



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 09:21 AM UTC

PDB ID : 6WXN / pdb_00006wxn
Title : EGFR(T790M/V948R) in complex with LN3844
Authors : Heppner, D.E.; Eck, M.J.
Deposited on : 2020-05-11
Resolution : 1.76 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

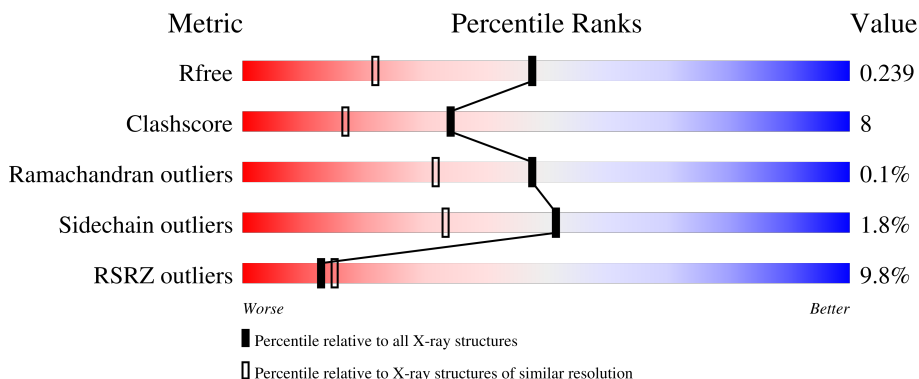
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	328	12% 73% 16% • 9%
1	B	328	6% 82% 9% • 8%
1	C	328	9% 72% 15% • 13%
1	D	328	7% 76% 12% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9883 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.

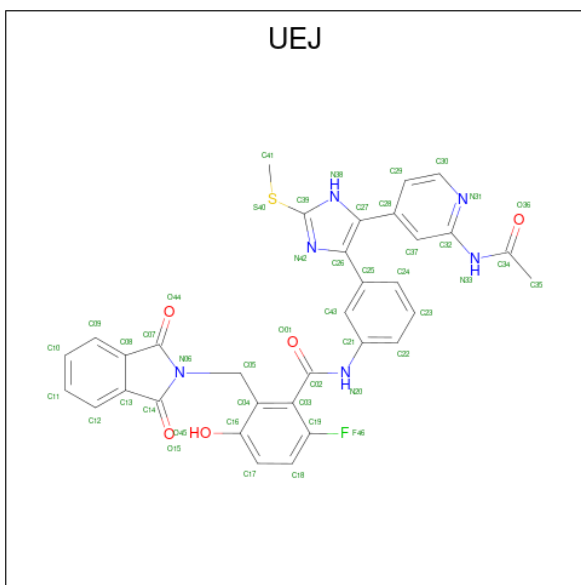
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	292	Total	C	N	O	S	0	1	0
			2358	1515	401	424	18			
1	A	298	Total	C	N	O	S	0	1	0
			2389	1531	403	436	19			
1	B	303	Total	C	N	O	S	0	1	0
			2448	1574	415	440	19			
1	C	286	Total	C	N	O	S	0	1	0
			2319	1489	390	421	19			

There are 8 discrepancies between the modelled and reference sequences:

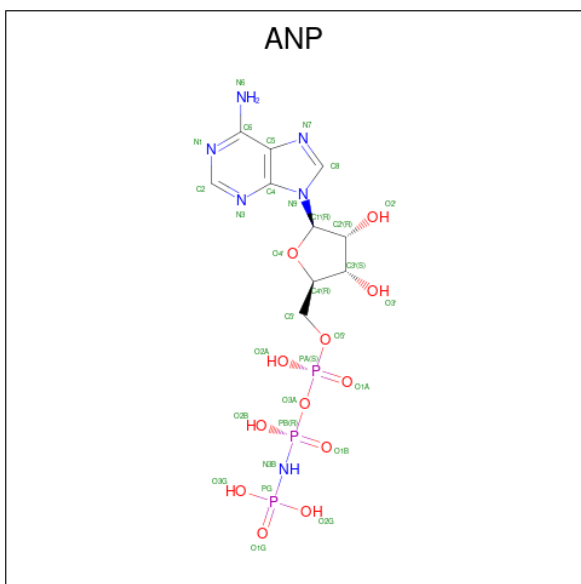
Chain	Residue	Modelled	Actual	Comment	Reference
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
B	948	ARG	VAL	engineered mutation	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533
C	948	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is N-(3-{5-[2-(acetylamino)pyridin-4-yl]-2-(methylsulfanyl)-1H-imidazol-4-yl}phenyl)-2-[(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)methyl]-6-fluoro-3-hydroxybenzamide (CCD ID: UEJ) (formula: C₃₃H₂₅FN₆O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	D	1	Total	C	F	N	O	S	0	0
			46	33	1	6	5	1		
2	C	1	Total	C	F	N	O	S	0	0
			46	33	1	6	5	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total 1	Cl 1	0	0

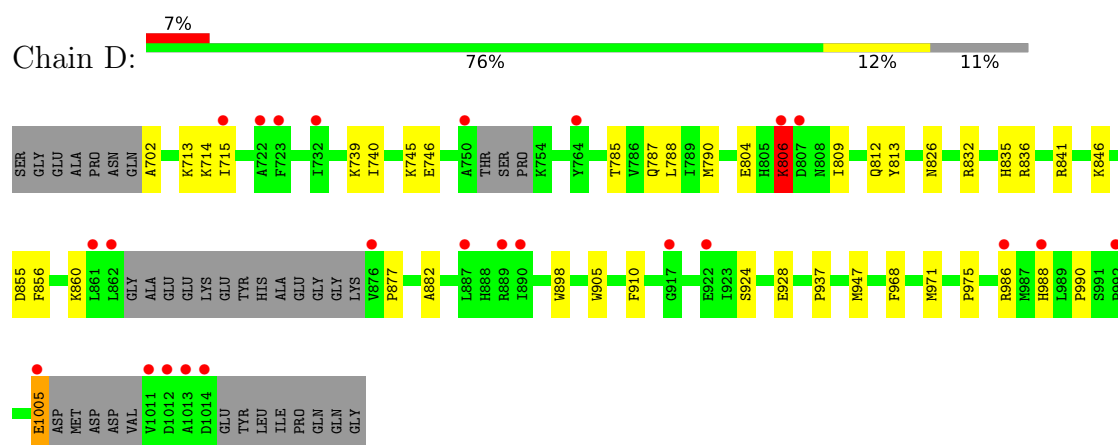
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	57	Total 57	O 57	0	0
6	A	44	Total 44	O 44	0	0
6	B	81	Total 81	O 81	0	0
6	C	62	Total 62	O 62	0	0

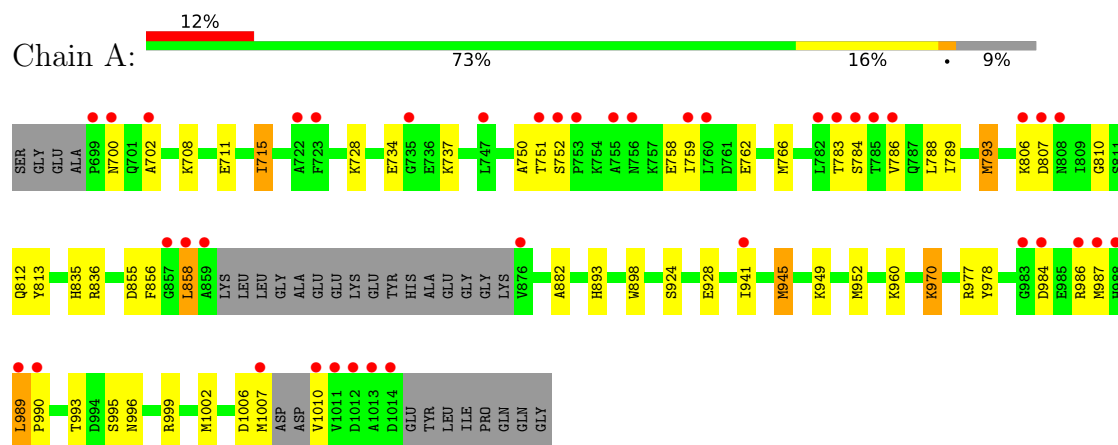
3 Residue-property plots [i](#)

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.

