



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2025 – 01:54 pm BST

PDB ID : 9QSR / pdb_00009qsr
Title : Protein Kinase CK2 and bivalent inhibitors
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Deposited on : 2025-04-07
Resolution : 2.83 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

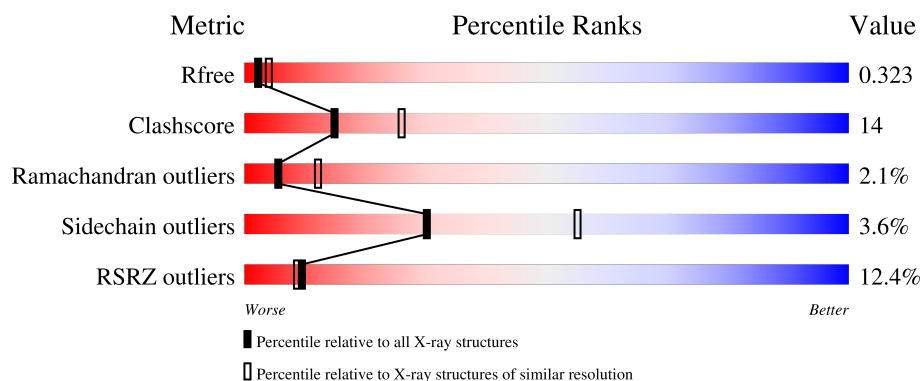
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.83 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}	164625	1367 (2.86-2.82)
Clashscore	180529	1455 (2.86-2.82)
Ramachandran outliers	177936	1422 (2.86-2.82)
Sidechain outliers	177891	1423 (2.86-2.82)
RSRZ outliers	164620	1368 (2.86-2.82)

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	359	
1	B	359	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5592 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	330	Total	C	N	O	S	0	0	0
			2731	1753	480	487	11			
1	B	330	Total	C	N	O	S	0	0	0
			2736	1754	483	488	11			

There are 44 discrepancies between the modelled and reference sequences:

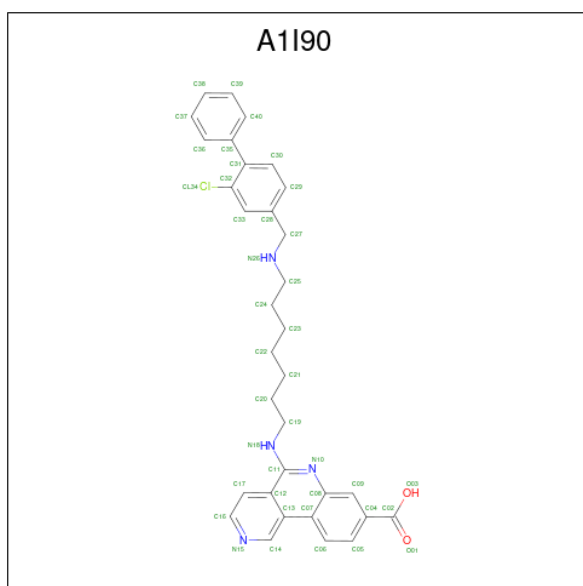
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP P68400
A	-20	HIS	-	expression tag	UNP P68400
A	-19	HIS	-	expression tag	UNP P68400
A	-18	HIS	-	expression tag	UNP P68400
A	-17	HIS	-	expression tag	UNP P68400
A	-16	HIS	-	expression tag	UNP P68400
A	-15	HIS	-	expression tag	UNP P68400
A	-14	SER	-	expression tag	UNP P68400
A	-13	SER	-	expression tag	UNP P68400
A	-12	GLY	-	expression tag	UNP P68400
A	-11	VAL	-	expression tag	UNP P68400
A	-10	ASP	-	expression tag	UNP P68400
A	-9	LEU	-	expression tag	UNP P68400
A	-8	GLY	-	expression tag	UNP P68400
A	-7	THR	-	expression tag	UNP P68400
A	-6	GLU	-	expression tag	UNP P68400
A	-5	ASN	-	expression tag	UNP P68400
A	-4	LEU	-	expression tag	UNP P68400
A	-3	TYR	-	expression tag	UNP P68400
A	-2	PHE	-	expression tag	UNP P68400
A	-1	GLN	-	expression tag	UNP P68400
A	0	SER	-	expression tag	UNP P68400
B	-21	MET	-	initiating methionine	UNP P68400
B	-20	HIS	-	expression tag	UNP P68400
B	-19	HIS	-	expression tag	UNP P68400

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	expression tag	UNP P68400
B	-17	HIS	-	expression tag	UNP P68400
B	-16	HIS	-	expression tag	UNP P68400
B	-15	HIS	-	expression tag	UNP P68400
B	-14	SER	-	expression tag	UNP P68400
B	-13	SER	-	expression tag	UNP P68400
B	-12	GLY	-	expression tag	UNP P68400
B	-11	VAL	-	expression tag	UNP P68400
B	-10	ASP	-	expression tag	UNP P68400
B	-9	LEU	-	expression tag	UNP P68400
B	-8	GLY	-	expression tag	UNP P68400
B	-7	THR	-	expression tag	UNP P68400
B	-6	GLU	-	expression tag	UNP P68400
B	-5	ASN	-	expression tag	UNP P68400
B	-4	LEU	-	expression tag	UNP P68400
B	-3	TYR	-	expression tag	UNP P68400
B	-2	PHE	-	expression tag	UNP P68400
B	-1	GLN	-	expression tag	UNP P68400
B	0	SER	-	expression tag	UNP P68400

