



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:39 AM UTC

PDB ID : 9EQ1 / pdb_00009eq1
Title : Crystal structure of human Casein Kinase II subunit alpha (CK2a1) in complex with allosteric ligand FGJM24
Authors : Kraemer, A.; Greco, F.; Moeckel, J.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on : 2024-03-20
Resolution : 3.00 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

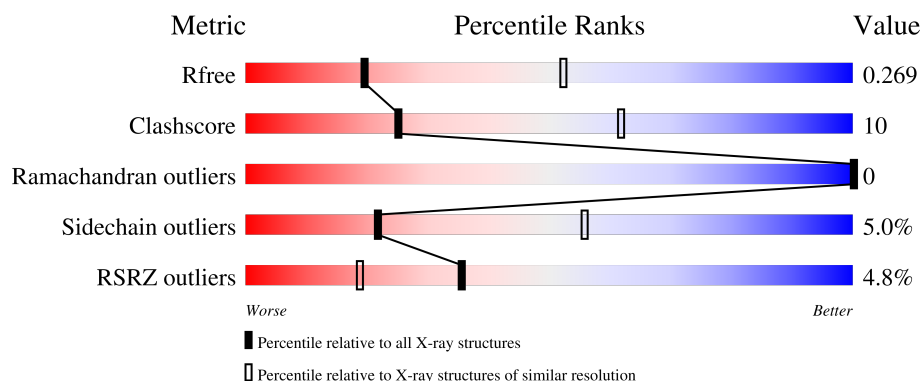
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	338	4% 76% 22% ..
1	B	338	5% 74% 22% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5648 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	331	Total	C	N	O	S	0	0	0
			2721	1748	468	494	11			
1	B	329	Total	C	N	O	S	0	0	0
			2738	1755	477	495	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P68400
B	0	SER	-	expression tag	UNP P68400

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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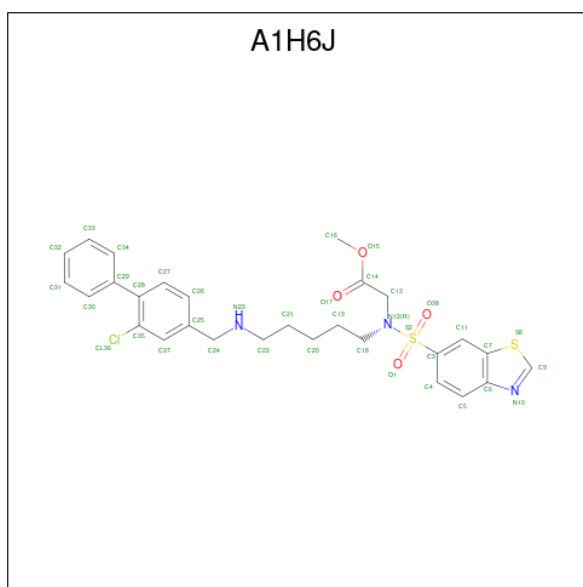
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is methyl 2-[1,3-benzothiazol-6-ylsulfonyl]-[5-[(3-chloranyl-4-phenyl-phenyl)methylamino]pentyl]amino]ethanoate (CCD ID: A1H6J) (formula: $C_{28}H_{30}ClN_3O_4S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0	0
			38	28	1	3	4	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	O	S	0	0
			38	28	1	3	4	2		

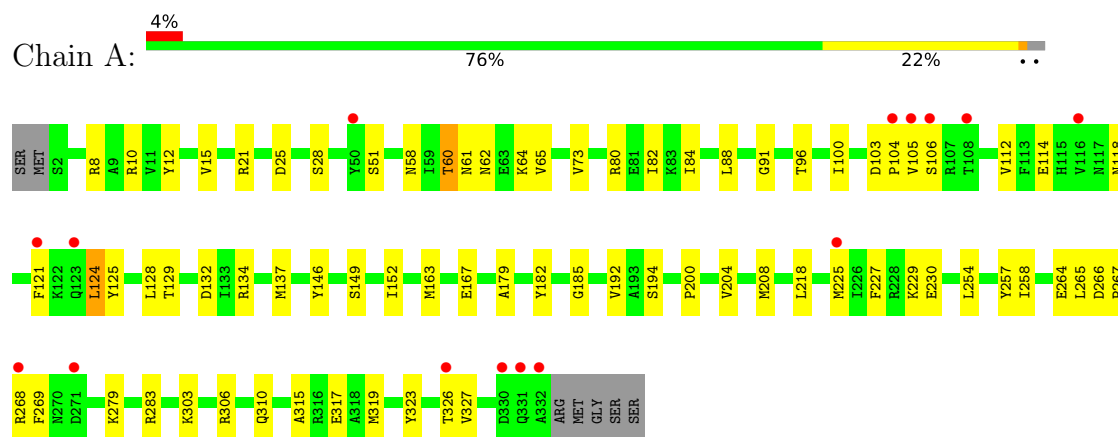
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	4	Total	O	0	0
			4	4		

