



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 07:26 PM UTC

PDB ID : 7YSE / pdb_00007yse
Title : Crystal structure of E. coli heterotetrameric GlyRS in complex with tRNA
Authors : Han, L.; Ju, Y.; Zhou, H.
Deposited on : 2022-08-12
Resolution : 2.91 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

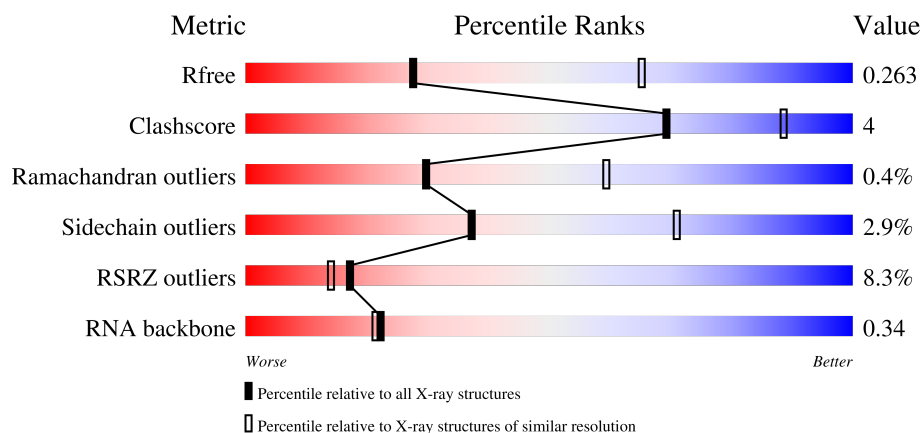
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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	303	89% 9% .
1	B	303	2% 92% 7% .
2	C	697	86% 6% 8%
2	D	697	21% 79% 12% . 8%

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Mol	Chain	Length	Quality of chain
3	E	76	3% 63% 32% 5%
3	F	76	7% 32% 43% 9% 16%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17368 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 Glycine-tRNA ligase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2386	1531	395	448	12			
1	B	299	Total	C	N	O	S	0	0	0
			2385	1528	394	451	12			

- Molecule 2 is a protein called Glycine-tRNA ligase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	641	Total	C	N	O	S	0	0	0
			4941	3134	856	934	17			
2	D	643	Total	C	N	O	S	0	0	0
			4628	2908	818	887	15			

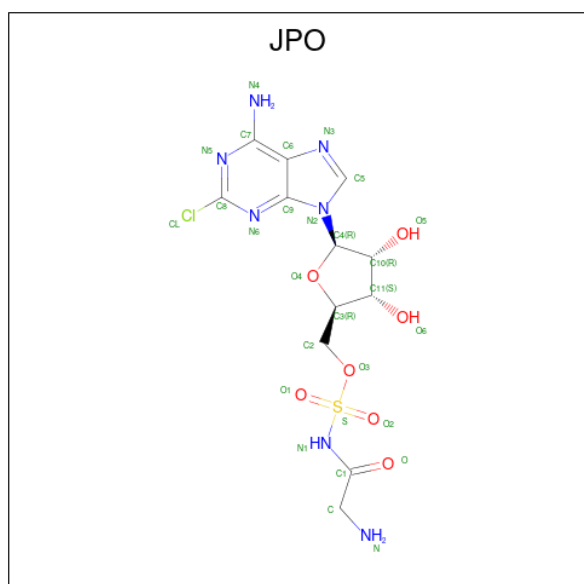
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	690	LEU	-	expression tag	UNP P00961
C	691	GLU	-	expression tag	UNP P00961
C	692	HIS	-	expression tag	UNP P00961
C	693	HIS	-	expression tag	UNP P00961
C	694	HIS	-	expression tag	UNP P00961
C	695	HIS	-	expression tag	UNP P00961
C	696	HIS	-	expression tag	UNP P00961
C	697	HIS	-	expression tag	UNP P00961
D	690	LEU	-	expression tag	UNP P00961
D	691	GLU	-	expression tag	UNP P00961
D	692	HIS	-	expression tag	UNP P00961
D	693	HIS	-	expression tag	UNP P00961
D	694	HIS	-	expression tag	UNP P00961
D	695	HIS	-	expression tag	UNP P00961
D	696	HIS	-	expression tag	UNP P00961
D	697	HIS	-	expression tag	UNP P00961

- Molecule 3 is a RNA chain called RNA (76-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	76	Total	C	N	O	P	0	0	0
			1608	714	285	533	76			
3	F	64	Total	C	N	O	P	0	0	0
			1344	594	242	444	64			

- Molecule 4 is [(2R,3S,4R,5R)-5-(6-azanyl-2-chloranyl-purin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methyl N-(2-azanylethanoyl)sulfamate (CCD ID: JPO) (formula: C₁₂H₁₆ClN₇O₇S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			28	12	1	7	7		
4	B	1	Total	C	Cl	N	O	0	0
			28	12	1	7	7		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	2	Total	Mg	0	0
			2	2		
5	D	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total 1	Mg 1	0	0

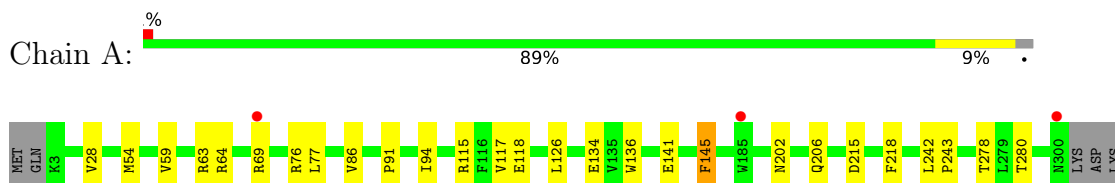
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	O 2	0	0
6	C	5	Total 5	O 5	0	0
6	D	3	Total 3	O 3	0	0
6	E	4	Total 4	O 4	0	0

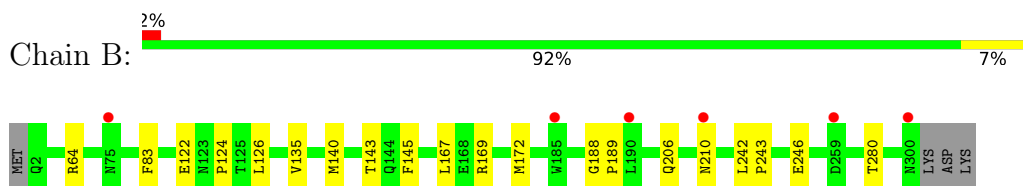
3 Residue-property plots

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.

