



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2021 – 06:03 PM EST

PDB ID : 6WA2
Title : Crystal structure of EGFR(T790M/V948R) in complex with LN3753
Authors : Heppner, D.E.; Eck, M.J.
Deposited on : 2020-03-24
Resolution : 2.40 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 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 : 2.23.2
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) : 2.23.2

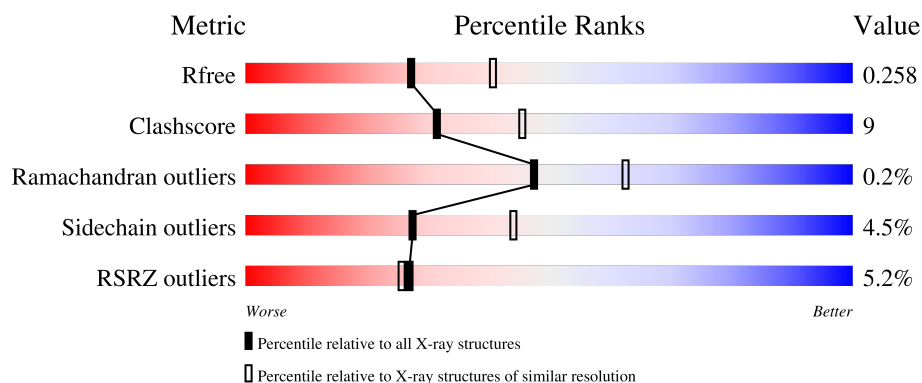
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	 3% 77% 14% • 8%
1	B	328	 4% 77% 17% • •
1	C	328	 9% 71% 18% • 9%
1	D	328	 4% 80% 14% • •

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	1302	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10285 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.

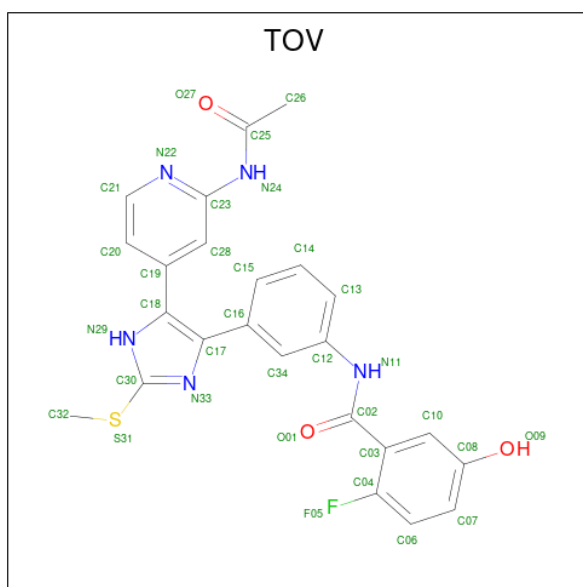
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	314	Total	C	N	O	S	0	1	0
			2530	1619	428	464	19			
1	A	302	Total	C	N	O	S	0	1	0
			2434	1562	413	440	19			
1	B	314	Total	C	N	O	S	0	1	0
			2527	1617	428	463	19			
1	C	300	Total	C	N	O	S	0	1	0
			2420	1552	410	439	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-fluoro-5-hydroxybenzamide (three-letter code: TOV) (formula: C₂₄H₂₀FN₅O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	F	N	O	S	
			34	24	1	5	3	1	0
2	A	1	Total	C	F	N	O	S	
			34	24	1	5	3	1	0
2	B	1	Total	C	F	N	O	S	
			34	24	1	5	3	1	0
2	C	1	Total	C	F	N	O	S	
			34	24	1	5	3	1	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total 1 Cl	0	0
3	B	1	Total 1 Cl	0	0
3	C	1	Total 1 Cl	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	56	Total 56 O	0	0
4	A	57	Total 57 O	0	0

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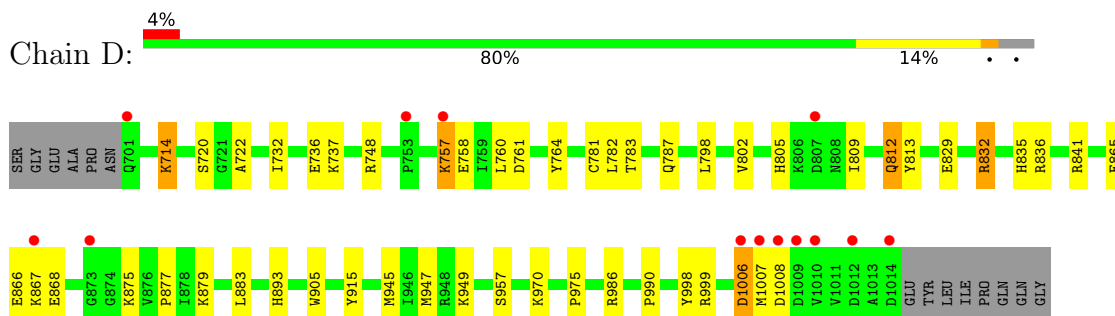
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	69	Total	O	0	0
			69	69		
4	C	53	Total	O	0	0
			53	53		

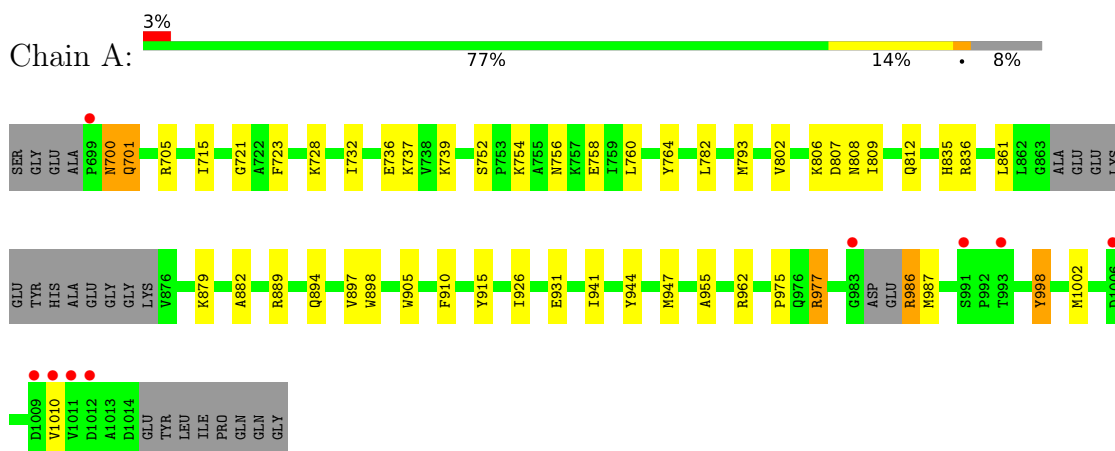
3 Residue-property plots [i](#)

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.

