



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:23 PM UTC

PDB ID : 9XU9 / pdb_00009xu9
Title : Crystal structure of EGFR T790M/C797S/L858R mutant in complex with (2-((5-chloro-2-((2-methoxy-4-(4-methylpiperazin-1-yl)-5-nitrophenyl)amino)pyrimidin-4-yl)amino)phenyl)dimethylphosphine oxide
Authors : Wang, Y.Y.; Ma, L.L.
Deposited on : 2025-11-24
Resolution : 2.84 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

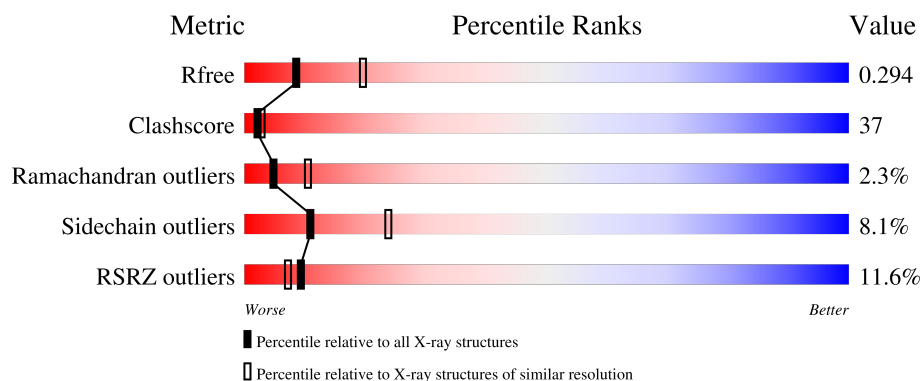
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	331	11% 42% 46% 6% 6%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2501 atoms, of which 29 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.

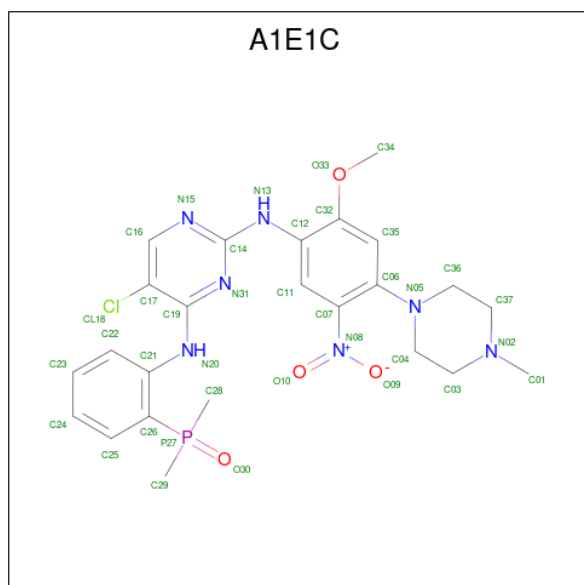
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2435	1562	413	443	17			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	692	GLY	-	expression tag	UNP P00533
A	693	SER	-	expression tag	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	797	SER	CYS	engineered mutation	UNP P00533
A	858	ARG	LEU	engineered mutation	UNP P00533

- Molecule 2 is 5-chloranyl- {N}4-(2-dimethylphosphorylphenyl)- {N}2-[2-methoxy-4-(4-methylpiperazin-1-yl)-5-nitro-phenyl]pyrimidine-2,4-diamine (CCD ID: A1E1C) (formula: C₂₄H₂₉ClN₇O₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Cl	H	N	O	P		
2	A	1	66	24	1	29	7	4	1	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	145.44Å 145.44Å 145.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.28 – 2.84 34.28 – 2.84	Depositor EDS
% Data completeness (in resolution range)	98.9 (34.28-2.84) 98.8 (34.28-2.84)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.85Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.228 , 0.294 0.228 , 0.294	Depositor DCC
R_{free} test set	1215 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	77.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.057 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2501	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: A1E1C

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	0.47	0/2486	0.70	1/3364 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	976	GLN	CA-CB-CG	-5.36	103.37	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	976	GLN	Peptide

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	2435	0	2432	182	0
2	A	37	29	0	3	0
All	All	2472	29	2432	182	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 37.

