



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:53 PM UTC

PDB ID : 7UKW / pdb_00007ukw
Title : EGFR(T790M/V948R) in complex with Lazertinib (YH25448)
Authors : Pham, C.D.; Heppner, D.E.
Deposited on : 2022-04-02
Resolution : 2.60 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

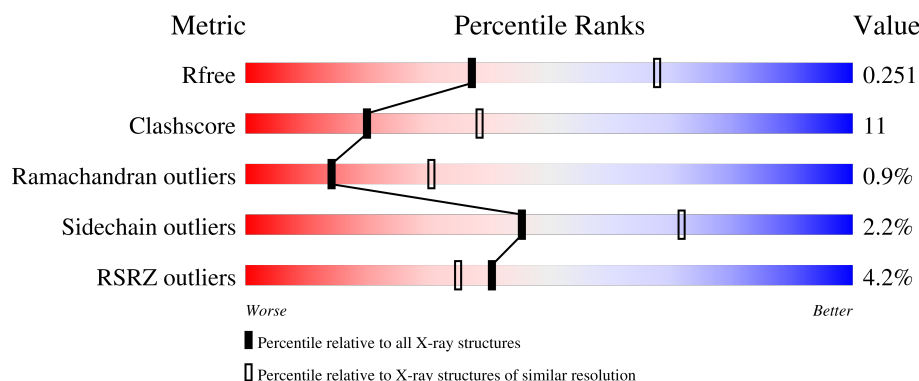
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	 4% 79% 14% 7%
1	B	328	 5% 60% 27% 11%
1	C	328	 3% 68% 19% 12%
1	D	328	 3% 67% 23% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9736 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.

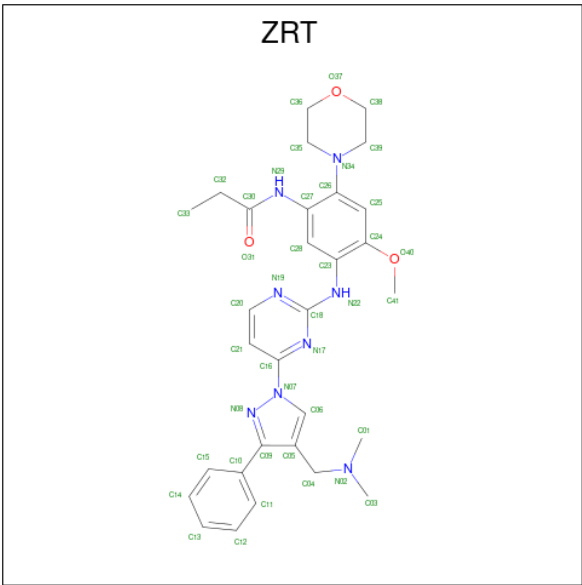
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	300	Total	C	N	O	S	0	1	0
			2421	1556	411	436	18			
1	A	306	Total	C	N	O	S	0	0	0
			2451	1574	417	442	18			
1	B	292	Total	C	N	O	S	0	0	0
			2336	1499	395	423	19			
1	C	287	Total	C	N	O	S	0	1	0
			2314	1489	394	413	18			

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-[5-[[[(4P)-4-{4-[(dimethylamino)methyl]-3-phenyl-1H-pyrazol-1-yl}]pyrimidin-2-yl]amino]-4-methoxy-2-(morpholin-4-yl)phenyl]propanamide (CCD ID: ZRT) (formula: C₃₀H₃₆N₈O₃) (labeled as "Ligand of Interest" by depositor).



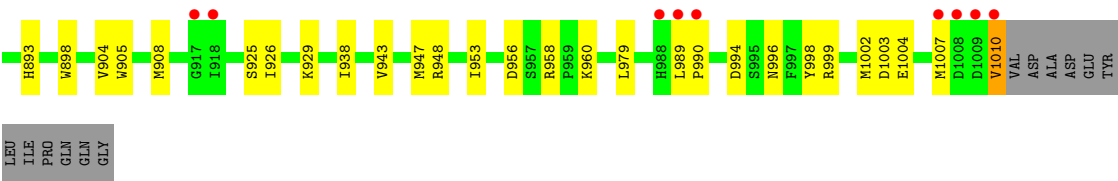
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			41	30	8	3		
2	C	1	Total	C	N	O	0	0
			41	30	8	3		

- Molecule 3 is water.

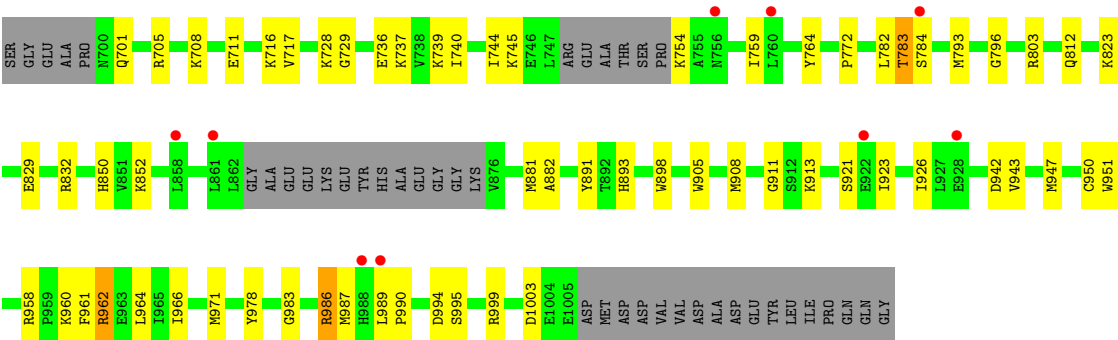
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	34	Total	O	0	0
			34	34		
3	A	36	Total	O	0	0
			36	36		
3	B	25	Total	O	0	0
			25	25		
3	C	37	Total	O	0	0
			37	37		