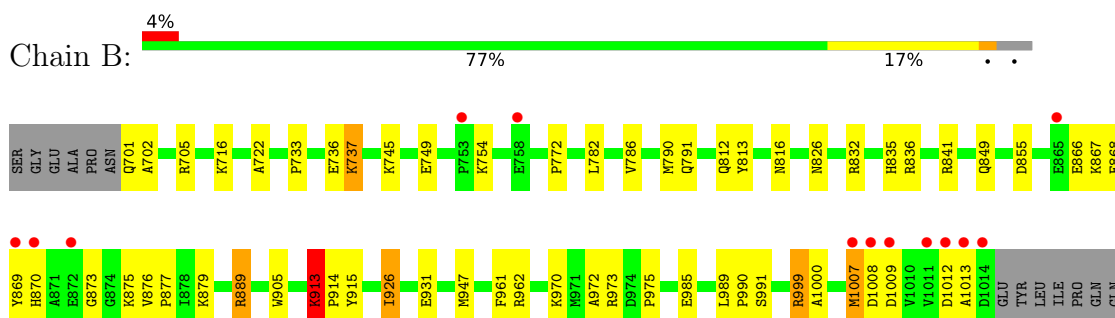
- Molecule 1: Epidermal growth factor receptor



- Molecule 1: Epidermal growth factor receptor

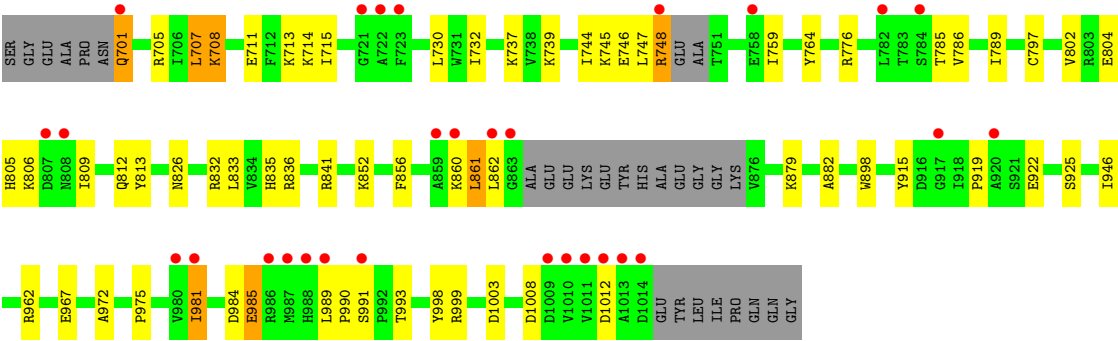


- Molecule 1: Epidermal growth factor receptor



GLY

● 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	71.36Å 102.47Å 87.68Å 90.00° 102.54° 90.00°	Depositor
Resolution (Å)	69.66 – 2.40 69.66 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.5 (69.66-2.40) 88.9 (69.66-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.41 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.221 , 0.258 0.221 , 0.258	Depositor DCC
R_{free} test set	2270 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10285	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8015e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TOV, CL

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	0.42	1/2486 (0.0%)	0.56	0/3361
1	B	0.37	1/2582 (0.0%)	0.51	0/3491
1	C	0.44	1/2471 (0.0%)	0.65	0/3340
1	D	0.39	0/2585	0.54	0/3495
All	All	0.41	3/10124 (0.0%)	0.57	0/13687

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	913	LYS	C-N	8.81	1.50	1.34
1	C	991	SER	C-N	7.36	1.48	1.34
1	A	752	SER	C-N	7.28	1.48	1.34

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	2434	0	2476	49	0
1	B	2527	0	2555	53	0
1	C	2420	0	2454	56	0
1	D	2530	0	2556	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	34	0	0	1	0
2	B	34	0	0	1	0
2	C	34	0	0	0	0
2	D	34	0	0	0	0
3	A	1	0	0	2	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	57	0	0	2	0
4	B	69	0	0	2	0
4	C	53	0	0	2	0
4	D	56	0	0	1	0
All	All	10285	0	10041	180	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 9.