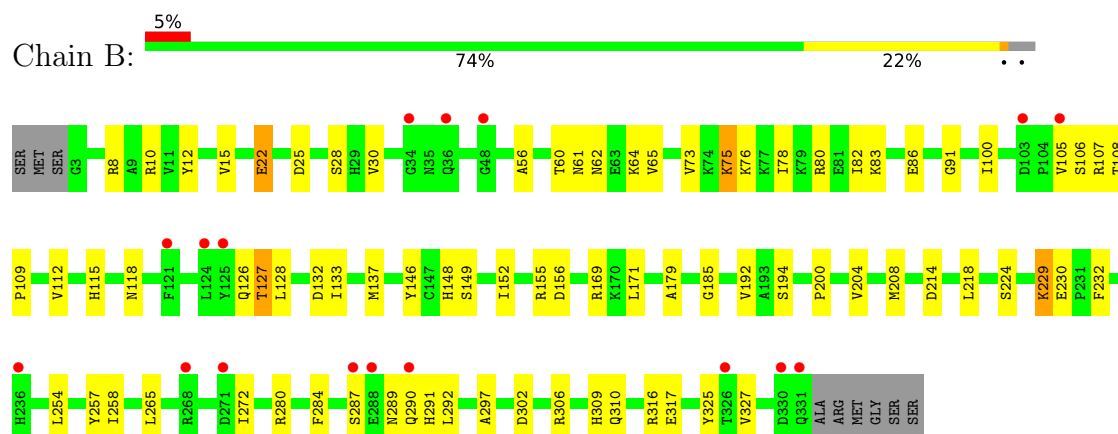
3 Residue-property plots [i](#)

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	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.74Å 126.74Å 125.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.62 – 3.00 89.62 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (89.62-3.00) 100.0 (89.62-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.210 , 0.251 0.227 , 0.269	Depositor DCC
R_{free} test set	976 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5648	wwPDB-VP
Average B, all atoms (Å ²)	65.0	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 32.27 % 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 9.6604e-04. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, A1H6J, SO4

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	0.62	0/2796	1.08	5/3796 (0.1%)
1	B	0.62	0/2811	1.10	7/3809 (0.2%)
All	All	0.62	0/5607	1.09	12/7605 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	ALA	N-CA-C	9.15	122.41	111.33
1	A	182	TYR	N-CA-CB	6.10	119.41	109.95
1	B	325	TYR	N-CA-CB	6.02	118.97	110.12
1	A	60	THR	CA-CB-OG1	-5.86	100.81	109.60
1	A	96	THR	CA-CB-OG1	-5.79	100.91	109.60
1	A	192	VAL	N-CA-C	-5.73	100.34	108.65
1	B	86	GLU	CB-CG-CD	5.71	122.30	112.60
1	B	156	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	60	THR	CA-CB-OG1	-5.65	101.13	109.60
1	A	227	PHE	N-CA-C	-5.41	106.72	113.38
1	B	284	PHE	N-CA-C	-5.09	106.48	113.30
1	B	287	SER	N-CA-C	-5.02	107.71	113.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2721	0	2591	63	0
1	B	2738	0	2645	44	0
2	A	35	0	0	4	0
2	B	60	0	0	1	0
3	A	4	0	6	0	0
3	B	4	0	6	1	0
4	A	38	0	0	4	0
4	B	38	0	0	2	0
5	A	6	0	0	0	0
5	B	4	0	0	0	0
All	All	5648	0	5248	105	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 10.

