



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:01 AM UTC

PDB ID : 4R5S / pdb_00004r5s
Title : Crystal structure of EGFR 696-1022 L858R in complex with FIIN-3
Authors : Zhu, S.J.; Yun, C.H.
Deposited on : 2014-08-22
Resolution : 3.00 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

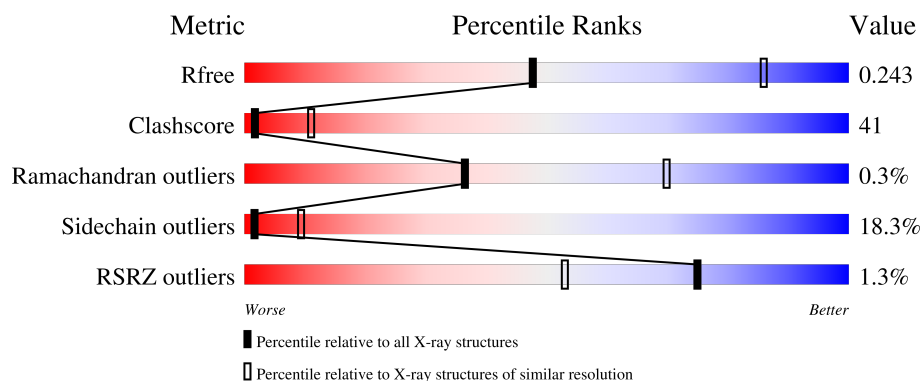
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2437 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.

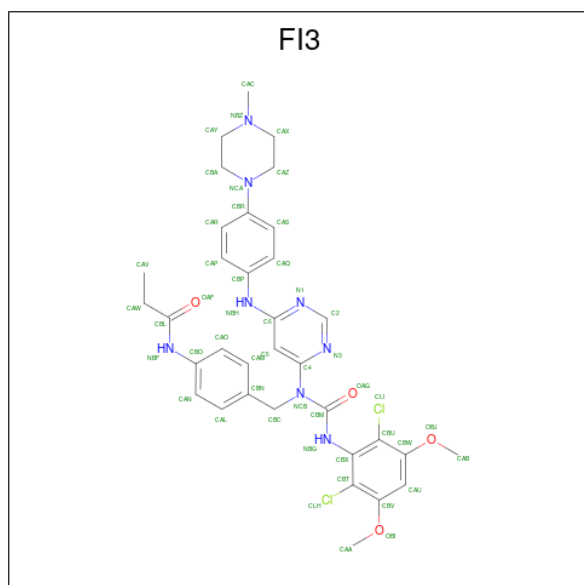
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	299	2367	1523	399	429	16	7	0	0

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	694	PRO	-	expression tag	UNP P00533
A	695	SER	-	expression tag	UNP P00533
A	858	ARG	LEU	engineered mutation	UNP P00533

- Molecule 2 is N-[4-({[(2,6-dichloro-3,5-dimethoxyphenyl)carbamoyl](6-{[4-(4-methylpiperazin-1-yl)phenyl]amino}pyrimidin-4-yl)amino}methyl)phenyl]propanamide (CCD ID: FI3) (formula: C₃₄H₃₈Cl₂N₈O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			48	34	2	8	4		

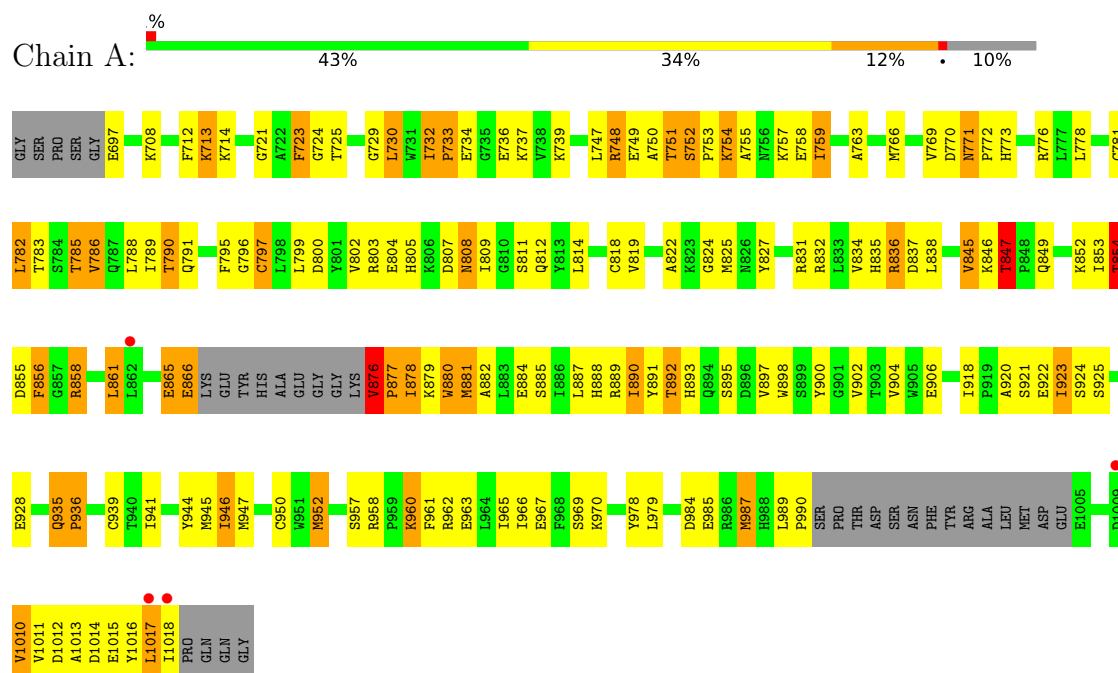
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		

