



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:01 PM UTC

PDB ID : 5CX9 / pdb_00005cx9
Title : Crystal structure of CK2alpha with (methyl 4-((3-(3-chloro-4-(phenyl)benzyl amino)propyl)amino)-4-oxobutanoate bound
Authors : Brear, P.; De Fusco, C.; Georgiou, K.H.; Spring, D.; Hyvonen, M.
Deposited on : 2015-07-28
Resolution : 1.73 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

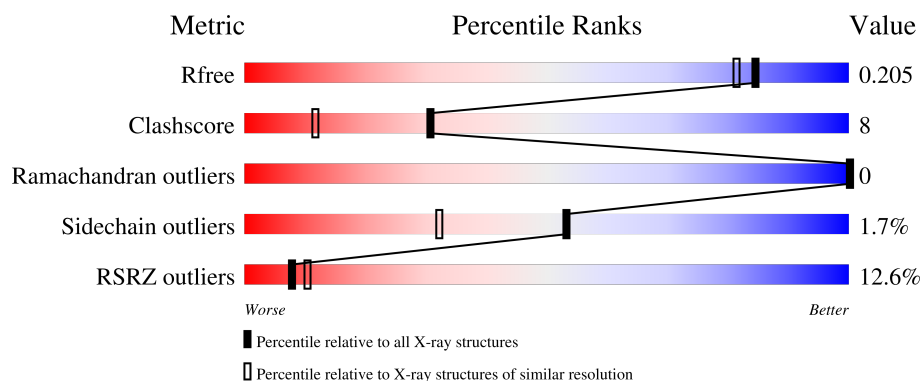
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	352	6% 83% 9% 7%
1	B	352	17% 81% 11% 8%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6033 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 Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	7	0
			2821	1804	495	511	11			
1	B	325	Total	C	N	O	S	0	4	0
			2773	1775	485	502	11			

There are 50 discrepancies between the modelled and reference sequences:

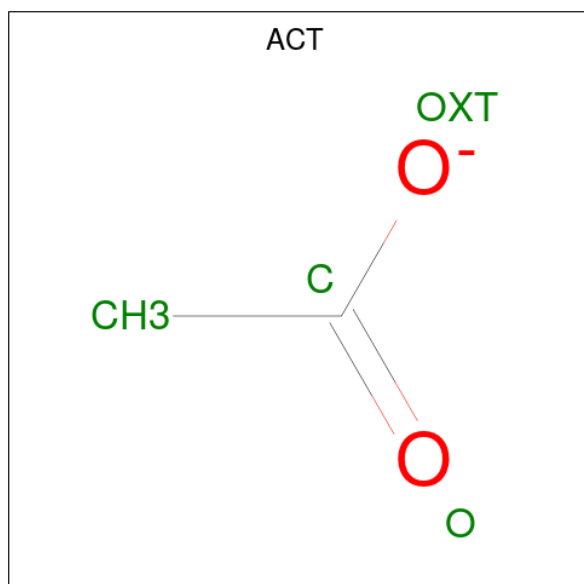
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLY	-	expression tag	UNP P68400
A	-21	SER	-	expression tag	UNP P68400
A	-20	MET	-	expression tag	UNP P68400
A	-19	ASP	-	expression tag	UNP P68400
A	-18	ILE	-	expression tag	UNP P68400
A	-17	GLU	-	expression tag	UNP P68400
A	-16	PHE	-	expression tag	UNP P68400
A	-15	ASP	-	expression tag	UNP P68400
A	-14	ASP	-	expression tag	UNP P68400
A	-13	ASP	-	expression tag	UNP P68400
A	-12	ALA	-	expression tag	UNP P68400
A	-11	ASP	-	expression tag	UNP P68400
A	-10	ASP	-	expression tag	UNP P68400
A	-9	ASP	-	expression tag	UNP P68400
A	-8	GLY	-	expression tag	UNP P68400
A	-7	SER	-	expression tag	UNP P68400
A	-6	GLY	-	expression tag	UNP P68400
A	-5	SER	-	expression tag	UNP P68400
A	-4	GLY	-	expression tag	UNP P68400
A	-3	SER	-	expression tag	UNP P68400
A	-2	GLY	-	expression tag	UNP P68400
A	-1	SER	-	expression tag	UNP P68400
A	0	GLY	-	expression tag	UNP P68400
A	1	SER	-	expression tag	UNP P68400
A	21	SER	ARG	engineered mutation	UNP P68400