All (105) 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:303:LYS:HA	1:A:306:ARG:HE	1.09	1.15
1:A:225:MET:HG3	4:A:409:A1H6J:C33	2.04	0.87
1:A:265:LEU:HD11	1:A:269:PHE:CD2	2.12	0.85
1:B:56:ALA:O	1:B:65:VAL:HG12	1.75	0.85
1:A:303:LYS:HA	1:A:306:ARG:NE	1.92	0.83
1:B:148:HIS:CD2	3:B:413:EDO:H12	2.18	0.78
1:A:80:ARG:NH2	2:A:407:SO4:O3	2.22	0.73
1:A:64:LYS:C	1:A:65:VAL:HG23	2.14	0.71
1:A:306:ARG:HH12	1:B:280:ARG:CD	2.07	0.67
1:A:80:ARG:HD3	1:A:179:ALA:O	1.95	0.66
1:A:8:ARG:NH2	1:A:208:MET:CE	2.59	0.66
1:B:78:ILE:HD13	1:B:109:PRO:HG2	1.79	0.65
1:B:80:ARG:HD3	1:B:179:ALA:O	1.97	0.64
1:B:56:ALA:O	1:B:65:VAL:CG1	2.46	0.63
1:A:64:LYS:O	1:A:65:VAL:HG23	2.02	0.59
1:A:265:LEU:CD1	1:A:269:PHE:CD2	2.84	0.58
1:A:64:LYS:O	1:A:65:VAL:CG2	2.51	0.58
1:A:105:VAL:HG23	1:A:106:SER:N	2.19	0.58
1:A:128:LEU:CD1	1:A:225:MET:HE1	2.35	0.57
1:A:265:LEU:HD11	1:A:269:PHE:CG	2.40	0.57
1:A:303:LYS:CA	1:A:306:ARG:HE	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:MET:HE1	4:A:409:A1H6J:CL36	2.43	0.56
1:B:185:GLY:HA2	1:B:208:MET:HE3	1.88	0.56
1:A:185:GLY:HA2	1:A:208:MET:HE3	1.88	0.56
1:A:84:ILE:HG23	1:A:152:ILE:HD13	1.88	0.55
1:B:25:ASP:O	1:B:28:SER:HB2	2.07	0.55
1:A:128:LEU:O	1:A:132:ASP:HB2	2.06	0.54
1:A:8:ARG:HH22	1:A:208:MET:CE	2.19	0.54
1:A:64:LYS:C	1:A:65:VAL:CG2	2.79	0.54
1:B:10:ARG:NH1	1:B:317:GLU:OE2	2.41	0.54
1:A:25:ASP:O	1:A:28:SER:HB2	2.08	0.54
1:A:105:VAL:HG23	1:A:106:SER:H	1.73	0.52
1:A:121:PHE:CZ	1:A:125:TYR:CD2	2.98	0.52
1:A:118:ASN:HB2	1:A:163:MET:CE	2.38	0.52
1:A:229:LYS:HE3	2:A:404:SO4:O2	2.11	0.51
1:B:148:HIS:HE1	1:B:214:ASP:OD2	1.93	0.50
1:B:232:PHE:O	2:B:409:SO4:O2	2.28	0.50
1:A:61:ASN:O	1:A:62:ASN:HB2	2.11	0.50
1:A:128:LEU:O	1:A:129:THR:OG1	2.26	0.50
1:A:91:GLY:HA3	1:A:146:TYR:CE2	2.47	0.50
1:A:265:LEU:HD21	1:A:269:PHE:HB3	1.93	0.50
1:A:279:LYS:NZ	2:A:406:SO4:O3	2.44	0.50
1:B:118:ASN:ND2	4:B:414:A1H6J:C21	2.75	0.50
1:A:266:ASP:O	1:A:267:PRO:C	2.53	0.49
1:B:200:PRO:O	1:B:204:VAL:HG22	2.12	0.49
1:A:10:ARG:NH1	1:A:317:GLU:OE2	2.45	0.49
1:B:155:ARG:NH1	1:B:192:VAL:HG11	2.27	0.49
1:A:65:VAL:CG1	1:A:112:VAL:CG1	2.90	0.49
1:B:316:ARG:HG2	1:B:316:ARG:HH21	1.77	0.49
1:B:8:ARG:NH2	1:B:208:MET:CE	2.76	0.49
1:B:65:VAL:CG2	1:B:112:VAL:CG1	2.91	0.49
1:A:200:PRO:O	1:A:204:VAL:HG22	2.13	0.49
1:B:61:ASN:O	1:B:62:ASN:HB2	2.12	0.49
1:B:137:MET:HE1	1:B:218:LEU:HG	1.95	0.48
1:B:302:ASP:O	1:B:306:ARG:HD3	2.13	0.48
1:B:82:ILE:HD13	1:B:100:ILE:HD13	1.95	0.48
