



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:39 AM UTC

PDB ID : 4PNK / pdb_00004pnk
Title : G protein-coupled receptor kinase 2 in complex with GSK180736A
Authors : Homan, K.T.; Larimore, K.M.; Elkins, J.; Knapp, S.; Tesmer, J.J.G.
Deposited on : 2014-05-23
Resolution : 2.56 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

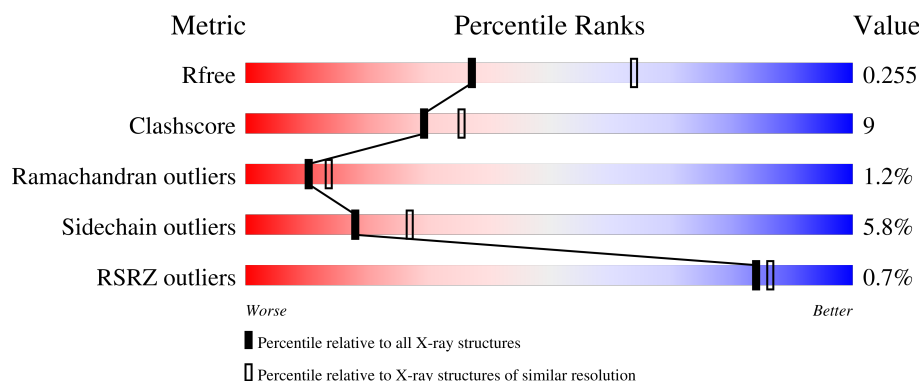
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	689	3% 64% 23% • 9%
2	B	340	77% 20% ••
3	G	71	3% 77% 8% • 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8322 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 Beta-adrenergic receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total	C	N	O	S	0	0	0
			5123	3265	896	927	35			

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	339	Total	C	N	O	S	0	2	0
			2619	1613	470	513	23			

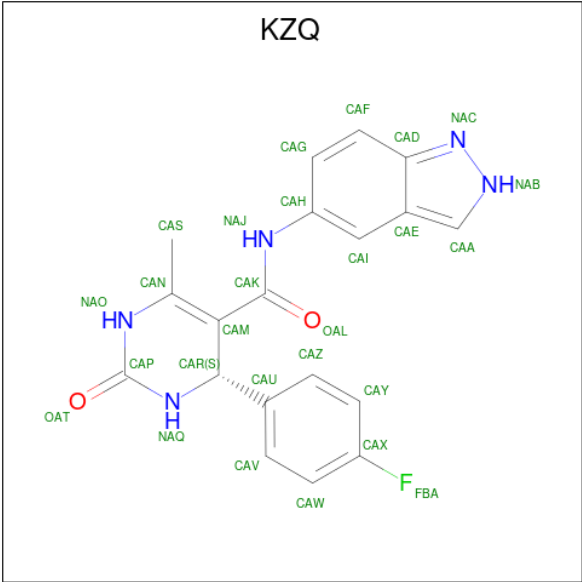
- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	62	Total	C	N	O	S	0	0	0
			484	307	84	90	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	68	SER	CYS	engineered mutation	UNP P63212

- Molecule 4 is (4S)-4-(4-fluorophenyl)-N-(2H-indazol-5-yl)-6-methyl-2-oxo-1,2,3,4-tetrahydro pyrimidine-5-carboxamide (CCD ID: KZQ) (formula: C₁₉H₁₆FN₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			27	19	1	5	2		