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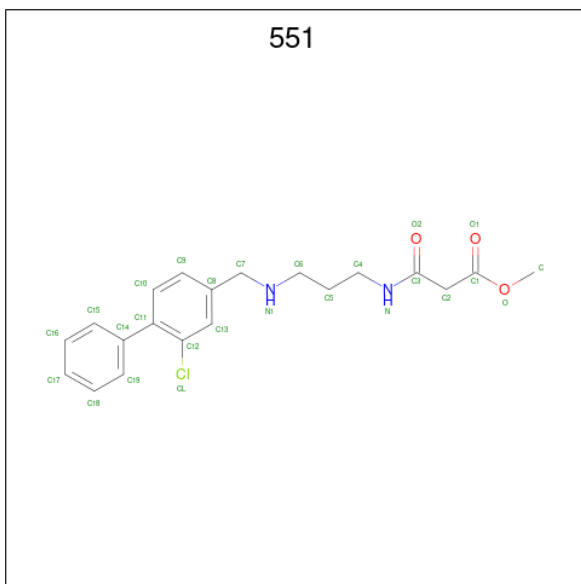
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLY	-	expression tag	UNP P68400
B	-21	SER	-	expression tag	UNP P68400
B	-20	MET	-	expression tag	UNP P68400
B	-19	ASP	-	expression tag	UNP P68400
B	-18	ILE	-	expression tag	UNP P68400
B	-17	GLU	-	expression tag	UNP P68400
B	-16	PHE	-	expression tag	UNP P68400
B	-15	ASP	-	expression tag	UNP P68400
B	-14	ASP	-	expression tag	UNP P68400
B	-13	ASP	-	expression tag	UNP P68400
B	-12	ALA	-	expression tag	UNP P68400
B	-11	ASP	-	expression tag	UNP P68400
B	-10	ASP	-	expression tag	UNP P68400
B	-9	ASP	-	expression tag	UNP P68400
B	-8	GLY	-	expression tag	UNP P68400
B	-7	SER	-	expression tag	UNP P68400
B	-6	GLY	-	expression tag	UNP P68400
B	-5	SER	-	expression tag	UNP P68400
B	-4	GLY	-	expression tag	UNP P68400
B	-3	SER	-	expression tag	UNP P68400
B	-2	GLY	-	expression tag	UNP P68400
B	-1	SER	-	expression tag	UNP P68400
B	0	GLY	-	expression tag	UNP P68400
B	1	SER	-	expression tag	UNP P68400
B	21	SER	ARG	engineered mutation	UNP P68400

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



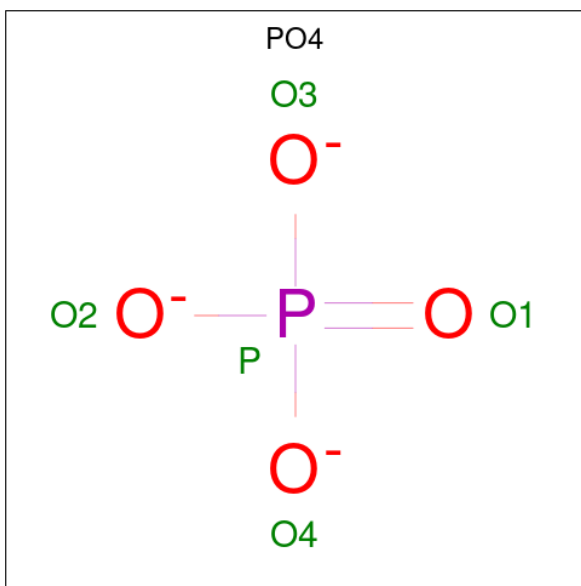
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

- Molecule 3 is methyl 3-[(3-[(2-chlorobiphenyl-4-yl)methyl]amino)propyl]amino]-3-oxopropionate (CCD ID: 551) (formula: C₂₀H₂₃ClN₂O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Cl N O 26 20 1 2 3	0	0
3	A	1	Total C Cl N 15 13 1 1	0	0
3	A	1	Total C Cl N 15 13 1 1	0	0
3	B	1	Total C Cl N O 26 20 1 2 3	0	0
3	B	1	Total C Cl N 15 13 1 1	0	0

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

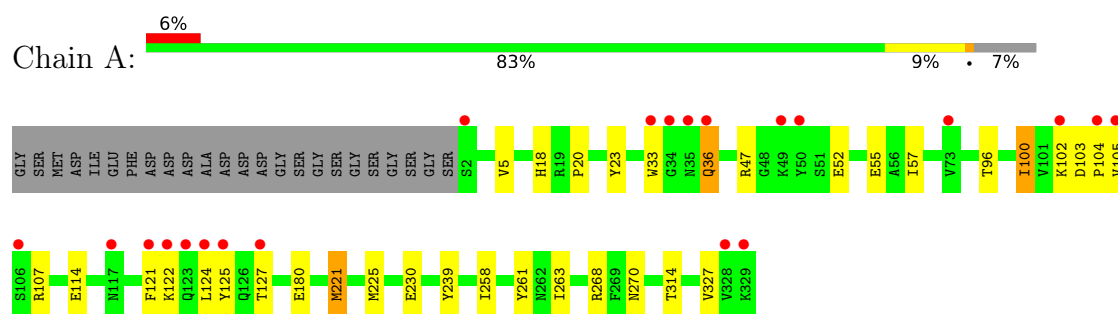
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	227	Total	O	0	0
			227	227		
5	B	86	Total	O	0	0
			86	86		

