



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2021 – 08:04 AM EDT

PDB ID : 7LGS  
Title : Structure of EGFR\_D770\_N771insNPG/V948R in complex with covalent inhibitor Osimertinib.  
Authors : Skene, R.J.; Lane, W.  
Deposited on : 2021-01-21  
Resolution : 3.10 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

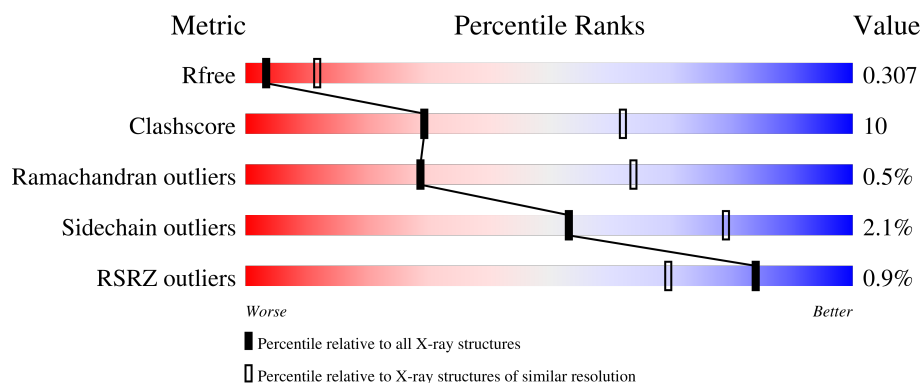
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 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	331	<div> <div>65%</div> <div>20%</div> <div>15%</div> </div>
1	B	331	<div> <div>57%</div> <div>29%</div> <div>• 14%</div> </div>
1	C	331	<div> <div>2%</div> <div>71%</div> <div>14%</div> <div>• 15%</div> </div>
1	D	331	<div> <div>2%</div> <div>68%</div> <div>16%</div> <div>• 16%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9394 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.

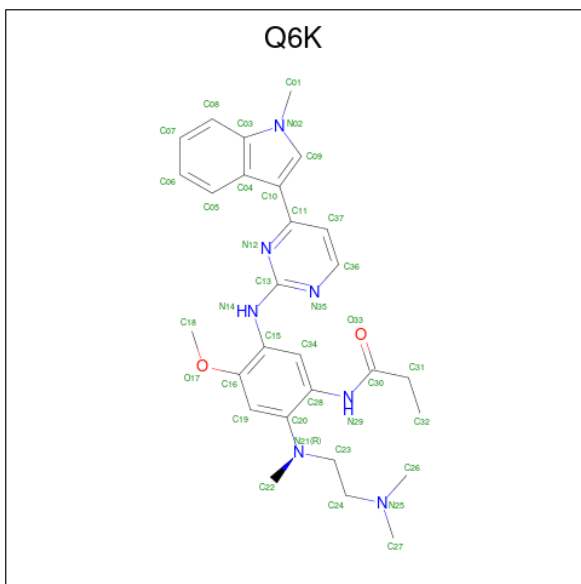
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2265	1461	387	402	15			
1	B	286	Total	C	N	O	S	0	1	0
			2294	1478	392	409	15			
1	C	283	Total	C	N	O	S	0	0	0
			2264	1460	385	404	15			
1	D	279	Total	C	N	O	S	0	0	0
			2233	1440	379	399	15			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	695	GLY	-	expression tag	UNP P00533
A	773	GLY	-	insertion	UNP P00533
A	774	ASN	-	insertion	UNP P00533
A	775	PRO	-	insertion	UNP P00533
A	951	ARG	VAL	engineered mutation	UNP P00533
B	695	GLY	-	expression tag	UNP P00533
B	773	GLY	-	insertion	UNP P00533
B	774	ASN	-	insertion	UNP P00533
B	775	PRO	-	insertion	UNP P00533
B	951	ARG	VAL	engineered mutation	UNP P00533
C	695	GLY	-	expression tag	UNP P00533
C	773	GLY	-	insertion	UNP P00533
C	774	ASN	-	insertion	UNP P00533
C	775	PRO	-	insertion	UNP P00533
C	951	ARG	VAL	engineered mutation	UNP P00533
D	695	GLY	-	expression tag	UNP P00533
D	773	GLY	-	insertion	UNP P00533
D	774	ASN	-	insertion	UNP P00533
D	775	PRO	-	insertion	UNP P00533
D	951	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is {N}-[2-[2-(dimethylamino)ethyl-methyl-amino]-4-methoxy-5-[[4-(1-methylindol-3-yl)pyrimidin-2-yl]amino]phenyl]propanamide (three-letter code: Q6K) (formula:  $C_{28}H_{35}N_7O_2$ ) (labeled as "Ligand of Interest" by depositor).



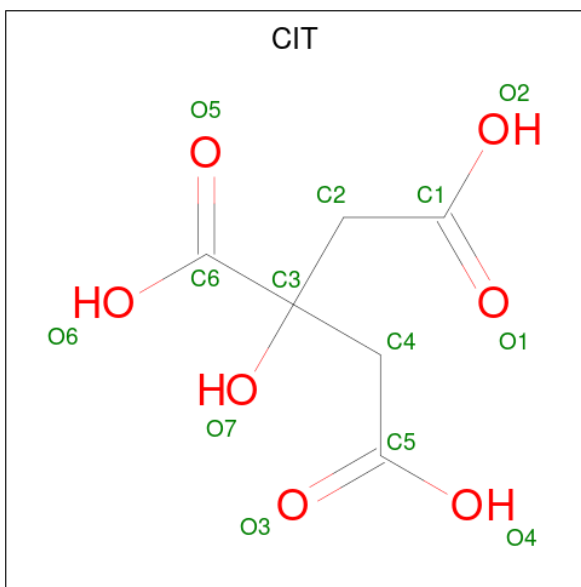
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			37	28	7	2		
2	B	1	Total	C	N	O	0	0
			37	28	7	2		
2	C	1	Total	C	N	O	0	0
			37	28	7	2		
2	D	1	Total	C	N	O	0	0
			37	28	7	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	6	7		

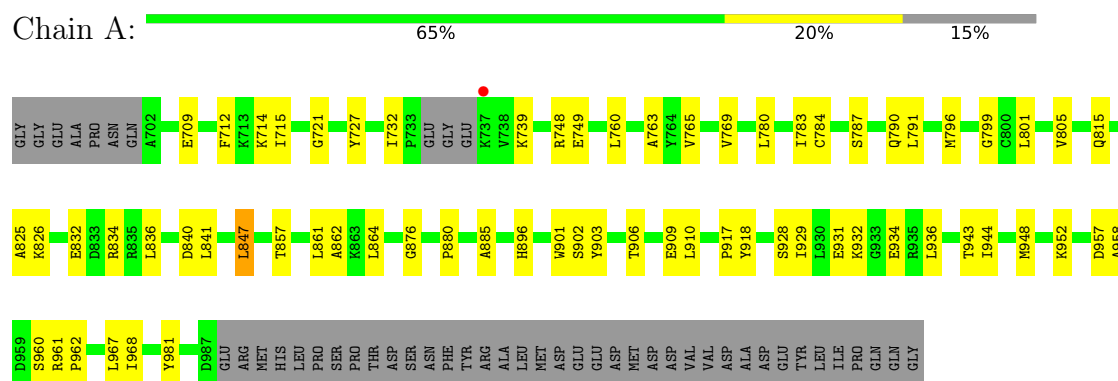
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	44	Total	O	0	0
			44	44		
5	B	46	Total	O	0	0
			46	46		
5	C	28	Total	O	0	0
			28	28		
5	D	35	Total	O	0	0
			35	35		