- Molecule 1: Epidermal growth factor receptor





● Molecule 1: Epidermal growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.05Å 101.80Å 87.35Å 90.00° 102.37° 90.00°	Depositor
Resolution (Å)	65.35 – 2.60 65.35 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (65.35-2.60) 93.5 (65.35-2.60)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.27 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.195 , 0.250 0.195 , 0.251	Depositor DCC
R_{free} test set	1992 reflections (5.30%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9736	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 24.28 % 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 3.9515e-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: ZRT

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	0/2504	0.41	1/3384 (0.0%)
1	B	0.44	0/2387	0.56	6/3231 (0.2%)
1	C	0.25	0/2363	0.40	0/3195
1	D	0.35	0/2472	0.54	3/3339 (0.1%)
All	All	0.33	0/9726	0.48	10/13149 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	755	ALA	N-CA-C	-9.58	100.16	112.23
1	B	754	LYS	N-CA-C	-8.13	102.41	113.30
1	D	876	VAL	CB-CA-C	7.25	118.57	110.52
1	A	751	THR	N-CA-C	-6.17	105.84	113.19
1	B	751	THR	N-CA-C	5.89	123.36	110.80
1	D	751	THR	CA-C-N	-5.43	117.88	123.10
1	D	751	THR	C-N-CA	-5.43	117.88	123.10
1	B	752	SER	N-CA-C	5.43	119.05	107.91
1	B	752	SER	CA-C-N	5.29	126.45	119.84
1	B	752	SER	C-N-CA	5.29	126.45	119.84

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	2451	0	2485	32	0
1	B	2336	0	2355	75	0
1	C	2314	0	2357	52	0
1	D	2421	0	2470	68	0
2	B	41	0	0	3	0
2	C	41	0	0	1	0
3	A	36	0	0	2	0
3	B	25	0	0	3	0
3	C	37	0	0	6	0
3	D	34	0	0	3	0
All	All	9736	0	9667	219	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 11.