- Molecule 2 is 5-[7-[(3-chloranyl-4-phenyl-phenyl)methylamino]heptylamino]benzo[c][2,6]naphthyridine-8-carboxylic acid (CCD ID: A1I90) (formula: C₃₃H₃₃ClN₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0
			40	33	1	4	2	

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	O	
			40	33	1	4	2	
							0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

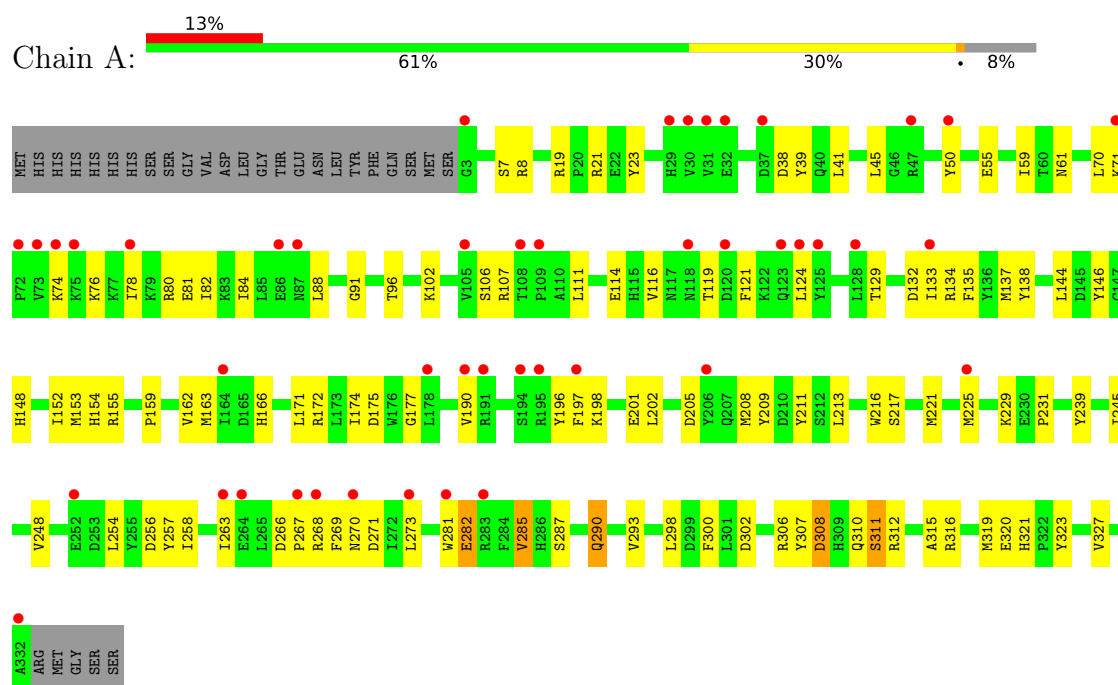
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O		
			6	6	0	0
4	B	9	Total	O		
			9	9	0	0

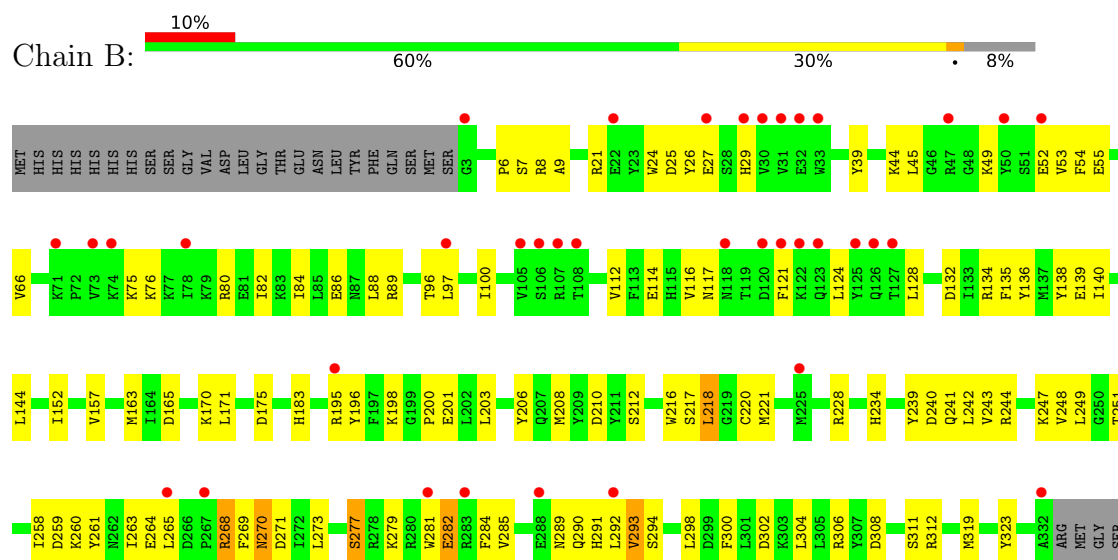
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Casein kinase II subunit alpha



• Molecule 1: Casein kinase II subunit alpha



SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.71Å 128.71Å 123.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.94 – 2.83 88.94 – 2.83	Depositor EDS
% Data completeness (in resolution range)	97.1 (88.94-2.83) 97.6 (88.94-2.83)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, R_{free}	0.268 , 0.326 0.267 , 0.323	Depositor DCC
R_{free} test set	1745 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	79.4	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5592	wwPDB-VP
Average B, all atoms (Å ²)	75.0	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 83.59 % 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 2.0847e-07. 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: A1I90, 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	0.41	0/2804	0.62	0/3799
1	B	0.45	0/2809	0.64	0/3806
All	All	0.43	0/5613	0.63	0/7605

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2731	0	2650	76	0
1	B	2736	0	2654	73	0
2	A	40	0	0	5	0
2	B	40	0	0	1	0
3	A	15	0	0	3	0
3	B	15	0	0	1	0
4	A	6	0	0	0	0
4	B	9	0	0	1	0
All	All	5592	0	5304	148	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 14.

