



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:55 PM UTC

PDB ID : 8A9G / pdb_00008a9g
Title : Binary complex of 14-3-3 zeta Glucocorticoid Receptor (GR) pT524 peptide stabilised by (R)-para chloropyrrolidone1
Authors : Munier, C.C.; Edman, K.; Perry, M.W.D.; Ottmann, C.
Deposited on : 2022-06-28
Resolution : 1.96 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

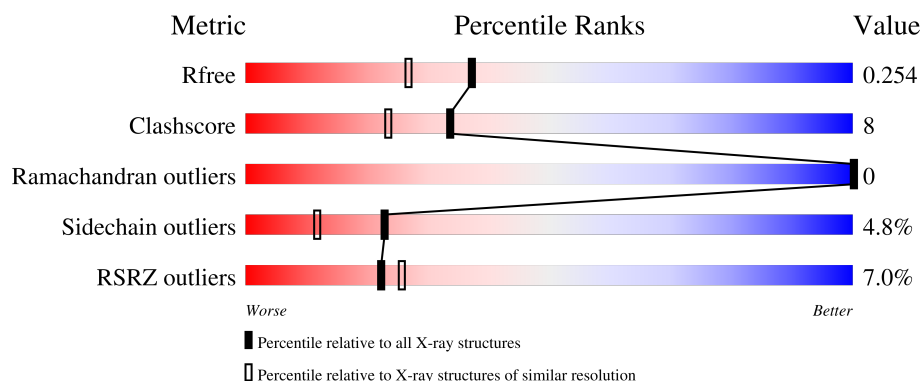
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	235	5% 64% 31% ..
1	B	235	4% 65% 28% ..
2	C	13	46% 77% 15% 8%
2	D	13	62% 92% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4269 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 14-3-3 protein zeta/delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	1	0
			1851	1158	310	373	10			
1	B	230	Total	C	N	O	S	0	0	0
			1843	1154	309	370	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P63104
A	-3	ALA	-	expression tag	UNP P63104
A	-2	MET	-	expression tag	UNP P63104
A	-1	GLY	-	expression tag	UNP P63104
A	0	SER	-	expression tag	UNP P63104
B	-4	GLY	-	expression tag	UNP P63104
B	-3	ALA	-	expression tag	UNP P63104
B	-2	MET	-	expression tag	UNP P63104
B	-1	GLY	-	expression tag	UNP P63104
B	0	SER	-	expression tag	UNP P63104

- Molecule 2 is a protein called Glucocorticoid receptor.

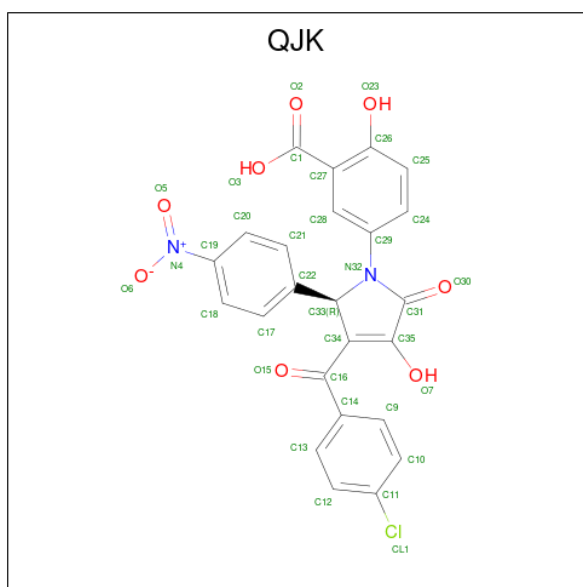
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	P	0	0	0
			92	58	13	20	1			
2	D	13	Total	C	N	O	P	0	0	0
			101	64	15	21	1			

- Molecule 3 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 5-[(2 {R})-3-(4-chlorophenyl)carbonyl-2-(4-nitrophenyl)-4-oxidanyl-5-oxidanylidene-2 {H}-pyrrol-1-yl]-2-oxidanyl-benzoic acid (CCD ID: QJK) (formula: $C_{24}H_{15}ClN_2O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			35	24	1	2	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	O	
			35	24	1	2	8	
							0	0

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	123	Total	O		
			123	123	0	0
6	B	135	Total	O		
			135	135	0	0
6	C	14	Total	O		
			14	14	0	0
6	D	11	Total	O		
			11	11	0	0

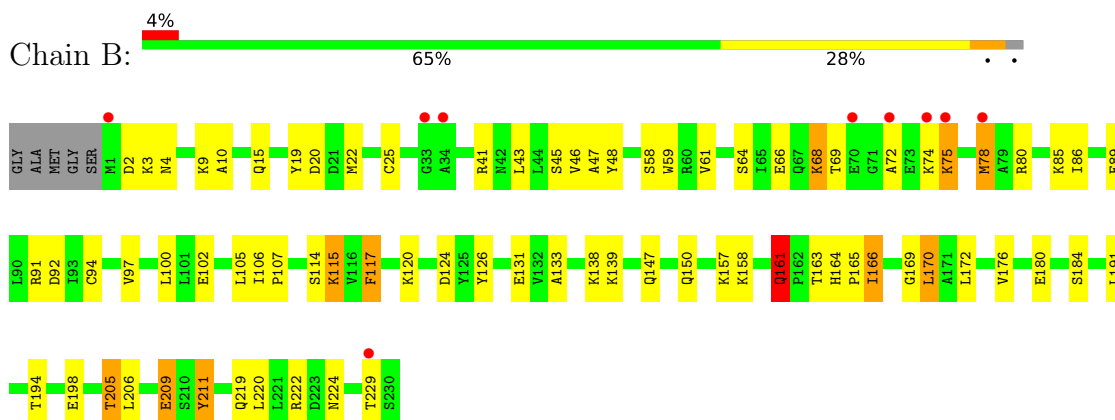
3 Residue-property plots

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.