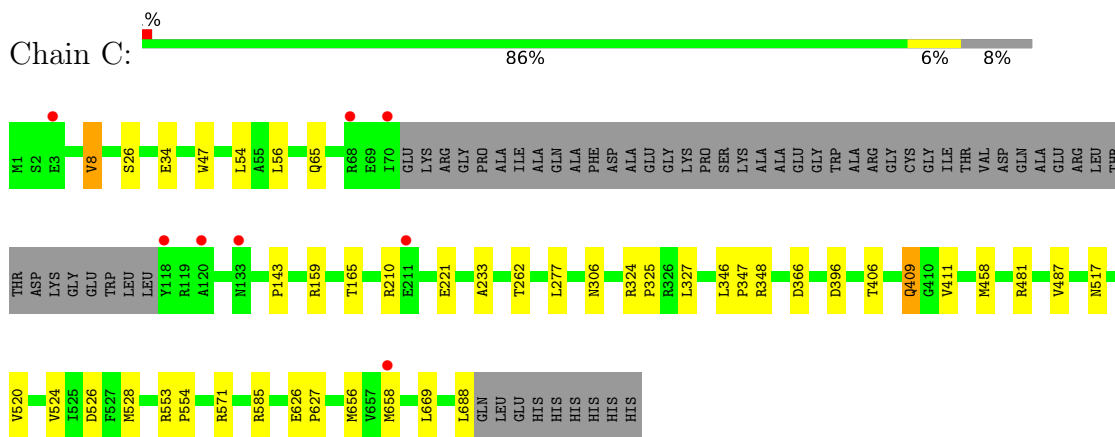
- Molecule 1: Glycine-tRNA ligase alpha subunit



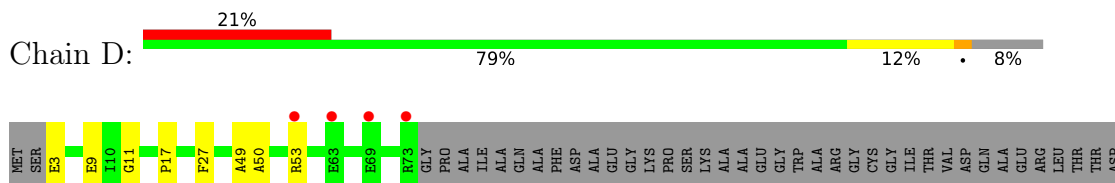
- Molecule 1: Glycine-tRNA ligase alpha subunit