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



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	147.92Å 147.92Å 147.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.77 – 3.00 46.77 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.77-3.00) 99.8 (46.77-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.202 , 0.239 0.213 , 0.243	Depositor DCC
R_{free} test set	524 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	93.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 76.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.041 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2437	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: FI3

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	0.91	5/2416 (0.2%)	1.06	15/3274 (0.5%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	935	GLN	C-N	6.17	1.40	1.33
1	A	732	ILE	C-N	5.62	1.40	1.33
1	A	877	PRO	N-CD	5.07	1.54	1.47
1	A	876	VAL	C-N	5.06	1.40	1.34
1	A	733	PRO	N-CD	5.01	1.54	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	847	THR	N-CA-C	-6.86	102.05	108.22
1	A	935	GLN	CA-C-N	-6.68	113.50	120.38
1	A	935	GLN	C-N-CA	-6.68	113.50	120.38
1	A	732	ILE	CA-C-N	-6.48	113.30	119.85
1	A	732	ILE	C-N-CA	-6.48	113.30	119.85
1	A	918	ILE	N-CA-C	6.37	115.91	108.96
1	A	854	THR	N-CA-C	6.32	116.91	108.38
1	A	808	ASN	N-CA-C	6.04	120.36	112.92
1	A	785	THR	N-CA-C	-5.93	102.54	110.55
1	A	876	VAL	CA-C-N	-5.49	112.95	119.05
1	A	876	VAL	C-N-CA	-5.49	112.95	119.05
1	A	757	LYS	N-CA-C	-5.44	105.45	111.71
1	A	936	PRO	CA-C-N	-5.41	113.04	119.05
1	A	936	PRO	C-N-CA	-5.41	113.04	119.05
1	A	771	ASN	N-CA-C	5.24	112.93	108.22

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2367	0	2392	185	0
2	A	48	0	36	15	0
3	A	22	0	0	2	0
All	All	2437	0	2428	197	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 41.