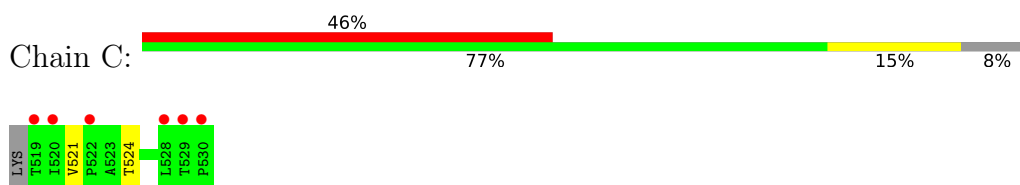
- Molecule 1: 14-3-3 protein zeta/delta



- Molecule 1: 14-3-3 protein zeta/delta

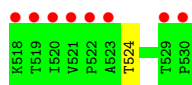


- Molecule 2: Glucocorticoid receptor



- Molecule 2: Glucocorticoid receptor

Chain D: 62% 92% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	57.35Å 78.07Å 122.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.85 – 1.96 65.85 – 1.96	Depositor EDS
% Data completeness (in resolution range)	78.7 (65.85-1.96) 79.4 (65.85-1.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.95Å)	Xtriage
Refinement program	BUSTER 2.11.8 (24-FEB-2021)	Depositor
R, R_{free}	0.250 , 0.261 0.236 , 0.254	Depositor DCC
R_{free} test set	1587 reflections (3.91%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.6	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	0.95	EDS
Total number of atoms	4269	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0096e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QJK, TPO, MG, BTB

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	1.91	34/1876 (1.8%)	1.19	8/2521 (0.3%)
1	B	1.94	42/1868 (2.2%)	1.22	10/2510 (0.4%)
2	C	0.64	0/82	0.97	0/112
2	D	0.77	0/91	0.86	0/123
All	All	1.89	76/3917 (1.9%)	1.19	18/5266 (0.3%)