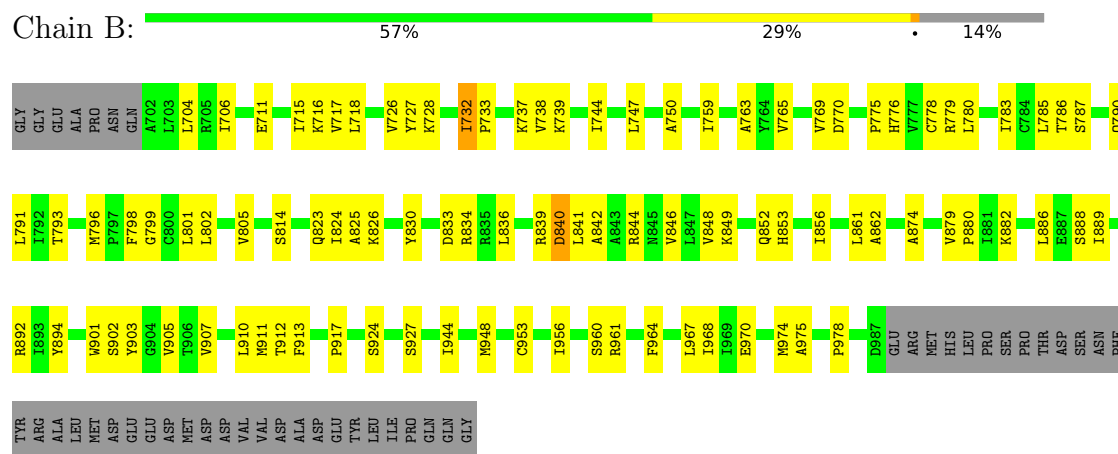
### 3 Residue-property plots

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

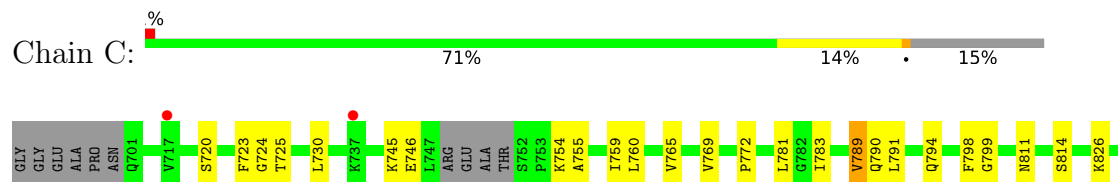
#### • Molecule 1: Epidermal growth factor receptor



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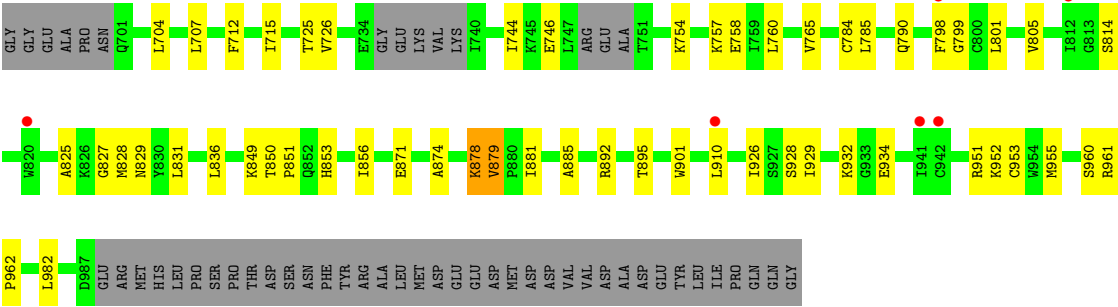


#### • Molecule 1: Epidermal growth factor receptor





● 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, $\alpha$ , $\beta$ , $\gamma$	60.66Å 132.10Å 85.81Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	49.01 – 3.10 48.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.2 (49.01-3.10) 88.3 (48.96-3.10)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.238 , 0.305 0.242 , 0.307	Depositor DCC
$R_{free}$ test set	1148 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.2	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 26.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.210 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9394	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EDO, Q6K, CIT

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	0.25	0/2315	0.56	0/3130
1	B	0.24	0/2349	0.55	0/3177
1	C	0.25	0/2314	0.51	0/3128
1	D	0.25	0/2282	0.51	0/3086
All	All	0.25	0/9260	0.53	0/12521

There are no bond length outliers.

There are no bond angle outliers.

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	2265	0	2329	46	0
1	B	2294	0	2352	69	0
1	C	2264	0	2321	29	0
1	D	2233	0	2283	33	0
2	A	37	0	0	3	0
2	B	37	0	0	4	0
2	C	37	0	0	3	0
2	D	37	0	0	2	0
3	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	24	0	0
3	C	4	0	6	0	0
4	B	13	0	5	1	0
5	A	44	0	0	0	0
5	B	46	0	0	1	0
5	C	28	0	0	0	0
5	D	35	0	0	0	0
All	All	9394	0	9326	177	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 10.