All (197) 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:754:LYS:HD2	1:A:754:LYS:C	1.50	1.33
1:A:754:LYS:HD2	1:A:754:LYS:O	1.39	1.18
1:A:809:ILE:HG21	1:A:814:LEU:HD21	1.31	1.05
1:A:854:THR:HG23	1:A:855:ASP:N	1.69	1.05
1:A:809:ILE:CG2	1:A:814:LEU:HD21	1.89	1.02
1:A:879:LYS:HB2	1:A:880:TRP:CE3	1.94	1.02
1:A:723:PHE:CD1	1:A:724:GLY:N	2.30	0.99
1:A:879:LYS:HB2	1:A:880:TRP:CZ3	2.00	0.96
2:A:1101:FI3:OAF	2:A:1101:FI3:H9	1.62	0.95
1:A:854:THR:CG2	1:A:855:ASP:N	2.31	0.94
2:A:1101:FI3:CAQ	2:A:1101:FI3:H21	1.98	0.93
1:A:772:PRO:O	1:A:852:LYS:HE3	1.69	0.93
1:A:935:GLN:HB2	1:A:944:TYR:CD2	2.07	0.90
1:A:754:LYS:C	1:A:754:LYS:CD	2.30	0.90
2:A:1101:FI3:H21	2:A:1101:FI3:H24	1.57	0.86
1:A:854:THR:HG23	1:A:855:ASP:H	1.38	0.86
1:A:855:ASP:HA	2:A:1101:FI3:H14	1.58	0.85
1:A:904:VAL:HG12	1:A:947:MET:HE2	1.58	0.85
1:A:752:SER:HB3	1:A:755:ALA:CB	2.10	0.82
1:A:952:MET:HE3	1:A:957:SER:HB3	1.61	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:SER:CB	1:A:755:ALA:CB	2.58	0.82
1:A:752:SER:OG	1:A:755:ALA:HB2	1.80	0.81
1:A:752:SER:OG	1:A:755:ALA:CB	2.30	0.80
1:A:723:PHE:CE1	1:A:724:GLY:O	2.34	0.79
1:A:935:GLN:HB2	1:A:944:TYR:CE2	2.18	0.79
1:A:834:VAL:HG22	1:A:893:HIS:HD2	1.47	0.78
1:A:807:ASP:O	1:A:987:MET:HE2	1.84	0.78
2:A:1101:FI3:CBM	2:A:1101:FI3:H8	2.14	0.77
1:A:920:ALA:HA	1:A:923:ILE:HD13	1.67	0.77
1:A:802:VAL:HA	1:A:809:ILE:HD11	1.67	0.76
1:A:771:ASN:CG	1:A:772:PRO:HD2	2.10	0.76
1:A:878:ILE:HA	1:A:881:MET:SD	2.26	0.76
1:A:752:SER:CB	1:A:755:ALA:HB2	2.16	0.75
1:A:752:SER:CB	1:A:755:ALA:HB3	2.18	0.74
1:A:809:ILE:HG21	1:A:814:LEU:CD2	2.13	0.73
1:A:865:GLU:O	1:A:866:GLU:HB2	1.89	0.71
1:A:795:PHE:HB2	1:A:845:VAL:HB	1.72	0.71
1:A:846:LYS:HG2	1:A:847:THR:HG23	1.72	0.71
1:A:752:SER:HB3	1:A:755:ALA:HB3	1.73	0.70
1:A:723:PHE:HD1	1:A:724:GLY:H	1.39	0.70
1:A:809:ILE:CG2	1:A:814:LEU:CD2	2.69	0.70
1:A:782:LEU:HD23	1:A:782:LEU:N	2.06	0.70
1:A:892:THR:H	1:A:895:SER:HB3	1.56	0.70
2:A:1101:FI3:H24	2:A:1101:FI3:C5	2.21	0.69
1:A:749:GLU:HA	1:A:785:THR:CG2	2.23	0.68
1:A:877:PRO:HG2	1:A:881:MET:HG2	1.75	0.68
1:A:878:ILE:CA	1:A:881:MET:HG3	2.24	0.68
1:A:936:PRO:HD2	1:A:939:CYS:SG	2.36	0.65
2:A:1101:FI3:OAF	2:A:1101:FI3:CAN	2.31	0.65
1:A:771:ASN:OD1	1:A:772:PRO:N	2.30	0.65
2:A:1101:FI3:NBG	2:A:1101:FI3:N3	2.30	0.65
1:A:752:SER:OG	1:A:755:ALA:N	2.30	0.64
1:A:733:PRO:HB2	1:A:736:GLU:CB	2.27	0.64
1:A:876:VAL:O	1:A:878:ILE:HG13	1.98	0.64
1:A:752:SER:HB3	1:A:755:ALA:HB2	1.78	0.63
1:A:781:CYS:C	1:A:782:LEU:HD23	2.25	0.62
1:A:819:VAL:O	1:A:822:ALA:N	2.32	0.62
1:A:960:LYS:HB2	1:A:963:GLU:HG3	1.81	0.61
1:A:825:MET:HE2	1:A:838:LEU:HD22	1.82	0.61
1:A:737:LYS:O	1:A:737:LYS:HG2	2.00	0.61
1:A:836:ARG:HG3	1:A:891:TYR:CD2	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:VAL:HG22	1:A:893:HIS:CD2	2.33	0.60
1:A:723:PHE:CG	1:A:724:GLY:N	2.68	0.60
1:A:730:LEU:HD13	1:A:739:LYS:HB3	1.83	0.60
1:A:786:VAL:O	1:A:786:VAL:CG2	2.49	0.60
1:A:877:PRO:C	1:A:878:ILE:HG13	2.26	0.60
1:A:846:LYS:HG2	1:A:847:THR:CG2	2.32	0.60
1:A:880:TRP:HE3	1:A:880:TRP:H	1.51	0.59
1:A:989:LEU:O	1:A:990:PRO:C	2.46	0.59
1:A:941:ILE:O	1:A:945:MET:HB2	2.04	0.58
1:A:771:ASN:OD1	1:A:772:PRO:HD2	2.01	0.58
2:A:1101:FI3:H7	3:A:1212:HOH:O	2.03	0.57
1:A:771:ASN:OD1	1:A:772:PRO:CD	2.53	0.57
1:A:878:ILE:N	1:A:881:MET:SD	2.78	0.57
1:A:891:TYR:CD1	1:A:891:TYR:N	2.73	0.57
1:A:771:ASN:CG	1:A:772:PRO:CD	2.78	0.57
1:A:878:ILE:H	1:A:881:MET:CG	2.18	0.56
1:A:880:TRP:CE3	1:A:880:TRP:N	2.73	0.56
1:A:831:ARG:NH2	3:A:1211:HOH:O	2.38	0.56
1:A:783:THR:C	1:A:785:THR:O	2.48	0.56
1:A:763:ALA:HB2	1:A:788:LEU:HD11	1.88	0.55
1:A:836:ARG:NH1	1:A:858:ARG:NH1	2.54	0.55
1:A:754:LYS:CE	1:A:755:ALA:HA	2.37	0.55
1:A:878:ILE:N	1:A:881:MET:HG3	2.21	0.55
1:A:853:ILE:HG22	1:A:854:THR:N	2.22	0.55
1:A:852:LYS:NZ	1:A:1014:ASP:OD2	2.39	0.54
1:A:878:ILE:CA	1:A:881:MET:SD	2.94	0.54
1:A:766:MET:HE1	1:A:790:THR:HG21	1.89	0.54
1:A:766:MET:O	1:A:769:VAL:HG22	2.08	0.54
1:A:836:ARG:NH2	1:A:836:ARG:HG2	2.22	0.54
1:A:713:LYS:N	1:A:713:LYS:CD	2.70	0.53
2:A:1101:FI3:CBM	2:A:1101:FI3:CAM	2.86	0.53
1:A:797:CYS:HB3	1:A:800:ASP:HB2	1.90	0.53
1:A:751:THR:O	1:A:753:PRO:HD3	2.09	0.52
1:A:807:ASP:O	1:A:987:MET:CE	2.56	0.52
1:A:855:ASP:HA	2:A:1101:FI3:CAA	2.36	0.52
1:A:712:PHE:C	1:A:713:LYS:HD2	2.35	0.52
1:A:878:ILE:HD12	1:A:920:ALA:HB1	1.91	0.52
1:A:755:ALA:O	1:A:758:GLU:HB3	2.10	0.52
1:A:723:PHE:HE1	1:A:724:GLY:O	1.92	0.51
1:A:809:ILE:HG22	1:A:814:LEU:HD21	1.82	0.51
