



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:12 AM UTC

PDB ID : 6QCJ / pdb_00006qcj
Title : Human Sirt6 in complex with ADP-ribose and the inhibitor catechin gallate
Authors : You, W.; Steegborn, C.
Deposited on : 2018-12-28
Resolution : 2.01 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

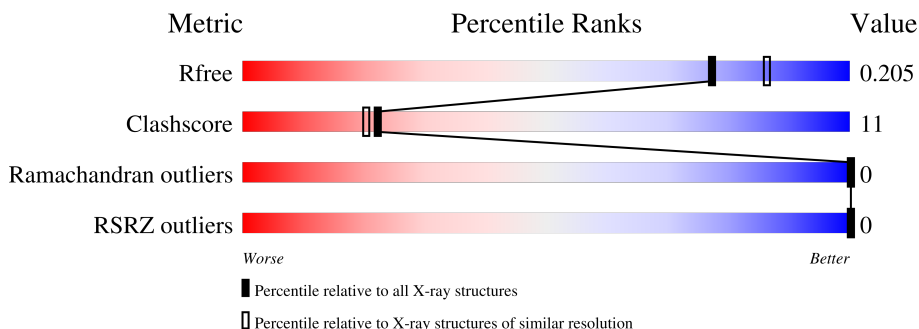
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	302	
1	B	302	

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
5	SO4	A	406	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4693 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.

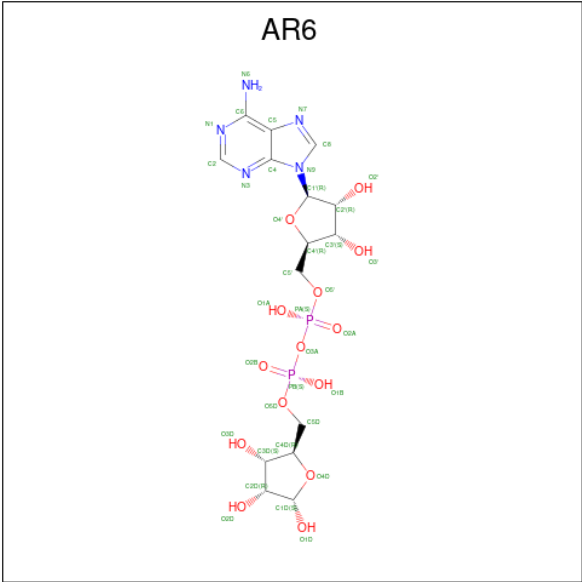
- Molecule 1 is a protein called NAD-dependent protein deacetylase sirtuin-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2202	1385	403	403	11			
1	B	277	Total	C	N	O	S	0	0	0
			2148	1352	392	393	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	GLY	-	expression tag	UNP Q8N6T7
A	8	ILE	-	expression tag	UNP Q8N6T7
A	9	ASP	-	expression tag	UNP Q8N6T7
A	10	PRO	-	expression tag	UNP Q8N6T7
A	11	PHE	-	expression tag	UNP Q8N6T7
A	12	THR	-	expression tag	UNP Q8N6T7
B	7	GLY	-	expression tag	UNP Q8N6T7
B	8	ILE	-	expression tag	UNP Q8N6T7
B	9	ASP	-	expression tag	UNP Q8N6T7
B	10	PRO	-	expression tag	UNP Q8N6T7
B	11	PHE	-	expression tag	UNP Q8N6T7
B	12	THR	-	expression tag	UNP Q8N6T7

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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



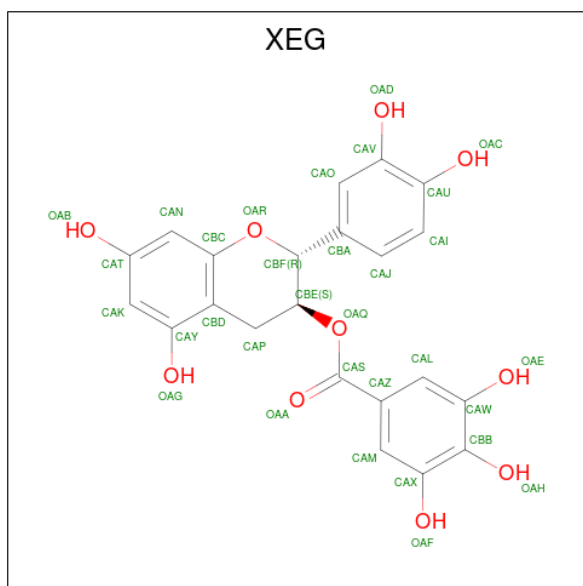
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 6 is (2R,3S)-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3,4-dihydro-2H-chromen-3-yl 3,4,5-trihydroxybenzoate (CCD ID: XEG) (formula: C₂₂H₁₈O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			32	22	10		
6	B	1	Total	C	O	0	0
			32	22	10		

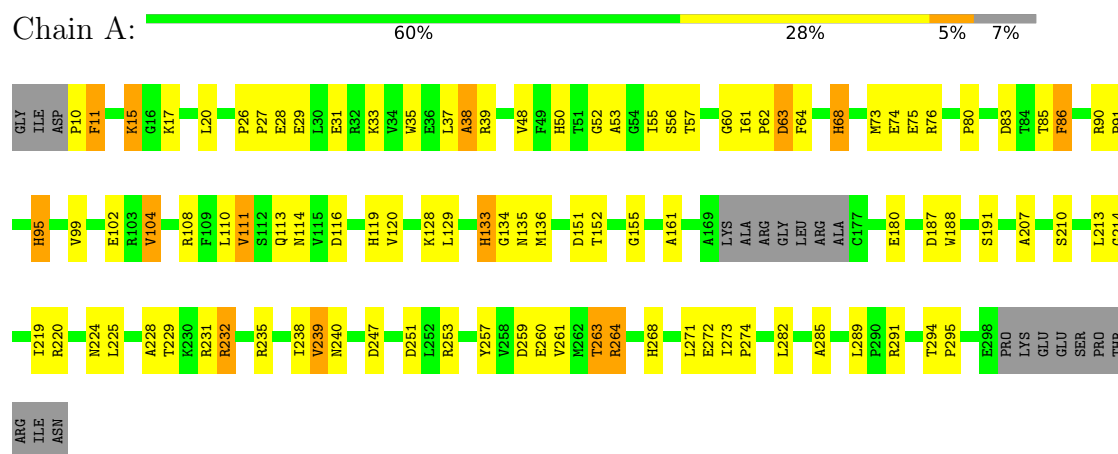
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	89	Total	O	0	0
			89	89		
7	B	77	Total	O	0	0
			77	77		

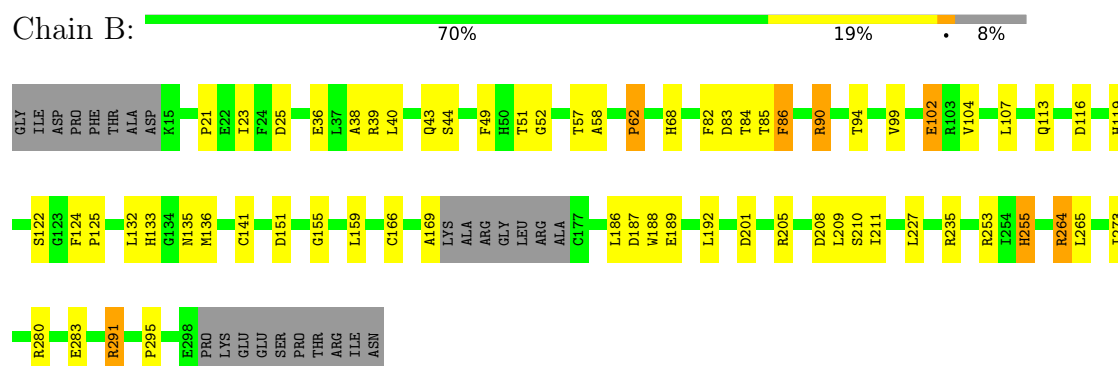
3 Residue-property plots [i](#)