All (177) 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:C:765:VAL:HG13	1:C:836:LEU:HD11	1.43	1.01
1:B:718:LEU:HD12	1:B:726:VAL:HG12	1.44	0.98
1:B:879:VAL:HG12	1:B:880:PRO:HD2	1.46	0.95
2:B:2703:Q6K:N29	2:B:2703:Q6K:C23	2.44	0.80
1:A:796:MET:HG3	1:A:847:LEU:HB3	1.62	0.80
1:B:786:THR:HG22	1:B:787:SER:H	1.46	0.80
2:C:1101:Q6K:C23	2:C:1101:Q6K:N29	2.45	0.79
1:B:805:VAL:HG11	1:B:910:LEU:HD22	1.65	0.78
1:B:785:LEU:HD22	1:D:760:LEU:HD21	1.66	0.77
1:A:847:LEU:CD2	1:A:857:THR:HG21	2.17	0.74
1:D:874:ALA:HB3	1:D:892:ARG:HB3	1.70	0.73
2:A:1101:Q6K:C23	2:A:1101:Q6K:N29	2.54	0.71
1:C:772:PRO:HD3	1:C:834:ARG:HH21	1.54	0.71
1:B:779:ARG:NH2	4:B:2705:CIT:O3	2.24	0.70
1:A:805:VAL:HG11	1:A:910:LEU:HD22	1.75	0.68
1:D:784:CYS:HB2	1:D:790:GLN:HB2	1.76	0.68
1:D:799:GLY:HA2	2:D:2500:Q6K:C34	2.25	0.67
1:A:841:LEU:HB3	1:A:902:SER:HB3	1.76	0.67
1:B:765:VAL:HG13	1:B:836:LEU:HD11	1.77	0.66
1:D:929:ILE:HG23	1:D:934:GLU:HB2	1.77	0.66
1:B:738:VAL:HG12	1:B:739:LYS:H	1.59	0.66
1:D:746:GLU:HB3	1:D:790:GLN:HG2	1.78	0.65
1:A:780:LEU:HD11	1:A:791:LEU:HD22	1.78	0.64
1:B:879:VAL:CG1	1:B:880:PRO:HD2	2.26	0.64
1:B:747:LEU:HG	1:B:759:ILE:HD12	1.80	0.63
1:C:781:LEU:HD11	1:C:794:GLN:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:ILE:HG22	1:A:791:LEU:HD23	1.82	0.62
1:C:907:VAL:O	1:C:911:MET:HG2	2.01	0.61
1:C:799:GLY:HA2	2:C:1101:Q6K:C34	2.30	0.61
1:B:732:ILE:HG23	1:B:739:LYS:HG2	1.82	0.60
1:B:799:GLY:HA2	2:B:2703:Q6K:C34	2.31	0.60
1:B:882:LYS:HD3	1:B:917:PRO:O	2.01	0.60
1:A:840:ASP:OD1	1:A:880:PRO:HG3	2.02	0.60
1:A:836:LEU:HD21	1:A:862:ALA:HB1	1.84	0.59
1:D:765:VAL:HG13	1:D:836:LEU:HD11	1.84	0.59
1:A:765:VAL:HG12	1:A:836:LEU:HD11	1.84	0.59
1:B:901:TRP:O	1:B:905:VAL:HG23	2.01	0.59
1:A:769:VAL:HG12	1:A:834:ARG:HB3	1.84	0.59
1:D:746:GLU:CB	1:D:790:GLN:HG2	2.33	0.59
1:A:765:VAL:CG1	1:A:836:LEU:HD11	2.32	0.59
1:B:769:VAL:HG12	1:B:834:ARG:HB3	1.83	0.59
1:A:826:LYS:HA	1:A:968:ILE:HD11	1.84	0.59
1:C:886:LEU:HD22	1:C:956:ILE:HD12	1.86	0.58
1:A:796:MET:CG	1:A:847:LEU:HB3	2.33	0.58
2:D:2500:Q6K:C23	2:D:2500:Q6K:N29	2.67	0.58
1:D:928:SER:O	1:D:932:LYS:HG2	2.04	0.57
1:B:715:ILE:HD12	1:B:728:LYS:HG2	1.86	0.56
1:A:815:GLN:HG3	1:B:852:GLN:HG2	1.88	0.56
1:A:748:ARG:HG2	1:A:749:GLU:HG2	1.88	0.56
1:B:836:LEU:HD21	1:B:862:ALA:HB1	1.88	0.56
1:A:721:GLY:O	1:A:748:ARG:NH2	2.38	0.56
1:A:957:ASP:OD2	1:A:960:SER:HB2	2.04	0.56
1:B:824:ILE:HG23	1:B:856:ILE:HD11	1.87	0.55
1:C:929:ILE:HG23	1:C:934:GLU:HB2	1.88	0.55
1:A:784:CYS:HB2	1:A:790:GLN:HB2	1.87	0.55
1:B:799:GLY:HA2	2:B:2703:Q6K:C15	2.36	0.55
1:B:826:LYS:HG3	1:B:968:ILE:HG12	1.89	0.55
1:D:801:LEU:HD13	1:D:910:LEU:HD21	1.89	0.55
1:A:847:LEU:HD21	1:A:857:THR:HG21	1.90	0.54
1:A:825:ALA:HB3	1:A:968:ILE:HG13	1.89	0.54
1:B:706:ILE:HD11	1:D:704:LEU:HD22	1.90	0.54
1:B:830:TYR:O	1:B:833:ASP:HB2	2.07	0.54
1:C:814:SER:OG	1:C:978:PRO:HB2	2.08	0.54
1:D:798:PHE:CE2	1:D:851:PRO:HD3	2.42	0.54
1:A:712:PHE:CE1	1:A:784:CYS:SG	3.01	0.54
1:D:825:ALA:O	1:D:829:ASN:HB2	2.08	0.54
1:A:714:LYS:HD3	1:A:727:TYR:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:787:SER:HA	1:D:757:LYS:NZ	2.23	0.53
1:B:796:MET:SD	1:B:849:LYS:HB2	2.49	0.53
1:B:763:ALA:HB2	1:B:791:LEU:HD21	1.91	0.52
1:B:841:LEU:HB3	1:B:902:SER:HB3	1.91	0.52
1:B:718:LEU:HD12	1:B:726:VAL:CG1	2.29	0.52
1:B:805:VAL:HG11	1:B:910:LEU:CD2	2.36	0.51
1:A:906:THR:O	1:A:909:GLU:HB2	2.10	0.51
1:B:841:LEU:HD23	1:B:903:TYR:HA	1.92	0.51
1:A:929:ILE:HG23	1:A:934:GLU:HB2	1.92	0.51
1:B:907:VAL:O	1:B:911:MET:HG2	2.11	0.51
1:C:769:VAL:HG12	1:C:834:ARG:HB3	1.93	0.51
1:A:847:LEU:CD2	1:A:857:THR:CG2	2.88	0.51
1:B:801:LEU:HB2	1:B:846:VAL:O	2.11	0.50
1:B:786:THR:HG22	1:B:787:SER:N	2.22	0.50
1:A:799:GLY:HA2	2:A:1101:Q6K:C15	2.41	0.50
1:B:953:CYS:O	1:B:961:ARG:HD3	2.12	0.49
1:A:903:TYR:CE2	1:A:967:LEU:HD22	2.48	0.49
1:D:871:GLU:HB3	1:D:895:THR:HG22	1.94	0.49
1:B:798:PHE:HB2	1:B:848:VAL:HB	1.95	0.49
1:B:776:HIS:CE1	1:B:823:GLN:HG2	2.47	0.49
1:C:746:GLU:HG3	1:C:790:GLN:HE21	1.77	0.49
1:A:763:ALA:HB2	1:A:791:LEU:HD21	1.95	0.48
1:C:754:LYS:HG3	1:C:755:ALA:N	2.28	0.48
1:B:912:THR:O	1:B:913:PHE:HB2	2.14	0.48
1:A:825:ALA:CB	1:A:968:ILE:HG13	2.43	0.48
1:C:799:GLY:HA2	2:C:1101:Q6K:C15	2.45	0.47
1:B:879:VAL:HG12	1:B:880:PRO:CD	2.33	0.47
1:D:955:MET:SD	1:D:960:SER:HB3	2.55	0.47
1:D:707:LEU:HD13	1:D:712:PHE:HZ	1.80	0.47
1:B:770:ASP:OD1	1:B:779:ARG:HD3	2.15	0.47
1:C:760:LEU:HD13	1:C:789:VAL:HG11	1.95	0.47
1:D:885:ALA:HA	1:D:901:TRP:CD2	2.50	0.46
1:D:952:LYS:HB3	1:D:962:PRO:HD3	1.97	0.46
1:A:885:ALA:HA	1:A:901:TRP:CD2	2.50	0.46
1:D:726:VAL:HA	1:D:744:ILE:O	2.15	0.46
1:B:840:ASP:HB2	1:B:861:LEU:HD22	1.96	0.46
1:B:726:VAL:HG21	2:B:2703:Q6K:C03	2.46	0.46
1:A:783:ILE:HA	1:A:790:GLN:O	2.16	0.46
1:B:747:LEU:O	1:B:750:ALA:HB2	2.16	0.46
1:B:944:ILE:HG13	1:B:948:MET:HG2	1.97	0.46
1:D:798:PHE:HD2	1:D:849:LYS:O	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:720:SER:HB2	1:C:725:THR:HG23	1.98	0.46
1:D:929:ILE:O	1:D:932:LYS:HB2	2.16	0.46
1:A:832:GLU:HA	1:A:896:HIS:CE1	2.51	0.45
1:A:748:ARG:HH11	1:A:748:ARG:HG3	1.81	0.45
1:B:839:ARG:HG2	1:B:894:TYR:CD2	2.52	0.45
1:D:828:MET:HA	1:D:831:LEU:HD12	1.99	0.45
1:A:958:ALA:O	1:A:961:ARG:HB2	2.16	0.45
1:C:723:PHE:CD2	1:C:724:GLY:N	2.84	0.45
1:B:964:PHE:HA	1:B:967:LEU:HD12	1.98	0.45
1:B:718:LEU:HD21	1:B:728:LYS:HB2	1.99	0.45
1:D:878:LYS:HD3	1:D:879:VAL:N	2.32	0.44
1:A:928:SER:HA	1:A:931:GLU:OE2	2.18	0.44
1:B:780:LEU:HD11	1:B:791:LEU:HD22	1.99	0.44
1:A:918:TYR:CE1	1:A:936:LEU:HG	2.52	0.44
1:C:723:PHE:CG	1:C:724:GLY:N	2.86	0.44
1:B:801:LEU:HG	1:B:910:LEU:HD21	2.00	0.44
1:C:798:PHE:HB2	1:C:848:VAL:HB	1.99	0.44
1:A:952:LYS:HB3	1:A:962:PRO:HD3	2.00	0.44
1:C:745:LYS:HD3	1:C:791:LEU:HD12	1.99	0.44
1:C:826:LYS:HA	1:C:968:ILE:HD11	2.01	0.43
1:C:836:LEU:HG	1:C:863:LYS:O	2.18	0.43
1:B:711:GLU:OE1	1:B:733:PRO:HA	2.17	0.43
1:B:704:LEU:HD12	1:B:704:LEU:HA	1.86	0.43
1:B:844:ARG:N	5:B:2801:HOH:O	2.49	0.43
1:A:799:GLY:HA2	2:A:1101:Q6K:C34	2.48	0.43
1:B:775:PRO:O	1:B:853:HIS:NE2	2.41	0.43
1:A:917:PRO:CB	1:A:936:LEU:HD21	2.49	0.43
1:A:929:ILE:O	1:A:932:LYS:HB2	2.19	0.43
1:D:801:LEU:O	1:D:805:VAL:HG22	2.19	0.43
1:B:889:ILE:HG21	1:B:927:SER:HB3	1.99	0.43
1:D:754:LYS:O	1:D:758:GLU:HG2	2.18	0.43
1:C:836:LEU:HD21	1:C:862:ALA:HB1	2.01	0.42
1:C:783:ILE:HG22	1:C:791:LEU:HD23	2.01	0.42
1:C:901:TRP:CE3	1:C:954:TRP:HA	2.55	0.42
1:D:814:SER:HB2	1:D:982:LEU:HB2	2.01	0.42
1:D:953:CYS:O	1:D:961:ARG:HD3	2.20	0.42
1:C:746:GLU:HG3	1:C:790:GLN:NE2	2.35	0.42
1:C:849:LYS:HD2	1:C:853:HIS:CD2	2.55	0.42
1:D:951:ARG:HA	1:D:951:ARG:HD2	1.81	0.42
1:B:814:SER:OG	1:B:978:PRO:HB2	2.19	0.42
1:B:825:ALA:CB	1:B:968:ILE:HG13	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:874:ALA:HB2	1:B:894:TYR:CE1	2.54	0.42
1:D:827:GLY:HA3	1:D:856:ILE:HD12	2.01	0.42
1:D:850:THR:H	1:D:853:HIS:HB3	1.85	0.42
1:A:944:ILE:HG13	1:A:948:MET:HG2	2.01	0.42
1:C:840:ASP:OD2	1:C:845:ASN:ND2	2.51	0.42
1:C:839:ARG:HD3	1:C:861:LEU:O	2.20	0.42
1:B:783:ILE:HA	1:B:790:GLN:O	2.20	0.41
1:B:802:LEU:O	1:B:805:VAL:HG22	2.20	0.41
1:B:842:ALA:O	1:B:846:VAL:HG23	2.20	0.41
1:B:886:LEU:HD22	1:B:956:ILE:HD12	2.01	0.41
1:B:975:ALA:O	1:B:978:PRO:HD3	2.20	0.41
1:A:732:ILE:HG23	1:A:739:LYS:HG2	2.02	0.41
1:A:943:THR:HG23	1:A:981:TYR:O	2.21	0.41
1:B:717:VAL:HA	1:B:727:TYR:HA	2.03	0.41
1:A:801:LEU:HG	1:A:910:LEU:HD21	2.02	0.41
1:B:970:GLU:O	1:B:974:MET:HG3	2.20	0.41
1:D:785:LEU:HD23	1:D:785:LEU:HA	1.95	0.41
1:B:825:ALA:HB3	1:B:968:ILE:HG13	2.03	0.41
1:A:840:ASP:HB2	1:A:861:LEU:HD12	2.03	0.41
1:B:786:THR:CG2	1:B:787:SER:H	2.27	0.41
1:B:726:VAL:HA	1:B:744:ILE:O	2.21	0.41
1:B:874:ALA:HB2	1:B:894:TYR:HE1	1.86	0.41
1:A:732:ILE:HG12	1:A:739:LYS:HG2	2.03	0.40
1:B:841:LEU:HD23	1:B:903:TYR:CA	2.51	0.40
1:B:888:SER:O	1:B:892:ARG:HA	2.21	0.40
1:C:921:ILE:HA	1:C:922:PRO:HD3	1.90	0.40
1:C:798:PHE:HB2	1:C:848:VAL:O	2.21	0.40
1:D:926:ILE:HD13	1:D:926:ILE:HA	1.86	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	279/331 (84%)	258 (92%)	19 (7%)	2 (1%)	22	57
1	B	285/331 (86%)	266 (93%)	16 (6%)	3 (1%)	14	46
1	C	279/331 (84%)	269 (96%)	10 (4%)	0	100	100
1	D	273/331 (82%)	261 (96%)	11 (4%)	1 (0%)	34	69
All	All	1116/1324 (84%)	1054 (94%)	56 (5%)	6 (0%)	29	64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	840	ASP
1	A	876	GLY
1	B	737	LYS
1	A	715	ILE
1	B	716	LYS
1	D	715	ILE