1:A:836:ARG:CG	1:A:836:ARG:HH21	2.23	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:ILE:C	1:A:891:TYR:CD1	2.88	0.51
2:A:1101:FI3:H8	2:A:1101:FI3:OAG	2.11	0.51
1:A:752:SER:O	1:A:755:ALA:N	2.43	0.51
1:A:936:PRO:HD2	1:A:939:CYS:HB2	1.92	0.50
1:A:961:PHE:O	1:A:965:ILE:HG13	2.12	0.50
1:A:855:ASP:O	1:A:855:ASP:OD1	2.30	0.50
1:A:846:LYS:NZ	1:A:1014:ASP:OD2	2.44	0.50
1:A:877:PRO:HG2	1:A:881:MET:CG	2.41	0.50
1:A:878:ILE:N	1:A:881:MET:CG	2.75	0.49
1:A:713:LYS:N	1:A:713:LYS:HD2	2.28	0.49
1:A:721:GLY:HA3	1:A:723:PHE:CE1	2.48	0.49
1:A:783:THR:O	1:A:785:THR:O	2.30	0.49
1:A:786:VAL:O	1:A:786:VAL:HG22	2.11	0.49
1:A:936:PRO:HD2	1:A:939:CYS:CB	2.42	0.49
1:A:748:ARG:O	1:A:750:ALA:O	2.30	0.48
1:A:967:GLU:OE1	1:A:970:LYS:NZ	2.44	0.48
1:A:978:TYR:O	1:A:979:LEU:HD23	2.13	0.48
1:A:878:ILE:HD12	1:A:920:ALA:CB	2.43	0.48
1:A:749:GLU:HA	1:A:785:THR:HG23	1.95	0.48
1:A:832:ARG:O	1:A:861:LEU:HD22	2.13	0.48
1:A:778:LEU:HB2	1:A:789:ILE:O	2.13	0.48
1:A:878:ILE:C	1:A:881:MET:HG3	2.38	0.48
1:A:796:GLY:O	1:A:845:VAL:HG23	2.13	0.47
1:A:748:ARG:HH11	1:A:748:ARG:HG3	1.80	0.47
1:A:902:VAL:O	1:A:906:GLU:HG3	2.13	0.47
1:A:877:PRO:C	1:A:878:ILE:CG1	2.86	0.47
1:A:805:HIS:N	1:A:805:HIS:ND1	2.62	0.47
1:A:836:ARG:HG2	1:A:836:ARG:HH21	1.79	0.47
1:A:861:LEU:HD22	1:A:861:LEU:HA	1.73	0.46
1:A:754:LYS:HD2	1:A:755:ALA:N	2.18	0.46
1:A:788:LEU:HD22	2:A:1101:FI3:OBJ	2.16	0.46
1:A:795:PHE:CE1	1:A:847:THR:HA	2.50	0.46
1:A:836:ARG:HB3	1:A:858:ARG:HB2	1.97	0.46
1:A:799:LEU:O	1:A:803:ARG:HG3	2.15	0.46
1:A:836:ARG:HH12	1:A:858:ARG:NH1	2.14	0.45
1:A:947:MET:O	1:A:950:CYS:HB2	2.17	0.45
1:A:878:ILE:CA	1:A:881:MET:CG	2.93	0.45
1:A:856:PHE:CD1	1:A:856:PHE:N	2.72	0.45
1:A:897:VAL:O	1:A:900:TYR:HB3	2.17	0.45
1:A:732:ILE:N	1:A:732:ILE:HD12	2.32	0.45
1:A:1013:ALA:C	1:A:1015:GLU:N	2.73	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:GLU:HB3	1:A:805:HIS:ND1	2.32	0.45
1:A:835:HIS:CE1	1:A:837:ASP:O	2.70	0.45
1:A:721:GLY:HA3	1:A:723:PHE:CD1	2.52	0.44
1:A:729:GLY:O	1:A:730:LEU:HD23	2.16	0.44
1:A:1016:TYR:C	1:A:1017:LEU:HG	2.41	0.44
1:A:877:PRO:O	1:A:879:LYS:N	2.42	0.44
1:A:749:GLU:O	1:A:751:THR:HG22	2.18	0.44
1:A:877:PRO:HG2	1:A:878:ILE:H	1.82	0.44
1:A:752:SER:O	1:A:755:ALA:HB3	2.18	0.44
1:A:770:ASP:OD1	1:A:776:ARG:NH1	2.50	0.44
1:A:759:ILE:HD12	1:A:759:ILE:HA	1.77	0.44
1:A:880:TRP:HE3	1:A:880:TRP:N	2.09	0.43
1:A:748:ARG:HG3	1:A:748:ARG:NH1	2.33	0.43
1:A:865:GLU:O	1:A:865:GLU:HG3	2.18	0.43
1:A:885:SER:O	1:A:889:ARG:N	2.49	0.43
1:A:924:SER:O	1:A:928:GLU:HG3	2.19	0.43
1:A:946:ILE:HD12	1:A:946:ILE:HA	1.76	0.43
1:A:811:SER:HB2	1:A:979:LEU:HB2	2.00	0.43
1:A:853:ILE:CG2	1:A:854:THR:N	2.82	0.43
1:A:818:CYS:O	1:A:819:VAL:C	2.57	0.43
1:A:824:GLY:O	1:A:827:TYR:HB3	2.18	0.43
1:A:946:ILE:HG22	1:A:947:MET:N	2.31	0.43
1:A:783:THR:OG1	1:A:785:THR:O	2.30	0.42
1:A:887:LEU:HB2	1:A:888:HIS:ND1	2.34	0.42
1:A:791:GLN:HE22	1:A:1014:ASP:CG	2.27	0.42
1:A:878:ILE:HA	1:A:881:MET:CG	2.50	0.42
1:A:962:ARG:O	1:A:966:ILE:HG13	2.20	0.42
1:A:836:ARG:NH2	1:A:891:TYR:CE2	2.87	0.42
1:A:952:MET:O	1:A:958:ARG:NH2	2.52	0.42
1:A:771:ASN:OD1	1:A:773:HIS:N	2.30	0.42
1:A:849:GLN:H	1:A:849:GLN:CD	2.28	0.42
1:A:712:PHE:C	1:A:713:LYS:CD	2.93	0.42
2:A:1101:FI3:H38	2:A:1101:FI3:H27	1.64	0.42
1:A:811:SER:HB3	1:A:984:ASP:OD2	2.19	0.41
1:A:877:PRO:O	1:A:878:ILE:HG13	2.20	0.41
1:A:836:ARG:CZ	1:A:858:ARG:NH1	2.83	0.41
1:A:892:THR:O	1:A:895:SER:HB3	2.21	0.41
1:A:754:LYS:CD	1:A:755:ALA:N	2.79	0.41
1:A:836:ARG:NH1	1:A:858:ARG:HH11	2.19	0.41
1:A:885:SER:HA	1:A:890:ILE:H	1.86	0.41
1:A:888:HIS:O	1:A:889:ARG:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:LEU:HD12	1:A:799:LEU:HA	1.85	0.41
1:A:865:GLU:O	1:A:866:GLU:CB	2.63	0.41
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.56	0.41
1:A:965:ILE:O	1:A:969:SER:HB2	2.21	0.41
2:A:1101:FI3:H25	2:A:1101:FI3:H29	1.78	0.41
1:A:713:LYS:HD2	1:A:713:LYS:HA	1.99	0.41
1:A:736:GLU:O	1:A:737:LYS:HB3	2.21	0.40
1:A:950:CYS:O	1:A:958:ARG:HG2	2.21	0.40
1:A:747:LEU:O	1:A:785:THR:HG21	2.21	0.40
1:A:808:ASN:HA	1:A:987:MET:HG2	2.02	0.40
1:A:771:ASN:HA	1:A:772:PRO:HD3	1.95	0.40
1:A:782:LEU:HD22	1:A:782:LEU:HA	1.85	0.40
1:A:1010:VAL:H	1:A:1010:VAL:HG12	1.58	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	293/331 (88%)	277 (94%)	15 (5%)	1 (0%)	36 70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	923	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	257/290 (89%)	210 (82%)	47 (18%)	2 9