All (180) 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:861:LEU:HD23	1:C:862:LEU:HG	1.30	1.13
1:D:832:ARG:HH21	1:D:832:ARG:HB3	1.12	1.11
1:A:809:ILE:O	1:A:986:ARG:HG3	1.48	1.11
1:C:748:ARG:HG3	1:C:748:ARG:HH21	1.19	1.03
1:C:981:ILE:HB	1:C:984:ASP:HB2	1.47	0.97
1:A:700:ASN:HD22	1:A:700:ASN:H	1.10	0.96
1:B:737:LYS:HE3	1:C:804:GLU:OE2	1.65	0.95
1:C:747:LEU:HD13	1:C:862:LEU:CD1	1.99	0.92
1:A:701:GLN:HG3	1:A:764:TYR:CE1	2.07	0.89
1:C:861:LEU:CD2	1:C:862:LEU:HG	2.05	0.87
1:A:754:LYS:HD3	1:A:758:GLU:OE1	1.77	0.84
1:C:861:LEU:HD23	1:C:862:LEU:CG	2.10	0.82
1:D:832:ARG:HB3	1:D:832:ARG:NH2	1.95	0.81
1:A:809:ILE:O	1:A:986:ARG:CG	2.29	0.80
1:C:747:LEU:HD13	1:C:862:LEU:HD13	1.62	0.80
1:B:913:LYS:HE2	1:B:914:PRO:HD2	1.63	0.79
1:C:946:ILE:HD11	1:C:967:GLU:OE2	1.83	0.79
1:D:758:GLU:HA	1:D:761:ASP:HB2	1.66	0.77
1:D:832:ARG:HH21	1:D:832:ARG:CB	1.97	0.76
1:A:977:ARG:O	1:A:977:ARG:HG3	1.85	0.76
1:A:700:ASN:HD22	1:A:700:ASN:N	1.85	0.75
1:C:747:LEU:HB2	1:C:786:VAL:HG23	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:720:SER:CB	1:B:832:ARG:NH1	2.50	0.74
1:B:889:ARG:HH11	1:B:889:ARG:CG	2.01	0.74
1:A:701:GLN:HG3	1:A:764:TYR:CZ	2.23	0.73
1:A:701:GLN:CG	1:A:764:TYR:CZ	2.71	0.73
1:B:913:LYS:HD3	1:B:914:PRO:HD2	1.71	0.73
1:C:746:GLU:HG3	1:C:785:THR:HG21	1.70	0.73
1:A:806:LYS:O	1:A:986:ARG:NH2	2.21	0.72
1:C:705:ARG:NH1	1:C:707:LEU:HD13	2.05	0.72
1:C:713:LYS:HD2	1:C:714:LYS:N	2.05	0.71
1:B:812:GLN:HG2	1:B:975:PRO:HG3	1.72	0.71
1:D:865:GLU:HG3	1:D:868:GLU:HG2	1.72	0.70
1:B:913:LYS:CE	1:B:914:PRO:HD2	2.22	0.70
1:C:747:LEU:HD12	1:C:786:VAL:CG2	2.21	0.70
1:C:732:ILE:HG12	1:C:739:LYS:HD3	1.76	0.68
1:D:720:SER:CB	1:B:832:ARG:HH12	2.05	0.68
1:C:981:ILE:HB	1:C:984:ASP:CB	2.23	0.67
1:B:812:GLN:NE2	1:B:972:ALA:O	2.28	0.67
1:C:879:LYS:HD3	1:C:915:TYR:HB2	1.76	0.66
1:C:759:ILE:HD13	1:C:786:VAL:HG11	1.76	0.66
1:A:812:GLN:HG2	1:A:975:PRO:HG3	1.78	0.65
1:C:748:ARG:HG3	1:C:748:ARG:NH2	1.97	0.65
1:A:754:LYS:CD	1:A:758:GLU:OE1	2.44	0.65
1:B:913:LYS:CD	1:B:914:PRO:HD2	2.27	0.65
1:C:747:LEU:HD13	1:C:862:LEU:HD11	1.79	0.64
1:D:720:SER:HB2	1:B:832:ARG:NH1	2.14	0.62
1:C:701:GLN:HB3	1:C:764:TYR:CE1	2.33	0.62
1:D:714:LYS:NZ	4:D:1402:HOH:O	2.32	0.62
1:A:701:GLN:CG	1:A:764:TYR:CE1	2.81	0.62
1:D:879:LYS:HD3	1:D:915:TYR:HB2	1.82	0.61
1:B:790:MET:HG2	1:B:791:GLN:N	2.15	0.61
1:D:999:ARG:HH22	1:D:1006:ASP:HA	1.66	0.60
1:B:745:LYS:NZ	1:B:855:ASP:OD2	2.34	0.60
1:B:866:GLU:OE2	1:B:870:HIS:NE2	2.31	0.60
1:C:852:LYS:NZ	4:C:1304:HOH:O	2.33	0.60
1:A:701:GLN:HG2	1:A:764:TYR:CZ	2.37	0.59
1:B:913:LYS:HD3	1:B:914:PRO:CD	2.32	0.59
1:A:808:ASN:O	1:A:987:MET:HG2	2.04	0.58
1:D:805:HIS:O	1:D:809:ILE:HG13	2.04	0.58
1:A:736:GLU:HA	1:A:736:GLU:OE1	2.04	0.58
1:B:772:PRO:HB3	1:B:1007:MET:HG2	1.86	0.58
1:B:737:LYS:O	1:B:737:LYS:HG3	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:LYS:HE3	1:A:861:LEU:O	2.03	0.57
1:A:732:ILE:HG12	1:A:739:LYS:HG2	1.86	0.57
1:B:889:ARG:HH11	1:B:889:ARG:HG2	1.67	0.57
1:D:722:ALA:O	1:D:748:ARG:NE	2.38	0.57
1:B:926:ILE:HG23	1:B:931:GLU:HB2	1.88	0.56
1:B:879:LYS:HD3	1:B:915:TYR:HB2	1.88	0.55
1:C:715:ILE:HG13	1:C:730:LEU:HG	1.88	0.55
1:A:807:ASP:HA	1:A:986:ARG:NH2	2.21	0.55
1:D:732:ILE:HD11	1:D:736:GLU:O	2.07	0.55
1:A:756:ASN:HD22	1:A:782:LEU:HD21	1.71	0.55
1:B:812:GLN:OE1	1:B:816:ASN:ND2	2.39	0.55
1:C:747:LEU:HD12	1:C:786:VAL:HG21	1.89	0.55
1:C:999:ARG:HA	1:C:1003:ASP:HB3	1.89	0.55
1:A:700:ASN:H	1:A:700:ASN:ND2	1.93	0.54
1:D:945:MET:O	1:D:949:LYS:HG3	2.07	0.54
1:A:793:MET:O	2:A:1301:TOV:N24	2.41	0.54
1:B:869:TYR:CD2	1:B:876:VAL:HG11	2.42	0.54
1:B:985:GLU:OE1	1:B:985:GLU:N	2.38	0.54
1:A:701:GLN:HG2	1:A:764:TYR:OH	2.08	0.53
1:C:836:ARG:CZ	1:C:860:LYS:HG3	2.39	0.53
1:C:746:GLU:CG	1:C:785:THR:HG21	2.36	0.53
1:D:760:LEU:O	1:D:764:TYR:CD2	2.62	0.53
1:A:808:ASN:O	1:A:986:ARG:HB2	2.09	0.53
1:A:926:ILE:HG23	1:A:931:GLU:HB2	1.91	0.52
1:B:701:GLN:N	4:B:1307:HOH:O	2.42	0.52
1:C:985:GLU:H	1:C:985:GLU:CD	2.12	0.52
1:C:826:ASN:ND2	4:C:1301:HOH:O	2.38	0.52
1:C:747:LEU:CD1	1:C:862:LEU:HD11	2.39	0.52
1:A:894:GLN:HA	1:A:894:GLN:OE1	2.08	0.52
1:A:894:GLN:CG	1:A:955:ALA:O	2.58	0.52
1:C:812:GLN:CG	1:C:975:PRO:HG3	2.39	0.52
1:D:841:ARG:HH12	1:D:877:PRO:HB3	1.74	0.51
1:C:813:TYR:OH	1:C:990:PRO:HD3	2.10	0.51
1:D:1007:MET:HG2	1:D:1008:ASP:N	2.26	0.51
1:B:867:LYS:O	1:B:867:LYS:HD3	2.11	0.50
1:A:802:VAL:HG22	1:A:910:PHE:HA	1.94	0.50
1:A:808:ASN:O	1:A:986:ARG:CB	2.60	0.50
1:A:879:LYS:HD3	1:A:915:TYR:HB2	1.94	0.50
1:C:707:LEU:HD12	1:C:711:GLU:OE2	2.12	0.50
1:B:835:HIS:O	1:B:836:ARG:HB2	2.12	0.49
1:C:812:GLN:NE2	1:C:972:ALA:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:865:GLU:HG3	1:D:868:GLU:CG	2.40	0.49
1:C:747:LEU:CD1	1:C:862:LEU:CD1	2.83	0.49
1:C:835:HIS:O	1:C:836:ARG:HB2	2.13	0.49
1:A:809:ILE:C	1:A:986:ARG:HG3	2.28	0.48
1:B:813:TYR:OH	1:B:990:PRO:HD3	2.13	0.48
1:D:812:GLN:HG2	1:D:975:PRO:HG3	1.96	0.48
1:A:721:GLY:HA3	3:A:1302:CL:CL	2.50	0.48
1:D:835:HIS:O	1:D:836:ARG:HB2	2.14	0.48
1:B:866:GLU:OE1	1:B:889:ARG:NH2	2.47	0.47
1:C:989:LEU:HB2	1:C:990:PRO:HD2	1.95	0.47
1:D:714:LYS:HE3	1:D:787:GLN:OE1	2.14	0.47
1:A:756:ASN:ND2	1:A:782:LEU:HD21	2.30	0.47
1:B:1000:ALA:HB2	1:C:776:ARG:HH21	1.80	0.47
1:A:835:HIS:O	1:A:836:ARG:HB2	2.15	0.46
1:B:790:MET:HE3	2:B:1202:TOV:C12	2.46	0.46
1:C:713:LYS:HD2	1:C:714:LYS:H	1.79	0.46
1:D:798:LEU:O	1:D:802:VAL:HG22	2.15	0.46
1:B:733:PRO:HB2	1:B:736:GLU:CG	2.46	0.46
1:D:905:TRP:HD1	1:D:947:MET:HE1	1.81	0.46
1:B:889:ARG:HH11	1:B:889:ARG:HG3	1.80	0.46
1:B:905:TRP:HD1	1:B:947:MET:HE1	1.81	0.45
1:C:747:LEU:HB2	1:C:786:VAL:CG2	2.41	0.45
1:A:715:ILE:HG12	1:A:728:LYS:O	2.17	0.45
1:B:813:TYR:CE2	1:B:989:LEU:HD23	2.52	0.45
1:A:723:PHE:HB2	3:A:1302:CL:CL	2.54	0.45
1:A:962:ARG:HE	1:A:962:ARG:HB3	1.57	0.45
1:B:913:LYS:HB2	1:B:913:LYS:HE3	1.71	0.45
1:C:744:ILE:HG12	1:C:789:ILE:HG13	1.99	0.44
1:A:879:LYS:HB3	1:A:915:TYR:HD2	1.83	0.44
1:D:757:LYS:O	1:D:760:LEU:HB2	2.17	0.44
1:A:700:ASN:N	1:A:700:ASN:ND2	2.60	0.44
1:B:999:ARG:NH2	4:B:1310:HOH:O	2.49	0.44
1:C:785:THR:HG22	1:C:786:VAL:N	2.32	0.44
1:A:705:ARG:NH1	4:A:1403:HOH:O	2.33	0.44
1:C:812:GLN:HG2	1:C:975:PRO:HG3	1.99	0.44
1:A:905:TRP:HD1	1:A:947:MET:HE1	1.83	0.44
1:A:941:ILE:HD12	1:A:944:TYR:HB3	2.00	0.44
1:C:747:LEU:HD12	1:C:786:VAL:HG23	2.00	0.44
1:C:919:PRO:HD2	1:C:922[A]:GLU:OE1	2.18	0.44
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.53	0.43
1:C:805:HIS:O	1:C:809:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:813:TYR:OH	1:D:990:PRO:HD3	2.18	0.43
1:A:1010:VAL:HG23	4:A:1425:HOH:O	2.18	0.43
1:C:732:ILE:HG12	1:C:739:LYS:CD	2.47	0.43
1:B:841:ARG:HH12	1:B:877:PRO:HB3	1.83	0.43
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.53	0.43
1:B:826:ASN:HB2	1:B:961:PHE:HB3	2.01	0.43
1:B:973:ARG:HA	1:B:1013:ALA:HA	2.01	0.43
1:B:705:ARG:HD3	1:C:993:THR:HG22	2.01	0.43
1:B:782:LEU:HD23	1:B:786:VAL:HG13	2.01	0.43
1:A:894:GLN:O	1:A:897:VAL:HB	2.20	0.42
1:C:812:GLN:OE1	1:C:1012:ASP:OD1	2.37	0.42
1:A:894:GLN:HG2	1:A:955:ALA:O	2.19	0.42
1:A:894:GLN:NE2	1:A:955:ALA:O	2.47	0.42
1:B:754:LYS:HA	1:B:754:LYS:HD3	1.80	0.42
1:A:998:TYR:O	1:A:1002:MET:HB2	2.20	0.41
1:B:989:LEU:HB3	1:B:990:PRO:HD2	2.02	0.41
1:C:802:VAL:HA	1:C:809:ILE:HD11	2.02	0.41
1:B:722:ALA:HB1	1:B:875:LYS:HA	2.01	0.41
1:D:720:SER:HB3	1:B:832:ARG:NH1	2.32	0.41
1:B:733:PRO:HB2	1:B:736:GLU:HG3	2.02	0.41
1:C:797:CYS:SG	1:C:841:ARG:HA	2.60	0.41
1:D:760:LEU:HG	1:D:782:LEU:HD11	2.03	0.41
1:C:708:LYS:HB2	1:C:708:LYS:HE2	1.71	0.41
1:B:832:ARG:HA	1:B:832:ARG:HD3	1.95	0.41
1:B:1012:ASP:OD1	1:B:1013:ALA:N	2.52	0.41
1:C:748:ARG:NH2	1:C:748:ARG:CG	2.72	0.41
1:A:987:MET:HG3	1:A:987:MET:O	2.21	0.40
1:B:702:ALA:O	1:C:993:THR:HA	2.21	0.40
1:B:868:GLU:HG3	1:B:876:VAL:HG23	2.03	0.40
1:C:833:LEU:HD13	1:C:856:PHE:CE2	2.55	0.40
1:D:829:GLU:HA	1:D:893:HIS:CE1	2.57	0.40
1:B:841:ARG:NH1	1:B:877:PRO:HB3	2.37	0.40
1:D:781:CYS:SG	1:D:783:THR:HG23	2.61	0.40
1:B:826:ASN:HD21	1:B:962:ARG:CZ	2.34	0.40
1:B:889:ARG:CG	1:B:889:ARG:NH1	2.71	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	297/328 (90%)	288 (97%)	9 (3%)	0	100	100
1	B	313/328 (95%)	304 (97%)	7 (2%)	2 (1%)	25	36
1	C	295/328 (90%)	286 (97%)	9 (3%)	0	100	100
1	D	313/328 (95%)	305 (97%)	8 (3%)	0	100	100
All	All	1218/1312 (93%)	1183 (97%)	33 (3%)	2 (0%)	47	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	749	GLU
1	B	873	GLY

