



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:12 PM UTC

PDB ID : 3K22 / pdb_00003k22
Title : Glucocorticoid Receptor with Bound alaninamide 10 with TIF2 peptide
Authors : Biggadike, K.B.; McLay, I.M.; Madauss, K.P.; Williams, S.P.; Bledsoe, R.K.
Deposited on : 2009-09-29
Resolution : 2.10 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

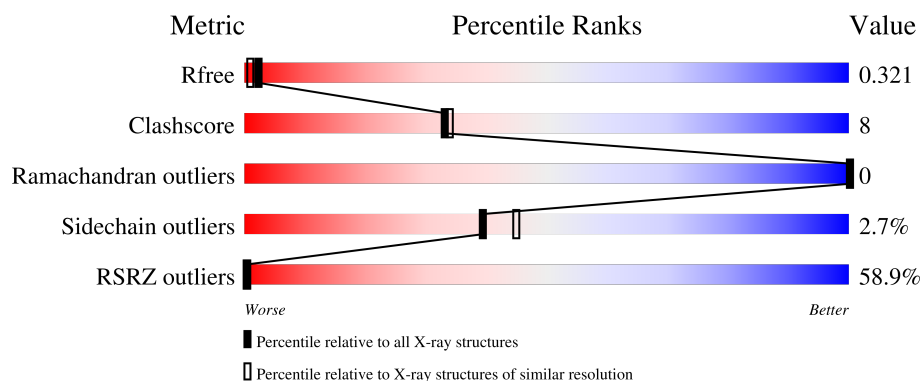
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	259	54% 82% 13% ..
1	B	259	59% 85% 10% ..
2	D	12	58% 75% 25%
2	H	12	75% 83% 8% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	JZS	B	1	-	-	X	-
4	JZR	A	1731	X	-	-	-
4	JZR	B	1731	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4352 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 Glucocorticoid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			2017	1306	331	364	16			
1	B	250	Total	C	N	O	S	0	0	0
			1979	1289	324	349	17			

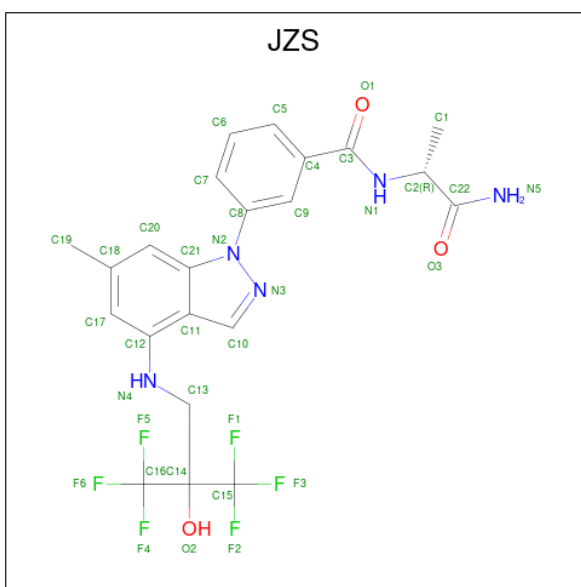
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	519	GLY	-	expression tag	UNP P04150
A	520	SER	-	expression tag	UNP P04150
A	602	TYR	PHE	engineered mutation	UNP P04150
A	638	GLY	CYS	engineered mutation	UNP P04150
B	519	GLY	-	expression tag	UNP P04150
B	520	SER	-	expression tag	UNP P04150
B	602	TYR	PHE	engineered mutation	UNP P04150
B	638	GLY	CYS	engineered mutation	UNP P04150

- Molecule 2 is a protein called Transcriptional Intermediary Factor 2.

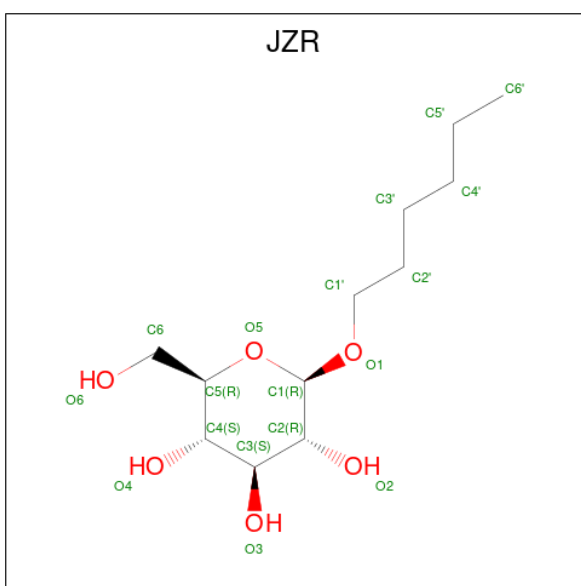
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	11	Total	C	N	O	0	0	0
			90	58	14	18			
2	D	12	Total	C	N	O	0	0	0
			96	62	17	17			

- Molecule 3 is N-[(1R)-2-amino-1-methyl-2-oxoethyl]-3-(6-methyl-4-[[3,3,3-trifluoro-2-hydroxy-2-(trifluoromethyl)propyl]amino]-1H-indazol-1-yl)benzamide (CCD ID: JZS) (formula: C₂₂H₂₁F₆N₅O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			36	22	6	5	3		
3	B	1	Total	C	F	N	O	0	0
			36	22	6	5	3		

- Molecule 4 is hexyl beta-D-glucopyranoside (CCD ID: JZR) (formula: $C_{12}H_{24}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			18	12	6		
4	B	1	Total	C	O	0	0
			18	12	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			18	12	6		

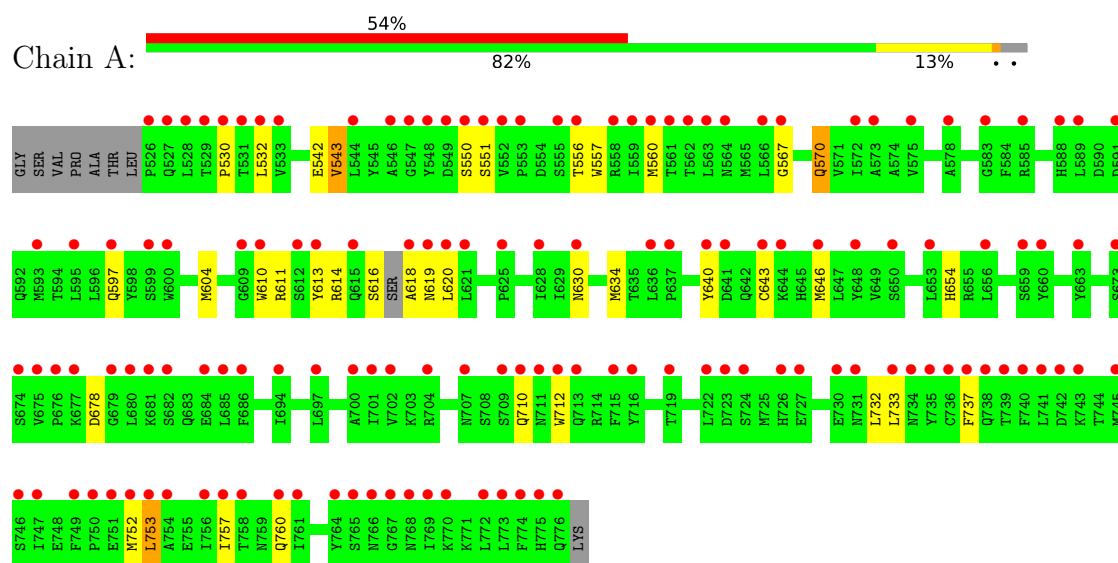
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		
5	B	13	Total	O	0	0
			13	13		