### 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	248/289 (86%)	243 (98%)	5 (2%)	55	80
1	B	251/289 (87%)	246 (98%)	5 (2%)	55	80
1	C	248/289 (86%)	241 (97%)	7 (3%)	43	73
1	D	245/289 (85%)	241 (98%)	4 (2%)	62	84
All	All	992/1156 (86%)	971 (98%)	21 (2%)	53	79

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	709	GLU
1	A	760	LEU
1	A	787	SER
1	A	847	LEU
1	A	864	LEU

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Mol	Chain	Res	Type
1	B	732	ILE
1	B	778	CYS
1	B	793	THR
1	B	924	SER
1	B	960	SER
1	C	730	LEU
1	C	759	ILE
1	C	789	VAL
1	C	811	ASN
1	C	836	LEU
1	C	945	ASP
1	C	954	TRP
1	D	725	THR
1	D	878	LYS
1	D	879	VAL
1	D	881	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	756	ASN
1	A	776	HIS
1	A	811	ASN
1	A	896	HIS
1	A	897	GLN
1	B	790	GLN
1	B	819	ASN
1	B	845	ASN
1	B	938	GLN
1	C	701	GLN
1	C	790	GLN
1	C	811	ASN
1	C	938	GLN
1	D	811	ASN
1	D	815	GLN

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

11 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	EDO	B	2701	-	3,3,3	0.04	0	2,2,2	0.17	0
2	Q6K	A	1101	1	38,40,40	0.98	2 (5%)	50,56,56	1.98	13 (26%)
3	EDO	C	1102	-	3,3,3	0.06	0	2,2,2	0.19	0
4	CIT	B	2705	-	3,12,12	0.66	0	3,17,17	0.56	0
2	Q6K	B	2703	1	38,40,40	0.95	2 (5%)	50,56,56	1.86	10 (20%)
3	EDO	B	2702	-	3,3,3	0.07	0	2,2,2	0.10	0
3	EDO	B	2704	-	3,3,3	0.05	0	2,2,2	0.25	0
2	Q6K	C	1101	1	38,40,40	0.98	2 (5%)	50,56,56	1.89	12 (24%)
3	EDO	A	1102	-	3,3,3	0.05	0	2,2,2	0.16	0
3	EDO	B	2706	-	3,3,3	0.06	0	2,2,2	0.25	0
2	Q6K	D	2500	1	38,40,40	0.92	1 (2%)	50,56,56	1.79	10 (20%)

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	EDO	B	2701	-	-	0/1/1/1	-
2	Q6K	A	1101	1	-	10/21/25/25	0/4/4/4
3	EDO	C	1102	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	B	2705	-	-	1/6/16/16	-
2	Q6K	B	2703	1	-	7/21/25/25	0/4/4/4
3	EDO	B	2702	-	-	1/1/1/1	-
3	EDO	B	2704	-	-	1/1/1/1	-
2	Q6K	C	1101	1	-	9/21/25/25	0/4/4/4
3	EDO	A	1102	-	-	1/1/1/1	-
3	EDO	B	2706	-	-	1/1/1/1	-
2	Q6K	D	2500	1	-	9/21/25/25	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	Q6K	C10-C11	-3.96	1.43	1.49
2	A	1101	Q6K	C10-C11	-3.79	1.44	1.49
2	B	2703	Q6K	C10-C11	-3.65	1.44	1.49
2	D	2500	Q6K	C10-C11	-3.42	1.44	1.49
2	A	1101	Q6K	C13-N14	2.15	1.40	1.36
2	B	2703	Q6K	C13-N14	2.04	1.40	1.36
2	C	1101	Q6K	C13-N14	2.00	1.40	1.36

