	2.08	0.54
1:B:61:GLU:CG	1:B:63:THR:OG1	2.54	0.54
1:B:190:PHE:CE2	1:B:232:ILE:CD1	2.92	0.52
1:A:163:ARG:HG2	1:A:165:TYR:CE1	2.45	0.52
1:A:249:SER:CB	5:A:502:HOH:O	2.57	0.52
1:A:114:TYR:N	1:A:114:TYR:CD2	2.78	0.51
1:A:173:GLU:HB3	1:A:178:LEU:HD12	1.92	0.51
1:A:134:LEU:O	1:A:138:LEU:N	2.40	0.51
1:B:139:TYR:CD1	1:B:140:PRO:HD2	2.46	0.51
1:B:315:TYR:CD2	1:B:316:ARG:HB3	2.47	0.50
1:A:244:PHE:CZ	1:B:295:PRO:HG2	2.46	0.50
1:A:204:TYR:CD1	1:A:228:VAL:HG11	2.47	0.50
1:A:72:GLN:HA	1:A:72:GLN:OE1	2.11	0.50
1:A:289:LYS:NZ	1:A:310:ASP:OD2	2.42	0.50
1:B:255:ASP:C	1:B:280:THR:HG23	2.37	0.49
1:A:243:PHE:O	1:A:247:MET:HB2	2.14	0.48
1:A:288:GLU:OE2	5:A:501:HOH:O	2.20	0.48
1:B:59:LEU:HD13	1:B:281:PRO:HG3	1.96	0.48
1:B:190:PHE:CE2	1:B:232:ILE:HD11	2.47	0.48
1:B:229:LYS:NZ	1:B:232:ILE:O	2.47	0.47
1:A:190:PHE:CD2	1:A:232:ILE:HD11	2.49	0.47
1:B:309:PHE:O	1:B:314:ALA:CB	2.63	0.46
1:B:124:PHE:CE2	1:B:227:LEU:HD23	2.50	0.46
1:A:242:ARG:HG3	1:A:242:ARG:HH11	1.80	0.46
1:A:268:PRO:O	1:A:271:SER:HB2	2.16	0.46
4:A:403:QUE:C9	5:A:507:HOH:O	2.64	0.46
1:A:59:LEU:HD11	1:A:281:PRO:HB3	1.98	0.45
1:A:113:PRO:HG2	1:A:114:TYR:CE2	2.52	0.45
1:A:163:ARG:NH1	1:A:181:GLU:O	2.49	0.45
1:A:150:TYR:O	1:A:153:ARG:HB3	2.17	0.45
1:A:139:TYR:CE1	1:A:141:GLY:HA2	2.52	0.45
1:A:129:GLU:HB2	1:A:130:PRO:CD	2.46	0.45
1:B:91:ALA:O	1:B:143:PHE:HD1	2.00	0.45
1:B:61:GLU:OE1	1:B:63:THR:OG1	2.28	0.44
1:A:257:LEU:HB2	1:A:282:ARG:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:CYS:O	1:B:225:GLN:HB2	2.18	0.44
1:A:123:TYR:CE1	1:A:127:HIS:HB2	2.52	0.44
1:A:247:MET:HE3	1:A:248:GLN:HG3	1.99	0.44
1:B:283:LEU:HD12	1:B:318:VAL:O	2.18	0.44
1:A:163:ARG:HD2	1:A:184:VAL:HG23	1.99	0.44
1:B:309:PHE:O	1:B:314:ALA:HB1	2.18	0.44
1:A:121:ILE:HD12	1:A:121:ILE:HA	1.86	0.43
1:B:84:GLY:C	1:B:261:GLY:O	2.61	0.43
1:B:109:LYS:O	1:B:111:HIS:CE1	2.71	0.43
1:B:91:ALA:O	1:B:143:PHE:CD1	2.71	0.43
1:B:208:TRP:CZ2	1:B:212:LYS:HE3	2.53	0.43
1:B:188:GLY:HA3	1:B:231:ASP:O	2.18	0.43
1:A:95:ASP:OD1	1:A:95:ASP:C	2.61	0.43
1:A:133:ALA:O	1:A:136:LYS:HG2	2.18	0.43
1:A:308:ASP:OD1	1:A:311:SER:HB3	2.19	0.43
1:A:60:ASP:OD1	1:A:60:ASP:C	2.61	0.43
1:A:215:SER:O	1:A:216:GLU:HB2	2.18	0.42
1:A:280:THR:HA	1:A:281:PRO:HD3	1.92	0.42
1:B:144:LYS:NZ	1:B:353:ASP:OD1	2.52	0.42
1:B:201:ARG:O	1:B:202:HIS:C	2.63	0.42
1:B:97:ARG:HG3	1:B:97:ARG:NH1	2.33	0.42
1:B:338:LYS:HE2	1:B:342:GLU:OE2	2.20	0.42
1:B:171:THR:O	1:B:175:ILE:HG13	2.19	0.42
1:A:123:TYR:CD1	1:A:123:TYR:C	2.98	0.41
1:A:153:ARG:O	1:A:156:LYS:HB3	2.20	0.41
1:B:114:TYR:OH	1:B:120:GLU:OE1	2.34	0.41
1:A:83:VAL:HG12	1:A:260:MET:HB2	2.02	0.41
1:B:208:TRP:O	1:B:212:LYS:HG2	2.20	0.41
1:A:194:HIS:HA	1:A:202:HIS:O	2.20	0.41
1:B:214:PHE:C	1:B:216:GLU:N	2.78	0.41
1:A:135:ALA:O	1:A:138:LEU:HB3	2.20	0.41
1:B:173:GLU:HB3	1:B:178:LEU:HD12	2.03	0.41
1:B:262:THR:HG23	1:B:264:LEU:HG	2.02	0.41
1:B:287:LYS:HG3	3:B:402:AR6:C2	2.50	0.41
1:B:204:TYR:CD2	1:B:208:TRP:CE2	3.09	0.41
1:B:129:GLU:N	1:B:130:PRO:CD	2.84	0.40
1:B:266:VAL:HG21	3:B:402:AR6:H4D	2.03	0.40
1:B:287:LYS:HG3	3:B:402:AR6:N3	2.36	0.40
1:B:354:ALA:O	1:B:355:GLN:C	2.64	0.40
1:B:95:ASP:C	1:B:95:ASP:OD1	2.64	0.40
1:B:130:PRO:O	1:B:131:PHE:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LYS:CB	1:B:219:PRO:HG3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/304 (98%)	280 (94%)	17 (6%)	0	100	100
1	B	298/304 (98%)	273 (92%)	25 (8%)	0	100	100
All	All	595/608 (98%)	553 (93%)	42 (7%)	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 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	260/265 (98%)	256 (98%)	4 (2%)	57	66
1	B	256/265 (97%)	253 (99%)	3 (1%)	63	72
All	All	516/530 (97%)	509 (99%)	7 (1%)	59	69