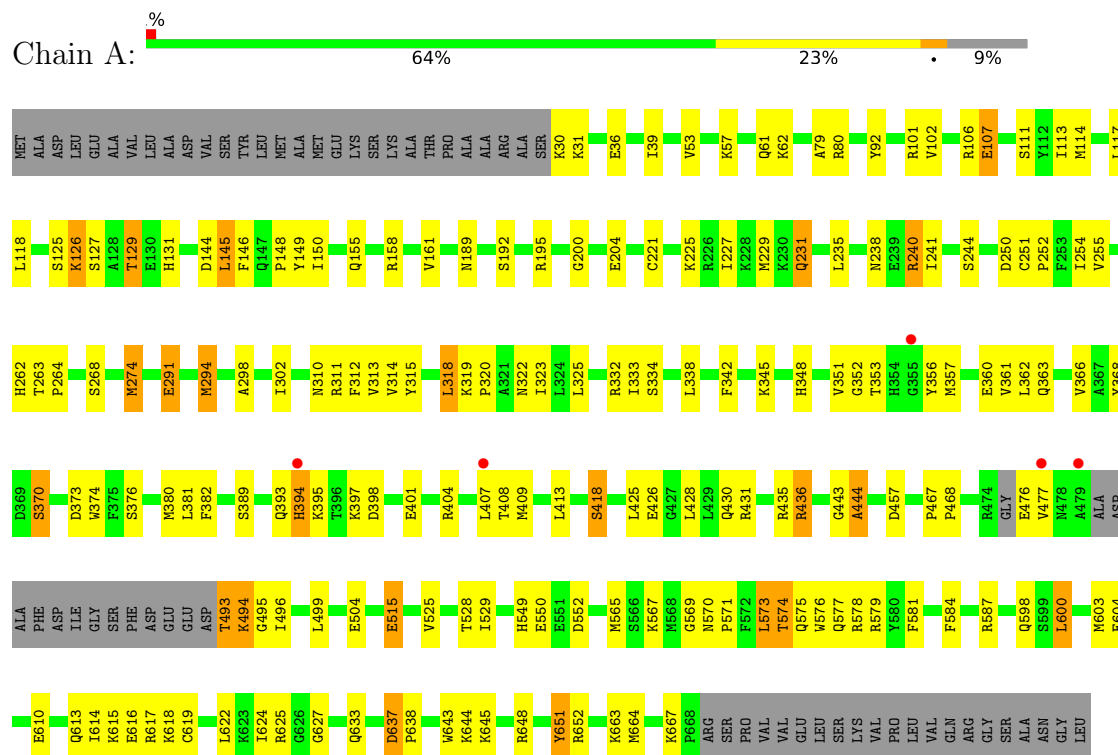
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	0
			35	35		
5	B	32	Total	O	0	0
			32	32		
5	G	2	Total	O	0	0
			2	2		

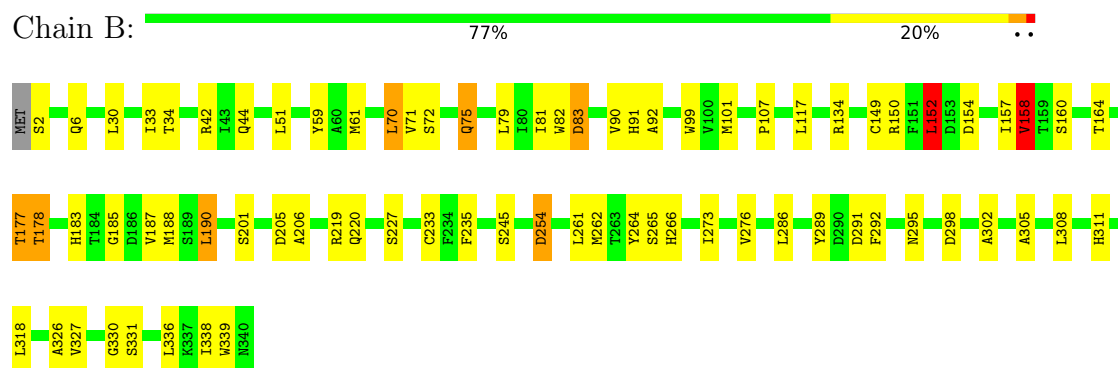
3 Residue-property plots

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.

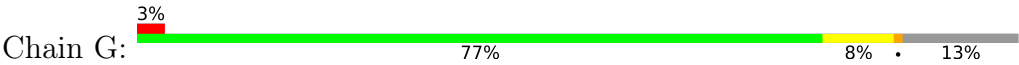
- Molecule 1: Beta-adrenergic receptor kinase 1



- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	61.44Å 241.40Å 212.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.55 – 2.56 24.55 – 2.56	Depositor EDS
% Data completeness (in resolution range)	97.5 (24.55-2.56) 97.7 (24.55-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.57Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.190 , 0.259 0.190 , 0.255	Depositor DCC
R_{free} test set	2565 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	77.3	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8322	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: KZQ

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	1.08	5/5238 (0.1%)	1.21	22/7038 (0.3%)
2	B	1.14	4/2666 (0.2%)	1.26	12/3613 (0.3%)
3	G	1.18	0/492	1.25	2/661 (0.3%)
All	All	1.11	9/8396 (0.1%)	1.23	36/11312 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	348	HIS	C-O	7.04	1.33	1.24
2	B	158	VAL	C-O	-6.34	1.17	1.24
1	A	325	LEU	C-O	-5.89	1.16	1.24
2	B	254	ASP	CA-C	-5.77	1.45	1.52
2	B	227	SER	C-O	-5.53	1.18	1.24
1	A	240	ARG	C-O	-5.30	1.17	1.24
1	A	600	LEU	C-O	-5.12	1.18	1.23
1	A	573	LEU	CA-C	5.09	1.59	1.52
2	B	295	ASN	C-O	5.08	1.29	1.23