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	270/288 (94%)	262 (97%)	8 (3%)	41	61
1	B	278/288 (96%)	266 (96%)	12 (4%)	29	46
1	C	268/288 (93%)	253 (94%)	15 (6%)	21	34
1	D	278/288 (96%)	264 (95%)	14 (5%)	24	40
All	All	1094/1152 (95%)	1045 (96%)	49 (4%)	27	44

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	714	LYS
1	D	737	LYS
1	D	757	LYS
1	D	812	GLN
1	D	832	ARG
1	D	866	GLU
1	D	867	LYS
1	D	875	LYS
1	D	883	LEU
1	D	957	SER
1	D	970	LYS
1	D	986	ARG
1	D	998	TYR
1	D	1006	ASP
1	A	700	ASN
1	A	701	GLN
1	A	737	LYS
1	A	760	LEU
1	A	889	ARG
1	A	977	ARG
1	A	986	ARG
1	A	998	TYR
1	B	716	LYS
1	B	737	LYS
1	B	849	GLN
1	B	889	ARG
1	B	913	LYS
1	B	926	ILE
1	B	970	LYS
1	B	991	SER
1	B	999	ARG
1	B	1007	MET
1	B	1008	ASP
1	B	1009	ASP
1	C	701	GLN
1	C	707	LEU
1	C	708	LYS
1	C	737	LYS
1	C	745	LYS
1	C	748	ARG
1	C	806	LYS
1	C	832	ARG
1	C	861	LEU

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Mol	Chain	Res	Type
1	C	925	SER
1	C	962	ARG
1	C	981	ILE
1	C	985	GLU
1	C	998	TYR
1	C	1008	ASP

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

Mol	Chain	Res	Type
1	A	700	ASN
1	A	756	ASN
1	C	812	GLN
1	C	849	GLN
1	C	988	HIS

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 monosaccharides 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	TOV	A	1301	-	35,37,37	2.19	10 (28%)	43,52,52	1.99	14 (32%)
2	TOV	B	1202	-	35,37,37	2.25	11 (31%)	43,52,52	2.31	12 (27%)
2	TOV	D	1301	-	35,37,37	2.20	10 (28%)	43,52,52	2.05	13 (30%)
2	TOV	C	1202	-	35,37,37	2.24	10 (28%)	43,52,52	2.02	12 (27%)