All (219) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:867:LYS:HE3	1:D:875:LYS:HG2	1.24	1.18
1:D:867:LYS:HE3	1:D:875:LYS:CG	1.76	1.15
1:C:962:ARG:NH2	1:C:966:ILE:HD11	1.65	1.11
1:C:754:LYS:HG2	1:C:759:ILE:HG13	1.31	1.09
1:D:722:ALA:HB1	1:D:875:LYS:HD2	1.36	1.06
1:D:867:LYS:CE	1:D:875:LYS:HG2	1.88	1.03
1:C:962:ARG:HH21	1:C:966:ILE:HD11	0.86	1.03
1:D:867:LYS:O	1:D:876:VAL:HG13	1.59	1.01
1:C:962:ARG:HH21	1:C:966:ILE:CD1	1.73	1.00
1:A:729:GLY:HA3	1:A:744:ILE:HD11	1.45	0.99
1:B:833:LEU:HD22	1:B:856:PHE:HZ	1.32	0.94
1:D:867:LYS:O	1:D:876:VAL:CG1	2.16	0.92
1:A:729:GLY:HA3	1:A:744:ILE:CD1	2.05	0.86
1:B:752:SER:HB3	1:B:756:ASN:OD1	1.80	0.82
1:D:867:LYS:HE3	1:D:875:LYS:HG3	1.61	0.81
1:C:793:MET:HE1	1:C:852:LYS:HD3	1.64	0.80
1:B:1007:MET:HE3	3:B:1223:HOH:O	1.80	0.80
1:B:999:ARG:HH21	1:B:1007:MET:HG2	1.48	0.78
1:C:812:GLN:CG	3:C:1215:HOH:O	2.33	0.77
1:C:986:ARG:HG3	1:C:986:ARG:HH11	1.50	0.76
1:D:722:ALA:HB1	1:D:875:LYS:CD	2.13	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:701:GLN:HA	1:C:764:TYR:CE1	2.20	0.75
1:C:986:ARG:HG3	1:C:986:ARG:NH1	2.00	0.75
1:B:752:SER:CB	1:B:756:ASN:OD1	2.34	0.74
1:B:833:LEU:HD22	1:B:856:PHE:CZ	2.21	0.74
1:D:867:LYS:HZ1	1:D:875:LYS:HE3	1.53	0.73
1:B:709:GLU:OE2	1:B:783:THR:CB	2.35	0.73
1:D:868:GLU:HG3	1:D:876:VAL:HG21	1.72	0.71
1:C:923:ILE:HD13	1:C:926:ILE:HD11	1.71	0.71
1:B:999:ARG:NH2	1:B:1007:MET:HG2	2.06	0.70
1:B:999:ARG:HH21	1:B:1007:MET:CG	2.06	0.69
1:C:754:LYS:HG2	1:C:759:ILE:CG1	2.16	0.69
1:C:908:MET:HE3	1:C:943:VAL:HG11	1.74	0.68
1:C:983:GLY:O	1:C:986:ARG:HG2	1.94	0.67
1:D:875:LYS:HD3	1:D:875:LYS:N	2.10	0.66
1:A:973:ARG:NH1	1:A:1012:ASP:O	2.25	0.66
1:D:832:ARG:HG3	1:D:832:ARG:HH11	1.61	0.66
1:A:730:LEU:HD22	1:A:739:LYS:HB2	1.78	0.66
1:D:913:LYS:HD2	1:D:914:PRO:HD2	1.78	0.66
1:D:726:VAL:HG22	1:D:745:LYS:HG3	1.77	0.65
1:D:925:SER:O	1:D:929:LYS:HE2	1.95	0.65
1:C:701:GLN:HA	1:C:764:TYR:HE1	1.60	0.65
1:D:756:ASN:ND2	3:D:1101:HOH:O	2.21	0.65
1:A:943:VAL:HG22	1:A:971:MET:HE1	1.78	0.65
1:B:831:ARG:HB2	1:B:833:LEU:HD12	1.78	0.65
1:C:995:SER:O	1:C:999:ARG:HG3	1.97	0.65
1:C:812:GLN:HG2	3:C:1215:HOH:O	1.96	0.64
1:C:812:GLN:HG3	3:C:1215:HOH:O	1.94	0.63
1:B:728:LYS:HG2	1:B:792:LEU:HD11	1.79	0.63
1:B:745:LYS:HE2	2:B:1101:ZRT:C14	2.29	0.63
1:B:724:GLY:H	1:B:745:LYS:HZ1	1.46	0.63
1:B:834:VAL:HG12	1:B:836:ARG:HG3	1.81	0.63
1:B:759:ILE:HD13	1:B:786:VAL:HG21	1.80	0.63
1:B:713:LYS:HD2	1:B:715:ILE:HD11	1.81	0.62
1:A:943:VAL:HG22	1:A:971:MET:CE	2.28	0.62
1:B:998:TYR:HD1	1:B:1002:MET:HE3	1.64	0.62
1:B:763:ALA:HA	1:B:766:MET:HE3	1.82	0.62
1:D:825:MET:HE2	1:D:838:LEU:HD22	1.82	0.61
1:B:989:LEU:HG	1:B:990:PRO:HD2	1.83	0.61
1:A:1011:VAL:N	3:A:1106:HOH:O	2.34	0.60
1:B:723:PHE:CB	1:B:745:LYS:HZ1	2.16	0.59
1:D:879:LYS:HD3	1:D:915:TYR:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:990:PRO:HB2	1:C:994:ASP:HB2	1.84	0.58
1:D:883:LEU:HD21	1:D:928:GLU:HG2	1.86	0.58
1:C:961:PHE:HA	1:C:964:LEU:HD12	1.86	0.58
1:B:908:MET:CE	1:B:943:VAL:HG11	2.33	0.58
1:D:949:LYS:NZ	3:D:1107:HOH:O	2.36	0.57
1:A:961:PHE:HA	1:A:964:LEU:HD12	1.86	0.57
1:C:796:GLY:HA2	2:C:1101:ZRT:C28	2.33	0.57
1:B:723:PHE:CB	1:B:745:LYS:CE	2.82	0.57
1:D:755:ALA:HB3	1:D:758:GLU:OE1	2.04	0.57
1:B:938:ILE:HG13	1:B:979:LEU:HD22	1.87	0.57
1:D:718:LEU:HD21	1:D:728:LYS:HB2	1.87	0.57
1:B:830:ASP:HB3	1:C:717:VAL:HG11	1.86	0.57
1:C:881:MET:HE3	1:C:891:TYR:OH	2.05	0.56
1:B:998:TYR:CD1	1:B:1002:MET:HE3	2.39	0.56
1:A:795:PHE:HE2	1:A:1002:MET:HE1	1.70	0.56
1:B:826:ASN:ND2	3:B:1205:HOH:O	2.39	0.56
1:B:884:GLU:OE2	1:B:958:ARG:NH1	2.23	0.56
1:C:729:GLY:HA3	1:C:744:ILE:HD12	1.88	0.56
1:C:962:ARG:NH2	1:C:966:ILE:CD1	2.49	0.56
1:B:726:VAL:HG22	1:B:745:LYS:HD3	1.88	0.55
1:A:768:SER:OG	1:A:831:ARG:NH2	2.24	0.54
1:D:812:GLN:OE1	1:D:975:PRO:HG3	2.08	0.54
1:B:724:GLY:HA3	1:B:746:GLU:O	2.08	0.54
1:D:752:SER:O	1:D:753:PRO:C	2.51	0.53
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.43	0.53
1:B:715:ILE:HG22	1:B:716:LYS:HD2	1.91	0.53
1:B:747:LEU:O	1:B:785:THR:HB	2.08	0.52
1:B:752:SER:HB2	1:B:756:ASN:OD1	2.09	0.52
1:D:825:MET:CE	1:D:838:LEU:HD22	2.39	0.52
1:B:835:HIS:C	1:B:836:ARG:HE	2.18	0.52
1:B:724:GLY:H	1:B:745:LYS:NZ	2.08	0.51
1:B:883:LEU:HD22	1:B:953:ILE:HD12	1.92	0.51
1:B:820:GLN:HE21	1:B:1010:VAL:HG21	1.76	0.51
1:B:877:PRO:O	1:B:881:MET:HG3	2.09	0.51
1:D:867:LYS:NZ	1:D:875:LYS:HG2	2.26	0.51
1:D:722:ALA:CB	1:D:875:LYS:HD2	2.23	0.50
1:D:715:ILE:HD11	1:D:730:LEU:HD12	1.94	0.50
1:D:1004:GLU:HB2	1:B:1004:GLU:HG3	1.93	0.50
1:D:908:MET:HG3	1:D:939:CYS:SG	2.52	0.50
1:C:832:ARG:NH1	3:C:1208:HOH:O	2.42	0.50
1:D:832:ARG:HG3	1:D:832:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:865:GLU:H	1:D:867:LYS:HD2	1.77	0.49
1:B:908:MET:HE3	1:B:943:VAL:HG11	1.93	0.49
1:B:708:LYS:HG3	1:B:710:THR:HG22	1.94	0.49
1:A:924:SER:O	1:A:928:GLU:HG3	2.11	0.49
1:C:950:CYS:O	1:C:958:ARG:HD3	2.12	0.49
1:C:701:GLN:HA	1:C:764:TYR:CD1	2.47	0.49
1:D:1000:ALA:HB2	1:B:776:ARG:HH12	1.77	0.49
1:B:996:ASN:ND2	3:B:1202:HOH:O	2.27	0.49
1:B:831:ARG:CB	1:B:833:LEU:HD12	2.42	0.49
1:D:809:ILE:HD12	1:D:817:TRP:HH2	1.78	0.48
