



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:54 AM EDT

PDB ID : 5RM8 / pdb_00005rm8
Title : PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 heli-
case in complex with Z1614545742
Authors : Newman, J.A.; Yosaatmadja, Y.; Douangamath, A.; Aimon, A.; Powell, A.J.;
Dias, A.; Fearon, D.; Dunnett, L.; Brandao-Neto, J.; Krojer, T.; Skyner, R.;
Gorrie-Stone, T.; Thompson, W.; von Delft, F.; Arrowsmith, C.H.; Edwards,
A.; Bountra, C.; Gileadi, O.
Deposited on : 2020-09-16
Resolution : 2.14 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)

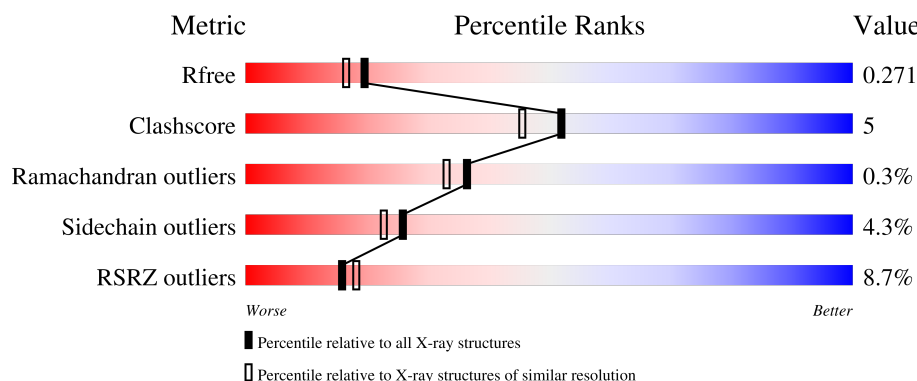
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	601	
1	B	601	

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

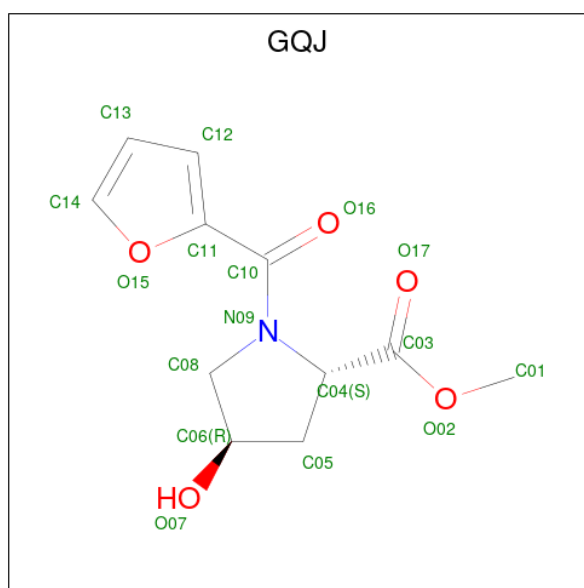
There are 5 unique types of molecules in this entry. The entry contains 9424 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	0
			4417	2816	737	832	32			
1	B	585	Total	C	N	O	S	0	1	0
			4508	2875	750	848	35			