All (148) 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:293:VAL:HG13	1:A:298:LEU:HD21	1.54	0.89
1:B:121:PHE:HA	1:B:124:LEU:HB3	1.64	0.80
1:A:258:ILE:HA	1:A:263:ILE:HD12	1.62	0.79
1:B:281:TRP:HE1	1:B:302:ASP:HB2	1.49	0.77
1:B:45:LEU:HD21	1:B:55:GLU:HB2	1.66	0.76
1:B:157:VAL:HG13	1:B:217:SER:HB2	1.67	0.75
1:A:306:ARG:NH2	1:B:282:GLU:OE2	2.21	0.73
1:A:308:ASP:HB3	1:A:311:SER:HB2	1.70	0.73
1:A:84:ILE:HG23	1:A:152:ILE:HD13	1.70	0.73
1:B:258:ILE:HG23	1:B:263:ILE:HB	1.72	0.72
1:A:216:TRP:HZ2	1:A:245:ILE:HD13	1.55	0.70
1:A:129:THR:HG23	1:A:132:ASP:H	1.57	0.70
1:B:21:ARG:NH2	1:B:25:ASP:OD2	2.24	0.68
1:B:195:ARG:HA	1:B:198:LYS:HD2	1.75	0.67
1:A:216:TRP:CZ2	1:A:245:ILE:HD13	2.29	0.67
1:B:308:ASP:HB3	1:B:311:SER:HB2	1.76	0.67
1:B:89:ARG:NH1	1:B:97:LEU:O	2.28	0.66
1:B:8:ARG:HH12	1:B:208:MET:HE3	1.60	0.66
1:B:290:GLN:O	1:B:292:LEU:N	2.30	0.64
1:B:7:SER:H	1:B:208:MET:HE2	1.63	0.64
1:A:163:MET:HE1	2:A:401:A1I90:C12	2.28	0.62
1:A:45:LEU:HD11	1:A:55:GLU:HB2	1.81	0.62
1:A:163:MET:HE1	2:A:401:A1I90:C11	2.29	0.61
1:A:269:PHE:O	1:A:271:ASP:N	2.34	0.61
1:B:264:GLU:OE1	1:B:264:GLU:N	2.30	0.59
1:A:209:TYR:CE1	1:A:213:LEU:HD12	2.37	0.59
1:A:281:TRP:HB3	1:A:298:LEU:HD12	1.85	0.59
1:A:80:ARG:NH1	3:A:402:SO4:O2	2.32	0.58
1:B:293:VAL:HG13	1:B:298:LEU:HD21	1.86	0.58
1:A:315:ALA:O	1:A:319:MET:HG3	2.04	0.58
1:A:78:ILE:O	1:A:82:ILE:HG13	2.03	0.58
1:A:190:VAL:HG11	1:A:205:ASP:HA	1.85	0.57
1:A:96:THR:HB	1:A:114:GLU:HB3	1.88	0.56
1:B:135:PHE:O	1:B:139:GLU:HG2	2.05	0.56
1:B:269:PHE:O	1:B:271:ASP:N	2.38	0.56
1:B:8:ARG:NH1	1:B:208:MET:HE3	2.22	0.55
1:B:294:SER:O	1:B:298:LEU:HD23	2.06	0.55
1:B:221:MET:HE1	2:B:403:A1I90:CL34	2.44	0.55
1:A:225:MET:HG3	2:A:401:A1I90:C39	2.37	0.54
1:B:24:TRP:CD1	1:B:24:TRP:H	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:GLU:OE1	1:B:312:ARG:NH2	2.29	0.54
1:B:138:TYR:CE1	1:B:319:MET:HB3	2.43	0.54
1:A:138:TYR:CE1	1:A:319:MET:HB3	2.43	0.53
1:B:234:HIS:O	1:B:244:ARG:NH1	2.41	0.53
1:B:300:PHE:CZ	1:B:304:LEU:HD11	2.43	0.53
1:A:266:ASP:OD1	1:A:267:PRO:HD2	2.09	0.53
1:B:6:PRO:HB3	1:B:208:MET:HE1	1.90	0.53
1:B:281:TRP:HB3	1:B:298:LEU:HD12	1.89	0.53
1:A:154:HIS:NE2	1:A:174:ILE:O	2.33	0.53
1:A:107:ARG:NH2	3:A:404:SO4:O2	2.42	0.53
1:A:129:THR:HG22	1:A:132:ASP:OD2	2.10	0.52
1:A:269:PHE:C	1:A:271:ASP:H	2.17	0.52
1:A:163:MET:HE2	1:A:174:ILE:HD13	1.91	0.52
1:A:148:HIS:CE1	1:A:211:TYR:HB3	2.45	0.52
1:A:198:LYS:NZ	3:A:403:SO4:O4	2.43	0.52
1:B:39:TYR:CE2	1:B:112:VAL:HG11	2.44	0.51
1:A:201:GLU:OE1	1:A:312:ARG:NH2	2.34	0.51
1:A:7:SER:O	1:A:8:ARG:HD2	2.11	0.50
1:B:281:TRP:CB	1:B:298:LEU:HD12	2.41	0.50
1:B:157:VAL:HG13	1:B:217:SER:CB	2.41	0.50
1:A:135:PHE:HA	1:A:327:VAL:HG11	1.93	0.50
1:A:268:ARG:HD2	1:A:268:ARG:H	1.74	0.50
1:B:49:LYS:N	1:B:49:LYS:HD3	2.27	0.50
1:B:44:LYS:HE2	1:B:54:PHE:CE2	2.47	0.50
1:B:117:ASN:O	1:B:165:ASP:HB2	2.11	0.50
1:B:206:TYR:CD1	1:B:263:ILE:HD11	2.46	0.49
1:B:96:THR:H	1:B:114:GLU:HG2	1.77	0.49
1:A:282:GLU:OE2	1:B:306:ARG:NH2	2.45	0.49
1:A:134:ARG:HG2	1:A:323:TYR:CZ	2.49	0.48
1:A:7:SER:C	1:A:8:ARG:HD2	2.39	0.48
1:B:84:ILE:HG23	1:B:152:ILE:HD13	1.95	0.48
1:A:70:LEU:HD21	1:A:111:LEU:HD13	1.96	0.48
1:B:144:LEU:HD11	1:B:218:LEU:HD13	1.94	0.47
1:A:163:MET:O	1:A:171:LEU:HA	2.15	0.47
1:A:257:TYR:CD2	1:A:307:TYR:HB3	2.50	0.47
1:A:121:PHE:HA	1:A:124:LEU:HB2	1.96	0.47