1:A:279:LYS:HB3	1:A:283:ARG:HD3	1.96	0.48
1:A:225:MET:CE	4:A:409:A1H6J:CL36	2.99	0.47
1:A:254:LEU:O	1:A:257:TYR:HB3	2.14	0.47
1:B:91:GLY:HA3	1:B:146:TYR:CE2	2.49	0.47
1:A:8:ARG:HH22	1:A:208:MET:HE1	1.80	0.47
1:A:283:ARG:NH1	2:A:401:SO4:O1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:SER:C	1:B:108:THR:N	2.72	0.46
1:A:8:ARG:NH2	1:A:208:MET:HE2	2.29	0.46
1:B:118:ASN:HD21	4:B:414:A1H6J:C21	2.27	0.46
1:A:315:ALA:O	1:A:319:MET:HG3	2.15	0.46
1:B:10:ARG:HD2	1:B:310:GLN:O	2.16	0.46
1:B:265:LEU:HD23	1:B:265:LEU:HA	1.75	0.46
1:A:124:LEU:O	1:A:128:LEU:HG	2.16	0.46
1:A:137:MET:HE1	1:A:218:LEU:HG	1.98	0.45
1:A:118:ASN:HB2	1:A:163:MET:HE3	1.98	0.45
1:B:128:LEU:O	1:B:132:ASP:HB2	2.16	0.45
1:A:82:ILE:HD13	1:A:100:ILE:HD13	1.98	0.45
1:B:289:ASN:O	1:B:290:GLN:C	2.59	0.45
1:B:254:LEU:O	1:B:257:TYR:HB3	2.17	0.45
1:B:128:LEU:HD23	1:B:128:LEU:HA	1.81	0.44
1:B:128:LEU:HD13	1:B:133:ILE:HG12	2.00	0.44
1:A:118:ASN:HB2	1:A:163:MET:HE2	2.00	0.44
1:A:124:LEU:HD12	1:A:124:LEU:HA	1.91	0.43
1:B:309:HIS:H	1:B:309:HIS:CD2	2.35	0.43
1:B:106:SER:O	1:B:107:ARG:C	2.61	0.43
1:A:58:ASN:OD1	1:A:60:THR:HB	2.19	0.43
1:A:306:ARG:HH12	1:B:280:ARG:NE	2.17	0.42
1:A:128:LEU:O	1:A:129:THR:CB	2.66	0.42
1:B:64:LYS:HG2	1:B:115:HIS:CD2	2.54	0.42
1:B:10:ARG:HH12	1:B:317:GLU:CD	2.28	0.42
1:B:224:SER:HB3	1:B:229:LYS:O	2.20	0.42
1:A:225:MET:CG	4:A:409:A1H6J:C33	2.89	0.42
1:B:127:THR:O	1:B:127:THR:CG2	2.67	0.42
1:A:124:LEU:HG	1:A:128:LEU:HD21	2.01	0.41
1:B:22:GLU:O	1:B:83:LYS:HE2	2.20	0.41
1:A:12:TYR:CD1	1:A:149:SER:HA	2.55	0.41
1:B:75:LYS:O	1:B:76:LYS:C	2.64	0.41
1:A:265:LEU:O	1:A:266:ASP:C	2.64	0.41
1:A:266:ASP:O	1:A:268:ARG:N	2.54	0.41
1:A:103:ASP:OD1	1:A:104:PRO:HD2	2.21	0.41
1:B:171:LEU:HD23	1:B:171:LEU:C	2.45	0.41
1:A:114:GLU:O	1:A:114:GLU:HG3	2.21	0.41
1:A:10:ARG:HD2	1:A:310:GLN:O	2.20	0.41
1:A:134:ARG:HG2	1:A:323:TYR:CZ	2.56	0.41
1:B:12:TYR:CD1	1:B:149:SER:HA	2.55	0.41
1:B:127:THR:O	1:B:127:THR:HG23	2.20	0.41
1:A:88:LEU:HD21	1:A:152:ILE:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:GLN:C	1:B:292:LEU:N	2.80	0.40
1:A:58:ASN:OD1	1:A:58:ASN:C	2.65	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	329/338 (97%)	312 (95%)	17 (5%)	0	100	100
1	B	327/338 (97%)	305 (93%)	22 (7%)	0	100	100
All	All	656/676 (97%)	617 (94%)	39 (6%)	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	287/310 (93%)	275 (96%)	12 (4%)	26	61
1	B	293/310 (94%)	276 (94%)	17 (6%)	18	51
All	All	580/620 (94%)	551 (95%)	29 (5%)	22	56

