



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:43 PM UTC

PDB ID : 7C7G / pdb_00007c7g
Title : Crystal structures of AKR1C3 ternary complex with NADP⁺ and the chromene derivative 2j
Authors : Irie, K.; Toyooka, N.; Endo, S.
Deposited on : 2020-05-25
Resolution : 1.86 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

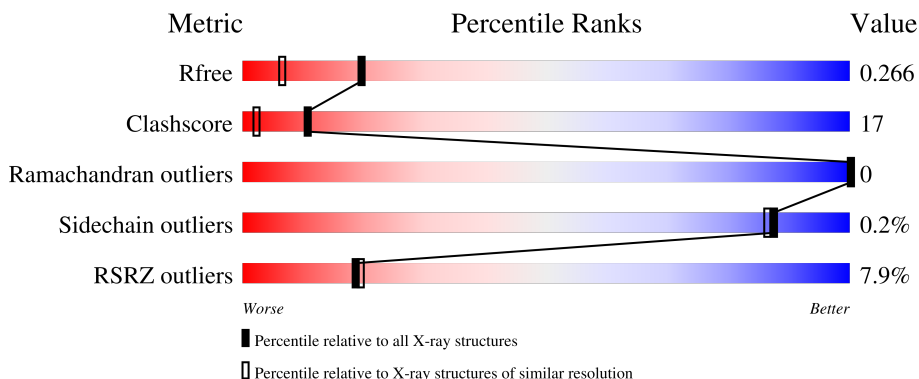
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	325	4% 78% 18% .
1	B	325	11% 74% 23% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5543 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.

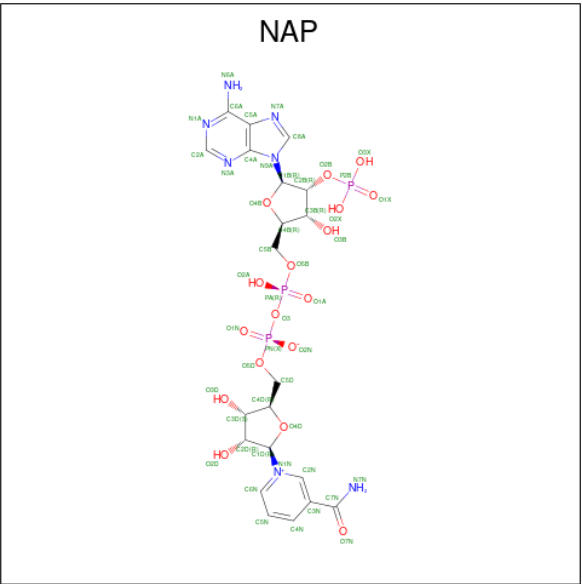
- Molecule 1 is a protein called Aldo-keto reductase family 1 member C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2534	1615	443	464	12			
1	B	318	Total	C	N	O	S	0	0	0
			2554	1627	443	472	12			

There are 4 discrepancies between the modelled and reference sequences:

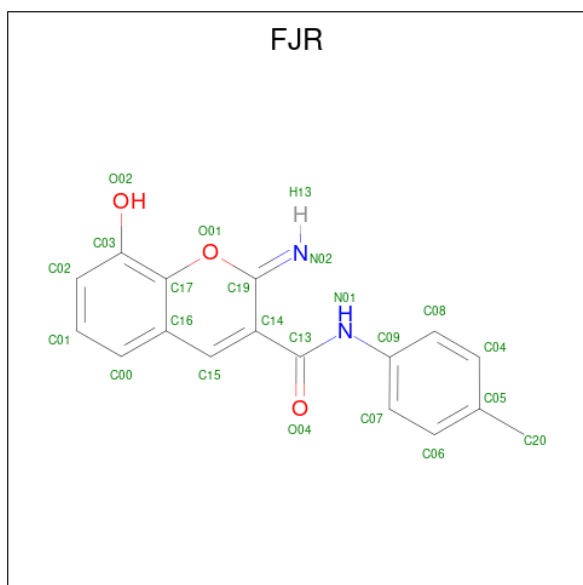
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42330
A	0	SER	-	expression tag	UNP P42330
B	-1	GLY	-	expression tag	UNP P42330
B	0	SER	-	expression tag	UNP P42330

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 2-azanylidene-N-(4-methylphenyl)-8-oxidanyl-chromene-3-carboxamide (CCD ID: FJR) (formula: C₁₇H₁₄N₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	17	2	3		
3	B	1	Total	C	N	O	0	0
			22	17	2	3		

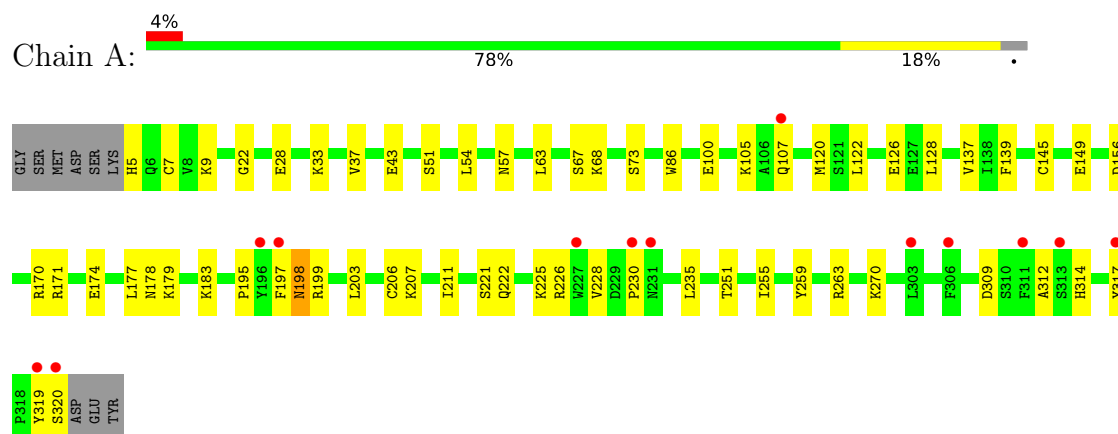
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	159	Total	O	0	0
			159	159		
4	B	156	Total	O	0	0
			156	156		

