



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:22 PM UTC

PDB ID : 4L39 / pdb_00004l39
Title : Crystal structure of GH3.12 from Arabidopsis thaliana in complex with AM-PCPP and salicylate
Authors : Zubieta, C.; Jez, J.M.; Brown, E.; Marcellin, R.; Kapp, U.; Round, A.; Westfall, C.
Deposited on : 2013-06-05
Resolution : 2.81 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

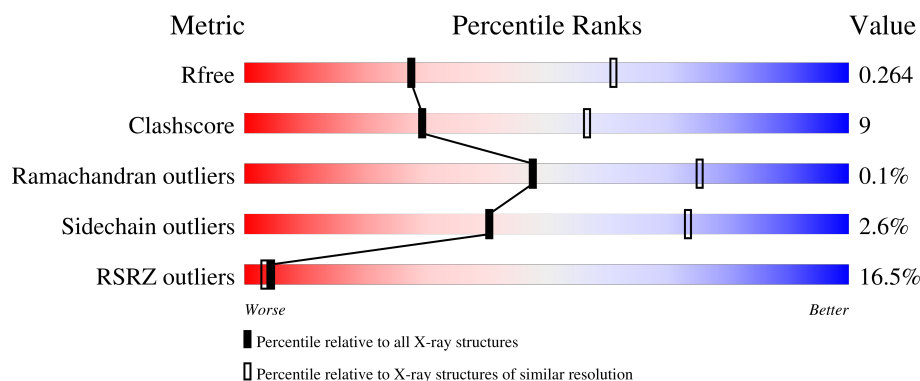
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	581	15% 78% 14% • 7%
1	B	581	16% 73% 19% • 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8660 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 4-substituted benzoates-glutamate ligase GH3.12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	7	0
			4153	2637	681	807	28			
1	B	542	Total	C	N	O	S	0	6	0
			4211	2672	681	831	27			

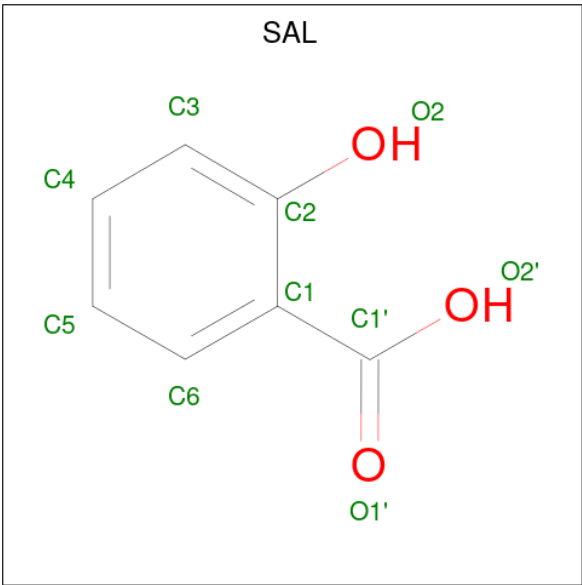
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q9LYU4
A	-4	SER	-	expression tag	UNP Q9LYU4
A	-3	HIS	-	expression tag	UNP Q9LYU4
A	-2	MET	-	expression tag	UNP Q9LYU4
A	-1	ALA	-	expression tag	UNP Q9LYU4
A	0	SER	-	expression tag	UNP Q9LYU4
B	-5	GLY	-	expression tag	UNP Q9LYU4
B	-4	SER	-	expression tag	UNP Q9LYU4
B	-3	HIS	-	expression tag	UNP Q9LYU4
B	-2	MET	-	expression tag	UNP Q9LYU4
B	-1	ALA	-	expression tag	UNP Q9LYU4
B	0	SER	-	expression tag	UNP Q9LYU4

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

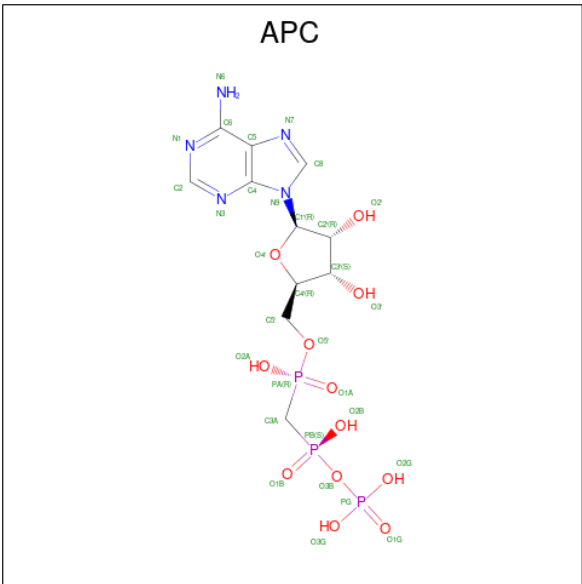
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2-HYDROXYBENZOIC ACID (CCD ID: SAL) (formula: C₇H₆O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	7	3		
3	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 4 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