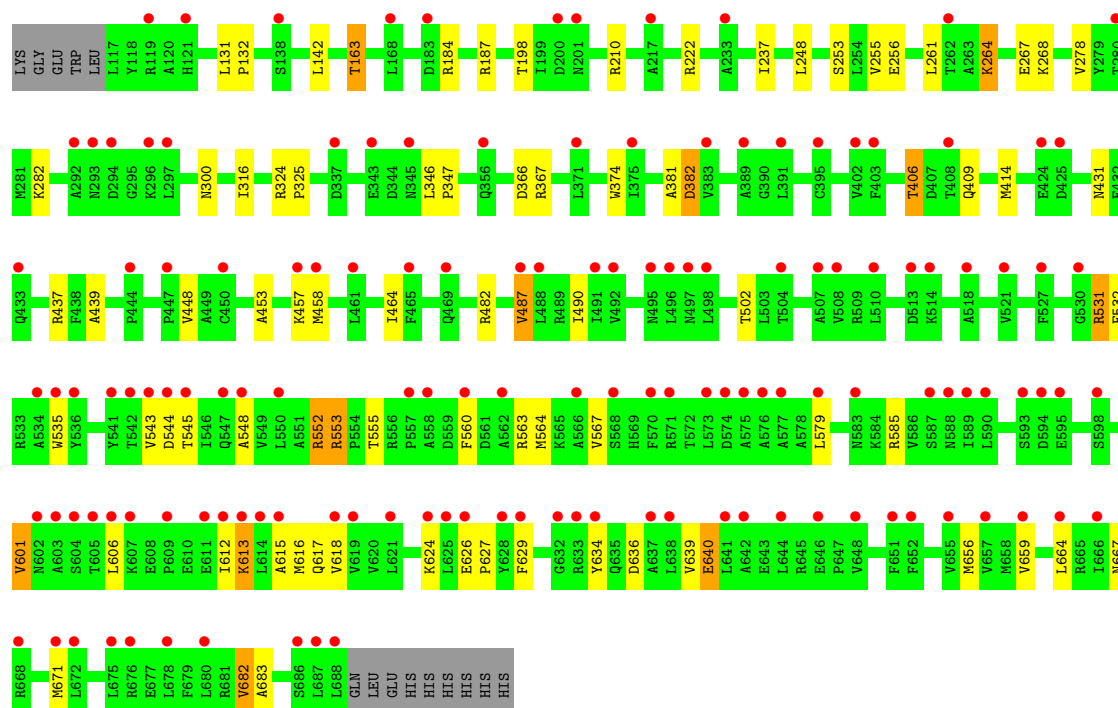


- Molecule 2: Glycine-tRNA ligase beta subunit

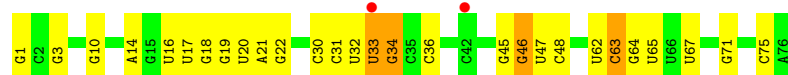


- Molecule 2: Glycine-tRNA ligase beta subunit

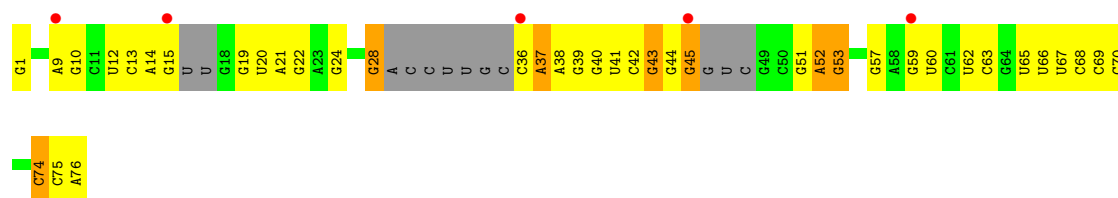




• Molecule 3: RNA (76-MER)



• Molecule 3: RNA (76-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	72.71Å 162.12Å 324.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.91 50.01 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.01-2.91) 99.9 (50.01-2.91)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.230 , 0.260 0.234 , 0.263	Depositor DCC
R_{free} test set	4395 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	72.2	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 74.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17368	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: JPO, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.97	0/2450	1.37	1/3337 (0.0%)
1	B	0.98	0/2449	1.40	0/3339
2	C	1.00	0/5027	1.50	1/6824 (0.0%)
2	D	1.08	0/4705	1.56	0/6419
3	E	0.47	1/1795 (0.1%)	0.81	4/2796 (0.1%)
3	F	0.44	1/1498 (0.1%)	0.73	0/2328
All	All	0.94	2/17924 (0.0%)	1.37	6/25043 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	G	OP3-P	6.50	1.61	1.48
3	F	1	G	OP3-P	6.37	1.61	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	46	G	C2'-C3'-O3'	5.74	118.11	109.50
3	E	3	G	C1'-C2'-O2'	5.60	116.80	108.40
2	C	366	ASP	CA-CB-CG	5.57	118.17	112.60
3	E	67	U	C1'-C2'-O2'	5.29	116.34	108.40
3	E	63	C	C3'-C2'-O2'	5.09	118.33	110.70
1	A	59	VAL	CA-C-O	-5.03	116.41	121.59

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	2386	0	2284	15	0
1	B	2385	0	2264	11	0
2	C	4941	0	4889	22	0
2	D	4628	0	4250	51	0
3	E	1608	0	814	7	0
3	F	1344	0	682	18	0
4	A	28	0	0	1	0
4	B	28	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	2	0	0	0	0
6	C	5	0	0	0	0
6	D	3	0	0	0	0
6	E	4	0	0	0	0
All	All	17368	0	15183	113	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 4.