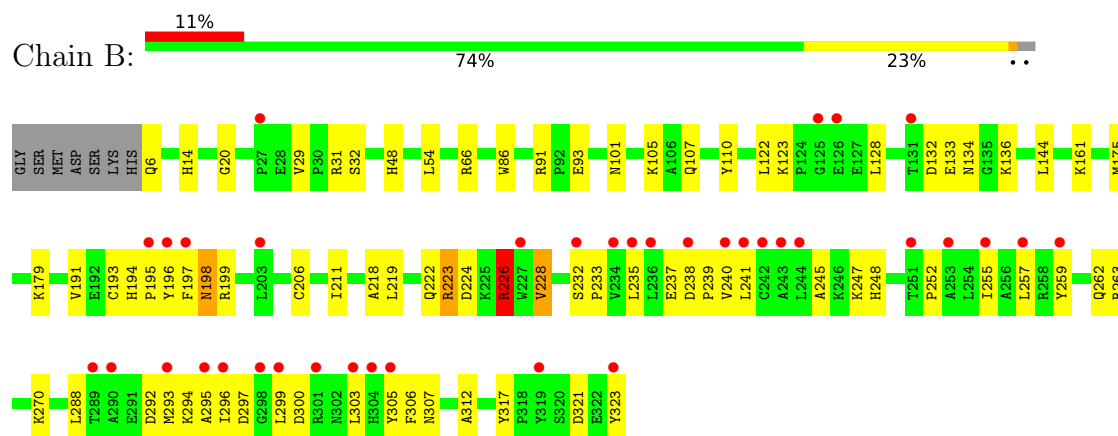
3 Residue-property plots [i](#)

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: Aldo-keto reductase family 1 member C3



- Molecule 1: Aldo-keto reductase family 1 member C3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	40.12Å 52.31Å 76.68Å 77.25° 86.16° 77.64°	Depositor
Resolution (Å)	46.30 – 1.86 46.30 – 1.86	Depositor EDS
% Data completeness (in resolution range)	96.7 (46.30-1.86) 96.7 (46.30-1.86)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.87Å)	Xtriage
Refinement program	PHENIX 1.13_2998, REFMAC 5	Depositor
R, R_{free}	0.219 , 0.265 0.220 , 0.266	Depositor DCC
R_{free} test set	2322 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5543	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% 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: NAP, FJR

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	0.39	0/2593	0.64	3/3509 (0.1%)
1	B	0.48	1/2613 (0.0%)	0.71	5/3535 (0.1%)
All	All	0.44	1/5206 (0.0%)	0.68	8/7044 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	223	ARG	CA-C	-5.95	1.45	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	ASN	N-CA-C	9.30	124.46	113.20
1	A	198	ASN	N-CA-C	8.18	122.83	113.01
1	A	221	SER	CB-CA-C	7.24	124.83	110.42
1	B	226	ARG	N-CA-C	6.81	118.70	111.28
1	B	123	LYS	CA-C-N	-5.50	113.47	120.23
1	B	123	LYS	C-N-CA	-5.50	113.47	120.23
1	A	228	VAL	N-CA-C	5.28	115.50	108.11
1	B	228	VAL	N-CA-C	5.09	115.46	108.12