All (182) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:ILE:HD11	1:A:786:VAL:HG21	1.35	1.08
1:A:876:VAL:HB	1:A:881:MET:HE1	1.07	1.04
1:A:876:VAL:CB	1:A:881:MET:HE1	1.89	1.02
1:A:876:VAL:HB	1:A:881:MET:CE	1.90	1.01
1:A:705:ARG:HG2	1:A:707:LEU:HD21	1.47	0.96
1:A:759:ILE:HD11	1:A:786:VAL:CG2	1.96	0.95
1:A:879:LYS:HE2	1:A:915:TYR:HB2	1.51	0.93
1:A:834:VAL:HG12	1:A:836:ARG:HG3	1.51	0.92
1:A:973:ARG:O	1:A:973:ARG:HD2	1.69	0.91
1:A:793:MET:HA	1:A:793:MET:HE2	1.55	0.89
1:A:924:SER:O	1:A:928:GLU:HG3	1.73	0.89
1:A:875:LYS:HD2	1:A:876:VAL:H	1.37	0.89
1:A:926:ILE:HD12	1:A:927:LEU:H	1.39	0.87
1:A:823:LYS:HG3	1:A:965:ILE:HD12	1.54	0.86
1:A:823:LYS:HE3	1:A:965:ILE:CD1	2.06	0.86
1:A:878:ILE:HA	1:A:881:MET:HE3	1.56	0.86
1:A:745:LYS:HE3	1:A:790:MET:HE1	1.59	0.83
1:A:740:ILE:HD11	1:A:1017:LEU:HG	1.60	0.83
1:A:823:LYS:HE3	1:A:965:ILE:HD11	1.60	0.82
1:A:759:ILE:HD12	1:A:760:LEU:N	1.96	0.81
1:A:926:ILE:HD12	1:A:927:LEU:N	1.95	0.81
1:A:920:ALA:HA	1:A:923:ILE:HG12	1.63	0.79
1:A:745:LYS:HE3	1:A:790:MET:CE	2.13	0.78
1:A:776:ARG:HG2	1:A:1018:ILE:HD11	1.68	0.74
1:A:759:ILE:O	1:A:762:GLU:N	2.21	0.73
1:A:705:ARG:HG2	1:A:707:LEU:CD2	2.19	0.73
1:A:811:SER:OG	1:A:975:PRO:HB2	1.89	0.72
1:A:893:HIS:O	1:A:896:ASP:HB2	1.89	0.72
1:A:766:MET:HE1	1:A:790:MET:SD	2.29	0.72
1:A:806:LYS:HG2	1:A:910:PHE:HB3	1.72	0.71
1:A:808:ASN:O	1:A:987:MET:HG2	1.91	0.70
1:A:776:ARG:CG	1:A:1018:ILE:HD11	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:SER:HB2	1:A:979:LEU:HB2	1.73	0.70
1:A:875:LYS:HD2	1:A:876:VAL:N	2.06	0.70
1:A:766:MET:HE3	1:A:777:LEU:HB2	1.75	0.68
1:A:982:GLN:H	1:A:982:GLN:CD	2.02	0.68
1:A:724:GLY:HA3	1:A:747:LEU:HA	1.75	0.68
1:A:878:ILE:CA	1:A:881:MET:HE3	2.26	0.65
1:A:744:ILE:HG23	1:A:789:ILE:CD1	2.26	0.65
1:A:973:ARG:HD2	1:A:973:ARG:C	2.21	0.65
1:A:877:PRO:HD2	1:A:881:MET:HE2	1.78	0.65
1:A:804:GLU:HB3	1:A:805:HIS:ND1	2.12	0.64
1:A:806:LYS:HA	1:A:910:PHE:CD2	2.33	0.64
1:A:829:GLU:HG3	1:A:893:HIS:CG	2.33	0.63
1:A:1017:LEU:O	1:A:1020:GLN:N	2.33	0.62
1:A:744:ILE:HG23	1:A:789:ILE:HD12	1.81	0.62
