



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:38 PM UTC

PDB ID : 1PY2 / pdb_00001py2
Title : Structure of a 60 nM Small Molecule Bound to a Hot Spot on IL-2
Authors : Thanos, C.D.; Randal, M.; Wells, J.A.
Deposited on : 2003-07-07
Resolution : 2.80 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

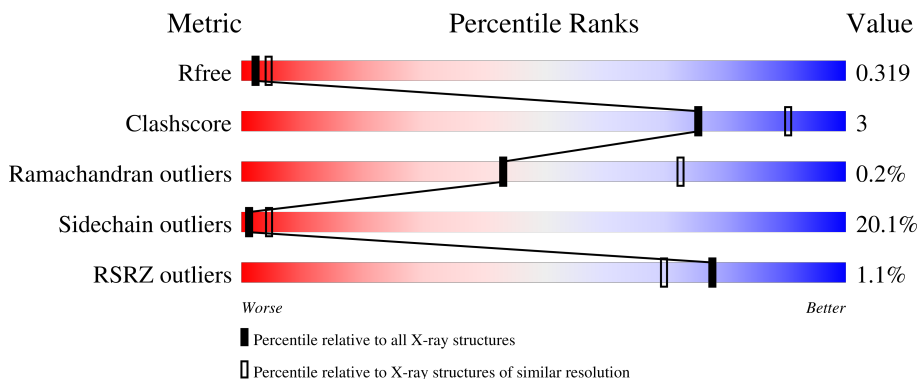
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	132	 % 63% 23% 11%
1	B	132	 2% 61% 18% 7% 12%
1	C	132	 % 58% 23% 6% 13%
1	D	132	 % 64% 23% 9%

2 Entry composition i

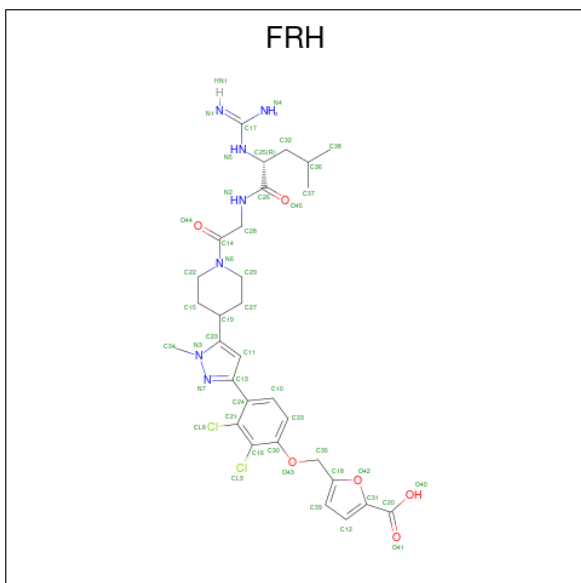
There are 3 unique types of molecules in this entry. The entry contains 4015 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Interleukin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	117	Total 959	C 623	N 152	O 177	S 7	50	0	0
1	B	116	Total 951	C 616	N 154	O 174	S 7	54	0	0
1	C	115	Total 944	C 610	N 152	O 175	S 7	48	0	0
1	D	120	Total 978	C 631	N 158	O 182	S 7	24	0	0

- Molecule 2 is 5-[2,3-DICHLORO-4-(5-{1-[2-(2-GUANIDINO-4-METHYL-PENTANOYLAMINO)-ACETYL]-PIPERIDIN-4-YL}-1-METHYL-1H-PYRAZOL-3-YL)-PHENOXYMETHYL]-FURAN-2-CARBOXYLIC ACID (CCD ID: FRH) (formula: $C_{30}H_{37}Cl_2N_7O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	A	1	Total 45	C 30	Cl 2	N 7	O 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	B	1	Total	C	Cl	N	O	0	0
			45	30	2	7	6		
2	C	1	Total	C	Cl	N	O	0	0
			45	30	2	7	6		
2	D	1	Total	C	Cl	N	O	0	0
			45	30	2	7	6		

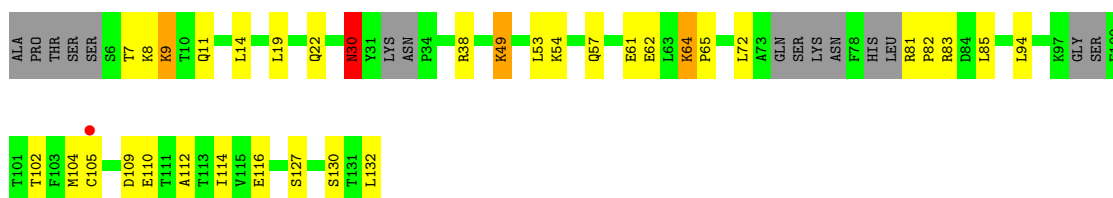
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	C	1	Total	Zn	0	0
			1	1		

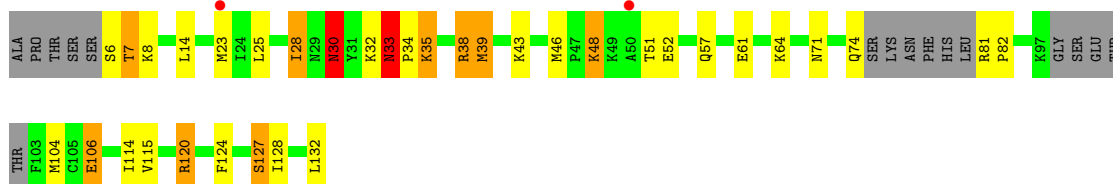
3 Residue-property plots [i](#)

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.