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	2534	0	2538	65	0
1	B	2554	0	2550	106	0
2	A	48	0	25	5	0
2	B	48	0	25	4	0
3	A	22	0	0	2	0
3	B	22	0	0	1	0
4	A	159	0	0	17	1
4	B	156	0	0	28	1
All	All	5543	0	5138	173	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (173) 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:196:TYR:CE1	1:B:299:LEU:HD13	1.23	1.64
1:B:196:TYR:CD1	1:B:299:LEU:CD1	1.86	1.59
1:B:196:TYR:CE1	1:B:299:LEU:CD1	1.91	1.51
1:B:238:ASP:OD2	1:B:299:LEU:HD22	1.12	1.22
1:A:222:GLN:NE2	1:A:270:LYS:HD3	1.56	1.18
1:B:238:ASP:CG	1:B:299:LEU:CD2	2.15	1.18
1:B:238:ASP:OD1	1:B:299:LEU:HD21	1.42	1.18
1:B:238:ASP:OD1	1:B:299:LEU:CD2	1.94	1.13
1:B:196:TYR:CD1	1:B:299:LEU:HD11	1.80	1.10
1:B:238:ASP:OD2	1:B:299:LEU:CD2	1.98	1.10
1:B:196:TYR:HD1	1:B:299:LEU:HD12	1.05	1.09
1:B:238:ASP:CG	1:B:299:LEU:HD22	1.76	1.08
1:B:196:TYR:HD1	1:B:299:LEU:CD1	1.43	1.04
1:B:196:TYR:CD1	1:B:299:LEU:HD13	1.75	0.98
1:B:198:ASN:HB2	1:B:263:ARG:HH12	1.29	0.97
1:B:252:PRO:HA	1:B:255:ILE:HD12	1.49	0.95
1:B:196:TYR:CD1	1:B:299:LEU:HD12	1.80	0.94
1:A:57:ASN:OD1	4:A:501:HOH:O	1.86	0.93
1:B:238:ASP:CG	1:B:299:LEU:HD21	1.86	0.89
1:B:245:ALA:HB2	1:B:255:ILE:HD11	1.55	0.88
1:A:225:LYS:HZ1	1:A:230:PRO:CB	1.88	0.87
1:B:196:TYR:CE1	1:B:299:LEU:HD11	1.95	0.85
1:A:222:GLN:HE21	1:A:270:LYS:HD3	1.41	0.84
1:A:225:LYS:HZ1	1:A:230:PRO:CG	1.90	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:HZ1	1:A:230:PRO:CD	1.91	0.82
1:A:225:LYS:NZ	1:A:230:PRO:HB3	1.96	0.81
1:A:225:LYS:NZ	1:A:230:PRO:HD3	1.94	0.81
1:B:91:ARG:NH1	4:B:504:HOH:O	2.05	0.80
1:B:196:TYR:HE1	1:B:299:LEU:CD1	1.55	0.80
1:B:224:ASP:OD1	1:B:226:ARG:HG2	1.83	0.78
1:A:5:HIS:O	4:A:502:HOH:O	2.01	0.78
1:A:7:CYS:SG	4:A:502:HOH:O	2.40	0.77
1:B:293:MET:SD	4:B:522:HOH:O	2.44	0.75
1:B:32:SER:OG	4:B:503:HOH:O	2.03	0.75
1:B:122:LEU:O	4:B:502:HOH:O	2.03	0.74
1:B:299:LEU:HD12	1:B:299:LEU:O	1.89	0.72
1:B:293:MET:SD	4:B:635:HOH:O	2.48	0.71
1:B:294:LYS:HG2	4:B:528:HOH:O	1.89	0.71
1:A:149:GLU:HG2	1:A:179:LYS:HE3	1.72	0.70
1:A:225:LYS:HZ1	1:A:230:PRO:HB3	1.50	0.70
1:B:132:ASP:CG	1:B:136:LYS:HG3	2.18	0.69
1:A:225:LYS:NZ	1:A:230:PRO:CD	2.54	0.69
1:A:225:LYS:NZ	1:A:230:PRO:CB	2.55	0.69
1:B:306:PHE:O	4:B:505:HOH:O	2.10	0.68
1:B:132:ASP:OD2	1:B:136:LYS:HG3	1.93	0.68
1:B:29:VAL:O	4:B:506:HOH:O	2.11	0.68
1:A:128:LEU:N	4:A:507:HOH:O	2.25	0.67
1:B:270:LYS:HB2	2:B:401:NAP:H52N	1.76	0.67
1:A:179:LYS:HA	4:A:512:HOH:O	1.95	0.66
1:B:293:MET:HB2	4:B:528:HOH:O	1.94	0.66
2:B:401:NAP:N6A	4:B:511:HOH:O	2.19	0.65
1:A:317:TYR:HE2	1:A:319:TYR:HB2	1.60	0.65
1:B:198:ASN:HB2	1:B:263:ARG:NH1	2.08	0.65
1:A:270:LYS:O	2:A:401:NAP:H8A	1.97	0.65
1:B:6:GLN:OE1	4:B:508:HOH:O	2.14	0.64
1:A:270:LYS:HB2	2:A:401:NAP:H52N	1.80	0.63
1:A:73:SER:OG	4:A:504:HOH:O	2.15	0.63
1:A:222:GLN:NE2	1:A:270:LYS:CD	2.48	0.62
1:A:178:ASN:C	4:A:512:HOH:O	2.41	0.62
1:A:206:CYS:HB3	1:A:211:ILE:O	2.00	0.62
1:A:225:LYS:HZ1	1:A:230:PRO:HD3	1.55	0.61
1:B:91:ARG:HD3	4:B:504:HOH:O	2.00	0.61
1:A:9:LYS:NZ	4:A:511:HOH:O	2.32	0.60
2:A:401:NAP:O2X	4:A:505:HOH:O	2.16	0.60
1:B:195:PRO:HD2	1:B:235:LEU:HD21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LYS:N	4:A:512:HOH:O	2.35	0.59
1:B:198:ASN:ND2	4:B:507:HOH:O	2.13	0.59
1:B:194:HIS:HB2	1:B:235:LEU:HD22	1.85	0.58
1:B:224:ASP:OD1	1:B:226:ARG:CG	2.51	0.58
1:B:132:ASP:OD2	1:B:136:LYS:CG	2.52	0.58
1:B:196:TYR:HE1	1:B:299:LEU:HD13	0.81	0.58
1:B:237:GLU:O	4:B:510:HOH:O	2.17	0.58
1:A:137:VAL:HG23	1:A:139:PHE:HE1	1.67	0.58
1:B:223:ARG:NE	4:B:501:HOH:O	1.86	0.57
1:A:225:LYS:HZ2	1:A:230:PRO:HD3	1.67	0.57
1:B:223:ARG:NH2	1:B:232:SER:O	2.35	0.57
1:A:179:LYS:CA	4:A:512:HOH:O	2.51	0.56
1:B:144:LEU:HB2	1:B:175:MET:HE1	1.87	0.56
1:B:247:LYS:NZ	1:B:292:ASP:OD1	2.38	0.56
1:B:240:VAL:HG11	1:B:295:ALA:C	2.30	0.56
1:B:307:ASN:ND2	4:B:521:HOH:O	2.38	0.56
1:B:179:LYS:NZ	4:B:512:HOH:O	2.22	0.55
1:A:198:ASN:HB2	1:A:263:ARG:NH2	2.22	0.55
1:B:262:GLN:NE2	4:B:522:HOH:O	2.40	0.55
1:A:43:GLU:OE2	1:A:68:LYS:NZ	2.38	0.54
1:B:101:ASN:O	1:B:105:LYS:HG3	2.06	0.54
1:B:259:TYR:CE1	1:B:263:ARG:HD2	2.43	0.54
1:A:195:PRO:HD2	1:A:235:LEU:HD11	1.89	0.54
1:B:238:ASP:HB3	1:B:241:LEU:HD12	1.90	0.54
1:B:194:HIS:CE1	1:B:197:PHE:HB3	2.43	0.53
1:B:259:TYR:O	1:B:263:ARG:HG3	2.08	0.53
1:A:259:TYR:O	1:A:263:ARG:HG3	2.09	0.53
1:B:245:ALA:CB	1:B:255:ILE:HD11	2.33	0.52
1:B:222:GLN:NE2	1:B:270:LYS:HD3	2.24	0.52
1:A:120:MET:HA	1:A:314:HIS:CE1	2.44	0.52
1:A:171:ARG:N	4:A:503:HOH:O	2.14	0.52
1:B:134:ASN:HB2	1:B:136:LYS:HZ3	1.74	0.52
1:A:203:LEU:HD11	1:A:207:LYS:HE3	1.90	0.52
1:A:197:PHE:CE1	1:A:199:ARG:NH1	2.78	0.51
1:B:132:ASP:OD2	1:B:136:LYS:HE2	2.11	0.51
1:A:312:ALA:HA	1:A:317:TYR:CD1	2.46	0.51
1:A:100:GLU:OE1	4:A:506:HOH:O	2.19	0.51
1:B:66:ARG:NH2	4:B:525:HOH:O	2.44	0.51
1:A:51:SER:OG	4:A:501:HOH:O	2.09	0.50
1:A:137:VAL:HG23	1:A:139:PHE:CE1	2.44	0.50
1:A:145:CYS:O	1:A:149:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLU:CG	1:A:179:LYS:HE3	2.43	0.49
1:B:66:ARG:HE	1:B:107:GLN:HB2	1.77	0.49
1:A:225:LYS:HZ3	1:A:230:PRO:HB3	1.77	0.49
1:B:110:TYR:CD1	1:B:161:LYS:HE2	2.48	0.49
1:B:307:ASN:CB	4:B:521:HOH:O	2.60	0.49
1:B:197:PHE:HB2	1:B:303:LEU:O	2.12	0.49
1:A:170:ARG:HD2	1:B:323:TYR:CZ	2.48	0.48
1:B:54:LEU:HD12	1:B:128:LEU:HD13	1.96	0.48
1:B:93:GLU:CD	1:B:93:GLU:H	2.22	0.48
1:B:294:LYS:N	4:B:528:HOH:O	2.47	0.47
1:B:288:LEU:HB3	1:B:292:ASP:HB2	1.96	0.47
1:B:20:GLY:HA2	1:B:48:HIS:HB3	1.97	0.47
3:B:402:FJR:N02	3:B:402:FJR:N01	2.63	0.47
1:B:132:ASP:CG	1:B:136:LYS:CG	2.88	0.46
1:B:133:GLU:HG2	1:B:134:ASN:N	2.30	0.46
1:A:251:THR:O	1:A:255:ILE:HG12	2.16	0.46
1:B:193:CYS:O	1:B:218:ALA:HA	2.15	0.46
1:A:28:GLU:OE2	1:A:226:ARG:NH1	2.48	0.46
1:B:228:VAL:HG22	1:B:305:TYR:O	2.16	0.46
1:A:126:GLU:HG3	4:A:544:HOH:O	2.16	0.45
1:B:196:TYR:O	1:B:300:ASP:OD1	2.34	0.45
1:A:270:LYS:HE2	2:A:401:NAP:H3B	1.99	0.45
1:A:174:GLU:HA	1:A:177:LEU:HD12	1.98	0.45
1:B:240:VAL:HG21	1:B:295:ALA:O	2.17	0.45
1:B:206:CYS:HB3	1:B:211:ILE:O	2.17	0.45
1:A:320:SER:HA	4:A:584:HOH:O	2.16	0.44
1:B:270:LYS:O	2:B:401:NAP:H8A	2.17	0.44
1:B:191:VAL:HB	1:B:199:ARG:HH12	1.81	0.44
1:A:105:LYS:O	1:A:107:GLN:NE2	2.49	0.44
1:A:63:LEU:O	1:A:67:SER:OG	2.33	0.44
1:B:239:PRO:HD3	4:B:510:HOH:O	2.17	0.44
1:B:194:HIS:O	1:B:197:PHE:N	2.49	0.44
1:B:196:TYR:C	4:B:513:HOH:O	2.61	0.44
1:B:194:HIS:O	1:B:195:PRO:C	2.59	0.43
1:B:226:ARG:HG2	1:B:226:ARG:H	1.37	0.43
1:B:247:LYS:HD2	1:B:248:HIS:CD2	2.53	0.43
1:A:170:ARG:HD2	1:B:323:TYR:CE2	2.54	0.43
1:A:320:SER:C	1:B:321:ASP:HB3	2.44	0.43
1:B:297:ASP:HA	4:B:507:HOH:O	2.19	0.42
1:B:240:VAL:HG11	1:B:296:ILE:N	2.34	0.42
1:A:122:LEU:HD21	3:A:402:FJR:C20	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ASP:OD2	1:A:183:LYS:NZ	2.38	0.42
1:A:33:LYS:O	1:A:37:VAL:HG22	2.20	0.42
1:B:54:LEU:HD22	1:B:86:TRP:CZ3	2.54	0.42
1:B:312:ALA:HA	1:B:317:TYR:CG	2.54	0.42
1:A:225:LYS:HD2	1:A:225:LYS:HA	1.77	0.42
1:B:134:ASN:HB2	1:B:136:LYS:NZ	2.35	0.42
1:B:195:PRO:HD2	1:B:235:LEU:CD2	2.48	0.42
1:B:219:LEU:HD21	1:B:257:LEU:HD21	2.01	0.42
1:A:22:GLY:HA3	2:A:401:NAP:H4D	2.01	0.42
1:A:309:ASP:OD1	1:A:309:ASP:N	2.53	0.41
1:B:241:LEU:O	1:B:255:ILE:HD13	2.20	0.41
1:A:197:PHE:CE1	1:A:199:ARG:HD3	2.54	0.41
2:B:401:NAP:H3D	2:B:401:NAP:O1N	2.20	0.41
1:A:170:ARG:HB3	4:A:503:HOH:O	2.19	0.41
1:B:132:ASP:OD1	1:B:136:LYS:CG	2.68	0.41
3:A:402:FJR:N02	3:A:402:FJR:N01	2.68	0.41
1:B:31:ARG:HG2	4:B:535:HOH:O	2.21	0.41
1:B:66:ARG:NE	1:B:107:GLN:HB2	2.35	0.41
1:A:54:LEU:HD22	1:A:86:TRP:CZ3	2.56	0.41
1:A:317:TYR:HE2	1:A:319:TYR:CB	2.32	0.41
1:B:132:ASP:OD1	1:B:136:LYS:HG3	2.21	0.41
1:B:14:HIS:HE1	4:B:537:HOH:O	2.04	0.41
1:B:122:LEU:HD23	1:B:122:LEU:HA	1.91	0.41
1:B:196:TYR:HE2	1:B:233:PRO:HB2	1.86	0.41
1:B:262:GLN:CD	4:B:514:HOH:O	2.65	0.40
1:B:306:PHE:HB2	4:B:519:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:586:HOH:O	4:B:579:HOH:O[1_556]	2.02	0.18