1:B:260:LYS:HD3	1:B:261:TYR:CE1	2.50	0.47
1:A:38:ASP:HB2	1:A:39:TYR:CE1	2.50	0.47
1:A:41:LEU:H	1:A:41:LEU:HD22	1.80	0.47
1:A:116:VAL:HG21	1:A:172:ARG:HG3	1.97	0.47
1:B:171:LEU:HD12	1:B:171:LEU:HA	1.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:PHE:C	1:B:271:ASP:H	2.23	0.47
2:A:401:A1I90:CL34	2:A:401:A1I90:C40	3.01	0.46
1:B:306:ARG:NH1	4:B:501:HOH:O	2.44	0.46
1:B:138:TYR:HE1	1:B:319:MET:HB3	1.80	0.46
1:A:45:LEU:HA	1:A:45:LEU:HD23	1.54	0.46
1:B:134:ARG:HG2	1:B:323:TYR:CE1	2.50	0.46
1:A:74:LYS:HE3	1:A:76:LYS:HD3	1.97	0.46
1:B:200:PRO:HD3	1:B:216:TRP:CE2	2.50	0.46
1:A:221:MET:HE3	1:A:221:MET:HB3	1.69	0.46
1:A:269:PHE:C	1:A:271:ASP:N	2.74	0.46
1:A:88:LEU:HD21	1:A:152:ILE:HD12	1.98	0.46
1:B:248:VAL:HG12	1:B:249:LEU:HD23	1.98	0.46
1:B:201:GLU:CD	1:B:312:ARG:HH22	2.19	0.45
1:A:19:ARG:HD3	1:A:23:TYR:CD2	2.51	0.45
1:A:71:LYS:HB3	1:A:71:LYS:HE2	1.70	0.45
1:A:287:SER:O	1:A:290:GLN:NE2	2.50	0.45
1:B:163:MET:O	1:B:171:LEU:HD12	2.17	0.45
1:A:81:GLU:HG3	1:A:177:GLY:HA2	1.99	0.44
1:A:266:ASP:OD1	1:A:268:ARG:HD2	2.18	0.44
1:B:27:GLU:H	1:B:27:GLU:HG2	1.50	0.44
1:B:82:ILE:O	1:B:86:GLU:HG3	2.17	0.44
1:A:91:GLY:HA3	1:A:146:TYR:CE2	2.53	0.44
1:B:290:GLN:C	1:B:292:LEU:H	2.26	0.44
1:A:201:GLU:HG2	1:A:202:LEU:H	1.83	0.44
1:B:270:ASN:OD1	1:B:270:ASN:N	2.51	0.43
1:B:282:GLU:H	1:B:282:GLU:HG3	1.47	0.43
1:B:265:LEU:HD23	1:B:265:LEU:HA	1.55	0.43
1:A:159:PRO:HD2	1:A:197:PHE:CZ	2.54	0.43
1:A:162:VAL:O	2:A:401:A1I90:N26	2.51	0.43
1:A:102:LYS:HD3	1:A:107:ARG:O	2.19	0.43
1:A:229:LYS:HG2	1:A:231:PRO:O	2.19	0.43
1:B:196:TYR:HA	1:B:241:GLN:NE2	2.34	0.43
1:B:80:ARG:NH1	3:B:402:SO4:O4	2.31	0.43
1:B:277:SER:OG	1:B:279:LYS:HE3	2.18	0.43
1:A:137:MET:HE3	1:A:137:MET:HB3	1.84	0.43
1:A:50:TYR:C	1:A:71:LYS:HB2	2.44	0.43
1:A:300:PHE:HB2	1:A:321:HIS:CE1	2.53	0.42
1:B:88:LEU:HD21	1:B:152:ILE:HD12	2.01	0.42
1:A:258:ILE:HA	1:A:263:ILE:CD1	2.42	0.42
1:A:282:GLU:HA	1:A:285:VAL:HG12	2.00	0.42
1:A:316:ARG:O	1:A:320:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:TYR:O	1:B:29:HIS:HB3	2.19	0.42
1:B:200:PRO:HD3	1:B:216:TRP:CD2	2.54	0.42
1:A:216:TRP:O	1:A:217:SER:C	2.61	0.42
1:B:9:ALA:HB2	1:B:210:ASP:HB2	2.01	0.42
1:B:240:ASP:HA	1:B:243:VAL:HG23	2.02	0.42
1:B:247:LYS:HB3	1:B:247:LYS:HE2	1.83	0.42
1:A:144:LEU:HD13	1:A:144:LEU:HA	1.93	0.42
1:A:129:THR:H	1:A:132:ASP:HB2	1.84	0.42
1:B:242:LEU:HD12	1:B:242:LEU:HA	1.86	0.42
1:B:136:TYR:O	1:B:140:ILE:HG12	2.18	0.41
1:A:196:TYR:CE2	1:A:231:PRO:HG3	2.56	0.41
1:B:289:ASN:C	1:B:289:ASN:OD1	2.63	0.41
1:A:308:ASP:OD1	1:A:310:GLN:HB2	2.21	0.41
1:B:216:TRP:NE1	1:B:220:CYS:SG	2.93	0.41
1:B:248:VAL:HG22	1:B:284:PHE:HZ	1.86	0.41
1:B:239:TYR:CE2	1:B:268:ARG:HD2	2.55	0.41
1:A:129:THR:O	1:A:133:ILE:HD12	2.21	0.41
1:A:208:MET:HE3	1:A:208:MET:HB2	1.72	0.41
1:B:116:VAL:HG13	1:B:170:LYS:NZ	2.36	0.41
1:B:210:ASP:OD1	1:B:212:SER:OG	2.37	0.40
1:A:153:MET:HE3	1:A:155:ARG:HD3	2.03	0.40
1:A:239:TYR:OH	1:A:266:ASP:OD2	2.27	0.40
1:A:119:THR:HG21	1:A:166:HIS:H	1.86	0.40
1:B:24:TRP:CE3	1:B:183:HIS:CE1	3.10	0.40
1:B:128:LEU:HD12	1:B:132:ASP:HB2	2.03	0.40
1:A:254:LEU:O	1:A:257:TYR:HB3	2.22	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	328/359 (91%)	297 (90%)	25 (8%)	6 (2%)	7	15
1	B	328/359 (91%)	294 (90%)	26 (8%)	8 (2%)	5	10
All	All	656/718 (91%)	591 (90%)	51 (8%)	14 (2%)	5	12