1:A:793:MET:HE2	1:A:793:MET:CA	2.28	0.62
1:A:825:MET:SD	1:A:853:ILE:HD13	2.40	0.61
1:A:753:PRO:HA	1:A:756:ASN:OD1	2.00	0.61
1:A:823:LYS:CG	1:A:965:ILE:HD12	2.29	0.61
1:A:714:LYS:NZ	1:A:787:GLN:OE1	2.33	0.60
1:A:869:TYR:HE2	1:A:871:ALA:HB2	1.66	0.60
1:A:900:TYR:CE2	1:A:964:LEU:HD13	2.37	0.60
1:A:759:ILE:HD12	1:A:760:LEU:H	1.65	0.59
1:A:938:ILE:HD12	1:A:938:ILE:N	2.17	0.59
1:A:745:LYS:NZ	1:A:762:GLU:OE2	2.35	0.59
1:A:919:PRO:HD2	1:A:922:GLU:CD	2.27	0.58
1:A:778:LEU:HD12	1:A:790:MET:C	2.28	0.58
1:A:789:ILE:N	1:A:789:ILE:HD13	2.19	0.58
1:A:983:GLY:O	1:A:987:MET:HE3	2.04	0.58
1:A:923:ILE:HA	1:A:926:ILE:HD11	1.86	0.57
1:A:759:ILE:HD13	1:A:788:LEU:HD21	1.87	0.56
1:A:793:MET:HB2	1:A:844:LEU:HD13	1.86	0.56
1:A:806:LYS:HA	1:A:910:PHE:HD2	1.70	0.56
1:A:747:LEU:HD13	1:A:759:ILE:HG21	1.87	0.56
1:A:877:PRO:CD	1:A:881:MET:HE2	2.34	0.56
1:A:938:ILE:HD12	1:A:938:ILE:H	1.69	0.56
1:A:876:VAL:CG2	1:A:881:MET:HE1	2.36	0.56
1:A:884:GLU:OE1	1:A:958:ARG:NH1	2.26	0.56
1:A:986:ARG:HD2	1:A:986:ARG:H	1.70	0.56
1:A:793:MET:HG3	1:A:844:LEU:HB3	1.88	0.56
1:A:1015:GLU:O	1:A:1018:ILE:HG22	2.07	0.55
1:A:882:ALA:HB1	1:A:884:GLU:OE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:935:GLN:HA	1:A:944:TYR:CE1	2.42	0.55
1:A:805:HIS:O	1:A:806:LYS:C	2.50	0.55
1:A:869:TYR:CE2	1:A:871:ALA:HB2	2.41	0.55
1:A:745:LYS:CE	1:A:790:MET:HE1	2.36	0.54
1:A:793:MET:HA	1:A:793:MET:CE	2.35	0.54
1:A:883:LEU:HD11	1:A:928:GLU:HG2	1.89	0.54
1:A:771:ASN:ND2	1:A:772:PRO:HD2	2.21	0.54
1:A:799:LEU:O	1:A:803:ARG:HG3	2.06	0.54
1:A:697:GLU:HG3	1:A:864:ALA:HB2	1.90	0.54
1:A:877:PRO:N	1:A:881:MET:HE2	2.23	0.53
1:A:888:HIS:O	1:A:890:ILE:HG12	2.08	0.53
1:A:919:PRO:HD2	1:A:922:GLU:OE1	2.09	0.53
1:A:713:LYS:O	1:A:713:LYS:HG3	2.09	0.53
1:A:945:MET:O	1:A:949:LYS:HG3	2.08	0.53
1:A:747:LEU:CD1	1:A:759:ILE:HG21	2.39	0.52
1:A:978:TYR:O	1:A:979:LEU:HD23	2.10	0.52
1:A:988:HIS:ND1	1:A:988:HIS:N	2.58	0.52
1:A:938:ILE:HG21	1:A:981:ILE:CD1	2.40	0.51
1:A:798:LEU:HD13	1:A:845:VAL:HG22	1.92	0.51
1:A:760:LEU:CD2	1:A:780:ILE:HD11	2.40	0.51