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	697	GLU
1	A	708	LYS
1	A	713	LYS
1	A	714	LYS
1	A	723	PHE
1	A	725	THR
1	A	730	LEU
1	A	734	GLU
1	A	748	ARG
1	A	751	THR
1	A	752	SER
1	A	754	LYS
1	A	759	ILE
1	A	782	LEU
1	A	786	VAL
1	A	790	THR
1	A	797	CYS
1	A	812	GLN
1	A	836	ARG
1	A	845	VAL
1	A	847	THR
1	A	854	THR
1	A	856	PHE
1	A	858	ARG
1	A	861	LEU
1	A	865	GLU
1	A	866	GLU
1	A	876	VAL
1	A	878	ILE
1	A	880	TRP
1	A	881	MET
1	A	884	GLU
1	A	890	ILE
1	A	892	THR
1	A	921	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	922	GLU
1	A	925	SER
1	A	946	ILE
1	A	952	MET
1	A	960	LYS
1	A	985	GLU
1	A	987	MET
1	A	1010	VAL
1	A	1011	VAL
1	A	1012	ASP
1	A	1017	LEU
1	A	1018	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	701	GLN
1	A	808	ASN
1	A	812	GLN
1	A	893	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	FI3	A	1101	1	52,52,52	2.29	13 (25%)	66,72,72	2.48	14 (21%)