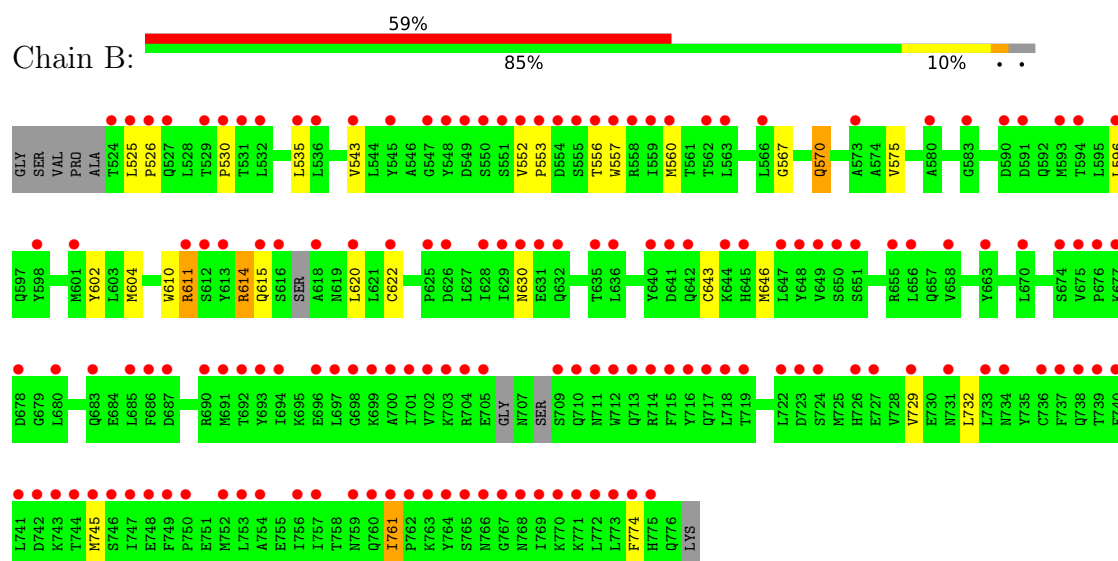
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

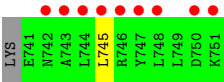
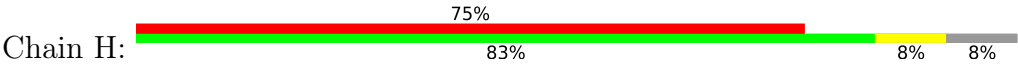
• Molecule 1: Glucocorticoid receptor



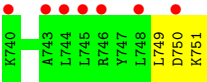
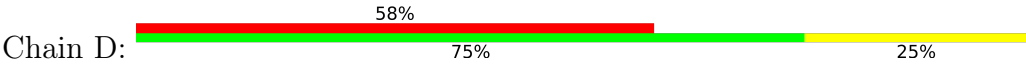
• Molecule 1: Glucocorticoid receptor



• Molecule 2: Transcriptional Intermediary Factor 2



● Molecule 2: Transcriptional Intermediary Factor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	127.60Å 127.60Å 78.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.85 – 2.10 19.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.85-2.10) 96.9 (19.85-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.98 (at 2.09Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.211 , 0.255 0.320 , 0.321	Depositor DCC
R_{free} test set	2889 reflections (7.03%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4352	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: JZR, JZS