1:A:919:PRO:O	1:A:922:GLU:OE1	2.29	0.51
1:A:781:CYS:HB3	1:A:787:GLN:HB2	1.92	0.51
1:A:904:VAL:O	1:A:908:MET:HG2	2.12	0.50
1:A:819:VAL:HG13	1:A:965:ILE:HG13	1.94	0.50
1:A:834:VAL:HG12	1:A:836:ARG:CG	2.32	0.50
1:A:752:SER:H	1:A:753:PRO:CD	2.25	0.49
1:A:706:ILE:HD13	1:A:780:ILE:CG2	2.43	0.49
1:A:697:GLU:O	1:A:698:ALA:HB3	2.12	0.48
1:A:742:VAL:HG12	1:A:778:LEU:HD13	1.95	0.48
1:A:750:ALA:HB1	1:A:753:PRO:HD2	1.96	0.48
1:A:886:ILE:O	1:A:886:ILE:HG22	2.14	0.48
1:A:781:CYS:CB	1:A:787:GLN:HB2	2.43	0.48
1:A:752:SER:H	1:A:753:PRO:HD2	1.79	0.47
1:A:884:GLU:HG2	1:A:885:SER:N	2.29	0.47
1:A:723:PHE:HB2	1:A:747:LEU:HD23	1.95	0.47
1:A:942:ASP:HB3	1:A:971:MET:HE2	1.96	0.47
1:A:726:VAL:HG11	2:A:1101:A1E1C:C22	2.44	0.47
1:A:938:ILE:HG21	1:A:981:ILE:HD11	1.96	0.47
1:A:1015:GLU:OE1	1:A:1015:GLU:C	2.57	0.47
1:A:749:GLU:HG2	1:A:754:LYS:HB2	1.97	0.47
1:A:788:LEU:HB2	1:A:790:MET:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:LYS:HG3	1:A:965:ILE:CD1	2.36	0.47
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.50	0.46
1:A:757:LYS:HD2	1:A:761:ASP:OD1	2.15	0.46
1:A:941:ILE:N	1:A:941:ILE:HD13	2.30	0.46
1:A:793:MET:HG3	1:A:844:LEU:CB	2.45	0.46
1:A:878:ILE:HG23	1:A:886:ILE:HD13	1.96	0.46
1:A:916:ASP:OD1	1:A:917:GLY:N	2.46	0.46
1:A:809:ILE:HD12	1:A:817:TRP:HH2	1.80	0.46
1:A:898:TRP:HE3	1:A:958:ARG:NH2	2.14	0.46
1:A:714:LYS:HD3	1:A:727:TYR:CG	2.50	0.46
1:A:781:CYS:O	1:A:786:VAL:HA	2.16	0.45
1:A:887:LEU:HB2	1:A:888:HIS:CD2	2.51	0.45
1:A:750:ALA:CB	1:A:753:PRO:HD2	2.45	0.45
1:A:759:ILE:CD1	1:A:786:VAL:CG2	2.83	0.45
1:A:788:LEU:C	1:A:789:ILE:HD13	2.42	0.45
1:A:832:ARG:NH2	1:A:863:GLY:O	2.50	0.45
1:A:867:LYS:O	1:A:892:THR:HG22	2.17	0.45
1:A:735:GLY:O	1:A:736:GLU:C	2.60	0.45
1:A:918:ILE:HG22	1:A:923:ILE:HD11	1.99	0.45
1:A:898:TRP:CE3	1:A:958:ARG:NH2	2.85	0.45
1:A:918:ILE:HG21	1:A:923:ILE:CD1	2.46	0.45
1:A:708:LYS:C	1:A:710:THR:N	2.74	0.44
1:A:709:GLU:O	1:A:709:GLU:HG3	2.16	0.44
1:A:723:PHE:O	1:A:747:LEU:HB3	2.17	0.44
1:A:751:THR:HG22	1:A:751:THR:O	2.17	0.44
1:A:789:ILE:C	1:A:790:MET:HG2	2.42	0.44