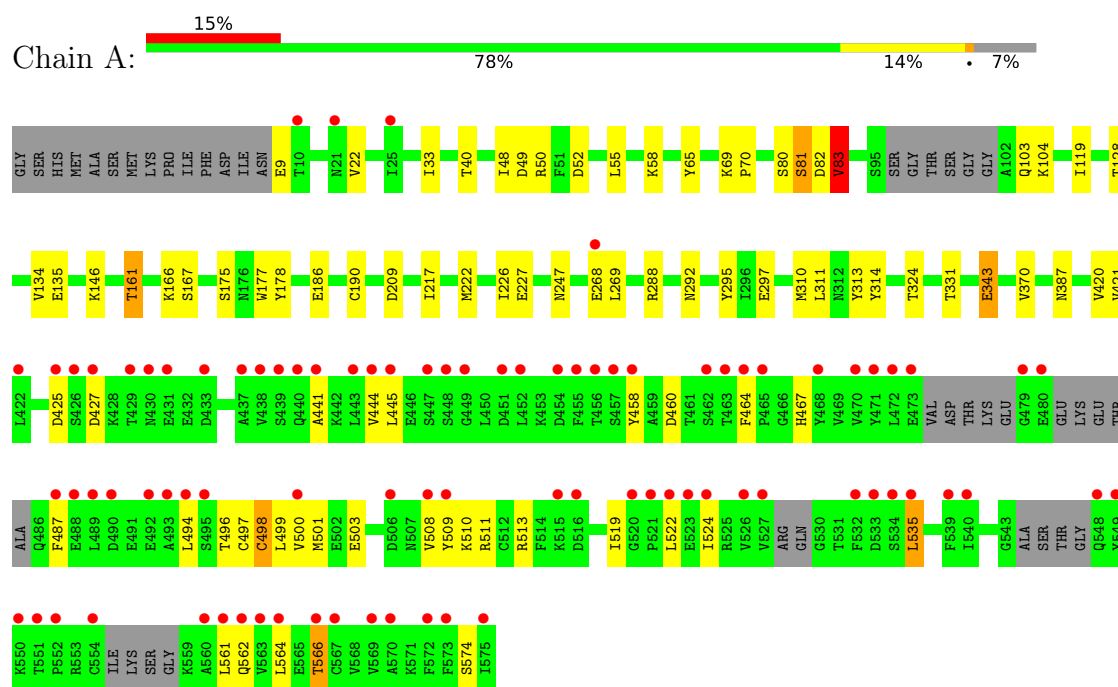
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	106	Total	O	0	0
			106	106		
5	B	107	Total	O	0	0
			107	107		

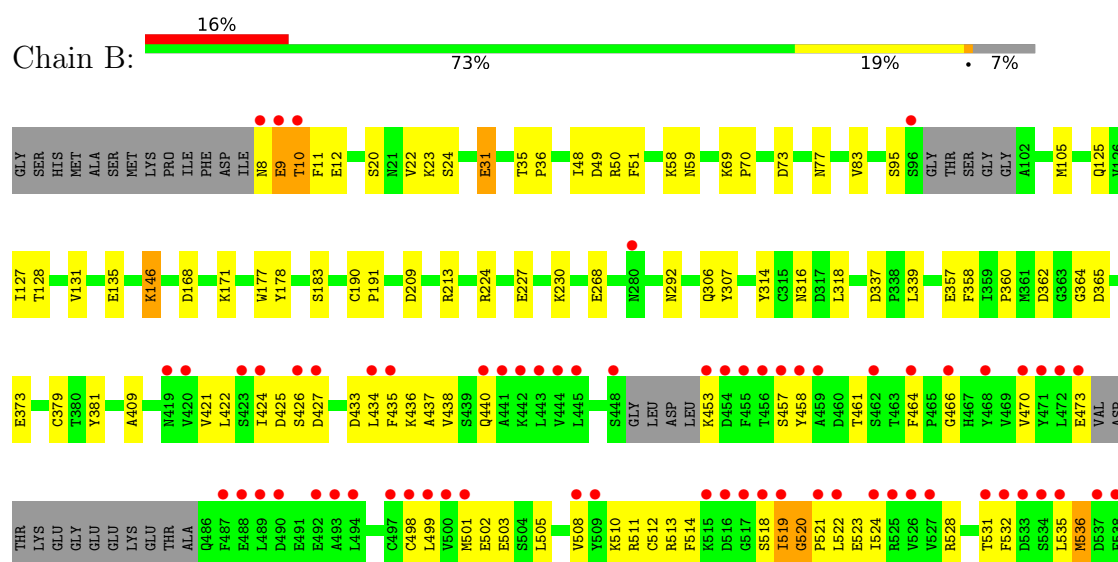
3 Residue-property plots [i](#)

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: 4-substituted benzoates-glutamate ligase GH3.12



- Molecule 1: 4-substituted benzoates-glutamate ligase GH3.12



F539	I540	S541	GLN	GLY	ALA	SER	T546	Q547	Q548	Y549	K550	T551	F552	H553	C554	T555	K556	S557	Q558	F559	A560	L561	Q562	V563	L564	E565	T566	C567	V568	V569	A570	R571	F572	F573	S574	ILE

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.36Å 114.09Å 157.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.00 – 2.81 58.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.00-2.81) 99.8 (58.00-2.81)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	0.26	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.198 , 0.267 0.198 , 0.264	Depositor DCC
R_{free} test set	1418 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8660	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7619e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAL, APC, MG

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	0.95	2/4251 (0.0%)	1.05	8/5770 (0.1%)
1	B	0.97	3/4309 (0.1%)	1.06	13/5850 (0.2%)
All	All	0.96	5/8560 (0.1%)	1.06	21/11620 (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	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	VAL	CA-CB	6.96	1.64	1.54
1	B	48	ILE	CA-CB	5.92	1.59	1.53
1	B	10	THR	CA-CB	5.68	1.59	1.53
1	B	409	ALA	CA-C	5.19	1.58	1.52
1	A	566	THR	CA-CB	5.06	1.61	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	440	GLN	N-CA-C	-7.69	103.87	113.55
1	B	127	ILE	N-CA-C	7.42	117.55	110.42
1	B	520	GLY	CA-C-N	7.16	128.78	119.84
1	B	520	GLY	C-N-CA	7.16	128.78	119.84
1	A	48	ILE	CB-CA-C	-6.54	105.22	112.68
1	A	487	PHE	N-CA-C	6.25	117.75	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	THR	N-CA-C	-6.13	104.86	113.20
1	A	288	ARG	N-CA-C	-6.07	106.00	113.41
1	A	387	ASN	N-CA-C	5.77	118.64	109.65
1	B	337	ASP	CA-C-N	5.61	125.08	119.24
1	B	337	ASP	C-N-CA	5.61	125.08	119.24
1	A	190	CYS	CA-C-N	5.42	124.93	119.19
1	A	190	CYS	C-N-CA	5.42	124.93	119.19
1	B	59	ASN	N-CA-C	5.40	119.95	112.45
1	A	81	SER	N-CA-C	-5.29	105.62	111.71
1	A	33	ILE	N-CA-C	-5.29	105.93	110.74
1	B	183	SER	CA-C-N	-5.27	114.53	119.85
1	B	183	SER	C-N-CA	-5.27	114.53	119.85
1	B	457	SER	N-CA-C	5.18	116.72	108.79
1	B	536	MET	N-CA-C	-5.06	107.66	113.88
1	B	9	GLU	N-CA-C	-5.05	105.48	111.69