All (113) 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)
2:D:634:TYR:HD1	2:D:682:VAL:HG22	1.17	1.08
2:D:634:TYR:CD1	2:D:682:VAL:HG22	2.04	0.92
2:D:629:PHE:HE1	2:D:682:VAL:HG23	1.52	0.74
2:D:414:MET:CB	2:D:431:ASN:HD21	2.10	0.65
2:D:659:VAL:HG21	2:D:664:LEU:HB2	1.80	0.64
2:D:545:THR:HG22	2:D:564:MET:SD	2.39	0.63
2:D:17:PRO:O	2:D:253:SER:HB2	2.02	0.59
1:B:242:LEU:HB2	1:B:243:PRO:HD3	1.86	0.57
2:C:658:MET:HE1	2:C:669:LEU:HD11	1.86	0.57
3:F:44:G:H2'	3:F:45:G:O4'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LEU:HB2	1:A:243:PRO:HD3	1.88	0.56
2:D:629:PHE:CE1	2:D:682:VAL:HG23	2.37	0.55
2:D:406:THR:HG21	3:F:74:C:H2'	1.89	0.55
2:D:629:PHE:HE1	2:D:682:VAL:CG2	2.18	0.54
1:A:54:MET:HE1	1:A:86:VAL:HG23	1.90	0.54
2:D:531:ARG:NH1	3:F:70:C:OP2	2.41	0.54
2:D:366:ASP:OD1	2:D:367:ARG:N	2.41	0.53
2:D:585:ARG:HA	3:F:37:A:O5'	2.08	0.53
2:D:601:VAL:HG21	2:D:671:MET:HG2	1.91	0.53
3:F:43:G:H2'	3:F:44:G:C8	2.44	0.53
1:B:126:LEU:HA	1:B:280:THR:HG21	1.90	0.53
2:C:233:ALA:HB1	2:C:262:THR:CG2	2.38	0.53
3:F:67:U:H2'	3:F:68:C:C6	2.44	0.53
2:D:324:ARG:HB2	2:D:325:PRO:HD3	1.91	0.52
2:C:396:ASP:OD1	2:C:409:GLN:O	2.27	0.52
2:D:264:LYS:HA	2:D:300:ASN:HA	1.92	0.52
1:A:126:LEU:HA	1:A:280:THR:HG21	1.92	0.52
2:D:545:THR:HG23	2:D:567:VAL:HB	1.90	0.52
3:F:51:G:H2'	3:F:51:G:N3	2.25	0.51
2:D:613:LYS:O	2:D:617:GLN:HG2	2.10	0.51
2:D:601:VAL:HG21	2:D:671:MET:CG	2.40	0.51
2:C:481:ARG:HD2	3:E:71:G:OP2	2.11	0.51
2:D:50:ALA:HB1	2:D:256:GLU:HG2	1.94	0.50
2:C:517:ASN:O	2:C:520:VAL:HG23	2.11	0.50
2:D:636:ASP:O	2:D:640:GLU:HG2	2.12	0.50
2:D:458:MET:HE1	2:D:487:VAL:HG21	1.93	0.49
2:D:346:LEU:N	2:D:347:PRO:HD2	2.28	0.49
3:E:33:U:H4'	3:E:34:G:OP1	2.12	0.49
1:A:134:GLU:HB2	1:A:141:GLU:HG3	1.96	0.48
2:C:626:GLU:HB3	2:C:627:PRO:HD3	1.95	0.48
2:D:53:ARG:NH1	2:D:256:GLU:OE2	2.47	0.48
2:D:548:ALA:HB1	2:D:683:ALA:HB1	1.95	0.48
1:A:215:ASP:OD1	1:A:218:PHE:HB2	2.15	0.47
2:D:612:ILE:O	2:D:616:MET:HG3	2.14	0.47
3:F:51:G:O2'	3:F:52:A:OP2	2.31	0.47
2:C:585:ARG:HG3	3:E:36:C:O2	2.15	0.47
2:D:615:ALA:HB2	2:D:671:MET:HE3	1.95	0.47
2:C:553:ARG:N	2:C:554:PRO:HD3	2.30	0.47
2:D:552:ARG:O	2:D:553:ARG:C	2.58	0.47
1:B:140:MET:HE3	1:B:169:ARG:HB3	1.96	0.46
1:A:76:ARG:C	1:A:77:LEU:HD12	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:553:ARG:O	2:D:555:THR:N	2.48	0.46
2:D:27:PHE:HB2	2:D:142:LEU:HD21	1.98	0.46
2:C:26:SER:OG	2:C:143:PRO:HD3	2.16	0.45
2:C:277:LEU:HD23	2:C:327:LEU:HD22	1.97	0.45
2:C:524:VAL:O	2:C:528:MET:HG3	2.16	0.45
2:D:543:VAL:HG11	3:F:12:U:H5'	1.99	0.45
2:D:381:ALA:O	2:D:382:ASP:C	2.59	0.45
3:F:65:U:H2'	3:F:66:U:C6	2.51	0.45
1:A:63:ARG:NH2	1:B:246:GLU:OE2	2.50	0.45
2:C:458:MET:HE1	2:C:487:VAL:HG11	1.97	0.45
2:D:616:MET:HB2	2:D:617:GLN:HE21	1.81	0.45
3:F:68:C:H2'	3:F:69:C:C6	2.51	0.45
1:B:206:GLN:O	1:B:210:ASN:ND2	2.49	0.45
2:C:571:ARG:HD3	2:C:688:LEU:HD13	1.97	0.45
2:D:606:LEU:HD23	2:D:667:ASN:HD21	1.81	0.45
1:A:202:ASN:O	1:A:206:GLN:HB2	2.17	0.44
2:D:11:GLY:HA3	2:D:163:THR:HB	1.99	0.44
1:A:91:PRO:HD2	1:A:94:ILE:HD12	1.98	0.44
2:D:656:MET:O	2:D:659:VAL:HG13	2.18	0.44
3:F:62:U:H2'	3:F:63:C:C6	2.52	0.44
2:D:49:ALA:O	2:D:222:ARG:NH2	2.48	0.44
2:D:53:ARG:NH2	2:D:187:ARG:O	2.51	0.44
3:F:28:G:N2	3:F:43:G:C4	2.86	0.44
1:A:117:VAL:HG21	1:A:136:TRP:CD2	2.53	0.43
2:C:346:LEU:N	2:C:347:PRO:CD	2.81	0.43
2:C:324:ARG:HB3	2:C:325:PRO:HD3	1.99	0.43
1:A:64:ARG:NH2	4:A:401:JPO:O1	2.50	0.43
1:A:145:PHE:C	1:A:145:PHE:CD1	2.97	0.43
1:B:135:VAL:HB	1:B:143:THR:HB	2.00	0.43
2:D:563:ARG:O	2:D:567:VAL:HG23	2.19	0.43
3:E:30:C:H2'	3:E:31:C:O4'	2.19	0.43
2:C:210:ARG:NH2	2:C:221:GLU:OE2	2.51	0.42
2:C:526:ASP:OD1	2:C:553:ARG:NH1	2.51	0.42
2:D:453:ALA:O	2:D:457:LYS:HG3	2.20	0.42
2:C:8:VAL:HA	2:C:165:THR:O	2.20	0.42
2:D:543:VAL:HG11	3:F:12:U:C5'	2.50	0.42
1:B:64:ARG:NH1	3:F:76:A:C8	2.87	0.42
1:B:188:GLY:O	1:B:189:PRO:C	2.63	0.42
2:D:634:TYR:HD1	2:D:682:VAL:CG2	2.07	0.42
3:F:44:G:C6	3:F:45:G:C5	3.08	0.42
2:D:414:MET:CB	2:D:431:ASN:ND2	2.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:GLU:C	1:B:124:PRO:HD3	2.45	0.41
2:D:374:TRP:CZ2	2:D:502:THR:HB	2.55	0.41
3:E:10:G:H2'	3:E:10:G:N3	2.34	0.41
1:A:115:ARG:HD3	2:C:306:ASN:HB2	2.02	0.41
1:B:169:ARG:O	1:B:172:MET:HB2	2.20	0.41
1:A:145:PHE:C	1:A:145:PHE:HD1	2.28	0.41
2:C:233:ALA:HB1	2:C:262:THR:HG21	2.01	0.41
2:D:278:VAL:O	2:D:282:LYS:N	2.52	0.41
2:D:437:ARG:O	2:D:482:ARG:HD3	2.20	0.41
3:F:52:A:H2'	3:F:53:G:O4'	2.21	0.41
1:A:118:GLU:OE2	2:C:159:ARG:NH2	2.53	0.40
3:E:64:G:H2'	3:E:65:U:O4'	2.20	0.40
3:F:36:C:H2'	3:F:37:A:C5	2.56	0.40
2:D:626:GLU:N	2:D:627:PRO:HD2	2.37	0.40
3:E:62:U:H2'	3:E:63:C:H6	1.86	0.40
2:C:47:TRP:HA	2:C:56:LEU:HD23	2.03	0.40
2:D:184:ARG:O	2:D:198:THR:HA	2.21	0.40
2:D:374:TRP:HZ2	2:D:502:THR:HB	1.87	0.40
1:B:83:PHE:HB2	1:B:167:LEU:HD21	2.04	0.40
2:D:616:MET:HB2	2:D:617:GLN:NE2	2.37	0.40
2:D:131:LEU:O	2:D:132:PRO:C	2.63	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	296/303 (98%)	288 (97%)	8 (3%)	0	100	100
1	B	297/303 (98%)	285 (96%)	12 (4%)	0	100	100
2	C	637/697 (91%)	618 (97%)	18 (3%)	1 (0%)	43	72
2	D	639/697 (92%)	561 (88%)	71 (11%)	7 (1%)	11	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1869/2000 (94%)	1752 (94%)	109 (6%)	8 (0%)	30 59