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	21	ARG
1	A	51	SER
1	A	73	VAL
1	A	124	LEU
1	A	167	GLU
1	A	194	SER
1	A	230	GLU
1	A	258	ILE
1	A	264	GLU
1	A	326	THR
1	A	327	VAL
1	B	15	VAL
1	B	22	GLU
1	B	30	VAL
1	B	73	VAL
1	B	75	LYS
1	B	105	VAL
1	B	126	GLN
1	B	127	THR
1	B	152	ILE
1	B	169	ARG
1	B	194	SER
1	B	229	LYS
1	B	230	GLU
1	B	258	ILE
1	B	272	ILE
1	B	291	HIS
1	B	327	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	29	HIS
1	A	115	HIS
1	A	126	GLN
1	A	234	HIS
1	A	238	ASN
1	A	291	HIS
1	B	18	HIS
1	B	35	ASN
1	B	115	HIS

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Mol	Chain	Res	Type
1	B	117	ASN
1	B	118	ASN
1	B	148	HIS
1	B	161	ASN
1	B	238	ASN
1	B	309	HIS
1	B	331	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

23 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	$\# Z > 2$
2	SO4	B	407	-	4,4,4	0.31	0	6,6,6	0.15	0
3	EDO	A	408	-	3,3,3	0.33	0	2,2,2	0.34	0
2	SO4	B	401	-	4,4,4	0.24	0	6,6,6	0.16	0
2	SO4	B	406	-	4,4,4	0.24	0	6,6,6	0.19	0
2	SO4	B	408	-	4,4,4	0.31	0	6,6,6	0.12	0
3	EDO	B	413	-	3,3,3	0.61	0	2,2,2	0.59	0
2	SO4	B	403	-	4,4,4	0.34	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A1H6J	B	414	-	41,41,41	0.47	0	52,56,56	0.87	1 (1%)
2	SO4	B	404	-	4,4,4	0.29	0	6,6,6	0.26	0
2	SO4	B	409	-	4,4,4	0.25	0	6,6,6	0.17	0
2	SO4	B	402	-	4,4,4	0.25	0	6,6,6	0.18	0
2	SO4	A	403	-	4,4,4	0.37	0	6,6,6	0.14	0
2	SO4	B	411	-	4,4,4	0.29	0	6,6,6	0.30	0
2	SO4	A	407	-	4,4,4	0.35	0	6,6,6	0.50	0
4	A1H6J	A	409	-	41,41,41	0.50	0	52,56,56	0.69	1 (1%)
2	SO4	A	401	-	4,4,4	0.32	0	6,6,6	0.15	0
2	SO4	A	406	-	4,4,4	0.49	0	6,6,6	0.38	0
2	SO4	B	410	-	4,4,4	0.28	0	6,6,6	0.08	0
2	SO4	B	412	-	4,4,4	0.42	0	6,6,6	0.06	0
2	SO4	A	404	-	4,4,4	0.33	0	6,6,6	0.06	0
2	SO4	B	405	-	4,4,4	0.29	0	6,6,6	0.16	0
2	SO4	A	402	-	4,4,4	0.38	0	6,6,6	0.17	0
2	SO4	A	405	-	4,4,4	0.30	0	6,6,6	0.14	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	EDO	A	408	-	-	0/1/1/1	-
3	EDO	B	413	-	-	0/1/1/1	-
4	A1H6J	A	409	-	-	14/32/32/32	0/4/4/4
4	A1H6J	B	414	-	-	16/32/32/32	0/4/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	414	A1H6J	C13-N12-C18	-3.80	107.52	116.84
4	A	409	A1H6J	C18-N12-S2	-2.55	112.65	117.88