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	TOV	A	1301	-	-	6/20/22/22	0/4/4/4
2	TOV	B	1202	-	-	3/20/22/22	0/4/4/4
2	TOV	D	1301	-	-	4/20/22/22	0/4/4/4
2	TOV	C	1202	-	-	6/20/22/22	0/4/4/4

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1202	TOV	C30-S31	7.22	1.81	1.75
2	B	1202	TOV	C30-S31	7.21	1.81	1.75
2	D	1301	TOV	C30-S31	6.99	1.81	1.75
2	A	1301	TOV	C30-S31	6.82	1.81	1.75
2	D	1301	TOV	C25-N24	5.54	1.46	1.36
2	A	1301	TOV	C25-N24	5.54	1.46	1.36
2	C	1202	TOV	C25-N24	5.52	1.46	1.36
2	B	1202	TOV	C25-N24	5.49	1.46	1.36
2	B	1202	TOV	C19-C18	4.17	1.53	1.49
2	C	1202	TOV	C16-C17	4.07	1.53	1.49
2	B	1202	TOV	C02-N11	3.84	1.46	1.35
2	A	1301	TOV	C16-C17	3.83	1.53	1.49
2	C	1202	TOV	C02-N11	3.75	1.45	1.35
2	D	1301	TOV	C02-N11	3.75	1.45	1.35
2	A	1301	TOV	C02-N11	3.73	1.45	1.35
2	B	1202	TOV	C16-C17	3.73	1.53	1.49
2	C	1202	TOV	C19-C18	3.72	1.53	1.49
2	A	1301	TOV	C19-C18	3.70	1.53	1.49
2	D	1301	TOV	C19-C18	3.57	1.53	1.49
2	D	1301	TOV	C16-C17	3.51	1.53	1.49
2	A	1301	TOV	C23-N24	2.73	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1202	TOV	C23-N24	2.72	1.46	1.40
2	B	1202	TOV	C23-N24	2.72	1.46	1.40
2	D	1301	TOV	C23-N24	2.70	1.46	1.40
2	D	1301	TOV	C18-C17	-2.68	1.37	1.44
2	A	1301	TOV	C18-C17	-2.58	1.37	1.44
2	B	1202	TOV	C18-C17	-2.54	1.37	1.44
2	C	1202	TOV	C18-C17	-2.53	1.37	1.44
2	D	1301	TOV	O01-C02	-2.41	1.18	1.23
2	D	1301	TOV	C18-N29	-2.41	1.31	1.37
2	C	1202	TOV	O01-C02	-2.38	1.18	1.23
2	C	1202	TOV	C18-N29	-2.38	1.31	1.37
2	B	1202	TOV	O01-C02	-2.35	1.18	1.23
2	A	1301	TOV	C18-N29	-2.35	1.31	1.37
2	A	1301	TOV	O01-C02	-2.35	1.18	1.23
2	B	1202	TOV	C18-N29	-2.24	1.31	1.37
2	A	1301	TOV	C17-N33	-2.23	1.31	1.37
2	D	1301	TOV	C17-N33	-2.22	1.31	1.37
2	B	1202	TOV	C17-N33	-2.19	1.32	1.37
2	C	1202	TOV	C17-N33	-2.06	1.32	1.37
2	B	1202	TOV	C12-N11	2.01	1.45	1.41

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1202	TOV	C32-S31-C30	10.99	110.47	102.27
2	D	1301	TOV	C32-S31-C30	8.38	108.53	102.27
2	C	1202	TOV	C32-S31-C30	8.18	108.38	102.27
2	A	1301	TOV	C32-S31-C30	6.59	107.19	102.27
2	C	1202	TOV	C21-N22-C23	3.57	122.29	117.22
2	A	1301	TOV	C21-N22-C23	3.54	122.25	117.22
2	B	1202	TOV	C21-N22-C23	3.54	122.25	117.22
2	A	1301	TOV	C15-C16-C17	3.47	126.11	120.61
2	D	1301	TOV	C21-N22-C23	3.46	122.12	117.22
2	B	1202	TOV	C15-C16-C17	3.15	125.59	120.61
2	B	1202	TOV	C04-C03-C02	-3.12	117.86	125.09
2	C	1202	TOV	C15-C16-C17	3.08	125.48	120.61
2	A	1301	TOV	C10-C03-C04	3.07	120.40	116.66
2	B	1202	TOV	C10-C03-C04	3.06	120.39	116.66
2	A	1301	TOV	C34-C16-C17	-3.06	114.26	120.15
2	D	1301	TOV	C10-C03-C04	3.03	120.35	116.66
2	A	1301	TOV	C04-C03-C02	-3.01	118.13	125.09
2	C	1202	TOV	C10-C03-C04	2.92	120.22	116.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1301	TOV	C15-C16-C17	2.90	125.21	120.61
2	D	1301	TOV	C34-C16-C17	-2.89	114.58	120.15
2	D	1301	TOV	C06-C04-C03	-2.88	119.97	123.11
2	B	1202	TOV	C34-C16-C17	-2.87	114.63	120.15
2	D	1301	TOV	C04-C03-C02	-2.81	118.59	125.09
2	B	1202	TOV	C06-C04-C03	-2.75	120.12	123.11
2	C	1202	TOV	C06-C04-C03	-2.74	120.12	123.11
2	A	1301	TOV	C06-C04-C03	-2.73	120.14	123.11
2	C	1202	TOV	C04-C03-C02	-2.67	118.91	125.09
2	A	1301	TOV	C26-C25-N24	2.62	118.83	114.98
2	A	1301	TOV	C28-C23-N22	-2.58	119.16	122.75
2	D	1301	TOV	C26-C25-N24	2.54	118.71	114.98
2	C	1202	TOV	C34-C16-C17	-2.52	115.29	120.15
2	C	1202	TOV	C26-C25-N24	2.52	118.68	114.98
2	B	1202	TOV	C20-C21-N22	-2.48	120.87	123.96
2	C	1202	TOV	C18-C17-N33	-2.48	107.08	113.76
2	D	1301	TOV	C28-C23-N22	-2.47	119.30	122.75
2	B	1202	TOV	C17-C18-N29	-2.47	107.09	113.76
2	C	1202	TOV	C28-C23-N22	-2.45	119.34	122.75
2	A	1301	TOV	C12-N11-C02	-2.44	120.24	126.58
2	B	1202	TOV	C26-C25-N24	2.43	118.55	114.98
2	C	1202	TOV	C20-C21-N22	-2.39	120.98	123.96
2	D	1301	TOV	C17-C18-N29	-2.37	107.35	113.76
2	B	1202	TOV	C28-C23-N22	-2.37	119.44	122.75
2	A	1301	TOV	C18-C17-N33	-2.36	107.39	113.76
2	A	1301	TOV	C17-C18-N29	-2.35	107.41	113.76
2	D	1301	TOV	C20-C21-N22	-2.28	121.12	123.96
2	C	1202	TOV	C17-C18-N29	-2.27	107.63	113.76
2	D	1301	TOV	C18-C17-N33	-2.26	107.66	113.76
2	A	1301	TOV	C20-C21-N22	-2.23	121.19	123.96
2	B	1202	TOV	C18-C17-N33	-2.23	107.75	113.76
2	D	1301	TOV	C23-N24-C25	-2.11	125.97	128.16
2	A	1301	TOV	C23-N24-C25	-2.07	126.01	128.16