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	382	ASP
2	C	409	GLN
2	D	409	GLN
2	D	439	ALA
2	D	544	ASP
2	D	553	ARG
2	D	682	VAL
2	D	618	VAL

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	250/261 (96%)	246 (98%)	4 (2%)	55 83
1	B	249/261 (95%)	248 (100%)	1 (0%)	84 94
2	C	506/574 (88%)	498 (98%)	8 (2%)	55 83
2	D	417/574 (73%)	389 (93%)	28 (7%)	15 43
All	All	1422/1670 (85%)	1381 (97%)	41 (3%)	37 71

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	69	ARG
1	A	145	PHE
1	A	278	THR
1	B	145	PHE
2	C	8	VAL
2	C	34	GLU

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Mol	Chain	Res	Type
2	C	54	LEU
2	C	65	GLN
2	C	348	ARG
2	C	406	THR
2	C	411	VAL
2	C	656	MET
2	D	3	GLU
2	D	9	GLU
2	D	163	THR
2	D	210	ARG
2	D	237	ILE
2	D	248	LEU
2	D	255	VAL
2	D	261	LEU
2	D	264	LYS
2	D	267	GLU
2	D	268	LYS
2	D	316	ILE
2	D	406	THR
2	D	448	VAL
2	D	464	ILE
2	D	487	VAL
2	D	490	ILE
2	D	531	ARG
2	D	532	PHE
2	D	535	TRP
2	D	552	ARG
2	D	560	PHE
2	D	579	LEU
2	D	601	VAL
2	D	613	LYS
2	D	624	LYS
2	D	639	VAL
2	D	640	GLU

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	95	GLN
1	A	123	ASN
1	A	144	GLN
1	A	202	ASN

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Mol	Chain	Res	Type
1	B	29	GLN
1	B	75	ASN
1	B	123	ASN
2	C	385	HIS
2	C	547	GLN
2	C	569	HIS
2	D	240	ASN
2	D	385	HIS
2	D	431	ASN
2	D	435	GLN
2	D	501	GLN
2	D	617	GLN
2	D	667	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	75/76 (98%)	16 (21%)	1 (1%)
3	F	60/76 (78%)	26 (43%)	0
All	All	135/152 (88%)	42 (31%)	1 (0%)

All (42) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	E	14	A
3	E	16	U
3	E	17	U
3	E	18	G
3	E	19	G
3	E	20	U
3	E	21	A
3	E	22	G
3	E	32	U
3	E	33	U
3	E	34	G
3	E	45	G
3	E	46	G
3	E	47	U
3	E	48	C
3	E	75	C
3	F	9	A

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Mol	Chain	Res	Type
3	F	10	G
3	F	13	C
3	F	14	A
3	F	15	G
3	F	19	G
3	F	20	U
3	F	21	A
3	F	22	G
3	F	24	G
3	F	28	G
3	F	37	A
3	F	38	A
3	F	39	G
3	F	40	G
3	F	41	U
3	F	42	C
3	F	43	G
3	F	45	G
3	F	52	A
3	F	53	G
3	F	57	G
3	F	59	G
3	F	60	U
3	F	74	C
3	F	75	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	E	46	G

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

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	JPO	B	401	-	29,30,30	0.26	0	40,45,45	0.35	0
4	JPO	A	401	-	29,30,30	0.27	0	40,45,45	0.33	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
4	JPO	B	401	-	-	6/16/33/33	0/3/3/3
4	JPO	A	401	-	-	3/16/33/33	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