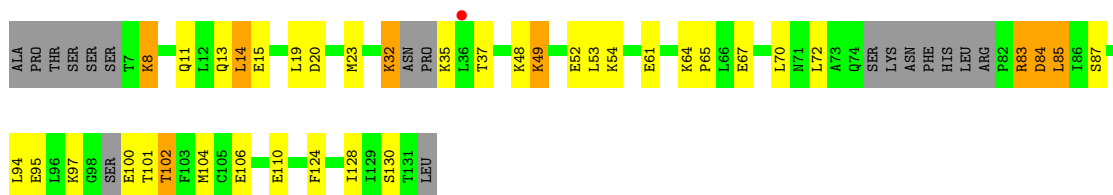
- Molecule 1: Interleukin-2



- Molecule 1: Interleukin-2



- Molecule 1: Interleukin-2



- Molecule 1: Interleukin-2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.98Å 52.45Å 89.47Å 90.00° 106.34° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (15.00-2.80) 97.7 (15.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.79Å)	Xtrriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.271 , 0.320 0.267 , 0.319	Depositor DCC
R_{free} test set	660 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtrriage
Anisotropy	0.183	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4015	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% 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: ZN, FRH

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	2.02	10/971 (1.0%)	1.75	14/1306 (1.1%)
1	B	2.72	10/964 (1.0%)	1.82	19/1299 (1.5%)
1	C	1.98	12/955 (1.3%)	1.37	17/1283 (1.3%)
1	D	1.64	7/991 (0.7%)	1.64	12/1336 (0.9%)
All	All	2.12	39/3881 (1.0%)	1.65	62/5224 (1.2%)

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	1
1	B	0	1
All	All	0	2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	32	LYS	CB-CG	68.17	3.56	1.52
1	A	49	LYS	CB-CG	37.87	2.66	1.52
1	D	102	THR	CB-OG1	36.00	2.01	1.43
1	C	83	ARG	CB-CG	35.82	2.60	1.52
1	A	30	ASN	CG-OD1	29.04	1.78	1.23
1	C	83	ARG	C-N	-27.08	1.00	1.33
1	B	64	LYS	CB-CG	23.70	2.23	1.52
1	B	7	THR	CA-CB	23.58	1.92	1.53
1	D	8	LYS	CB-CG	21.77	2.17	1.52
1	C	37	THR	CB-OG1	20.75	1.76	1.43
1	A	94	LEU	CB-CG	-20.23	1.12	1.53
1	B	104	MET	CB-CG	19.93	2.12	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	30	ASN	CB-CG	19.64	2.01	1.52
1	C	84	ASP	C-N	-19.54	1.06	1.33
1	D	11	GLN	CB-CG	17.31	2.04	1.52
1	A	130	SER	CB-OG	-16.00	1.10	1.42
1	A	83	ARG	CB-CG	-15.05	1.07	1.52
1	A	127	SER	CB-OG	-14.96	1.12	1.42
1	C	49	LYS	CG-CD	13.50	1.93	1.52
1	D	52	GLU	CB-CG	-13.23	1.12	1.52
1	D	8	LYS	CD-CE	12.38	1.89	1.52
1	C	110	GLU	CB-CG	11.80	1.87	1.52
1	A	7	THR	CB-CG2	11.51	1.90	1.52
1	B	35	LYS	CB-CG	-10.31	1.21	1.52
1	A	8	LYS	CB-CG	-9.88	1.22	1.52
1	B	64	LYS	CA-CB	-9.40	1.41	1.53
1	C	85	LEU	N-CA	9.29	1.58	1.46
1	A	64	LYS	CB-CG	-9.27	1.24	1.52
1	B	71	ASN	CB-CG	-9.05	1.29	1.52
1	C	8	LYS	CD-CE	8.69	1.78	1.52
1	C	35	LYS	CB-CG	8.09	1.76	1.52
1	B	74	GLN	CB-CG	7.88	1.76	1.52
1	C	100	GLU	CB-CG	-7.87	1.28	1.52
1	B	33	ASN	CB-CG	7.79	1.71	1.52
1	D	6	SER	CA-CB	-7.60	1.38	1.53
1	C	32	LYS	CB-CG	7.31	1.74	1.52
1	A	85	LEU	CB-CG	7.25	1.68	1.53
1	C	54	LYS	CB-CG	-7.08	1.31	1.52
1	D	100	GLU	CB-CG	-6.56	1.32	1.52

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	ASN	OD1-CG-ND2	-31.44	91.16	122.60
1	D	100	GLU	CA-CB-CG	-26.76	60.58	114.10
1	B	32	LYS	CA-CB-CG	-25.58	62.94	114.10
1	D	100	GLU	CB-CG-CD	-22.15	74.94	112.60
1	A	8	LYS	CA-CB-CG	-21.25	71.60	114.10
1	A	9	LYS	CG-CD-CE	21.16	159.97	111.30
1	B	7	THR	N-CA-CB	20.83	142.57	110.28
1	B	30	ASN	CA-CB-CG	20.25	132.84	112.60
1	B	33	ASN	CB-CG-ND2	18.95	144.83	116.40
1	D	8	LYS	CB-CG-CD	17.19	150.84	111.30
1	D	8	LYS	CD-CE-NZ	-17.17	56.95	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	8	LYS	CG-CD-CE	-17.08	72.01	111.30
1	A	8	LYS	CB-CG-CD	-16.88	72.47	111.30
1	C	37	THR	CA-CB-OG1	-15.55	86.28	109.60
1	B	64	LYS	CB-CG-CD	-15.11	76.55	111.30
1	B	71	ASN	CA-CB-CG	14.90	127.50	112.60
1	B	33	ASN	CB-CG-OD1	-14.73	91.34	120.80
1	A	49	LYS	CA-CB-CG	-14.30	85.50	114.10
1	B	48	LYS	CA-CB-CG	13.77	141.63	114.10
1	D	102	THR	OG1-CB-CG2	-13.41	82.48	109.30
1	C	83	ARG	CA-CB-CG	-13.09	87.91	114.10
1	A	30	ASN	CB-CG-OD1	-12.39	96.03	120.80
1	A	64	LYS	CA-CB-CG	12.34	138.77	114.10
1	C	84	ASP	O-C-N	-11.99	109.28	121.87
1	A	7	THR	OG1-CB-CG2	-11.31	86.68	109.30
1	C	85	LEU	N-CA-C	-11.31	86.71	110.80
1	D	8	LYS	CA-CB-CG	-10.78	92.53	114.10
1	B	106	GLU	CB-CG-CD	-10.26	95.17	112.60
1	C	83	ARG	O-C-N	10.23	134.46	122.79
1	C	32	LYS	CA-CB-CG	-9.86	94.37	114.10
1	C	37	THR	CA-CB-CG2	-9.70	94.00	110.50
1	B	7	THR	CA-CB-CG2	9.46	126.58	110.50
1	C	37	THR	OG1-CB-CG2	-9.45	90.41	109.30
1	D	104	MET	CA-CB-CG	-9.22	95.66	114.10
1	D	11	GLN	OE1-CD-NE2	-8.79	113.81	122.60
1	B	30	ASN	CB-CG-ND2	-8.62	103.47	116.40
1	C	52	GLU	CA-CB-CG	-8.15	97.80	114.10
1	D	6	SER	N-CA-CB	8.12	124.30	110.50
1	A	9	LYS	CD-CE-NZ	7.96	137.37	111.90
1	C	85	LEU	N-CA-CB	7.46	123.09	110.49
1	C	83	ARG	CA-C-N	-7.25	112.27	125.02
1	C	83	ARG	C-N-CA	-7.25	112.27	125.02
1	D	11	GLN	CG-CD-NE2	6.91	126.77	116.40
1	C	100	GLU	CA-CB-CG	-6.67	100.76	114.10
1	C	8	LYS	CG-CD-CE	-6.41	96.56	111.30
1	B	127	SER	CA-CB-OG	6.39	123.87	111.10
1	A	54	LYS	CA-CB-CG	-6.37	101.37	114.10
1	A	94	LEU	CB-CG-CD2	-6.24	91.97	110.70
1	B	64	LYS	CA-CB-CG	-6.07	101.97	114.10
1	A	64	LYS	CB-CG-CD	-6.01	97.47	111.30
1	B	57	GLN	CA-CB-CG	-5.98	102.13	114.10
1	B	32	LYS	CB-CG-CD	-5.88	97.79	111.30
1	B	64	LYS	N-CA-CB	5.88	118.57	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	THR	CA-CB-OG1	-5.83	100.85	109.60
1	B	74	GLN	CA-CB-CG	-5.77	102.55	114.10
1	D	102	THR	CA-CB-OG1	-5.70	101.06	109.60
1	C	95	GLU	CA-CB-CG	-5.45	103.21	114.10
1	C	95	GLU	CB-CG-CD	-5.45	103.34	112.60
1	A	83	ARG	CD-NE-CZ	-5.28	117.01	124.40
1	B	7	THR	CB-CA-C	-5.27	100.56	110.67
1	C	110	GLU	CA-CB-CG	-5.19	103.71	114.10
1	A	83	ARG	CG-CD-NE	-5.10	100.78	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	30	ASN	Sidechain
1	B	30	ASN	Sidechain