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	520	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4153	0	3910	56	0
1	B	4211	0	4003	84	0
2	A	1	0	0	0	0
3	A	10	0	5	0	0
3	B	10	0	5	0	0
4	A	31	0	14	1	0
4	B	31	0	14	0	0
5	A	106	0	0	2	0
5	B	107	0	0	6	0
All	All	8660	0	7951	140	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 9.

All (140) 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:501:MET:HE2	1:A:522:LEU:HD21	1.46	0.96
1:A:310:MET:HE2	1:A:314:TYR:CZ	2.10	0.86
1:B:8:ASN:N	5:B:739:HOH:O	2.12	0.82
1:B:513:ARG:NH2	1:B:521:PRO:HA	1.95	0.81
1:A:562:GLN:O	1:A:566:THR:HG23	1.84	0.77
1:A:535:LEU:HD13	1:A:564:LEU:HD21	1.67	0.75
1:B:512:CYS:SG	1:B:518:SER:OG	2.42	0.73
1:B:427:ASP:HA	1:B:508:VAL:HG11	1.69	0.72
1:B:513:ARG:HD3	1:B:519:ILE:HB	1.74	0.69
1:A:310:MET:CE	1:A:314:TYR:CZ	2.74	0.69
1:B:31:GLU:HG2	1:B:51:PHE:CE2	2.28	0.68
1:B:453:LYS:N	1:B:473:GLU:O	2.29	0.66
1:A:65:TYR:CE1	1:A:104:LYS:HD2	2.31	0.66
1:B:49:ASP:OD1	1:B:50:ARG:NH1	2.29	0.66
1:A:80:SER:O	1:A:83:VAL:HG13	1.97	0.64
1:B:20:SER:O	5:B:718:HOH:O	2.14	0.64
1:B:499:LEU:HD23	1:B:502:GLU:HG3	1.79	0.64
1:A:445:LEU:HD11	1:A:497:CYS:SG	2.38	0.64
1:B:268:GLU:OE2	5:B:774:HOH:O	2.14	0.63
1:B:562:GLN:O	1:B:566:THR:OG1	2.09	0.63
1:B:532:PHE:HA	1:B:535:LEU:HB3	1.80	0.62
1:B:437:ALA:HB1	1:B:501:MET:HG2	1.81	0.61
1:B:513:ARG:HH11	1:B:519:ILE:HB	1.67	0.60
1:B:522:LEU:HD12	1:B:523:GLU:N	2.19	0.58
1:A:227:GLU:HG3	1:A:464:PHE:CG	2.38	0.58
1:B:427:ASP:HB3	1:B:508:VAL:HG12	1.85	0.58
1:A:146:LYS:HZ1	1:A:511:ARG:HD2	1.68	0.58
1:A:501:MET:HE2	1:A:522:LEU:CD2	2.29	0.58
1:A:310:MET:HE2	1:A:314:TYR:CE2	2.39	0.58
1:B:12:GLU:N	1:B:12:GLU:OE1	2.37	0.58
1:B:470:VAL:HG23	1:B:522:LEU:HD11	1.86	0.57
1:B:421:VAL:HG23	1:B:422:LEU:HD12	1.85	0.57
1:B:499:LEU:HD23	1:B:502:GLU:CG	2.35	0.57
1:A:445:LEU:CD1	1:A:497:CYS:SG	2.93	0.56
1:B:307:TYR:OH	1:B:424:ILE:O	2.23	0.56
1:B:513:ARG:NH1	1:B:519:ILE:HG22	2.20	0.56
1:B:35:THR:O	5:B:738:HOH:O	2.17	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ARG:HA	1:A:519:ILE:HB	1.88	0.55
1:B:513:ARG:HH22	1:B:521:PRO:HA	1.68	0.55
1:B:178:TYR:O	1:B:213:ARG:NH2	2.41	0.54
1:B:499:LEU:CD2	1:B:502:GLU:HG3	2.37	0.54
1:B:373:GLU:N	1:B:373:GLU:OE1	2.41	0.53
1:B:458:TYR:CE1	1:B:561:LEU:HD11	2.43	0.53
1:A:501:MET:CE	1:A:522:LEU:HD21	2.29	0.52
1:B:9:GLU:C	1:B:11:PHE:H	2.17	0.52
1:B:513:ARG:HH11	1:B:519:ILE:CB	2.22	0.52
1:B:427:ASP:HA	1:B:508:VAL:CG1	2.38	0.52
1:A:268[A]:GLU:HG2	1:A:269:LEU:N	2.25	0.52
1:A:535:LEU:HD12	1:A:564:LEU:HD11	1.92	0.51
1:B:23:LYS:HD3	1:B:373:GLU:HG3	1.93	0.51
1:B:131:VAL:HG22	1:B:339:LEU:HD21	1.93	0.51
1:B:511:ARG:HG3	1:B:512:CYS:N	2.26	0.50
1:A:161:THR:HG21	1:A:217:ILE:HD11	1.94	0.50
1:B:22:VAL:N	5:B:718:HOH:O	2.44	0.50
1:B:23:LYS:HD2	1:B:373:GLU:OE2	2.11	0.50
1:A:103:GLN:OE1	1:A:508:VAL:HG12	2.12	0.49
1:B:458:TYR:CE1	1:B:561:LEU:CD1	2.96	0.48
1:A:427:ASP:CB	1:A:509:TYR:HA	2.43	0.48
1:A:441:ALA:O	1:A:444:VAL:HG22	2.14	0.48
1:A:460:ASP:OD1	1:A:467:HIS:N	2.45	0.48
1:B:435:PHE:HA	1:B:438:VAL:HG22	1.95	0.47
1:B:560:ALA:O	1:B:563:VAL:HG22	2.13	0.47
1:A:310:MET:CE	1:A:314:TYR:CE2	2.97	0.47
1:B:557:SER:O	1:B:561:LEU:HD13	2.15	0.47
1:B:528:ARG:N	1:B:531:THR:OG1	2.47	0.47
1:B:532:PHE:O	1:B:536:MET:N	2.47	0.47
1:B:73:ASP:O	1:B:77:ASN:ND2	2.48	0.46
1:B:501:MET:O	1:B:505:LEU:HD13	2.14	0.46