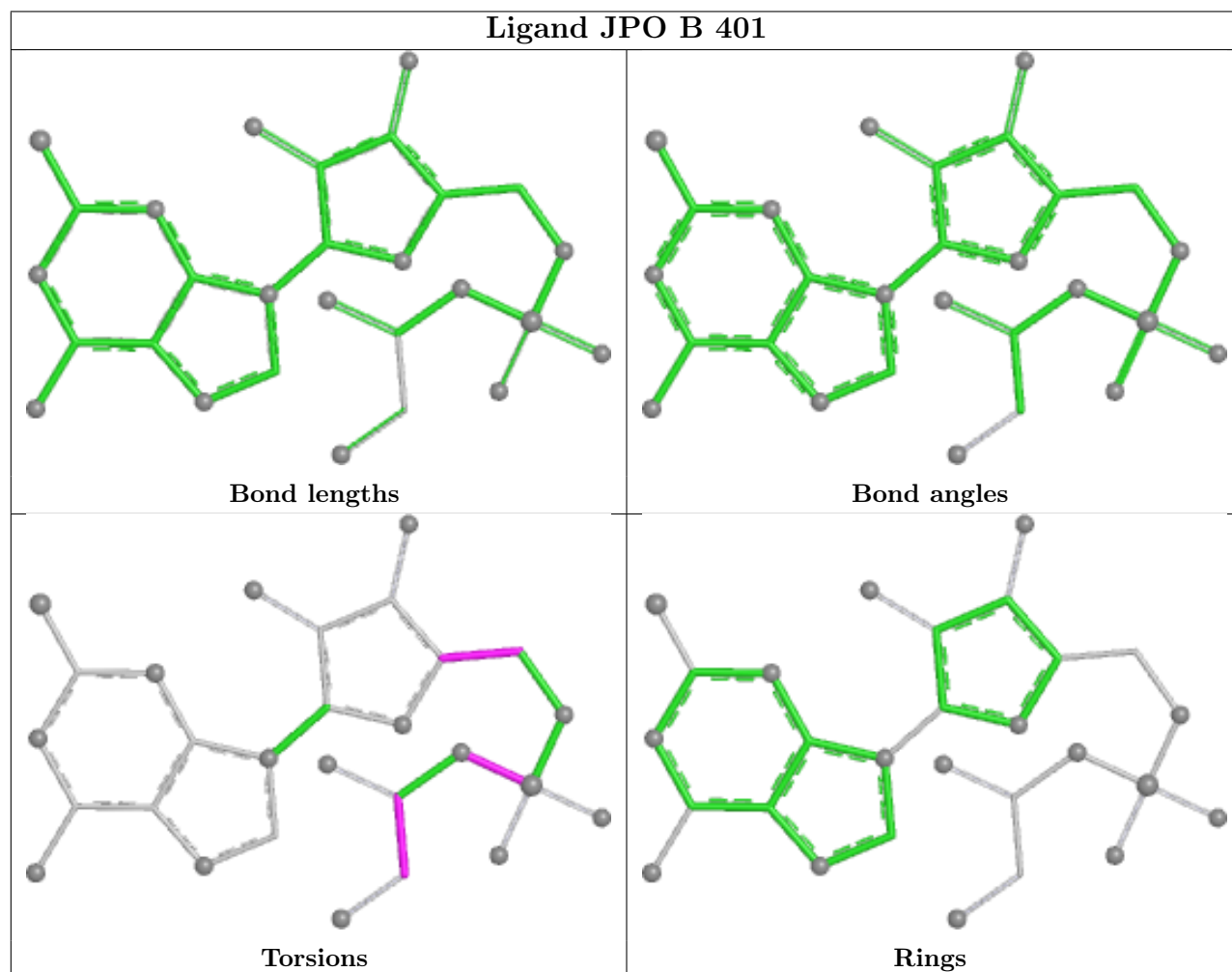
Mol	Chain	Res	Type	Atoms
4	A	401	JPO	O3-C2-C3-O4
4	A	401	JPO	O3-C2-C3-C11
4	A	401	JPO	C1-N1-S-O2
4	B	401	JPO	N-C-C1-N1
4	B	401	JPO	O3-C2-C3-O4
4	B	401	JPO	O3-C2-C3-C11
4	B	401	JPO	C1-N1-S-O1
4	B	401	JPO	N-C-C1-O
4	B	401	JPO	C1-N1-S-O2