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	76	LYS
1	A	21	ARG
1	A	61	ASN
1	A	175	ASP
1	A	270	ASN
1	A	273	LEU
1	B	75	LYS
1	B	270	ASN
1	B	291	HIS
1	B	52	GLU
1	B	268	ARG
1	A	308	ASP
1	B	175	ASP
1	B	228	ARG

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	290/329 (88%)	281 (97%)	9 (3%)	35	60
1	B	291/329 (88%)	279 (96%)	12 (4%)	26	50
All	All	581/658 (88%)	560 (96%)	21 (4%)	30	55

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ILE
1	A	106	SER

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Mol	Chain	Res	Type
1	A	248	VAL
1	A	256	ASP
1	A	282	GLU
1	A	285	VAL
1	A	290	GLN
1	A	302	ASP
1	A	311	SER
1	B	53	VAL
1	B	66	VAL
1	B	100	ILE
1	B	203	LEU
1	B	218	LEU
1	B	251	THR
1	B	259	ASP
1	B	273	LEU
1	B	277	SER
1	B	282	GLU
1	B	285	VAL
1	B	293	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	331	GLN
1	B	18	HIS
1	B	117	ASN
1	B	148	HIS
1	B	276	HIS
1	B	331	GLN

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](#)

8 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	SO4	A	403	-	4,4,4	0.17	0	6,6,6	0.14	0
3	SO4	B	402	-	4,4,4	0.36	0	6,6,6	0.29	0
3	SO4	A	402	-	4,4,4	0.14	0	6,6,6	0.26	0
2	A1I90	B	403	-	43,44,44	1.43	4 (9%)	55,59,59	1.67	6 (10%)
3	SO4	A	404	-	4,4,4	0.12	0	6,6,6	0.19	0
3	SO4	B	401	-	4,4,4	0.30	0	6,6,6	0.29	0
2	A1I90	A	401	-	43,44,44	1.57	4 (9%)	55,59,59	1.61	8 (14%)
3	SO4	B	404	-	4,4,4	0.15	0	6,6,6	0.42	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
2	A1I90	A	401	-	-	12/21/21/21	0/5/5/5
2	A1I90	B	403	-	-	12/21/21/21	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	A1I90	C11-N18	5.90	1.45	1.34
2	B	403	A1I90	C11-N18	5.72	1.45	1.34
2	A	401	A1I90	C04-C02	4.58	1.59	1.49
2	A	401	A1I90	C08-N10	3.06	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	A1I90	C04-C02	2.85	1.55	1.49
2	B	403	A1I90	C08-N10	2.70	1.42	1.37
2	A	401	A1I90	O03-C02	-2.41	1.23	1.30
2	B	403	A1I90	O03-C02	-2.39	1.23	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	A1I90	C33-C32-C31	6.80	126.74	121.91
2	A	401	A1I90	C33-C32-C31	5.67	125.94	121.91
2	B	403	A1I90	C31-C32-CL34	-4.57	114.20	120.75
2	A	401	A1I90	C30-C31-C35	4.12	126.82	118.68
2	B	403	A1I90	C30-C31-C32	-4.09	113.10	117.63
2	A	401	A1I90	C30-C31-C32	-3.65	113.59	117.63
2	A	401	A1I90	C31-C32-CL34	-3.63	115.55	120.75
2	B	403	A1I90	C30-C31-C35	3.47	125.54	118.68
2	A	401	A1I90	C19-N18-C11	2.92	127.80	122.89
2	A	401	A1I90	C20-C19-N18	2.52	118.25	111.49
2	A	401	A1I90	C35-C31-C32	-2.40	119.49	123.53
2	B	403	A1I90	C29-C28-C33	-2.17	115.50	118.54
2	B	403	A1I90	C14-C13-C12	-2.11	114.69	117.37
2	A	401	A1I90	C29-C28-C33	-2.01	115.72	118.54