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	GLU
1	A	190	PHE
1	A	197	SER
1	A	311	SER
1	B	139	TYR
1	B	195	CYS
1	B	316	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	HIS
1	B	167	GLN
1	B	292	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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
4	QUE	A	403	-	24,24,24	0.72	0	36,36,36	1.46	4 (11%)
3	AR6	B	402	-	39,39,39	0.94	2 (5%)	56,60,60	1.45	11 (19%)
3	AR6	A	402	-	39,39,39	1.38	3 (7%)	56,60,60	1.23	7 (12%)

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
4	QUE	A	403	-	-	4/4/4/4	0/3/3/3
3	AR6	B	402	-	-	6/22/54/54	0/4/4/4
3	AR6	A	402	-	-	1/22/54/54	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	AR6	O4D-C1D	-5.70	1.36	1.43
3	A	402	AR6	PB-O3A	3.60	1.63	1.59
3	A	402	AR6	PA-O3A	3.30	1.63	1.59
3	B	402	AR6	O4D-C1D	2.54	1.46	1.43
3	B	402	AR6	PB-O3A	2.27	1.62	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	QUE	O12-C11-C14	4.58	117.28	110.87
4	A	403	QUE	C14-C11-C10	-4.27	121.72	128.44
3	B	402	AR6	O1A-PA-O2A	3.78	130.05	112.44
3	A	402	AR6	O3A-PB-O2B	-3.27	100.87	110.70
3	A	402	AR6	C1D-C2D-C3D	-3.21	98.34	102.29
3	B	402	AR6	O1D-C1D-C2D	3.02	124.15	110.25
3	B	402	AR6	O3A-PA-O2A	-2.97	101.77	110.70
3	B	402	AR6	O3D-C3D-C2D	2.91	121.13	111.82
3	B	402	AR6	O2D-C2D-C1D	2.90	119.93	111.85
3	B	402	AR6	O4'-C1'-N9	-2.81	102.69	108.09
3	B	402	AR6	O3D-C3D-C4D	-2.78	103.09	111.08
4	A	403	QUE	C2-C3-C9	2.66	125.38	121.45
3	A	402	AR6	O3'-C3'-C4'	2.64	118.65	111.08
3	A	402	AR6	O1B-PB-O3A	-2.37	100.87	107.27
3	B	402	AR6	C4-N9-C8	2.35	108.21	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	AR6	C2D-C3D-C4D	-2.34	98.09	102.61
3	A	402	AR6	C2D-C3D-C4D	-2.27	98.22	102.61
3	A	402	AR6	O1B-PB-O2B	2.20	122.66	112.44
3	B	402	AR6	C1D-C2D-C3D	2.19	104.98	102.29
3	B	402	AR6	O1B-PB-O3A	2.15	113.09	107.27
4	A	403	QUE	O23-C18-C17	2.10	124.02	118.42
3	A	402	AR6	O1B-PB-O5D	2.01	116.68	107.57