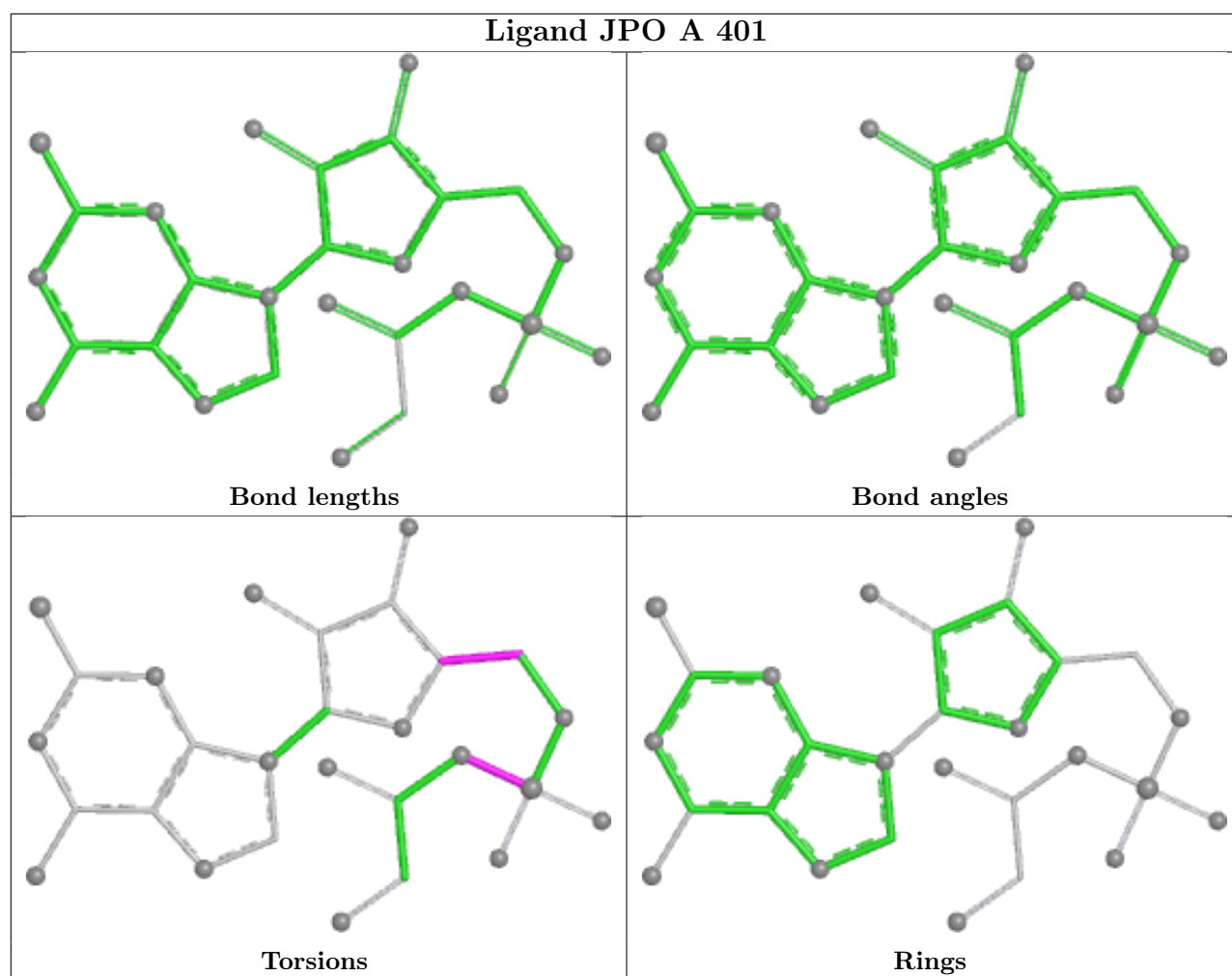
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	JPO	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	298/303 (98%)	0.12	3 (1%) 79 73	45, 61, 89, 118	0
1	B	299/303 (98%)	0.23	6 (2%) 65 56	53, 75, 100, 119	0
2	C	641/697 (91%)	0.17	8 (1%) 76 69	45, 65, 88, 143	0
2	D	643/697 (92%)	1.31	143 (22%) 2 2	74, 115, 146, 163	0
3	E	76/76 (100%)	0.13	2 (2%) 57 48	43, 76, 147, 168	0
3	F	64/76 (84%)	0.76	5 (7%) 19 16	74, 135, 182, 198	0
All	All	2021/2152 (93%)	0.55	167 (8%) 17 14	43, 76, 141, 198	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	615	ALA	7.8
2	D	688	LEU	6.1
2	D	605	THR	6.0
2	D	641	LEU	6.0
2	D	604	SER	5.8
2	D	450	CYS	5.4
2	D	73	ARG	5.2
2	D	614	LEU	5.2
2	D	633	ARG	5.0
2	D	686	SER	4.9
2	D	611	GLU	4.8
1	A	300	ASN	4.6
2	D	651	PHE	4.5
2	C	70	ILE	4.4
2	D	402	VAL	4.2
2	D	602	ASN	4.1
2	D	574	ASP	4.0
2	D	672	LEU	4.0
2	D	606	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	634	TYR	3.9
2	D	487	VAL	3.9
2	C	118	TYR	3.8
2	D	573	LEU	3.7
2	D	589	ILE	3.7
3	F	59	G	3.6
2	D	465	PHE	3.5
2	D	513	ASP	3.5
2	D	504	THR	3.4
2	D	375	ILE	3.4
2	D	575	ALA	3.4
1	B	300	ASN	3.4
2	D	492	VAL	3.4
2	D	294	ASP	3.4
2	D	652	PHE	3.4
2	D	293	ASN	3.3
2	D	687	LEU	3.3
2	D	632	GLY	3.3
2	D	570	PHE	3.3
2	D	403	PHE	3.2
2	D	547	GLN	3.2
2	D	666	ILE	3.2
2	D	542	THR	3.2
2	D	183	ASP	3.2
2	D	678	LEU	3.1
2	D	548	ALA	3.1
2	D	657	VAL	3.1
2	D	642	ALA	3.1
2	D	618	VAL	3.1
2	D	648	VAL	3.1
2	C	68	ARG	3.1
2	D	507	ALA	3.0
2	D	544	ASP	3.0
2	D	625	LEU	3.0
2	D	576	ALA	3.0
2	D	680	LEU	3.0
2	D	603	ALA	3.0
2	D	469	GLN	2.9
2	D	296	LYS	2.9
2	D	588	ASN	2.9
2	D	510	LEU	2.9
2	D	595	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	629	PHE	2.9
2	D	521	VAL	2.9
2	D	383	VAL	2.8
2	D	508	VAL	2.8
1	B	190	LEU	2.8
2	D	498	LEU	2.8
1	B	75	ASN	2.8
2	D	593	SER	2.8
2	D	624	LYS	2.8
2	D	536	TYR	2.8
2	D	562	ALA	2.8
2	D	568	SER	2.8
1	A	185	TRP	2.7
2	D	577	ALA	2.7
2	D	579	LEU	2.7
2	D	425	ASP	2.7
2	D	395	CYS	2.7
2	D	566	ALA	2.7
2	D	637	ALA	2.7
2	D	613	LYS	2.7
1	A	69	ARG	2.7
2	D	121	HIS	2.7
2	D	583	ASN	2.7
2	D	594	ASP	2.7
2	D	262	THR	2.6
2	D	433	GLN	2.6
2	D	461	LEU	2.6
2	D	488	LEU	2.6
2	D	543	VAL	2.6
2	D	659	VAL	2.6
2	D	535	TRP	2.6
2	D	676	ARG	2.5
3	F	9	A	2.5
2	D	541	TYR	2.5
2	D	612	ILE	2.5
2	D	534	ALA	2.5
2	D	598	SER	2.5
2	D	557	PRO	2.5
2	D	280	THR	2.5
2	C	120	ALA	2.5
2	D	497	ASN	2.5
2	D	628	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	233	ALA	2.5
2	D	664	LEU	2.5
2	D	646	GLU	2.5
2	D	217	ALA	2.5
2	C	658	MET	2.4
2	D	391	LEU	2.4
2	D	621	LEU	2.4
2	D	671	MET	2.4
2	D	675	LEU	2.4
2	D	491	ILE	2.4
2	D	69	GLU	2.4
3	E	42	C	2.4
2	D	447	PRO	2.4
2	D	655	VAL	2.4
2	D	63	GLU	2.4
2	D	337	ASP	2.4
2	D	571	ARG	2.4
1	B	185	TRP	2.4
2	D	292	ALA	2.4
2	D	389	ALA	2.3
2	D	297	LEU	2.3
2	D	590	LEU	2.3
2	D	644	LEU	2.3
2	C	133	ASN	2.3
2	D	626	GLU	2.3
1	B	259	ASP	2.3
3	E	33	U	2.3
2	D	560	PHE	2.3
2	D	200	ASP	2.3
2	D	607	LYS	2.3
2	D	201	ASN	2.2
2	D	424	GLU	2.2
2	D	550	LEU	2.2
2	D	138	SER	2.2
2	D	527	PHE	2.2
2	D	343	GLU	2.2
1	B	210	ASN	2.2
2	D	408	THR	2.2
2	D	495	ASN	2.2
3	F	36	C	2.2
2	D	587	SER	2.2
2	D	457	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	53	ARG	2.2
2	D	444	PRO	2.2
2	D	496	LEU	2.2
2	D	558	ALA	2.2
2	D	345	ASN	2.1
3	F	45	G	2.1
2	D	371	LEU	2.1
2	D	609	PRO	2.1
2	D	545	THR	2.1
2	C	3	GLU	2.1
2	C	211	GLU	2.1
2	D	356	GLN	2.1
2	D	518	ALA	2.1
2	D	168	LEU	2.0
2	D	530	GLY	2.0
2	D	638	LEU	2.0
2	D	119	ARG	2.0
2	D	668	ARG	2.0
2	D	514	LYS	2.0
3	F	15	G	2.0
2	D	458	MET	2.0
2	D	619	VAL	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
5	MG	A	402	1/1	0.88	0.32	58,58,58,58	0