1:A:933:LEU:O	1:A:944:TYR:OH	2.30	0.44
1:A:877:PRO:C	1:A:881:MET:HE3	2.42	0.44
1:A:923:ILE:O	1:A:926:ILE:HD12	2.18	0.44
1:A:944:TYR:O	1:A:948:VAL:HG23	2.17	0.44
1:A:918:ILE:CG2	1:A:923:ILE:CD1	2.95	0.43
1:A:965:ILE:O	1:A:969:SER:HB2	2.18	0.43
1:A:827:TYR:O	1:A:830:ASP:HB2	2.18	0.43
1:A:925:SER:O	1:A:929:LYS:HG2	2.18	0.43
1:A:985:GLU:C	1:A:987:MET:H	2.25	0.43
1:A:985:GLU:H	1:A:985:GLU:HG2	1.34	0.43
1:A:782:LEU:HD12	1:A:782:LEU:HA	1.77	0.43
1:A:820:GLN:OE1	1:A:851:VAL:HG22	2.19	0.43
1:A:823:LYS:CD	1:A:965:ILE:HD12	2.48	0.43
1:A:783:THR:O	1:A:784:SER:C	2.62	0.42
1:A:780:ILE:HD13	1:A:780:ILE:HG21	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:ARG:HG3	1:A:842:ASN:N	2.33	0.42
1:A:955:ALA:HB2	1:A:958:ARG:NH1	2.34	0.42
1:A:877:PRO:C	1:A:881:MET:CE	2.91	0.42
1:A:1009:ASP:O	1:A:1010:VAL:CB	2.67	0.42
1:A:919:PRO:HD2	1:A:922:GLU:OE2	2.20	0.42
1:A:760:LEU:HD21	1:A:780:ILE:HD11	2.01	0.42
1:A:875:LYS:CD	1:A:876:VAL:H	2.18	0.42
1:A:793:MET:O	2:A:1101:A1E1C:N13	2.52	0.42
1:A:886:ILE:O	1:A:886:ILE:CG2	2.68	0.42
1:A:705:ARG:O	1:A:780:ILE:HG22	2.20	0.42
1:A:1005:GLU:O	1:A:1007:MET:SD	2.78	0.42
1:A:815:LEU:O	1:A:818:CYS:HB2	2.20	0.42
1:A:937:PRO:HD2	1:A:938:ILE:HD12	2.01	0.41
1:A:796:GLY:HA2	2:A:1101:A1E1C:C11	2.51	0.41
1:A:708:LYS:O	1:A:710:THR:N	2.53	0.41
1:A:709:GLU:HA	1:A:712:PHE:CZ	2.56	0.41
1:A:750:ALA:N	1:A:754:LYS:HB3	2.36	0.41
1:A:795:PHE:HB2	1:A:845:VAL:HG12	2.01	0.41
1:A:842:ASN:O	1:A:854:THR:HG22	2.21	0.41
1:A:878:ILE:N	1:A:881:MET:HE3	2.35	0.41
1:A:946:ILE:O	1:A:947:MET:C	2.63	0.41
1:A:1015:GLU:C	1:A:1015:GLU:CD	2.89	0.41
1:A:714:LYS:HD2	1:A:727:TYR:CD1	2.56	0.41
1:A:806:LYS:C	1:A:808:ASN:H	2.29	0.40
1:A:761:ASP:O	1:A:764:TYR:HB3	2.20	0.40
1:A:756:ASN:O	1:A:757:LYS:HB2	2.22	0.40
1:A:788:LEU:HD23	1:A:788:LEU:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	306/331 (92%)	257 (84%)	42 (14%)	7 (2%)	5	10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	752	SER
1	A	1007	MET
1	A	702	ALA
1	A	736	GLU
1	A	1014	ASP
1	A	807	ASP
1	A	1010	VAL