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	A1I90	C20-C19-N18-C11
2	B	403	A1I90	C20-C19-N18-C11
2	B	403	A1I90	C28-C27-N26-C25
2	A	401	A1I90	C23-C24-C25-N26
2	B	403	A1I90	N18-C19-C20-C21
2	A	401	A1I90	O01-C02-C04-C05
2	A	401	A1I90	O03-C02-C04-C05
2	A	401	A1I90	O01-C02-C04-C09
2	A	401	A1I90	O03-C02-C04-C09
2	A	401	A1I90	N18-C19-C20-C21
2	A	401	A1I90	N10-C11-N18-C19
2	A	401	A1I90	C22-C23-C24-C25
2	A	401	A1I90	C20-C21-C22-C23
2	A	401	A1I90	C12-C11-N18-C19
2	B	403	A1I90	C19-C20-C21-C22

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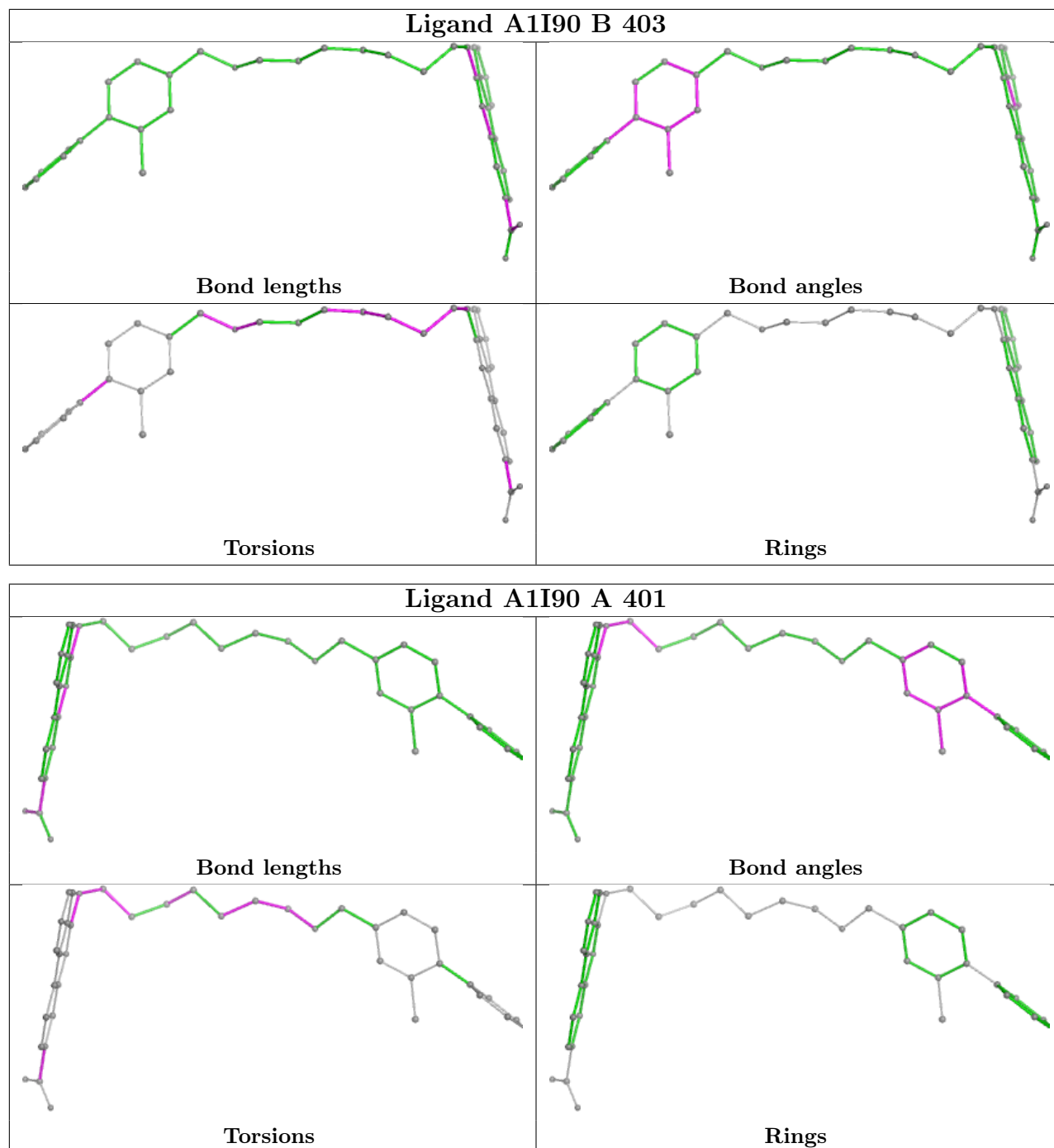
Mol	Chain	Res	Type	Atoms
2	B	403	A1I90	C32-C31-C35-C40
2	B	403	A1I90	O01-C02-C04-C05
2	B	403	A1I90	O01-C02-C04-C09
2	B	403	A1I90	C21-C22-C23-C24
2	A	401	A1I90	C24-C25-N26-C27
2	B	403	A1I90	O03-C02-C04-C05
2	B	403	A1I90	O03-C02-C04-C09
2	B	403	A1I90	C24-C25-N26-C27
2	B	403	A1I90	C20-C21-C22-C23