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: NAD-dependent protein deacetylase sirtuin-6



- Molecule 1: NAD-dependent protein deacetylase sirtuin-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	91.92Å 91.92Å 144.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.96 – 2.01 45.96 – 2.01	Depositor EDS
% Data completeness (in resolution range)	98.9 (45.96-2.01) 98.9 (45.96-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.163 , 0.199 (Not available) , 0.205	Depositor DCC
R_{free} test set	2100 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.720	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.428 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.561 for H, K, L 0.439 for -K, -H, -L	Depositor
Outliers	0 of 45089 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4693	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: EDO, ZN, SO4, AR6, XEG

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	1.47	26/2251 (1.2%)	1.71	37/3054 (1.2%)
1	B	1.37	17/2195 (0.8%)	1.65	24/2980 (0.8%)
All	All	1.42	43/4446 (1.0%)	1.68	61/6034 (1.0%)

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

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	VAL	C-O	9.52	1.34	1.24
1	A	85	THR	C-O	8.34	1.34	1.23
1	A	95	HIS	CE1-NE2	8.24	1.40	1.32
1	A	48	VAL	C-O	8.15	1.32	1.24
1	A	83	ASP	C-O	8.02	1.35	1.23
1	A	56	SER	CA-CB	-7.53	1.43	1.54
1	B	209	LEU	C-O	7.25	1.32	1.23
1	B	235	ARG	C-O	7.23	1.32	1.23
1	B	264	ARG	C-N	-6.86	1.25	1.33
1	B	86	PHE	C-O	6.69	1.32	1.24
1	A	219	ILE	C-O	6.54	1.31	1.24
1	A	272	GLU	C-O	6.49	1.31	1.23
1	A	214	GLY	C-O	6.37	1.32	1.24
1	A	52	GLY	C-O	6.17	1.29	1.23
1	B	102	GLU	C-O	6.17	1.31	1.24
1	A	210	SER	CA-CB	-6.16	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	SER	CA-CB	-6.06	1.44	1.53
1	B	273	ILE	N-CA	6.05	1.50	1.46
1	A	75	GLU	C-O	6.04	1.31	1.24
1	A	135	ASN	C-O	6.01	1.31	1.23
1	A	91	PRO	C-O	-5.97	1.15	1.23
1	B	52	GLY	C-O	5.89	1.30	1.23
1	B	62	PRO	C-O	-5.87	1.17	1.23
1	A	114	ASN	N-CA	5.66	1.53	1.46
1	A	133	HIS	CE1-NE2	5.62	1.38	1.32
1	A	282	LEU	C-O	5.59	1.30	1.24
1	A	133	HIS	ND1-CE1	-5.58	1.26	1.32
1	B	211	ILE	C-O	-5.57	1.18	1.24
1	A	61	ILE	N-CA	5.41	1.51	1.46
1	A	68	HIS	CE1-NE2	5.38	1.38	1.32
1	A	80	PRO	C-O	-5.36	1.17	1.23
1	B	291	ARG	N-CA	5.33	1.50	1.45
1	A	152	THR	C-O	5.32	1.30	1.23
1	A	64	PHE	C-O	5.24	1.30	1.23
1	A	27	PRO	C-O	-5.24	1.17	1.24
1	A	86	PHE	C-O	5.24	1.30	1.24
1	B	264	ARG	C-O	-5.14	1.18	1.24
1	B	99	VAL	C-O	5.11	1.29	1.24
1	B	295	PRO	C-O	5.10	1.29	1.23
1	A	99	VAL	C-O	5.09	1.29	1.24
1	B	57	THR	C-O	-5.08	1.17	1.24
1	B	210	SER	C-O	5.04	1.29	1.24
1	B	159	LEU	C-O	5.02	1.30	1.23

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ARG	CG-CD-NE	-8.96	92.30	112.00
1	A	116	ASP	CA-CB-CG	8.46	121.06	112.60
1	A	57	THR	CA-CB-OG1	7.78	121.27	109.60
1	A	104	VAL	N-CA-C	-7.54	105.20	112.29
1	B	280	ARG	CG-CD-NE	-7.37	95.80	112.00
1	B	94	THR	CA-CB-OG1	-7.19	98.81	109.60
1	A	52	GLY	O-C-N	6.86	131.40	123.51
1	A	111	VAL	CA-C-O	-6.64	113.03	120.74
1	B	116	ASP	CA-CB-CG	6.60	119.20	112.60
1	B	264	ARG	CG-CD-NE	-6.54	97.61	112.00
1	B	94	THR	CA-C-O	-6.45	113.99	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	ASP	N-CA-C	-6.42	105.08	113.17
1	A	53	ALA	CA-C-N	6.23	127.97	120.13
1	A	53	ALA	C-N-CA	6.23	127.97	120.13
1	A	57	THR	N-CA-CB	5.99	119.44	110.22
1	B	264	ARG	O-C-N	-5.97	115.34	122.15
1	A	104	VAL	O-C-N	5.83	127.34	122.09
1	B	273	ILE	CA-C-O	5.77	122.35	119.12
1	B	208	ASP	N-CA-C	-5.74	106.91	114.31
1	B	90	ARG	CB-CA-C	5.74	116.62	108.76
1	A	90	ARG	CA-C-O	5.70	124.98	120.19
1	B	255	HIS	CA-C-N	5.68	128.76	121.27
1	B	255	HIS	C-N-CA	5.68	128.76	121.27
1	A	38	ALA	CA-C-N	5.66	128.14	120.38
1	A	38	ALA	C-N-CA	5.66	128.14	120.38
1	A	83	ASP	N-CA-C	-5.66	106.03	113.17
1	B	62	PRO	CA-C-O	-5.61	114.82	121.67
1	A	151	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	52	GLY	CA-C-N	5.59	128.33	120.28
1	A	52	GLY	C-N-CA	5.59	128.33	120.28
1	A	11	PHE	CA-C-N	5.59	130.18	120.68
1	A	11	PHE	C-N-CA	5.59	130.18	120.68
1	B	135	ASN	CB-CA-C	5.58	118.39	110.24
1	A	52	GLY	CA-C-O	-5.57	115.16	121.68
1	A	219	ILE	O-C-N	5.49	129.13	123.03
1	A	134	GLY	CA-C-N	5.48	130.52	121.86
1	A	134	GLY	C-N-CA	5.48	130.52	121.86
1	A	238	ILE	N-CA-CB	-5.47	104.81	111.21
1	B	124	PHE	CB-CA-C	5.46	117.99	109.42
1	A	63	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	273	ILE	CB-CA-C	5.42	117.24	110.95
1	A	263	THR	CA-C-N	5.40	127.52	120.28
1	A	263	THR	C-N-CA	5.40	127.52	120.28
1	B	151	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	132	LEU	CA-C-O	-5.38	114.84	120.55
1	A	50	HIS	CA-C-O	-5.19	114.61	120.32
1	B	57	THR	CA-C-O	-5.19	114.23	120.10
1	B	125	PRO	CB-CA-C	-5.17	105.93	111.56
1	A	257	TYR	CA-C-O	-5.15	115.05	120.92
1	A	15	LYS	N-CA-C	-5.12	106.88	112.72
1	A	10	PRO	CA-C-N	5.11	127.13	120.28
1	A	10	PRO	C-N-CA	5.11	127.13	120.28
1	A	191	SER	CA-C-N	5.11	127.50	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	SER	C-N-CA	5.11	127.50	120.39
1	B	264	ARG	CA-C-N	-5.09	113.83	120.44
1	B	264	ARG	C-N-CA	-5.09	113.83	120.44
1	A	134	GLY	O-C-N	5.07	127.93	122.86
1	A	120	VAL	CA-C-N	5.02	127.94	120.31
1	A	120	VAL	C-N-CA	5.02	127.94	120.31
1	B	38	ALA	CA-C-N	5.01	126.99	120.28
1	B	38	ALA	C-N-CA	5.01	126.99	120.28