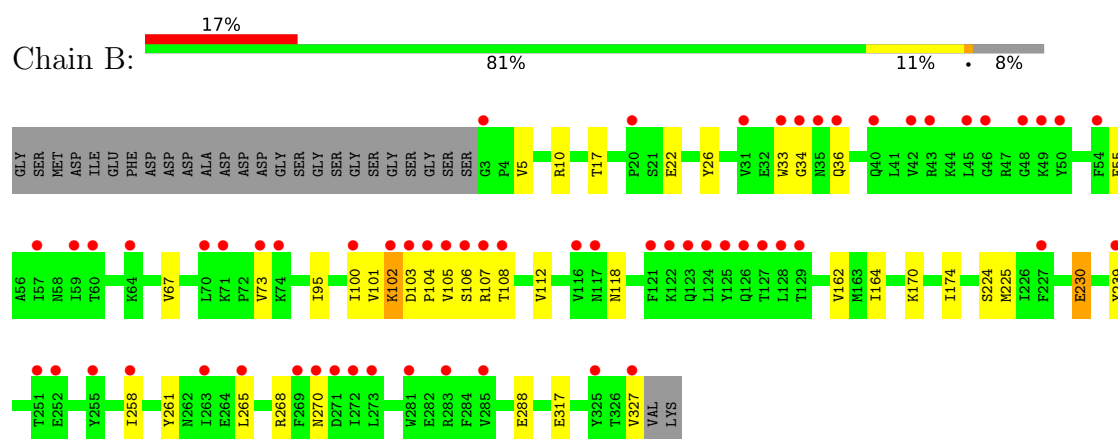
3 Residue-property plots [i](#)

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: Casein kinase II subunit alpha



- Molecule 1: Casein kinase II subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	64.68Å 68.13Å 334.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.46 – 1.73 46.46 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.46-1.73) 99.7 (46.46-1.73)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.73Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.189 , 0.198 0.191 , 0.205	Depositor DCC
R_{free} test set	3904 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.066 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6033	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ACT, 551

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	1.02	5/2896 (0.2%)	1.02	4/3916 (0.1%)
1	B	0.86	0/2848	1.09	6/3854 (0.2%)
All	All	0.94	5/5744 (0.1%)	1.06	10/7770 (0.1%)

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	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	MET	SD-CE	-7.63	1.60	1.79
1	A	100	ILE	C-O	-5.95	1.18	1.24
1	A	180	GLU	C-O	-5.88	1.16	1.23
1	A	270	ASN	C-O	-5.49	1.17	1.24
1	A	230	GLU	C-O	-5.47	1.18	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	VAL	N-CA-C	6.17	117.19	111.45
1	B	270	ASN	N-CA-C	5.97	118.28	111.11
1	B	26	TYR	N-CA-C	5.88	118.47	111.71
1	B	108	THR	CA-C-N	-5.86	113.93	120.14
1	B	108	THR	C-N-CA	-5.86	113.93	120.14
1	A	270	ASN	N-CA-C	5.68	117.93	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	GLU	N-CA-C	-5.52	100.68	109.96
1	B	55	GLU	N-CA-C	-5.45	100.81	109.96
1	A	314	THR	N-CA-C	-5.19	103.83	110.53
1	B	34	GLY	N-CA-C	-5.04	102.90	112.27

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	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	2821	0	2755	34	0
1	B	2773	0	2701	61	0
2	A	16	0	12	0	0
2	B	8	0	6	0	0
3	A	56	0	0	6	0
3	B	41	0	0	6	0
4	A	5	0	0	0	0
5	A	227	0	0	0	0
5	B	86	0	0	1	0
All	All	6033	0	5474	93	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 8.