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	QUE	C10-C11-C14-C15
3	B	402	AR6	O4D-C4D-C5D-O5D
4	A	403	QUE	C10-C11-C14-C19
3	B	402	AR6	C3D-C4D-C5D-O5D
4	A	403	QUE	O12-C11-C14-C15
3	A	402	AR6	C5D-O5D-PB-O2B
3	B	402	AR6	C5'-O5'-PA-O2A
3	B	402	AR6	C5D-O5D-PB-O2B
3	B	402	AR6	O4'-C4'-C5'-O5'
3	B	402	AR6	PB-O3A-PA-O1A
4	A	403	QUE	O12-C11-C14-C19

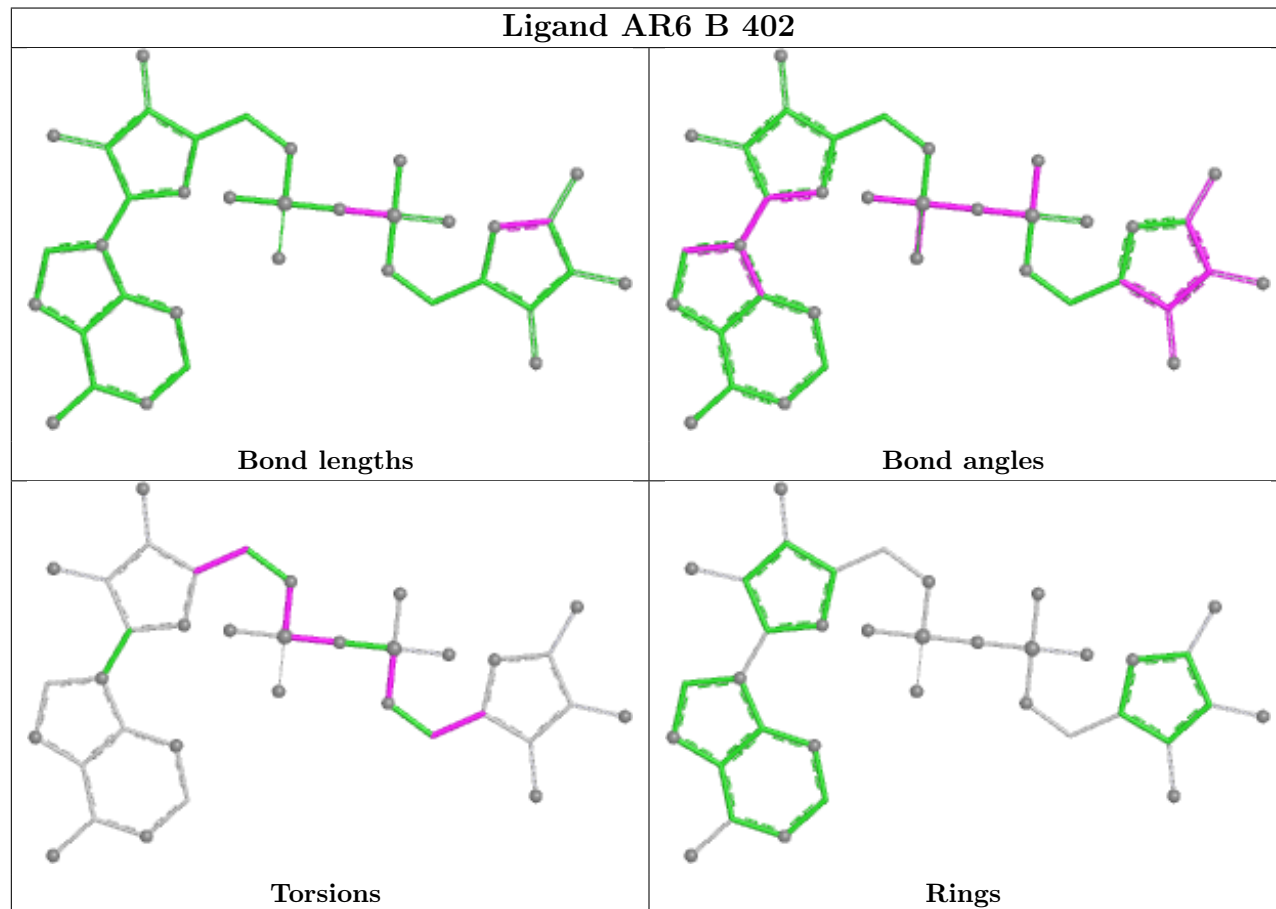
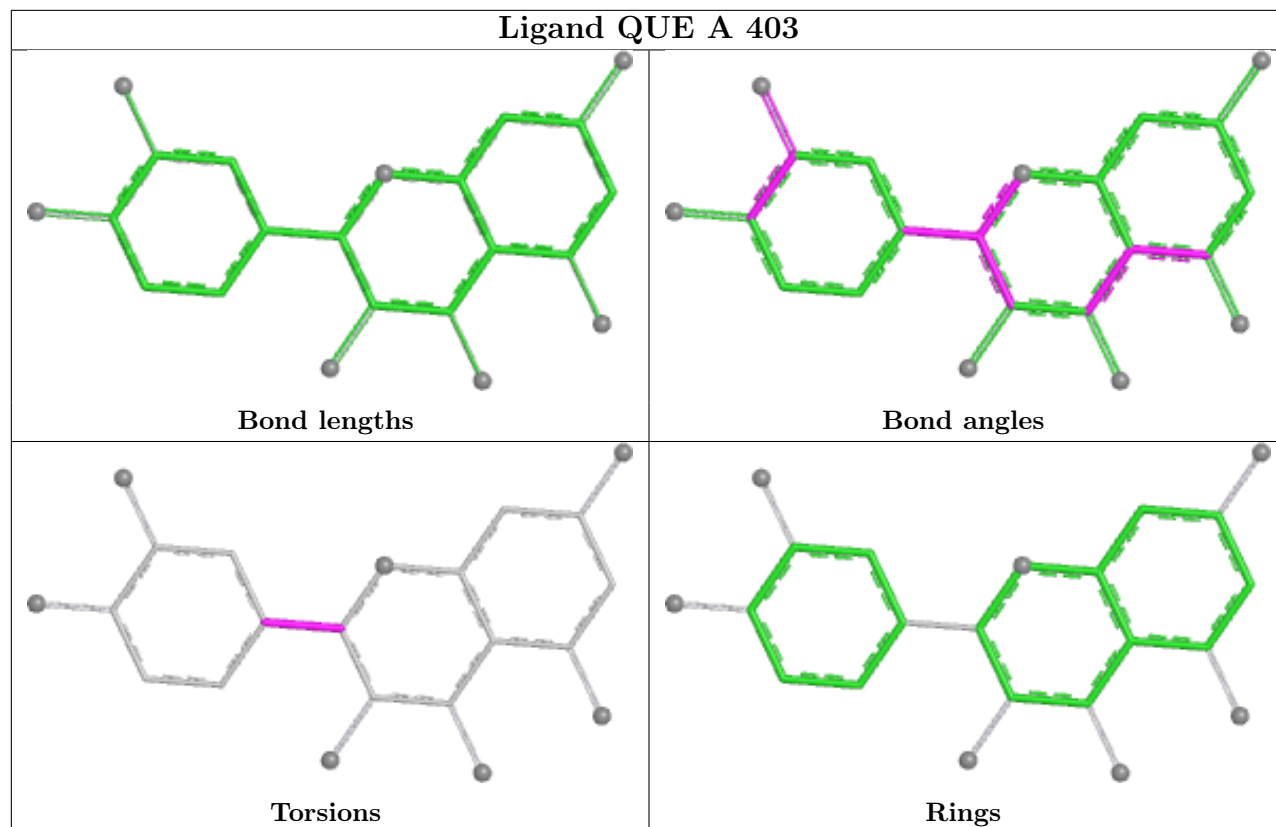
There are no ring outliers.