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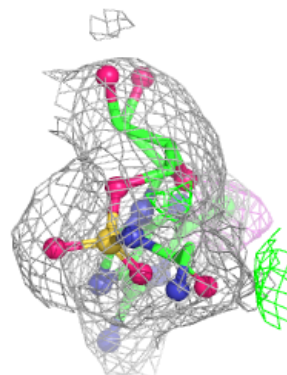
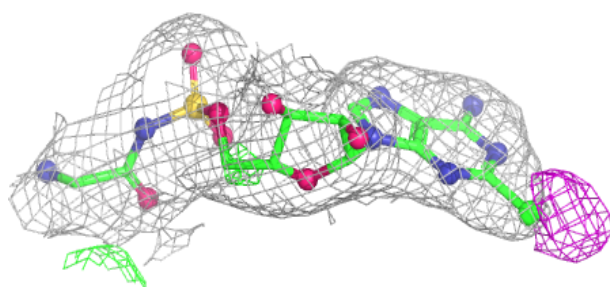
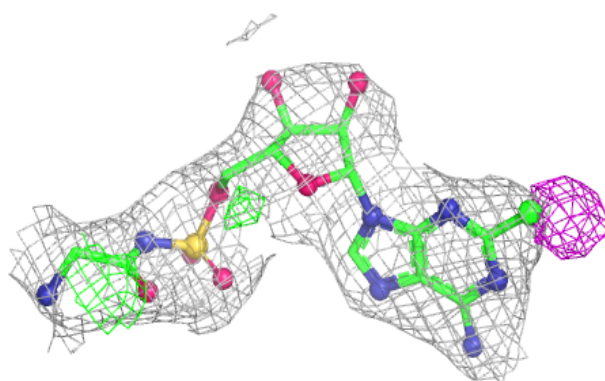
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	D	701	1/1	0.89	0.22	84,84,84,84	0
4	JPO	B	401	28/28	0.92	0.12	76,84,86,97	0
5	MG	B	402	1/1	0.95	0.21	65,65,65,65	0
4	JPO	A	401	28/28	0.95	0.12	62,71,76,84	0
5	MG	E	101	1/1	0.95	0.53	68,68,68,68	0
5	MG	C	701	1/1	0.96	0.39	75,75,75,75	0
5	MG	C	702	1/1	0.96	0.26	64,64,64,64	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.

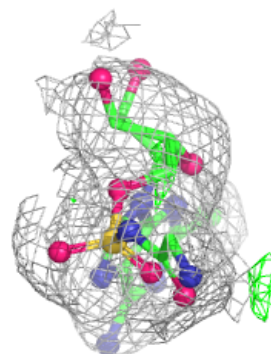
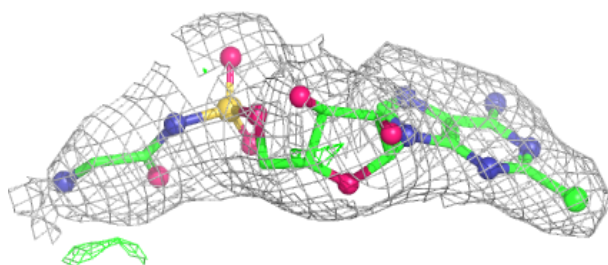
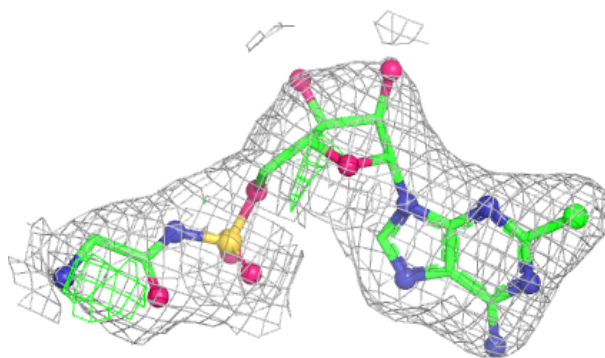
Electron density around JPO B 401:

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



Electron density around JPO A 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.