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	106	ILE	C-O	-8.52	1.17	1.24
1	A	117	PHE	C-O	-6.87	1.16	1.24
1	B	170	LEU	C-O	-6.48	1.16	1.24
1	B	176	VAL	C-O	-6.48	1.16	1.24
1	B	91	ARG	C-O	-6.42	1.16	1.24
1	A	43	LEU	C-O	-6.26	1.16	1.24
1	A	99	SER	C-O	-6.07	1.16	1.24
1	B	150	GLN	C-O	-5.96	1.17	1.24
1	B	97	VAL	C-O	-5.88	1.17	1.24
1	A	22	MET	C-O	-5.88	1.17	1.24
1	A	131	GLU	C-O	-5.86	1.16	1.24
1	B	124	ASP	C-O	-5.82	1.17	1.24
1	B	43	LEU	C-O	-5.79	1.17	1.24
1	A	170	LEU	C-O	-5.77	1.17	1.24
1	B	94	CYS	C-O	-5.74	1.17	1.24
1	B	46	VAL	C-O	-5.72	1.17	1.24
1	A	172	LEU	C-O	-5.72	1.17	1.24
1	B	58	SER	C-O	-5.71	1.17	1.24
1	B	169	GLY	C-O	-5.70	1.17	1.23
1	A	91	ARG	C-O	-5.70	1.17	1.24
1	A	174	PHE	C-O	-5.70	1.17	1.24
1	A	162	PRO	C-O	-5.67	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	GLN	C-O	-5.60	1.17	1.24
1	B	20	ASP	C-O	-5.57	1.17	1.24
1	B	45	SER	C-O	-5.53	1.17	1.24
1	B	59	TRP	C-O	-5.50	1.17	1.24
1	B	224	ASN	C-O	-5.47	1.17	1.24
1	B	147	GLN	C-O	-5.46	1.17	1.24
1	A	95	ASN	C-O	-5.45	1.17	1.24
1	B	48	TYR	C-O	-5.41	1.17	1.24
1	A	55	ARG	C-O	-5.40	1.17	1.24
1	B	184	SER	C-O	-5.40	1.18	1.24
1	A	90	LEU	C-O	-5.37	1.18	1.24
1	A	114	SER	C-O	-5.35	1.17	1.24
1	B	92	ASP	C-O	-5.34	1.17	1.24
1	A	107	PRO	C-O	-5.33	1.17	1.24
1	A	153	PHE	C-O	-5.31	1.18	1.24
1	A	61	VAL	C-O	-5.29	1.18	1.24
1	B	61	VAL	C-O	-5.29	1.18	1.24
1	A	40	GLU	C-O	-5.28	1.17	1.24
1	B	19	TYR	C-O	-5.28	1.17	1.24
1	B	85	LYS	C-O	-5.27	1.18	1.24
1	B	117	PHE	C-O	-5.27	1.18	1.24
1	B	105	LEU	C-O	-5.26	1.18	1.24
1	B	114	SER	C-O	-5.26	1.17	1.24
1	B	222	ARG	C-O	-5.26	1.18	1.24
1	A	54	ALA	C-O	-5.25	1.18	1.24
1	A	105	LEU	C-O	-5.24	1.18	1.24
1	B	126	TYR	C-O	-5.23	1.17	1.24
1	A	148	ALA	C-O	-5.22	1.18	1.24
1	B	211	TYR	C-O	-5.21	1.17	1.24
1	B	47	ALA	C-O	-5.21	1.18	1.24
1	A	125	TYR	C-O	-5.20	1.17	1.24
1	B	100	LEU	C-O	-5.20	1.18	1.24
1	B	89	GLU	C-O	-5.20	1.18	1.24
1	B	107	PRO	C-O	-5.17	1.17	1.24
1	B	102	GLU	C-O	-5.16	1.18	1.24
1	B	69	THR	N-CA	-5.15	1.40	1.46
1	A	50	ASN	C-O	-5.15	1.18	1.24
1	B	86	ILE	C-O	-5.13	1.18	1.24
1	A	25	CYS	C-O	-5.13	1.18	1.24
1	A	42	ASN	C-O	-5.10	1.17	1.24
1	B	220	LEU	C-O	-5.09	1.18	1.24
1	B	172	LEU	C-O	-5.08	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	LEU	C-O	-5.07	1.18	1.24
1	A	29	VAL	C-O	-5.06	1.18	1.24
1	B	166	ILE	C-O	-5.06	1.18	1.24
1	A	219	GLN	C-O	-5.05	1.17	1.24
1	A	216	LEU	C-O	-5.05	1.18	1.24
1	B	219	GLN	C-O	-5.04	1.18	1.24
1	A	150	GLN	C-O	-5.03	1.18	1.24
1	B	165	PRO	C-O	-5.03	1.17	1.24
1	A	110	SER	C-O	-5.02	1.17	1.24
1	B	131	GLU	C-O	-5.02	1.17	1.24
1	A	101	LEU	C-O	-5.01	1.18	1.24
1	A	123	GLY	CA-C	5.01	1.57	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	LEU	N-CA-C	10.90	122.91	111.14
1	B	158	LYS	N-CA-C	8.99	121.16	111.36
1	A	138	LYS	N-CA-C	7.72	119.33	111.07
1	B	211	TYR	N-CA-C	7.31	120.11	111.71
1	B	75	LYS	CB-CA-C	-6.69	100.66	110.96
1	A	210	SER	N-CA-C	6.51	120.44	111.71
1	A	158	LYS	N-CA-C	6.35	117.99	111.14
1	B	105	LEU	N-CA-C	6.20	117.91	111.03
1	B	209	GLU	N-CA-C	5.99	118.76	111.82
1	B	180	GLU	N-CA-C	5.95	119.72	112.23
1	B	161	GLN	CA-C-N	5.81	125.48	119.56
1	B	161	GLN	C-N-CA	5.81	125.48	119.56
1	B	2	ASP	N-CA-C	5.66	117.53	111.36
1	A	78	MET	N-CA-C	-5.57	105.13	111.14
1	A	73	GLU	N-CA-C	5.54	122.59	110.80
1	B	19	TYR	N-CA-C	5.11	117.75	111.82
1	A	126	TYR	N-CA-C	-5.04	105.88	112.23
1	A	156	SER	N-CA-C	5.04	116.77	111.28

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	1851	0	1836	35	0
1	B	1843	0	1833	26	0
2	C	92	0	94	0	0
2	D	101	0	107	0	0
3	A	14	0	19	1	0
3	B	14	0	19	0	0
4	A	35	0	0	0	0
4	B	35	0	0	0	0
5	B	1	0	0	0	0
6	A	123	0	0	0	0
6	B	135	0	0	0	0
6	C	14	0	0	0	0
6	D	11	0	0	0	0
All	All	4269	0	3908	61	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 8.