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	LYS	N-CA-C	-7.58	99.24	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	92	ALA	CA-C-N	-7.15	115.58	123.02
2	B	92	ALA	C-N-CA	-7.15	115.58	123.02
1	A	584	PHE	CA-C-N	-6.75	112.85	119.87
1	A	584	PHE	C-N-CA	-6.75	112.85	119.87
1	A	496	ILE	N-CA-C	6.35	118.77	109.63
2	B	235	PHE	N-CA-C	-6.33	101.35	110.08
2	B	265	SER	N-CA-C	6.32	118.12	108.07
1	A	477	VAL	N-CA-C	6.17	116.28	110.30
1	A	418	SER	CA-C-N	6.17	126.62	119.47
1	A	418	SER	C-N-CA	6.17	126.62	119.47
1	A	550	GLU	N-CA-C	6.10	120.34	112.41
1	A	499	LEU	N-CA-C	6.02	118.09	110.33
3	G	32	LYS	N-CA-C	-5.90	104.76	111.14
1	A	251	CYS	N-CA-C	-5.83	101.16	109.62
2	B	152	LEU	N-CA-C	-5.65	103.91	112.04
1	A	291	GLU	N-CA-C	-5.56	105.22	111.28
2	B	188	MET	CB-CA-C	-5.56	99.68	109.02
1	A	495	GLY	CA-C-N	5.50	127.88	120.50
1	A	495	GLY	C-N-CA	5.50	127.88	120.50
1	A	496	ILE	CB-CA-C	-5.49	102.36	111.32
2	B	154	ASP	N-CA-C	5.36	119.31	112.34
1	A	637	ASP	CA-C-N	-5.31	113.26	119.32
1	A	637	ASP	C-N-CA	-5.31	113.26	119.32
3	G	66	PHE	N-CA-C	5.30	117.16	108.52
1	A	413	LEU	CA-C-N	5.29	125.29	119.90
1	A	413	LEU	C-N-CA	5.29	125.29	119.90
2	B	157	ILE	N-CA-C	5.23	115.90	108.42
2	B	326	ALA	N-CA-C	5.18	116.95	109.07
1	A	569	GLY	N-CA-C	-5.14	101.00	113.18
2	B	33	ILE	N-CA-C	5.09	116.42	110.62
1	A	333	ILE	CB-CA-C	-5.07	103.77	111.33
1	A	274	MET	CB-CA-C	-5.05	104.85	111.82
2	B	6	GLN	N-CA-C	5.04	117.43	111.33
1	A	652	ARG	N-CA-C	5.04	116.46	111.07
2	B	190	LEU	N-CA-C	5.02	116.61	109.14

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	494	LYS	Peptide
1	A	616	GLU	Peptide

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	5123	0	5114	96	0
2	B	2619	0	2518	44	0
3	G	484	0	496	2	0
4	A	27	0	16	3	0
5	A	35	0	0	3	0
5	B	32	0	0	2	0
5	G	2	0	0	0	0
All	All	8322	0	8144	141	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 9.