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	VAL	Mainchain
1	A	232	ARG	Peptide
1	A	271	LEU	Mainchain
1	A	62	PRO	Mainchain
1	A	68	HIS	Mainchain

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	2202	0	2208	54	1
1	B	2148	0	2149	33	0
2	A	36	0	21	2	0
2	B	36	0	20	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	6	0	0
5	A	15	0	0	3	0
5	B	20	0	0	1	0
6	A	32	0	15	6	0
6	B	32	0	16	8	0
7	A	89	0	0	17	0
7	B	77	0	0	12	0
All	All	4693	0	4435	95	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 11.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:HG	7:A:514:HOH:O	1.50	1.09
1:A:20:LEU:HD13	7:A:538:HOH:O	1.71	0.90
1:B:49:PHE:HB3	7:B:565:HOH:O	1.70	0.88
1:A:220:ARG:HG3	5:A:406:SO4:O3	1.74	0.87
1:A:232:ARG:NH1	5:A:405:SO4:O4	2.11	0.83
1:A:95:HIS:CE1	7:A:505:HOH:O	2.29	0.83
1:A:136:MET:HG2	6:A:407:XEG:CAL	2.09	0.82
1:B:227:LEU:HB3	7:B:572:HOH:O	1.83	0.79
6:B:407:XEG:OAA	6:B:407:XEG:OAR	2.01	0.77
1:A:289:LEU:O	7:A:501:HOH:O	2.02	0.77
1:A:31:GLU:OE2	1:A:264:ARG:NH1	2.22	0.72
1:A:155:GLY:N	6:A:407:XEG:OAH	2.22	0.72
1:B:25:ASP:OD1	1:B:255:HIS:HB2	1.89	0.72
1:A:228:ALA:O	1:A:231:ARG:HG2	1.90	0.71
1:A:95:HIS:ND1	7:A:505:HOH:O	2.24	0.70
1:A:60:GLY:CA	7:B:509:HOH:O	2.38	0.70
6:A:407:XEG:OAD	7:A:502:HOH:O	2.06	0.69
1:B:51:THR:HG23	7:B:565:HOH:O	1.93	0.69
1:A:239:VAL:HG12	7:A:512:HOH:O	1.95	0.67
1:B:136:MET:HG2	6:B:407:XEG:HAL	1.79	0.64
1:B:169:ALA:O	7:B:501:HOH:O	2.15	0.63
1:B:227:LEU:CB	7:B:572:HOH:O	2.44	0.62
1:A:28:GLU:HB2	7:A:568:HOH:O	1.99	0.62
1:B:186:LEU:HD11	1:B:192:LEU:HA	1.83	0.61
1:B:201:ASP:OD2	1:B:205:ARG:NE	2.31	0.61
1:B:84:THR:OG1	1:B:85:THR:N	2.33	0.61
1:B:283:GLU:OE1	7:B:502:HOH:O	2.16	0.61
1:A:104:VAL:O	1:A:291:ARG:NH2	2.35	0.60
1:A:60:GLY:HA2	7:B:509:HOH:O	2.00	0.60
1:B:104:VAL:O	1:B:291:ARG:NH2	2.35	0.60
6:B:407:XEG:HAP	6:B:407:XEG:HAJ	1.85	0.58
1:A:239:VAL:C	7:A:512:HOH:O	2.46	0.58
6:B:407:XEG:OAA	6:B:407:XEG:CBF	2.51	0.58
1:A:259:ASP:O	1:A:263:THR:HG23	2.03	0.58
6:A:407:XEG:HAJ	6:A:407:XEG:CBD	2.34	0.57
1:B:21:PRO:HB3	7:B:570:HOH:O	2.04	0.56
1:A:161:ALA:HB2	1:A:180:GLU:OE1	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ARG:NH2	5:B:404:SO4:O4	2.38	0.56
1:A:17:LYS:HB3	1:A:20:LEU:HD11	1.88	0.56
1:A:240:ASN:N	7:A:512:HOH:O	2.38	0.55
1:A:39:ARG:HD2	7:A:583:HOH:O	2.07	0.55
1:A:86:PHE:CD2	1:A:136:MET:HE1	2.42	0.54
1:B:119:HIS:O	1:B:122:SER:OG	2.22	0.53
1:A:108:ARG:NH1	7:A:513:HOH:O	2.41	0.53
1:A:95:HIS:O	7:A:504:HOH:O	2.19	0.52
1:A:128:LYS:HE3	1:A:285:ALA:CB	2.40	0.51
1:A:224:ASN:ND2	5:A:406:SO4:O3	2.43	0.51
1:A:113:GLN:HG2	1:A:133:HIS:CE1	2.46	0.51
1:B:40:LEU:O	1:B:44:SER:OG	2.27	0.51
1:B:39:ARG:NH1	1:B:43:GLN:OE1	2.44	0.51
1:B:86:PHE:CD2	1:B:136:MET:HE1	2.46	0.50
1:A:73:MET:HE2	1:B:68:HIS:CE1	2.47	0.50
6:B:407:XEG:CAM	7:B:564:HOH:O	2.60	0.49
1:B:58:ALA:HA	7:B:509:HOH:O	2.13	0.48
6:B:407:XEG:OAR	6:B:407:XEG:CAS	2.61	0.48
1:A:35:TRP:CE2	1:A:268:HIS:CE1	3.02	0.48
1:A:136:MET:HG2	6:A:407:XEG:HAL	1.93	0.47
1:A:15:LYS:NZ	1:A:74:GLU:OE1	2.47	0.47
1:A:264:ARG:N	7:A:518:HOH:O	2.48	0.47
1:A:102:GLU:OE2	1:A:128:LYS:NZ	2.33	0.47
1:A:86:PHE:CE2	1:A:136:MET:HE1	2.50	0.46
1:B:62:PRO:HD2	1:B:82:PHE:CE2	2.50	0.46
1:A:294:THR:CG2	1:A:295:PRO:HD2	2.46	0.45
1:B:23:ILE:HB	1:B:255:HIS:CD2	2.51	0.45
1:B:264:ARG:O	1:B:265:LEU:C	2.58	0.45
1:B:141:CYS:SG	1:B:166:CYS:HB2	2.57	0.44
1:A:55:ILE:HD12	7:A:505:HOH:O	2.17	0.44
1:B:90:ARG:NH1	7:B:516:HOH:O	2.50	0.44
1:B:189:GLU:OE1	1:B:189:GLU:N	2.44	0.44
1:A:76:ARG:HG2	7:A:575:HOH:O	2.18	0.43
1:A:29:GLU:O	1:A:33:LYS:HG3	2.18	0.43
1:A:187:ASP:CG	1:A:188:TRP:H	2.26	0.43
1:B:187:ASP:OD1	1:B:188:TRP:N	2.42	0.42
1:A:37:LEU:O	1:A:38:ALA:C	2.62	0.42
1:A:110:LEU:HD21	1:A:119:HIS:CE1	2.54	0.42
1:A:273:ILE:HA	1:A:274:PRO:HD3	1.89	0.42
1:B:62:PRO:HD2	1:B:82:PHE:CD2	2.54	0.42
1:B:113:GLN:HG2	1:B:133:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:GLU:HA	1:B:107:LEU:HB3	2.01	0.42
1:A:207:ALA:HB3	1:A:229:THR:HG23	2.01	0.41
1:B:201:ASP:O	1:B:205:ARG:HG3	2.20	0.41
1:B:36:GLU:OE2	1:B:39:ARG:NH2	2.54	0.41
1:B:155:GLY:HA2	6:B:407:XEG:OAH	2.20	0.41
1:A:294:THR:HG22	1:A:295:PRO:HD2	2.01	0.41
2:A:401:AR6:H2	7:A:512:HOH:O	2.20	0.41
1:A:155:GLY:CA	6:A:407:XEG:OAH	2.69	0.41
1:A:26:PRO:HD2	1:A:29:GLU:HB3	2.01	0.41
1:A:63:ASP:OD2	2:A:401:AR6:H2'	2.21	0.41
1:A:260:GLU:O	1:A:261:VAL:C	2.64	0.41
6:B:407:XEG:HAJ	6:B:407:XEG:CAP	2.48	0.41
1:A:29:GLU:CG	1:A:33:LYS:HE3	2.51	0.41
1:A:110:LEU:O	1:A:129:LEU:HA	2.20	0.40
1:A:225:LEU:HD23	1:A:225:LEU:HA	1.94	0.40
1:A:247:ASP:HB3	1:A:253:ARG:HD3	2.04	0.40
1:A:235:ARG:HA	1:A:251:ASP:OD2	2.22	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)
1:A:11:PHE:O	1:A:17:LYS:CE[2_565]	2.17	0.03