All (61) 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:64:SER:O	1:B:68:LYS:HD3	1.66	0.94
1:B:161:GLN:HG2	1:B:205:THR:CG2	1.99	0.92
1:A:78:MET:HA	1:A:78:MET:HE3	1.48	0.92
1:B:161:GLN:HG2	1:B:205:THR:HG23	1.51	0.90
1:B:163:THR:OG1	1:B:205:THR:HG22	1.73	0.89
1:A:56:ARG:O	1:A:60:ARG:HG3	1.71	0.88
1:A:153:PHE:CZ	1:A:157:LYS:HE3	2.14	0.83
1:A:225:LEU:O	1:A:229:THR:HG23	1.79	0.81
1:A:69:THR:HG21	1:A:75:LYS:HE2	1.68	0.76
1:A:65:ILE:O	1:A:69:THR:HG23	1.87	0.74
1:A:77:GLN:O	1:A:81:GLU:HG3	1.87	0.73
1:A:106:ILE:O	1:A:115:LYS:NZ	2.22	0.72
1:A:164:HIS:HD2	1:A:166:ILE:H	1.38	0.72
1:B:163:THR:OG1	1:B:205:THR:CG2	2.38	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:PHE:CE2	1:A:157:LYS:HE3	2.28	0.69
1:A:102:GLU:HG3	1:A:103:LYS:HD3	1.76	0.67
1:B:163:THR:HG1	1:B:205:THR:HG22	1.58	0.66
1:B:194:THR:O	1:B:198:GLU:HG3	1.96	0.64
1:A:78:MET:HA	1:A:78:MET:CE	2.24	0.62
1:A:106:ILE:N	1:A:107:PRO:HD2	2.15	0.62
1:A:194:THR:O	1:A:198:GLU:HG3	2.01	0.60
1:A:178:TYR:CD1	1:A:182:LEU:HD12	2.36	0.60
1:A:153:PHE:CZ	1:A:157:LYS:CE	2.83	0.60
1:B:161:GLN:HG2	1:B:205:THR:HG21	1.82	0.55
1:B:66:GLU:OE2	1:B:80:ARG:HG3	2.07	0.54
1:A:160:MET:CE	1:A:164:HIS:CG	2.91	0.53
1:B:164:HIS:HD2	1:B:166:ILE:H	1.57	0.52
1:A:213:ASP:O	1:A:217:ILE:HG13	2.09	0.52
1:A:25:CYS:O	1:A:29:VAL:HG23	2.10	0.51
1:B:9:LYS:HD3	1:B:25:CYS:SG	2.51	0.51
1:B:209:GLU:O	1:B:209:GLU:HG2	2.11	0.51
1:A:3:LYS:HB2	1:A:32:GLN:OE1	2.11	0.50
1:A:3:LYS:HG3	1:A:29:VAL:HG13	1.95	0.48
1:B:72:ALA:HB1	1:B:75:LYS:HG3	1.96	0.48
1:A:178:TYR:HD1	1:A:182:LEU:HD12	1.78	0.48
1:B:133:ALA:HB3	1:B:138:LYS:HG3	1.95	0.48
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.79	0.47
3:A:301:BTB:H41	3:A:301:BTB:H71	1.52	0.47
1:A:83:ARG:HG2	1:A:83:ARG:NH1	2.30	0.47
1:B:161:GLN:CG	1:B:205:THR:HG21	2.45	0.46
1:A:102:GLU:CG	1:A:103:LYS:HD3	2.43	0.46
1:B:120:LYS:HD2	1:B:170:LEU:HA	1.97	0.46
1:A:160:MET:CE	1:A:164:HIS:CD2	2.98	0.46
1:B:139:LYS:N	1:B:139:LYS:HD3	2.31	0.45
1:B:41:ARG:HD2	1:B:117:PHE:CD1	2.52	0.45
1:A:106:ILE:N	1:A:107:PRO:CD	2.80	0.45
1:B:115:LYS:HB2	1:B:115:LYS:HE2	1.70	0.45
1:B:163:THR:HB	1:B:206:LEU:HD23	1.99	0.44
1:B:157:LYS:NZ	1:B:198:GLU:OE2	2.51	0.44
1:B:206:LEU:HD13	1:B:211:TYR:HB2	1.99	0.43
1:A:8:GLN:HG3	1:B:78:MET:HE1	2.00	0.42
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.76	0.42
1:B:10:ALA:O	1:B:22:MET:HG3	2.20	0.42
1:A:132:VAL:O	1:A:132:VAL:HG23	2.20	0.42
1:A:103:LYS:HA	1:A:103:LYS:HD2	1.87	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:HIS:CD2	1:A:166:ILE:H	2.26	0.41
1:B:191:LEU:C	1:B:191:LEU:HD23	2.46	0.41
1:A:126:TYR:HB3	1:A:145:SER:HB2	2.03	0.41
1:A:127:ARG:HG3	1:A:181:ILE:HG13	2.03	0.41
1:B:161:GLN:CG	1:B:205:THR:CG2	2.87	0.40
1:A:219:GLN:O	1:A:219:GLN:HG3	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	229/235 (97%)	225 (98%)	4 (2%)	0	100	100
1	B	228/235 (97%)	222 (97%)	6 (3%)	0	100	100
2	C	9/13 (69%)	9 (100%)	0	0	100	100
2	D	10/13 (77%)	9 (90%)	1 (10%)	0	100	100
All	All	476/496 (96%)	465 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	201/202 (100%)	192 (96%)	9 (4%)	24	14
1	B	200/202 (99%)	190 (95%)	10 (5%)	22	11
2	C	10/11 (91%)	9 (90%)	1 (10%)	7	1
2	D	11/11 (100%)	11 (100%)	0	100	100
All	All	422/426 (99%)	402 (95%)	20 (5%)	23	12