All (93) 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:36:GLN:HE21	1:B:103[B]:ASP:CA	1.42	1.31
1:B:36:GLN:NE2	1:B:103[A]:ASP:OD1	1.65	1.30
1:B:36:GLN:NE2	1:B:103[A]:ASP:HA	1.50	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:GLN:NE2	1:B:103[B]:ASP:CB	2.01	1.23
1:B:258:ILE:HD13	1:B:265:LEU:CD1	1.73	1.18
1:B:36:GLN:NE2	1:B:103[B]:ASP:HA	1.62	1.15
1:B:36:GLN:NE2	1:B:103[B]:ASP:HB2	1.61	1.12
1:A:221:MET:HE1	3:A:405:551:CL	1.90	1.08
1:B:258:ILE:HD13	1:B:265:LEU:HD13	1.36	1.05
1:B:36:GLN:HE22	1:B:103[B]:ASP:HB2	1.13	1.03
1:A:221:MET:CE	3:A:405:551:CL	2.44	1.03
1:A:36:GLN:HG2	1:A:104:PRO:HD3	1.38	1.02
1:B:36:GLN:HE21	1:B:103[B]:ASP:HA	0.88	1.01
1:B:224:SER:HB2	1:B:230:GLU:HG2	1.47	0.96
1:A:36:GLN:HE21	1:A:103:ASP:HA	1.32	0.95
1:B:36:GLN:CG	1:B:104:PRO:HD3	1.96	0.95
1:A:33:TRP:CE3	1:A:100:ILE:HG22	2.05	0.91
1:B:258:ILE:HD13	1:B:265:LEU:HD11	1.50	0.89
1:B:36:GLN:HE21	1:B:103[A]:ASP:HA	0.81	0.89
1:B:162:VAL:HG11	3:B:403:551:CL	2.11	0.87
1:B:36:GLN:NE2	1:B:103[B]:ASP:CA	2.17	0.86
1:A:36:GLN:CG	1:A:104:PRO:HD3	2.05	0.85
1:A:36:GLN:NE2	1:A:103:ASP:HA	1.92	0.85
1:B:258:ILE:CD1	1:B:265:LEU:HD13	2.09	0.83
1:B:36:GLN:HG2	1:B:104:PRO:HD3	1.59	0.82
1:A:36:GLN:NE2	3:A:406:551:C10	2.39	0.81
1:B:10:ARG:NH2	1:B:317:GLU:OE2	2.14	0.81
1:B:17:THR:HG22	5:B:536:HOH:O	1.81	0.80
1:B:36:GLN:HE22	1:B:103[A]:ASP:CG	1.86	0.79
1:B:162:VAL:CG1	3:B:403:551:CL	2.72	0.75
1:A:225:MET:HG3	3:A:405:551:C16	2.18	0.73
1:B:258:ILE:CD1	1:B:265:LEU:CD1	2.61	0.72
1:A:121:PHE:HD2	1:A:125:TYR:CE2	2.08	0.71
1:B:36:GLN:NE2	1:B:104:PRO:CD	2.55	0.70
1:A:36:GLN:HE21	1:A:104:PRO:CD	2.05	0.70
1:A:36:GLN:NE2	1:A:104:PRO:CD	2.56	0.68
1:B:258:ILE:HG21	1:B:265:LEU:HD11	1.74	0.68
1:B:103[A]:ASP:HB3	1:B:106[A]:SER:HB3	1.77	0.66
1:B:36:GLN:HE22	1:B:103[B]:ASP:CB	1.85	0.63
1:B:10:ARG:HH22	1:B:317:GLU:CD	2.08	0.62
1:A:102:LYS:HD3	1:A:107:ARG:O	2.00	0.61
1:A:36:GLN:NE2	1:A:104:PRO:HD2	2.17	0.59
1:B:225:MET:HG3	3:B:403:551:C16	2.32	0.59
1:A:33:TRP:CZ3	1:A:100:ILE:CG2	2.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TRP:CE3	1:A:100:ILE:CG2	2.84	0.58
1:B:36:GLN:CD	1:B:104:PRO:HD3	2.29	0.58
1:A:36:GLN:HE21	1:A:103:ASP:CA	2.11	0.57
1:B:103[A]:ASP:O	1:B:107:ARG:N	2.36	0.57
1:A:221:MET:HE3	3:A:405:551:CL	2.38	0.57
1:B:103[A]:ASP:OD2	1:B:106[A]:SER:HB2	2.05	0.56
1:A:121:PHE:N	1:A:121:PHE:CD1	2.73	0.56
1:A:33:TRP:CZ3	1:A:100:ILE:HG22	2.42	0.55
1:A:47:ARG:HG2	1:A:52:GLU:HG3	1.90	0.54
1:B:36:GLN:NE2	1:B:103[B]:ASP:HB3	2.12	0.53
1:A:23:TYR:HB2	1:B:105:VAL:HG22	1.91	0.53
1:B:36:GLN:NE2	1:B:104:PRO:HD2	2.24	0.52
1:B:36:GLN:NE2	1:B:103[A]:ASP:CA	2.32	0.52
1:B:36:GLN:HE21	1:B:104:PRO:CD	2.22	0.51
1:B:103[A]:ASP:CB	1:B:106[A]:SER:HB3	2.40	0.51
1:B:102:LYS:HD3	1:B:107:ARG:O	2.09	0.51
1:A:20:PRO:HD2	1:B:105:VAL:HG21	1.93	0.50
1:B:36:GLN:HE21	1:B:103[B]:ASP:C	2.15	0.50
1:B:36:GLN:HG2	1:B:103[B]:ASP:HA	1.94	0.49
1:B:118:ASN:HD22	1:B:164:ILE:H	1.61	0.49
1:B:36:GLN:CD	1:B:104:PRO:CD	2.86	0.48
1:A:36:GLN:HE22	3:A:406:551:C10	2.21	0.48
1:B:36:GLN:NE2	1:B:103[A]:ASP:CG	2.46	0.48
1:A:36:GLN:NE2	1:A:104:PRO:HD3	2.29	0.47
1:B:239:TYR:CZ	1:B:268:ARG:HD3	2.49	0.47
1:A:239:TYR:CZ	1:A:268:ARG:HD3	2.50	0.47
1:B:36:GLN:NE2	1:B:104:PRO:HD3	2.30	0.47
1:B:162:VAL:CB	3:B:403:551:CL	3.02	0.45
1:B:36:GLN:CD	1:B:103[B]:ASP:HA	2.37	0.45
1:B:33:TRP:NE1	1:B:100:ILE:HG22	2.32	0.45
1:B:162:VAL:HB	3:B:403:551:CL	2.54	0.45
1:B:67:VAL:HG22	1:B:112:VAL:HG22	1.99	0.44
1:A:121:PHE:O	1:A:122:LYS:C	2.61	0.44
1:A:121:PHE:O	1:A:124:LEU:N	2.46	0.43
1:B:36:GLN:NE2	3:B:404:551:C10	2.79	0.43
1:B:102:LYS:HG2	1:B:107:ARG:O	2.19	0.43
1:B:36:GLN:HG3	1:B:104:PRO:HD3	1.94	0.42
1:B:103[B]:ASP:O	1:B:107:ARG:N	2.47	0.42
1:B:5:VAL:HB	1:B:261:TYR:HA	2.01	0.42
1:B:103[A]:ASP:HB3	1:B:106[A]:SER:CB	2.48	0.41
1:B:106[A]:SER:O	1:B:107:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLN:CD	1:A:104:PRO:HD3	2.45	0.41
1:A:121:PHE:HD2	1:A:125:TYR:CZ	2.38	0.41
1:B:33:TRP:HD1	1:B:101:VAL:C	2.28	0.41
1:A:96:THR:H	1:A:114[A]:GLU:HG2	1.86	0.41
1:A:5:VAL:HB	1:A:261:TYR:HA	2.03	0.41
1:A:258:ILE:HG23	1:A:263:ILE:O	2.21	0.40
1:A:124:LEU:HD23	1:A:127:THR:OG1	2.22	0.40
1:B:95:ILE:HB	1:B:174:ILE:HG22	2.03	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	333/352 (95%)	326 (98%)	7 (2%)	0	100	100
1	B	327/352 (93%)	320 (98%)	7 (2%)	0	100	100
All	All	660/704 (94%)	646 (98%)	14 (2%)	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	309/319 (97%)	306 (99%)	3 (1%)	68	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	303/319 (95%)	296 (98%)	7 (2%)	44	20
All	All	612/638 (96%)	602 (98%)	10 (2%)	53	35