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	0.48	0/2061	0.70	0/2789
1	B	0.48	0/2022	0.71	1/2741 (0.0%)
2	D	0.47	0/96	0.55	0/127
2	H	0.46	0/90	0.69	0/119
All	All	0.48	0/4269	0.70	1/5776 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	761	ILE	CB-CA-C	-5.84	108.15	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2017	0	2013	37	1
1	B	1979	0	1949	31	1
2	D	96	0	97	2	0
2	H	90	0	87	1	0
3	A	36	0	21	5	0
3	B	36	0	21	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	18	0	24	2	0
4	B	36	0	48	1	0
5	A	31	0	0	0	0
5	B	13	0	0	0	0
All	All	4352	0	4260	67	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (67) 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:A:604:MET:HE2	3:A:1:JZS:H9	1.27	1.16
1:A:556:THR:HG22	1:A:560:MET:HE2	1.37	1.06
1:B:604:MET:HE2	3:B:1:JZS:H9	1.39	1.04
1:B:556:THR:HG22	1:B:560:MET:HE2	1.47	0.97
1:A:570:GLN:HG2	3:A:1:JZS:HN5	1.37	0.89
1:B:604:MET:CE	3:B:1:JZS:H9	2.03	0.88
1:B:557:TRP:HA	1:B:560:MET:HE3	1.61	0.83
1:B:570:GLN:HB3	1:B:604:MET:HE3	1.58	0.82
1:A:530:PRO:HB3	1:B:535:LEU:HD12	1.62	0.81
1:A:604:MET:HE2	3:A:1:JZS:C9	2.13	0.77
1:B:745:MET:HE1	4:B:1731:JZR:O3	1.84	0.77
1:A:567:GLY:HA2	1:A:604:MET:HE1	1.66	0.76
1:B:646:MET:HE2	1:B:732:LEU:HD21	1.68	0.75
1:A:570:GLN:HG2	3:A:1:JZS:N5	2.02	0.74
1:B:570:GLN:HG3	3:B:1:JZS:N5	2.01	0.74
1:B:604:MET:HE2	3:B:1:JZS:C9	2.16	0.74
1:B:570:GLN:CB	1:B:604:MET:HE3	2.17	0.73
1:B:567:GLY:HA2	1:B:604:MET:HE1	1.72	0.72
1:A:557:TRP:HA	1:A:560:MET:HE3	1.71	0.70
1:A:556:THR:CG2	1:A:560:MET:HE2	2.20	0.67
1:B:570:GLN:HG2	3:B:1:JZS:C9	2.25	0.66
1:A:532:LEU:HD13	1:B:530:PRO:HD3	1.80	0.62
1:A:570:GLN:HB3	1:A:604:MET:HE3	1.81	0.62
1:B:570:GLN:HG2	3:B:1:JZS:C3	2.30	0.61
1:A:646:MET:HE1	4:A:1731:JZR:H6'B	1.83	0.60
1:A:616:SER:HG	1:A:618:ALA:N	2.00	0.60
1:A:610:TRP:CZ2	1:A:614:ARG:HD2	2.39	0.57
1:B:570:GLN:HG3	3:B:1:JZS:HN5	1.69	0.57
1:B:646:MET:HE2	1:B:732:LEU:CD2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:CYS:HA	1:B:646:MET:HE3	1.86	0.56
1:A:634:MET:HE2	1:A:640:TYR:HA	1.86	0.56
1:B:570:GLN:HG2	3:B:1:JZS:C4	2.34	0.56
1:A:646:MET:HE2	1:A:732:LEU:HD22	1.88	0.55
1:B:556:THR:CG2	1:B:560:MET:HE2	2.30	0.53
1:A:634:MET:HE1	1:A:643:CYS:HB2	1.91	0.52
1:A:753:LEU:HD22	1:A:757:ILE:HD11	1.94	0.50
1:B:610:TRP:CZ2	1:B:614:ARG:HD3	2.45	0.50
1:B:575:VAL:HG22	1:B:596:LEU:HD13	1.95	0.49
1:A:543:VAL:HG23	1:A:611:ARG:CZ	2.43	0.49
1:A:646:MET:HE2	1:A:732:LEU:CD2	2.44	0.48
1:A:646:MET:HE1	4:A:1731:JZR:C6'	2.44	0.47
1:A:620:LEU:HD22	1:A:630:ASN:HA	1.96	0.47
1:B:602:TYR:CG	1:B:729:VAL:HG21	2.51	0.46
2:D:750:ASP:O	2:D:751:LYS:C	2.58	0.46
1:A:597:GLN:HB3	1:A:760:GLN:NE2	2.30	0.46
1:A:557:TRP:CA	1:A:560:MET:HE3	2.44	0.45
1:B:620:LEU:HD22	1:B:630:ASN:HA	1.99	0.45
1:A:634:MET:HE1	1:A:643:CYS:CB	2.47	0.45
1:A:634:MET:HE3	1:A:634:MET:HA	1.97	0.45
1:A:733:LEU:HD22	1:A:737:PHE:CZ	2.52	0.44
1:A:604:MET:HA	3:A:1:JZS:O1	2.18	0.44
1:B:611:ARG:HG2	1:B:622:CYS:O	2.17	0.44
1:A:752:MET:HE3	1:A:752:MET:HA	2.00	0.44
1:A:570:GLN:HB3	1:A:604:MET:CE	2.47	0.44
1:A:753:LEU:HD22	1:A:757:ILE:CD1	2.48	0.44
1:B:596:LEU:CD1	2:D:749:LEU:HD21	2.47	0.44
1:A:619:ASN:O	1:A:620:LEU:HD23	2.19	0.43
1:B:525:LEU:N	1:B:526:PRO:CD	2.81	0.42
1:A:550:SER:O	1:A:551:SER:C	2.61	0.42
1:A:613:TYR:CE1	1:A:654:HIS:HA	2.54	0.42
1:A:752:MET:HE1	2:H:745:LEU:HB2	2.01	0.42
1:B:552:VAL:HG13	1:B:553:PRO:HD2	2.01	0.41
1:A:570:GLN:HE21	1:A:570:GLN:HB2	1.59	0.41
1:B:570:GLN:CG	3:B:1:JZS:C3	2.99	0.41
1:B:602:TYR:CD2	1:B:729:VAL:HG21	2.56	0.41
1:B:604:MET:HE3	3:B:1:JZS:H9	1.96	0.41
1:A:737:PHE:CD2	1:A:757:ILE:HG23	2.56	0.41

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:TRP:NE1	1:B:774:PHE:O[4_565]	2.13	0.07

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	246/259 (95%)	237 (96%)	9 (4%)	0	100	100
1	B	243/259 (94%)	239 (98%)	4 (2%)	0	100	100
2	D	10/12 (83%)	9 (90%)	1 (10%)	0	100	100
2	H	9/12 (75%)	9 (100%)	0	0	100	100
All	All	508/542 (94%)	494 (97%)	14 (3%)	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	220/236 (93%)	214 (97%)	6 (3%)	39	45
1	B	208/236 (88%)	202 (97%)	6 (3%)	37	42
2	D	9/11 (82%)	9 (100%)	0	100	100
2	H	8/11 (73%)	8 (100%)	0	100	100
All	All	445/494 (90%)	433 (97%)	12 (3%)	39	45

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	542	GLU
1	A	543	VAL
1	A	570	GLN
1	A	678	ASP
1	A	710	GLN
1	A	753	LEU
1	B	543	VAL
1	B	570	GLN
1	B	611	ARG
1	B	614	ARG
1	B	615	GLN
1	B	761	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	570	GLN
1	A	717	GLN
1	A	760	GLN
1	B	760	GLN
1	B	776	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	JZS	B	1	-	37,38,38	1.66	6 (16%)	54,59,59	1.56	9 (16%)
4	JZR	B	778	-	18,18,18	0.76	1 (5%)	23,23,23	0.94	1 (4%)
4	JZR	A	1731	-	18,18,18	0.71	1 (5%)	23,23,23	2.15	3 (13%)
4	JZR	B	1731	-	18,18,18	0.74	1 (5%)	23,23,23	2.24	5 (21%)
3	JZS	A	1	-	37,38,38	1.67	6 (16%)	54,59,59	1.45	8 (14%)