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	258/290 (89%)	237 (92%)	21 (8%)	11	24

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

Mol	Chain	Res	Type
1	A	708	LYS
1	A	720	SER
1	A	732	ILE
1	A	759	ILE
1	A	768	SER
1	A	775	CYS
1	A	781	CYS
1	A	782	LEU
1	A	789	ILE
1	A	807	ASP
1	A	832	ARG
1	A	849	GLN
1	A	875	LYS
1	A	883	LEU

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Mol	Chain	Res	Type
1	A	921	SER
1	A	924	SER
1	A	929	LYS
1	A	988	HIS
1	A	1008	ASP
1	A	1018	ILE
1	A	1020	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	870	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
2	A1E1C	A	1101	-	38,40,40	3.18	20 (52%)	47,58,58	2.50	19 (40%)

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	A1E1C	A	1101	-	-	9/22/34/34	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	A1E1C	P27-C28	-8.64	1.70	1.79
2	A	1101	A1E1C	P27-C29	8.63	1.89	1.79
2	A	1101	A1E1C	C14-N13	4.74	1.46	1.36
2	A	1101	A1E1C	C04-N05	4.69	1.54	1.46
2	A	1101	A1E1C	C07-N08	4.57	1.54	1.45
2	A	1101	A1E1C	C19-N20	4.33	1.44	1.36
2	A	1101	A1E1C	C36-N05	4.27	1.54	1.46
2	A	1101	A1E1C	C25-C26	3.36	1.44	1.40
2	A	1101	A1E1C	C35-C32	3.10	1.44	1.38
2	A	1101	A1E1C	C35-C06	3.04	1.44	1.39
2	A	1101	A1E1C	C12-N13	2.91	1.47	1.39
2	A	1101	A1E1C	C14-N15	2.89	1.38	1.34
2	A	1101	A1E1C	C04-C03	2.79	1.61	1.51
2	A	1101	A1E1C	O33-C32	2.78	1.41	1.37
2	A	1101	A1E1C	C21-N20	2.69	1.47	1.39
2	A	1101	A1E1C	C23-C24	2.69	1.44	1.38
2	A	1101	A1E1C	O09-N08	-2.66	1.17	1.35
2	A	1101	A1E1C	C22-C21	2.41	1.43	1.39
2	A	1101	A1E1C	C11-C12	2.29	1.43	1.39
2	A	1101	A1E1C	C24-C25	2.10	1.42	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	A1E1C	N15-C14-N31	-6.57	120.06	126.42
2	A	1101	A1E1C	C01-N02-C03	-6.44	98.37	110.63
2	A	1101	A1E1C	O33-C32-C12	4.90	120.92	114.81
2	A	1101	A1E1C	O30-P27-C28	-4.87	102.83	112.71
2	A	1101	A1E1C	C17-C19-N31	-4.02	117.12	121.01
2	A	1101	A1E1C	C11-C12-C32	-3.64	114.68	118.95
2	A	1101	A1E1C	C17-C19-N20	3.58	123.43	120.23
2	A	1101	A1E1C	C01-N02-C37	-3.41	104.13	110.63
2	A	1101	A1E1C	C06-C35-C32	3.16	124.70	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	A1E1C	O33-C32-C35	-3.04	118.85	124.08
2	A	1101	A1E1C	C12-C11-C07	3.02	124.49	116.35
2	A	1101	A1E1C	C32-C12-N13	3.01	124.81	118.10
2	A	1101	A1E1C	P27-C26-C25	2.80	126.07	115.45
2	A	1101	A1E1C	C34-O33-C32	-2.76	113.46	117.51
2	A	1101	A1E1C	C14-N31-C19	2.65	122.86	116.36
2	A	1101	A1E1C	O10-N08-C07	-2.46	114.82	119.03
2	A	1101	A1E1C	C23-C22-C21	2.35	123.46	118.69
2	A	1101	A1E1C	C23-C24-C25	-2.33	117.37	120.24
2	A	1101	A1E1C	C12-N13-C14	-2.27	122.30	129.22