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	57	ILE
1	A	327	VAL
1	B	22	GLU
1	B	73	VAL
1	B	102	LYS
1	B	170	LYS
1	B	230	GLU
1	B	288	GLU
1	B	327	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	160	HIS
1	A	207	GLN
1	A	286	HIS
1	B	29	HIS
1	B	118	ASN
1	B	126	GLN
1	B	207	GLN
1	B	234	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

12 ligands are modelled in this entry.

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	$\# Z > 2$
3	551	A	405	-	27,27,27	0.17	0	33,34,34	0.18	0
2	ACT	A	403	-	3,3,3	0.94	0	3,3,3	0.84	0
2	ACT	B	402	-	3,3,3	1.59	1 (33%)	3,3,3	0.78	0
2	ACT	A	401	-	3,3,3	1.40	0	3,3,3	0.94	0
2	ACT	A	402	-	3,3,3	1.03	0	3,3,3	1.18	0
4	PO4	A	408	-	4,4,4	2.58	2 (50%)	6,6,6	0.85	0
2	ACT	A	404	-	3,3,3	1.38	0	3,3,3	0.90	0
2	ACT	B	401	-	3,3,3	1.03	0	3,3,3	1.08	0
3	551	A	406	-	16,16,27	0.12	0	21,21,34	0.24	0
3	551	B	403	-	27,27,27	0.18	0	33,34,34	0.18	0
3	551	B	404	-	16,16,27	0.09	0	21,21,34	0.19	0
3	551	A	407	-	16,16,27	0.09	0	21,21,34	0.21	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	551	A	405	-	-	4/19/19/19	0/2/2/2
3	551	A	406	-	-	0/6/6/19	0/2/2/2
3	551	B	403	-	-	7/19/19/19	0/2/2/2
3	551	B	404	-	-	0/6/6/19	0/2/2/2
3	551	A	407	-	-	1/6/6/19	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	408	PO4	P-O1	4.23	1.60	1.50
2	B	402	ACT	CH3-C	2.33	1.58	1.49
4	A	408	PO4	P-O3	2.18	1.61	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	405	551	C2-C1-O-C
3	B	403	551	C12-C11-C14-C15
3	B	403	551	C12-C11-C14-C19
3	A	405	551	O1-C1-O-C
3	A	405	551	N-C4-C5-C6
3	B	403	551	C2-C1-O-C
3	B	403	551	O1-C1-C2-C3
3	B	403	551	O1-C1-O-C
3	B	403	551	C10-C11-C14-C19
3	B	403	551	C10-C11-C14-C15
3	A	405	551	O1-C1-C2-C3
3	A	407	551	N1-C7-C8-C13