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	314/325 (97%)	306 (98%)	8 (2%)	0	100	100
1	B	316/325 (97%)	303 (96%)	13 (4%)	0	100	100
All	All	630/650 (97%)	609 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	280/288 (97%)	280 (100%)	0	100	100
1	B	282/288 (98%)	281 (100%)	1 (0%)	84	82
All	All	562/576 (98%)	561 (100%)	1 (0%)	87	86

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	226	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	B	14	HIS
1	B	222	GLN
1	B	231	ASN

5.3.3 RNA ⓘ

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](#)

4 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	FJR	A	402	-	23,24,24	1.29	3 (13%)	31,34,34	1.46	5 (16%)
2	NAP	A	401	-	50,52,52	1.19	4 (8%)	71,80,80	1.66	13 (18%)
3	FJR	B	402	-	23,24,24	1.35	3 (13%)	31,34,34	1.10	3 (9%)
2	NAP	B	401	-	50,52,52	1.35	7 (14%)	71,80,80	1.56	14 (19%)

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	FJR	A	402	-	-	2/8/8/8	0/3/3/3
2	NAP	A	401	-	-	5/35/67/67	0/5/5/5
3	FJR	B	402	-	-	0/8/8/8	0/3/3/3
2	NAP	B	401	-	-	3/35/67/67	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	C5A-C4A	4.93	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAP	PN-O3	4.84	1.64	1.59
2	B	401	NAP	C5A-C4A	4.56	1.47	1.39
3	B	402	FJR	C19-N02	4.27	1.36	1.24
3	A	402	FJR	C19-N02	4.24	1.36	1.24
3	B	402	FJR	C09-N01	-3.09	1.35	1.41
3	A	402	FJR	C09-N01	-2.76	1.36	1.41
2	B	401	NAP	C5A-C6A	2.67	1.48	1.41
2	A	401	NAP	C8A-N7A	2.65	1.36	1.31
2	A	401	NAP	C5A-C6A	2.59	1.48	1.41
2	B	401	NAP	C4A-N9A	-2.20	1.33	1.37
2	A	401	NAP	O4D-C1D	2.13	1.43	1.40
2	B	401	NAP	C8A-N7A	2.13	1.35	1.31
2	B	401	NAP	PA-O3	2.11	1.61	1.59
2	B	401	NAP	C5A-N7A	-2.11	1.35	1.39
3	B	402	FJR	C16-C15	-2.09	1.39	1.43
3	A	402	FJR	C15-C14	2.04	1.40	1.35