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	959	0	988	3	2
1	B	951	0	987	12	4
1	C	944	0	979	4	2
1	D	978	0	1008	2	4
2	A	45	0	35	0	0
2	B	45	0	35	5	0
2	C	45	0	35	0	0
2	D	45	0	35	1	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	4015	0	4102	22	6

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 3.

All (22) 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:33:ASN:HB2	1:B:34:PRO:HD3	1.56	0.88
1:B:33:ASN:CB	1:B:34:PRO:HD3	2.21	0.70
1:B:33:ASN:HB2	1:B:34:PRO:CD	2.24	0.67
1:C:83:ARG:O	1:C:84:ASP:HB2	1.96	0.65
1:D:64:LYS:HB2	1:D:65:PRO:HD3	1.87	0.57
1:B:38:ARG:HD2	2:B:301:FRH:C33	2.40	0.51
1:A:112:ALA:HB1	1:A:116:GLU:HB3	1.93	0.50
1:B:35:LYS:NZ	2:B:301:FRH:H352	2.28	0.49
1:D:60:GLU:HA	1:D:63:LEU:HD12	1.96	0.47
1:C:64:LYS:HB3	1:C:65:PRO:HD3	1.97	0.46
1:A:62:GLU:C	1:A:65:PRO:HD2	2.40	0.46
1:C:124:PHE:O	1:C:128:ILE:HG12	2.17	0.45
2:D:501:FRH:H281	2:D:501:FRH:H292	1.80	0.43
1:B:38:ARG:CD	2:B:301:FRH:C10	2.97	0.43
1:B:46:MET:HE3	1:B:120:ARG:HH11	1.84	0.42
1:C:14:LEU:HD11	1:C:53:LEU:HD21	2.01	0.42
1:B:38:ARG:CD	2:B:301:FRH:C33	2.98	0.42
1:A:81:ARG:HA	1:A:82:PRO:HD3	1.88	0.41
1:B:81:ARG:HA	1:B:82:PRO:HD3	1.87	0.41
1:B:35:LYS:HZ1	2:B:301:FRH:H352	1.85	0.41
1:B:28:ILE:HG23	1:B:39:MET:HE1	2.02	0.40
1:B:124:PHE:O	1:B:128:ILE:HG12	2.21	0.40

All (6) 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:72:LEU:CD2	1:D:100:GLU:OE2[2_646]	1.07	1.13
1:B:52:GLU:OE1	1:C:102:THR:OG1[2_656]	1.41	0.79
1:B:52:GLU:CD	1:C:102:THR:OG1[2_656]	2.01	0.19
1:A:72:LEU:CD2	1:D:100:GLU:CD[2_646]	2.11	0.09
1:B:8:LYS:NZ	1:D:26:ASN:OD1[1_655]	2.16	0.04
1:B:8:LYS:CE	1:D:26:ASN:OD1[1_655]	2.17	0.03

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	108/132 (82%)	107 (99%)	1 (1%)	0	100	100
1	B	110/132 (83%)	107 (97%)	2 (2%)	1 (1%)	14	41
1	C	107/132 (81%)	105 (98%)	2 (2%)	0	100	100
1	D	114/132 (86%)	113 (99%)	1 (1%)	0	100	100
All	All	439/528 (83%)	432 (98%)	6 (1%)	1 (0%)	43	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	33	ASN

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	111/125 (89%)	92 (83%)	19 (17%)	2	7
1	B	110/125 (88%)	90 (82%)	20 (18%)	2	6
1	C	109/125 (87%)	85 (78%)	24 (22%)	1	3
1	D	113/125 (90%)	87 (77%)	26 (23%)	1	3
All	All	443/500 (89%)	354 (80%)	89 (20%)	1	4

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	11	GLN
1	A	14	LEU
1	A	19	LEU
1	A	22	GLN
1	A	30	ASN
1	A	38	ARG