1:B:230:LYS:NZ	1:B:314:TYR:OH	2.46	0.46
1:A:166:LYS:HA	1:A:166:LYS:HD2	1.81	0.46
1:A:119:ILE:HG13	1:A:331:THR:HG21	1.98	0.46
1:A:247:ASN:ND2	5:A:762:HOH:O	2.46	0.46
1:A:458:TYR:CE1	1:A:561:LEU:HD11	2.50	0.46
1:A:9:GLU:N	5:A:775:HOH:O	2.48	0.46
1:B:318:LEU:O	5:B:736:HOH:O	2.21	0.46
1:A:498:CYS:HB2	1:A:574:SER:HB3	1.97	0.45
1:B:373:GLU:H	1:B:373:GLU:CD	2.25	0.45
1:A:499:LEU:O	1:A:503:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:SER:O	1:B:95:SER:OG	2.28	0.45
1:B:168:ASP:HA	1:B:171:LYS:HG2	1.99	0.45
1:A:499:LEU:HB3	1:A:574:SER:HB2	1.99	0.45
1:B:357:GLU:C	1:B:358:PHE:CD1	2.95	0.45
1:B:521:PRO:O	1:B:573:PHE:HD1	1.99	0.45
1:A:324:THR:O	4:A:603:APC:N6	2.50	0.44
1:A:498:CYS:HB3	1:A:524:ILE:HD12	1.99	0.44
1:B:360:PRO:HB3	1:B:365:ASP:HB3	1.99	0.44
1:A:343:GLU:H	1:A:343:GLU:CD	2.26	0.44
1:A:494:LEU:HD12	1:A:497:CYS:SG	2.58	0.44
1:A:209:ASP:O	1:A:292:ASN:ND2	2.46	0.44
1:B:362:ASP:OD1	1:B:364:GLY:N	2.50	0.44
1:B:433:ASP:HB2	1:B:436:LYS:CE	2.48	0.44
1:A:222:MET:HE3	1:A:226:ILE:HD11	2.00	0.43
1:A:420:VAL:HG12	1:A:421:VAL:N	2.33	0.43
1:B:35:THR:N	1:B:36:PRO:HD2	2.32	0.43
1:A:128[B]:THR:HG21	1:A:135:GLU:OE2	2.19	0.43
1:B:146:LYS:HD2	1:B:511:ARG:NH2	2.33	0.43
1:A:177:TRP:CG	1:A:178:TYR:N	2.87	0.43
1:A:496:THR:HA	1:A:499:LEU:HG	2.00	0.43
1:B:433:ASP:CB	1:B:436:LYS:HE2	2.49	0.43
1:B:521:PRO:HB2	1:B:574:SER:HB2	2.01	0.43
1:A:186:GLU:OE1	1:A:186:GLU:N	2.48	0.42
1:A:40:THR:HA	1:A:82:ASP:O	2.19	0.42
1:A:52:ASP:HB3	1:A:55:LEU:HB3	2.01	0.42
1:A:177:TRP:CD2	1:A:178:TYR:N	2.88	0.42
1:B:503:GLU:HA	1:B:510:LYS:CE	2.49	0.42
1:A:535:LEU:O	1:A:535:LEU:HG	2.20	0.42
1:B:146:LYS:HE2	1:B:511:ARG:HH22	1.85	0.42
1:B:224:ARG:HD3	1:B:464:PHE:HZ	1.84	0.42
1:A:295:TYR:CE2	1:A:297:GLU:HB2	2.55	0.42
1:A:501:MET:HE3	1:A:501:MET:HB3	1.87	0.42
1:A:522:LEU:C	1:A:522:LEU:HD23	2.44	0.42
1:B:227:GLU:HG3	1:B:464:PHE:CD1	2.54	0.42
1:B:498:CYS:SG	1:B:524:ILE:CD1	3.08	0.42
1:A:509:TYR:CD2	1:A:510:LYS:N	2.87	0.41
1:B:69:LYS:N	1:B:70:PRO:CD	2.83	0.41
1:B:209:ASP:O	1:B:292:ASN:ND2	2.45	0.41
1:B:135:GLU:HG2	1:B:177:TRP:CD1	2.54	0.41
1:B:425:ASP:CG	1:B:426:SER:H	2.28	0.41
1:A:310:MET:HE1	1:A:313:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:LEU:CD1	1:A:564:LEU:HD21	2.42	0.41
1:B:379:CYS:HB2	1:B:381:TYR:CE2	2.56	0.41
1:B:523:GLU:HA	1:B:572:PHE:O	2.21	0.41
1:B:9:GLU:HG2	1:B:10:THR:N	2.35	0.41
1:B:434:LEU:O	1:B:438:VAL:HG22	2.21	0.41
1:B:466:GLY:O	1:B:519:ILE:HG23	2.21	0.41
1:B:561:LEU:O	1:B:565:GLU:N	2.46	0.41
1:A:49:ASP:OD1	1:A:50:ARG:NH1	2.54	0.41
1:A:69:LYS:N	1:A:70:PRO:CD	2.84	0.41
1:B:306:GLN:CD	1:B:461:THR:HG21	2.45	0.41
1:B:470:VAL:HG11	1:B:501:MET:HE1	2.03	0.40
1:A:460:ASP:OD2	1:A:467:HIS:NE2	2.54	0.40
1:B:190:CYS:HA	1:B:191:PRO:HD3	1.98	0.40
1:B:433:ASP:OD1	1:B:433:ASP:C	2.64	0.40
1:A:310:MET:CE	1:A:314:TYR:CE1	3.04	0.40
1:B:8:ASN:O	1:B:12:GLU:OE1	2.38	0.40
1:B:177:TRP:CG	1:B:178:TYR:N	2.89	0.40
1:B:513:ARG:HG3	1:B:514:PHE:CD1	2.57	0.40
1:B:9:GLU:C	1:B:11:PHE:N	2.80	0.40
1:B:11:PHE:HB2	1:B:125:GLN:OE1	2.21	0.40
1:B:458:TYR:CE1	1:B:555:ILE:CB	3.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	534/581 (92%)	506 (95%)	27 (5%)	1 (0%)	43	71
1	B	537/581 (92%)	507 (94%)	30 (6%)	0	100	100
All	All	1071/1162 (92%)	1013 (95%)	57 (5%)	1 (0%)	48	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	425	ASP