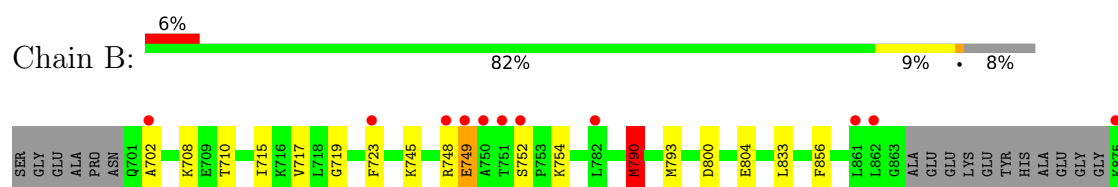
- Molecule 1: Epidermal growth factor receptor

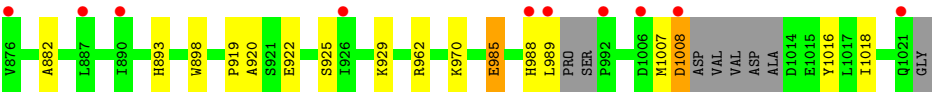


- Molecule 1: Epidermal growth factor receptor

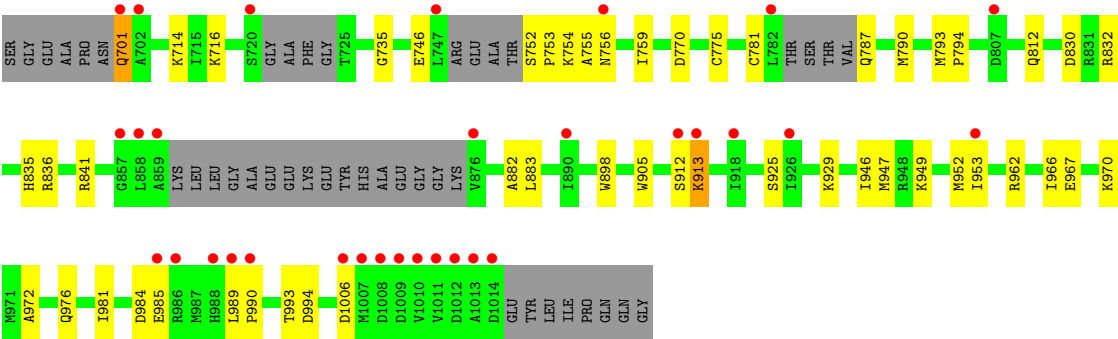


- Molecule 1: Epidermal growth factor receptor





● Molecule 1: Epidermal growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.91Å 102.74Å 87.31Å 90.00° 101.20° 90.00°	Depositor
Resolution (Å)	65.78 – 1.76 65.78 – 1.76	Depositor EDS
% Data completeness (in resolution range)	97.1 (65.78-1.76) 90.8 (65.78-1.76)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.208 , 0.235 0.211 , 0.239	Depositor DCC
R_{free} test set	6019 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9883	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.30% 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: CL, UEJ, MG, ANP

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	0.68	3/2439 (0.1%)	0.82	7/3300 (0.2%)
1	B	0.66	4/2499 (0.2%)	0.72	6/3375 (0.2%)
1	C	0.72	9/2366 (0.4%)	0.86	10/3196 (0.3%)
1	D	0.49	2/2406 (0.1%)	0.61	1/3250 (0.0%)
All	All	0.64	18/9710 (0.2%)	0.76	24/13121 (0.2%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	913	LYS	C-N	12.79	1.50	1.33
1	A	793	MET	C-N	11.96	1.48	1.33
1	A	989	LEU	C-N	11.38	1.48	1.33
1	B	793	MET	C-N	11.18	1.47	1.33
1	C	793	MET	C-N	10.91	1.46	1.33
1	C	753	PRO	C-O	-7.34	1.14	1.24
1	D	739	LYS	C-O	-6.76	1.16	1.24
1	C	1006	ASP	C-O	-6.55	1.16	1.24
1	C	781	CYS	C-O	-6.42	1.16	1.24
1	B	790	MET	C-O	-6.18	1.16	1.23
1	D	809	ILE	C-O	-6.05	1.17	1.24
1	C	746	GLU	C-O	-6.00	1.17	1.24
1	C	841	ARG	C-O	-5.95	1.16	1.24
1	C	832	ARG	C-O	-5.73	1.16	1.23
1	B	988	HIS	C-O	-5.66	1.17	1.24
1	C	754	LYS	C-O	-5.48	1.17	1.24
1	A	945	MET	C-O	-5.40	1.17	1.24
1	B	1018	ILE	C-O	-5.32	1.18	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	913	LYS	CA-C-N	17.30	137.06	119.76
1	C	913	LYS	C-N-CA	17.30	137.06	119.76
1	A	989	LEU	CA-C-N	9.87	130.48	119.92
1	A	989	LEU	C-N-CA	9.87	130.48	119.92
1	B	793	MET	CA-C-N	8.88	128.61	119.56
1	B	793	MET	C-N-CA	8.88	128.61	119.56
1	A	793	MET	CA-C-N	8.81	128.54	119.56
1	A	793	MET	C-N-CA	8.81	128.54	119.56
1	C	793	MET	CA-C-N	8.66	128.39	119.56
1	C	793	MET	C-N-CA	8.66	128.39	119.56
1	A	989	LEU	O-C-N	-8.49	112.19	121.53
1	C	793	MET	O-C-N	-6.64	114.14	120.85
1	D	1005	GLU	CB-CG-CD	6.18	123.10	112.60
1	C	793	MET	CB-CA-C	-5.61	105.39	110.44
1	B	793	MET	O-C-N	-5.46	114.73	120.68
1	C	755	ALA	CA-C-N	-5.42	111.47	122.31
1	C	755	ALA	C-N-CA	-5.42	111.47	122.31
1	B	1008	ASP	CB-CA-C	5.30	120.18	110.10
1	C	752	SER	CA-C-N	5.29	124.75	119.24
1	C	752	SER	C-N-CA	5.29	124.75	119.24
1	A	715	ILE	CA-C-O	-5.20	114.28	120.78
1	B	1007	MET	CA-C-N	5.15	130.97	121.70
1	B	1007	MET	C-N-CA	5.15	130.97	121.70
1	A	793	MET	O-C-N	-5.14	115.38	120.83