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Mol	Chain	Res	Type
1	A	49	LYS
1	A	53	LEU
1	A	57	GLN
1	A	61	GLU
1	A	64	LYS
1	A	102	THR
1	A	104	MET
1	A	105	CYS
1	A	109	ASP
1	A	110	GLU
1	A	114	ILE
1	A	132	LEU
1	B	6	SER
1	B	7	THR
1	B	14	LEU
1	B	23	MET
1	B	25	LEU
1	B	28	ILE
1	B	30	ASN
1	B	33	ASN
1	B	38	ARG
1	B	39	MET
1	B	43	LYS
1	B	48	LYS
1	B	51	THR
1	B	61	GLU
1	B	106	GLU
1	B	114	ILE
1	B	115	VAL
1	B	120	ARG
1	B	127	SER
1	B	132	LEU
1	C	8	LYS
1	C	11	GLN
1	C	13	GLN
1	C	14	LEU
1	C	15	GLU
1	C	19	LEU
1	C	20	ASP
1	C	23	MET
1	C	32	LYS
1	C	48	LYS

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Mol	Chain	Res	Type
1	C	49	LYS
1	C	61	GLU
1	C	67	GLU
1	C	70	LEU
1	C	72	LEU
1	C	85	LEU
1	C	87	SER
1	C	94	LEU
1	C	97	LYS
1	C	101	THR
1	C	102	THR
1	C	104	MET
1	C	106	GLU
1	C	130	SER
1	D	6	SER
1	D	7	THR
1	D	8	LYS
1	D	14	LEU
1	D	19	LEU
1	D	23	MET
1	D	30	ASN
1	D	32	LYS
1	D	38	ARG
1	D	39	MET
1	D	43	LYS
1	D	49	LYS
1	D	51	THR
1	D	54	LYS
1	D	56	LEU
1	D	60	GLU
1	D	61	GLU
1	D	71	ASN
1	D	83	ARG
1	D	85	LEU
1	D	95	GLU
1	D	97	LYS
1	D	101	THR
1	D	106	GLU
1	D	109	ASP
1	D	130	SER

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	71	ASN
1	A	119	ASN
1	A	126	GLN
1	C	57	GLN
1	C	71	ASN
1	C	74	GLN
1	C	90	ASN
1	C	119	ASN
1	D	22	GLN
1	D	71	ASN
1	D	90	ASN

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](#)

Of 7 ligands modelled in this entry, 3 are 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
2	FRH	B	301	-	48,48,48	2.12	10 (20%)	63,68,68	2.09	12 (19%)
2	FRH	A	201	-	48,48,48	2.12	10 (20%)	63,68,68	2.09	12 (19%)
2	FRH	C	401	-	48,48,48	2.16	10 (20%)	63,68,68	2.09	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FRH	D	501	-	48,48,48	2.14	10 (20%)	63,68,68	2.15	15 (23%)

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	FRH	B	301	-	-	10/38/48/48	0/4/4/4
2	FRH	A	201	-	-	9/38/48/48	0/4/4/4
2	FRH	C	401	-	-	20/38/48/48	0/4/4/4
2	FRH	D	501	-	-	12/38/48/48	0/4/4/4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FRH	C11-C13	-8.53	1.27	1.40
2	D	501	FRH	C11-C13	-8.32	1.27	1.40
2	B	301	FRH	C11-C13	-8.30	1.27	1.40
2	A	201	FRH	C11-C13	-8.25	1.27	1.40
2	C	401	FRH	C11-C23	-7.79	1.26	1.37
2	D	501	FRH	C11-C23	-7.64	1.27	1.37
2	B	301	FRH	C11-C23	-7.42	1.27	1.37
2	A	201	FRH	C11-C23	-7.42	1.27	1.37
2	B	301	FRH	O42-C31	3.63	1.44	1.38
2	A	201	FRH	O42-C31	3.61	1.44	1.38
2	C	401	FRH	C12-C39	-3.60	1.27	1.39
2	A	201	FRH	C12-C39	-3.60	1.27	1.39
2	D	501	FRH	C12-C39	-3.58	1.27	1.39
2	B	301	FRH	C12-C39	-3.58	1.27	1.39
2	C	401	FRH	O42-C31	3.57	1.44	1.38
2	D	501	FRH	O42-C31	3.56	1.44	1.38
2	D	501	FRH	C21-CL8	3.43	1.80	1.72
2	B	301	FRH	C21-CL8	3.42	1.80	1.72
2	A	201	FRH	C16-CL9	3.41	1.80	1.72
2	C	401	FRH	C21-CL8	3.38	1.80	1.72
2	B	301	FRH	C16-CL9	3.38	1.80	1.72
2	C	401	FRH	C16-CL9	3.35	1.79	1.72
2	D	501	FRH	C16-CL9	3.34	1.79	1.72
2	A	201	FRH	C21-CL8	3.32	1.79	1.72
2	A	201	FRH	N3-N7	-3.22	1.30	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FRH	N3-N7	-3.21	1.30	1.36
2	B	301	FRH	N3-N7	-3.10	1.30	1.36
2	C	401	FRH	N3-N7	-2.96	1.31	1.36
2	D	501	FRH	C23-N3	-2.72	1.32	1.35
2	A	201	FRH	C39-C18	-2.67	1.26	1.34
2	B	301	FRH	C39-C18	-2.67	1.26	1.34
2	D	501	FRH	C39-C18	-2.64	1.26	1.34
2	C	401	FRH	C39-C18	-2.60	1.27	1.34
2	C	401	FRH	C23-N3	-2.38	1.33	1.35
2	A	201	FRH	C23-N3	-2.36	1.33	1.35
2	B	301	FRH	C23-N3	-2.31	1.33	1.35
2	B	301	FRH	O42-C18	2.06	1.44	1.38
2	D	501	FRH	O42-C18	2.06	1.44	1.38
2	C	401	FRH	O42-C18	2.05	1.44	1.38
2	A	201	FRH	O42-C18	2.04	1.44	1.38