All (141) 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:B:42:ARG:NH2	5:B:417:HOH:O	1.89	1.06
2:B:42:ARG:CZ	5:B:417:HOH:O	2.15	0.89
1:A:493:THR:O	1:A:494:LYS:CE	2.28	0.82
1:A:357:MET:HE3	1:A:362:LEU:HD21	1.65	0.79
1:A:493:THR:O	1:A:494:LYS:HE3	1.82	0.79
1:A:131:HIS:CD2	1:A:148:PRO:HG2	2.24	0.73
1:A:587:ARG:HD2	1:A:600:LEU:HD22	1.74	0.68
1:A:294:MET:HE3	1:A:381:LEU:HD13	1.77	0.67
2:B:59:TYR:CE2	2:B:75:GLN:HB2	2.29	0.67
1:A:235:LEU:HD11	1:A:338:LEU:HD23	1.77	0.65
1:A:515:GLU:HB2	5:A:804:HOH:O	1.98	0.64
2:B:177:THR:HG22	2:B:178:THR:OG1	1.99	0.63
1:A:291:GLU:OE2	1:A:418:SER:OG	2.18	0.62
1:A:430:GLN:HG3	1:A:435:ARG:O	1.99	0.62
1:A:126:LYS:HG3	1:A:127:SER:N	2.14	0.61
1:A:144:ASP:O	1:A:145:LEU:C	2.43	0.61
1:A:314:VAL:HG12	1:A:370:SER:HA	1.83	0.60
1:A:235:LEU:CD1	1:A:338:LEU:HD23	2.33	0.59
1:A:274:MET:H	4:A:701:KZQ:HNAB	1.49	0.59
2:B:254:ASP:HB2	2:B:261:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:MET:HE3	2:B:101:MET:HG3	1.85	0.58
1:A:263:THR:HB	1:A:264:PRO:CD	2.34	0.57
1:A:573:LEU:O	1:A:574:THR:C	2.47	0.57
2:B:160:SER:HB3	2:B:190:LEU:HD23	1.88	0.56
1:A:493:THR:O	1:A:494:LYS:CD	2.54	0.56
2:B:71:VAL:HG23	2:B:81:ILE:HG12	1.88	0.55
1:A:356:TYR:O	1:A:376:SER:OG	2.21	0.55
2:B:70:LEU:O	2:B:70:LEU:HG	2.05	0.55
2:B:177:THR:HG22	2:B:178:THR:N	2.20	0.55
1:A:617:ARG:HG2	1:A:633:GLN:NE2	2.21	0.55
2:B:30:LEU:O	2:B:34:THR:HG23	2.06	0.54
1:A:195:ARG:HD3	1:A:476:GLU:OE1	2.08	0.54
1:A:238:ASN:HA	1:A:241:ILE:HD12	1.89	0.54
2:B:262:MET:SD	2:B:302:ALA:HB2	2.48	0.54
1:A:525:VAL:O	1:A:529:ILE:HG12	2.09	0.53
2:B:276:VAL:HA	2:B:286:LEU:O	2.08	0.53
1:A:323:ILE:HG13	1:A:380:MET:HE1	1.91	0.53
1:A:603:MET:HB3	1:A:651:TYR:HA	1.91	0.52
1:A:92:TYR:CD1	1:A:92:TYR:C	2.87	0.52
4:A:701:KZQ:OAL	4:A:701:KZQ:HAG	2.10	0.52
2:B:83:ASP:OD1	2:B:83:ASP:C	2.53	0.52
2:B:42:ARG:HD3	2:B:44:GLN:HG2	1.91	0.51
1:A:637:ASP:HB2	1:A:638:PRO:HD3	1.93	0.51
2:B:164:THR:HA	2:B:187:VAL:HG23	1.92	0.51
1:A:374:TRP:HA	1:A:374:TRP:CE3	2.46	0.51
2:B:298:ASP:C	2:B:298:ASP:OD1	2.54	0.50
1:A:667:LYS:HE3	5:A:835:HOH:O	2.12	0.49
1:A:318:LEU:HB3	1:A:376:SER:HB3	1.94	0.49
1:A:53:VAL:HG12	1:A:53:VAL:O	2.12	0.49
1:A:614:ILE:O	1:A:615:LYS:C	2.55	0.49
1:A:107:GLU:O	1:A:111:SER:HB3	2.12	0.49
1:A:443:GLY:O	1:A:444:ALA:C	2.56	0.49
1:A:604:GLU:HG3	5:A:830:HOH:O	2.12	0.49
1:A:579:ARG:HB2	1:A:581:PHE:CE1	2.47	0.48
1:A:644:LYS:HE3	1:A:648:ARG:CZ	2.44	0.48
2:B:51:LEU:HB3	2:B:82:TRP:CZ3	2.47	0.48
1:A:576:TRP:CZ3	1:A:633:GLN:HB2	2.48	0.48
2:B:99:TRP:HB3	2:B:117:LEU:HG	1.96	0.48
2:B:164:THR:HG22	2:B:185:GLY:C	2.39	0.48
1:A:600:LEU:C	1:A:600:LEU:HD12	2.39	0.47
3:G:59:ASN:ND2	3:G:62:ARG:HG2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LEU:O	1:A:426:GLU:C	2.56	0.47
2:B:292:PHE:CD1	2:B:292:PHE:N	2.82	0.47
1:A:401:GLU:HG2	1:A:404:ARG:HE	1.78	0.47
2:B:59:TYR:HE2	2:B:75:GLN:HB2	1.74	0.47
1:A:274:MET:HE2	1:A:332:ARG:HB2	1.97	0.47
1:A:360:GLU:HG3	1:A:368:TYR:HB3	1.97	0.47
1:A:149:TYR:O	1:A:150:ILE:C	2.56	0.47
1:A:312:PHE:HA	1:A:342:PHE:CE1	2.50	0.47
2:B:61:MET:HE3	2:B:70:LEU:HD13	1.98	0.46
2:B:311:HIS:CE1	2:B:331:SER:HB2	2.50	0.46
1:A:393:GLN:HG3	1:A:394:HIS:H	1.81	0.46
1:A:573:LEU:C	1:A:575:GLN:N	2.69	0.46
1:A:319:LYS:HE2	1:A:353:THR:OG1	2.15	0.45
2:B:152:LEU:HD21	2:B:158:VAL:CG2	2.46	0.45
1:A:30:LYS:HG2	1:A:31:LYS:N	2.31	0.45
1:A:274:MET:SD	1:A:332:ARG:HD2	2.55	0.45