- Molecule 2 is methyl (2 {S},4 {R})-1-(furan-2-ylcarbonyl)-4-oxidanyl-pyrrolidine-2-carboxylate (CCD ID: GQJ) (formula: C₁₁H₁₃NO₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	11	1	5		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Zn	0	0
			3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Zn	0	0
			3	3		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	204	Total	O	0	0
			204	204		
5	B	252	Total	O	0	0
			252	252		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.25Å 70.28Å 85.49Å 102.90° 96.06° 112.34°	Depositor
Resolution (Å)	81.46 – 2.14 81.46 – 2.14	Depositor EDS
% Data completeness (in resolution range)	96.6 (81.46-2.14) 96.6 (81.46-2.14)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.14Å)	Xtriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, R_{free}	0.167 , 0.248 0.193 , 0.271	Depositor DCC
R_{free} test set	3345 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9424	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.89	1/4517 (0.0%)	1.15	14/6156 (0.2%)
1	B	0.89	0/4610	1.14	15/6283 (0.2%)
All	All	0.89	1/9127 (0.0%)	1.14	29/12439 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	474	MET	CA-C	-5.44	1.46	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	VAL	CA-C-N	8.00	130.99	120.28
1	B	103	VAL	C-N-CA	8.00	130.99	120.28
1	A	466	ASP	CA-CB-CG	7.52	120.12	112.60
1	A	256	LEU	N-CA-C	-7.21	104.11	113.12
1	A	591	GLU	CA-C-N	6.45	133.31	121.70
1	A	591	GLU	C-N-CA	6.45	133.31	121.70
1	B	45	VAL	N-CA-C	-6.33	104.33	110.72
1	A	179	ASN	CA-CB-CG	6.22	118.82	112.60
1	B	214	THR	CA-C-N	6.09	133.17	121.54
1	B	214	THR	C-N-CA	6.09	133.17	121.54
1	B	319	GLU	CB-CG-CD	6.05	122.88	112.60
1	B	373	PHE	CA-CB-CG	5.70	119.50	113.80
1	A	183	THR	CB-CA-C	5.65	119.46	110.19
1	B	561	PHE	CA-CB-CG	-5.62	108.18	113.80
1	A	587	PHE	CA-CB-CG	5.60	119.40	113.80
1	B	507	ARG	CG-CD-NE	-5.59	99.70	112.00
1	B	464	HIS	N-CA-C	-5.54	106.19	113.12
1	A	561	PHE	CA-CB-CG	-5.54	108.26	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	ASN	CA-CB-CG	5.34	117.94	112.60
1	B	580	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	373	PHE	CA-CB-CG	5.26	119.06	113.80
1	B	350	SER	CA-C-N	5.20	127.97	120.38
1	B	350	SER	C-N-CA	5.20	127.97	120.38
1	B	95	ASN	CA-CB-CG	5.19	117.79	112.60
1	A	516	ASN	CA-CB-CG	5.18	117.78	112.60
1	A	405	LEU	N-CA-C	5.17	116.39	109.83
1	B	174	PRO	O-C-N	5.12	123.56	121.15
1	A	314	VAL	CA-C-N	5.04	127.04	120.28
1	A	314	VAL	C-N-CA	5.04	127.04	120.28

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	4417	0	4322	50	0
1	B	4508	0	4425	41	0
2	A	17	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	10	0	0	1	0
4	B	10	0	0	0	0
5	A	204	0	0	1	0
5	B	252	0	0	2	0
All	All	9424	0	8747	90	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 5.