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	FRH	O42-C18-C35	10.66	126.17	116.30
2	A	201	FRH	O42-C18-C35	10.58	126.09	116.30
2	D	501	FRH	O42-C18-C35	10.13	125.67	116.30
2	C	401	FRH	O42-C18-C35	10.12	125.66	116.30
2	D	501	FRH	C31-O42-C18	-6.00	101.77	106.59
2	B	301	FRH	C31-O42-C18	-5.37	102.28	106.59
2	A	201	FRH	C31-O42-C18	-5.36	102.28	106.59
2	C	401	FRH	C39-C12-C31	4.95	111.36	106.94
2	A	201	FRH	C39-C12-C31	4.51	110.97	106.94
2	B	301	FRH	C39-C12-C31	4.50	110.96	106.94
2	C	401	FRH	C31-O42-C18	-4.47	103.00	106.59
2	D	501	FRH	O42-C31-C12	-4.41	104.57	109.68
2	C	401	FRH	C12-C39-C18	4.18	112.90	107.12
2	A	201	FRH	O42-C31-C12	-4.12	104.90	109.68
2	D	501	FRH	C39-C12-C31	4.10	110.61	106.94
2	C	401	FRH	O42-C31-C12	-4.04	104.99	109.68
2	B	301	FRH	O42-C31-C12	-4.00	105.04	109.68
2	D	501	FRH	O43-C30-C16	3.94	122.11	115.77
2	B	301	FRH	C12-C39-C18	3.77	112.34	107.12
2	A	201	FRH	C12-C39-C18	3.69	112.22	107.12
2	C	401	FRH	C13-N7-N3	-3.63	102.84	105.11
2	A	201	FRH	C13-N7-N3	-3.58	102.87	105.11
2	C	401	FRH	C21-C24-C13	-3.48	120.36	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	FRH	C13-C11-C23	3.46	112.14	106.24
2	A	201	FRH	C13-C11-C23	3.44	112.11	106.24
2	D	501	FRH	C13-N7-N3	-3.43	102.97	105.11
2	B	301	FRH	C13-N7-N3	-3.34	103.03	105.11
2	C	401	FRH	C13-C11-C23	3.32	111.90	106.24
2	D	501	FRH	C13-C11-C23	3.31	111.89	106.24
2	D	501	FRH	C12-C39-C18	3.13	111.46	107.12
2	D	501	FRH	C35-O43-C30	2.73	123.29	117.60
2	B	301	FRH	C35-O43-C30	2.64	123.10	117.60
2	A	201	FRH	C11-C13-N7	-2.56	108.29	111.11
2	D	501	FRH	O43-C30-C33	-2.55	118.38	123.95
2	D	501	FRH	C21-C24-C13	-2.48	121.74	125.16
2	B	301	FRH	C11-C13-N7	-2.38	108.49	111.11
2	C	401	FRH	O40-C20-C31	2.37	119.43	114.06
2	D	501	FRH	C15-C22-N6	-2.35	106.06	110.66
2	C	401	FRH	C27-C29-N6	-2.32	106.11	110.66
2	B	301	FRH	C21-C24-C13	-2.32	121.97	125.16
2	C	401	FRH	C15-C22-N6	-2.27	106.22	110.66
2	C	401	FRH	C11-C13-N7	-2.26	108.62	111.11
2	A	201	FRH	C21-C24-C13	-2.25	122.06	125.16
2	A	201	FRH	C35-O43-C30	2.25	122.30	117.60
2	C	401	FRH	C35-O43-C30	2.22	122.23	117.60
2	B	301	FRH	O40-C20-C31	2.16	118.95	114.06
2	D	501	FRH	O42-C18-C39	-2.13	105.90	109.52
2	A	201	FRH	O43-C30-C16	2.12	119.17	115.77
2	C	401	FRH	O43-C30-C16	2.09	119.13	115.77
2	B	301	FRH	C35-C18-C39	-2.06	126.69	133.53
2	D	501	FRH	O40-C20-C31	2.04	118.68	114.06
2	C	401	FRH	C35-C18-C39	-2.04	126.76	133.53
2	D	501	FRH	C11-C13-N7	-2.03	108.88	111.11
2	A	201	FRH	C35-C18-C39	-2.01	126.84	133.53

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	FRH	N4-C17-N5-C25
2	A	201	FRH	N1-C17-N5-C25
2	A	201	FRH	O42-C18-C35-O43
2	B	301	FRH	N4-C17-N5-C25
2	B	301	FRH	N1-C17-N5-C25
2	B	301	FRH	C39-C18-C35-O43

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Mol	Chain	Res	Type	Atoms
2	B	301	FRH	O42-C18-C35-O43
2	B	301	FRH	O40-C20-C31-O42
2	B	301	FRH	O41-C20-C31-O42
2	B	301	FRH	O40-C20-C31-C12
2	B	301	FRH	O41-C20-C31-C12
2	C	401	FRH	C28-C14-N6-C22
2	C	401	FRH	C28-C14-N6-C29
2	C	401	FRH	O44-C14-N6-C29
2	C	401	FRH	O42-C18-C35-O43
2	C	401	FRH	O40-C20-C31-O42
2	C	401	FRH	O41-C20-C31-O42
2	C	401	FRH	O40-C20-C31-C12
2	C	401	FRH	O41-C20-C31-C12
2	D	501	FRH	C16-C30-O43-C35
2	D	501	FRH	O40-C20-C31-O42
2	D	501	FRH	O41-C20-C31-O42
2	D	501	FRH	O40-C20-C31-C12
2	D	501	FRH	O41-C20-C31-C12
2	B	301	FRH	C26-C25-C32-C36
2	C	401	FRH	O44-C14-N6-C22
2	D	501	FRH	N5-C25-C32-C36
2	B	301	FRH	N5-C25-C32-C36
2	C	401	FRH	C16-C30-O43-C35
2	D	501	FRH	C26-C25-C32-C36
2	A	201	FRH	C16-C30-O43-C35
2	C	401	FRH	N5-C25-C32-C36
2	C	401	FRH	C26-C25-C32-C36
2	D	501	FRH	C25-C32-C36-C37
2	A	201	FRH	N5-C25-C32-C36
2	A	201	FRH	C39-C18-C35-O43
2	A	201	FRH	C26-C25-C32-C36
2	D	501	FRH	C25-C32-C36-C38
2	C	401	FRH	N1-C17-N5-C25
2	D	501	FRH	C33-C30-O43-C35
2	C	401	FRH	C32-C25-C26-O45
2	C	401	FRH	C33-C30-O43-C35
2	C	401	FRH	N4-C17-N5-C25
2	C	401	FRH	C32-C25-C26-N2
2	C	401	FRH	C39-C18-C35-O43
2	A	201	FRH	C33-C30-O43-C35
2	D	501	FRH	C14-C28-N2-C26
2	C	401	FRH	C15-C19-C23-C11