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAP	C5A-C4A-N3A	-5.46	119.20	126.72
2	B	401	NAP	C5A-C4A-N3A	-4.81	120.09	126.72
2	A	401	NAP	N3A-C4A-N9A	4.52	134.86	127.17
2	B	401	NAP	N3A-C4A-N9A	4.36	134.58	127.17
3	A	402	FJR	C17-O01-C19	-4.13	121.03	122.22
2	A	401	NAP	C2A-N3A-C4A	3.80	121.12	111.83
2	B	401	NAP	C4A-N9A-C8A	3.67	109.59	105.74
2	A	401	NAP	N3A-C2A-N1A	-3.66	123.03	128.58
2	A	401	NAP	C2B-C1B-N9A	-3.58	107.86	113.75
2	B	401	NAP	N3A-C2A-N1A	-3.30	123.58	128.58
2	B	401	NAP	C2A-N3A-C4A	3.22	119.69	111.83
2	A	401	NAP	C4A-N9A-C8A	3.05	108.94	105.74
2	A	401	NAP	C4A-C5A-N7A	-3.02	107.13	110.58
2	A	401	NAP	O3-PN-O1N	-2.86	102.10	110.70
2	B	401	NAP	C4A-C5A-N7A	-2.82	107.35	110.58
2	A	401	NAP	O2A-PA-O3	2.82	114.89	107.27
3	A	402	FJR	O01-C17-C03	2.71	119.31	116.21
3	A	402	FJR	C17-C16-C15	2.65	120.69	117.80
2	B	401	NAP	O2A-PA-O3	2.63	114.38	107.27
3	A	402	FJR	C14-C13-N01	2.44	119.05	115.61
2	A	401	NAP	C5A-N7A-C8A	2.31	107.08	103.45
2	B	401	NAP	C2A-N1A-C6A	2.27	122.46	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAP	C6A-C5A-N7A	2.25	136.43	132.09
2	B	401	NAP	N9A-C8A-N7A	-2.23	110.77	113.94
2	B	401	NAP	C5A-N7A-C8A	2.22	106.95	103.45
3	A	402	FJR	C15-C14-C13	2.20	120.47	118.23
2	B	401	NAP	O3-PN-O1N	-2.19	104.12	110.70
2	B	401	NAP	O3X-P2B-O2X	2.18	115.99	107.80
2	A	401	NAP	C2B-C3B-C4B	2.16	106.63	101.99
3	B	402	FJR	O01-C17-C03	2.15	118.66	116.21
2	A	401	NAP	N9A-C8A-N7A	-2.14	110.90	113.94
2	B	401	NAP	O7N-C7N-C3N	-2.10	117.03	119.60
3	B	402	FJR	C15-C14-C13	2.10	120.37	118.23
2	B	401	NAP	C3N-C7N-N7N	2.06	120.28	117.74
3	B	402	FJR	C17-C16-C15	2.05	120.04	117.80

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAP	O4D-C1D-N1N-C6N
2	B	401	NAP	O4D-C1D-N1N-C6N
2	A	401	NAP	PA-O3-PN-O5D
2	B	401	NAP	PA-O3-PN-O5D
3	A	402	FJR	C08-C09-N01-C13
3	A	402	FJR	C07-C09-N01-C13
2	B	401	NAP	C4D-C5D-O5D-PN
2	A	401	NAP	C4D-C5D-O5D-PN
2	A	401	NAP	O4D-C1D-N1N-C2N
2	A	401	NAP	C2B-C1B-N9A-C8A

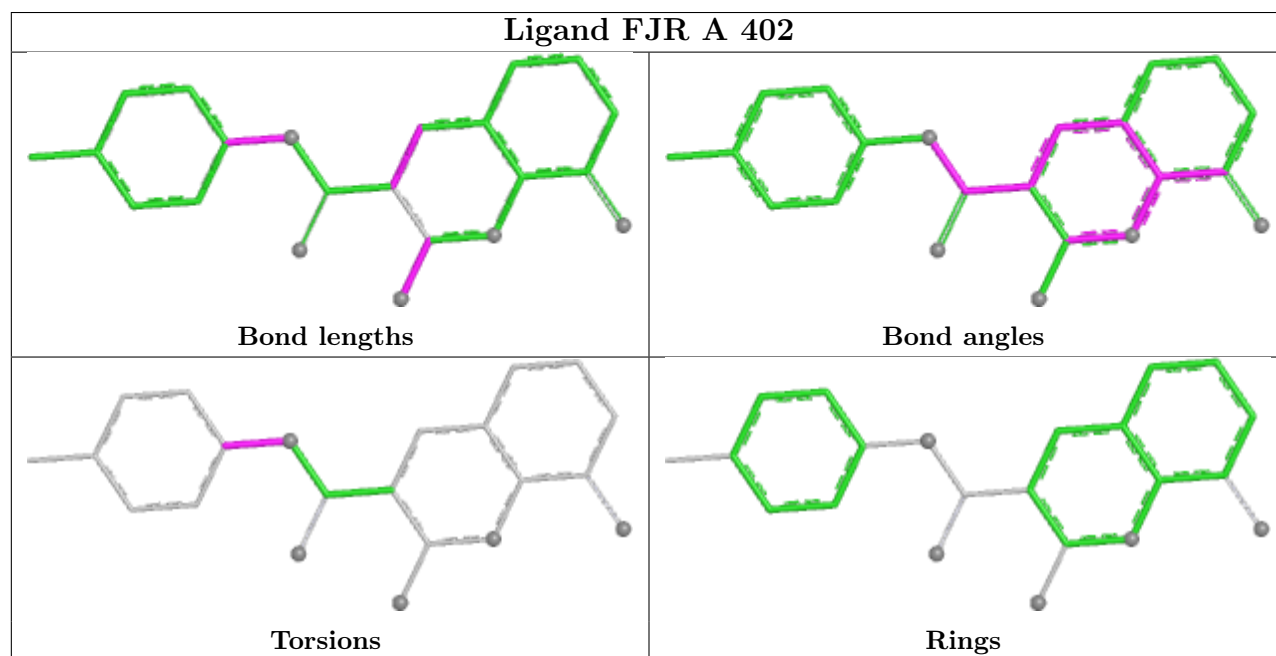
There are no ring outliers.