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	409	A1H6J	C14-C13-N12-S2

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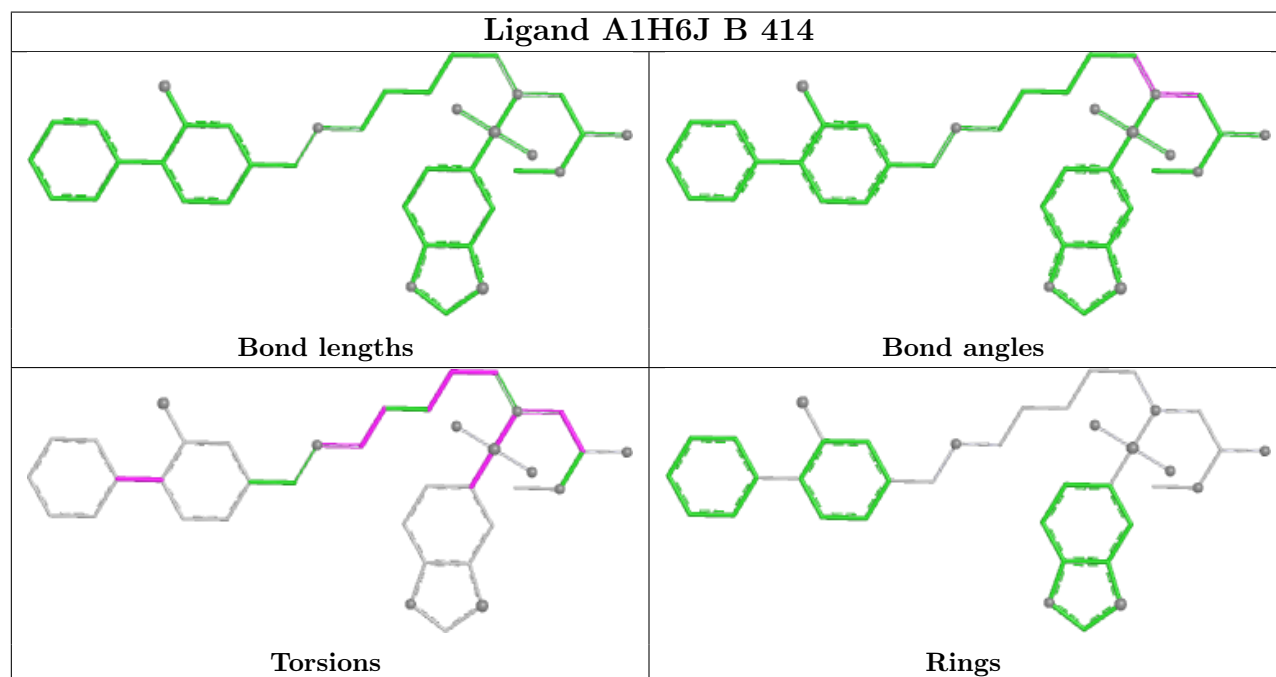
Mol	Chain	Res	Type	Atoms
4	A	409	A1H6J	C14-C13-N12-C18
4	A	409	A1H6J	C19-C18-N12-S2
4	A	409	A1H6J	C19-C18-N12-C13
4	A	409	A1H6J	N12-C13-C14-O15
4	B	414	A1H6J	C14-C13-N12-C18
4	A	409	A1H6J	C13-N12-S2-O1
4	A	409	A1H6J	C13-N12-S2-C3
4	B	414	A1H6J	C20-C21-C22-N23
4	A	409	A1H6J	C25-C24-N23-C22
4	B	414	A1H6J	C13-N12-S2-O1
4	A	409	A1H6J	C19-C20-C21-C22
4	B	414	A1H6J	C18-C19-C20-C21
4	B	414	A1H6J	C13-N12-S2-C3
4	A	409	A1H6J	C21-C22-N23-C24
4	A	409	A1H6J	N12-C13-C14-O17
4	B	414	A1H6J	C14-C13-N12-S2
4	A	409	A1H6J	N12-C18-C19-C20
4	B	414	A1H6J	N12-C18-C19-C20
4	B	414	A1H6J	C4-C3-S2-O38
4	B	414	A1H6J	C35-C28-C29-C30
4	B	414	A1H6J	N12-C13-C14-O17
4	A	409	A1H6J	C11-C3-S2-O38
4	B	414	A1H6J	C27-C28-C29-C30
4	B	414	A1H6J	C27-C28-C29-C34
4	B	414	A1H6J	N12-C13-C14-O15
4	B	414	A1H6J	C21-C22-N23-C24
4	B	414	A1H6J	C4-C3-S2-N12
4	B	414	A1H6J	C11-C3-S2-O38
4	A	409	A1H6J	C4-C3-S2-O38