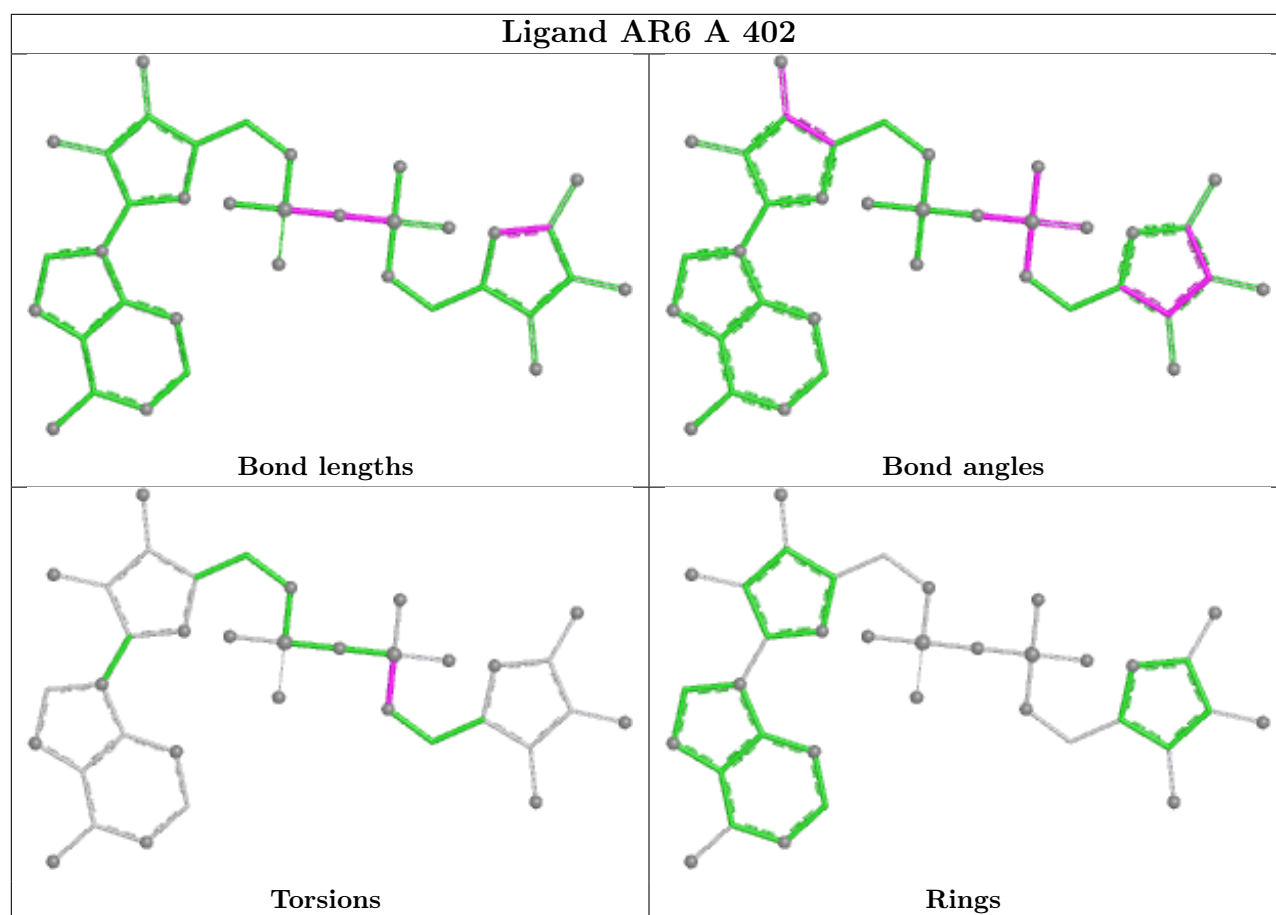
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	QUE	1	0
3	B	402	AR6	4	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	299/304 (98%)	0.73	21 (7%) 22 20	31, 48, 74, 104	0
1	B	300/304 (98%)	0.95	29 (9%) 13 12	31, 54, 86, 97	0
All	All	599/608 (98%)	0.84	50 (8%) 17 15	31, 51, 83, 104	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	141	GLY	6.1
1	A	140	PRO	5.7
1	A	138	LEU	4.3
1	B	206	LEU	4.3
1	B	349	HIS	4.1
1	B	198	ALA	3.9
1	A	191	TYR	3.8
1	B	138	LEU	3.6
1	A	213	ILE	3.2
1	B	315	TYR	2.9
1	B	139	TYR	2.8
1	A	141	GLY	2.7
1	A	206	LEU	2.7
1	B	352	ILE	2.7
1	A	198	ALA	2.6
1	B	142	GLN	2.6
1	B	208	TRP	2.6
1	B	293	SER	2.5
1	A	354	ALA	2.5
1	B	140	PRO	2.4
1	B	214	PHE	2.4
1	B	56	GLU	2.4
1	A	252	LEU	2.4
1	A	214	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	234	PHE	2.4
1	A	355	GLN	2.4
1	B	304	GLY	2.3
1	B	57	ARG	2.3
1	B	217	VAL	2.3
1	B	128	PRO	2.3
1	B	132	PHE	2.2
1	A	352	ILE	2.2
1	B	144	LYS	2.2
1	B	292	GLN	2.2
1	A	232	ILE	2.2
1	B	58	LEU	2.2
1	A	238	SER	2.2
1	B	350	ALA	2.2
1	A	139	TYR	2.1
1	A	266	VAL	2.1
1	A	217	VAL	2.1
1	B	258	LEU	2.1
1	A	142	GLN	2.1
1	B	321	LEU	2.1
1	A	126	LYS	2.0
1	A	312	LYS	2.0
1	B	100	SER	2.0
1	B	290	ALA	2.0
1	B	273	ILE	2.0
1	B	136	LYS	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](#)