1:B:720:SER:HB3	1:B:725:THR:HG23	1.95	0.48
1:B:925:SER:O	1:B:929:LYS:HG2	2.13	0.48
1:D:705:ARG:NH1	1:B:994:ASP:OD1	2.46	0.48
1:C:989:LEU:HB3	1:C:990:PRO:HD2	1.95	0.48
1:C:942:ASP:HB3	1:C:971:MET:HE3	1.95	0.48
1:B:782:LEU:HD23	1:B:782:LEU:HA	1.55	0.48
1:B:904:VAL:O	1:B:908:MET:HG2	2.14	0.48
1:D:929:LYS:HD3	1:D:929:LYS:N	2.28	0.48
1:A:998:TYR:CE1	1:A:1002:MET:SD	3.07	0.48
1:B:796:GLY:HA2	2:B:1101:ZRT:C28	2.43	0.48
1:B:745:LYS:HB3	1:B:788:LEU:HB2	1.94	0.48
1:B:877:PRO:HB2	1:B:880:TRP:HB2	1.94	0.47
1:C:823:LYS:NZ	3:C:1206:HOH:O	2.37	0.47
1:D:804:GLU:OE1	1:D:805:HIS:CE1	2.67	0.47
1:A:812:GLN:HG2	1:A:975:PRO:HG3	1.96	0.47
1:C:986:ARG:HH11	1:C:986:ARG:CG	2.18	0.47
1:D:1001:LEU:HD21	1:B:742:VAL:HG12	1.95	0.47
1:D:751:THR:HG21	1:D:864:ALA:C	2.39	0.47
1:C:905:TRP:HD1	1:C:947:MET:HE1	1.79	0.46
1:D:948:ARG:HD2	1:D:948:ARG:HA	1.71	0.46
1:A:750:ALA:C	1:A:752:SER:H	2.24	0.46
1:D:812:GLN:NE2	1:D:1011:VAL:O	2.49	0.46
1:B:766:MET:O	1:B:769:VAL:HG22	2.16	0.46
1:B:793:MET:CE	1:B:852:LYS:HD3	2.46	0.46
1:C:905:TRP:CD1	1:C:947:MET:HE1	2.51	0.46
1:B:960:LYS:HD2	1:B:960:LYS:HA	1.65	0.46
1:B:724:GLY:N	1:B:745:LYS:HZ1	2.12	0.46
1:D:812:GLN:NE2	1:D:816:ASN:OD1	2.49	0.46
1:D:905:TRP:HB2	1:D:947:MET:HE3	1.97	0.46
1:A:790:MET:HE3	1:A:790:MET:HB3	1.86	0.46
1:D:861:LEU:HD12	1:D:862:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:882:ALA:HA	1:D:898:TRP:CD2	2.51	0.45
1:C:701:GLN:CA	1:C:764:TYR:HE1	2.27	0.45
1:A:729:GLY:HA3	1:A:744:ILE:HD12	1.95	0.45
1:D:836:ARG:HG2	1:D:891:TYR:CG	2.51	0.45
1:B:762:GLU:O	1:B:766:MET:HG3	2.16	0.45
1:D:836:ARG:HG2	1:D:891:TYR:CD1	2.52	0.45
1:A:752:SER:HA	1:A:753:PRO:HD3	1.87	0.45
1:A:925:SER:OG	3:A:1101:HOH:O	2.21	0.45
1:D:976:GLN:NE2	3:D:1108:HOH:O	2.49	0.45
1:A:900:TYR:O	1:A:904:VAL:HG23	2.17	0.45
1:B:795:PHE:HB2	1:B:845:VAL:O	2.16	0.45
1:B:829:GLU:HG3	1:B:893:HIS:CG	2.52	0.45
1:B:990:PRO:HB2	1:B:994:ASP:HB2	1.98	0.44
1:B:750:ALA:O	1:B:752:SER:N	2.49	0.44
1:D:783:THR:OG1	1:D:784:SER:N	2.50	0.44
1:A:752:SER:O	1:A:754:LYS:N	2.46	0.44
1:A:795:PHE:CE2	1:A:1002:MET:HE1	2.50	0.44
1:C:913:LYS:NZ	1:C:913:LYS:HB3	2.33	0.44
1:D:867:LYS:O	1:D:876:VAL:HG11	2.12	0.44
1:B:813:TYR:OH	1:B:990:PRO:HD3	2.18	0.44
1:C:772:PRO:O	1:C:850:HIS:NE2	2.51	0.44
1:C:783:THR:OG1	1:C:784:SER:N	2.49	0.44
1:A:1002:MET:HE3	1:C:740:ILE:HG12	2.00	0.44
1:C:803:ARG:HG3	1:C:911:GLY:HA3	2.00	0.44
1:D:755:ALA:O	1:D:759:ILE:HG13	2.18	0.44
1:D:790:MET:HE3	1:D:790:MET:HB3	1.87	0.44
1:C:971:MET:HE2	1:C:978:TYR:HB3	1.99	0.44
1:C:850:HIS:ND1	1:C:1003:ASP:OD2	2.34	0.44
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.52	0.44
1:C:705:ARG:NH2	1:C:711:GLU:OE1	2.50	0.43
1:C:708:LYS:O	1:C:711:GLU:HG2	2.18	0.43
1:A:836:ARG:HG2	1:A:891:TYR:CD1	2.53	0.43
1:C:793:MET:CE	1:C:852:LYS:HD3	2.40	0.43
1:D:825:MET:HE2	1:D:838:LEU:HD13	1.99	0.43
1:C:716:LYS:HE3	1:C:728:LYS:HD3	2.01	0.43
1:B:755:ALA:O	1:B:759:ILE:HD12	2.19	0.43
1:D:788:LEU:HD11	1:D:858:LEU:HD21	2.01	0.43
1:C:962:ARG:HD2	1:C:962:ARG:HA	1.68	0.42
1:D:793:MET:HE1	1:D:852:LYS:HD3	2.01	0.42
1:C:736:GLU:C	1:C:737:LYS:HD2	2.43	0.42
1:A:998:TYR:HE1	1:A:1002:MET:SD	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:723:PHE:CB	1:B:745:LYS:NZ	2.81	0.42
1:B:791:GLN:H	1:B:791:GLN:HG3	1.72	0.42
1:D:750:ALA:CB	1:D:862:LEU:HA	2.49	0.42
1:D:858:LEU:HD23	1:D:858:LEU:HA	1.87	0.42
1:D:1012:ASP:OD1	1:D:1012:ASP:N	2.53	0.42
1:B:725:THR:HB	1:B:727:TYR:CE1	2.55	0.42
1:B:714:LYS:HG2	1:B:727:TYR:CG	2.54	0.42
1:B:948:ARG:HA	1:B:948:ARG:HD2	1.85	0.42
1:C:739:LYS:NZ	3:C:1213:HOH:O	2.52	0.42
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.54	0.42
1:C:947:MET:HE2	1:C:951:TRP:CH2	2.55	0.42
1:A:750:ALA:C	1:A:752:SER:N	2.78	0.41
1:A:943:VAL:O	1:A:947:MET:HG3	2.19	0.41
1:D:823:LYS:HA	1:D:965:ILE:HD11	2.01	0.41
1:B:718:LEU:HD22	2:B:1101:ZRT:C25	2.49	0.41
1:B:905:TRP:HB2	1:B:947:MET:HE3	2.02	0.41
1:B:999:ARG:HA	1:B:1003:ASP:HB3	2.01	0.41
1:C:829:GLU:HG3	1:C:893:HIS:HB3	2.02	0.41
1:D:816:ASN:O	1:D:820:GLN:HG3	2.21	0.41
1:A:797:CYS:HA	1:A:844:LEU:HA	2.03	0.41
1:D:803:ARG:HG3	1:D:911:GLY:HA3	2.02	0.41
1:D:734:GLU:O	1:D:736:GLU:HG2	2.20	0.41
1:D:867:LYS:HZ3	1:D:867:LYS:HG2	1.66	0.41
1:D:962:ARG:NH2	1:A:718:LEU:O	2.54	0.41
1:D:811:SER:HB3	1:D:981:ILE:HD12	2.02	0.41
1:D:750:ALA:HB1	1:D:862:LEU:HA	2.03	0.41
1:A:745:LYS:HB3	1:A:788:LEU:HB2	2.03	0.41
1:B:746:GLU:HG3	1:B:787:GLN:HG2	2.02	0.41
1:B:785:THR:O	1:B:786:VAL:C	2.64	0.41
1:D:962:ARG:NH2	1:A:719:GLY:HA2	2.36	0.40
1:D:825:MET:CE	1:D:838:LEU:HB2	2.51	0.40
1:A:944:TYR:CZ	1:A:948:ARG:HD3	2.56	0.40
1:C:737:LYS:HD2	1:C:737:LYS:N	2.35	0.40
1:B:812:GLN:HG2	1:B:989:LEU:HD22	2.02	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	300/328 (92%)	289 (96%)	9 (3%)	2 (1%)	18	38
1	B	288/328 (88%)	267 (93%)	17 (6%)	4 (1%)	9	19
1	C	282/328 (86%)	273 (97%)	8 (3%)	1 (0%)	30	51
1	D	295/328 (90%)	273 (92%)	19 (6%)	3 (1%)	12	28
All	All	1165/1312 (89%)	1102 (95%)	53 (4%)	10 (1%)	14	30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	806	LYS
1	A	806	LYS
1	B	722	ALA
1	B	751	THR
1	B	753	PRO
1	D	923	ILE
1	A	783	THR
1	C	783	THR
1	B	783	THR
1	D	753	PRO