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	278/302 (92%)	270 (97%)	8 (3%)	0	100	100
1	B	273/302 (90%)	263 (96%)	10 (4%)	0	100	100
All	All	551/604 (91%)	533 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	406	-	4,4,4	0.39	0	6,6,6	0.18	0
2	AR6	A	401	-	39,39,39	2.48	13 (33%)	56,60,60	2.02	18 (32%)
5	SO4	A	405	-	4,4,4	0.38	0	6,6,6	0.12	0
5	SO4	B	406	-	4,4,4	0.20	0	6,6,6	0.34	0
6	XEG	A	407	-	35,35,35	1.26	3 (8%)	52,52,52	1.88	18 (34%)
5	SO4	A	404	-	4,4,4	0.47	0	6,6,6	0.34	0
5	SO4	B	404	-	4,4,4	0.30	0	6,6,6	0.09	0
5	SO4	B	405	-	4,4,4	0.34	0	6,6,6	0.13	0
4	EDO	A	403	-	3,3,3	0.41	0	2,2,2	0.13	0
5	SO4	B	403	-	4,4,4	0.61	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AR6	B	401	-	39,39,39	2.81	13 (33%)	56,60,60	2.18	16 (28%)
6	XEG	B	407	-	35,35,35	0.73	0	52,52,52	1.24	5 (9%)

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	AR6	A	401	-	-	3/22/54/54	0/4/4/4
6	XEG	A	407	-	-	3/12/24/24	0/4/4/4
4	EDO	A	403	-	-	1/1/1/1	-
2	AR6	B	401	-	-	3/22/54/54	0/4/4/4
6	XEG	B	407	-	-	3/12/24/24	0/4/4/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	AR6	PB-O3A	13.06	1.73	1.59
2	A	401	AR6	C3'-C2'	6.60	1.71	1.53
2	A	401	AR6	PB-O3A	6.48	1.66	1.59
2	A	401	AR6	C1'-N9	4.52	1.58	1.46
2	B	401	AR6	C3D-C4D	4.45	1.64	1.53
2	A	401	AR6	O3D-C3D	4.25	1.53	1.43
2	B	401	AR6	C6-N6	4.09	1.44	1.34
2	B	401	AR6	C2-N3	4.03	1.41	1.33
6	A	407	XEG	OAQ-CBE	3.93	1.52	1.46
2	A	401	AR6	C1D-C2D	3.85	1.57	1.52
2	A	401	AR6	C2-N1	3.70	1.40	1.33
2	B	401	AR6	C3'-C2'	3.40	1.62	1.53
6	A	407	XEG	OAR-CBF	3.27	1.50	1.45
2	B	401	AR6	C2-N1	3.16	1.39	1.33
2	A	401	AR6	O4'-C1'	3.08	1.49	1.42
2	A	401	AR6	C5'-C4'	3.02	1.60	1.51
2	A	401	AR6	C2-N3	2.98	1.39	1.33
2	A	401	AR6	C6-N6	2.83	1.41	1.34
2	A	401	AR6	C3D-C4D	2.56	1.59	1.53
6	A	407	XEG	CBA-CBF	2.42	1.55	1.51
2	B	401	AR6	C3'-C4'	-2.30	1.47	1.53
2	B	401	AR6	C1'-N9	2.29	1.52	1.46
2	A	401	AR6	C5-C6	-2.29	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	AR6	O4D-C1D	-2.24	1.40	1.43
2	B	401	AR6	C5-C6	-2.20	1.34	1.41
2	B	401	AR6	C8-N9	-2.20	1.33	1.37
2	B	401	AR6	C5-N7	-2.17	1.35	1.39
2	A	401	AR6	O1D-C1D	2.13	1.46	1.39
2	B	401	AR6	C4-N9	-2.02	1.33	1.37