5.3.2 Protein sidechains ⓘ

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	445/527 (84%)	431 (97%)	14 (3%)	35	69
1	B	465/527 (88%)	455 (98%)	10 (2%)	45	77
All	All	910/1054 (86%)	886 (97%)	24 (3%)	40	73

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	58	LYS
1	A	81	SER
1	A	83	VAL
1	A	134	VAL
1	A	161	THR
1	A	167	SER
1	A	175	SER
1	A	311	LEU
1	A	343	GLU
1	A	370	VAL
1	A	498	CYS
1	A	500	VAL
1	A	535	LEU
1	B	24[B]	SER
1	B	31	GLU
1	B	58	LYS
1	B	83	VAL
1	B	105	MET
1	B	128[A]	THR
1	B	128[B]	THR
1	B	146	LYS

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Mol	Chain	Res	Type
1	B	316	ASN
1	B	519	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	193	ASN

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, 1 is monoatomic - leaving 4 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	APC	B	602	-	29,33,33	1.67	6 (20%)	44,52,52	2.30	12 (27%)
3	SAL	B	601	-	10,10,10	1.18	1 (10%)	13,13,13	1.25	2 (15%)
4	APC	A	603	2	29,33,33	1.77	6 (20%)	44,52,52	2.24	14 (31%)
3	SAL	A	602	-	10,10,10	1.14	0	13,13,13	1.76	4 (30%)

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	APC	B	602	-	-	1/19/38/38	0/3/3/3
3	SAL	B	601	-	-	0/4/4/4	0/1/1/1
4	APC	A	603	2	-	1/19/38/38	0/3/3/3
3	SAL	A	602	-	-	0/4/4/4	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	APC	O4'-C1'	4.06	1.51	1.42
4	A	603	APC	O4'-C1'	3.89	1.51	1.42
4	A	603	APC	C5-N7	-3.79	1.32	1.39
4	B	602	APC	C5-N7	-3.65	1.32	1.39
4	A	603	APC	C2'-C3'	-3.60	1.43	1.53
4	A	603	APC	O4'-C4'	3.02	1.51	1.45
4	A	603	APC	C3'-C4'	-2.64	1.46	1.53
3	B	601	SAL	O2-C2	2.63	1.41	1.36
4	B	602	APC	O4'-C4'	2.60	1.50	1.45
4	B	602	APC	C2'-C3'	-2.53	1.46	1.53
4	A	603	APC	C1'-N9	-2.41	1.39	1.46
4	B	602	APC	C1'-N9	-2.30	1.40	1.46
4	B	602	APC	C6-N6	2.24	1.39	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	APC	N3-C2-N1	-7.05	117.91	128.58
4	B	602	APC	N3-C2-N1	-6.19	119.21	128.58
4	B	602	APC	C5-C4-N3	-5.41	119.27	126.72
4	B	602	APC	O4'-C1'-N9	4.94	117.58	108.09
4	B	602	APC	C3'-C2'-C1'	4.82	110.59	101.46
4	A	603	APC	C5-C4-N3	-4.80	120.11	126.72
4	B	602	APC	N3-C4-N9	4.61	135.01	127.17
4	A	603	APC	N3-C4-N9	4.49	134.80	127.17
4	A	603	APC	C3'-C2'-C1'	3.98	108.99	101.46
4	B	602	APC	C2'-C1'-N9	-3.94	103.52	113.30
4	A	603	APC	C2-N3-C4	3.91	121.37	111.83
4	B	602	APC	C2-N3-C4	3.79	121.09	111.83
4	B	602	APC	C5-N7-C8	3.77	109.38	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	APC	C5-N7-C8	3.72	109.29	103.45
3	A	602	SAL	C2-C1-C1'	3.66	123.75	120.00
4	A	603	APC	O2'-C2'-C3'	-2.90	102.54	111.82
4	A	603	APC	C5'-C4'-C3'	-2.87	104.87	115.21
4	A	603	APC	N9-C8-N7	-2.76	110.03	113.94
3	B	601	SAL	C2-C1-C1'	2.73	122.80	120.00
4	B	602	APC	N9-C8-N7	-2.64	110.19	113.94
3	A	602	SAL	C3-C2-C1	2.59	122.58	119.89
3	A	602	SAL	O2'-C1'-C1	2.57	122.60	115.28
4	B	602	APC	C4-C5-N7	-2.55	107.67	110.58
4	A	603	APC	O4'-C1'-N9	2.51	112.91	108.09
4	A	603	APC	C4'-O4'-C1'	-2.51	103.93	109.47
4	A	603	APC	C2-N1-C6	2.41	122.69	118.73
3	A	602	SAL	O2'-C1'-O1'	-2.27	118.47	123.35
4	B	602	APC	C2-N1-C6	2.19	122.33	118.73
3	B	601	SAL	O2'-C1'-C1	2.18	121.48	115.28
4	B	602	APC	O4'-C4'-C3'	2.13	109.39	105.15
4	A	603	APC	C4-C5-N7	-2.12	108.16	110.58
4	A	603	APC	C2'-C1'-N9	-2.04	108.23	113.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	APC	C5'-O5'-PA-O1A
4	B	602	APC	C4'-C5'-O5'-PA