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	JZS	B	1	-	-	4/40/40/40	0/3/3/3
4	JZR	B	778	-	-	6/9/29/29	0/1/1/1
4	JZR	A	1731	-	1/1/5/5	4/9/29/29	0/1/1/1
4	JZR	B	1731	-	1/1/5/5	5/9/29/29	0/1/1/1
3	JZS	A	1	-	-	6/40/40/40	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	JZS	N2-N3	-4.11	1.33	1.38
3	A	1	JZS	N2-N3	-4.10	1.33	1.38
3	A	1	JZS	C11-C12	-4.09	1.38	1.41
3	B	1	JZS	C11-C21	-3.91	1.37	1.41
3	B	1	JZS	C11-C12	-3.90	1.38	1.41
3	A	1	JZS	C11-C21	-3.86	1.37	1.41
3	A	1	JZS	C16-C14	-3.04	1.49	1.53
3	B	1	JZS	C15-C14	-2.97	1.49	1.53
3	B	1	JZS	C8-N2	-2.96	1.38	1.42
3	A	1	JZS	C8-N2	-2.86	1.39	1.42
3	A	1	JZS	C15-C14	-2.71	1.50	1.53
4	B	778	JZR	O1-C1	2.71	1.44	1.40
4	B	1731	JZR	O1-C1	2.60	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1731	JZR	O1-C1	2.60	1.44	1.40
3	B	1	JZS	C16-C14	-2.59	1.50	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1731	JZR	O1-C1-C2	7.57	119.77	108.27
4	B	1731	JZR	O1-C1-C2	6.33	117.89	108.27
4	B	1731	JZR	O5-C1-C2	5.26	121.19	110.37
4	B	1731	JZR	O5-C1-O1	4.40	120.45	110.04
4	A	1731	JZR	O5-C1-C2	4.40	119.40	110.37
4	A	1731	JZR	O5-C1-O1	4.24	120.06	110.04
3	B	1	JZS	C17-C12-C11	-4.11	114.84	120.47
3	A	1	JZS	C17-C12-C11	-3.96	115.06	120.47
3	B	1	JZS	C20-C18-C17	3.88	122.42	118.11
3	A	1	JZS	C20-C18-C17	3.85	122.39	118.11
3	B	1	JZS	C10-N3-N2	-3.72	103.77	106.14
4	B	1731	JZR	C1-O5-C5	3.60	120.74	113.72
3	A	1	JZS	C21-C20-C18	-3.45	114.39	120.62
3	B	1	JZS	C21-C20-C18	-3.33	114.60	120.62
3	A	1	JZS	C10-N3-N2	-3.20	104.10	106.14
4	B	778	JZR	O1-C1-C2	2.96	112.77	108.27
3	B	1	JZS	C21-N2-N3	2.80	113.58	111.33
3	A	1	JZS	C21-N2-N3	2.51	113.34	111.33
3	B	1	JZS	C8-N2-N3	-2.49	117.06	119.15
3	B	1	JZS	C21-C11-C12	2.42	121.70	118.29
4	B	1731	JZR	O5-C5-C4	2.40	114.02	109.70
3	B	1	JZS	C5-C4-C9	2.39	122.01	119.25
3	A	1	JZS	C5-C4-C9	2.33	121.94	119.25
3	A	1	JZS	O2-C14-C13	-2.25	108.47	112.65
3	B	1	JZS	O2-C14-C13	-2.13	108.70	112.65
3	A	1	JZS	C21-C11-C12	2.10	121.25	118.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1731	JZR	C1
4	B	1731	JZR	C1

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1731	JZR	O5-C1-O1-C1'
4	B	1731	JZR	O5-C1-O1-C1'
4	B	778	JZR	C2'-C1'-O1-C1
4	B	778	JZR	O5-C1-O1-C1'
4	B	778	JZR	C4-C5-C6-O6
4	B	1731	JZR	C2'-C1'-O1-C1
3	B	1	JZS	C7-C8-N2-N3
4	B	778	JZR	C1'-C2'-C3'-C4'
4	B	778	JZR	O5-C5-C6-O6
4	A	1731	JZR	C1'-C2'-C3'-C4'
3	A	1	JZS	C7-C8-N2-N3
3	A	1	JZS	C9-C8-N2-N3
3	B	1	JZS	C9-C8-N2-N3
4	B	778	JZR	O1-C1'-C2'-C3'
4	A	1731	JZR	C3'-C4'-C5'-C6'
3	A	1	JZS	C9-C8-N2-C21
4	B	1731	JZR	C2'-C3'-C4'-C5'
4	A	1731	JZR	C2'-C3'-C4'-C5'
3	A	1	JZS	C7-C8-N2-C21
4	B	1731	JZR	C3'-C4'-C5'-C6'
3	A	1	JZS	C15-C14-C16-F4
3	B	1	JZS	C7-C8-N2-C21
3	B	1	JZS	C9-C8-N2-C21
4	B	1731	JZR	O1-C1'-C2'-C3'
3	A	1	JZS	C15-C14-C16-F5

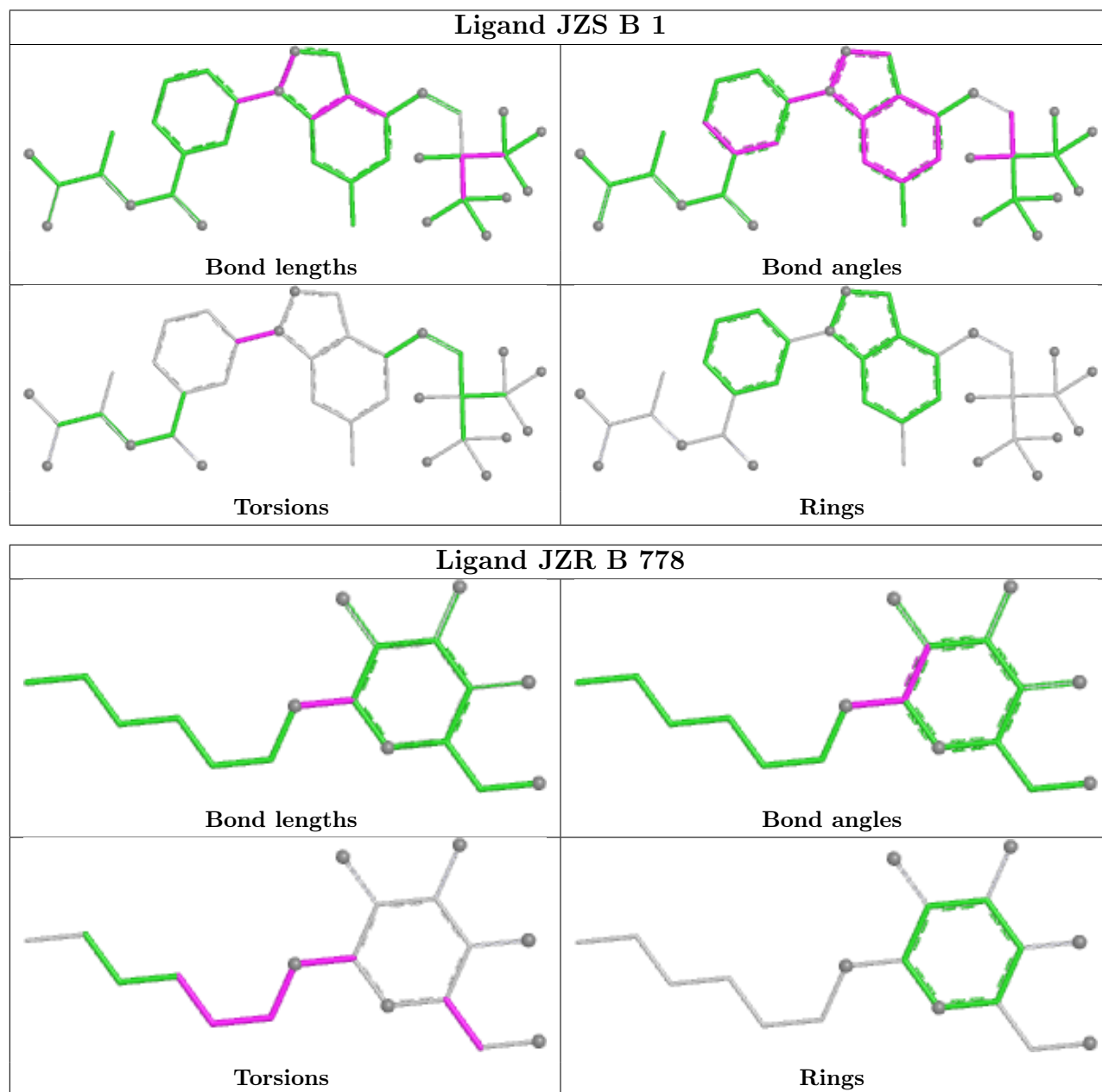
There are no ring outliers.