1:A:311:ARG:O	1:A:313:VAL:HG23	2.16	0.45
1:A:408:THR:HA	1:A:431:ARG:HD3	1.98	0.45
2:B:61:MET:CE	2:B:70:LEU:HD13	2.46	0.45
1:A:129:THR:HG23	1:A:149:TYR:OH	2.17	0.45
1:A:613:GLN:NE2	1:A:618:LYS:HG3	2.31	0.45
1:A:382:PHE:C	1:A:382:PHE:CD1	2.96	0.44
2:B:318:LEU:C	2:B:318:LEU:HD12	2.42	0.44
2:B:30:LEU:HD12	3:G:34:ALA:HB1	2.00	0.44
1:A:254:ILE:HG22	1:A:255:VAL:N	2.33	0.44
1:A:570:ASN:HB3	1:A:573:LEU:HD12	1.99	0.44
1:A:155:GLN:HG2	1:A:158:ARG:HH21	1.82	0.44
2:B:90:VAL:HG12	2:B:91:HIS:CD2	2.52	0.44
1:A:79:ALA:O	1:A:80:ARG:C	2.61	0.44
1:A:294:MET:HE2	1:A:298:ALA:HB2	1.99	0.43
1:A:315:TYR:OH	1:A:322:ASN:HB3	2.18	0.43
1:A:144:ASP:O	1:A:146:PHE:N	2.51	0.43
1:A:315:TYR:N	1:A:373:ASP:OD2	2.42	0.43
1:A:61:GLN:O	1:A:62:LYS:C	2.60	0.43
1:A:637:ASP:O	1:A:638:PRO:C	2.60	0.43
1:A:263:THR:HB	1:A:264:PRO:HD2	2.00	0.43
1:A:397:LYS:O	1:A:398:ASP:C	2.61	0.43
1:A:252:PRO:HA	1:A:332:ARG:NH2	2.33	0.43
2:B:233[B]:CYS:SG	2:B:276:VAL:HG23	2.58	0.43
2:B:152:LEU:N	2:B:152:LEU:HD23	2.32	0.43
2:B:291:ASP:OD1	2:B:291:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:GLN:HB3	1:A:366:VAL:HG21	2.01	0.43
2:B:183:HIS:HE2	2:B:201:SER:HG	1.67	0.43
1:A:315:TYR:OH	1:A:334:SER:O	2.33	0.42
2:B:273:ILE:HG13	2:B:289:TYR:CE2	2.54	0.42
2:B:219:ARG:C	2:B:220:GLN:HG3	2.44	0.42
1:A:428:LEU:O	1:A:436:ARG:HD3	2.20	0.42
1:A:570:ASN:HA	1:A:571:PRO:HD2	1.81	0.42
1:A:598:GLN:HA	1:A:598:GLN:OE1	2.20	0.42
1:A:312:PHE:HA	1:A:342:PHE:CZ	2.54	0.42
1:A:318:LEU:HD12	1:A:319:LYS:N	2.34	0.42
1:A:294:MET:O	1:A:294:MET:HG2	2.20	0.42
1:A:625:ARG:C	1:A:627:GLY:H	2.28	0.42
2:B:262:MET:HG2	2:B:264:TYR:CZ	2.55	0.42
2:B:134:ARG:HA	2:B:134:ARG:HD3	1.89	0.42
1:A:467:PRO:HA	1:A:468:PRO:HD3	1.81	0.41
1:A:581:PHE:N	1:A:581:PHE:CD1	2.88	0.41
1:A:101:ARG:O	1:A:102:VAL:C	2.62	0.41
1:A:294:MET:CE	1:A:298:ALA:HB2	2.49	0.41
1:A:565:MET:HE3	1:A:643:TRP:CD1	2.56	0.41
2:B:42:ARG:HG2	2:B:305:ALA:O	2.19	0.41
1:A:114:MET:HE2	1:A:118:LEU:HD11	2.02	0.41
1:A:125:SER:O	1:A:129:THR:OG1	2.39	0.41
1:A:200:GLY:O	4:A:701:KZQ:CAX	2.69	0.41
1:A:430:GLN:O	1:A:431:ARG:C	2.62	0.41
2:B:327:VAL:HB	2:B:339:TRP:HB2	2.02	0.41
1:A:225:LYS:C	1:A:227:ILE:N	2.78	0.41
1:A:310:ASN:HD22	1:A:310:ASN:HA	1.56	0.41
1:A:319:LYS:O	1:A:320:PRO:C	2.64	0.41
1:A:361:VAL:HA	1:A:368:TYR:CE2	2.56	0.41
1:A:381:LEU:O	1:A:382:PHE:C	2.64	0.41
2:B:205:ASP:O	2:B:206:ALA:HB3	2.20	0.41
2:B:219:ARG:O	2:B:220:GLN:HG3	2.20	0.41
2:B:330:GLY:CA	2:B:336:LEU:HD23	2.51	0.41
1:A:351:VAL:HG12	1:A:352:GLY:N	2.35	0.40
1:A:644:LYS:O	1:A:645:LYS:C	2.62	0.40
2:B:72:SER:O	2:B:79:LEU:HA	2.21	0.40
2:B:149:CYS:O	2:B:150:ARG:NH1	2.55	0.40
1:A:36:GLU:O	1:A:39:ILE:HG22	2.22	0.40
1:A:624:ILE:HG22	1:A:625:ARG:H	1.87	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	619/689 (90%)	548 (88%)	60 (10%)	11 (2%)	6	8
2	B	339/340 (100%)	309 (91%)	30 (9%)	0	100	100
3	G	60/71 (84%)	57 (95%)	2 (3%)	1 (2%)	7	8
All	All	1018/1100 (92%)	914 (90%)	92 (9%)	12 (1%)	10	14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	ASP
1	A	444	ALA
3	G	62	ARG
1	A	145	LEU
1	A	407	LEU
1	A	229	MET
1	A	370	SER
1	A	395	LYS
1	A	231	GLN
1	A	394	HIS
1	A	409	MET
1	A	113	ILE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	560/609 (92%)	523 (93%)	37 (7%)	15	21
2	B	284/283 (100%)	271 (95%)	13 (5%)	24	35
3	G	51/58 (88%)	49 (96%)	2 (4%)	28	41
All	All	895/950 (94%)	843 (94%)	52 (6%)	18	27