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	FI3	A	1101	1	-	3/34/44/44	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	FI3	CBC-CBN	-7.59	1.37	1.51
2	A	1101	FI3	CBU-CLI	-6.04	1.60	1.72
2	A	1101	FI3	CBX-NBG	-5.61	1.33	1.43
2	A	1101	FI3	C4-NCB	-5.22	1.32	1.41
2	A	1101	FI3	CBT-CLH	-5.11	1.62	1.72
2	A	1101	FI3	CBO-NBF	-4.53	1.32	1.41
2	A	1101	FI3	CBP-NBH	-3.83	1.32	1.40
2	A	1101	FI3	C6-NBH	-3.53	1.32	1.38
2	A	1101	FI3	C2-N3	2.53	1.38	1.33
2	A	1101	FI3	CBM-NCB	-2.48	1.34	1.39
2	A	1101	FI3	C2-N1	2.37	1.38	1.33
2	A	1101	FI3	CBR-NCA	-2.12	1.33	1.38
2	A	1101	FI3	OBJ-CBW	-2.05	1.33	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	FI3	CAB-OBJ-CBW	-9.52	103.54	117.51
2	A	1101	FI3	CAA-OBI-CBV	-7.78	106.11	117.51
2	A	1101	FI3	C2-N3-C4	6.57	120.46	114.95
2	A	1101	FI3	N1-C2-N3	-6.16	119.26	128.58
2	A	1101	FI3	CBO-NBF-CBL	-6.03	116.85	127.52
2	A	1101	FI3	NBG-CBM-NCB	3.84	119.84	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	FI3	CBA-NCA-CAZ	3.81	120.13	111.57
2	A	1101	FI3	CBN-CBC-NCB	-3.38	107.97	113.46
2	A	1101	FI3	C6-C5-C4	3.35	119.32	116.64
2	A	1101	FI3	CBX-NBG-CBM	-3.32	115.96	122.43
2	A	1101	FI3	CBP-NBH-C6	-3.28	120.32	128.75
2	A	1101	FI3	N3-C4-NCB	2.83	119.66	114.77
2	A	1101	FI3	OBJ-CBW-CAU	-2.25	120.20	124.08
2	A	1101	FI3	C5-C6-N1	-2.00	120.29	122.92