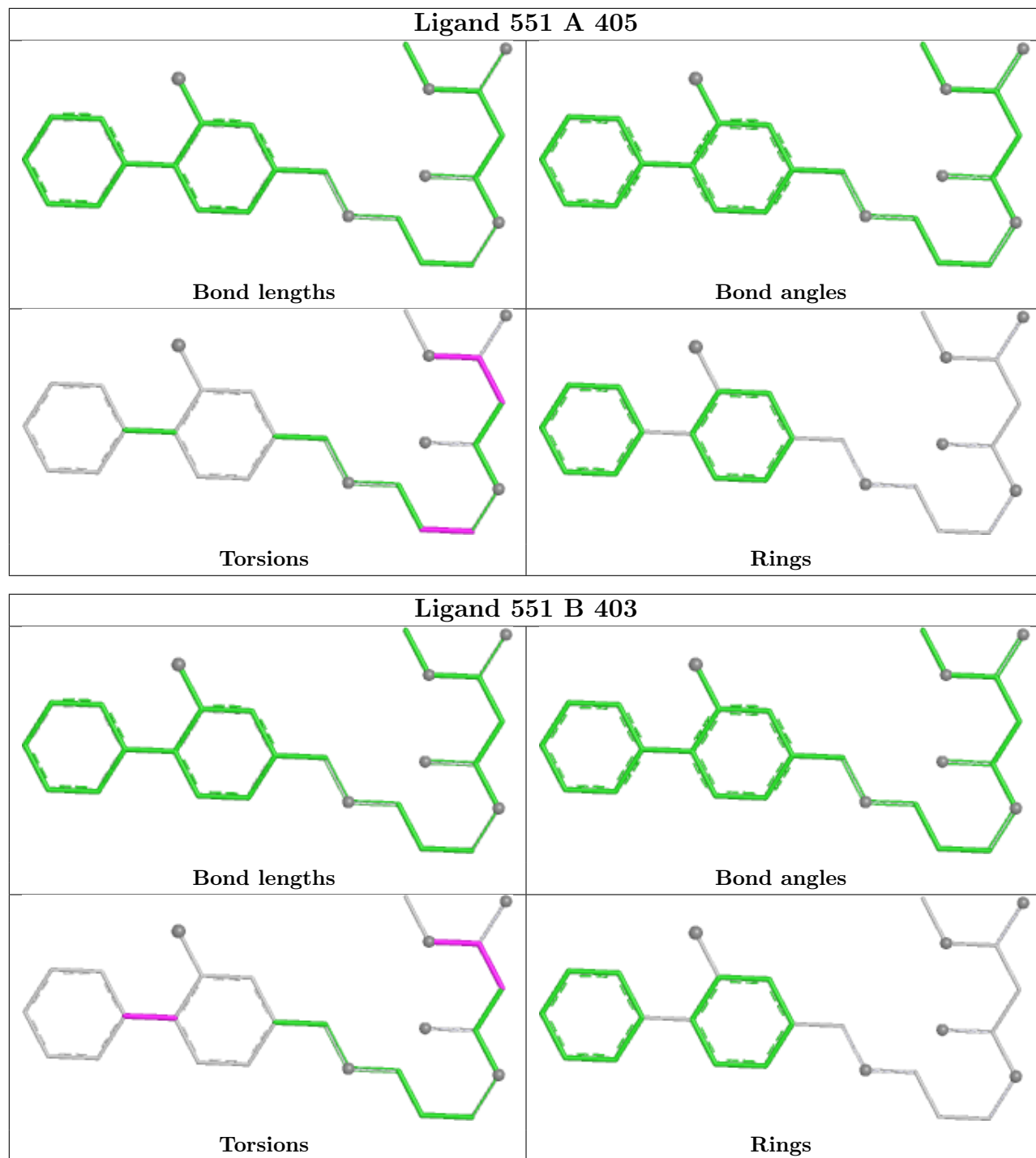
There are no ring outliers.