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	268/288 (93%)	265 (99%)	3 (1%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	257/288 (89%)	251 (98%)	6 (2%)	44	71
1	C	255/288 (88%)	248 (97%)	7 (3%)	39	67
1	D	267/288 (93%)	259 (97%)	8 (3%)	36	64
All	All	1047/1152 (91%)	1023 (98%)	24 (2%)	45	71

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	713	LYS
1	D	749	GLU
1	D	867	LYS
1	D	868	GLU
1	D	876	VAL
1	D	922[A]	GLU
1	D	922[B]	GLU
1	D	925	SER
1	A	962	ARG
1	A	985	GLU
1	A	995	SER
1	B	749	GLU
1	B	754	LYS
1	B	784	SER
1	B	926	ILE
1	B	956	ASP
1	B	1010	VAL
1	C	745	LYS
1	C	782	LEU
1	C	921	SER
1	C	960	LYS
1	C	962	ARG
1	C	986	ARG
1	C	987	MET

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

Mol	Chain	Res	Type
1	D	805	HIS
1	D	976	GLN
1	A	894	GLN
1	A	988	HIS

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Mol	Chain	Res	Type
1	B	787	GLN
1	B	812	GLN
1	B	826	ASN
1	C	756	ASN
1	C	791	GLN
1	C	808	ASN

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](#)

2 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	$\# Z > 2$
2	ZRT	C	1101	1	44,45,45	1.52	8 (18%)	56,62,62	2.16	15 (26%)
2	ZRT	B	1101	1	44,45,45	1.64	8 (18%)	56,62,62	2.26	15 (26%)