There are no chirality outliers.

All (3) torsion outliers are listed below:

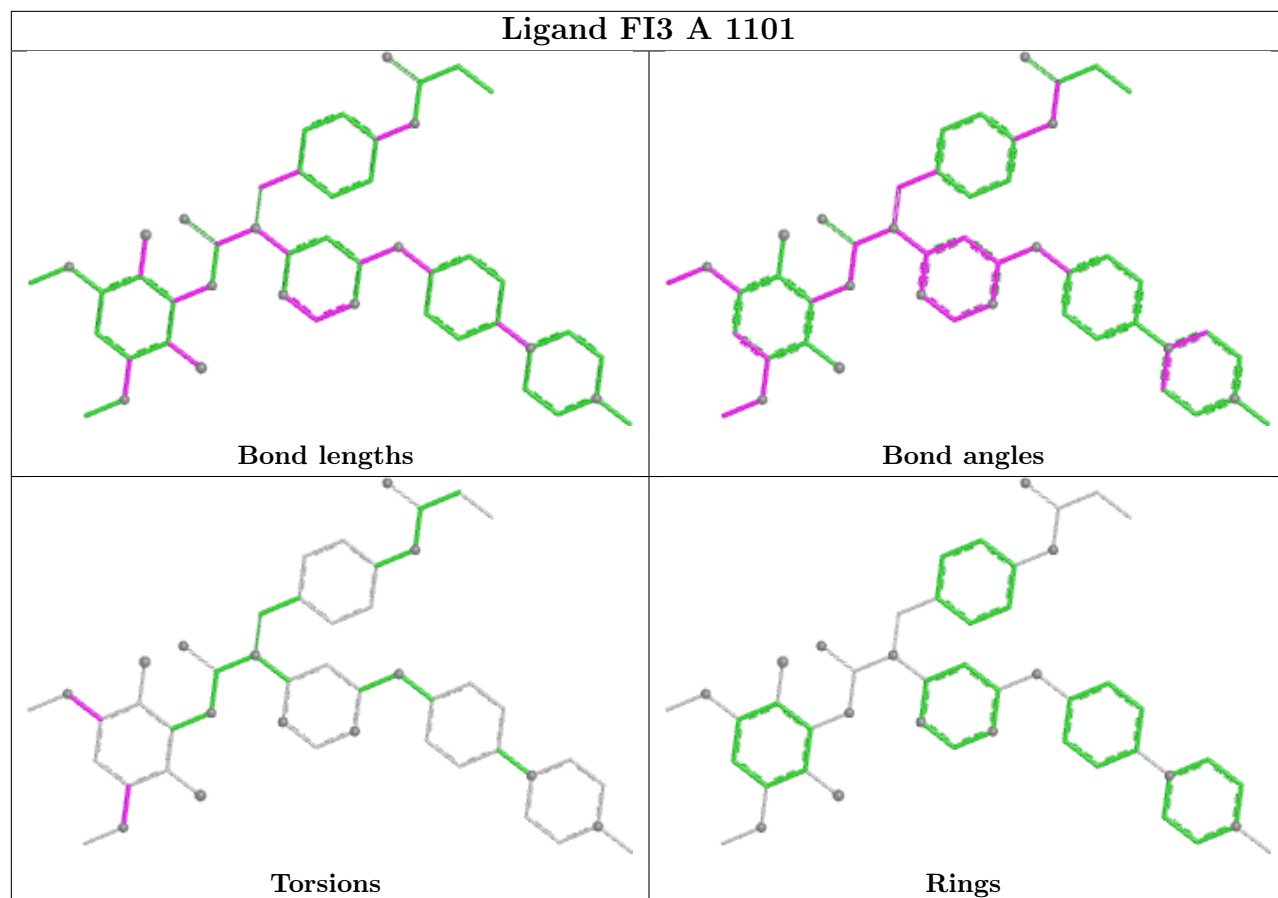
Mol	Chain	Res	Type	Atoms
2	A	1101	FI3	CBT-CBV-OBI-CAA
2	A	1101	FI3	CAU-CBV-OBI-CAA
2	A	1101	FI3	CBU-CBW-OBJ-CAB

There are no ring outliers.