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	Q6K	C18-O17-C16	-8.32	104.96	117.53
2	C	1101	Q6K	C18-O17-C16	-7.85	105.69	117.53
2	B	2703	Q6K	C18-O17-C16	-7.83	105.71	117.53
2	D	2500	Q6K	C18-O17-C16	-7.59	106.08	117.53
2	A	1101	Q6K	N35-C13-N12	-4.05	122.71	126.55
2	C	1101	Q6K	N35-C13-N12	-3.46	123.27	126.55
2	D	2500	Q6K	C11-C10-C04	3.44	130.62	123.90
2	B	2703	Q6K	N35-C13-N12	-3.40	123.32	126.55
2	A	1101	Q6K	C36-C37-C11	-3.38	114.03	117.22
2	B	2703	Q6K	C11-C10-C04	3.31	130.38	123.90
2	B	2703	Q6K	O17-C16-C15	3.18	118.70	114.80
2	D	2500	Q6K	N35-C13-N12	-3.15	123.56	126.55
2	D	2500	Q6K	C19-C20-N21	-3.05	116.82	120.93
2	C	1101	Q6K	C36-C37-C11	-3.01	114.38	117.22
2	A	1101	Q6K	C19-C20-N21	-2.97	116.93	120.93
2	D	2500	Q6K	O17-C16-C15	2.95	118.42	114.80
2	C	1101	Q6K	C19-C20-N21	-2.83	117.12	120.93
2	C	1101	Q6K	C11-C10-C04	2.79	129.35	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2703	Q6K	C36-C37-C11	-2.78	114.60	117.22
2	C	1101	Q6K	O17-C16-C15	2.73	118.15	114.80
2	B	2703	Q6K	O17-C16-C19	-2.72	119.44	124.12
2	C	1101	Q6K	C34-C15-N14	2.71	126.68	121.05
2	B	2703	Q6K	O33-C30-N29	2.70	128.55	123.63
2	D	2500	Q6K	C22-N21-C20	-2.68	108.52	115.89
2	A	1101	Q6K	C34-C15-N14	2.67	126.59	121.05
2	A	1101	Q6K	C11-C10-C04	2.66	129.09	123.90
2	A	1101	Q6K	O17-C16-C15	2.62	118.01	114.80
2	C	1101	Q6K	C22-N21-C20	-2.60	108.74	115.89
2	A	1101	Q6K	C36-N35-C13	2.51	117.68	115.45
2	A	1101	Q6K	O17-C16-C19	-2.51	119.81	124.12
2	A	1101	Q6K	C19-C20-C28	-2.50	116.34	120.04
2	A	1101	Q6K	O33-C30-N29	2.50	128.19	123.63
2	D	2500	Q6K	C36-C37-C11	-2.48	114.88	117.22
2	C	1101	Q6K	O17-C16-C19	-2.40	119.99	124.12
2	C	1101	Q6K	C36-N35-C13	2.39	117.57	115.45
2	B	2703	Q6K	C22-N21-C20	-2.36	109.39	115.89
2	D	2500	Q6K	O17-C16-C19	-2.36	120.06	124.12
2	C	1101	Q6K	O33-C30-N29	2.34	127.89	123.63
2	B	2703	Q6K	C36-N35-C13	2.27	117.47	115.45
2	B	2703	Q6K	C19-C20-N21	-2.09	118.11	120.93
2	D	2500	Q6K	O33-C30-N29	2.08	127.43	123.63
2	A	1101	Q6K	C22-N21-C20	-2.02	110.33	115.89
2	C	1101	Q6K	C19-C20-C28	-2.01	117.07	120.04
2	A	1101	Q6K	C34-C15-C16	-2.01	116.48	118.91
2	D	2500	Q6K	C36-N35-C13	2.00	117.23	115.45

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	Q6K	C19-C20-N21-C22
2	B	2703	Q6K	C19-C20-N21-C23
2	D	2500	Q6K	C15-C16-O17-C18
2	A	1101	Q6K	C15-C16-O17-C18
2	C	1101	Q6K	C15-C16-O17-C18
2	D	2500	Q6K	C31-C30-N29-C28
2	D	2500	Q6K	C19-C16-O17-C18
2	B	2703	Q6K	C19-C16-O17-C18
2	A	1101	Q6K	C19-C16-O17-C18
2	C	1101	Q6K	C19-C16-O17-C18

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Mol	Chain	Res	Type	Atoms
2	B	2703	Q6K	C15-C16-O17-C18
2	D	2500	Q6K	O33-C30-N29-C28
3	B	2702	EDO	O1-C1-C2-O2
2	A	1101	Q6K	N21-C23-C24-N25
2	C	1101	Q6K	C28-C20-N21-C23
2	D	2500	Q6K	C28-C20-N21-C22
2	C	1101	Q6K	C23-C24-N25-C26
2	C	1101	Q6K	C23-C24-N25-C27
2	D	2500	Q6K	C23-C24-N25-C27
3	A	1102	EDO	O1-C1-C2-O2
2	D	2500	Q6K	C23-C24-N25-C26
2	A	1101	Q6K	C28-C20-N21-C22
2	A	1101	Q6K	C23-C24-N25-C26
2	A	1101	Q6K	C19-C20-N21-C23
2	C	1101	Q6K	C19-C20-N21-C22
2	C	1101	Q6K	C19-C20-N21-C23
2	D	2500	Q6K	C19-C20-N21-C22
4	B	2705	CIT	C1-C2-C3-C6
2	A	1101	Q6K	C23-C24-N25-C27
3	B	2704	EDO	O1-C1-C2-O2
2	A	1101	Q6K	C28-C20-N21-C23
2	B	2703	Q6K	N21-C23-C24-N25
2	C	1101	Q6K	C28-C20-N21-C22
2	C	1101	Q6K	N21-C23-C24-N25
3	B	2706	EDO	O1-C1-C2-O2
2	A	1101	Q6K	C24-C23-N21-C22
2	B	2703	Q6K	C24-C23-N21-C22
2	D	2500	Q6K	C34-C15-N14-C13
2	B	2703	Q6K	C28-C20-N21-C22
2	B	2703	Q6K	C19-C20-N21-C22

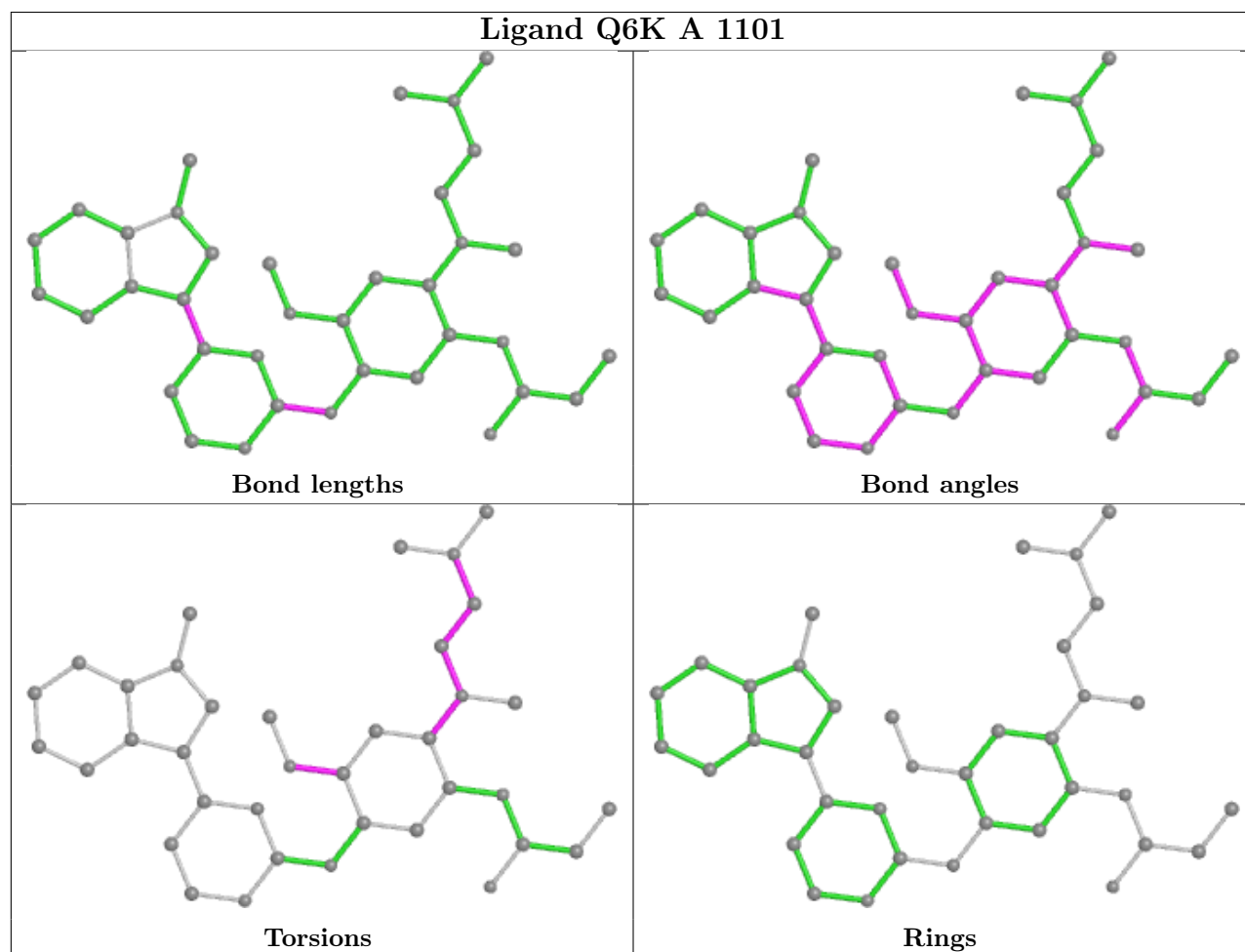
There are no ring outliers.