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	ZRT	C	1101	1	-	12/28/36/36	0/5/5/5
2	ZRT	B	1101	1	-	5/28/36/36	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	ZRT	C30-N29	4.74	1.45	1.35
2	C	1101	ZRT	C30-N29	4.64	1.45	1.35
2	B	1101	ZRT	C33-C32	-4.52	1.32	1.51
2	B	1101	ZRT	C18-N22	4.16	1.45	1.36
2	C	1101	ZRT	C18-N22	3.56	1.44	1.36
2	B	1101	ZRT	C04-C05	3.17	1.54	1.51
2	B	1101	ZRT	C10-C09	2.97	1.52	1.48
2	C	1101	ZRT	C10-C09	2.66	1.52	1.48
2	C	1101	ZRT	C06-N07	-2.56	1.31	1.35
2	C	1101	ZRT	C18-N19	-2.51	1.31	1.34
2	C	1101	ZRT	C04-C05	2.48	1.53	1.51
2	C	1101	ZRT	O31-C30	-2.43	1.18	1.23
2	B	1101	ZRT	C27-N29	2.32	1.46	1.41
2	B	1101	ZRT	C06-N07	-2.31	1.31	1.35
2	B	1101	ZRT	O31-C30	-2.22	1.18	1.23
2	C	1101	ZRT	C26-N34	2.16	1.46	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	ZRT	C20-N19-C18	7.90	122.02	115.42
2	C	1101	ZRT	C20-N19-C18	7.69	121.84	115.42
2	B	1101	ZRT	N19-C18-N17	-4.90	121.68	126.42
2	C	1101	ZRT	C33-C32-C30	4.87	129.28	113.29
2	B	1101	ZRT	N17-C16-N07	4.80	120.87	114.25
2	B	1101	ZRT	C21-C20-N19	-4.79	118.10	123.97
2	C	1101	ZRT	C21-C20-N19	-4.59	118.35	123.97
2	C	1101	ZRT	N19-C18-N17	-4.40	122.17	126.42
2	B	1101	ZRT	O40-C24-C23	4.35	120.23	114.81
2	B	1101	ZRT	C05-C09-N08	-4.20	107.42	111.62
2	C	1101	ZRT	N17-C16-N07	4.16	119.99	114.25
2	C	1101	ZRT	O40-C24-C23	4.03	119.83	114.81
2	B	1101	ZRT	C25-C26-N34	-3.70	117.20	122.59
2	C	1101	ZRT	C05-C09-N08	-3.69	107.93	111.62
2	B	1101	ZRT	C41-O40-C24	-3.63	112.18	117.51
2	C	1101	ZRT	C10-C09-N08	3.49	124.21	118.99
2	B	1101	ZRT	C09-N08-N07	3.18	107.48	104.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	ZRT	C16-N07-N08	2.69	122.94	119.96
2	B	1101	ZRT	C16-N07-N08	2.68	122.93	119.96
2	C	1101	ZRT	C41-O40-C24	-2.65	113.63	117.51
2	B	1101	ZRT	O40-C24-C25	-2.62	119.56	124.08
2	B	1101	ZRT	C20-C21-C16	2.40	118.29	115.94
2	B	1101	ZRT	C39-N34-C35	-2.40	106.18	111.57
2	B	1101	ZRT	C38-O37-C36	2.37	117.53	109.88
2	C	1101	ZRT	O40-C24-C25	-2.36	120.00	124.08
2	C	1101	ZRT	C25-C26-N34	-2.33	119.20	122.59
2	C	1101	ZRT	C39-N34-C26	2.26	121.56	116.19
2	C	1101	ZRT	C39-N34-C35	-2.24	106.52	111.57
2	C	1101	ZRT	C09-N08-N07	2.19	106.67	104.89
2	B	1101	ZRT	C33-C32-C30	2.11	120.23	113.29

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	ZRT	C23-C24-O40-C41
2	B	1101	ZRT	C25-C24-O40-C41
2	C	1101	ZRT	C21-C16-N07-C06
2	C	1101	ZRT	C21-C16-N07-N08
2	C	1101	ZRT	N17-C16-N07-N08
2	C	1101	ZRT	N17-C16-N07-C06
2	C	1101	ZRT	C23-C24-O40-C41
2	C	1101	ZRT	C25-C24-O40-C41
2	B	1101	ZRT	C25-C26-N34-C39
2	C	1101	ZRT	N08-C09-C10-C11
2	B	1101	ZRT	C25-C26-N34-C35
2	C	1101	ZRT	N08-C09-C10-C15
2	B	1101	ZRT	N02-C04-C05-C09
2	C	1101	ZRT	C05-C09-C10-C11
2	C	1101	ZRT	C05-C09-C10-C15
2	C	1101	ZRT	N29-C30-C32-C33
2	C	1101	ZRT	O31-C30-C32-C33

There are no ring outliers.

2 monomers are involved in 4 short contacts:

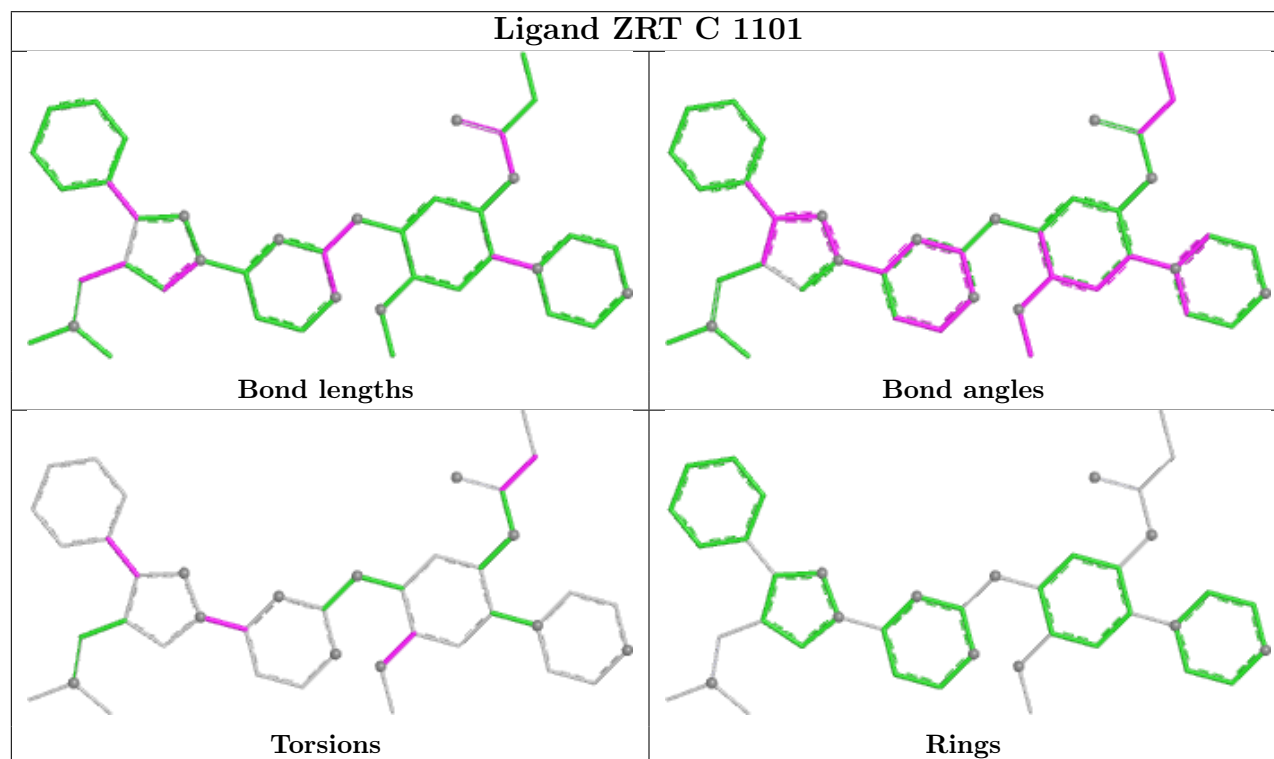
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1101	ZRT	1	0