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	106	ARG
1	A	107	GLU
1	A	117	LEU
1	A	126	LYS
1	A	129	THR
1	A	161	VAL
1	A	189	ASN
1	A	192	SER
1	A	204	GLU
1	A	221	CYS
1	A	231	GLN
1	A	240	ARG
1	A	244	SER
1	A	262	HIS
1	A	268	SER
1	A	294	MET
1	A	302	ILE
1	A	318	LEU
1	A	345	LYS
1	A	389	SER
1	A	436	ARG
1	A	457	ASP
1	A	493	THR
1	A	504	GLU
1	A	515	GLU
1	A	528	THR
1	A	549	HIS
1	A	552	ASP
1	A	574	THR
1	A	577	GLN

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Mol	Chain	Res	Type
1	A	578	ARG
1	A	610	GLU
1	A	619	CYS
1	A	622	LEU
1	A	651	TYR
1	A	663	LYS
2	B	2	SER
2	B	70	LEU
2	B	75	GLN
2	B	83	ASP
2	B	107	PRO
2	B	152	LEU
2	B	158	VAL
2	B	177	THR
2	B	178	THR
2	B	245	SER
2	B	266	HIS
2	B	308	LEU
2	B	338	ILE
3	G	47	GLU
3	G	51	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	131	HIS
1	A	147	GLN
1	A	189	ASN
1	A	309	HIS
1	A	310	ASN
1	A	330	HIS
1	A	633	GLN
2	B	9	GLN
2	B	110	ASN
2	B	155	ASN
2	B	239	ASN
3	G	11	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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$
4	KZQ	A	701	-	28,30,30	1.97	7 (25%)	37,43,43	3.01	14 (37%)