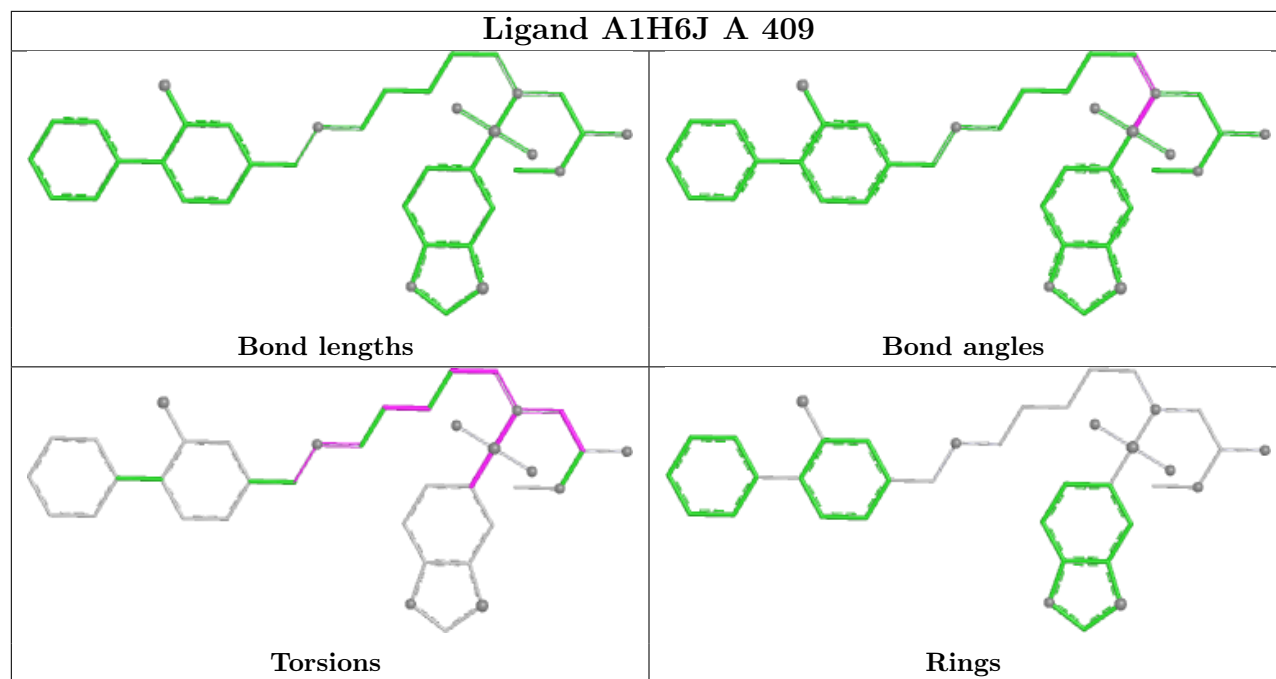
There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	413	EDO	1	0
4	B	414	A1H6J	2	0
2	B	409	SO4	1	0
2	A	407	SO4	1	0
4	A	409	A1H6J	4	0
2	A	401	SO4	1	0
2	A	406	SO4	1	0
2	A	404	SO4	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	331/338 (97%)	0.06	15 (4%)	38 20	30, 58, 102, 137	0
1	B	329/338 (97%)	0.12	17 (5%)	33 17	30, 60, 105, 136	0
All	All	660/676 (97%)	0.09	32 (4%)	35 19	30, 59, 104, 137	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	271	ASP	4.4
1	A	108	THR	4.0
1	A	105	VAL	3.8
1	A	121	PHE	3.8
1	A	271	ASP	3.8
1	A	330	ASP	3.7
1	B	48	GLY	3.6
1	B	236	HIS	3.2
1	B	36	GLN	3.2
1	B	121	PHE	3.2
1	A	123	GLN	3.1
1	B	124	LEU	2.9
1	A	331	GLN	2.8
1	A	225	MET	2.8
1	A	326	THR	2.8
1	A	268	ARG	2.7
1	B	34	GLY	2.7
1	A	332	ALA	2.5
1	B	326	THR	2.3
1	A	116	VAL	2.3
1	B	125	TYR	2.3
1	B	268	ARG	2.3
1	B	290	GLN	2.3
1	B	330	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	106	SER	2.2
1	B	287	SER	2.1
1	B	331	GLN	2.1
1	B	103	ASP	2.1
1	A	104	PRO	2.1
1	B	288	GLU	2.0
1	B	105	VAL	2.0
1	A	50	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	SO4	B	408	5/5	0.43	0.13	119,132,142,160	0
2	SO4	B	405	5/5	0.58	0.15	113,125,154,169	0
2	SO4	A	405	5/5	0.62	0.11	112,127,138,148	0
2	SO4	B	404	5/5	0.64	0.14	84,109,130,145	0
2	SO4	B	406	5/5	0.70	0.13	104,107,120,127	0
2	SO4	B	409	5/5	0.74	0.16	100,131,142,152	0
2	SO4	B	410	5/5	0.74	0.18	102,107,132,138	0
2	SO4	B	407	5/5	0.75	0.18	126,153,172,180	0
2	SO4	B	403	5/5	0.76	0.10	115,131,142,148	0
2	SO4	A	406	5/5	0.78	0.12	70,82,110,149	0
2	SO4	B	402	5/5	0.80	0.14	72,89,103,128	0
2	SO4	A	404	5/5	0.81	0.14	137,137,155,163	0
2	SO4	A	403	5/5	0.82	0.11	72,87,92,98	0
2	SO4	B	401	5/5	0.83	0.19	96,102,125,154	0
4	A1H6J	A	409	38/38	0.85	0.18	53,84,117,136	0