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	SO4	1	0
3	B	402	SO4	1	0
3	A	402	SO4	1	0
2	B	403	A1I90	1	0
3	A	404	SO4	1	0
2	A	401	A1I90	5	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	330/359 (91%)	0.96	45 (13%) 8 7	51, 74, 108, 167	1 (0%)
1	B	330/359 (91%)	0.86	37 (11%) 11 10	42, 69, 106, 155	3 (0%)
All	All	660/718 (91%)	0.91	82 (12%) 9 9	42, 71, 108, 167	4 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	125	TYR	5.0
1	A	120	ASP	4.4
1	B	32	GLU	4.2
1	B	127	THR	4.1
1	B	126	GLN	3.8
1	B	29	HIS	3.7
1	A	124	LEU	3.6
1	A	73	VAL	3.6
1	A	74	LYS	3.6
1	A	270	ASN	3.6
1	A	32	GLU	3.5
1	A	72	PRO	3.5
1	B	123	GLN	3.5
1	A	30	VAL	3.5
1	B	106	SER	3.4
1	B	78	ILE	3.3
1	B	50	TYR	3.2
1	B	31	VAL	3.1
1	A	195	ARG	3.1
1	A	191	ARG	3.1
1	B	73	VAL	3.0
1	A	123	GLN	2.9
1	B	107	ARG	2.9
1	A	267	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	50	TYR	2.8
1	B	22	GLU	2.8
1	A	3	GLY	2.8
1	B	120	ASP	2.8
1	A	190	VAL	2.8
1	B	288	GLU	2.8
1	A	105	VAL	2.7
1	A	125	TYR	2.7
1	A	273	LEU	2.7
1	A	118	ASN	2.7
1	B	283	ARG	2.7
1	A	283	ARG	2.7
1	B	105	VAL	2.6
1	A	108	THR	2.6
1	A	86	GLU	2.6
1	B	122	LYS	2.6
1	A	197	PHE	2.6
1	A	71	LYS	2.5
1	A	87	ASN	2.5
1	A	281	TRP	2.5
1	A	47	ARG	2.5
1	A	31	VAL	2.4
1	B	108	THR	2.4
1	A	268	ARG	2.4
1	A	78	ILE	2.4
1	A	225	MET	2.3
1	A	194	SER	2.3
1	A	178	LEU	2.3
1	A	37	ASP	2.3
1	B	265	LEU	2.3
1	B	267	PRO	2.3
1	B	118	ASN	2.3
1	B	292	LEU	2.3
1	A	75	LYS	2.3
1	A	332	ALA	2.2
1	B	52	GLU	2.2
1	A	133	ILE	2.2
1	B	121	PHE	2.2
1	B	195	ARG	2.2
1	B	27	GLU	2.2
1	A	206	TYR	2.2
1	A	264	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	30	VAL	2.2
1	B	225	MET	2.2
1	A	29	HIS	2.1
1	B	47	ARG	2.1
1	B	74	LYS	2.1
1	B	33	TRP	2.1
1	B	71	LYS	2.1
1	A	128	LEU	2.1
1	A	164	ILE	2.1
1	A	263	ILE	2.1
1	B	3	GLY	2.1
1	B	97	LEU	2.1
1	A	252	GLU	2.1
1	B	332	ALA	2.0
1	B	281	TRP	2.0
1	A	109	PRO	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.

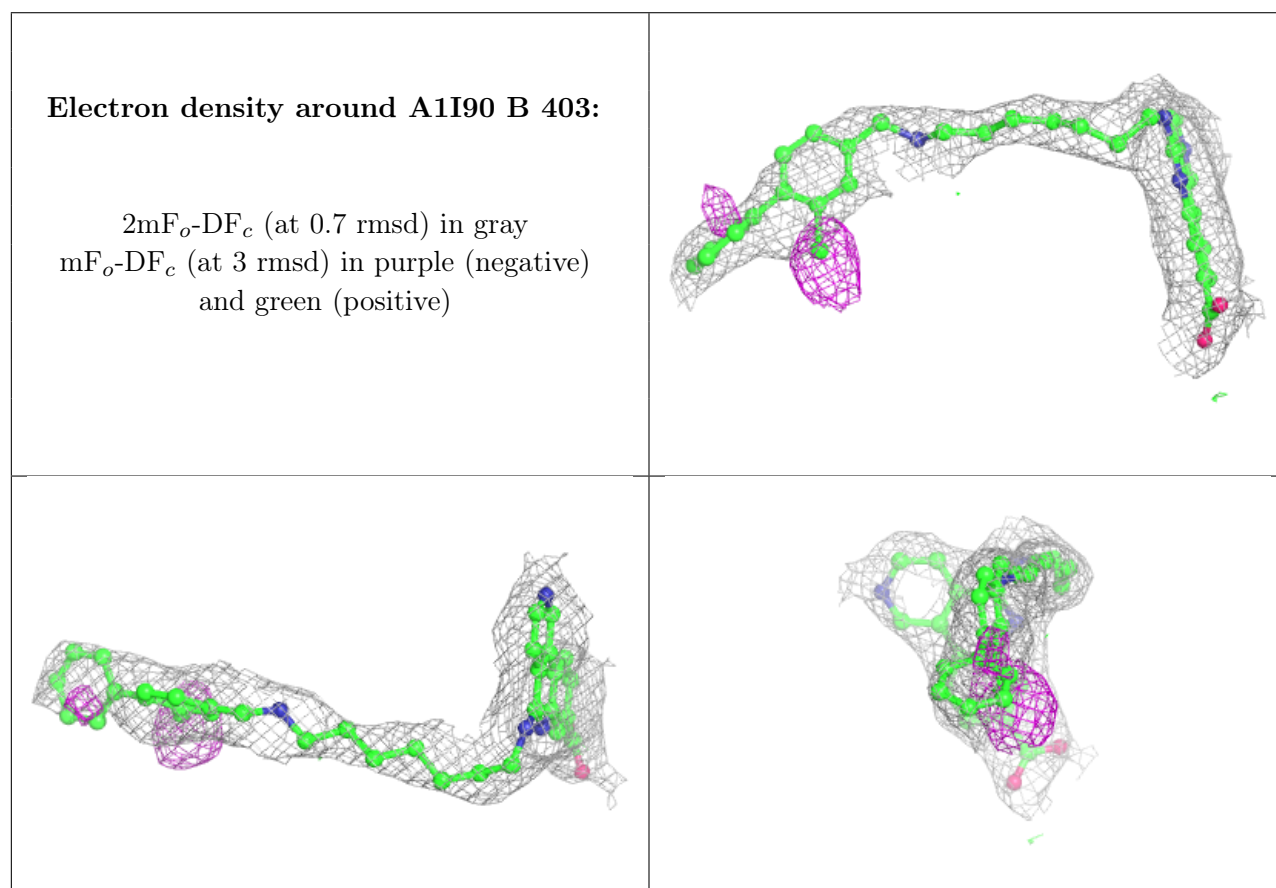
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	404	5/5	0.38	0.18	109,112,113,118	0
3	SO4	A	403	5/5	0.57	0.39	96,100,107,111	0
3	SO4	B	404	5/5	0.66	0.20	72,73,78,78	5
3	SO4	B	401	5/5	0.78	0.32	72,75,80,81	0
2	A1I90	B	403	40/40	0.81	0.17	51,65,73,80	0
2	A1I90	A	401	40/40	0.84	0.17	56,67,79,81	0
3	SO4	A	402	5/5	0.84	0.19	78,84,89,90	0