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	67	GLN
1	A	78	MET
1	A	103	LYS
1	A	113	GLU
1	A	141	ILE
1	A	147	GLN
1	A	207	SER
1	A	227	LEU
1	B	3	LYS
1	B	4	ASN
1	B	15	GLN
1	B	68	LYS
1	B	74	LYS
1	B	78	MET
1	B	115	LYS
1	B	161	GLN
1	B	205	THR
1	B	229	THR
2	C	521	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	38	ASN
1	A	111	GLN
1	A	144	GLN
1	A	161	GLN
1	A	164	HIS
1	B	15	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	67	GLN
1	B	146	GLN
1	B	147	GLN
1	B	164	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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$
2	TPO	C	524	2	8,10,11	1.34	1 (12%)	10,14,16	1.35	2 (20%)
2	TPO	D	524	2	8,10,11	1.07	1 (12%)	10,14,16	1.65	4 (40%)

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	TPO	C	524	2	-	2/9/11/13	-
2	TPO	D	524	2	-	3/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	524	TPO	P-OG1	-3.41	1.53	1.59
2	D	524	TPO	P-OG1	-2.69	1.54	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	524	TPO	O3P-P-OG1	2.87	117.05	105.85
2	D	524	TPO	P-OG1-CB	-2.39	116.84	123.33
2	C	524	TPO	OG1-P-O1P	2.23	117.29	109.33
2	D	524	TPO	OG1-P-O1P	-2.15	101.66	109.33
2	D	524	TPO	O-C-CA	-2.13	119.28	124.77
2	C	524	TPO	O-C-CA	-2.08	119.42	124.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	524	TPO	N-CA-CB-CG2
2	D	524	TPO	CB-OG1-P-O1P
2	C	524	TPO	O-C-CA-CB
2	D	524	TPO	O-C-CA-CB
2	C	524	TPO	N-CA-CB-CG2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
3	BTB	B	301	-	13,13,13	1.35	2 (15%)	7,16,16	1.41	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	QJK	A	302	-	38,38,38	0.80	0	53,56,56	2.24	7 (13%)
3	BTB	A	301	-	13,13,13	1.33	1 (7%)	7,16,16	1.43	1 (14%)
4	QJK	B	303	5	38,38,38	0.83	2 (5%)	53,56,56	2.31	9 (16%)

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	BTB	B	301	-	-	4/21/21/21	-
4	QJK	A	302	-	-	6/22/44/44	0/4/4/4
3	BTB	A	301	-	-	10/21/21/21	-
4	QJK	B	303	5	-	1/22/44/44	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	BTB	C2-N	3.67	1.55	1.48
3	B	301	BTB	C2-N	3.55	1.55	1.48
4	B	303	QJK	C35-C34	2.30	1.36	1.34
4	B	303	QJK	C31-N32	-2.16	1.35	1.37
3	B	301	BTB	C7-N	2.05	1.50	1.48

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	303	QJK	C33-C34-C35	-9.19	105.18	109.83
4	A	302	QJK	C33-C34-C35	-8.47	105.55	109.83
4	A	302	QJK	C34-C33-N32	7.28	107.28	101.99
4	B	303	QJK	C34-C33-N32	7.15	107.19	101.99
4	A	302	QJK	C35-C31-N32	6.54	110.17	105.89
4	B	303	QJK	C35-C31-N32	6.34	110.04	105.89
4	A	302	QJK	C33-N32-C31	-5.88	107.16	112.06
4	B	303	QJK	C33-N32-C31	-5.59	107.40	112.06
4	B	303	QJK	C29-N32-C33	5.01	126.87	121.74
4	A	302	QJK	C29-N32-C33	3.93	125.77	121.74
4	A	302	QJK	O7-C35-C34	-3.13	125.37	131.51
4	B	303	QJK	O7-C35-C34	-2.97	125.68	131.51
3	A	301	BTB	O4-C4-C2	2.61	117.54	111.40
4	B	303	QJK	O3-C1-C27	2.26	121.72	115.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	303	QJK	C14-C16-C34	2.24	125.04	120.95
4	B	303	QJK	O3-C1-O2	-2.21	118.60	123.35
4	A	302	QJK	C28-C27-C26	2.15	120.75	118.72
3	B	301	BTB	O1-C1-C2	2.11	116.36	111.40
3	B	301	BTB	O4-C4-C2	2.00	116.12	111.40

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	BTB	C1-C2-C4-O4
3	A	301	BTB	C3-C2-C4-O4
3	A	301	BTB	N-C2-C4-O4
3	A	301	BTB	C1-C2-N-C5
3	A	301	BTB	C3-C2-N-C5
3	A	301	BTB	C4-C2-N-C5
3	A	301	BTB	C4-C2-N-C7
3	A	301	BTB	N-C5-C6-O6
3	B	301	BTB	O1-C1-C2-C4
3	B	301	BTB	N-C7-C8-O8
4	A	302	QJK	O3-C1-C27-C26
3	B	301	BTB	N-C5-C6-O6
4	A	302	QJK	O2-C1-C27-C26
4	A	302	QJK	C20-C19-N4-O5
3	A	301	BTB	C3-C2-N-C7
4	A	302	QJK	C18-C19-N4-O5
4	B	303	QJK	O3-C1-C27-C26
3	A	301	BTB	C1-C2-N-C7
3	B	301	BTB	O1-C1-C2-N
4	A	302	QJK	O15-C16-C34-C33
4	A	302	QJK	O15-C16-C34-C35