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	KZQ	A	701	-	-	1/12/28/28	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	KZQ	CAF-CAD	-4.96	1.34	1.40
4	A	701	KZQ	CAR-CAM	-4.60	1.47	1.51
4	A	701	KZQ	CAN-CAM	2.92	1.39	1.35
4	A	701	KZQ	CAN-NAO	-2.88	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	KZQ	CAD-CAE	-2.81	1.38	1.43
4	A	701	KZQ	NAB-NAC	-2.77	1.30	1.36
4	A	701	KZQ	CAU-CAR	-2.40	1.49	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	KZQ	CAU-CAR-CAM	-8.81	100.92	112.84
4	A	701	KZQ	CAS-CAN-CAM	-7.46	120.19	127.61
4	A	701	KZQ	NAO-CAP-NAQ	6.53	122.61	116.06
4	A	701	KZQ	CAS-CAN-NAO	5.03	119.27	113.42
4	A	701	KZQ	OAL-CAK-CAM	-4.18	113.74	121.32
4	A	701	KZQ	CAN-NAO-CAP	-3.77	120.78	123.70
4	A	701	KZQ	CAF-CAG-CAH	3.73	124.60	120.30
4	A	701	KZQ	CAE-CAA-NAB	-3.51	105.73	108.93
4	A	701	KZQ	CAM-CAR-NAQ	3.43	112.05	109.07
4	A	701	KZQ	CAG-CAF-CAD	-2.93	117.30	120.80
4	A	701	KZQ	OAT-CAP-NAQ	-2.68	118.00	122.99
4	A	701	KZQ	OAL-CAK-NAJ	2.61	130.09	123.89
4	A	701	KZQ	CAH-CAI-CAE	-2.61	116.70	120.30
4	A	701	KZQ	CAD-NAC-NAB	2.40	110.36	105.24

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	KZQ	NAJ-CAK-CAM-CAN

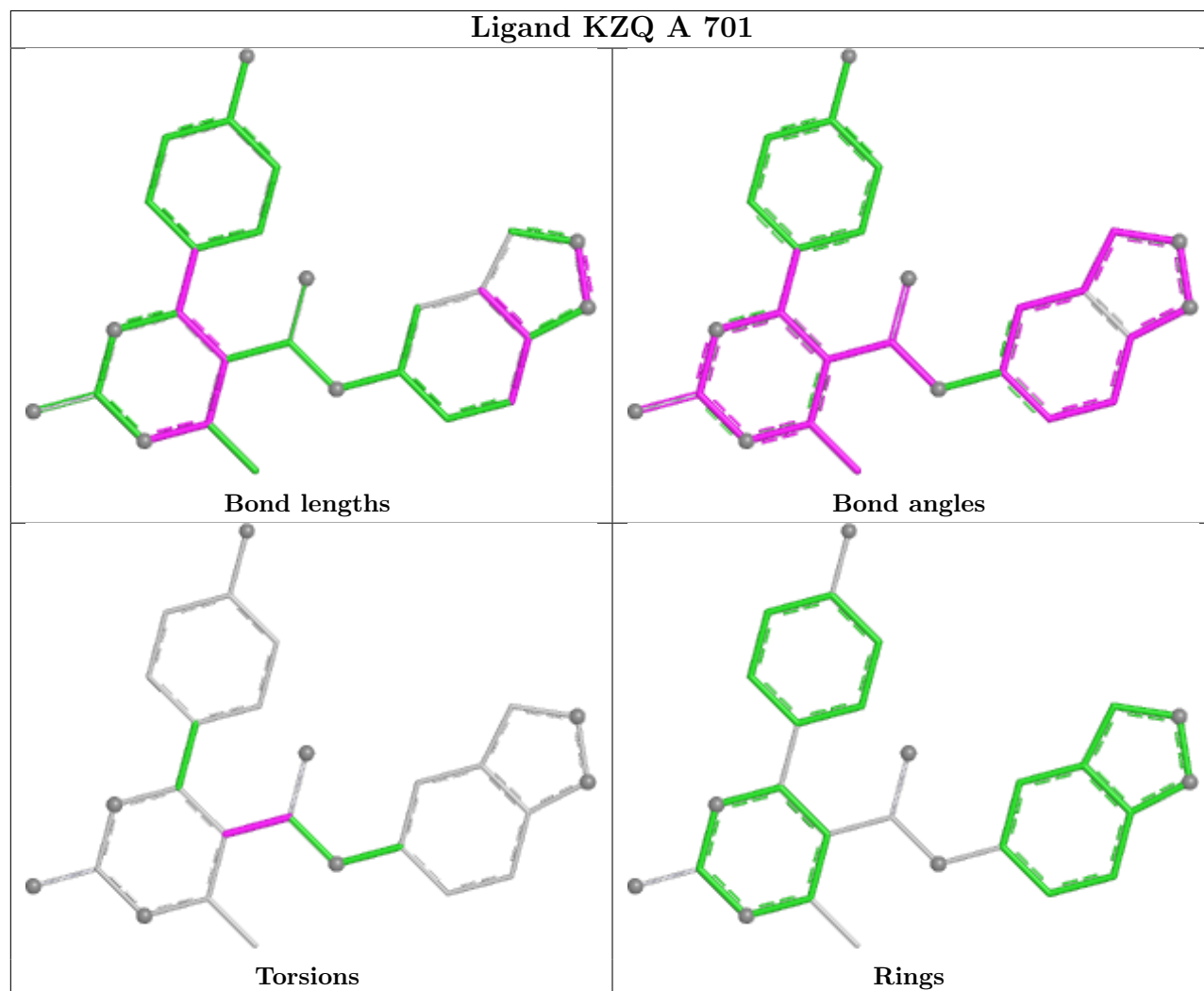
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	KZQ	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	625/689 (90%)	-0.32	5 (0%) 82 85	61, 102, 179, 246	0
2	B	339/340 (99%)	-0.58	0 100 100	34, 81, 121, 175	2 (0%)
3	G	62/71 (87%)	-0.21	2 (3%) 50 51	73, 105, 172, 202	0
All	All	1026/1100 (93%)	-0.40	7 (0%) 84 86	34, 93, 172, 246	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	477	VAL	5.2
1	A	479	ALA	4.6
3	G	65	LYS	2.3
3	G	7	ALA	2.2
1	A	394	HIS	2.1
1	A	407	LEU	2.1
1	A	355	GLY	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.