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	2389	0	2417	47	0
1	B	2448	0	2485	25	0
1	C	2319	0	2348	38	0
1	D	2358	0	2404	47	0
2	C	46	0	0	0	0
2	D	46	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	13	1	0
4	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	44	0	0	3	0
6	B	81	0	0	3	0
6	C	62	0	0	3	0
6	D	57	0	0	3	0
All	All	9883	0	9667	147	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 (147) 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:D:836:ARG:NH2	1:D:860:LYS:HE2	1.34	1.35
1:D:836:ARG:CZ	1:D:860:LYS:HE2	1.71	1.20
1:D:832:ARG:HG3	1:B:749:GLU:HB3	1.34	1.09
1:D:836:ARG:NE	1:D:860:LYS:HE3	1.76	1.00
1:D:836:ARG:HH21	1:D:860:LYS:HE2	1.19	0.99
1:D:836:ARG:CZ	1:D:860:LYS:CE	2.41	0.98
1:D:836:ARG:NE	1:D:860:LYS:CE	2.29	0.94
1:C:701:GLN:N	1:C:701:GLN:OE1	2.05	0.89
1:D:836:ARG:NH2	1:D:860:LYS:CE	2.31	0.86
1:A:810:GLY:HA2	1:A:987:MET:HE3	1.60	0.82
1:A:810:GLY:CA	1:A:987:MET:HE3	2.13	0.79
1:D:740:ILE:HG13	1:A:1002:MET:HE2	1.63	0.78
1:D:905:TRP:HD1	1:D:947:MET:HE1	1.49	0.78
1:C:976:GLN:HE22	1:C:985:GLU:HG2	1.47	0.77
1:D:713:LYS:HD2	1:D:715:ILE:HD11	1.68	0.75
1:A:715:ILE:HD11	1:A:728:LYS:HD3	1.69	0.74
1:A:810:GLY:HA2	1:A:987:MET:CE	2.19	0.72
1:D:1005:GLU:O	1:D:1005:GLU:HG3	1.87	0.72
1:D:806:LYS:O	1:D:806:LYS:HD3	1.90	0.72
1:A:960:LYS:HD3	6:A:1117:HOH:O	1.88	0.72
1:D:836:ARG:HE	1:D:860:LYS:HE3	1.55	0.71
1:A:984:ASP:HA	1:A:987:MET:HE2	1.73	0.71
1:A:858:LEU:C	1:A:858:LEU:HD13	2.17	0.69
1:D:836:ARG:HE	1:D:860:LYS:CE	2.03	0.68
1:D:836:ARG:NE	1:D:860:LYS:HE2	2.01	0.68
1:D:806:LYS:O	1:D:910:PHE:CD1	2.46	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:826:ASN:ND2	6:D:1201:HOH:O	2.26	0.68
1:D:804:GLU:OE1	1:A:737:LYS:HD3	1.97	0.65
1:A:812:GLN:HG2	1:A:989:LEU:HG	1.80	0.64
1:C:989:LEU:HB3	1:C:990:PRO:HD2	1.80	0.64
1:D:968:PHE:HA	1:D:971:MET:HE3	1.79	0.63
1:D:806:LYS:O	1:D:910:PHE:CG	2.52	0.63
1:A:858:LEU:O	1:A:858:LEU:HD22	1.99	0.62
1:D:905:TRP:CD1	1:D:947:MET:HE1	2.33	0.62
1:A:858:LEU:H	1:A:858:LEU:HD12	1.64	0.62
1:D:832:ARG:HG3	1:B:749:GLU:CB	2.20	0.61
1:A:759:ILE:HG21	1:A:786:VAL:HG21	1.82	0.61
1:C:905:TRP:HD1	1:C:947:MET:HE1	1.65	0.61
1:D:812:GLN:HG2	1:D:975:PRO:HG3	1.82	0.60
1:C:925:SER:O	1:C:929:LYS:HG2	2.00	0.60
1:B:717:VAL:HG23	6:B:1251:HOH:O	2.00	0.60
1:B:893:HIS:HD2	6:B:1232:HOH:O	1.83	0.60
1:B:919:PRO:HB2	1:B:922[A]:GLU:HG3	1.84	0.60
1:C:794:PRO:HD2	6:C:1423:HOH:O	2.01	0.60
1:A:941:ILE:O	1:A:945:MET:HG3	2.02	0.60
1:B:922[B]:GLU:OE2	1:B:922[B]:GLU:HA	1.95	0.60
1:C:905:TRP:HZ3	1:C:912:SER:O	1.84	0.59
1:D:856:PHE:O	2:D:1101:UEJ:O45	2.20	0.59
1:D:790:MET:HE3	2:D:1101:UEJ:C21	2.32	0.59
1:A:762:GLU:O	1:A:766:MET:HG2	2.02	0.59
1:A:708:LYS:HE2	1:A:734:GLU:OE1	2.03	0.58
1:A:924:SER:O	1:A:928:GLU:HG3	2.02	0.58
1:B:962:ARG:HG2	1:B:962:ARG:HH11	1.66	0.58
1:B:723:PHE:HB2	6:B:1207:HOH:O	2.04	0.58
1:B:989:LEU:HD22	1:C:735:GLY:HA3	1.86	0.57
1:B:985:GLU:CD	1:B:985:GLU:H	2.10	0.57
1:A:751:THR:N	1:A:784:SER:O	2.38	0.57
1:D:836:ARG:HH21	1:D:860:LYS:CE	2.07	0.56
1:C:812:GLN:HG2	1:C:989:LEU:CD1	2.36	0.56
1:A:986:ARG:CZ	1:A:986:ARG:HB3	2.36	0.56
1:C:812:GLN:HG2	1:C:989:LEU:HG	1.88	0.56
1:D:846:LYS:NZ	1:D:1005:GLU:HG2	2.22	0.55
1:B:962:ARG:HG2	1:B:962:ARG:NH1	2.21	0.55
1:D:745:LYS:NZ	1:D:855:ASP:OD2	2.40	0.55
1:B:989:LEU:CD2	1:C:735:GLY:HA3	2.37	0.55
1:D:836:ARG:CZ	1:D:860:LYS:HG3	2.38	0.53
1:A:858:LEU:N	1:A:858:LEU:CD1	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:905:TRP:HB2	1:C:947:MET:HE3	1.91	0.53
1:A:996:ASN:OD1	1:A:999:ARG:NH1	2.43	0.52
1:C:756:ASN:HA	1:C:759:ILE:HB	1.91	0.52
1:C:990:PRO:HB2	1:C:994:ASP:HB2	1.91	0.52
1:B:800:ASP:O	1:B:804:GLU:HG3	2.10	0.52
1:C:905:TRP:CZ3	1:C:912:SER:O	2.63	0.52
1:A:858:LEU:H	1:A:858:LEU:CD1	2.23	0.51
1:A:858:LEU:HD12	1:A:858:LEU:N	2.24	0.51
1:D:714:LYS:NZ	1:D:787:GLN:OE1	2.34	0.51
1:D:924:SER:O	1:D:928:GLU:HG3	2.11	0.50
1:C:714:LYS:NZ	1:C:787:GLN:OE1	2.40	0.50
1:D:806:LYS:CD	1:D:806:LYS:C	2.85	0.50
1:A:995:SER:OG	1:A:999:ARG:NH2	2.45	0.50
1:C:883:LEU:HD22	1:C:953:ILE:HD12	1.93	0.49
1:A:812:GLN:CG	1:A:989:LEU:HG	2.42	0.49
1:A:806:LYS:HD3	1:A:807:ASP:OD1	2.12	0.49
1:D:806:LYS:HD3	1:D:806:LYS:C	2.37	0.49
1:C:966:ILE:O	1:C:970:LYS:HG3	2.12	0.49
1:C:701:GLN:N	1:C:701:GLN:CD	2.72	0.48
1:A:924:SER:HB3	6:A:1103:HOH:O	2.12	0.48
1:A:986:ARG:HH11	1:A:986:ARG:HG3	1.79	0.48
1:A:758:GLU:HA	1:A:758:GLU:OE1	2.13	0.48
1:C:812:GLN:HG2	1:C:989:LEU:CG	2.44	0.48
1:A:858:LEU:C	1:A:858:LEU:CD1	2.82	0.47
1:D:836:ARG:NH1	1:D:860:LYS:HG3	2.29	0.47
1:A:813:TYR:OH	1:A:990:PRO:HD3	2.15	0.47
1:D:882:ALA:HA	1:D:898:TRP:CD2	2.50	0.47
1:C:949:LYS:HA	1:C:952:MET:HE2	1.96	0.47
1:C:905:TRP:CD1	1:C:947:MET:HE1	2.46	0.46
1:C:946:ILE:HD11	1:C:967:GLU:HG2	1.97	0.46
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.50	0.46
1:A:858:LEU:HD13	1:A:858:LEU:O	2.16	0.46
1:C:835:HIS:O	1:C:836:ARG:HB2	2.16	0.46
1:D:813:TYR:OH	1:D:990:PRO:HD3	2.15	0.46
1:D:860:LYS:HD2	6:D:1244:HOH:O	2.16	0.45
1:C:976:GLN:NE2	1:C:985:GLU:HG2	2.25	0.45
1:A:835:HIS:CD2	1:A:856:PHE:HB3	2.52	0.45
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.51	0.45
1:C:716:LYS:CE	6:C:1418:HOH:O	2.64	0.45
1:A:750:ALA:HB1	1:A:784:SER:OG	2.16	0.45
1:B:989:LEU:HD21	1:C:735:GLY:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:HIS:HD2	6:A:1120:HOH:O	1.99	0.45
1:A:708:LYS:O	1:A:711:GLU:HG2	2.18	0.44
1:B:745:LYS:HB2	1:B:790:MET:HE1	1.99	0.44
1:D:788:LEU:HD13	2:D:1101:UEJ:C07	2.48	0.43
1:D:841:ARG:HH12	1:D:877:PRO:HB3	1.83	0.43
1:D:905:TRP:HB2	1:D:947:MET:HE3	2.00	0.43
1:A:855:ASP:O	1:A:858:LEU:HD11	2.18	0.43
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.54	0.43
1:B:719:GLY:HA3	3:B:1101:ANP:H4'	2.00	0.43
1:A:949:LYS:O	1:A:952:MET:HG2	2.18	0.43
1:B:833:LEU:HD13	1:B:856:PHE:CZ	2.54	0.43
1:B:920:ALA:C	1:B:922[B]:GLU:H	2.25	0.43
1:C:812:GLN:NE2	1:C:972:ALA:O	2.51	0.43
1:D:937:PRO:HD2	6:D:1241:HOH:O	2.18	0.43
1:D:746:GLU:OE2	1:D:785:THR:HG21	2.17	0.43
1:A:835:HIS:O	1:A:836:ARG:HB2	2.19	0.42
1:D:702:ALA:HA	1:A:993:THR:OG1	2.20	0.42
1:A:898:TRP:CD1	1:A:898:TRP:C	2.98	0.42
1:C:775:CYS:SG	1:C:790:MET:HE1	2.60	0.42
1:C:830:ASP:OD2	1:C:962:ARG:NH2	2.51	0.42
1:C:883:LEU:HD23	1:C:953:ILE:HG23	2.01	0.42
1:C:989:LEU:HB3	1:C:990:PRO:CD	2.49	0.42
1:C:794:PRO:CD	6:C:1423:HOH:O	2.63	0.41
1:D:835:HIS:O	1:D:836:ARG:HB2	2.20	0.41
1:A:970:LYS:HE2	1:A:970:LYS:HB2	1.33	0.41
1:B:748:ARG:NH2	1:B:748:ARG:HG2	2.35	0.41
1:D:841:ARG:NH1	1:D:877:PRO:HB3	2.36	0.41
1:D:988:HIS:CD2	1:D:988:HIS:H	2.39	0.41
1:B:702:ALA:O	1:C:993:THR:HA	2.20	0.41
1:B:715:ILE:HD13	1:B:715:ILE:HA	1.96	0.41
1:A:977:ARG:HD3	1:A:978:TYR:CZ	2.56	0.41
1:B:708:LYS:HG3	1:B:710:THR:OG1	2.21	0.41
1:B:925:SER:O	1:B:929:LYS:HG3	2.21	0.41
1:C:812:GLN:HG2	1:C:989:LEU:HD11	2.03	0.41
1:A:788:LEU:C	1:A:789:ILE:HD12	2.46	0.40
1:A:945:MET:HE2	1:A:945:MET:HB3	1.84	0.40
1:A:700:ASN:ND2	1:A:702:ALA:H	2.19	0.40
1:B:1016:TYR:CD1	1:C:770:ASP:HB3	2.56	0.40
1:C:981:ILE:O	1:C:984:ASP:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	293/328 (89%)	285 (97%)	8 (3%)	0	100	100
1	B	296/328 (90%)	290 (98%)	6 (2%)	0	100	100
1	C	277/328 (84%)	272 (98%)	5 (2%)	0	100	100
1	D	285/328 (87%)	279 (98%)	5 (2%)	1 (0%)	30	15
All	All	1151/1312 (88%)	1126 (98%)	24 (2%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	806	LYS