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1301	TOV	N11-C02-C03-C04
2	D	1301	TOV	C15-C16-C17-N33
2	A	1301	TOV	N11-C02-C03-C04
2	C	1202	TOV	N11-C02-C03-C04

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Mol	Chain	Res	Type	Atoms
2	D	1301	TOV	C34-C16-C17-N33
2	A	1301	TOV	O01-C02-C03-C04
2	C	1202	TOV	O01-C02-C03-C04
2	B	1202	TOV	N11-C02-C03-C04
2	A	1301	TOV	C34-C12-N11-C02
2	C	1202	TOV	C34-C12-N11-C02
2	B	1202	TOV	C15-C16-C17-N33
2	D	1301	TOV	O01-C02-C03-C04
2	A	1301	TOV	C13-C12-N11-C02
2	C	1202	TOV	C13-C12-N11-C02
2	B	1202	TOV	C34-C16-C17-N33
2	C	1202	TOV	C15-C16-C17-N33
2	A	1301	TOV	C15-C16-C17-N33
2	C	1202	TOV	C34-C16-C17-N33
2	A	1301	TOV	C34-C16-C17-N33

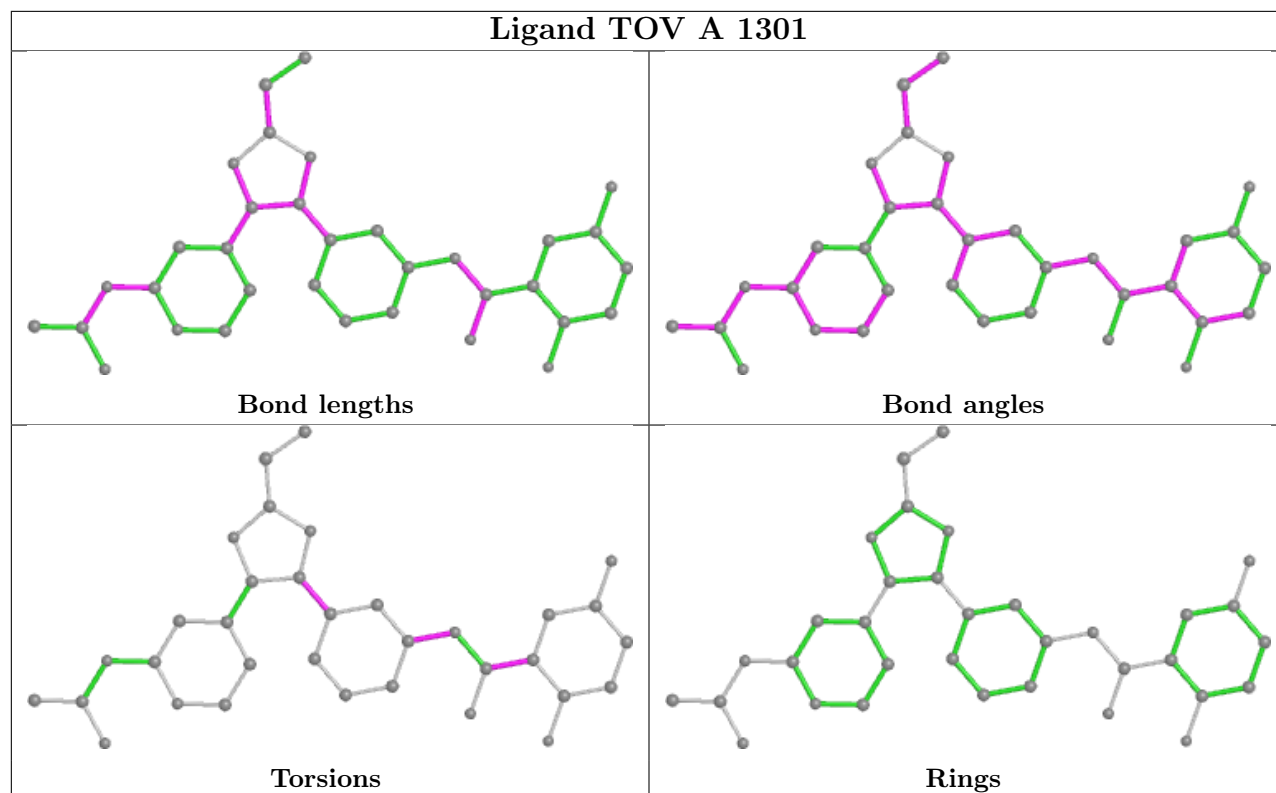
There are no ring outliers.

2 monomers are involved in 2 short contacts:

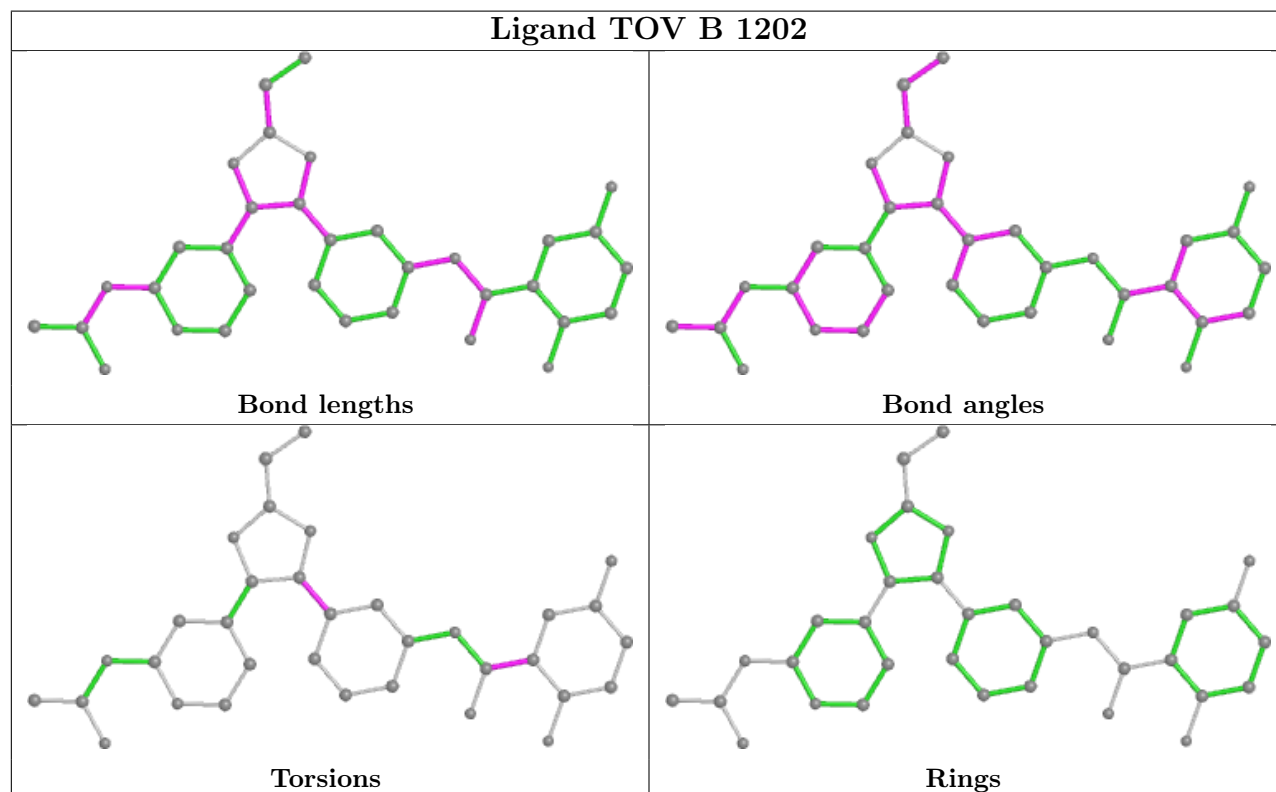
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	TOV	1	0
2	B	1202	TOV	1	0