All (90) 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:27:CYS:SG	5:B:899:HOH:O	2.18	1.01
1:A:326:PRO:HB2	1:A:329:LYS:HZ3	1.53	0.74
1:A:326:PRO:HG2	1:A:329:LYS:NZ	2.05	0.72
1:B:12:THR:HG21	1:B:26:CYS:HA	1.73	0.69
1:A:12:THR:HG21	1:A:26:CYS:HA	1.73	0.69
1:B:162:GLU:HG2	1:B:210:VAL:HG22	1.74	0.69
1:A:331:SER:HB2	1:A:353:GLU:HG3	1.77	0.67
1:B:163:LEU:HD11	1:B:219:LEU:HD11	1.75	0.66
1:A:163:LEU:HD11	1:A:200:PHE:HE2	1.63	0.64
1:A:326:PRO:HG2	1:A:329:LYS:HZ1	1.65	0.61
1:B:13:SER:O	1:B:44:SER:HA	2.00	0.61
1:A:158:LEU:HD11	1:A:164:HIS:CE1	2.37	0.59
1:A:326:PRO:CB	1:A:329:LYS:HZ3	2.16	0.57
1:A:579:ARG:HG2	5:A:973:HOH:O	2.05	0.56
1:B:228:THR:HG22	1:B:230:HIS:CE1	2.40	0.56
1:B:12:THR:CG2	1:B:26:CYS:HA	2.36	0.56
1:B:474[B]:MET:HG2	1:B:590:LEU:HB2	1.87	0.56
1:B:157:VAL:HG23	1:B:221:VAL:HG23	1.89	0.55
1:A:12:THR:CG2	1:A:26:CYS:HA	2.38	0.54
1:A:326:PRO:HB2	1:A:329:LYS:NZ	2.23	0.53
1:B:510:VAL:HG21	1:B:541:TYR:CD1	2.43	0.53
1:B:16:CYS:O	1:B:22:ARG:HA	2.09	0.52
1:A:498:GLU:HG3	1:A:502:ARG:NH2	2.24	0.52
1:A:132:LEU:O	1:A:136:GLU:HG3	2.10	0.52
1:A:176:LEU:HD22	1:A:200:PHE:HB2	1.92	0.51
1:B:100:SER:HB2	1:B:103:VAL:HG23	1.92	0.51
1:B:511:PHE:HB3	1:B:530:THR:HG22	1.93	0.50
1:A:163:LEU:HD11	1:A:200:PHE:CE2	2.45	0.49
1:B:371:VAL:HG23	1:B:393:ALA:HB2	1.94	0.49
1:A:326:PRO:CG	1:A:329:LYS:HZ3	2.26	0.49
1:B:451:THR:HG21	1:B:585:LEU:HD23	1.95	0.49
1:B:279:THR:HB	1:B:429:MET:CE	2.43	0.49
1:A:326:PRO:HG2	1:A:329:LYS:HZ3	1.76	0.48
1:A:244:GLU:HB2	1:A:276:LYS:HB2	1.95	0.48
1:A:510:VAL:HG21	1:A:541:TYR:CD1	2.47	0.48
1:B:15:ARG:HG3	1:B:24:PHE:CD2	2.49	0.48
1:A:326:PRO:CG	1:A:329:LYS:NZ	2.76	0.48
1:B:228:THR:HG22	1:B:230:HIS:NE2	2.29	0.48
1:A:16:CYS:O	1:A:22:ARG:HA	2.13	0.47
1:A:215:THR:HG22	1:B:193:VAL:HG21	1.96	0.47
1:B:8:CYS:SG	1:B:99:GLY:N	2.87	0.47
1:B:279:THR:HB	1:B:429:MET:HE2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:TYR:HE2	1:A:211:TYR:HD1	1.61	0.47
1:A:371:VAL:HG23	1:A:393:ALA:HB2	1.96	0.47
1:A:140:ALA:HA	1:A:232:VAL:HG21	1.96	0.47
1:A:519:ASN:HB3	1:A:530:THR:CG2	2.45	0.47
1:B:195:ILE:HG23	1:B:195:ILE:O	2.15	0.47
1:B:480:ILE:HD11	5:B:838:HOH:O	2.14	0.46
1:B:196:GLY:HA3	1:B:215:THR:HG21	1.98	0.46
1:A:531:GLN:HG3	1:A:535:SER:OG	2.15	0.46
1:A:120:TYR:CE2	1:A:409:ARG:HG2	2.51	0.46
1:A:7:LEU:HD13	1:A:103:VAL:HG22	1.97	0.46
1:B:65:LEU:HD23	1:B:81:PHE:CZ	2.51	0.46
1:A:451:THR:HG21	1:A:585:LEU:HD23	1.99	0.45
1:B:185:TYR:CE2	1:B:194:GLN:HG2	2.51	0.45
1:A:14:LEU:HB2	1:A:25:LEU:O	2.17	0.45
1:B:77:PRO:HB2	1:B:78:PRO:HD2	1.98	0.45
1:B:244:GLU:HB2	1:B:276:LYS:HB2	1.99	0.45
1:A:279:THR:HB	1:A:429:MET:CE	2.46	0.45
1:A:280:LEU:HD11	1:A:438:LEU:HG	1.99	0.45
1:B:445:PRO:HB3	1:B:468:SER:HB3	1.99	0.45
1:B:13:SER:HB3	1:B:92:LEU:HB2	1.99	0.45
1:A:158:LEU:HD11	1:A:164:HIS:ND1	2.32	0.45
1:A:445:PRO:HB3	1:A:468:SER:HB3	1.98	0.44
1:A:284:PRO:HA	4:A:706:PO4:O2	2.18	0.44
1:A:519:ASN:HB3	1:A:530:THR:HG23	1.99	0.44
1:B:14:LEU:HB2	1:B:25:LEU:O	2.17	0.44
1:A:367:THR:HG22	1:A:392:ARG:HB3	1.99	0.44
1:A:297:LEU:HD11	1:A:324:TYR:HB3	2.00	0.44
1:A:163:LEU:HG	1:A:211:TYR:HB3	2.01	0.43
1:B:182:PHE:HB3	1:B:225:PHE:HB3	1.99	0.43
1:A:151:ILE:HG12	1:A:226:VAL:HG22	2.00	0.43
1:B:120:TYR:CE2	1:B:409:ARG:HG2	2.53	0.43
1:B:228:THR:CG2	1:B:230:HIS:CE1	3.01	0.43
1:A:255:THR:HG23	1:A:300:PRO:HG3	2.01	0.43
1:A:140:ALA:O	1:A:144:THR:HG23	2.19	0.43
1:A:326:PRO:CB	1:A:329:LYS:NZ	2.80	0.43
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.54	0.43
1:B:333:ILE:HB	1:B:358:CYS:SG	2.59	0.43
1:A:512:ILE:O	1:A:546:PHE:HA	2.19	0.42
1:A:263:SER:HA	1:A:266:VAL:HG13	2.01	0.42
1:B:474[B]:MET:HE2	1:B:474[B]:MET:HB3	1.93	0.42
1:A:31:TYR:O	1:A:35:ILE:HG22	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ILE:HG12	1:A:425:VAL:HG11	2.01	0.41
1:B:297:LEU:HD11	1:B:324:TYR:HB3	2.01	0.41
1:B:376:ILE:HG12	1:B:425:VAL:HG11	2.03	0.41
1:A:279:THR:HB	1:A:429:MET:HE2	2.01	0.41
1:B:49:VAL:HG23	1:B:58:THR:HG22	2.02	0.41
1:A:591:GLU:O	1:A:592:ILE:HB	2.21	0.40
1:B:512:ILE:O	1:B:546:PHE:HA	2.21	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	564/601 (94%)	541 (96%)	20 (4%)	3 (0%)	24	19
1	B	580/601 (96%)	552 (95%)	27 (5%)	1 (0%)	43	42
All	All	1144/1202 (95%)	1093 (96%)	47 (4%)	4 (0%)	36	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	VAL
1	A	195	ILE
1	A	219	LEU
1	B	215	THR