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	AR6	O1D-C1D-O4D	-6.06	103.39	111.12
2	B	401	AR6	N3-C2-N1	-5.99	119.52	128.58
2	B	401	AR6	C4-C5-N7	-5.31	104.51	110.58
2	A	401	AR6	C4-C5-N7	-5.30	104.52	110.58
2	A	401	AR6	C5-N7-C8	4.61	110.70	103.45
6	A	407	XEG	CBE-OAQ-CAS	4.19	126.42	117.33
2	B	401	AR6	C1D-C2D-C3D	-4.03	97.33	102.29
2	A	401	AR6	C2'-C1'-N9	4.01	123.26	113.30
2	A	401	AR6	O3'-C3'-C4'	3.98	122.50	111.08
6	A	407	XEG	OAQ-CAS-CAZ	3.93	118.22	111.90
2	B	401	AR6	C5-N7-C8	3.87	109.53	103.45
2	A	401	AR6	N9-C8-N7	-3.75	108.61	113.94
2	A	401	AR6	N3-C2-N1	-3.75	122.91	128.58
2	B	401	AR6	C2-N1-C6	3.72	124.85	118.73
2	B	401	AR6	O4'-C4'-C3'	3.68	112.45	105.15
6	A	407	XEG	OAR-CBF-CBE	-3.60	99.45	109.13
6	B	407	XEG	CBA-CBF-CBE	3.39	122.12	113.70
2	B	401	AR6	O4'-C1'-N9	-3.26	101.83	108.09
2	A	401	AR6	C1D-C2D-C3D	-3.23	98.32	102.29
2	B	401	AR6	N9-C8-N7	-3.22	109.36	113.94
6	A	407	XEG	CAM-CAZ-CAS	3.21	126.33	120.09
6	A	407	XEG	CAJ-CBA-CAO	-3.14	115.09	118.74
6	B	407	XEG	OAB-CAT-CAN	-3.14	111.64	119.85
6	A	407	XEG	CBA-CBF-CBE	3.11	121.42	113.70
2	A	401	AR6	O1D-C1D-O4D	-3.05	107.23	111.12
6	A	407	XEG	OAR-CBF-CBA	3.00	113.84	107.44
2	B	401	AR6	C5-C4-N9	2.93	109.01	105.81
6	A	407	XEG	CAL-CAZ-CAS	-2.85	114.55	120.09
2	B	401	AR6	C2'-C1'-N9	2.82	120.30	113.30
2	A	401	AR6	C5-C4-N3	-2.81	122.85	126.72
2	A	401	AR6	C4-N9-C1'	-2.80	120.09	126.63
6	B	407	XEG	OAB-CAT-CAK	2.72	126.98	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	407	XEG	CAP-CBE-CBF	-2.68	104.69	110.16
6	B	407	XEG	OAE-CAW-CAL	2.67	126.67	119.45
6	A	407	XEG	CAJ-CBA-CBF	2.65	125.56	120.62
2	A	401	AR6	C4-N9-C8	2.62	108.49	105.74
6	A	407	XEG	OAC-CAU-CAI	2.61	126.38	119.36
2	B	401	AR6	C4-N9-C1'	-2.61	120.53	126.63
6	B	407	XEG	CBE-OAQ-CAS	2.59	122.96	117.33
2	B	401	AR6	C6-C5-C4	2.58	120.70	117.18
2	A	401	AR6	O5D-C5D-C4D	-2.54	100.33	108.99
6	A	407	XEG	CAI-CAU-CAV	-2.53	116.96	119.66
2	A	401	AR6	O4'-C1'-N9	-2.49	103.31	108.09
2	A	401	AR6	O3'-C3'-C2'	-2.46	103.94	111.82
6	A	407	XEG	OAF-CAX-CAM	2.45	126.05	119.45
6	A	407	XEG	CAP-CBD-CBC	-2.30	117.24	121.01
2	A	401	AR6	O4D-C4D-C5D	2.20	116.38	109.33
2	B	401	AR6	C1'-N9-C8	2.19	131.95	127.09
2	A	401	AR6	C6-C5-C4	2.17	120.14	117.18
6	A	407	XEG	CAO-CAV-CAU	2.16	121.89	119.89
2	B	401	AR6	O2'-C2'-C3'	-2.09	105.10	111.82
6	A	407	XEG	CAZ-CAL-CAW	2.07	121.90	120.09
6	A	407	XEG	OAF-CAX-CBB	-2.07	112.57	117.90
6	A	407	XEG	OAQ-CBE-CAP	2.05	114.90	109.09
2	A	401	AR6	O2'-C2'-C3'	-2.05	105.25	111.82
2	B	401	AR6	O3D-C3D-C4D	2.04	116.95	111.08
2	A	401	AR6	O4'-C4'-C3'	2.03	109.19	105.15

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	AR6	C5D-O5D-PB-O2B
6	A	407	XEG	CAZ-CAS-OAQ-CBE
6	B	407	XEG	CBF-CBE-OAQ-CAS
6	A	407	XEG	OAA-CAS-OAQ-CBE
6	A	407	XEG	CBF-CBE-OAQ-CAS
6	B	407	XEG	CAZ-CAS-OAQ-CBE
6	B	407	XEG	OAA-CAS-OAQ-CBE
2	A	401	AR6	C2'-C1'-N9-C8
2	B	401	AR6	C5D-O5D-PB-O2B
2	A	401	AR6	O4'-C1'-N9-C8
4	A	403	EDO	O1-C1-C2-O2
2	B	401	AR6	O4'-C4'-C5'-O5'

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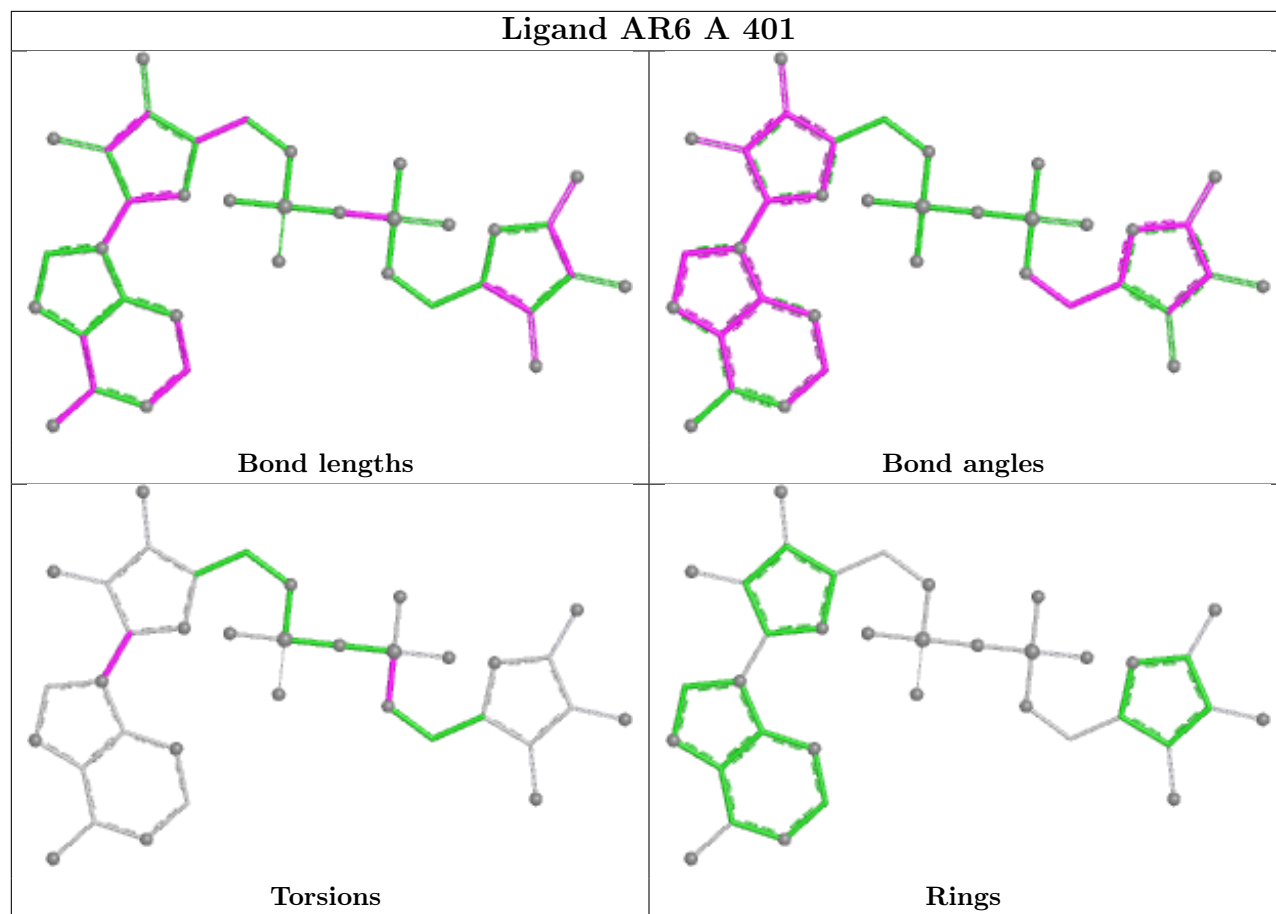
Mol	Chain	Res	Type	Atoms
2	B	401	AR6	PA-O3A-PB-O1B