5.3.2 Protein sidechains

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	264/288 (92%)	256 (97%)	8 (3%)	36	16
1	B	269/288 (93%)	262 (97%)	7 (3%)	40	20
1	C	258/288 (90%)	256 (99%)	2 (1%)	73	64
1	D	260/288 (90%)	258 (99%)	2 (1%)	73	64
All	All	1051/1152 (91%)	1032 (98%)	19 (2%)	51	33

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	806	LYS
1	D	986	ARG
1	A	752	SER
1	A	783	THR
1	A	793	MET
1	A	858	LEU
1	A	970	LYS
1	A	1006	ASP
1	A	1007	MET
1	A	1010	VAL
1	B	749	GLU
1	B	752	SER
1	B	754	LYS
1	B	790	MET
1	B	970	LYS
1	B	985	GLU
1	B	1008	ASP
1	C	701	GLN
1	C	913	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	805	HIS
1	D	826	ASN
1	D	988	HIS
1	A	893	HIS
1	A	982	GLN
1	B	849	GLN
1	B	893	HIS
1	C	701	GLN
1	C	812	GLN
1	C	976	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	UEJ	D	1101	-	51,51,51	5.58	34 (66%)	68,74,74	2.08	20 (29%)
3	ANP	B	1101	4	33,33,33	1.36	4 (12%)	45,52,52	1.86	3 (6%)
2	UEJ	C	1301	-	51,51,51	5.41	36 (70%)	68,74,74	1.79	20 (29%)

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	UEJ	D	1101	-	-	2/26/42/42	0/6/6/6
3	ANP	B	1101	4	-	4/18/38/38	0/3/3/3
2	UEJ	C	1301	-	-	7/26/42/42	0/6/6/6