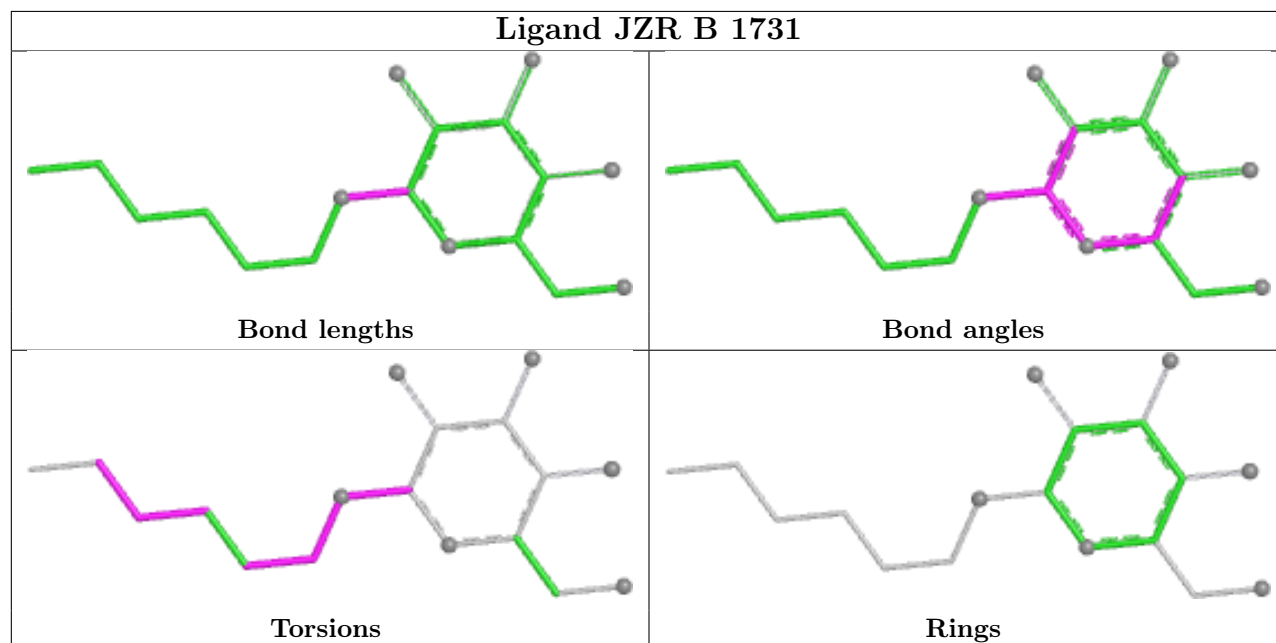
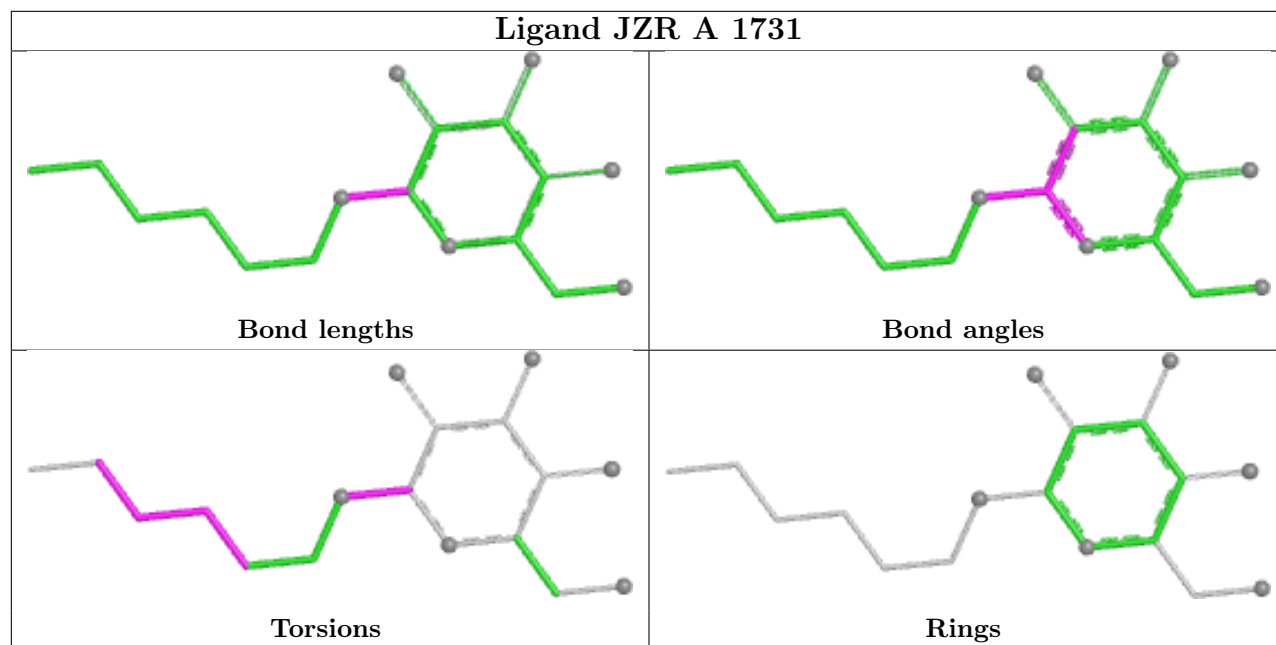
4 monomers are involved in 18 short contacts:

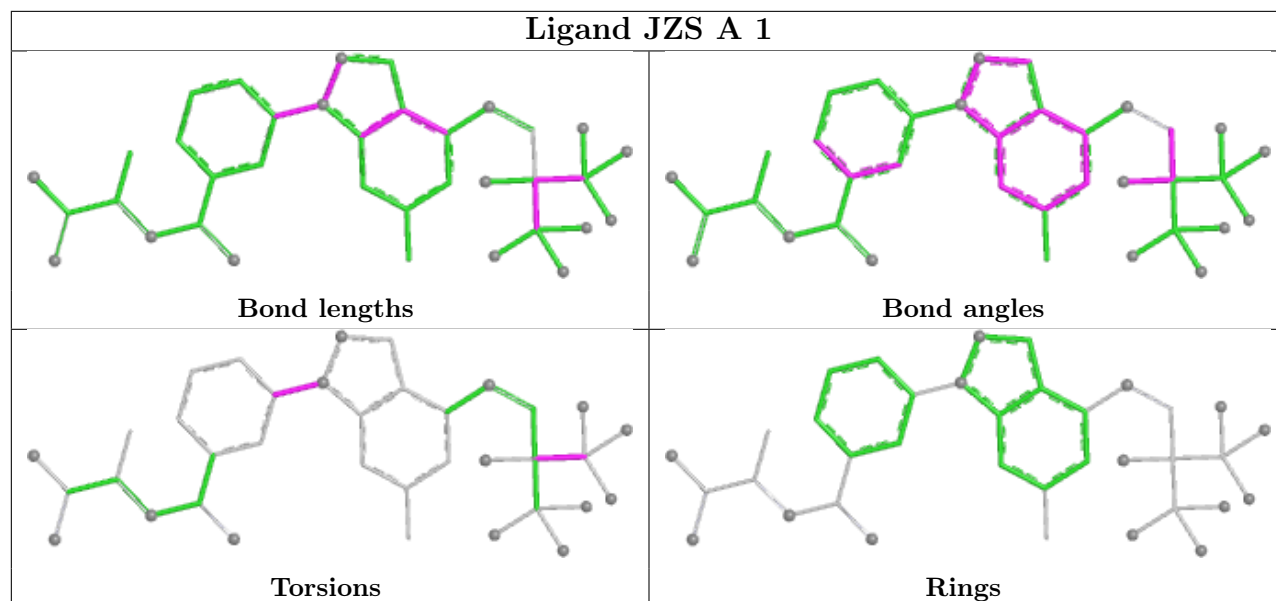
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	JZS	10	0
4	A	1731	JZR	2	0
4	B	1731	JZR	1	0
3	A	1	JZS	5	0

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	250/259 (96%)	2.17	139 (55%) 0 0	42, 56, 71, 80	1 (0%)
1	B	250/259 (96%)	2.42	153 (61%) 0 0	45, 59, 74, 83	0
2	D	12/12 (100%)	2.17	7 (58%) 0 0	58, 62, 69, 70	0
2	H	11/12 (91%)	2.23	9 (81%) 0 0	58, 61, 67, 69	0
All	All	523/542 (96%)	2.29	308 (58%) 0 0	42, 58, 73, 83	1 (0%)