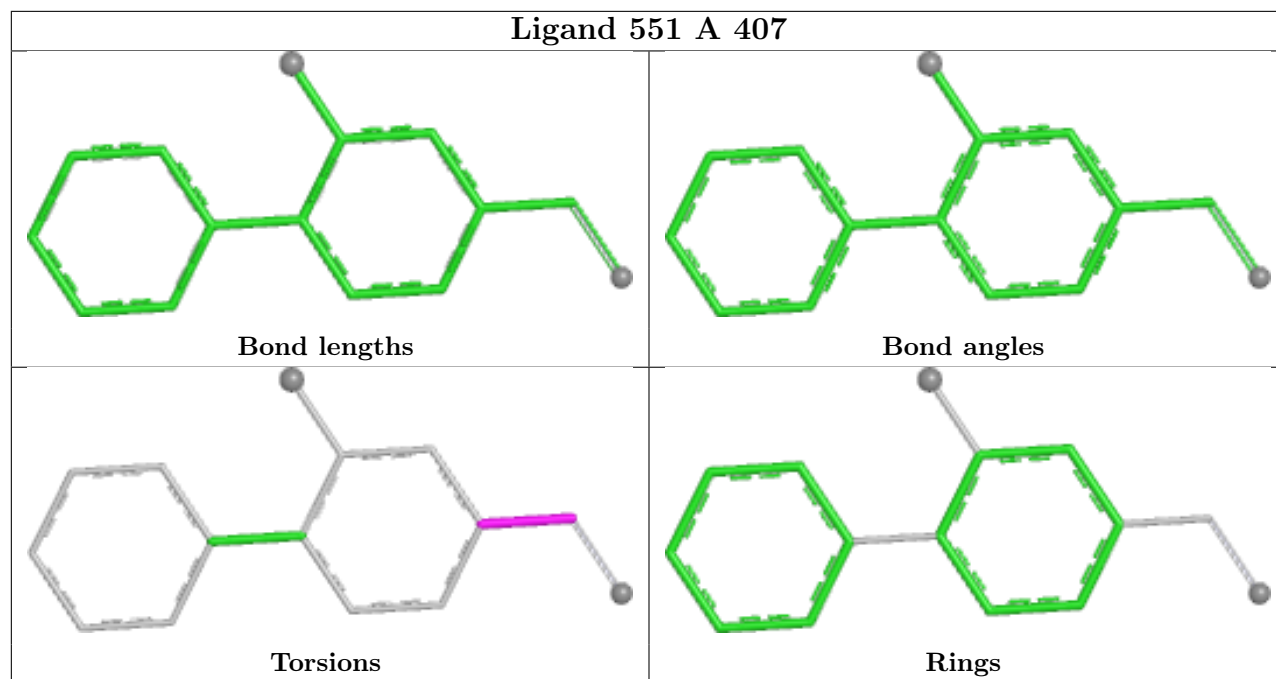
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	405	551	4	0
3	A	406	551	2	0
3	B	403	551	5	0
3	B	404	551	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	328/352 (93%)	0.12	21 (6%) 25 31	9, 26, 58, 101	7 (2%)
1	B	325/352 (92%)	1.09	61 (18%) 3 4	25, 54, 90, 109	4 (1%)
All	All	653/704 (92%)	0.60	82 (12%) 8 10	9, 39, 83, 109	11 (1%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	105	VAL	6.2
1	A	125	TYR	6.0
1	B	104	PRO	5.2
1	A	121	PHE	5.2
1	A	124	LEU	5.2
1	B	33	TRP	5.1
1	B	327	VAL	5.1
1	B	121	PHE	4.9
1	A	33	TRP	4.5
1	A	104	PRO	4.3
1	B	124	LEU	4.2
1	B	50	TYR	4.1
1	B	125	TYR	4.1
1	A	105	VAL	4.1
1	B	36	GLN	3.9
1	B	265	LEU	3.9
1	B	57	ILE	3.6
1	B	107	ARG	3.5
1	A	35	ASN	3.4
1	B	103[A]	ASP	3.4
1	A	329	LYS	3.4
1	B	127	THR	3.4
1	A	50	TYR	3.3
1	B	122	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	122	LYS	3.2
1	A	123	GLN	3.1
1	A	49	LYS	3.1
1	A	328	VAL	3.0
1	A	36	GLN	3.0
1	A	34	GLY	3.0
1	B	269	PHE	3.0
1	B	128	LEU	2.9
1	B	123	GLN	2.9
1	B	106[A]	SER	2.9
1	B	258	ILE	2.9
1	B	116	VAL	2.8
1	A	106	SER	2.8
1	A	117	ASN	2.8
1	B	73	VAL	2.8
1	B	31	VAL	2.7
1	B	74	LYS	2.7
1	B	255	TYR	2.7
1	B	272	ILE	2.6
1	B	102	LYS	2.6
1	B	3	GLY	2.5
1	B	35	ASN	2.5
1	B	59	ILE	2.5
1	B	46	GLY	2.5
1	B	64	LYS	2.5
1	B	270	ASN	2.5
1	A	73	VAL	2.5
1	B	281	TRP	2.4
1	B	126	GLN	2.4
1	B	129	THR	2.4
1	B	45	LEU	2.4
1	B	54	PHE	2.4
1	B	283	ARG	2.4
1	B	71	LYS	2.3
1	B	100	ILE	2.3
1	B	285	VAL	2.3
1	A	2	SER	2.3
1	B	271	ASP	2.3
1	B	49	LYS	2.3
1	A	127	THR	2.3
1	B	252	GLU	2.2
1	B	43	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	108	THR	2.2
1	B	273	LEU	2.1
1	B	60	THR	2.1
1	B	227	PHE	2.1
1	B	40[A]	GLN	2.1
1	B	117	ASN	2.1
1	B	239	TYR	2.1
1	B	325	TYR	2.1
1	B	34	GLY	2.1
1	B	48	GLY	2.1
1	B	42	VAL	2.1
1	B	251	THR	2.1
1	A	102	LYS	2.1
1	B	70	LEU	2.0
1	B	20	PRO	2.0
1	B	263	ILE	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
2	ACT	A	404	4/4	0.56	0.22	53,55,55,55	0
3	551	A	405	26/26	0.67	0.24	55,57,73,74	0
3	551	A	406	15/26	0.67	0.18	47,56,64,65	0
3	551	B	404	15/26	0.68	0.26	32,32,33,33	15
3	551	B	403	26/26	0.73	0.19	56,75,80,87	0
2	ACT	B	402	4/4	0.85	0.16	35,38,42,44	0
2	ACT	B	401	4/4	0.88	0.12	47,49,49,49	0