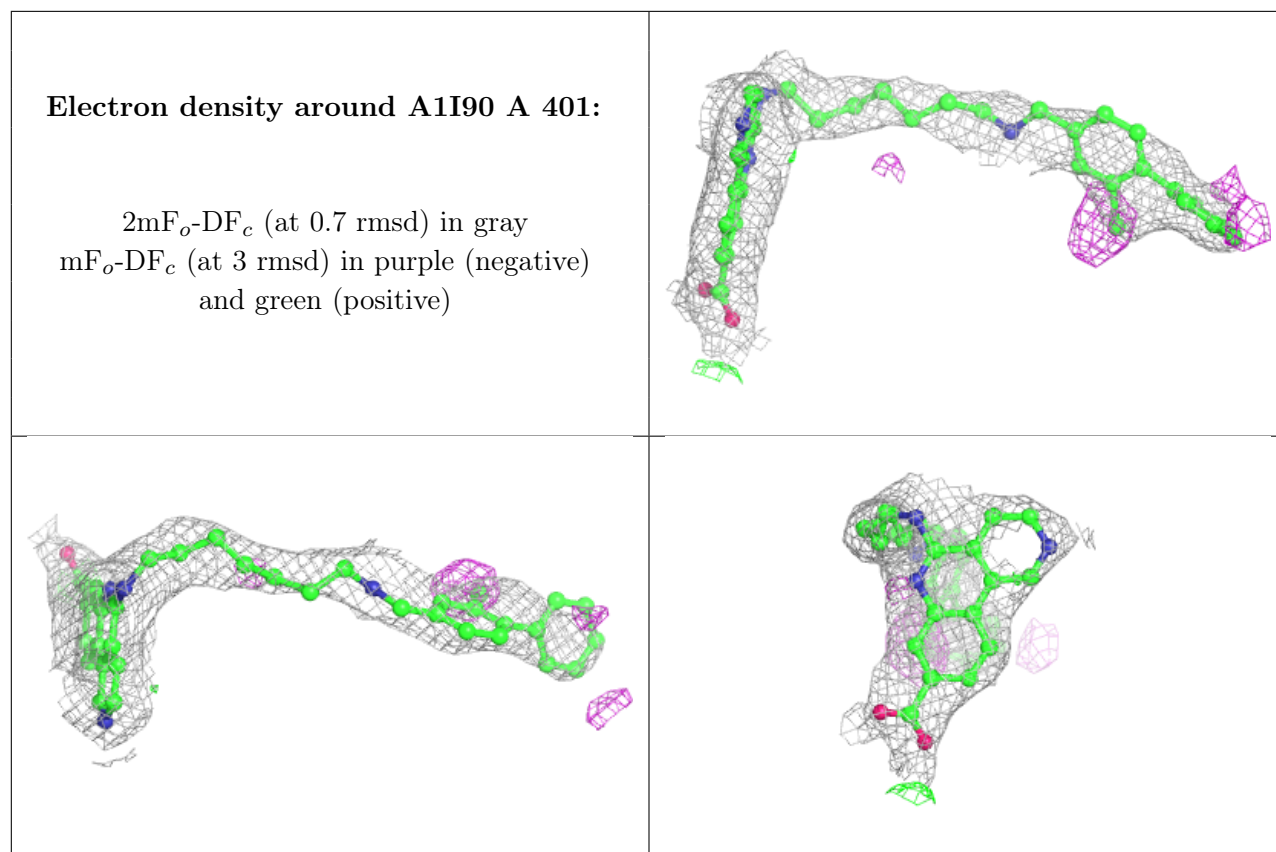
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	B	402	5/5	0.85	0.18	73,74,82,82	0

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.