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	485/523 (93%)	466 (96%)	19 (4%)	28	26
1	B	498/523 (95%)	475 (95%)	23 (5%)	24	20
All	All	983/1046 (94%)	941 (96%)	42 (4%)	26	23

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	76	LYS
1	A	81	PHE
1	A	162	GLU
1	A	173	ARG
1	A	179	ASN
1	A	209	VAL
1	A	217	TYR
1	A	255	THR
1	A	289	SER
1	A	301	SER
1	A	344	ASP
1	A	432	ILE
1	A	516	ASN
1	A	530	THR
1	A	531	GLN
1	A	551	GLU
1	A	589	SER
1	A	592	ILE
1	B	11	GLN
1	B	12	THR
1	B	69	SER
1	B	76	LYS
1	B	92	LEU
1	B	95	ASN
1	B	96	THR
1	B	98	VAL
1	B	103	VAL
1	B	124	ASN
1	B	155	ARG
1	B	158	LEU
1	B	188	THR
1	B	192	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	195	ILE
1	B	199	THR
1	B	219	LEU
1	B	289	SER
1	B	301	SER
1	B	353	GLU
1	B	432	ILE
1	B	486	SER
1	B	551	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	164	HIS
1	A	177	ASN
1	A	179	ASN
1	A	245	HIS
1	A	275	GLN
1	A	404	GLN
1	A	459	ASN
1	A	464	HIS
1	A	516	ASN
1	B	51	ASN
1	B	116	ASN
1	B	164	HIS
1	B	177	ASN
1	B	245	HIS
1	B	268	ASN
1	B	404	GLN
1	B	459	ASN
1	B	516	ASN

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](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	PO4	B	704	-	4,4,4	2.53	1 (25%)	6,6,6	0.51	0
2	GQJ	A	701	-	18,18,18	0.45	0	25,25,25	0.59	0
4	PO4	A	705	-	4,4,4	2.64	2 (50%)	6,6,6	0.71	0
4	PO4	B	705	-	4,4,4	2.50	1 (25%)	6,6,6	0.53	0
4	PO4	A	706	-	4,4,4	2.54	2 (50%)	6,6,6	0.80	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	GQJ	A	701	-	-	1/14/26/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	705	PO4	P-O1	4.48	1.61	1.50
4	B	704	PO4	P-O1	4.25	1.60	1.50
4	A	706	PO4	P-O1	4.21	1.60	1.50
4	B	705	PO4	P-O1	4.17	1.60	1.50
4	A	705	PO4	P-O3	2.05	1.60	1.54
4	A	706	PO4	P-O3	2.03	1.60	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