All (308) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	556	THR	6.9
1	B	551	SER	6.5
1	B	616	SER	6.2
1	B	525	LEU	5.9
1	B	524	THR	5.7
1	B	773	LEU	5.6
1	B	764	TYR	5.6
1	A	615	GLN	5.2
1	A	556	THR	5.0
1	B	716	TYR	4.9
1	A	754	ALA	4.8
1	A	741	LEU	4.7
1	B	552	VAL	4.7
1	B	765	SER	4.7
1	A	765	SER	4.5
1	B	754	ALA	4.5
1	B	702	VAL	4.5
1	A	550	SER	4.4
1	A	764	TYR	4.4
2	D	740	LYS	4.4
1	B	709	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	747	ILE	4.4
1	B	750	PRO	4.3
1	B	559	ILE	4.3
1	B	747	ILE	4.3
1	A	761	ILE	4.2
1	B	698	GLY	4.1
1	A	702	VAL	4.0
1	A	526	PRO	4.0
1	B	550	SER	3.9
1	A	773	LEU	3.9
1	B	711	ASN	3.9
1	B	772	LEU	3.8
1	B	557	TRP	3.8
1	B	723	ASP	3.8
1	A	551	SER	3.7
1	A	766	ASN	3.7
1	B	699	LYS	3.7
1	A	684	GLU	3.7
1	B	745	MET	3.7
1	B	560	MET	3.7
1	A	724	SER	3.7
1	A	613	TYR	3.6
1	B	676	PRO	3.6
1	A	648	TYR	3.6
1	B	640	TYR	3.6
1	A	746	SER	3.6
1	B	712	TRP	3.6
1	B	626	ASP	3.6
1	B	763	LYS	3.6
1	A	555	SER	3.6
1	B	558	ARG	3.5
1	B	526	PRO	3.5
1	B	553	PRO	3.5
1	B	590	ASP	3.5
1	B	548	TYR	3.5
1	B	680	LEU	3.5
1	A	529	THR	3.5
1	A	756	ILE	3.4
1	A	768	ASN	3.4
1	B	675	VAL	3.4
1	B	741	LEU	3.4
1	A	758	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	756	ILE	3.4
1	A	751	GLU	3.3
1	B	648	TYR	3.3
1	B	748	GLU	3.3
1	B	743	LYS	3.3
1	B	739	THR	3.3
1	B	701	ILE	3.3
1	A	656	LEU	3.3
1	B	733	LEU	3.3
1	B	774	PHE	3.3
1	A	588	HIS	3.3
1	A	735	TYR	3.3
1	B	628	ILE	3.3
1	A	646	MET	3.3
1	A	562	THR	3.2
1	A	583	GLY	3.2
1	A	774	PHE	3.2
1	B	641	ASP	3.2
1	B	529	THR	3.2
1	B	767	GLY	3.2
1	A	730	GLU	3.2
1	A	776	GLN	3.2
1	B	757	ILE	3.2
1	B	591	ASP	3.2
1	B	691	MET	3.2
1	A	700	ALA	3.1
1	B	543	VAL	3.1
1	B	697	LEU	3.1
1	B	613	TYR	3.1
1	B	612	SER	3.1
1	A	618	ALA	3.1
1	B	752	MET	3.1
1	A	630	ASN	3.1
1	B	630	ASN	3.1
1	B	636	LEU	3.1
1	A	757	ILE	3.1
1	A	742	ASP	3.1
1	B	770	LYS	3.1
1	A	713	GLN	3.1
1	A	619	ASN	3.0
1	B	647	LEU	3.0
1	B	759	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	560	MET	3.0
1	A	531	THR	3.0
1	A	659	SER	3.0
1	A	533	VAL	3.0
1	B	685	LEU	3.0
1	A	572	ILE	3.0
1	B	749	PHE	3.0
1	B	580	ALA	2.9
1	B	670	LEU	2.9
1	A	737	PHE	2.9
1	B	693	TYR	2.9
1	A	712	TRP	2.9
1	B	573	ALA	2.9
1	A	772	LEU	2.9
1	A	715	PHE	2.9
1	B	700	ALA	2.9
1	B	718	LEU	2.9
1	A	723	ASP	2.9
1	B	622	CYS	2.9
1	B	713	GLN	2.9
1	A	673	SER	2.8
1	A	752	MET	2.8
1	B	549	ASP	2.8
1	B	601	MET	2.8
1	B	761	ILE	2.8
1	B	555	SER	2.8
1	A	745	MET	2.8
1	A	749	PHE	2.8
1	A	595	LEU	2.8
1	B	656	LEU	2.8
1	B	719	THR	2.8
1	A	628	ILE	2.8
1	B	618	ALA	2.8
2	D	745	LEU	2.8
1	B	762	PRO	2.8
1	A	675	VAL	2.8
1	A	564	ASN	2.7
1	B	611	ARG	2.7
1	A	694	ILE	2.7
1	A	701	ILE	2.7
2	H	746	ARG	2.7
1	A	738	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	750	PRO	2.7
1	B	527	GLN	2.7
1	B	686	PHE	2.7
1	B	535	LEU	2.7
1	B	705	GLU	2.7
1	A	548	TYR	2.7
1	A	716	TYR	2.7
1	B	734	ASN	2.7
1	B	768	ASN	2.7
1	B	742	ASP	2.7
1	B	642	GLN	2.6
1	A	620	LEU	2.6
1	B	690	ARG	2.6
1	B	744	THR	2.6
1	B	625	PRO	2.6
1	A	641	ASP	2.6
1	A	546	ALA	2.6
1	B	644	LYS	2.6
1	B	650	SER	2.6
1	B	737	PHE	2.6
1	B	714	ARG	2.6
1	A	726	HIS	2.6
1	B	766	ASN	2.6
1	A	553	PRO	2.6
2	H	745	LEU	2.6
1	A	575	VAL	2.5
1	B	736	CYS	2.5
1	B	775	HIS	2.5
1	A	719	THR	2.5
1	B	724	SER	2.5
1	A	532	LEU	2.5
1	B	545	TYR	2.5
1	B	717	GLN	2.5
1	B	696	GLU	2.5
1	A	563	LEU	2.5
1	A	636	LEU	2.5
1	B	753	LEU	2.5
2	H	748	LEU	2.5
1	B	629	ILE	2.5
1	B	694	ILE	2.5
1	A	734	ASN	2.5
1	B	530	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	704	ARG	2.5
1	A	591	ASP	2.4
1	A	709	SER	2.4
1	B	674	SER	2.4
1	A	530	PRO	2.4
2	H	743	ALA	2.4
1	A	680	LEU	2.4
1	B	566	LEU	2.4
1	B	596	LEU	2.4
1	B	722	LEU	2.4
1	B	771	LYS	2.4
1	B	740	PHE	2.4
1	A	727	GLU	2.4
1	B	710	GLN	2.4
1	A	549	ASP	2.4
1	A	610	TRP	2.4
1	A	663	TYR	2.4
1	A	674	SER	2.4
1	B	651	SER	2.4
2	H	747	TYR	2.4
1	A	637	PRO	2.4
1	A	609	GLY	2.4
1	B	635	THR	2.4
1	B	598	TYR	2.3
1	A	621	LEU	2.3
1	A	707	ASN	2.3
1	A	731	ASN	2.3
1	B	532	LEU	2.3
1	A	547	GLY	2.3
1	A	686	PHE	2.3
1	A	740	PHE	2.3
1	B	703	LYS	2.3
1	A	682	SER	2.3
1	B	658	VAL	2.3
1	A	739	THR	2.3
1	A	527	GLN	2.3
1	A	600	TRP	2.3
1	B	615	GLN	2.3
2	H	744	LEU	2.3
2	D	748	LEU	2.3
1	A	612	SER	2.3
1	A	710	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	562	THR	2.3
1	A	643	CYS	2.3
1	A	544	LEU	2.3
1	A	589	LEU	2.3
1	A	722	LEU	2.3
1	A	767	GLY	2.3
1	A	743	LYS	2.3
1	B	760	GLN	2.3
1	B	729	VAL	2.3
2	D	746	ARG	2.3
2	H	750	ASP	2.3
2	D	743	ALA	2.3
1	B	547	GLY	2.3
1	A	653	LEU	2.3
1	A	753	LEU	2.3
1	B	715	PHE	2.2
1	A	559	ILE	2.2
1	B	531	THR	2.2
1	B	704	ARG	2.2
1	A	736	CYS	2.2
2	D	744	LEU	2.2
1	A	650	SER	2.2
1	A	677	LYS	2.2
1	A	711	ASN	2.2
1	B	769	ILE	2.2
2	H	742	ASN	2.2
1	B	687	ASP	2.2
2	D	750	ASP	2.2
1	A	679	GLY	2.2
1	A	733	LEU	2.2
1	B	726	HIS	2.2
1	B	677	LYS	2.2
1	A	552	VAL	2.2
1	A	697	LEU	2.2
1	B	563	LEU	2.2
1	A	585	ARG	2.2
1	B	746	SER	2.2
2	H	751	LYS	2.2
1	A	660	TYR	2.1
1	B	731	ASN	2.1
1	B	554	ASP	2.1
1	B	678	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	561	THR	2.1
1	B	594	THR	2.1
1	B	692	THR	2.1
1	A	760	GLN	2.1
1	A	567	GLY	2.1
1	B	649	VAL	2.1
1	B	655	ARG	2.1
1	A	599	SER	2.1
1	B	536	LEU	2.1
1	A	640	TYR	2.1
1	B	645	HIS	2.1
1	A	769	ILE	2.1
1	A	644	LYS	2.1
1	A	578	ALA	2.1
1	A	593	MET	2.1
1	B	727	GLU	2.1
1	B	683	GLN	2.1
1	A	625	PRO	2.1
1	B	583	GLY	2.1
1	A	573	ALA	2.1
1	B	593	MET	2.0
1	A	528	LEU	2.0
1	A	566	LEU	2.0
1	B	620	LEU	2.0
1	A	558	ARG	2.0
1	A	775	HIS	2.0
1	A	681	LYS	2.0
1	A	770	LYS	2.0
1	B	631	GLU	2.0
1	A	597	GLN	2.0
1	A	685	LEU	2.0
1	B	632	GLN	2.0
1	B	738	GLN	2.0
1	A	676	PRO	2.0
1	B	663	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](#)

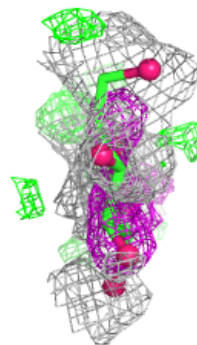
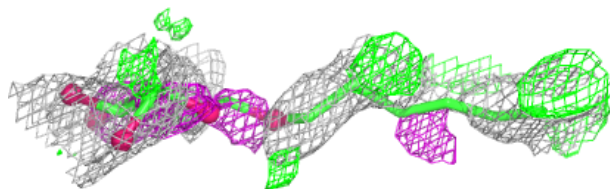
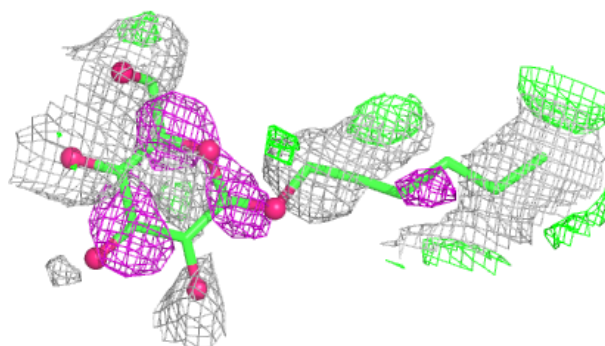
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	JZR	B	778	18/18	0.31	0.28	65,70,71,71	0
4	JZR	B	1731	18/18	0.68	0.21	80,82,83,83	0
4	JZR	A	1731	18/18	0.69	0.20	69,72,73,74	0
3	JZS	B	1	36/36	0.89	0.10	39,42,46,47	0
3	JZS	A	1	36/36	0.89	0.10	41,42,45,46	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.