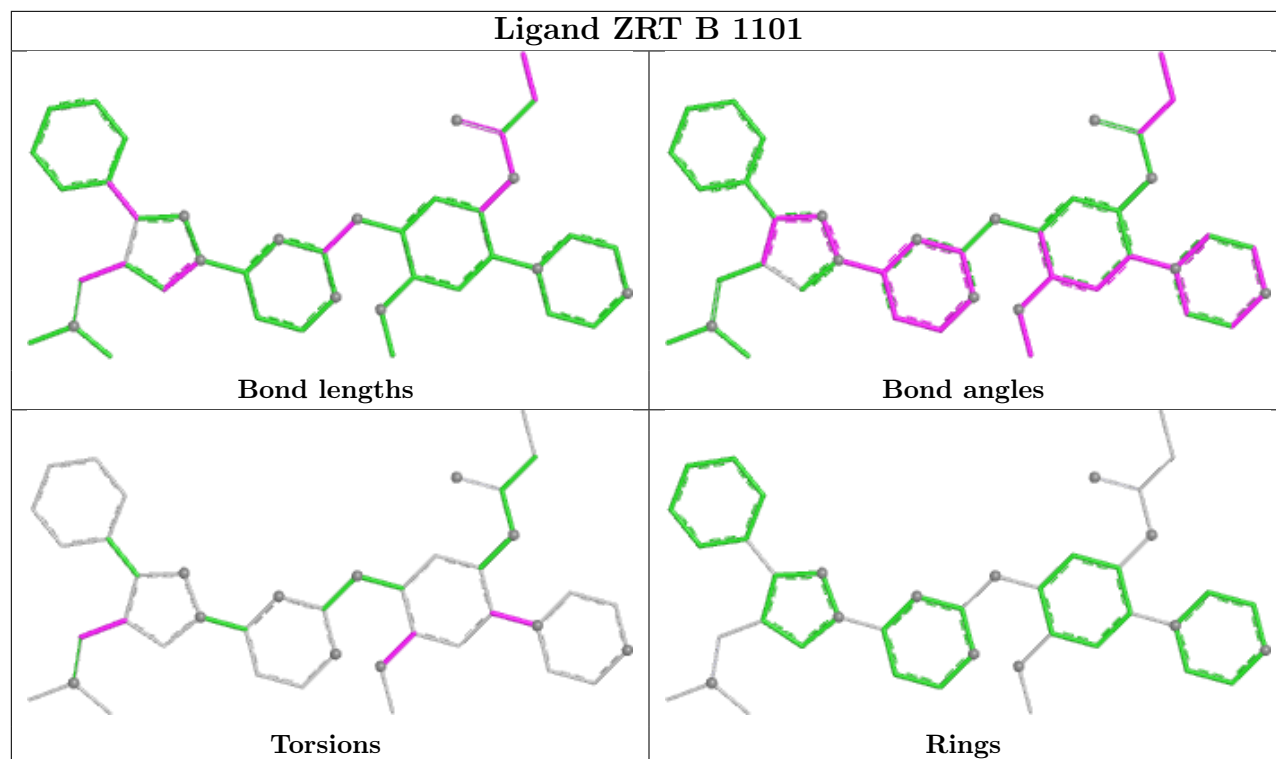
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	ZRT	3	0

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	306/328 (93%)	0.39	13 (4%) 40 35	26, 40, 65, 82	0
1	B	292/328 (89%)	0.51	18 (6%) 26 21	28, 44, 74, 100	0
1	C	287/328 (87%)	0.40	9 (3%) 51 45	24, 42, 69, 90	1 (0%)
1	D	300/328 (91%)	0.36	10 (3%) 49 43	23, 41, 72, 88	1 (0%)
All	All	1185/1312 (90%)	0.41	50 (4%) 40 35	23, 42, 70, 100	2 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1010	VAL	4.4
1	B	989	LEU	4.4
1	B	858	LEU	4.0
1	B	786	VAL	3.8
1	C	922[A]	GLU	3.6
1	B	1008	ASP	3.6
1	B	753	PRO	3.6
1	A	917	GLY	3.3
1	B	918	ILE	3.2
1	A	783	THR	3.2
1	B	782	LEU	3.1
1	B	988	HIS	3.1
1	A	782	LEU	3.0
1	D	751	THR	2.8
1	A	702	ALA	2.8
1	C	858	LEU	2.8
1	D	866	GLU	2.8
1	B	1007	MET	2.8
1	A	868	GLU	2.7
1	B	751	THR	2.6
1	A	807	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	807	ASP	2.6
1	B	1009	ASP	2.6
1	A	873	GLY	2.5
1	C	756	ASN	2.5
1	B	784	SER	2.5
1	A	874	GLY	2.4
1	C	988	HIS	2.4
1	D	987	MET	2.4
1	D	990	PRO	2.3
1	D	988	HIS	2.3
1	A	784	SER	2.3
1	B	722	ALA	2.3
1	A	988	HIS	2.2
1	B	990	PRO	2.2
1	D	750	ALA	2.2
1	B	917	GLY	2.2
1	C	760	LEU	2.2
1	B	758	GLU	2.1
1	B	747	LEU	2.1
1	A	756	ASN	2.1
1	C	861	LEU	2.1
1	C	989	LEU	2.1
1	C	928	GLU	2.0
1	D	752	SER	2.0
1	A	757	LYS	2.0
1	D	986	ARG	2.0
1	D	755	ALA	2.0
1	C	784	SER	2.0
1	A	861	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