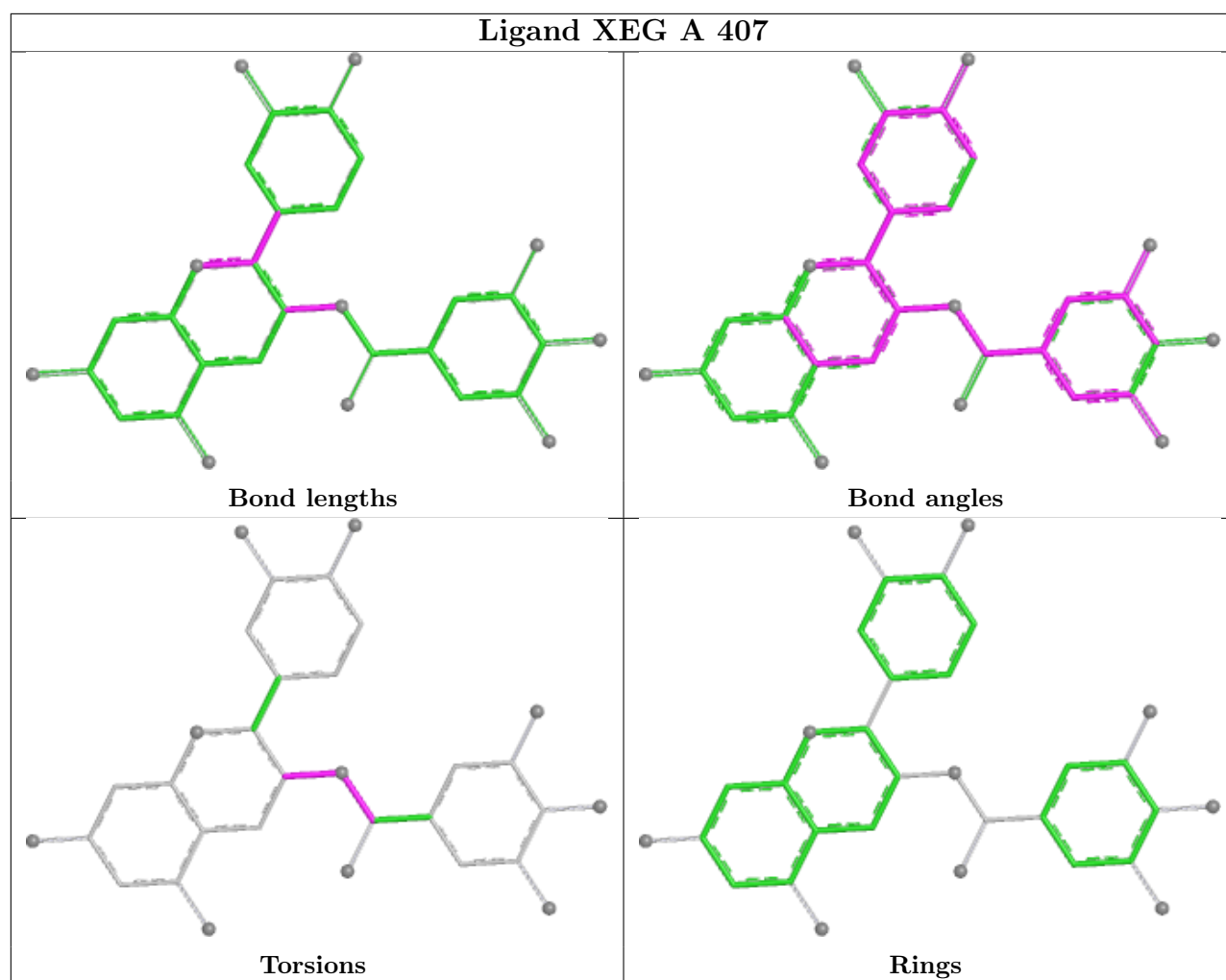
There are no ring outliers.

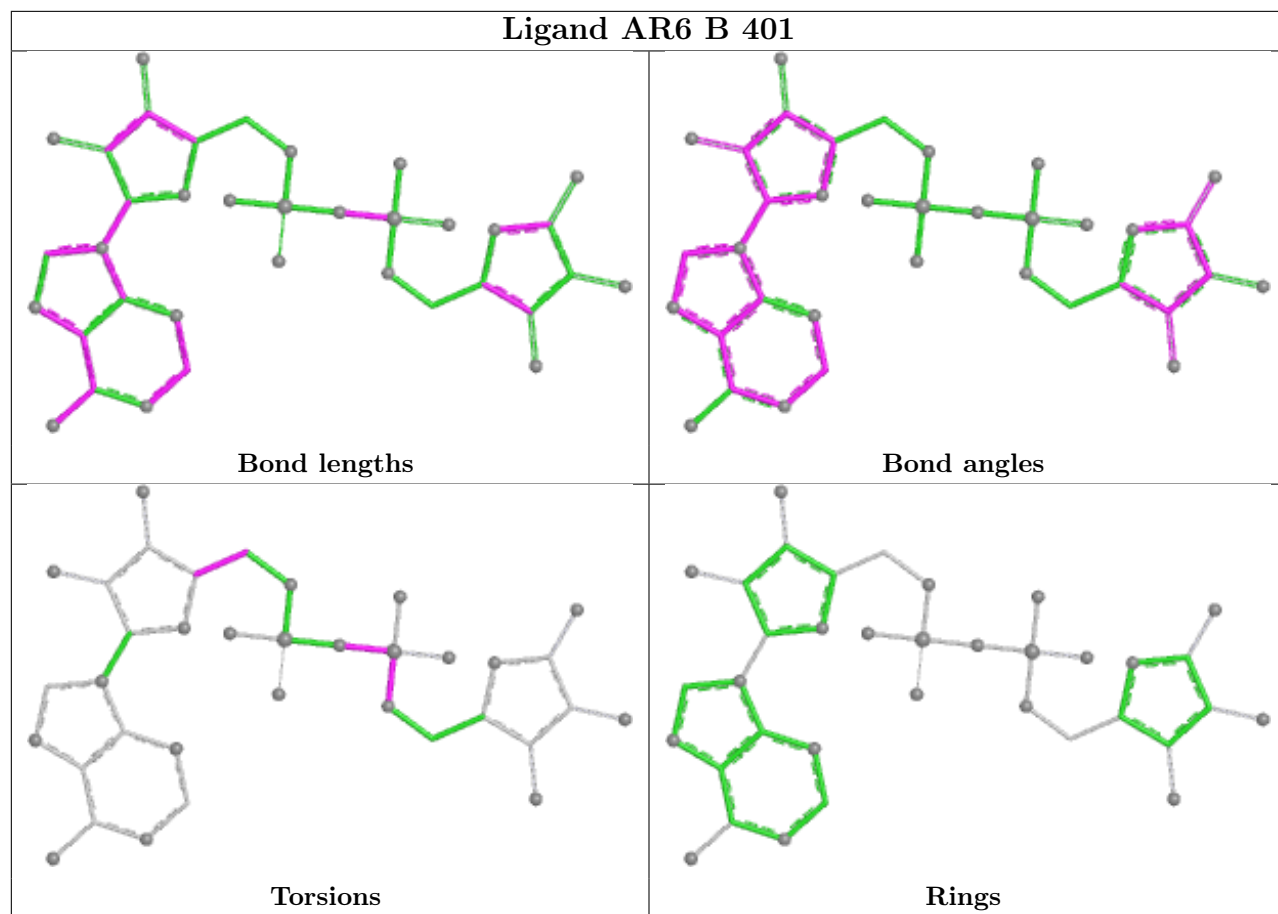
6 monomers are involved in 20 short contacts:

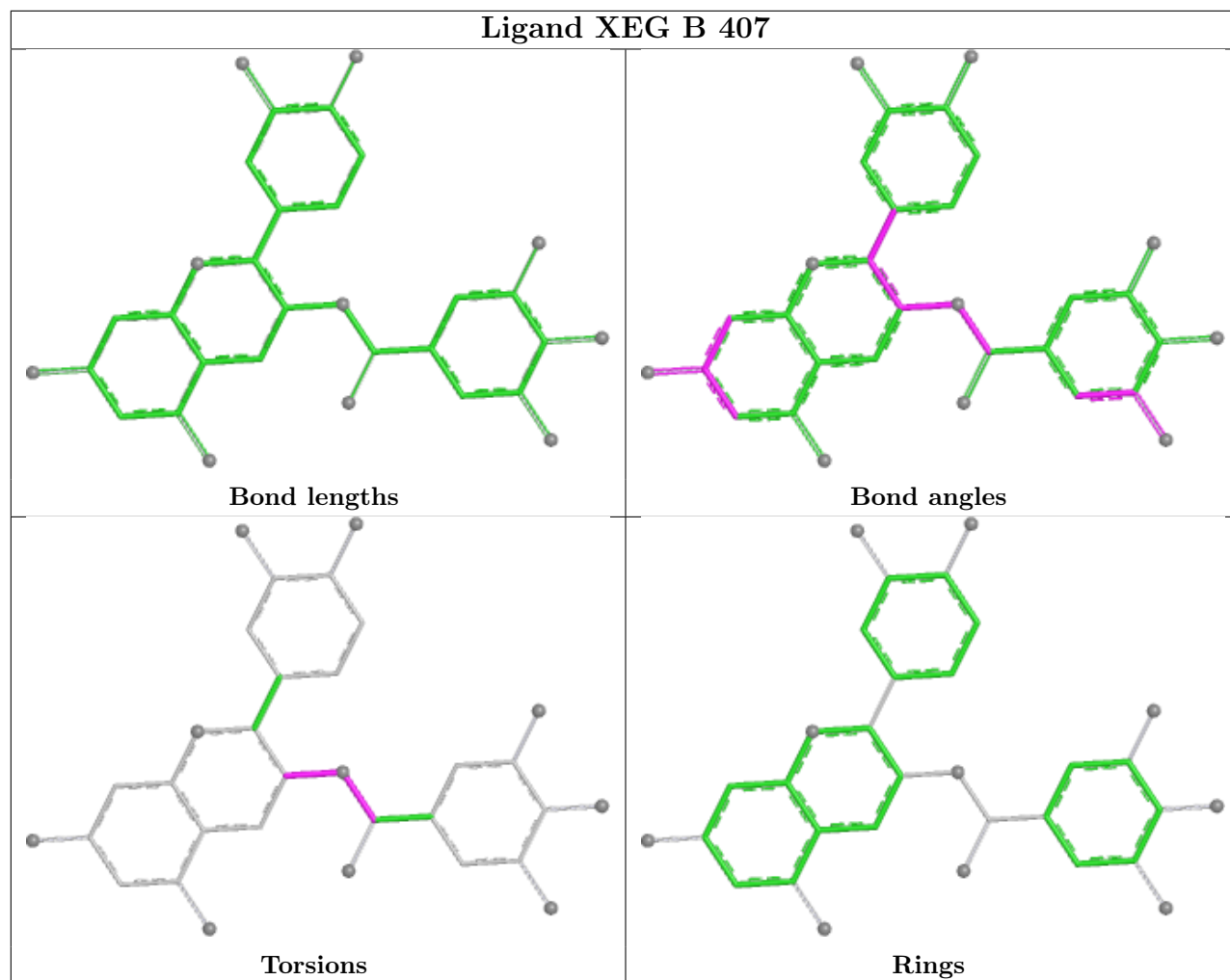
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	406	SO4	2	0
2	A	401	AR6	2	0
5	A	405	SO4	1	0
6	A	407	XEG	6	0
5	B	404	SO4	1	0
6	B	407	XEG	8	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	282/302 (93%)	-0.92	0 100 100	18, 36, 58, 82	0
1	B	277/302 (91%)	-0.83	0 100 100	24, 41, 64, 89	0
All	All	559/604 (92%)	-0.87	0 100 100	18, 40, 61, 89	0

There are no RSRZ outliers to report.

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.

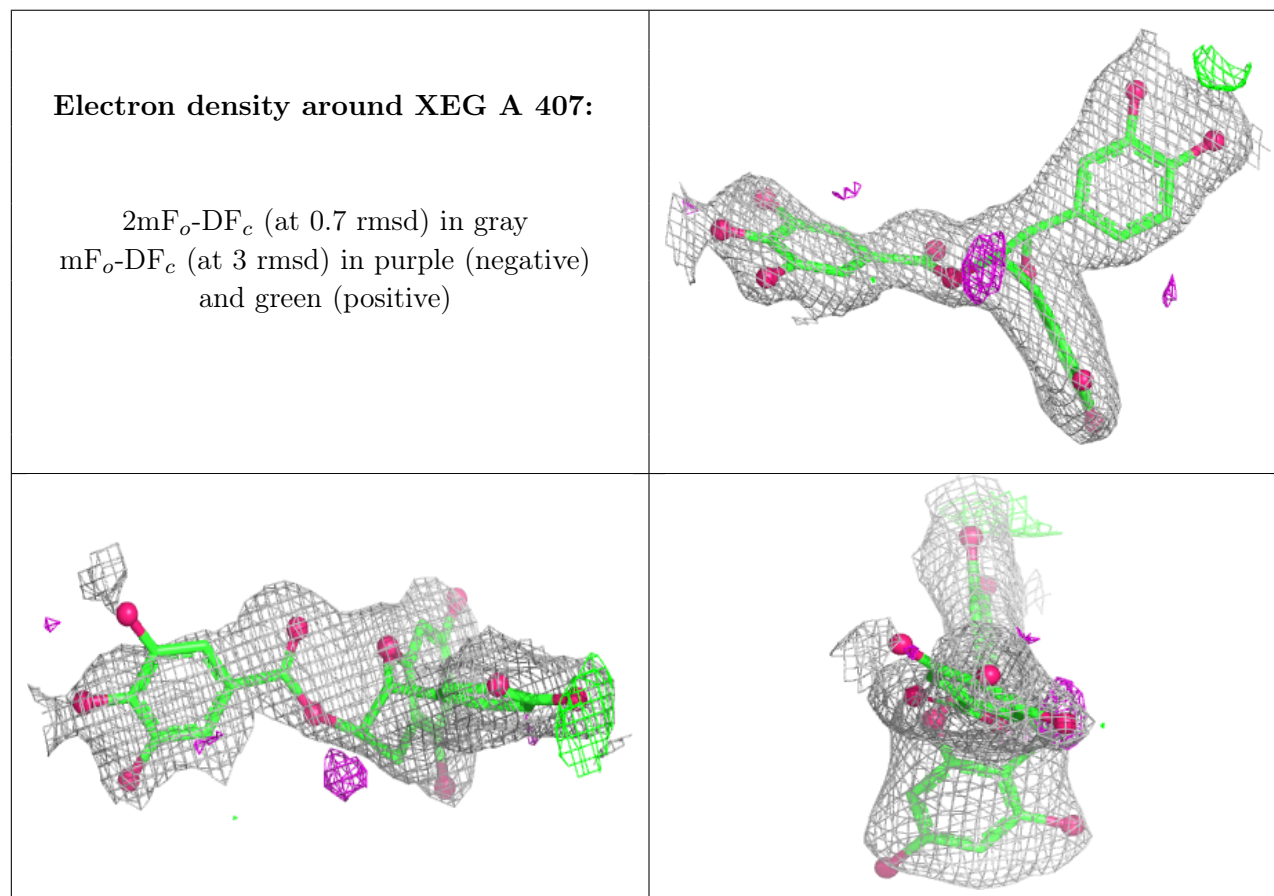
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	403	4/4	0.97	0.08	48,51,52,53	0
5	SO4	A	406	5/5	0.97	0.05	60,60,72,86	0
5	SO4	A	405	5/5	0.98	0.07	93,98,102,109	0
5	SO4	A	404	5/5	0.98	0.04	48,50,57,67	0
5	SO4	B	404	5/5	0.98	0.04	50,51,64,65	0
5	SO4	B	406	5/5	0.98	0.06	36,46,54,62	0
6	XEG	A	407	32/32	0.98	0.06	29,41,74,79	0