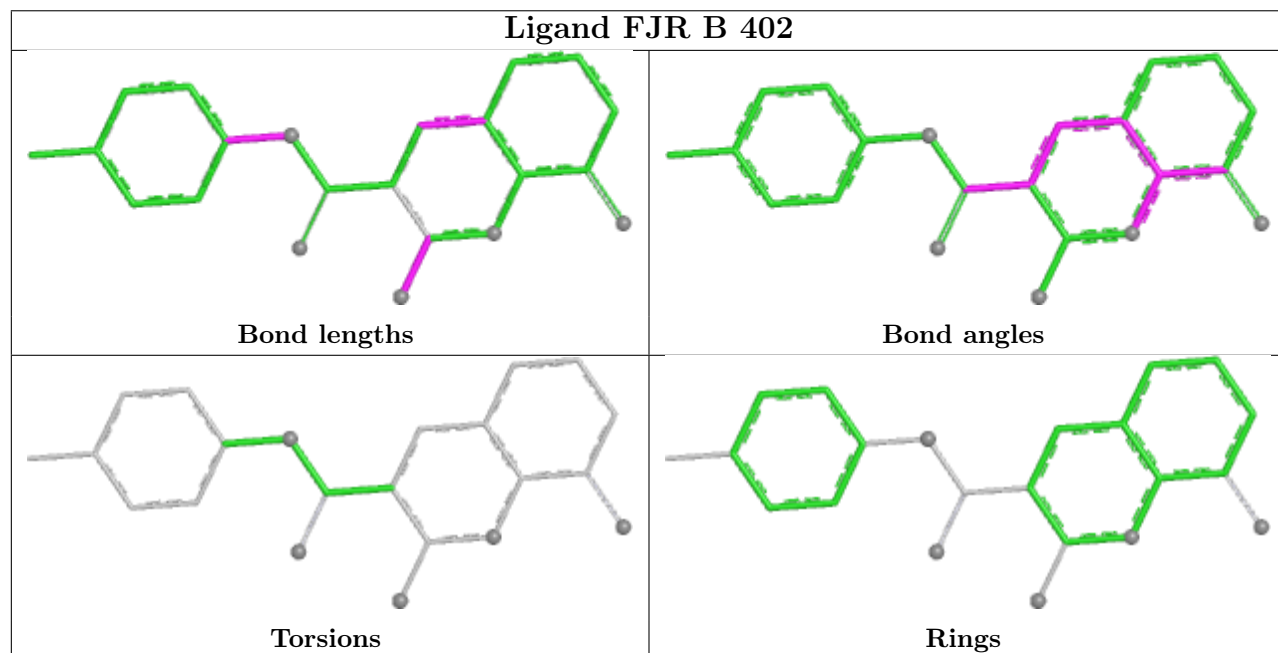
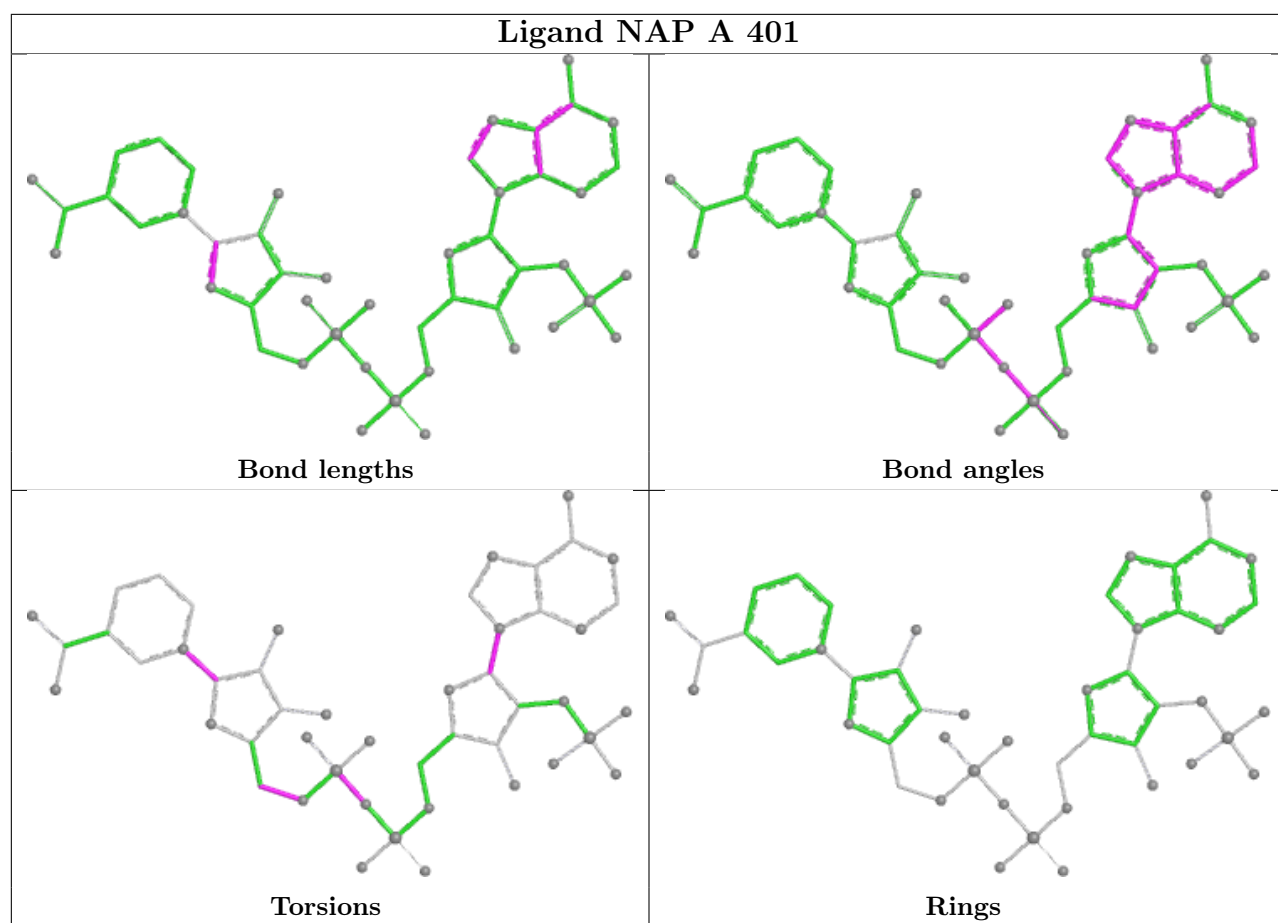
4 monomers are involved in 12 short contacts:

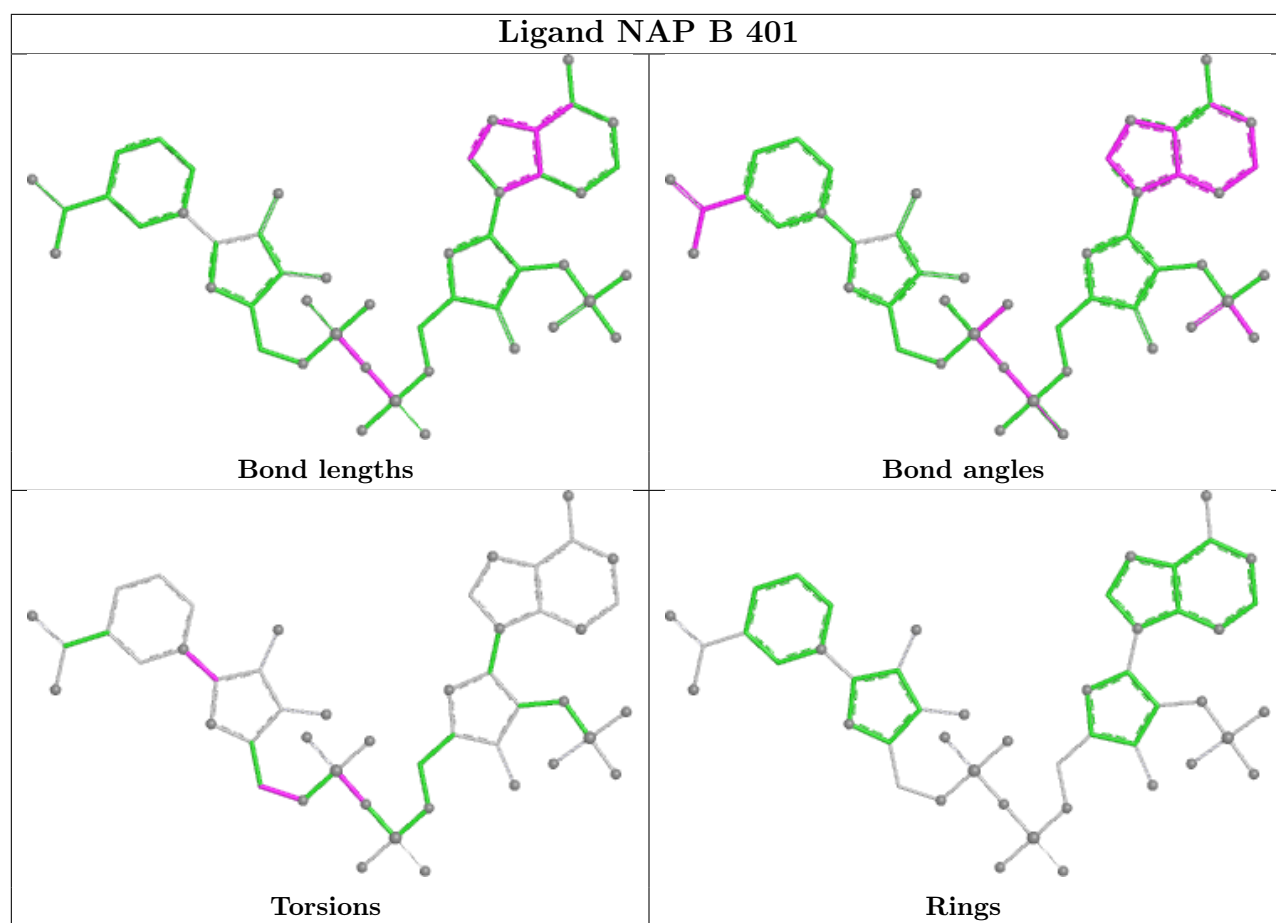
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	FJR	2	0
2	A	401	NAP	5	0
3	B	402	FJR	1	0
2	B	401	NAP	4	0

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	316/325 (97%)	0.57	13 (4%) 41 45	24, 40, 64, 76	0
1	B	318/325 (97%)	0.72	37 (11%) 9 9	21, 41, 65, 76	0
All	All	634/650 (97%)	0.65	50 (7%) 18 19	21, 40, 65, 76	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	299	LEU	4.8
1	B	236	LEU	4.0
1	A	319	TYR	3.9
1	B	296	ILE	3.8
1	B	290	ALA	3.6
1	A	320	SER	3.3
1	B	240	VAL	3.3
1	A	196	TYR	3.1
1	B	234	VAL	3.1
1	B	241	LEU	3.1
1	B	196	TYR	3.0
1	B	295	ALA	3.0
1	A	311	PHE	2.9
1	B	259	TYR	2.9
1	B	131	THR	2.9
1	A	197	PHE	2.8
1	B	244	LEU	2.7
1	B	243	ALA	2.6
1	A	107	GLN	2.6
1	B	298	GLY	2.6
1	B	253	ALA	2.6
1	B	235	LEU	2.5
1	B	289	THR	2.5
1	B	238	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	27	PRO	2.5
1	B	242	CYS	2.4
1	B	323	TYR	2.4
1	B	227	TRP	2.4
1	B	232	SER	2.4
1	B	303	LEU	2.3
1	B	305	TYR	2.3
1	B	257	LEU	2.3
1	B	251	THR	2.3
1	B	197	PHE	2.3
1	B	319	TYR	2.3
1	B	195	PRO	2.2
1	A	303	LEU	2.2
1	B	293	MET	2.2
1	A	231	ASN	2.2
1	B	304	HIS	2.2
1	B	126	GLU	2.1
1	A	313	SER	2.1
1	B	125	GLY	2.1
1	A	317	TYR	2.1
1	A	227	TRP	2.1
1	B	255	ILE	2.0
1	A	230	PRO	2.0
1	B	203	LEU	2.0
1	A	306	PHE	2.0
1	B	301	ARG	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](#)

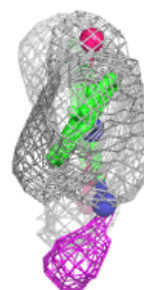
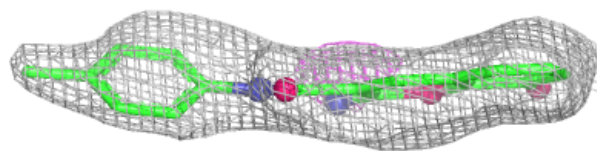
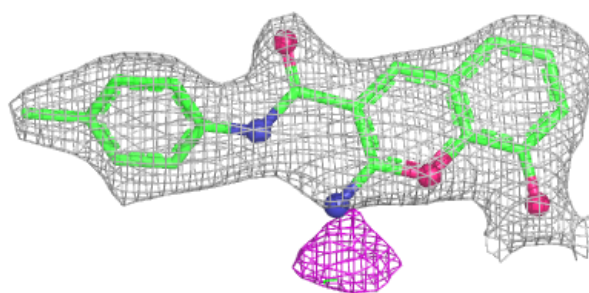
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	FJR	B	402	22/22	0.90	0.10	32,43,49,50	0
3	FJR	A	402	22/22	0.92	0.09	36,48,52,54	0
2	NAP	B	401	48/48	0.94	0.08	27,38,46,48	0
2	NAP	A	401	48/48	0.97	0.06	27,34,39,41	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.