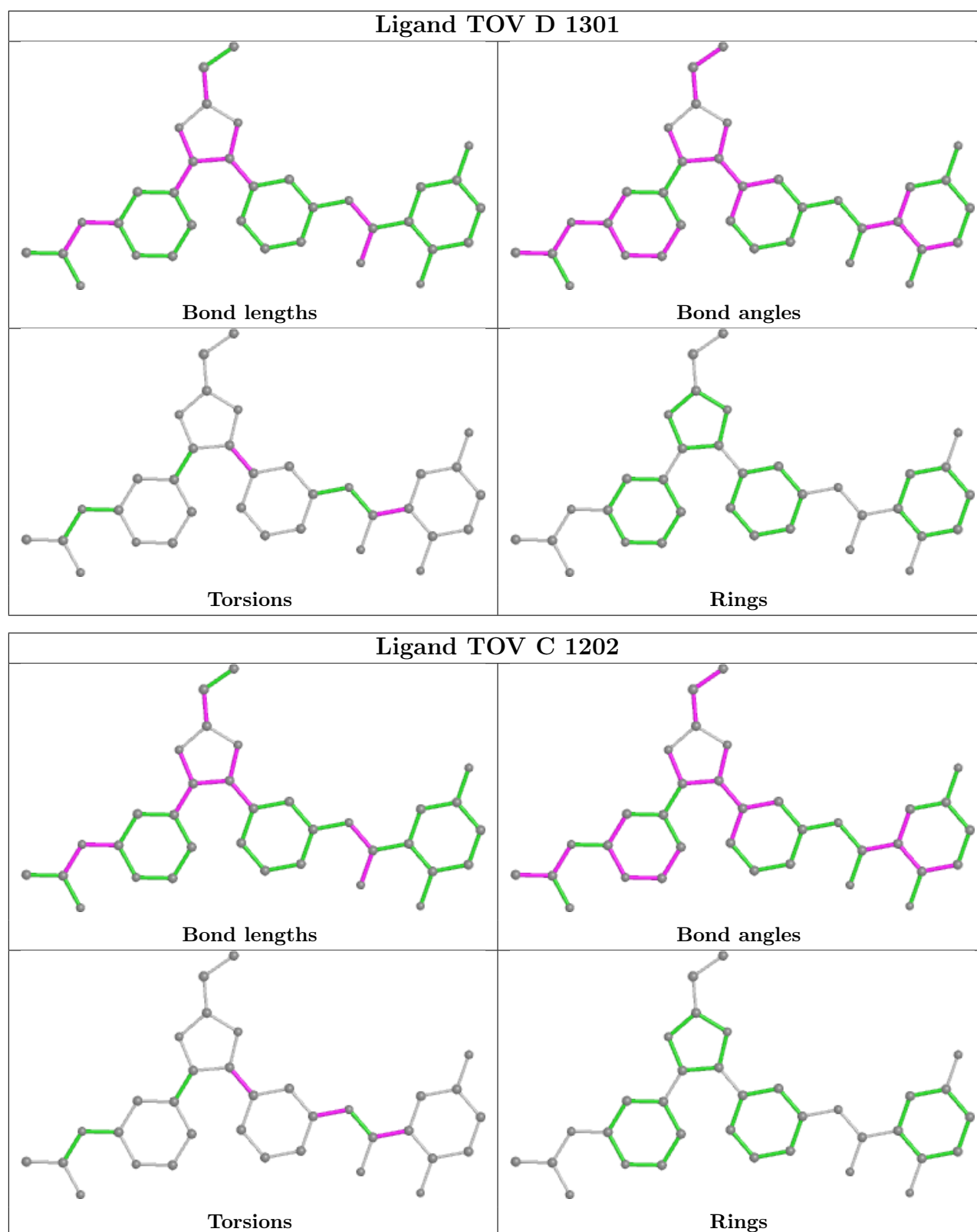
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand TOV A 1301



Ligand TOV B 1202





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	302/328 (92%)	0.16	9 (2%) 50 49	25, 42, 68, 87	0
1	B	314/328 (95%)	0.21	13 (4%) 37 36	26, 44, 82, 115	0
1	C	300/328 (91%)	0.31	29 (9%) 7 7	24, 46, 80, 102	0
1	D	314/328 (95%)	0.21	13 (4%) 37 36	24, 44, 83, 116	0
All	All	1230/1312 (93%)	0.22	64 (5%) 27 26	24, 44, 80, 116	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1012	ASP	6.9
1	D	1008	ASP	5.6
1	D	753	PRO	5.0
1	B	1013	ALA	4.9
1	C	1012	ASP	4.5
1	C	1013	ALA	4.4
1	B	1008	ASP	4.4
1	A	983	GLY	4.3
1	C	723	PHE	4.3
1	D	873	GLY	4.3
1	D	867	LYS	4.3
1	B	870	HIS	4.1
1	C	1009	ASP	4.0
1	B	753	PRO	3.9
1	D	1012	ASP	3.8
1	D	701	GLN	3.8
1	A	1012	ASP	3.6
1	C	1014	ASP	3.4
1	A	699	PRO	3.3
1	A	1010	VAL	3.3
1	D	1009	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	1010	VAL	3.2
1	B	1009	ASP	3.2
1	C	989	LEU	3.0
1	B	1007	MET	2.9
1	D	1007	MET	2.9
1	C	981	ILE	2.9
1	A	991	SER	2.9
1	B	1014	ASP	2.8
1	B	758	GLU	2.8
1	B	872	GLU	2.8
1	D	1014	ASP	2.8
1	C	1010	VAL	2.7
1	C	784	SER	2.7
1	C	808	ASN	2.6
1	C	859	ALA	2.6
1	C	980	VAL	2.5
1	C	987	MET	2.5
1	C	988	HIS	2.5
1	C	1011	VAL	2.5
1	D	807	ASP	2.5
1	A	993	THR	2.4
1	A	1011	VAL	2.4
1	B	1011	VAL	2.3
1	C	701	GLN	2.3
1	C	862	LEU	2.3
1	D	1006	ASP	2.3
1	C	722	ALA	2.2
1	C	920	ALA	2.2
1	C	917	GLY	2.2
1	C	860	LYS	2.2
1	C	748	ARG	2.2
1	A	1009	ASP	2.2
1	A	1006	ASP	2.2
1	B	865	GLU	2.2
1	B	869	TYR	2.1
1	C	986	ARG	2.1
1	C	991	SER	2.1
1	C	721	GLY	2.1
1	C	758	GLU	2.1
1	C	807	ASP	2.1
1	C	782	LEU	2.1
1	C	863	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	757	LYS	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 monosaccharides in this entry.