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	UEJ	C12-C13	10.26	1.55	1.39
2	D	1101	UEJ	C09-C08	10.08	1.55	1.39
2	C	1301	UEJ	C09-C08	9.84	1.54	1.39
2	C	1301	UEJ	C12-C13	9.62	1.54	1.39
2	D	1101	UEJ	C24-C25	9.00	1.53	1.39
2	C	1301	UEJ	C18-C17	8.73	1.52	1.38
2	D	1101	UEJ	C18-C17	8.72	1.52	1.38
2	D	1101	UEJ	C07-N06	8.32	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	UEJ	C11-C12	8.32	1.53	1.38
2	D	1101	UEJ	C10-C09	8.31	1.53	1.38
2	C	1301	UEJ	C23-C22	8.24	1.53	1.38
2	D	1101	UEJ	C23-C24	8.24	1.53	1.38
2	D	1101	UEJ	C23-C22	8.23	1.53	1.38
2	C	1301	UEJ	C11-C12	8.14	1.52	1.38
2	D	1101	UEJ	C22-C21	8.04	1.52	1.39
2	C	1301	UEJ	C10-C09	8.01	1.52	1.38
2	D	1101	UEJ	C14-N06	7.91	1.49	1.39
2	C	1301	UEJ	C23-C24	7.82	1.52	1.38
2	C	1301	UEJ	C24-C25	7.78	1.51	1.39
2	C	1301	UEJ	C07-N06	7.74	1.49	1.39
2	C	1301	UEJ	C32-N31	7.59	1.47	1.34
2	C	1301	UEJ	C17-C16	7.51	1.52	1.39
2	C	1301	UEJ	C22-C21	7.48	1.51	1.39
2	C	1301	UEJ	C16-C04	7.34	1.52	1.40
2	D	1101	UEJ	C32-N31	7.24	1.47	1.34
2	D	1101	UEJ	C17-C16	7.15	1.51	1.39
2	D	1101	UEJ	C16-C04	7.13	1.52	1.40
2	C	1301	UEJ	C43-C25	7.10	1.50	1.39
2	D	1101	UEJ	C43-C25	7.01	1.50	1.39
2	D	1101	UEJ	C03-C19	6.97	1.51	1.39
2	C	1301	UEJ	C03-C19	6.89	1.50	1.39
2	C	1301	UEJ	C14-N06	6.88	1.48	1.39
2	D	1101	UEJ	C18-C19	6.83	1.51	1.37
2	C	1301	UEJ	C29-C30	6.79	1.51	1.38
2	D	1101	UEJ	C11-C10	6.77	1.53	1.38
2	D	1101	UEJ	C43-C21	6.74	1.50	1.39
2	C	1301	UEJ	C18-C19	6.72	1.51	1.37
2	C	1301	UEJ	C11-C10	6.55	1.52	1.38
2	C	1301	UEJ	C43-C21	6.53	1.50	1.39
2	C	1301	UEJ	C30-N31	6.41	1.48	1.34
2	D	1101	UEJ	C29-C28	6.33	1.49	1.39
2	D	1101	UEJ	C30-N31	6.28	1.47	1.34
2	D	1101	UEJ	C29-C30	6.24	1.50	1.38
2	C	1301	UEJ	C29-C28	6.24	1.48	1.39
2	C	1301	UEJ	C37-C28	6.05	1.48	1.39
2	D	1101	UEJ	C37-C28	6.04	1.48	1.39
2	D	1101	UEJ	C03-C04	5.94	1.51	1.40
2	C	1301	UEJ	C03-C04	5.37	1.50	1.40
2	D	1101	UEJ	C34-N33	5.19	1.45	1.36
2	C	1301	UEJ	C34-N33	4.85	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	UEJ	C37-C32	4.65	1.51	1.39
2	C	1301	UEJ	C26-N42	-4.64	1.31	1.38
2	C	1301	UEJ	C08-C13	4.39	1.48	1.39
2	D	1101	UEJ	C26-N42	-4.31	1.31	1.38
2	C	1301	UEJ	C37-C32	4.22	1.50	1.39
2	D	1101	UEJ	C08-C13	4.08	1.48	1.39
3	B	1101	ANP	PG-O2G	-4.07	1.46	1.56
2	D	1101	UEJ	C39-S40	3.56	1.80	1.75
3	B	1101	ANP	PG-O3G	-3.47	1.47	1.56
2	D	1101	UEJ	C27-N38	-3.45	1.31	1.37
2	C	1301	UEJ	C27-N38	-3.44	1.31	1.37
2	D	1101	UEJ	C08-C07	3.14	1.53	1.48
3	B	1101	ANP	PB-O2B	-3.04	1.48	1.56
2	C	1301	UEJ	C39-S40	2.99	1.80	1.75
2	D	1101	UEJ	C13-C14	2.64	1.53	1.48
3	B	1101	ANP	PG-N3B	-2.62	1.56	1.63
2	C	1301	UEJ	C13-C14	2.52	1.52	1.48
2	D	1101	UEJ	C25-C26	2.52	1.51	1.48
2	D	1101	UEJ	C02-N20	2.46	1.42	1.35
2	C	1301	UEJ	C05-N06	-2.27	1.43	1.47
2	C	1301	UEJ	C08-C07	2.05	1.52	1.48
2	C	1301	UEJ	O15-C14	-2.05	1.18	1.22
2	C	1301	UEJ	C27-C26	-2.04	1.35	1.38
2	C	1301	UEJ	C02-N20	2.02	1.41	1.35

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1101	ANP	O1B-PB-N3B	10.64	127.44	111.77
2	D	1101	UEJ	C19-C03-C02	-6.61	112.18	122.21
2	C	1301	UEJ	C19-C03-C02	-4.62	115.20	122.21
2	D	1101	UEJ	C41-S40-C39	4.44	109.47	102.27
2	D	1101	UEJ	C07-N06-C14	-4.42	108.25	112.02
2	C	1301	UEJ	C43-C25-C26	-4.32	111.71	120.51
2	D	1101	UEJ	C43-C25-C26	-4.09	112.17	120.51
2	D	1101	UEJ	C24-C25-C26	3.95	127.21	120.74
3	B	1101	ANP	O2B-PB-O1B	3.81	118.05	109.87
2	D	1101	UEJ	C30-N31-C32	3.75	122.56	117.21
2	D	1101	UEJ	C29-C30-N31	-3.57	119.60	123.97
2	D	1101	UEJ	C37-C32-N31	-3.39	118.47	122.92
2	D	1101	UEJ	C32-N33-C34	-3.32	124.77	128.16
2	D	1101	UEJ	C05-N06-C07	3.24	127.77	123.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	UEJ	C13-C14-N06	3.22	108.27	105.88
3	B	1101	ANP	O2G-PG-O1G	-3.21	105.41	113.45
2	C	1301	UEJ	S40-C39-N38	3.17	126.51	119.66
2	C	1301	UEJ	C07-N06-C14	-3.16	109.32	112.02
2	C	1301	UEJ	C24-C25-C43	3.06	122.79	119.25
2	D	1101	UEJ	S40-C39-N38	3.00	126.15	119.66
2	C	1301	UEJ	O01-C02-C03	2.92	125.35	121.06
2	C	1301	UEJ	C24-C25-C26	2.90	125.50	120.74
2	C	1301	UEJ	C04-C05-N06	-2.88	108.33	113.68
2	C	1301	UEJ	C03-C02-N20	-2.81	109.65	114.81
2	C	1301	UEJ	C37-C32-N31	-2.80	119.25	122.92
2	D	1101	UEJ	C28-C27-C26	-2.72	128.37	133.06
2	D	1101	UEJ	F46-C19-C18	2.69	124.91	118.65
2	C	1301	UEJ	C05-C04-C16	2.67	123.60	120.22
2	D	1101	UEJ	C26-C27-N38	2.67	108.89	105.63
2	D	1101	UEJ	C18-C19-C03	-2.60	118.72	123.48
2	C	1301	UEJ	C30-N31-C32	2.59	120.91	117.21
2	C	1301	UEJ	C29-C28-C37	2.56	122.21	119.25
2	D	1101	UEJ	C43-C21-N20	-2.53	111.92	120.13
2	D	1101	UEJ	C29-C28-C37	2.52	122.17	119.25
2	C	1301	UEJ	F46-C19-C18	2.47	124.40	118.65
2	C	1301	UEJ	C29-C30-N31	-2.47	120.95	123.97
2	C	1301	UEJ	C28-C27-C26	-2.41	128.90	133.06
2	C	1301	UEJ	C26-C27-N38	2.28	108.41	105.63
2	D	1101	UEJ	O01-C02-C03	2.26	124.38	121.06
2	D	1101	UEJ	C08-C07-N06	2.18	107.50	105.88
2	C	1301	UEJ	C32-N33-C34	-2.18	125.93	128.16
2	C	1301	UEJ	C23-C24-C25	-2.16	118.24	120.36
2	C	1301	UEJ	C43-C21-N20	-2.10	113.31	120.13