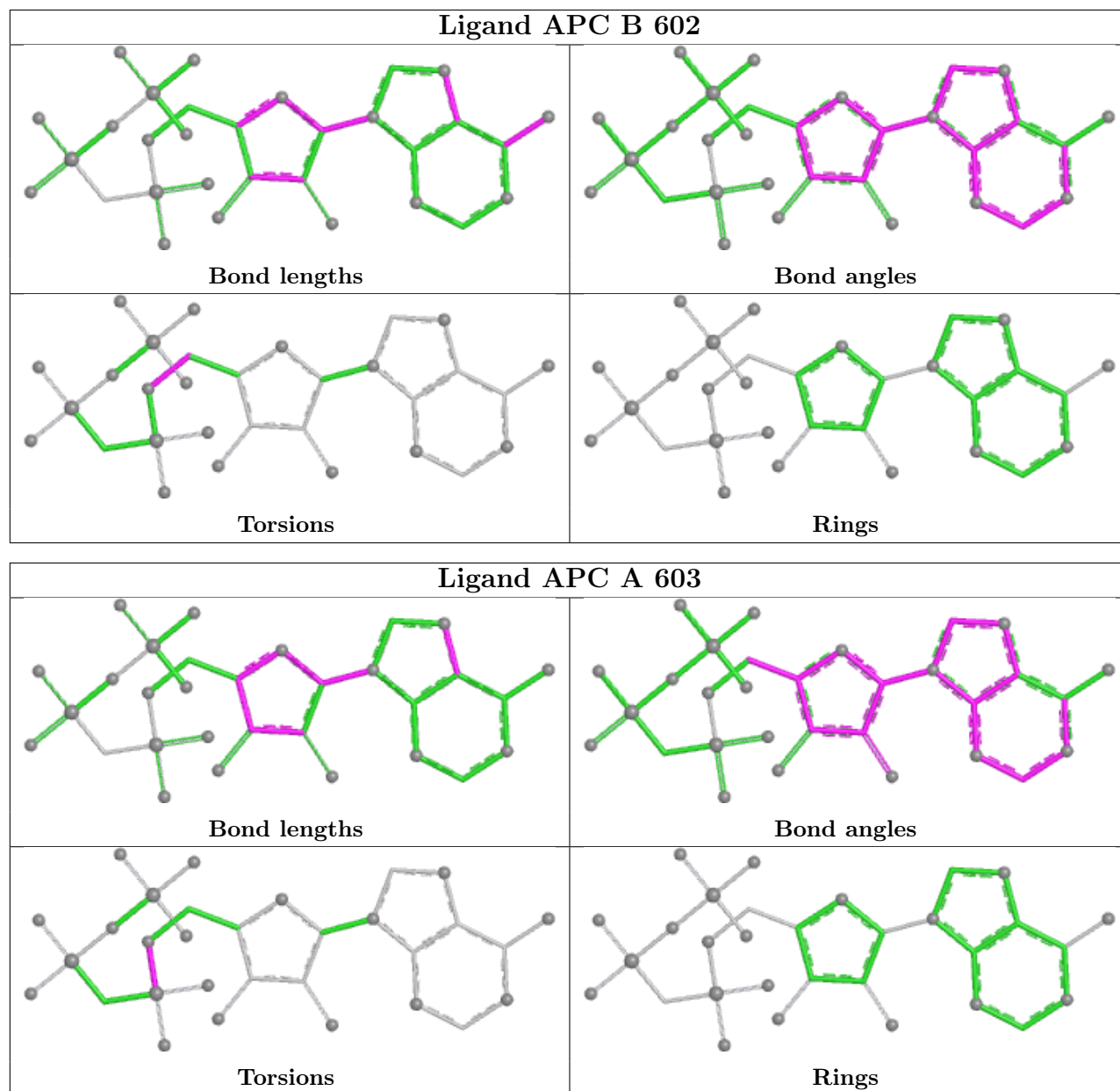
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	APC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	541/581 (93%)	0.05	86 (15%) 5 3	7, 20, 138, 155	7 (1%)
1	B	542/581 (93%)	0.09	93 (17%) 4 3	6, 21, 160, 182	5 (0%)
All	All	1083/1162 (93%)	0.07	179 (16%) 4 3	6, 21, 150, 182	12 (1%)