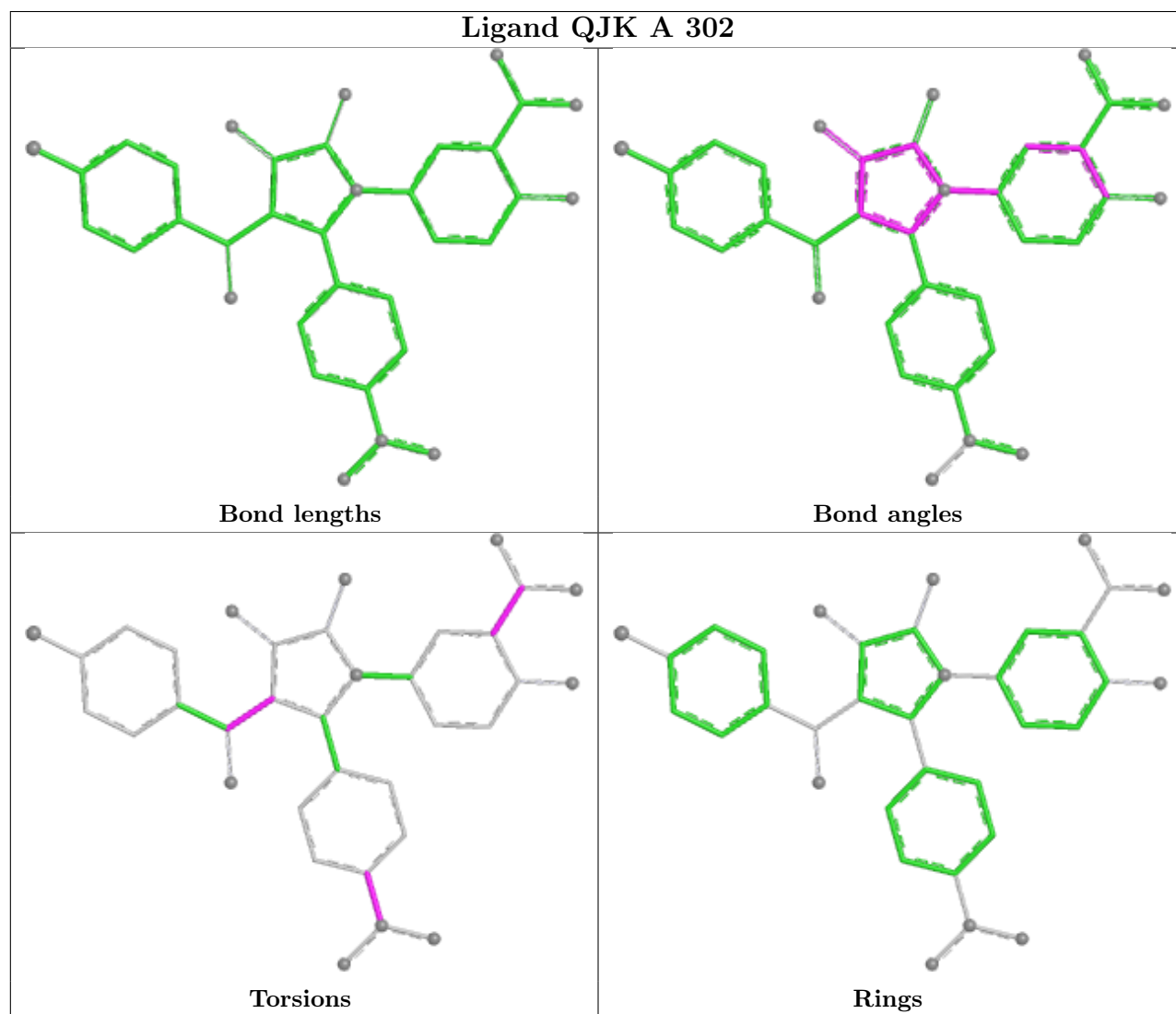
There are no ring outliers.