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1301	UEJ	N38-C39-S40-C41
2	C	1301	UEJ	N42-C39-S40-C41
3	B	1101	ANP	PB-N3B-PG-O1G
3	B	1101	ANP	PG-N3B-PB-O1B
3	B	1101	ANP	PG-N3B-PB-O3A
2	D	1101	UEJ	N42-C39-S40-C41
2	D	1101	UEJ	N38-C39-S40-C41
2	C	1301	UEJ	C43-C25-C26-C27

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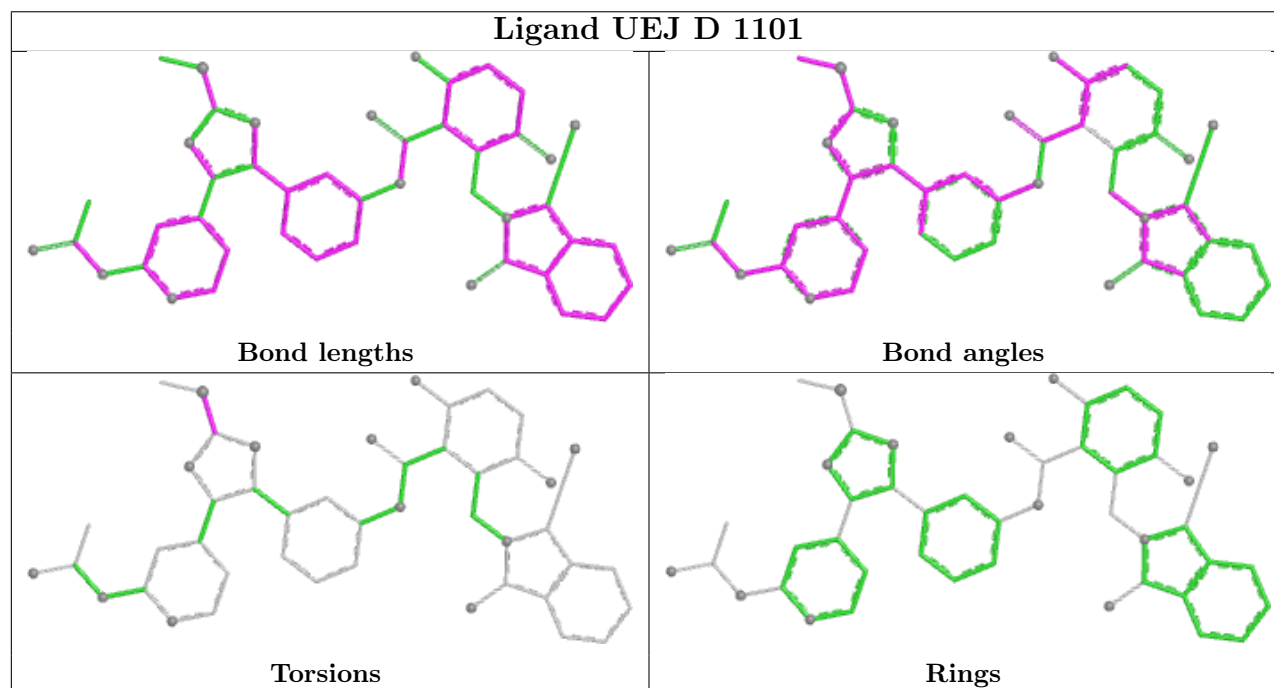
Mol	Chain	Res	Type	Atoms
2	C	1301	UEJ	C24-C25-C26-C27
3	B	1101	ANP	PB-O3A-PA-O1A
2	C	1301	UEJ	C43-C25-C26-N42
2	C	1301	UEJ	C04-C05-N06-C14
2	C	1301	UEJ	C24-C25-C26-N42