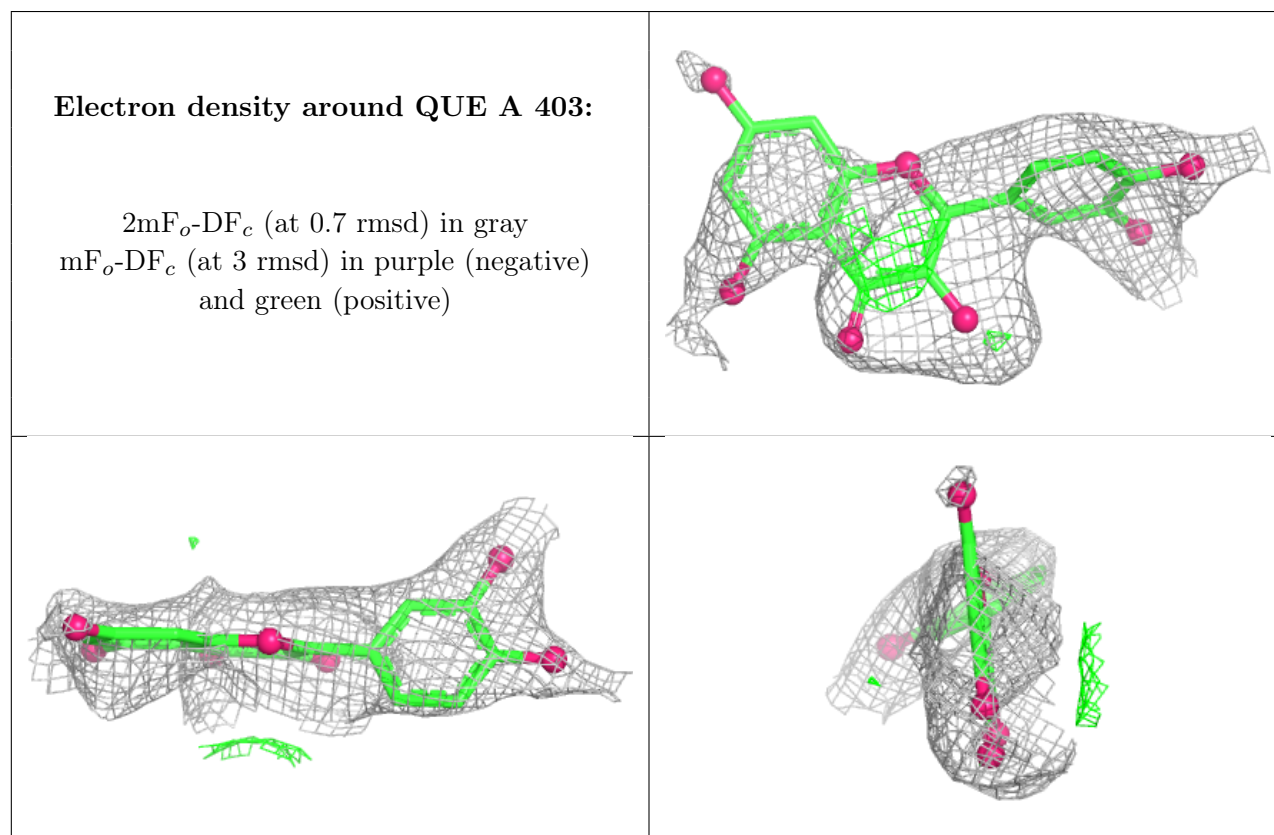
There are no oligosaccharides in this entry.