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21[A]	ASN	5.8
1	B	8	ASN	5.7
1	B	546	THR	5.2
1	B	535	LEU	4.6
1	B	444	VAL	4.6
1	A	444	VAL	4.4
1	B	560	ALA	4.3
1	A	572	PHE	4.3
1	B	564	LEU	4.3
1	B	518	SER	4.3
1	A	480	GLU	4.2
1	A	573	PHE	4.2
1	A	563	VAL	4.1
1	B	434	LEU	4.0
1	B	426	SER	4.0
1	A	494	LEU	3.9
1	A	462	SER	3.9
1	B	509	TYR	3.8
1	B	494	LEU	3.8
1	A	454	ASP	3.8
1	B	552	PRO	3.7
1	A	516	ASP	3.6
1	B	471	TYR	3.6
1	A	445	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	456	THR	3.5
1	A	551	THR	3.5
1	B	457	SER	3.5
1	A	433	ASP	3.5
1	B	96	SER	3.4
1	B	462	SER	3.4
1	B	497	CYS	3.4
1	A	533	ASP	3.4
1	B	554	CYS	3.4
1	A	25	ILE	3.4
1	A	524	ILE	3.3
1	B	548	GLN	3.3
1	B	549	TYR	3.3
1	A	493	ALA	3.3
1	B	563	VAL	3.3
1	B	569	VAL	3.3
1	B	454	ASP	3.3
1	B	445	LEU	3.3
1	B	561	LEU	3.3
1	B	539	PHE	3.3
1	A	441	ALA	3.2
1	B	551	THR	3.2
1	A	564	LEU	3.2
1	B	10	THR	3.2
1	B	419	ASN	3.2
1	A	508	VAL	3.1
1	A	489	LEU	3.1
1	A	268[A]	GLU	3.1
1	A	429	THR	3.1
1	B	524	ILE	3.1
1	B	521	PRO	3.1
1	B	498	CYS	3.1
1	B	547	GLY	3.1
1	A	468	TYR	3.0
1	B	499	LEU	3.0
1	A	470	VAL	3.0
1	A	447	SER	3.0
1	A	527	VAL	3.0
1	B	538	PHE	3.0
1	A	440	GLN	3.0
1	A	479	GLY	3.0
1	B	280	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	488	GLU	3.0
1	A	443	LEU	2.9
1	B	566	THR	2.9
1	A	567	CYS	2.9
1	B	508	VAL	2.9
1	B	573	PHE	2.9
1	A	561	LEU	2.9
1	A	509	TYR	2.9
1	B	9	GLU	2.9
1	A	437	ALA	2.9
1	A	439	SER	2.9
1	B	532	PHE	2.9
1	A	448	SER	2.8
1	A	575	ILE	2.8
1	B	423	SER	2.8
1	A	473	GLU	2.8
1	A	456	THR	2.8
1	B	517	GLY	2.8
1	A	526	VAL	2.7
1	A	532	PHE	2.7
1	B	525	ARG	2.7
1	A	487	PHE	2.7
1	A	554	CYS	2.7
1	A	560	ALA	2.7
1	B	557	SER	2.7
1	A	539	PHE	2.7
1	B	464	PHE	2.7
1	B	487	PHE	2.7
1	B	490	ASP	2.7
1	B	427	ASP	2.7
1	B	443	LEU	2.7
1	B	448	SER	2.7
1	A	520	GLY	2.6
1	B	531	THR	2.6
1	B	522	LEU	2.6
1	A	534	SER	2.6
1	B	472	LEU	2.6
1	A	492	GLU	2.6
1	B	540	ILE	2.6
1	A	490	ASP	2.6
1	B	526	VAL	2.6
1	B	574	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	535	LEU	2.5
1	B	489	LEU	2.5
1	B	565	GLU	2.5
1	B	516	ASP	2.5
1	A	463	THR	2.5
1	B	473	GLU	2.5
1	A	464	PHE	2.5
1	B	459	ALA	2.5
1	B	556	LYS	2.5
1	B	558	GLY	2.5
1	A	550	LYS	2.5
1	B	440	GLN	2.5
1	A	515	LYS	2.5
1	B	453	LYS	2.5
1	A	427	ASP	2.4
1	A	451	ASP	2.4
1	A	562	GLN	2.4
1	A	522	LEU	2.4
1	B	470	VAL	2.4
1	B	553	ARG	2.4
1	B	515	LYS	2.4
1	A	430	ASN	2.4
1	A	570	ALA	2.4
1	A	566	THR	2.4
1	B	501	MET	2.4
1	A	540	ILE	2.4
1	A	548	GLN	2.3
1	B	534	SER	2.3
1	A	452	LEU	2.3
1	B	519	ILE	2.3
1	A	465	PRO	2.3
1	B	455	PHE	2.3
1	A	549	TYR	2.3
1	B	550	LYS	2.3
1	B	527	VAL	2.3
1	B	537	ASP	2.3
1	B	567	CYS	2.3
1	B	555	ILE	2.3
1	A	457	SER	2.3
1	A	449	GLY	2.3
1	B	424	ILE	2.2
1	A	458	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	492	GLU	2.2
1	A	569	VAL	2.2
1	B	466	GLY	2.2
1	B	493	ALA	2.2
1	A	500	VAL	2.2
1	B	420	VAL	2.2
1	B	442	LYS	2.2
1	B	468	TYR	2.2
1	A	426	SER	2.2
1	B	500	VAL	2.1
1	A	472	LEU	2.1
1	A	471	TYR	2.1
1	B	458	TYR	2.1
1	B	570	ALA	2.1
1	A	552	PRO	2.1
1	B	435	PHE	2.1
1	A	488	GLU	2.1
1	A	523	GLU	2.1
1	A	495	SER	2.0
1	A	438	VAL	2.0
1	A	455	PHE	2.0
1	A	10	THR	2.0
1	A	425	ASP	2.0
1	B	441	ALA	2.0
1	A	431	GLU	2.0
1	A	521	PRO	2.0
1	A	422	LEU	2.0
1	A	506	ASP	2.0
1	B	533	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