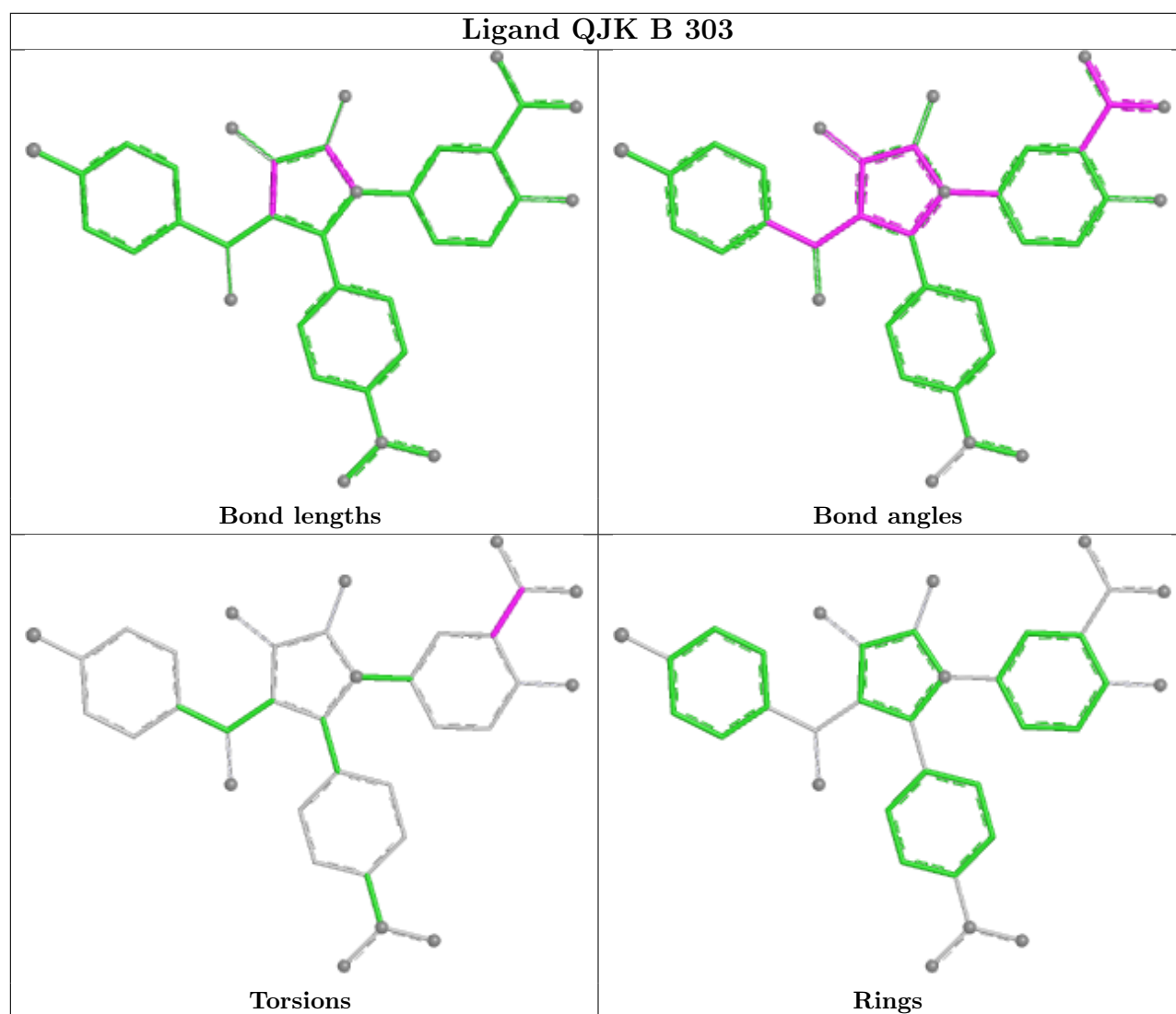
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	BTB	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	230/235 (97%)	0.58	11 (4%) 35 41	18, 42, 70, 82	1 (0%)
1	B	230/235 (97%)	0.41	9 (3%) 43 50	17, 39, 76, 95	0
2	C	11/13 (84%)	2.57	6 (54%) 0 0	44, 61, 72, 76	0
2	D	12/13 (92%)	2.60	8 (66%) 0 0	41, 57, 79, 91	0
All	All	483/496 (97%)	0.60	34 (7%) 22 26	17, 41, 74, 95	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	528	LEU	5.3
2	D	519	THR	4.6
2	D	520	ILE	4.6
2	C	520	ILE	4.3
1	A	1	MET	4.0
1	A	71	GLY	4.0
2	C	529	THR	3.9
2	C	530	PRO	3.9
2	D	529	THR	3.7
1	A	3	LYS	3.7
1	B	34	ALA	3.7
2	D	521	VAL	3.7
1	B	78	MET	3.4
2	C	519	THR	2.8
1	A	209	GLU	2.8
2	D	518	LYS	2.7
2	D	522	PRO	2.7
1	B	72	ALA	2.6
1	B	74	LYS	2.6
2	D	530	PRO	2.4
1	B	70	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	229	THR	2.4
2	C	522	PRO	2.3
1	A	181	ILE	2.3
1	B	33	GLY	2.3
1	A	157	LYS	2.3
1	A	208	GLU	2.3
1	B	1	MET	2.3
2	D	523	ALA	2.2
1	B	75	LYS	2.2
1	A	73	GLU	2.1
1	A	2	ASP	2.1
1	A	72	ALA	2.1
1	A	102	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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	TPO	D	524	11/12	0.94	0.10	32,39,42,44	0
2	TPO	C	524	11/12	0.96	0.10	29,34,42,43	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BTB	A	301	14/14	0.59	0.21	73,73,74,74	0
3	BTB	B	301	14/14	0.66	0.23	87,87,88,88	0
4	QJK	A	302	35/35	0.74	0.20	91,92,93,93	0

Continued on next page...