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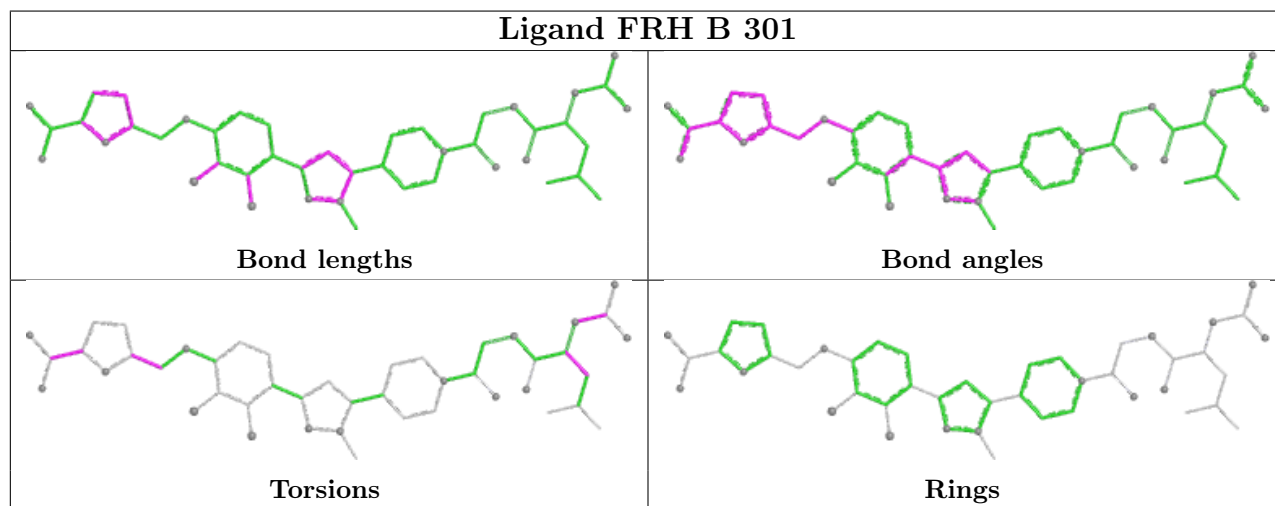
Mol	Chain	Res	Type	Atoms
2	C	401	FRH	C15-C19-C23-N3
2	D	501	FRH	C15-C19-C23-N3
2	A	201	FRH	C14-C28-N2-C26

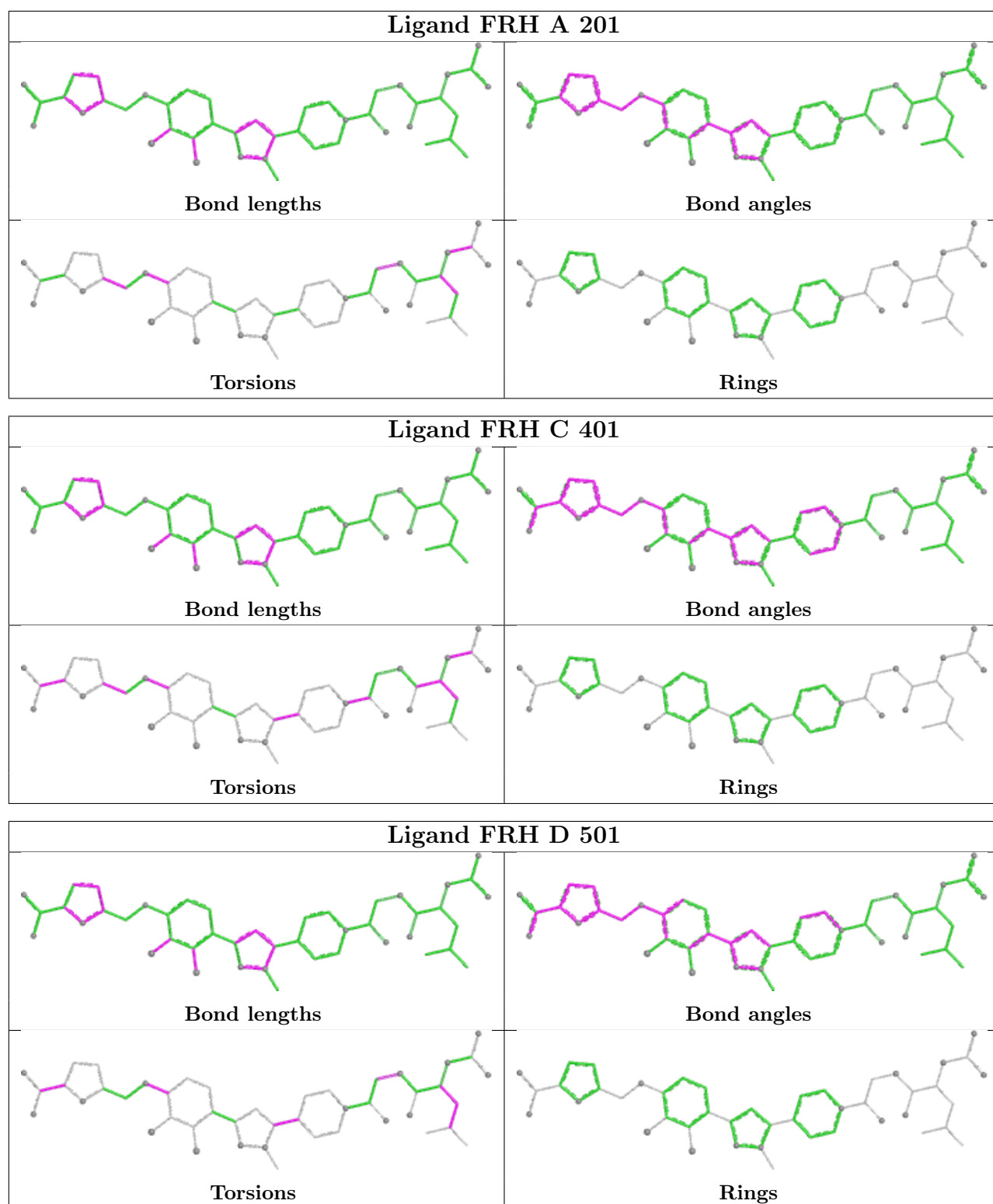
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	FRH	5	0
2	D	501	FRH	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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	84:ASP	C	85:LEU	N	1.06
1	C	83:ARG	C	84:ASP	N	1.00