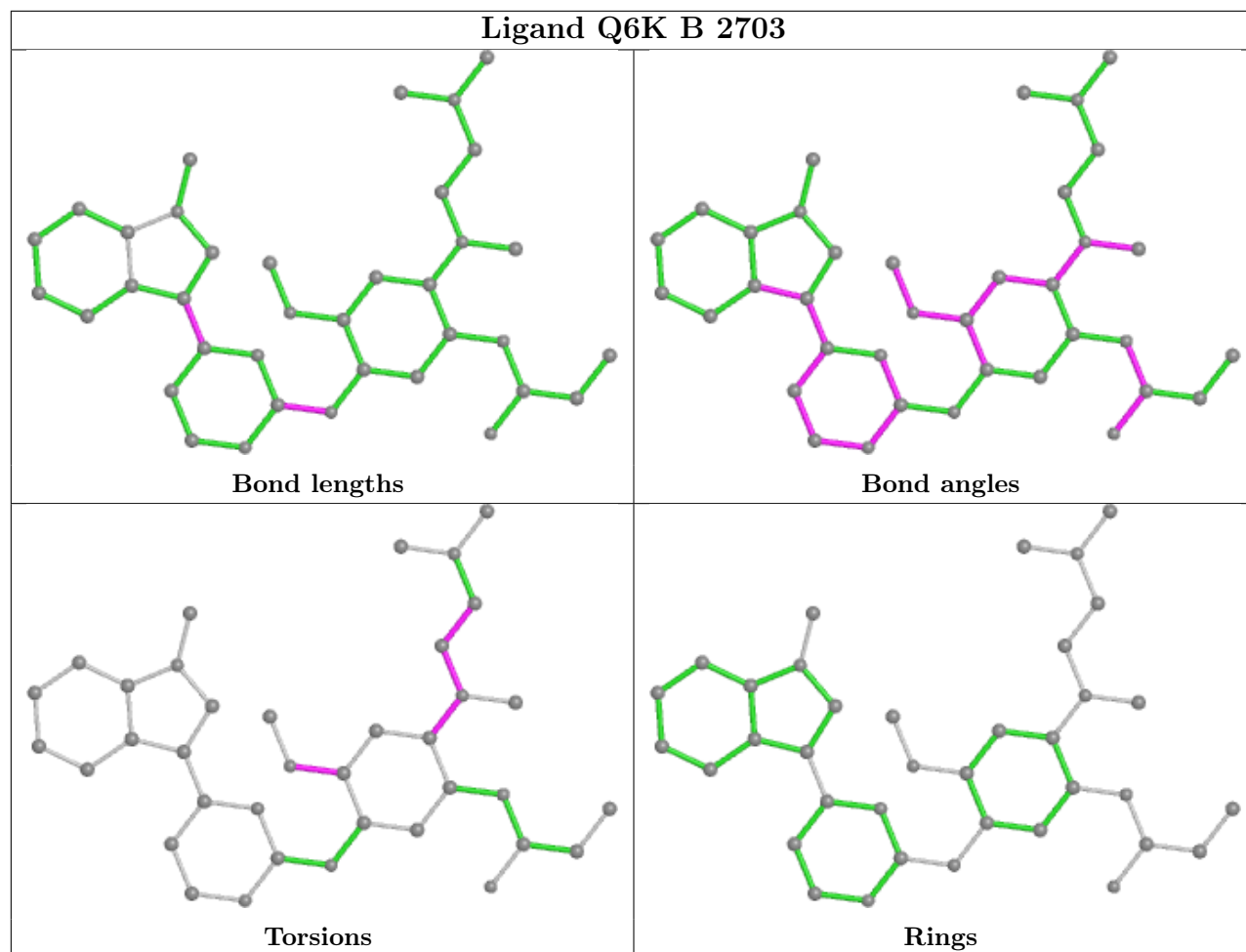
5 monomers are involved in 13 short contacts:

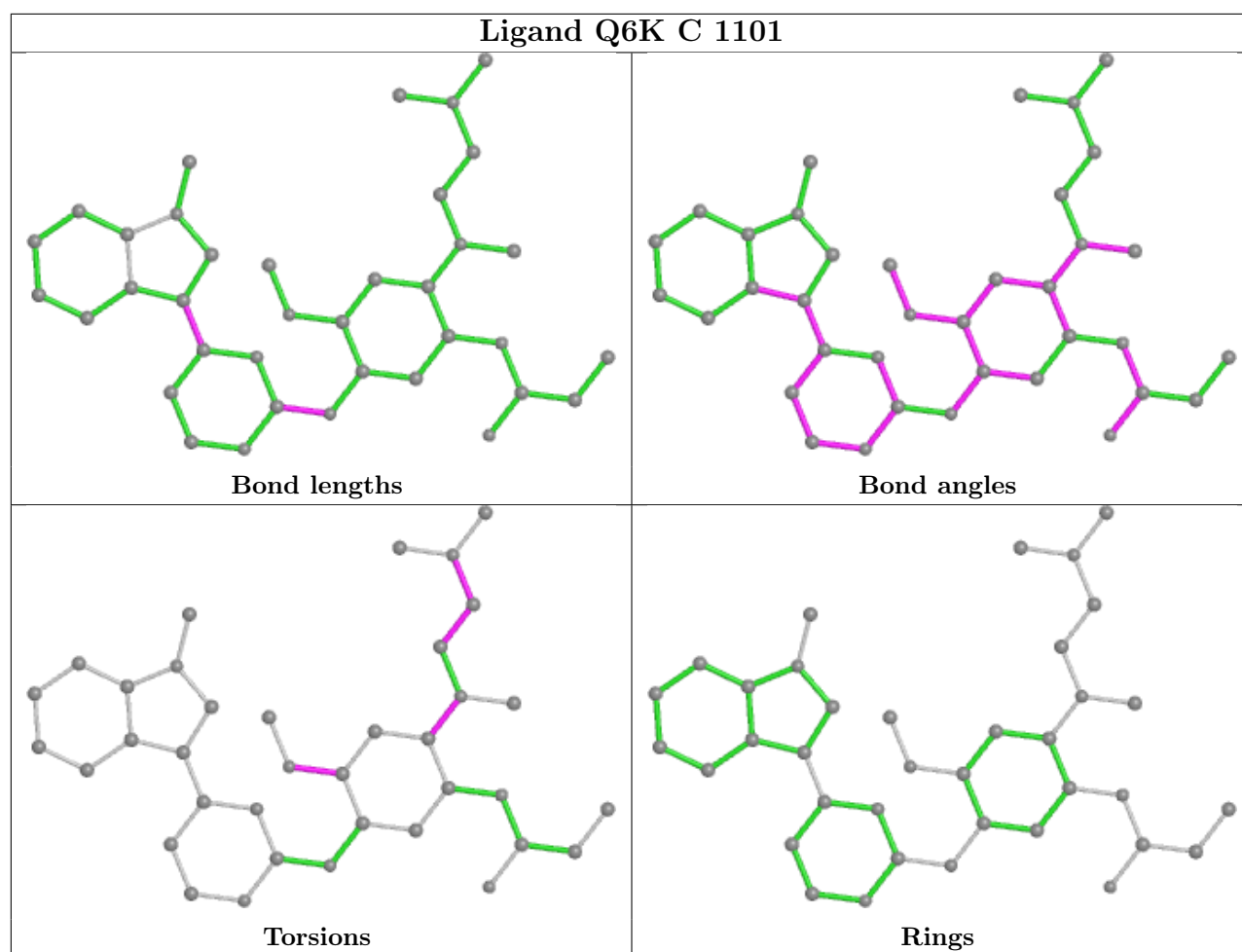
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	Q6K	3	0
4	B	2705	CIT	1	0
2	B	2703	Q6K	4	0
2	C	1101	Q6K	3	0
2	D	2500	Q6K	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