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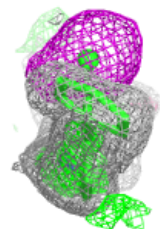
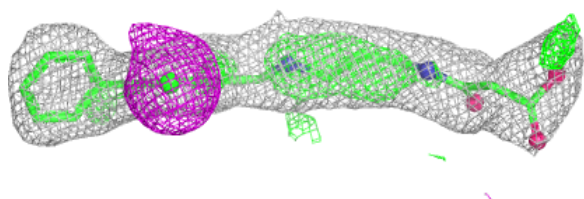
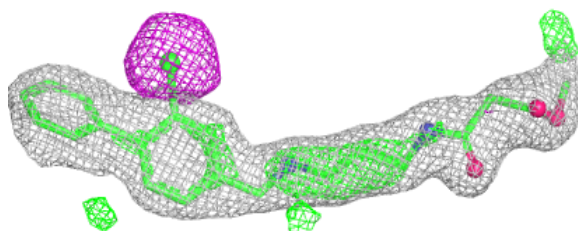
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	551	A	407	15/26	0.88	0.14	63,64,66,69	0
2	ACT	A	403	4/4	0.89	0.15	42,42,43,46	0
4	PO4	A	408	5/5	0.89	0.10	43,44,50,54	0
2	ACT	A	401	4/4	0.93	0.10	26,27,30,30	0
2	ACT	A	402	4/4	0.97	0.07	30,33,34,35	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.

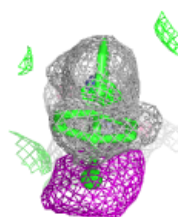
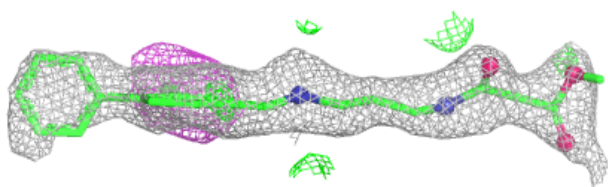
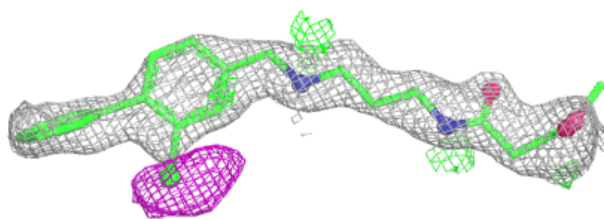
Electron density around 551 A 405:

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

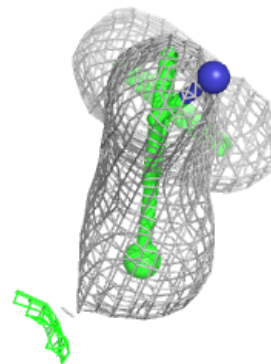
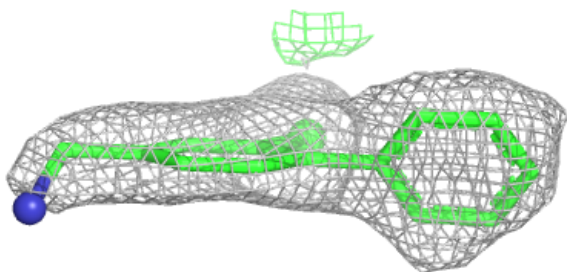
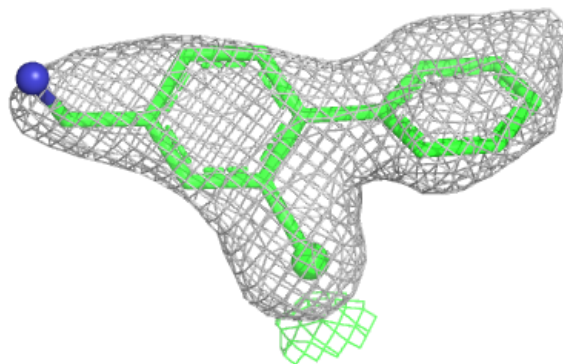


Electron density around 551 B 403:

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

**Electron density around 551 A 407:**

$2mF_o-DF_c$ (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.