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.

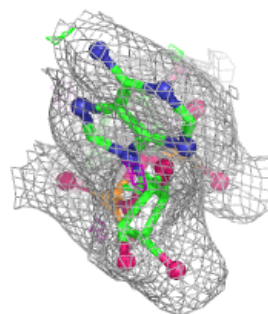
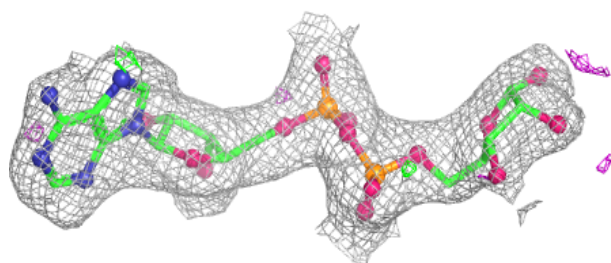
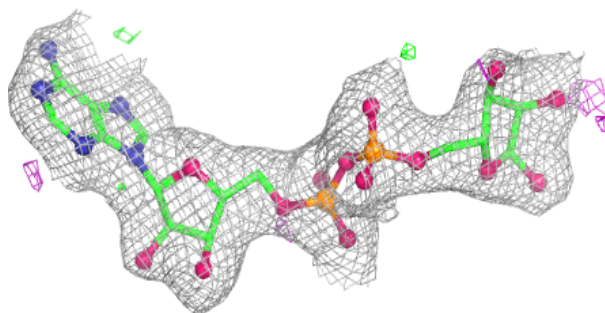
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	QUE	A	403	22/22	0.68	0.19	60,74,81,83	0
3	AR6	B	402	36/36	0.95	0.07	23,34,42,47	0
3	AR6	A	402	36/36	0.96	0.06	22,33,42,46	0
2	ZN	B	401	1/1	0.97	0.06	81,81,81,81	0
2	ZN	A	401	1/1	0.99	0.03	60,60,60,60	0

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.

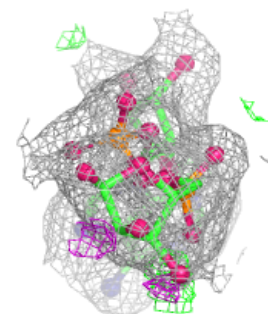
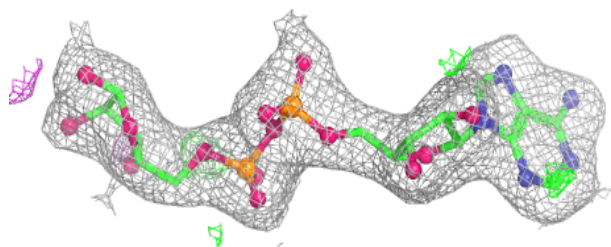
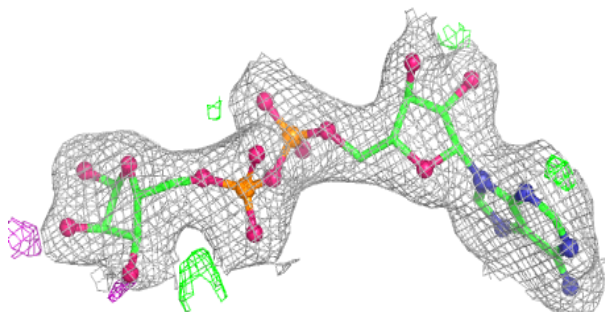


Electron density around AR6 B 402:

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

**Electron density around AR6 A 402:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.