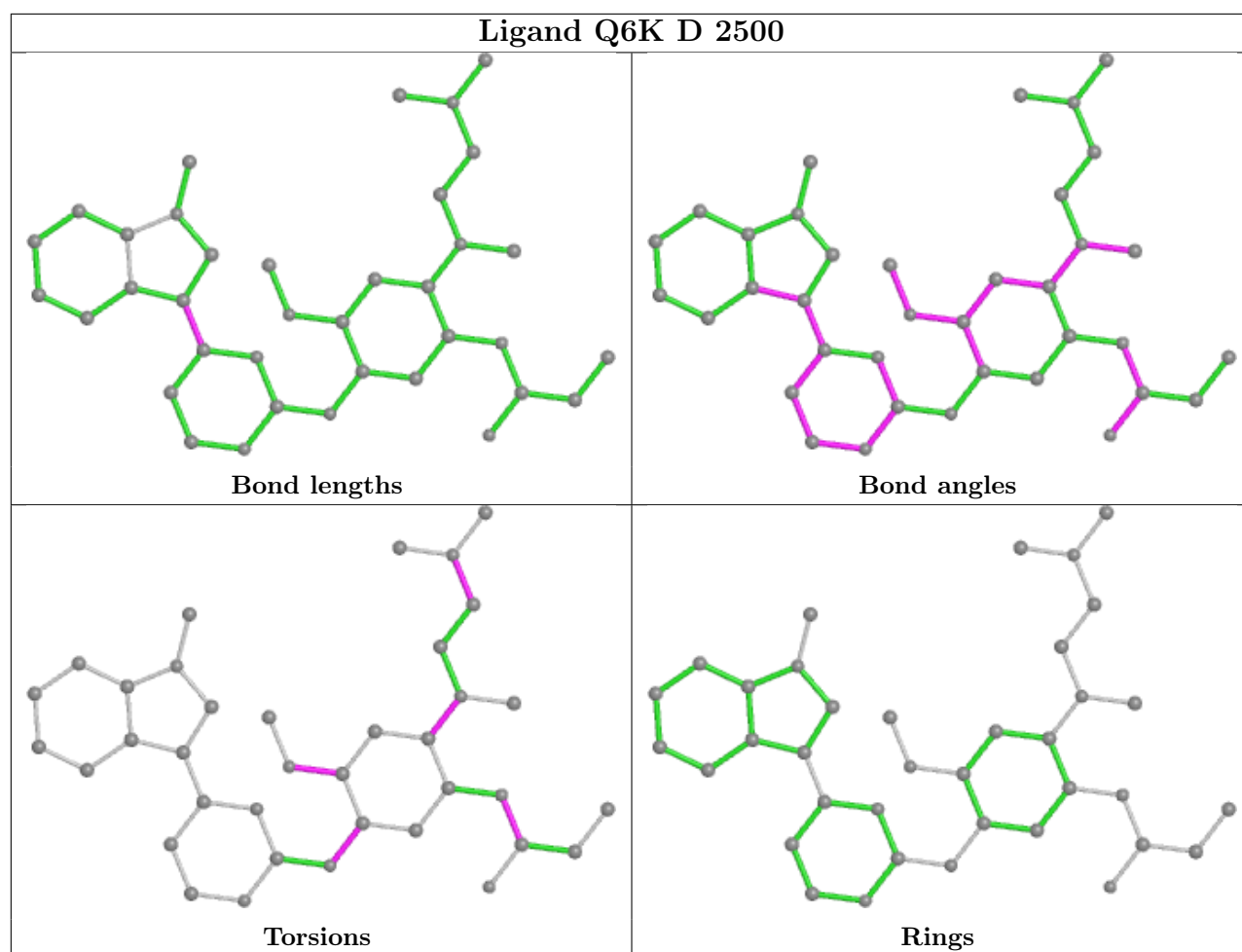
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	283/331 (85%)	-0.28	1 (0%) 92 84	43, 67, 107, 142	0
1	B	286/331 (86%)	-0.28	0 100 100	43, 71, 108, 151	0
1	C	283/331 (85%)	-0.12	3 (1%) 80 64	62, 91, 124, 156	0
1	D	279/331 (84%)	-0.12	6 (2%) 62 41	65, 97, 134, 149	0
All	All	1131/1324 (85%)	-0.20	10 (0%) 84 69	43, 83, 125, 156	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	737	LYS	3.3
1	D	798	PHE	3.1
1	A	737	LYS	2.7
1	D	941	ILE	2.5
1	C	851	PRO	2.5
1	D	910	LEU	2.4
1	C	717	VAL	2.1
1	D	812	ILE	2.0
1	D	820	TRP	2.0
1	D	942	CYS	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 monosaccharides in this entry.

## 6.4 Ligands

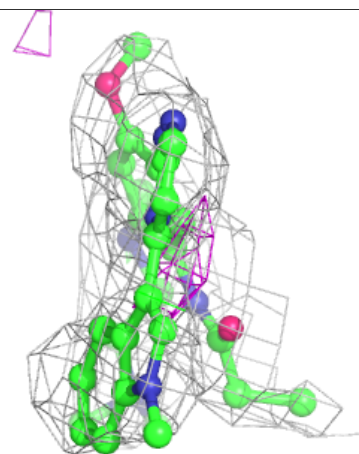
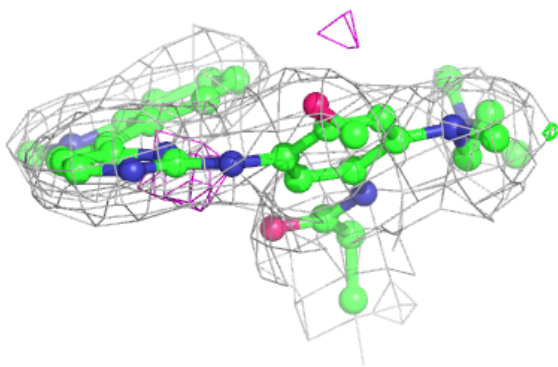
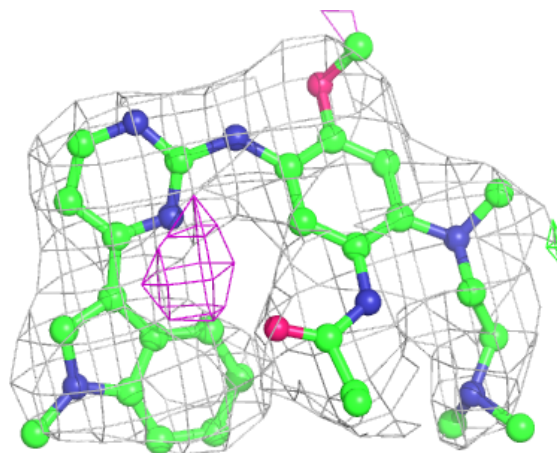
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	EDO	B	2706	4/4	0.86	0.18	61,64,65,66	0
3	EDO	B	2704	4/4	0.88	0.22	73,73,73,75	0
4	CIT	B	2705	13/13	0.88	0.16	67,80,83,84	0
3	EDO	B	2701	4/4	0.89	0.20	56,57,58,58	0
2	Q6K	A	1101	37/37	0.93	0.26	61,66,80,82	0
3	EDO	C	1102	4/4	0.93	0.12	72,72,72,72	0
2	Q6K	D	2500	37/37	0.93	0.27	86,111,121,123	0
3	EDO	A	1102	4/4	0.94	0.12	47,48,49,49	0
2	Q6K	B	2703	37/37	0.94	0.24	54,66,88,90	0
2	Q6K	C	1101	37/37	0.95	0.25	84,93,116,118	0
3	EDO	B	2702	4/4	0.96	0.16	50,51,51,51	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.