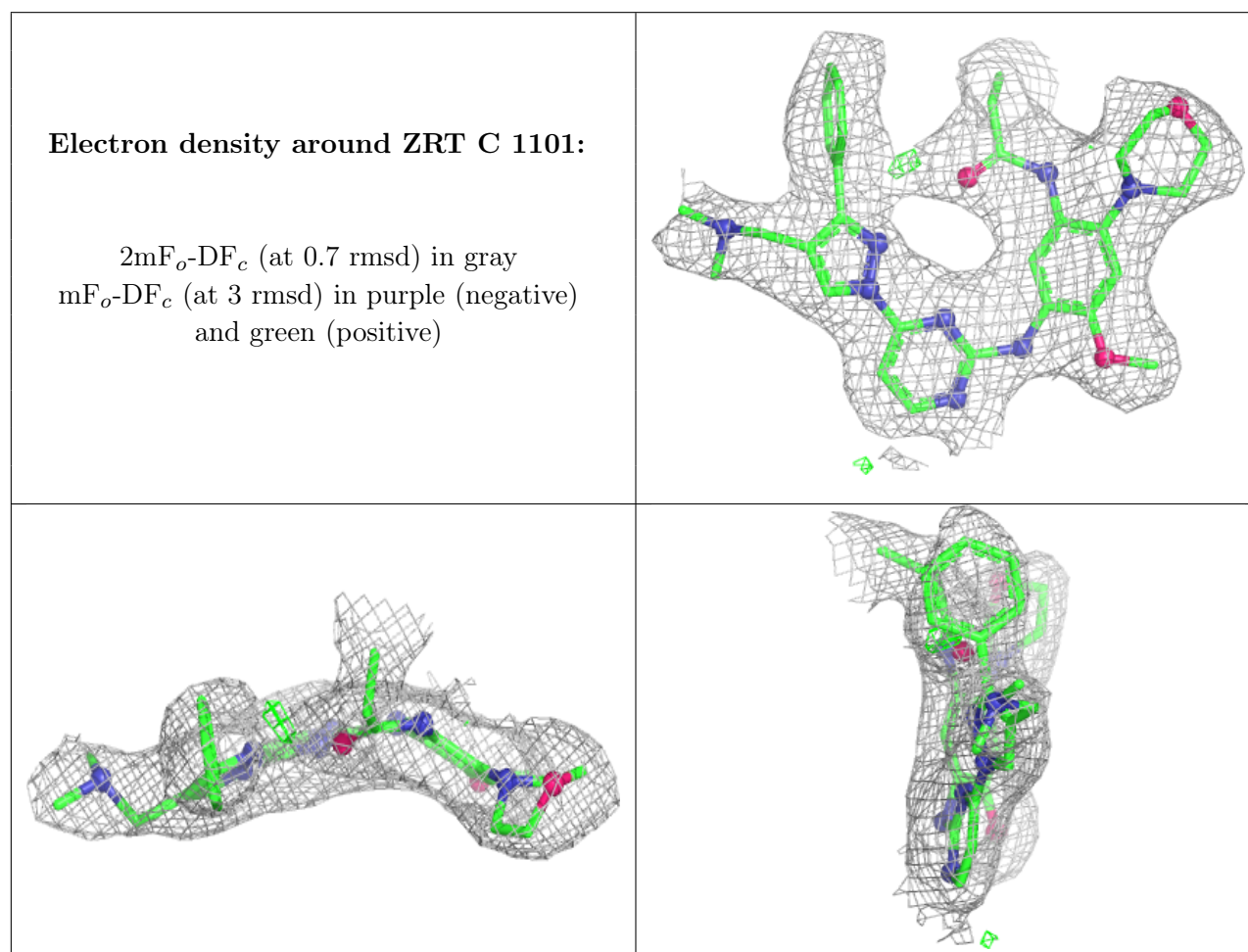
There are no oligosaccharides in this entry.

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, 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.

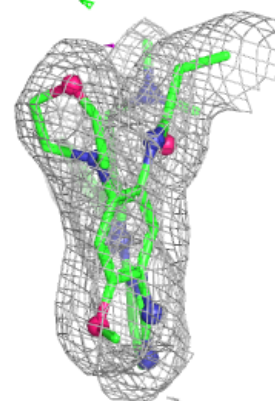
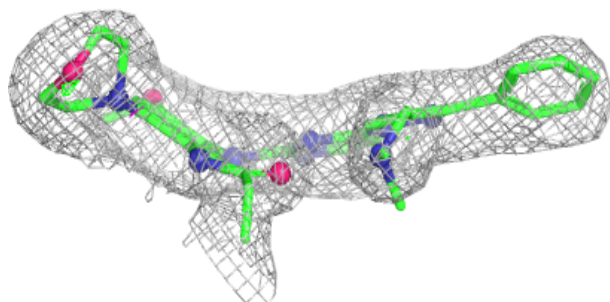
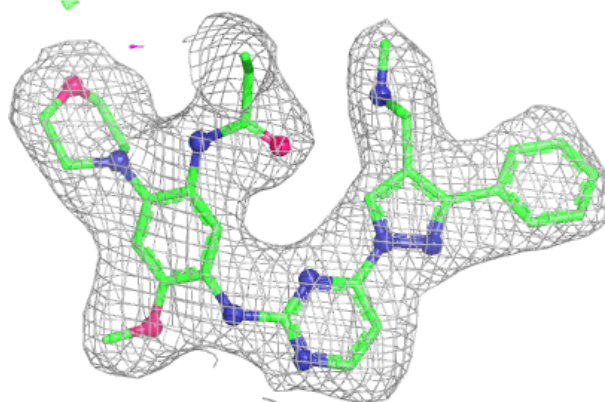
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZRT	C	1101	41/41	0.88	0.12	33,46,64,70	0
2	ZRT	B	1101	41/41	0.93	0.10	24,37,47,52	0

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 ZRT B 1101:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.