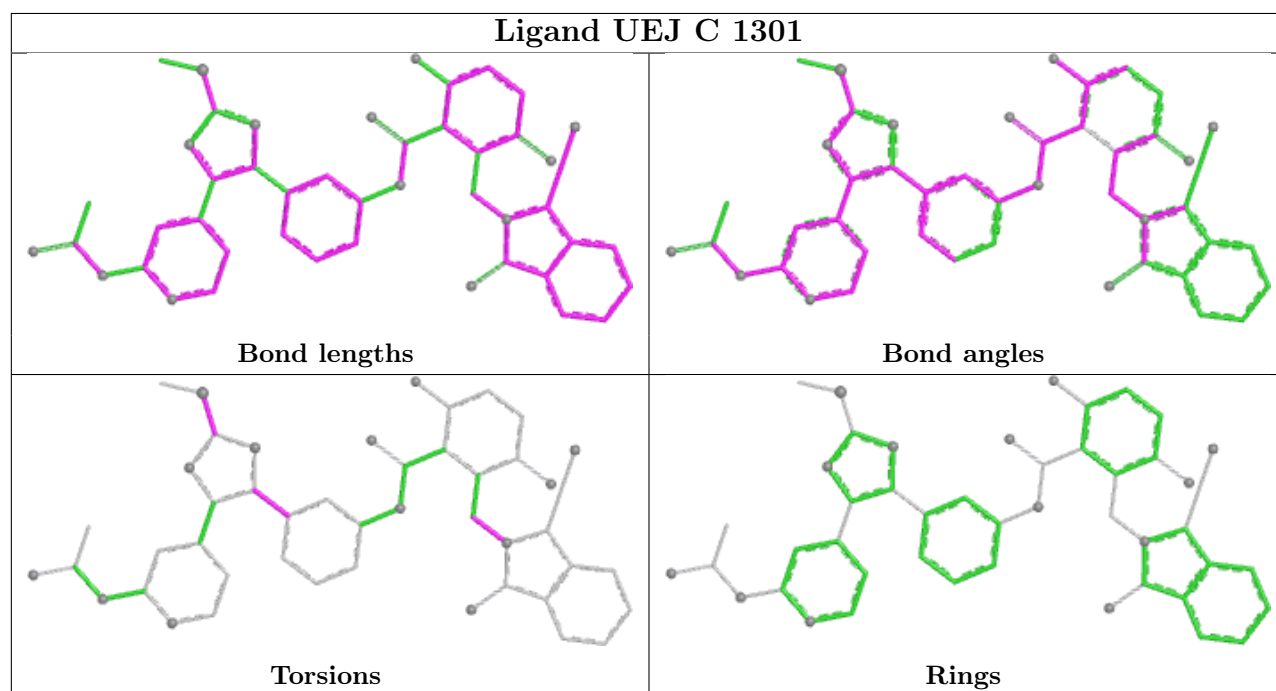
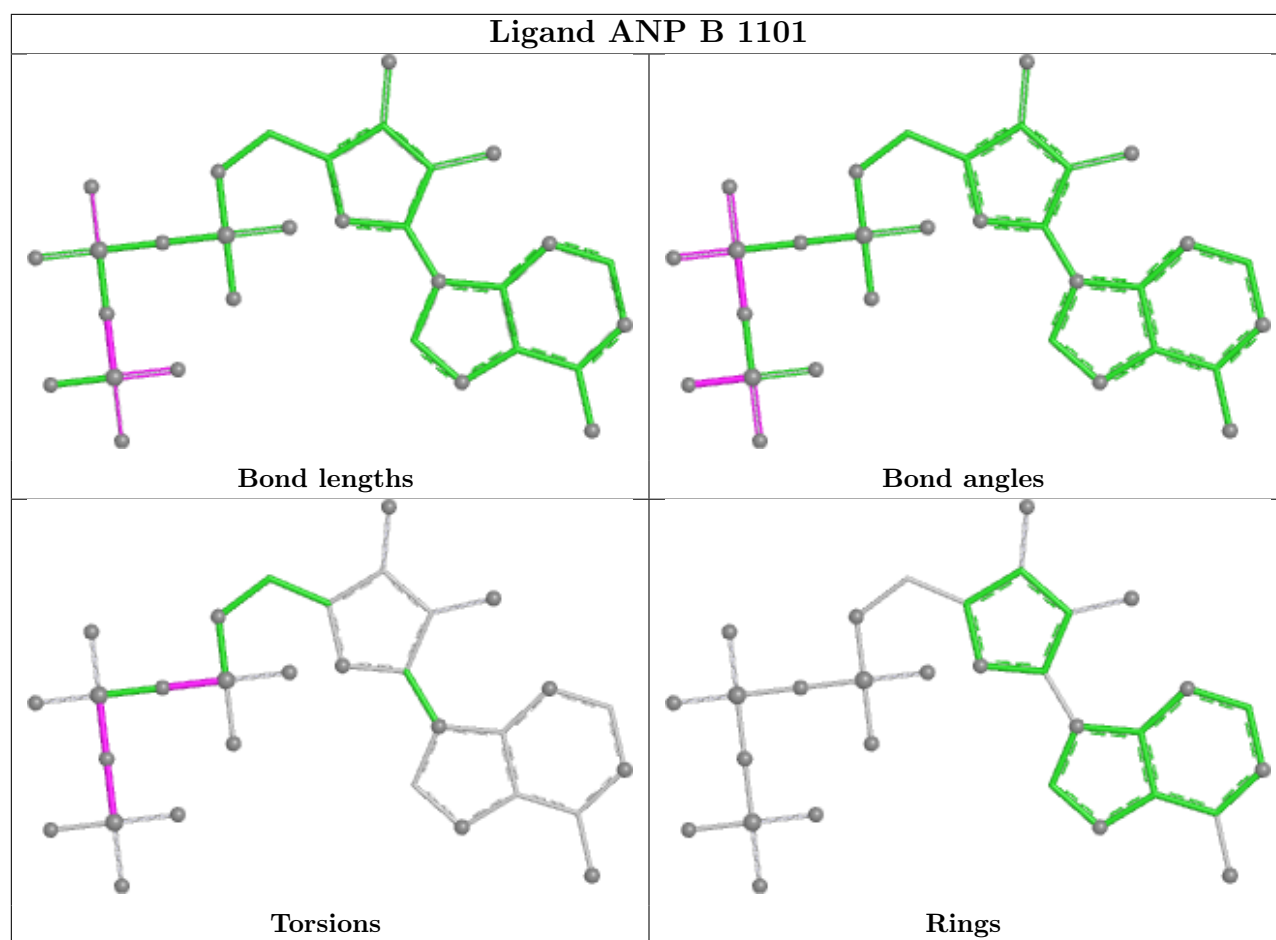
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1101	UEJ	3	0
3	B	1101	ANP	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	298/328 (90%)	0.85	40 (13%) 7 8	18, 34, 64, 84	1 (0%)
1	B	303/328 (92%)	0.54	21 (6%) 23 26	19, 31, 50, 75	1 (0%)
1	C	286/328 (87%)	0.76	31 (10%) 11 12	18, 33, 55, 82	1 (0%)
1	D	292/328 (89%)	0.69	24 (8%) 17 21	19, 34, 56, 79	1 (0%)
All	All	1179/1312 (89%)	0.71	116 (9%) 13 15	18, 33, 59, 84	4 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1010	VAL	6.2
1	D	750	ALA	5.6
1	C	1013	ALA	5.2
1	A	1011	VAL	5.2
1	C	859	ALA	5.2
1	B	750	ALA	5.1
1	B	1008	ASP	5.1
1	A	989	LEU	4.9
1	A	699	PRO	4.8
1	A	859	ALA	4.7
1	D	1013	ALA	4.5
1	A	858	LEU	4.5
1	C	858	LEU	4.5
1	C	1014	ASP	4.4
1	D	861	LEU	4.3
1	A	723	PHE	4.2
1	A	1013	ALA	4.2
1	C	1006	ASP	4.2
1	C	720	SER	4.1
1	C	1010	VAL	4.0
1	C	857	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	990	PRO	3.9
1	D	862	LEU	3.8
1	B	751	THR	3.8
1	B	989	LEU	3.7
1	C	988	HIS	3.7
1	C	918	ILE	3.7
1	A	876	VAL	3.6
1	A	783	THR	3.6
1	D	722	ALA	3.6
1	B	723	PHE	3.5
1	C	1008	ASP	3.5
1	A	722	ALA	3.4
1	C	913	LYS	3.4
1	C	1011	VAL	3.4
1	A	755	ALA	3.3
1	D	917	GLY	3.3
1	C	1007	MET	3.2
1	A	753	PRO	3.2
1	B	887	LEU	3.2
1	D	723	PHE	3.2
1	B	861	LEU	3.2
1	C	1012	ASP	3.2
1	D	988	HIS	3.2
1	A	988	HIS	3.1
1	B	992	PRO	3.1
1	A	751	THR	3.1
1	A	1012	ASP	3.1
1	B	862	LEU	3.0
1	C	782	LEU	3.0
1	D	1005	GLU	3.0
1	A	752	SER	3.0
1	D	1014	ASP	2.9
1	C	912	SER	2.9
1	D	922[A]	GLU	2.9
1	B	988	HIS	2.9
1	D	806	LYS	2.9
1	A	702	ALA	2.8
1	D	1012	ASP	2.8
1	C	989	LEU	2.8
1	A	785	THR	2.8
1	D	1011	VAL	2.8
1	C	890	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	752	SER	2.8
1	D	876	VAL	2.8
1	B	1021	GLN	2.8
1	C	756	ASN	2.7
1	A	857	GLY	2.7
1	A	1007	MET	2.7
1	D	986	ARG	2.7
1	A	941	ILE	2.7
1	C	807	ASP	2.7
1	C	701	GLN	2.7
1	A	700	ASN	2.6
1	C	702	ALA	2.6
1	A	784	SER	2.6
1	A	807	ASP	2.6
1	B	1006	ASP	2.6
1	D	889	ARG	2.6
1	B	890	ILE	2.5
1	A	808	ASN	2.5
1	C	985	GLU	2.5
1	A	782	LEU	2.5
1	A	786	VAL	2.5
1	D	890	ILE	2.5
1	D	992	PRO	2.5
1	C	876	VAL	2.5
1	B	876	VAL	2.5
1	D	807	ASP	2.4
1	D	715	ILE	2.4
1	A	983	GLY	2.4
1	A	987	MET	2.4
1	A	735	GLY	2.4
1	A	756	ASN	2.4
1	A	747	LEU	2.4
1	A	1014	ASP	2.3
1	A	760	LEU	2.3
1	D	764	TYR	2.3
1	B	875	LYS	2.3
1	C	990	PRO	2.3
1	A	986	ARG	2.3
1	C	986	ARG	2.2
1	B	782	LEU	2.2
1	A	984	ASP	2.2
1	D	732	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	748	ARG	2.2
1	C	1009	ASP	2.2
1	D	887	LEU	2.2
1	C	747	LEU	2.2
1	A	806	LYS	2.1
1	B	749	GLU	2.1
1	B	926	ILE	2.1
1	C	953	ILE	2.1
1	A	759	ILE	2.0
1	C	926	ILE	2.0
1	B	702	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