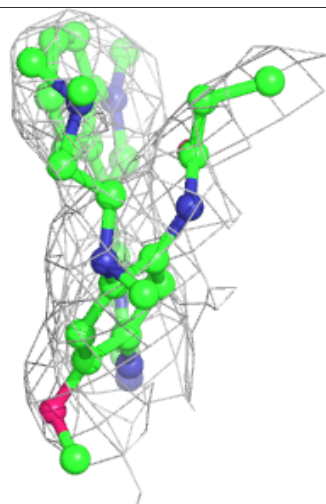
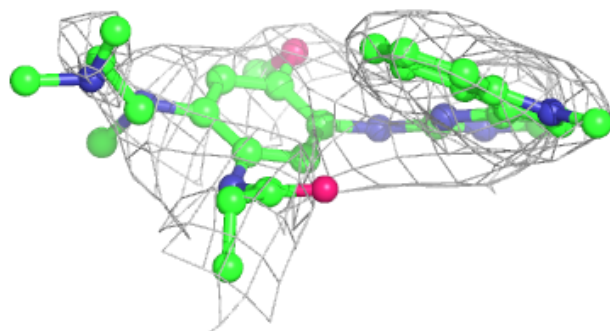
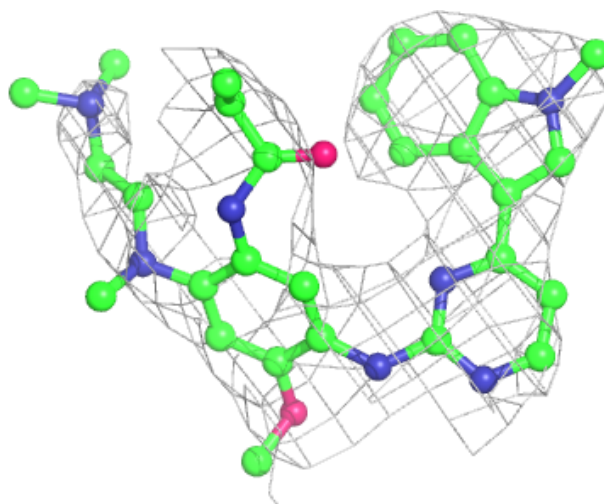
**Electron density around Q6K A 1101:**

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



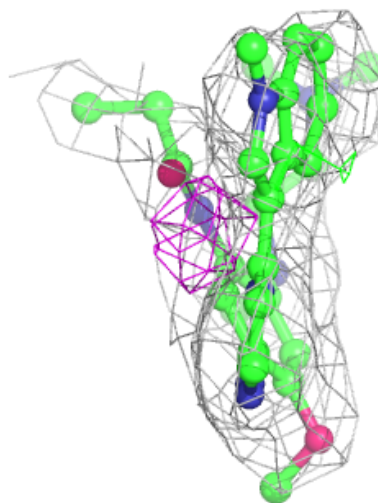
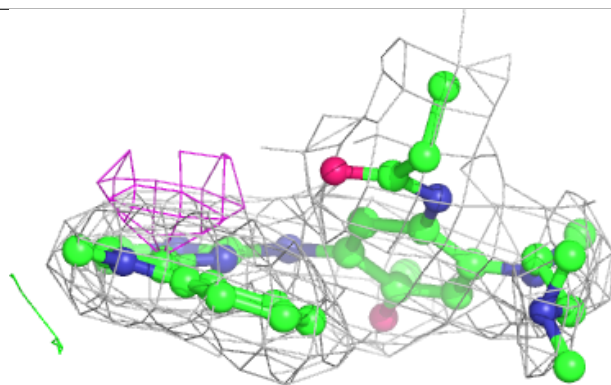
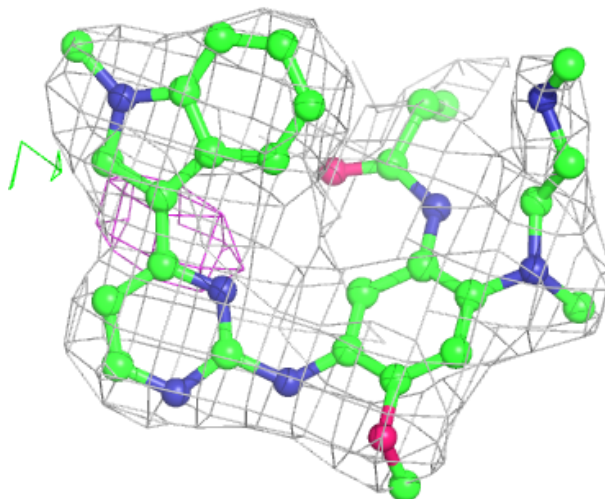
**Electron density around Q6K D 2500:**

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



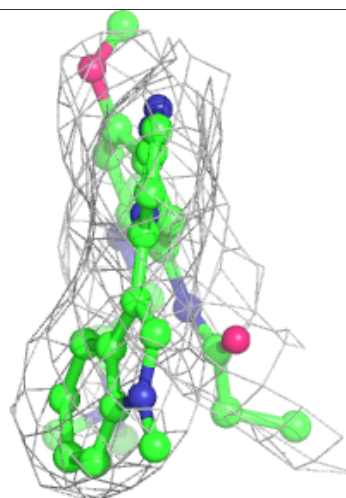
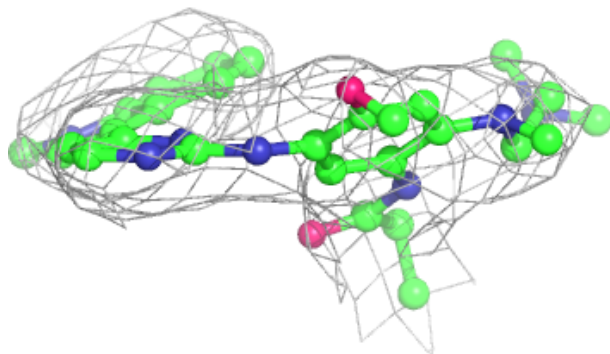
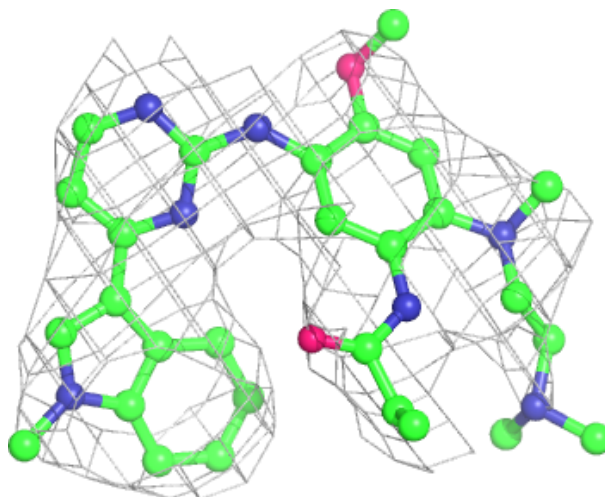
**Electron density around Q6K B 2703:**

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



**Electron density around Q6K C 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.