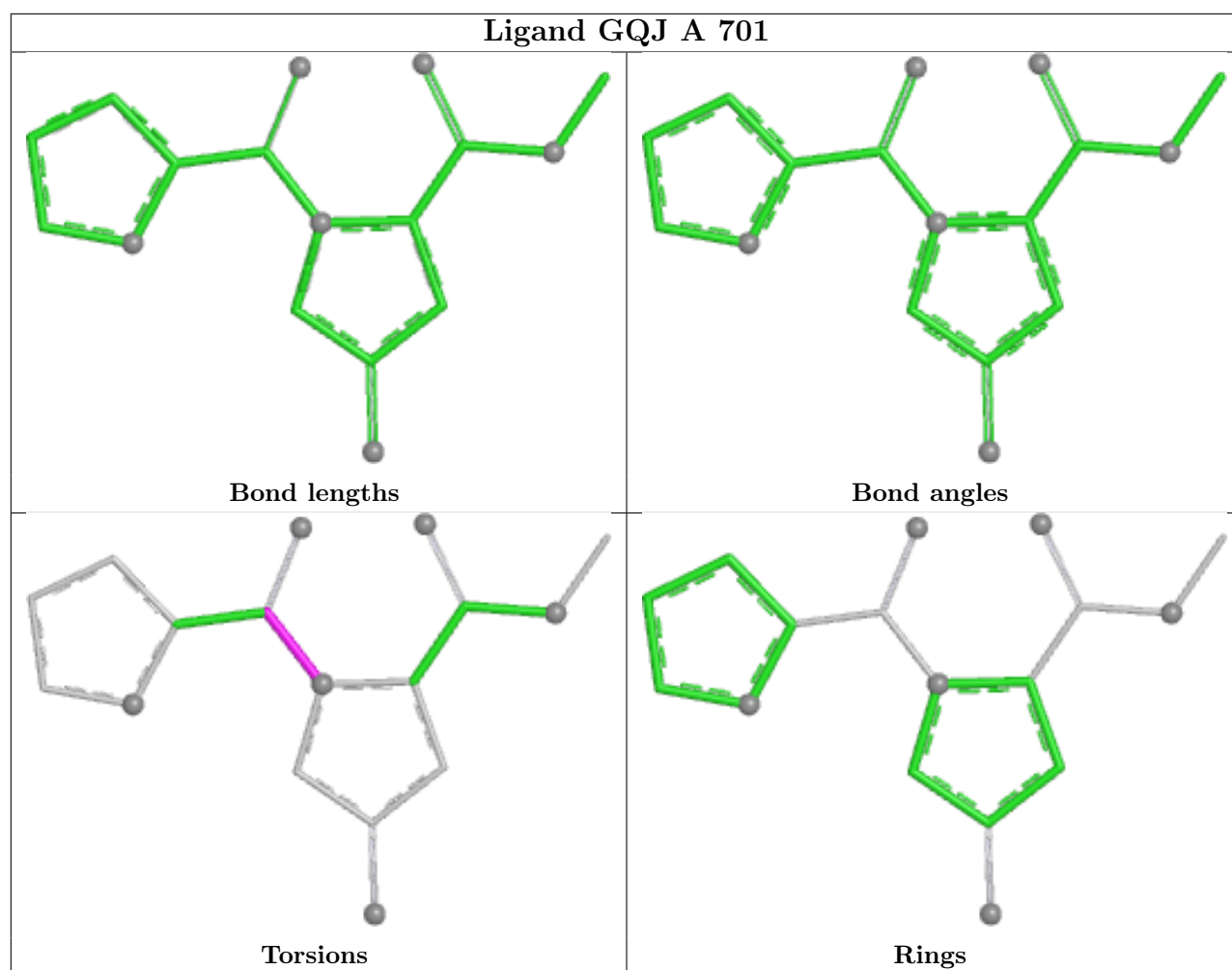
Mol	Chain	Res	Type	Atoms
2	A	701	GQJ	C11-C10-N09-C04