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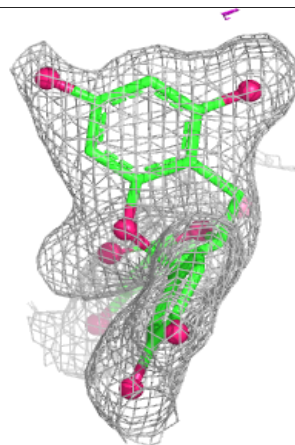
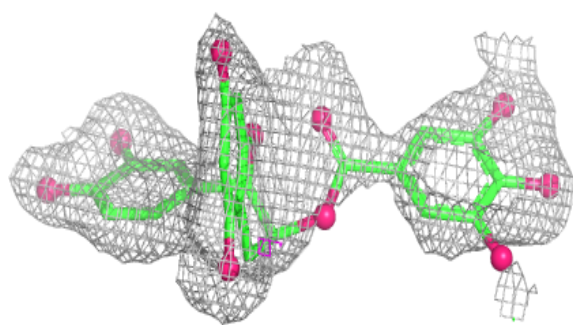
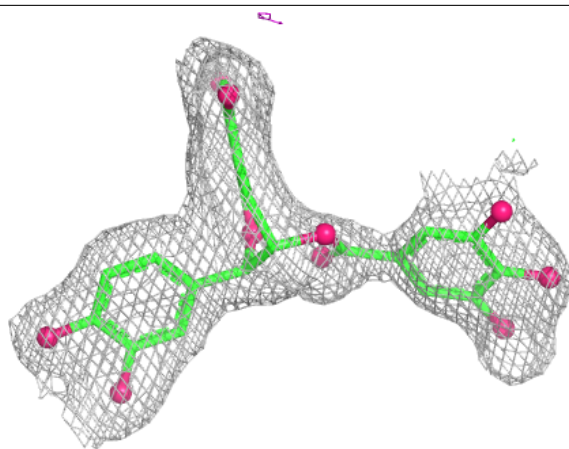
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	XEG	B	407	32/32	0.98	0.05	32,50,73,81	0
5	SO4	B	405	5/5	0.99	0.04	60,65,74,74	0
2	AR6	B	401	36/36	0.99	0.04	22,34,42,46	0
5	SO4	B	403	5/5	0.99	0.05	34,39,41,54	0
2	AR6	A	401	36/36	0.99	0.04	12,26,34,37	0
3	ZN	A	402	1/1	1.00	0.01	52,52,52,52	0
3	ZN	B	402	1/1	1.00	0.01	56,56,56,56	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.

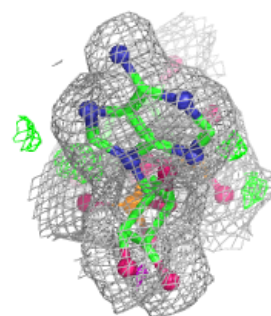
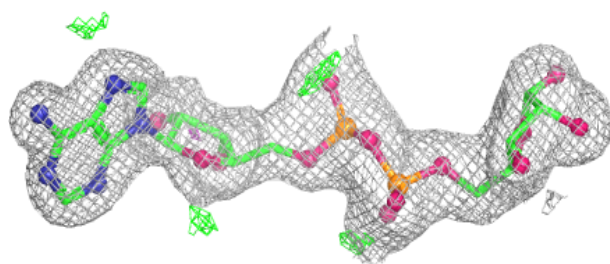
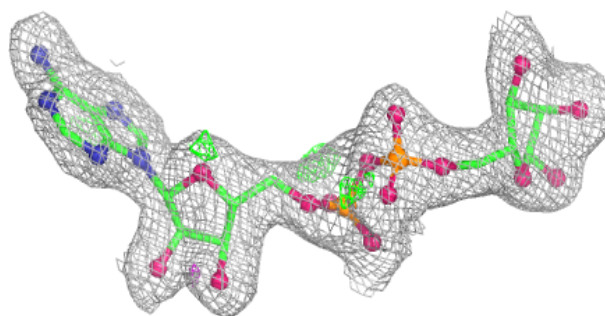


Electron density around XEG B 407:

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

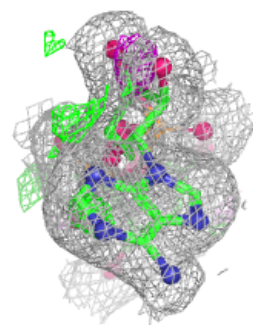
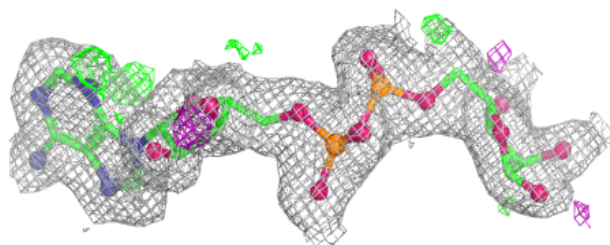
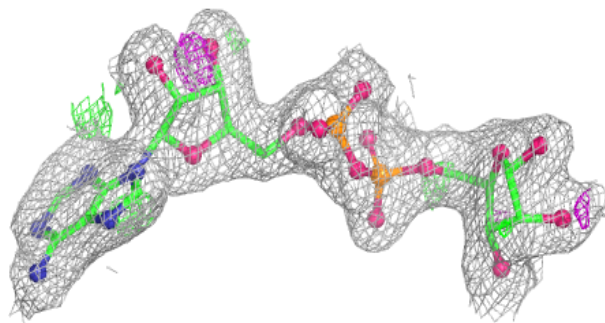
**Electron density around AR6 B 401:**

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



Electron density around AR6 A 401:

$2mF_o-DF_c$ (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.