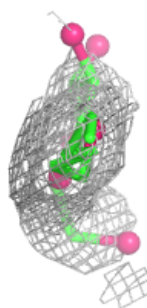
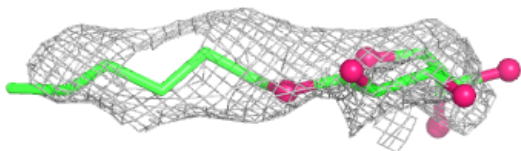
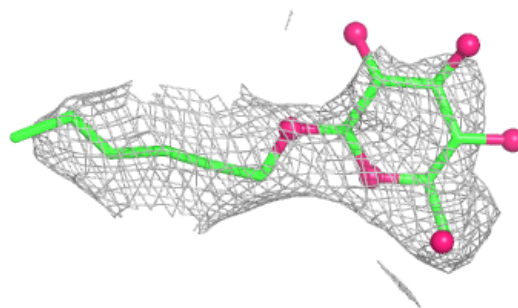
Electron density around JZR B 778:

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

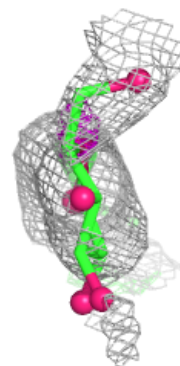
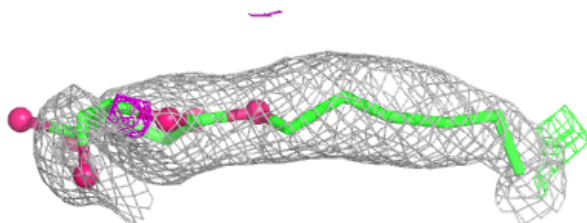
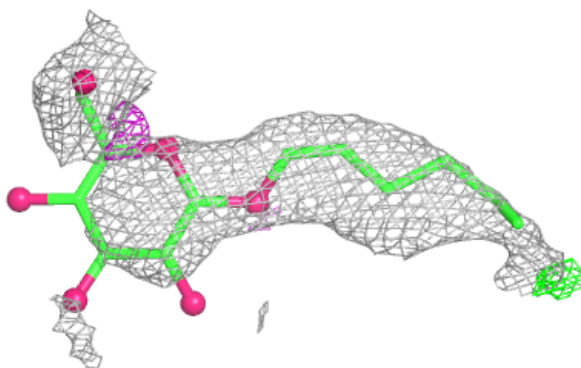


Electron density around JZR B 1731:

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

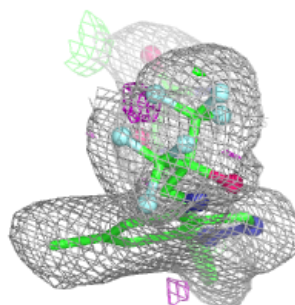
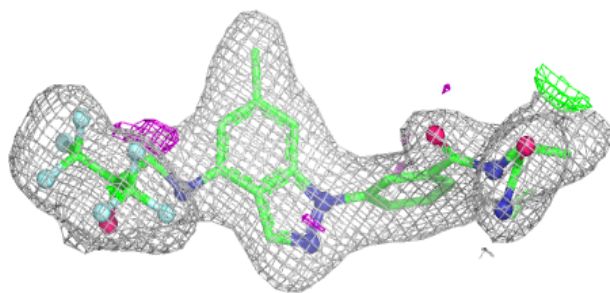
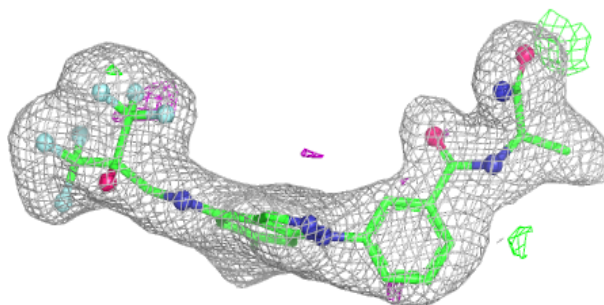
**Electron density around JZR A 1731:**

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

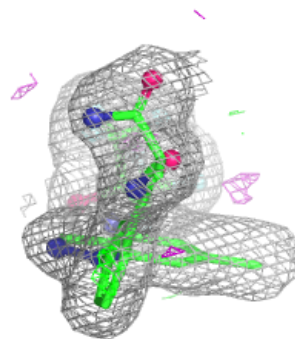
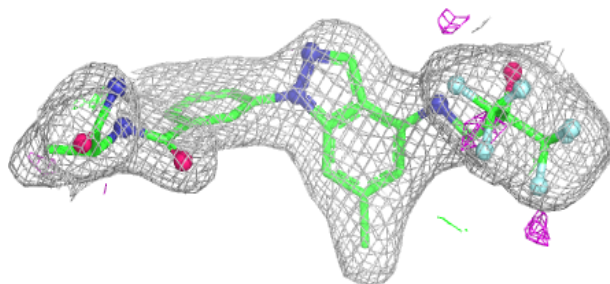
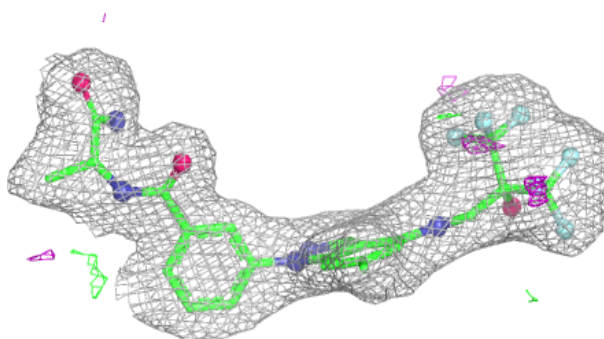


Electron density around JZS B 1:

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

**Electron density around JZS A 1:**

$2mF_o-DF_c$ (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.