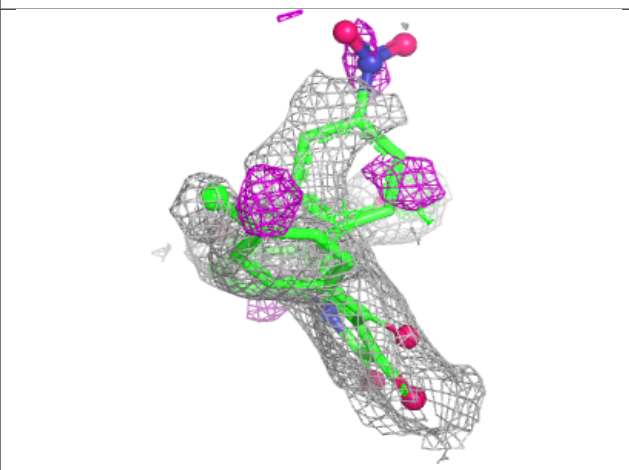
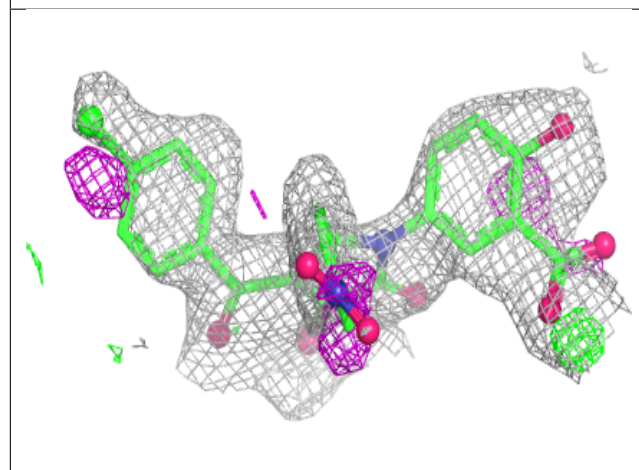
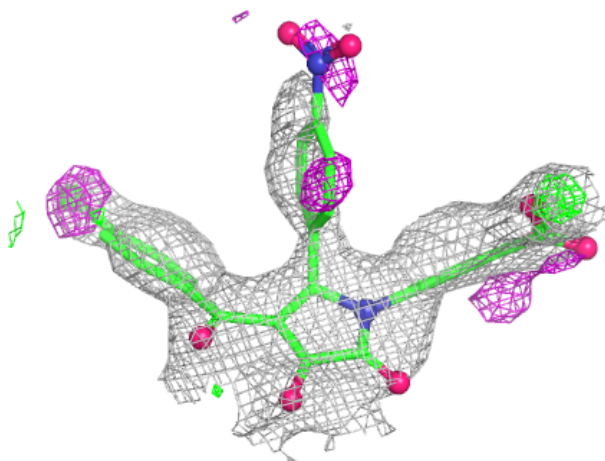
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	QJK	B	303	35/35	0.79	0.16	78,78,79,79	0
5	MG	B	302	1/1	0.79	0.10	88,88,88,88	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.

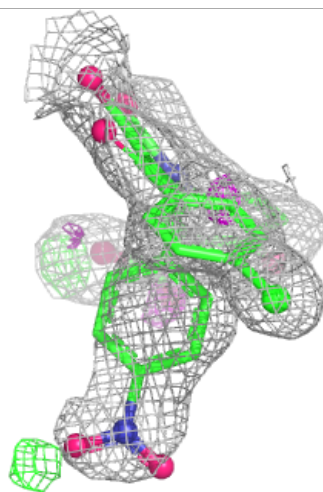
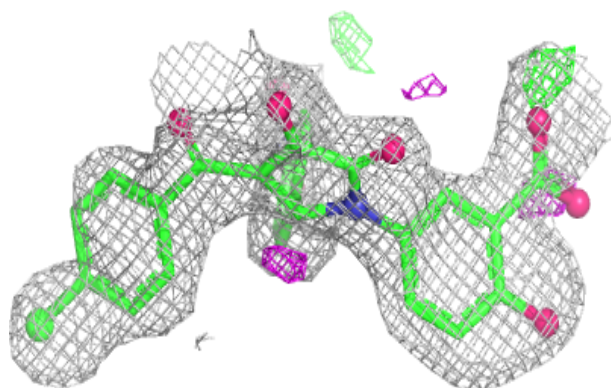
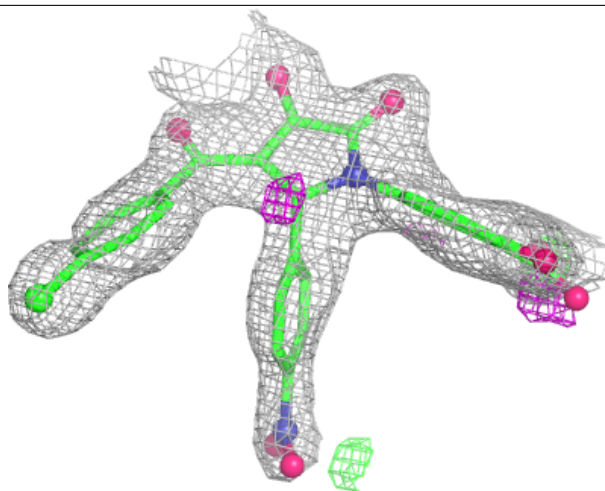
Electron density around QJK A 302:

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 QJK B 303:

$2mF_o-DF_c$ (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.