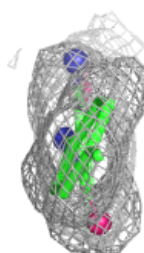
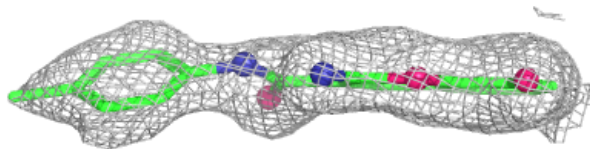
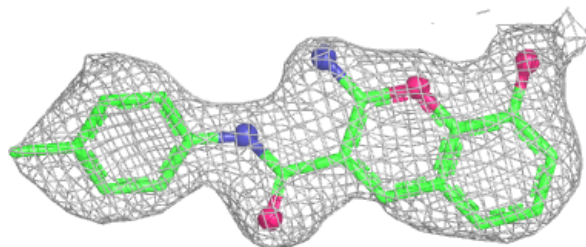
Electron density around FJR B 402:

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

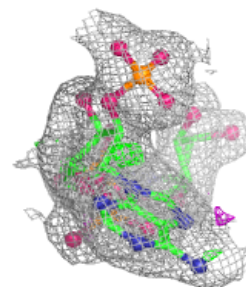
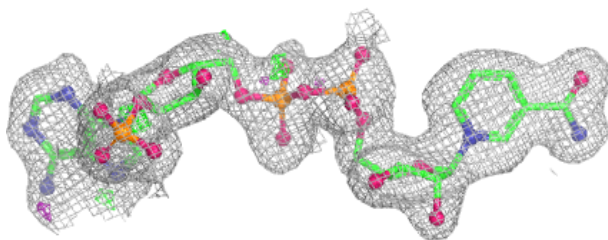
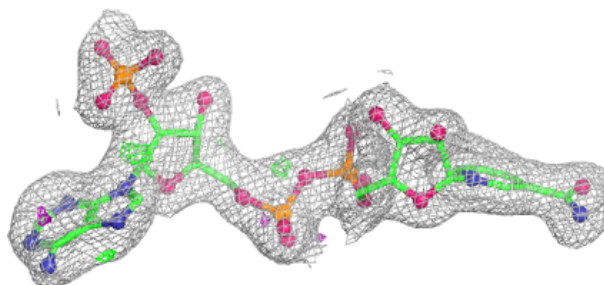


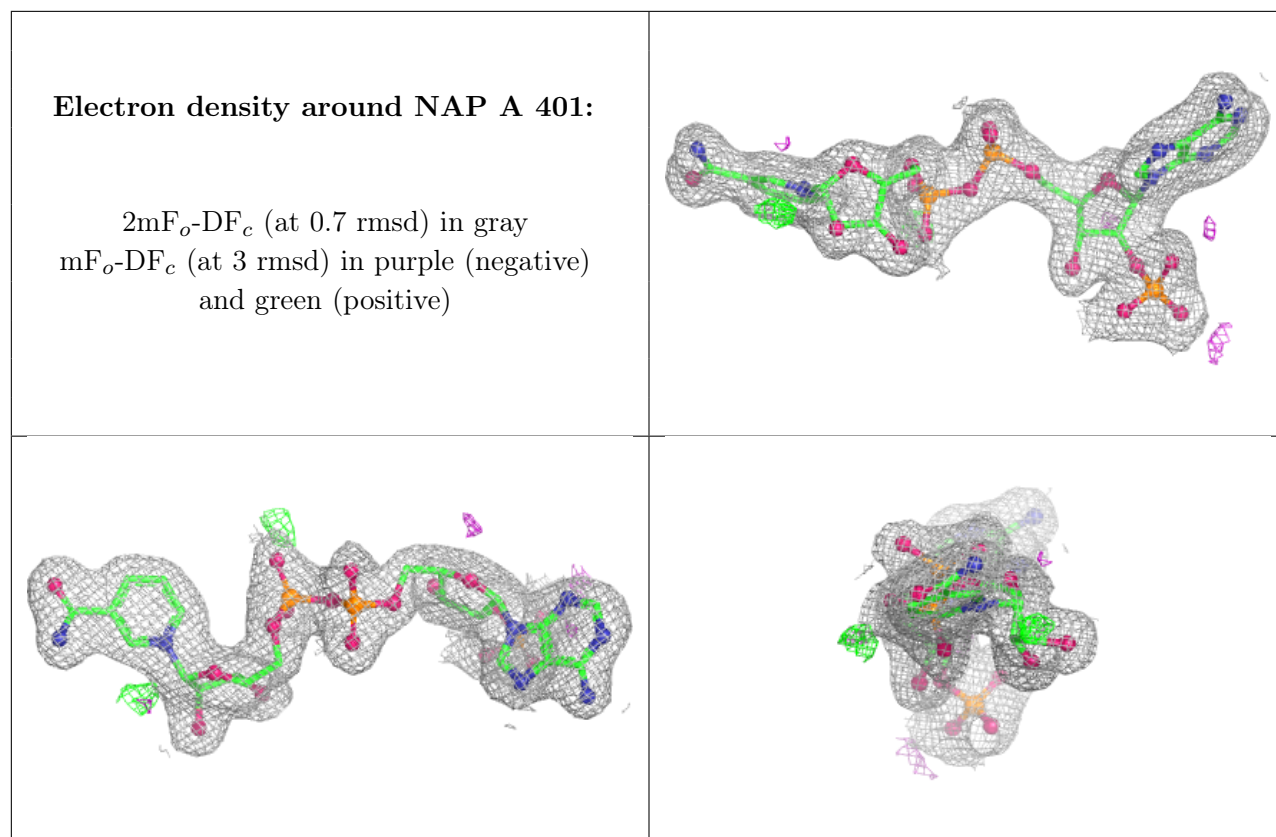
Electron density around FJR A 402:

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

**Electron density around NAP B 401:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.