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	706	PO4	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	572/601 (95%)	0.80	74 (12%) 7 9	36, 71, 142, 167	0
1	B	585/601 (97%)	0.35	27 (4%) 37 42	25, 55, 104, 143	1 (0%)
All	All	1157/1202 (96%)	0.58	101 (8%) 16 18	25, 62, 132, 167	1 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	PHE	5.6
1	A	209	VAL	5.0
1	A	592	ILE	5.0
1	A	169	VAL	4.3
1	A	195	ILE	4.0
1	A	219	LEU	3.9
1	A	208	ALA	3.9
1	A	340	VAL	3.8
1	A	167	TRP	3.7
1	A	165	LEU	3.7
1	A	6	VAL	3.7
1	B	2	VAL	3.5
1	A	258	ILE	3.4
1	A	170	GLY	3.4
1	A	210	VAL	3.4
1	A	504	PRO	3.4
1	A	393	ALA	3.4
1	A	226	VAL	3.3
1	A	151	ILE	3.3
1	A	94	LYS	3.2
1	A	247	VAL	3.1
1	A	92	LEU	3.1
1	A	182	PHE	3.1
1	A	149	TYR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	202	LYS	3.1
1	B	340	VAL	3.0
1	A	266	VAL	3.0
1	A	224	TYR	2.9
1	B	217	TYR	2.9
1	A	1	ALA	2.9
1	A	157	VAL	2.9
1	A	81	PHE	2.9
1	A	152	ALA	2.9
1	A	221	VAL	2.8
1	A	200	PHE	2.8
1	A	185	TYR	2.8
1	B	214	THR	2.8
1	A	89	VAL	2.8
1	A	508	LYS	2.7
1	A	163	LEU	2.7
1	A	220	ASN	2.7
1	B	336	ALA	2.7
1	A	217	TYR	2.6
1	A	103	VAL	2.6
1	A	181	VAL	2.6
1	A	2	VAL	2.6
1	B	91	GLY	2.6
1	A	176	LEU	2.6
1	A	198	TYR	2.6
1	A	336	ALA	2.6
1	B	187	VAL	2.5
1	A	7	LEU	2.5
1	A	145	PHE	2.5
1	A	49	VAL	2.5
1	A	90	PHE	2.5
1	A	184	GLY	2.5
1	B	67	GLY	2.5
1	B	592	ILE	2.5
1	B	97	CYS	2.4
1	B	203	GLY	2.4
1	A	85	ALA	2.4
1	B	176	LEU	2.4
1	B	42	VAL	2.4
1	A	153	THR	2.4
1	A	222	GLY	2.4
1	B	12	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	98	VAL	2.3
1	A	174	PRO	2.3
1	B	46	ASN	2.3
1	A	215	THR	2.3
1	A	70	TYR	2.3
1	A	396	TYR	2.3
1	A	154	VAL	2.2
1	A	237	ALA	2.2
1	A	48	TYR	2.2
1	B	208	ALA	2.2
1	A	93	TYR	2.2
1	A	45	VAL	2.2
1	A	352	LEU	2.2
1	B	7	LEU	2.2
1	A	339	ARG	2.2
1	B	16	CYS	2.1
1	A	218	LYS	2.1
1	A	179	ASN	2.1
1	B	463	ALA	2.1
1	A	199	THR	2.1
1	A	231	THR	2.1
1	B	78	PRO	2.1
1	B	45	VAL	2.1
1	B	193	VAL	2.1
1	A	147	LEU	2.1
1	B	36	SER	2.1
1	A	84	CYS	2.1
1	A	180	TYR	2.1
1	A	304	ILE	2.1
1	B	215	THR	2.0
1	B	196	GLY	2.0
1	A	241	VAL	2.0
1	A	326	PRO	2.0
1	B	54	GLY	2.0
1	A	31	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 [i](#)