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	117/132 (88%)	0.11	1 (0%) 81 74	20, 49, 84, 96	16 (13%)
1	B	116/132 (87%)	0.05	2 (1%) 69 60	18, 51, 78, 91	15 (12%)
1	C	115/132 (87%)	0.16	1 (0%) 81 74	27, 54, 83, 102	13 (11%)
1	D	120/132 (90%)	0.11	1 (0%) 82 75	32, 54, 77, 84	8 (6%)
All	All	468/528 (88%)	0.11	5 (1%) 78 70	18, 53, 81, 102	52 (11%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	ALA	2.4
1	A	105	CYS	2.4
1	C	36	LEU	2.4
1	B	23	MET	2.3
1	D	110	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

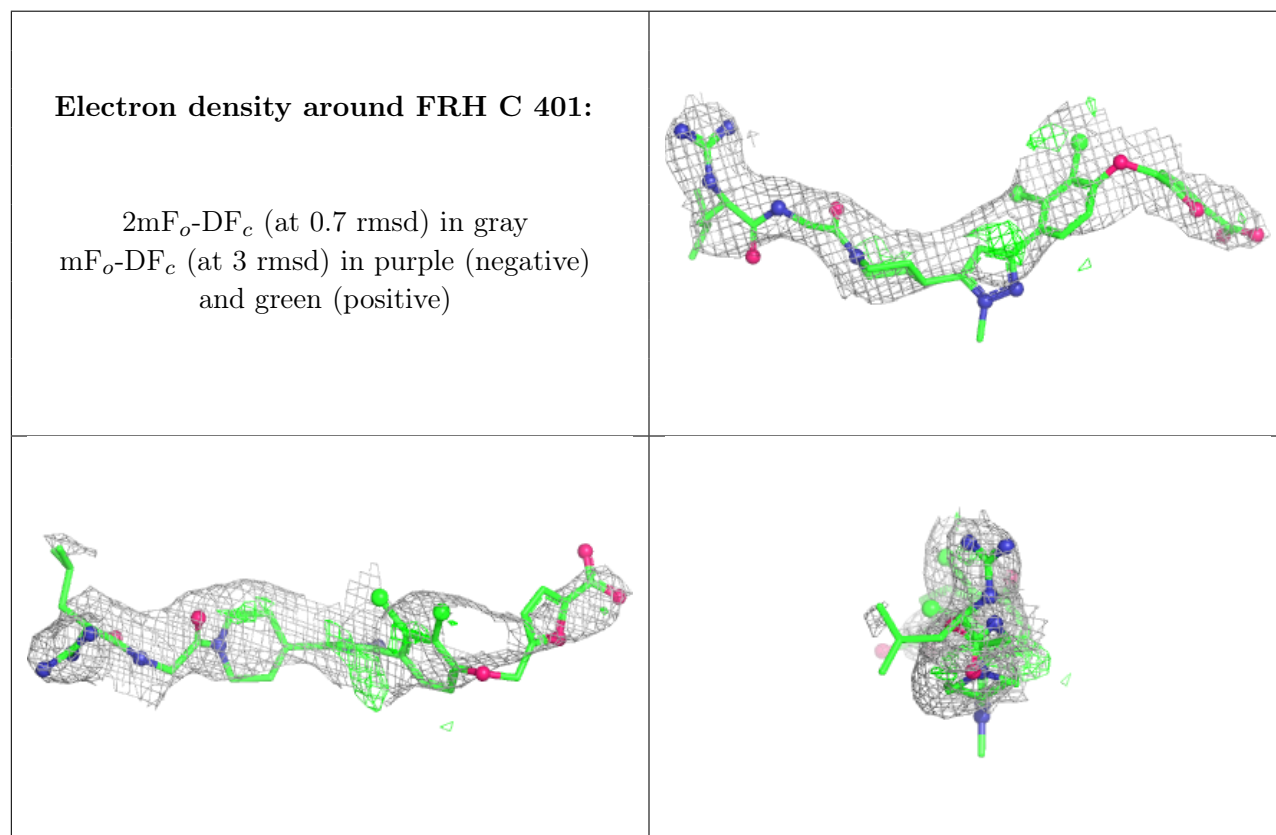
6.4 Ligands [i](#)