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	A1E1C	C21-C26-P27-O30
2	A	1101	A1E1C	C12-C32-O33-C34
2	A	1101	A1E1C	C35-C32-O33-C34
2	A	1101	A1E1C	C35-C06-N05-C36
2	A	1101	A1E1C	C35-C06-N05-C04
2	A	1101	A1E1C	C25-C26-P27-C28
2	A	1101	A1E1C	C07-C06-N05-C04
2	A	1101	A1E1C	C25-C26-P27-O30
2	A	1101	A1E1C	C07-C06-N05-C36

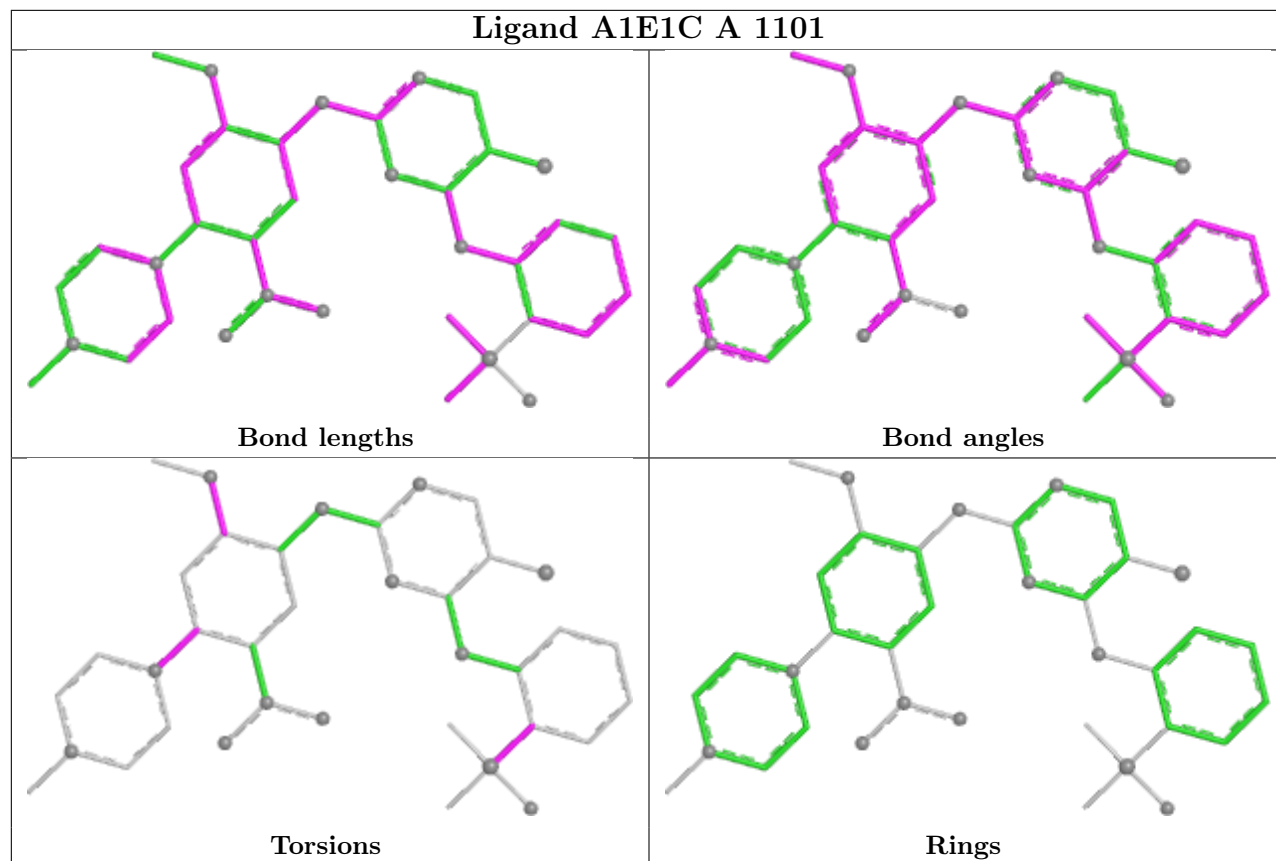
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	A1E1C	3	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	310/331 (93%)	0.57	36 (11%) 9 7	45, 65, 105, 130	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ARG	6.5
1	A	758	GLU	5.3
1	A	1018	ILE	4.1
1	A	1019	PRO	3.9
1	A	747	LEU	3.8
1	A	755	ALA	3.7
1	A	722	ALA	3.6
1	A	753	PRO	3.4
1	A	988	HIS	3.4
1	A	1007	MET	3.3
1	A	751	THR	3.3
1	A	785	THR	3.2
1	A	723	PHE	3.1
1	A	986	ARG	3.1
1	A	756	ASN	3.0
1	A	1012	ASP	3.0
1	A	863	GLY	2.9
1	A	873	GLY	2.9
1	A	752	SER	2.8
1	A	867	LYS	2.8
1	A	1015	GLU	2.7
1	A	696	GLY	2.7
1	A	1014	ASP	2.6
1	A	926	ILE	2.6
1	A	1005	GLU	2.6
1	A	776	ARG	2.3
1	A	1004	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	759	ILE	2.3
1	A	750	ALA	2.2
1	A	864	ALA	2.2
1	A	749	GLU	2.1
1	A	754	LYS	2.1
1	A	757	LYS	2.1
1	A	1008	ASP	2.1
1	A	874	GLY	2.0
1	A	721	GLY	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](#)