6.4 Ligands [i](#)

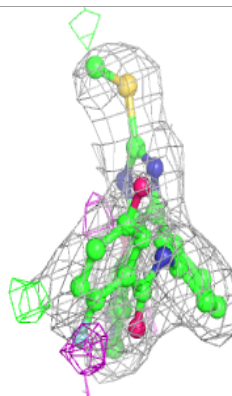
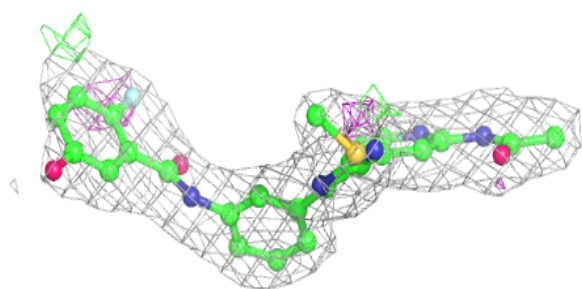
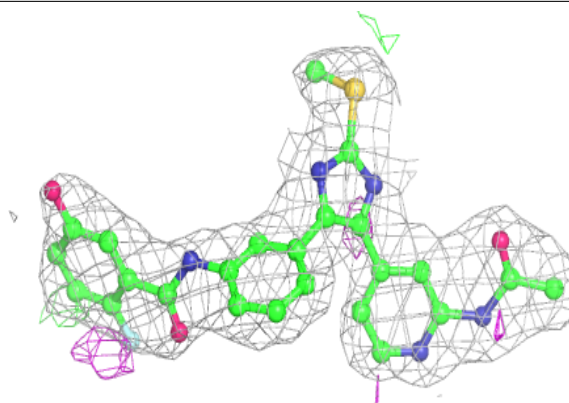
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	C	1201	1/1	0.62	0.30	94,94,94,94	0
3	CL	A	1302	1/1	0.87	0.14	63,63,63,63	0
3	CL	B	1201	1/1	0.89	0.08	67,67,67,67	0
2	TOV	C	1202	34/34	0.89	0.18	26,42,51,61	0
2	TOV	A	1301	34/34	0.92	0.18	22,38,46,58	0
2	TOV	D	1301	34/34	0.94	0.17	32,40,51,66	0
2	TOV	B	1202	34/34	0.94	0.16	26,38,45,59	0

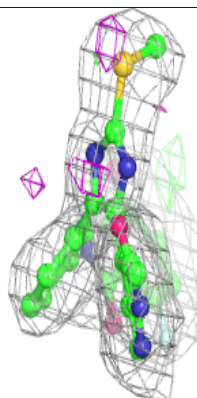
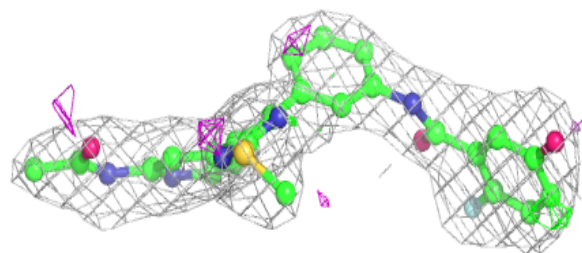
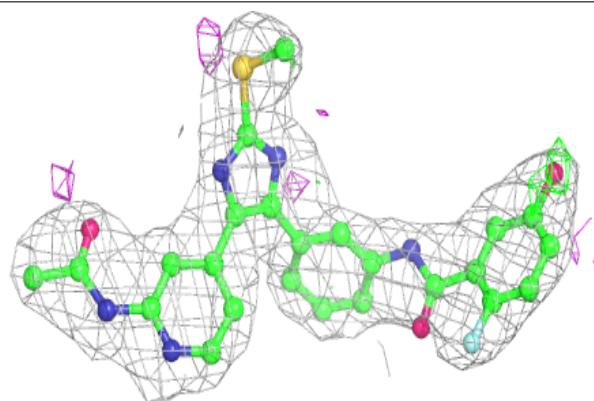
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TOV C 1202:

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

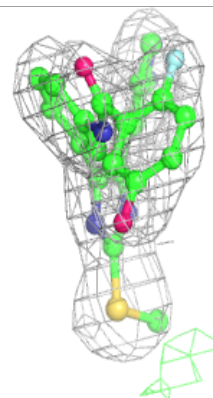
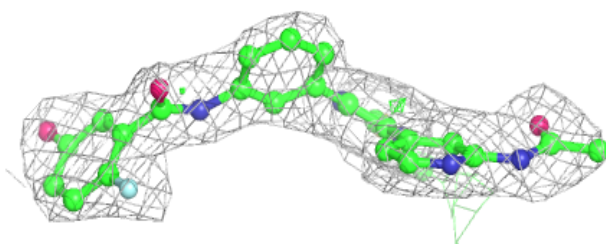
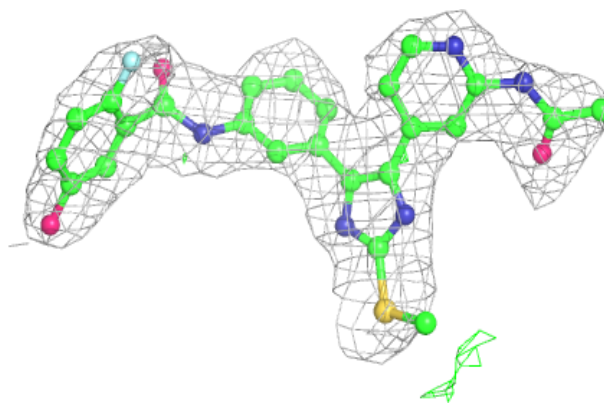
**Electron density around TOV A 1301:**

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

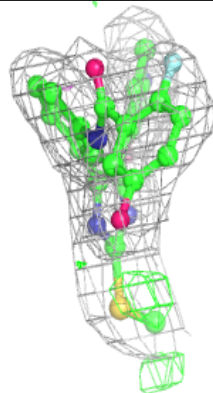
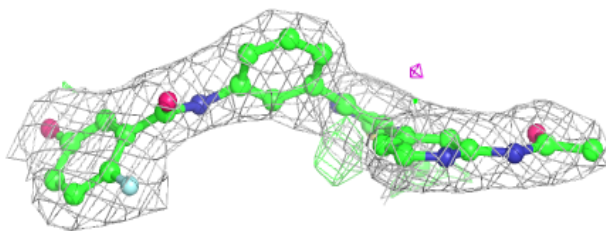
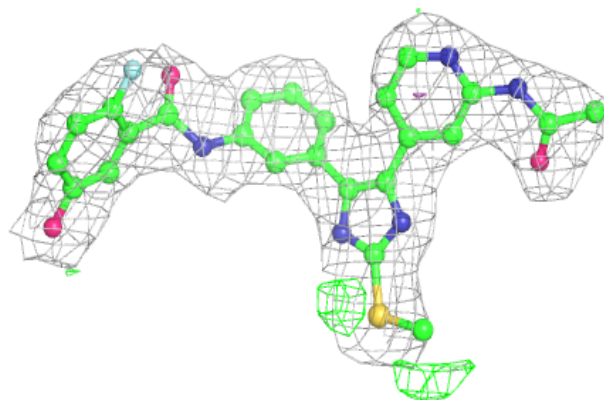


Electron density around TOV D 1301:

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

**Electron density around TOV B 1202:**

$2mF_o-DF_c$ (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.