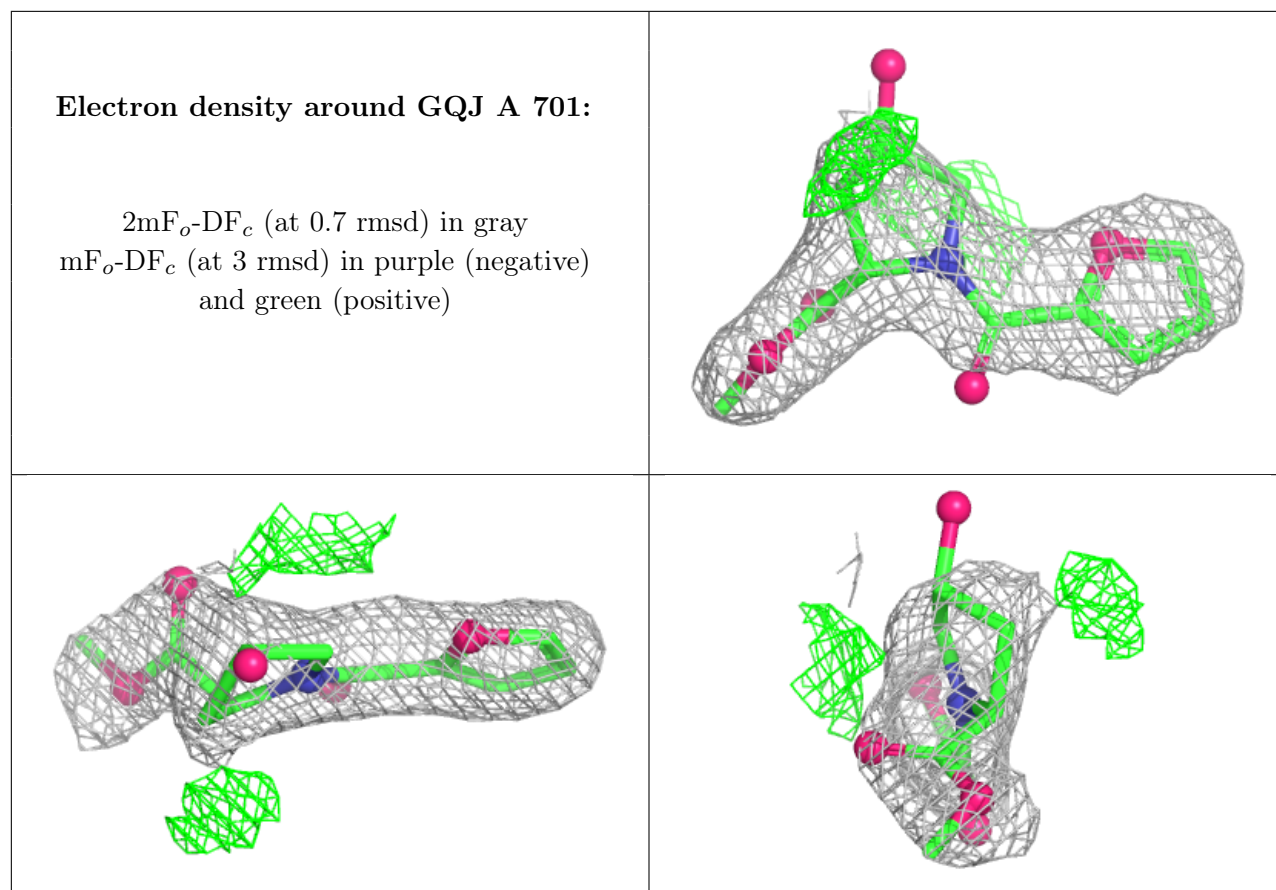
There are no oligosaccharides in this entry.

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
2	GQJ	A	701	17/17	0.87	0.21	46,50,56,56	17
4	PO4	B	704	5/5	0.97	0.06	53,54,55,56	0
4	PO4	B	705	5/5	0.97	0.07	50,51,57,58	0
4	PO4	A	705	5/5	0.98	0.05	46,48,50,51	0
4	PO4	A	706	5/5	0.98	0.06	44,46,49,51	0
3	ZN	A	704	1/1	0.99	0.03	110,110,110,110	0
3	ZN	B	702	1/1	0.99	0.05	79,79,79,79	0
3	ZN	A	702	1/1	0.99	0.04	69,69,69,69	0
3	ZN	A	703	1/1	1.00	0.03	67,67,67,67	0
3	ZN	B	703	1/1	1.00	0.05	95,95,95,95	0
3	ZN	B	701	1/1	1.00	0.02	42,42,42,42	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 ⓘ

There are no such residues in this entry.