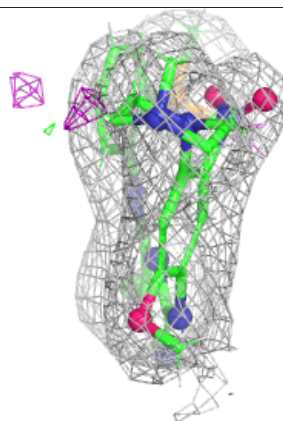
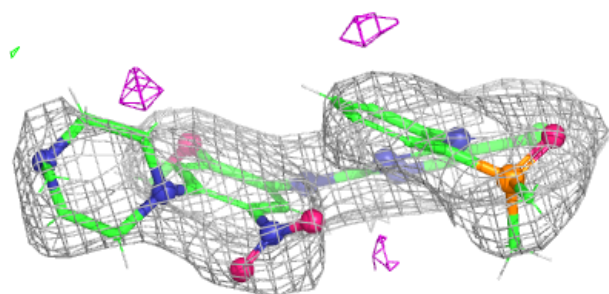
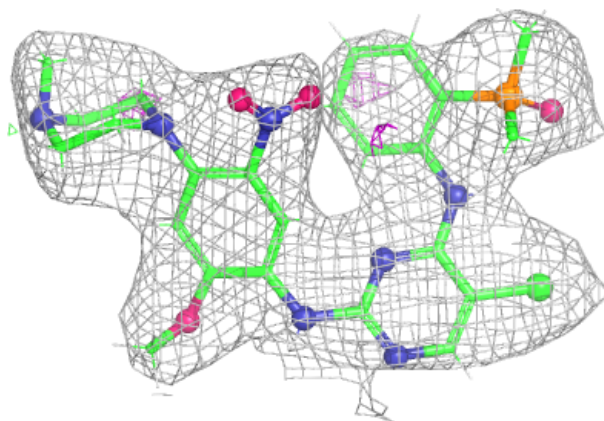
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	A1E1C	A	1101	37/37	0.92	0.10	53,77,102,110	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 A1E1C 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.