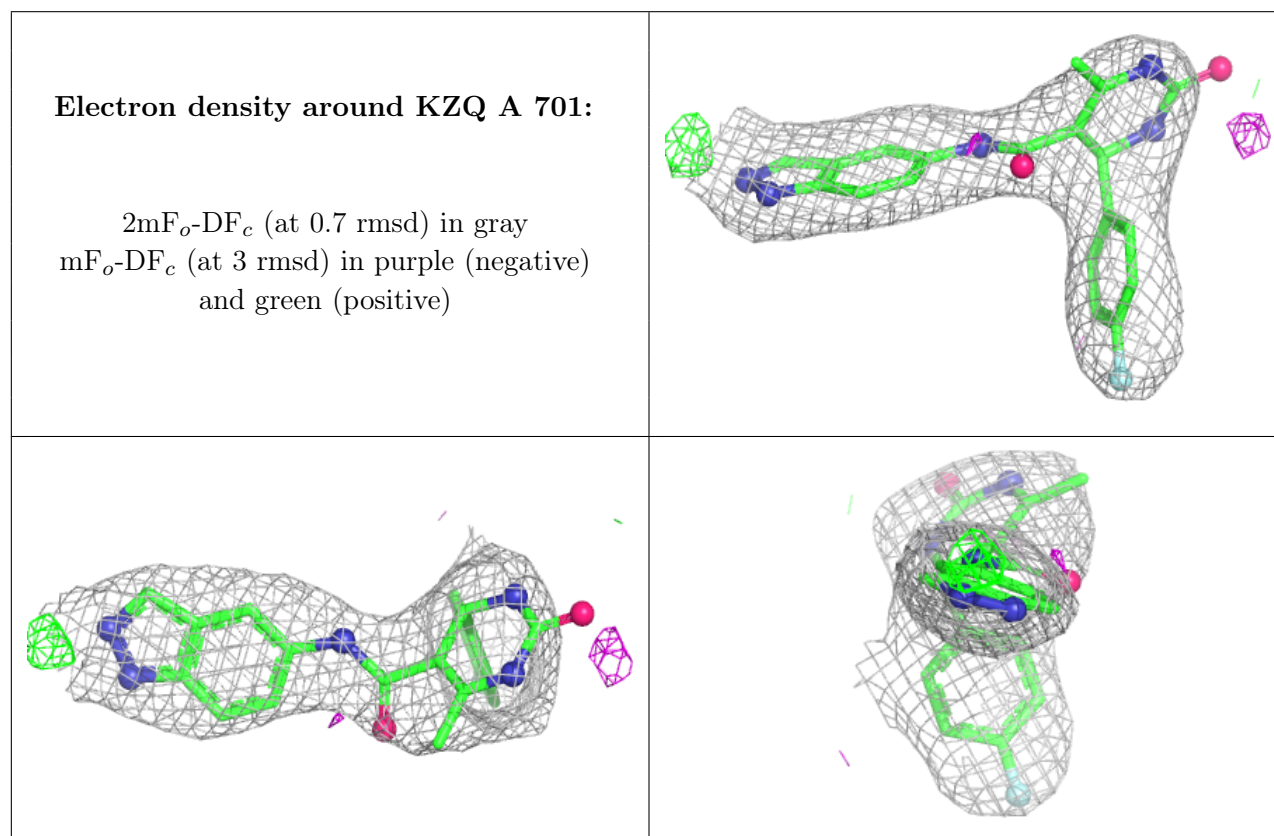
6.4 Ligands [i](#)

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
4	KZQ	A	701	27/27	0.94	0.08	74,101,125,145	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.