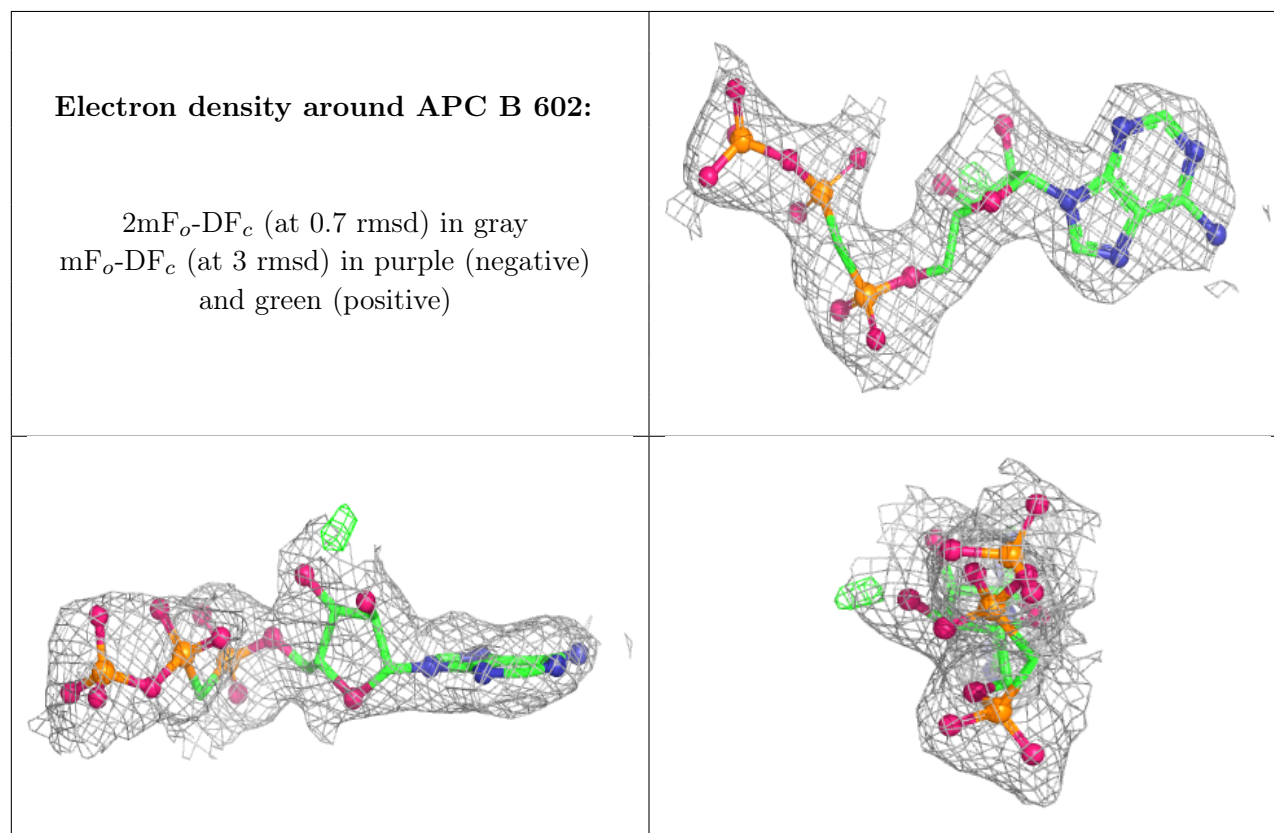
There are no oligosaccharides in this entry.

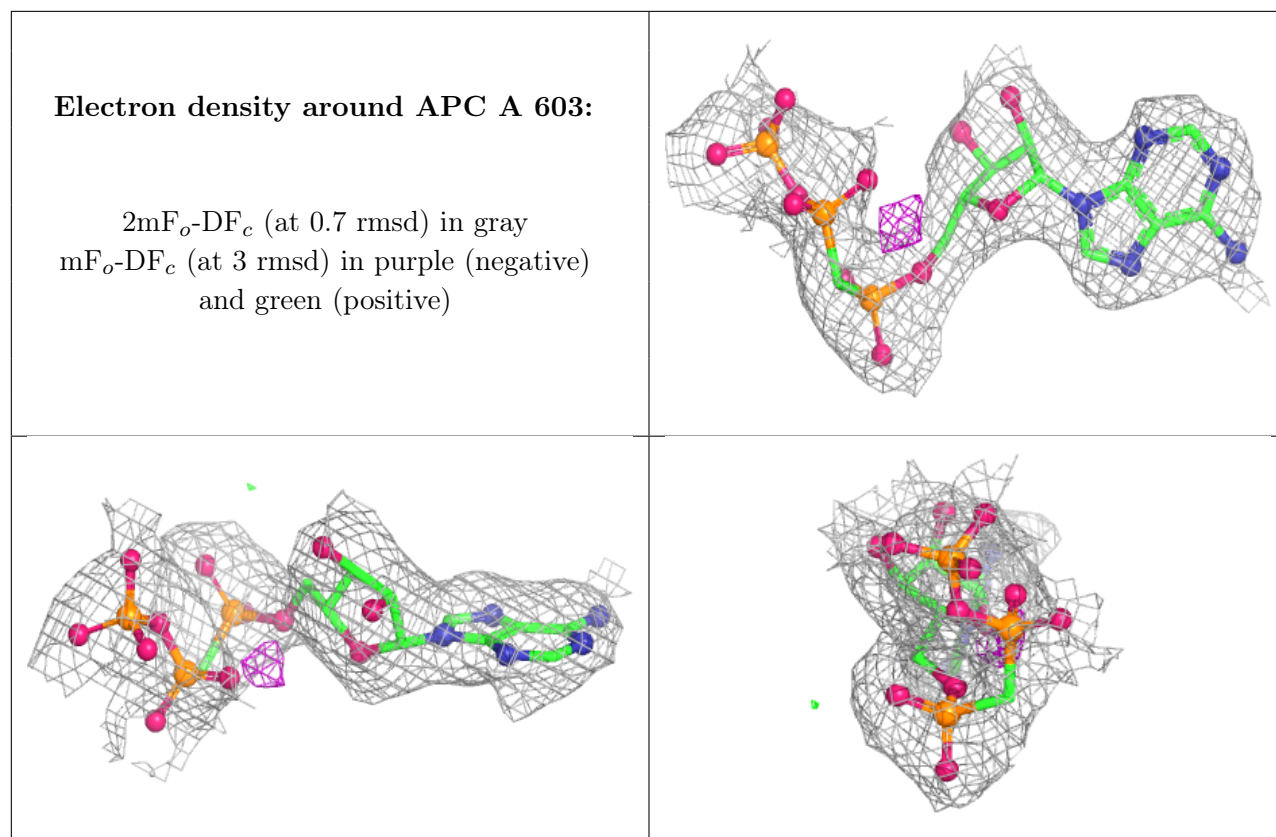
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	601	1/1	0.84	0.08	44,44,44,44	0
3	SAL	B	601	10/10	0.91	0.13	35,46,51,59	0
4	APC	B	602	31/31	0.91	0.08	21,39,74,83	0
4	APC	A	603	31/31	0.92	0.08	15,30,78,84	0
3	SAL	A	602	10/10	0.92	0.11	17,38,46,51	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.