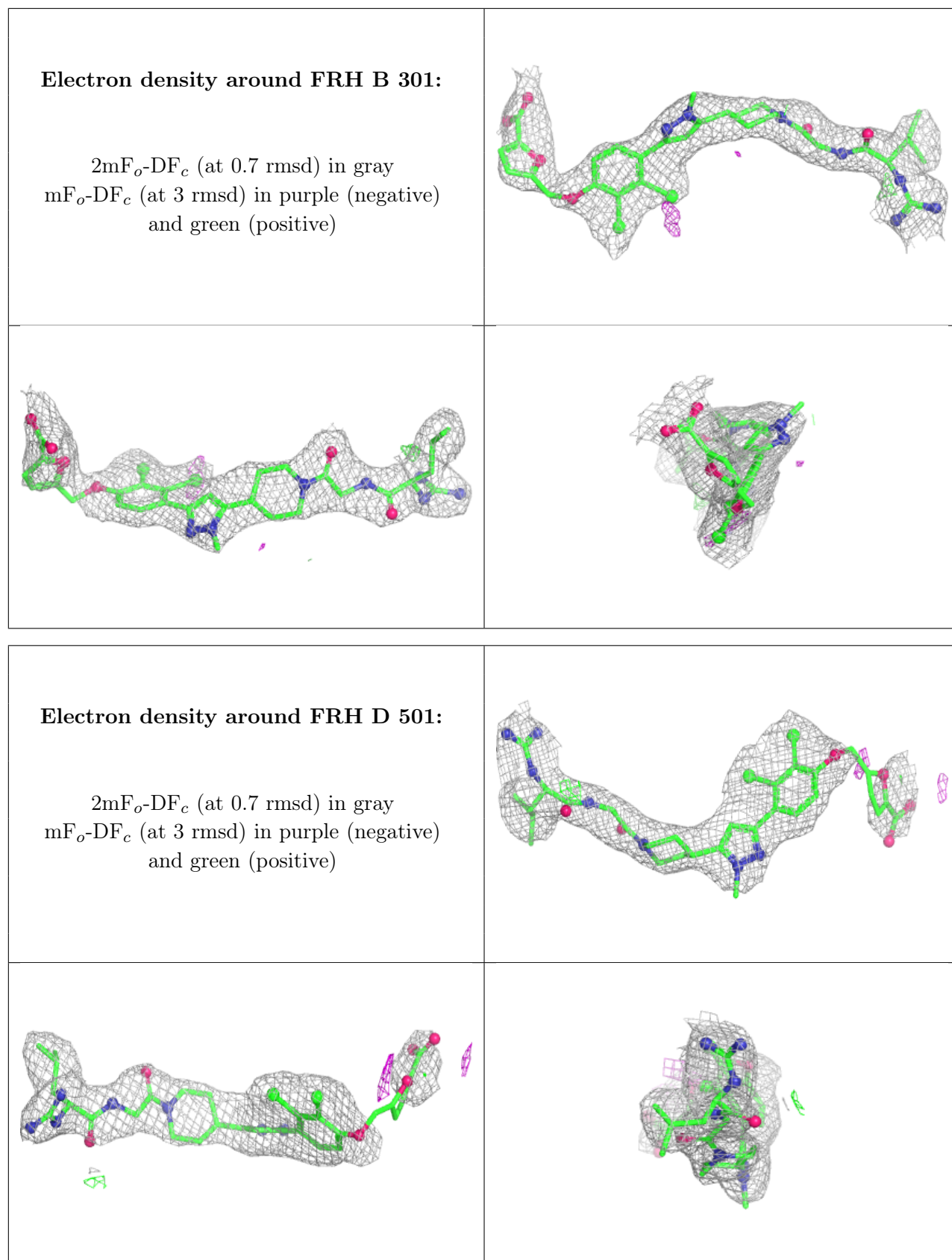
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

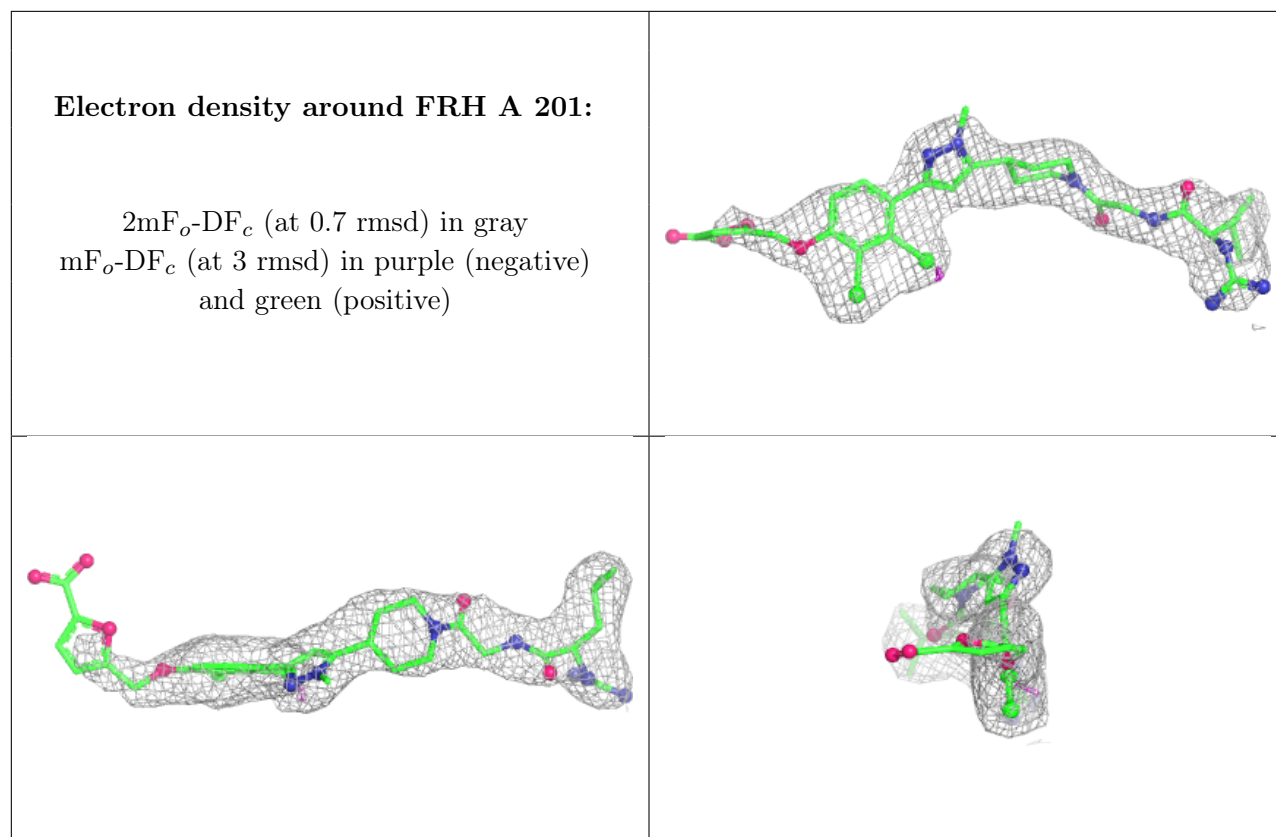
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	B	801	1/1	0.56	0.26	155,155,155,155	0
3	ZN	C	701	1/1	0.63	0.29	137,137,137,137	0
2	FRH	C	401	45/45	0.76	0.18	49,115,147,155	0
3	ZN	B	601	1/1	0.79	0.24	116,116,116,116	0
2	FRH	B	301	45/45	0.84	0.10	35,56,96,110	0
2	FRH	D	501	45/45	0.88	0.12	43,63,116,137	0
2	FRH	A	201	45/45	0.88	0.10	35,55,106,127	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 [i](#)

There are no such residues in this entry.