1 monomer is involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	FI3	15	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, 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	299/331 (90%)	-0.11	4 (1%) 75 53	49, 72, 122, 177	6 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1017	LEU	2.9
1	A	862	LEU	2.7
1	A	1009	ASP	2.5
1	A	1018	ILE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

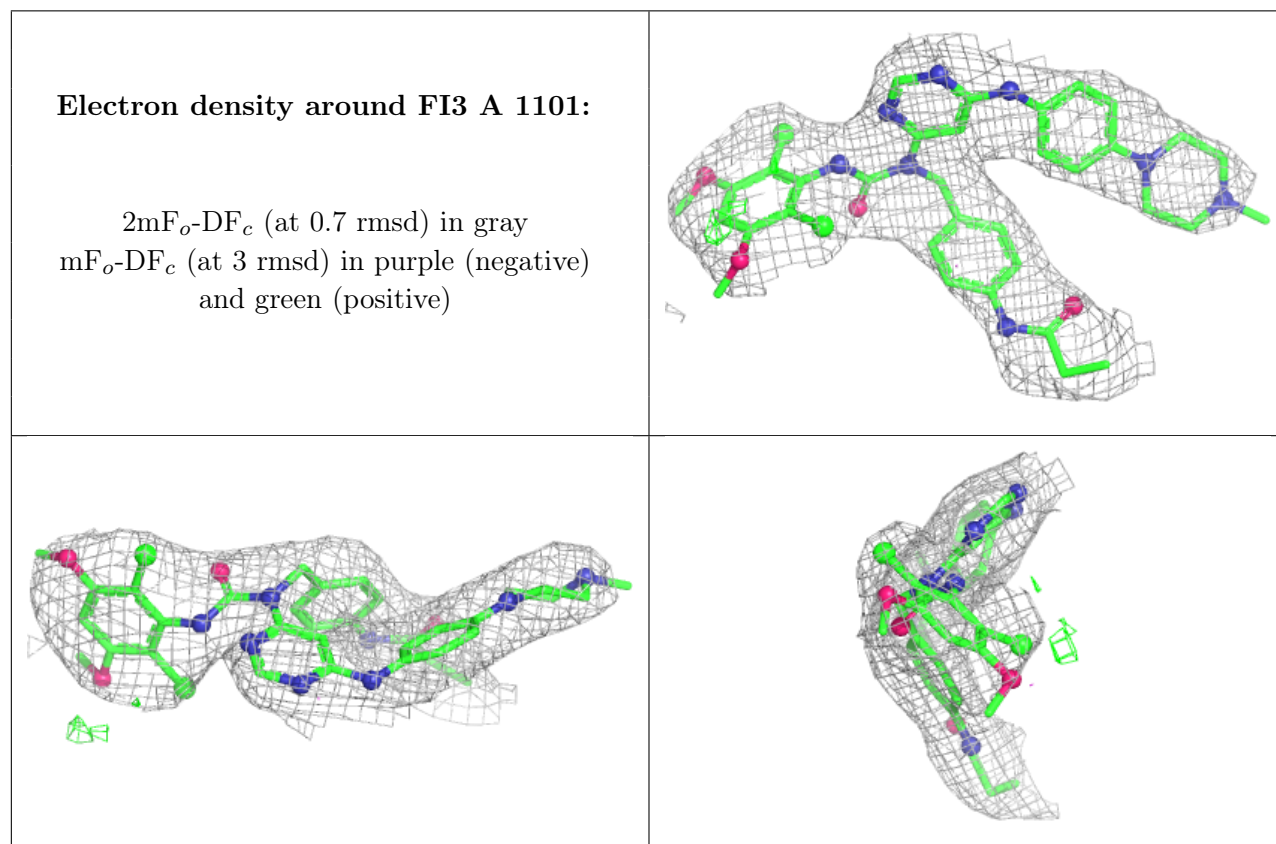
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FI3	A	1101	48/48	0.91	0.10	65,81,97,104	3

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.