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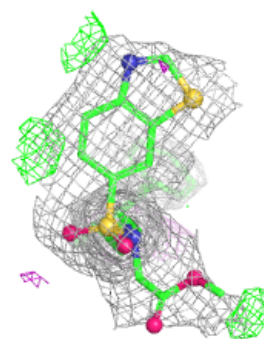
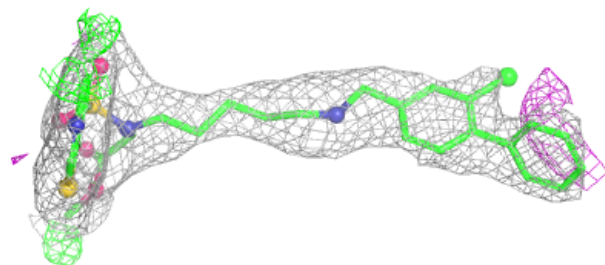
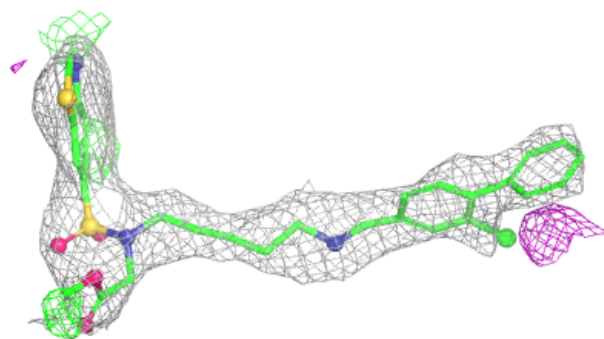
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	408	4/4	0.86	0.18	76,79,87,90	0
4	A1H6J	B	414	38/38	0.87	0.20	62,84,120,135	0
2	SO4	A	402	5/5	0.88	0.10	90,94,96,98	0
2	SO4	B	412	5/5	0.89	0.13	60,69,73,78	0
2	SO4	B	411	5/5	0.91	0.07	77,82,85,86	0
3	EDO	B	413	4/4	0.93	0.12	38,47,50,54	0
2	SO4	A	401	5/5	0.94	0.18	74,80,101,103	0
2	SO4	A	407	5/5	0.95	0.08	55,57,58,59	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.

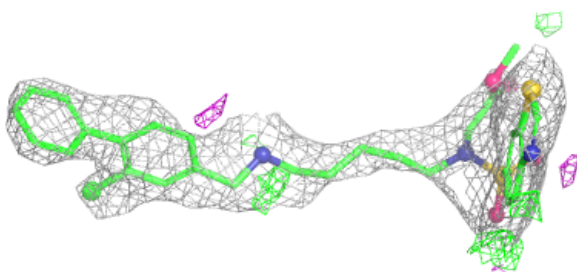
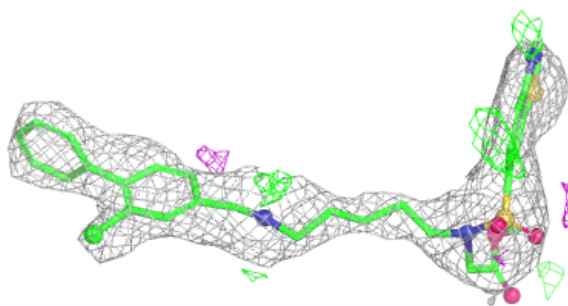
Electron density around A1H6J A 409:

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 A1H6J B 414:

$2mF_o-DF_c$ (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.