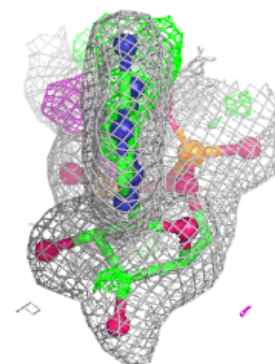
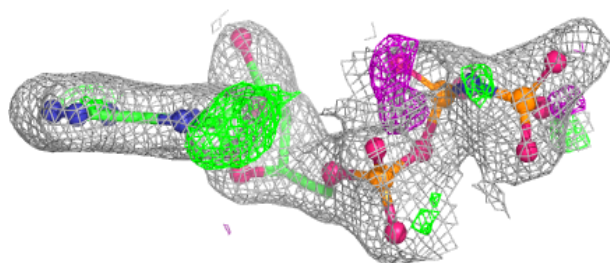
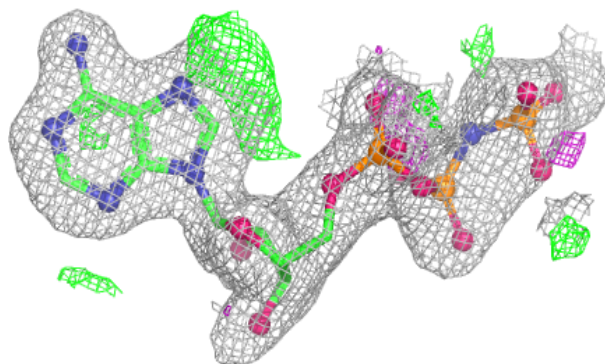
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ANP	B	1101	31/31	0.89	0.12	20,33,40,49	31
2	UEJ	D	1101	46/46	0.91	0.10	27,34,47,50	0
2	UEJ	C	1301	46/46	0.94	0.09	22,28,40,45	0
4	MG	B	1102	1/1	0.96	0.17	35,35,35,35	0
5	CL	C	1302	1/1	0.96	0.08	44,44,44,44	0

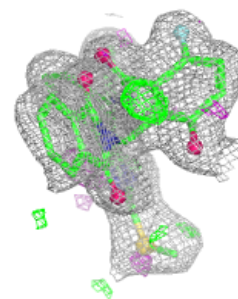
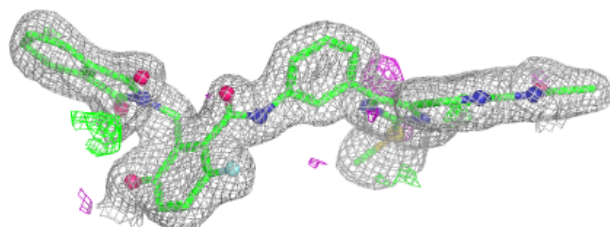
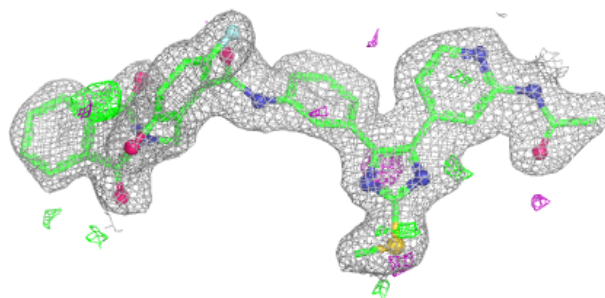
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

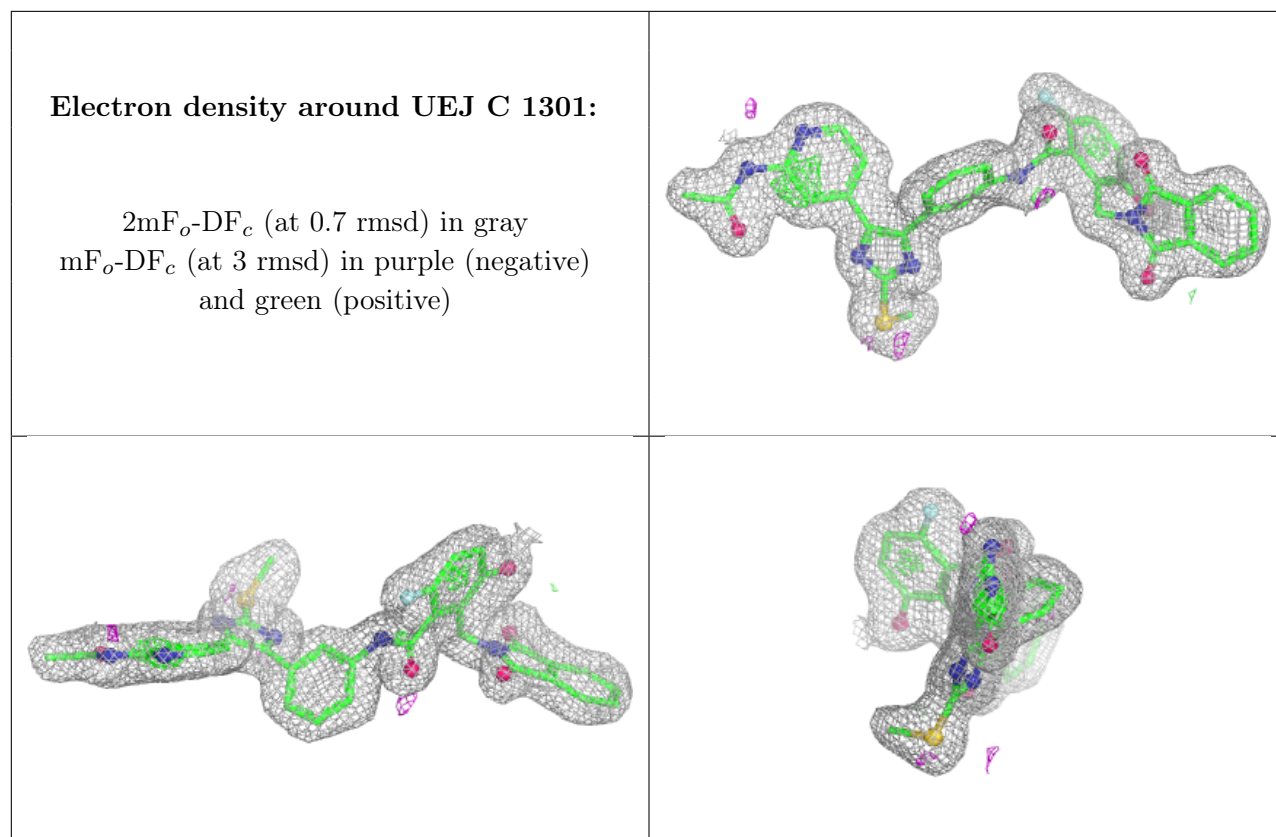
Electron density around ANP B 1101:

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

**Electron density around UEJ D 1101:**

$2mF_o-DF_c$ (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.