



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 10:05 AM EDT

PDB ID : 8F1W  
Title : EGFR(T790M/V948R) kinase in complex with poziotinib  
Authors : Beyett, T.S.; Eck, M.J.  
Deposited on : 2022-11-06  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

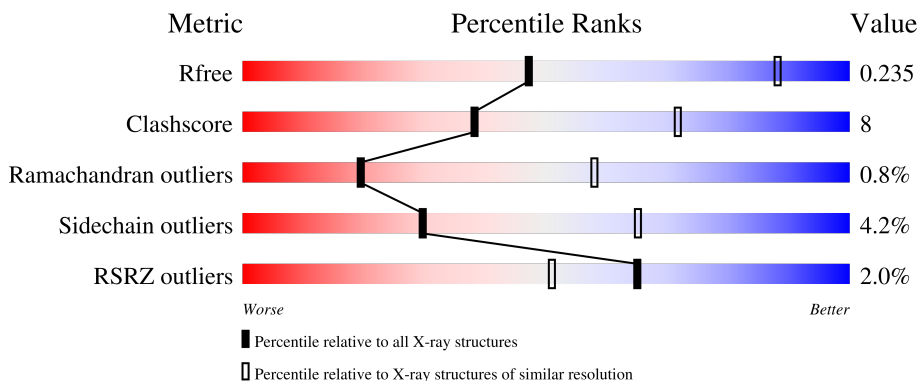
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	331	 72% 17% • 8%
1	B	331	 71% 14% •• 13%
1	C	331	 74% 11% • 12%
1	D	331	 75% 15% • 8%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9658 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.

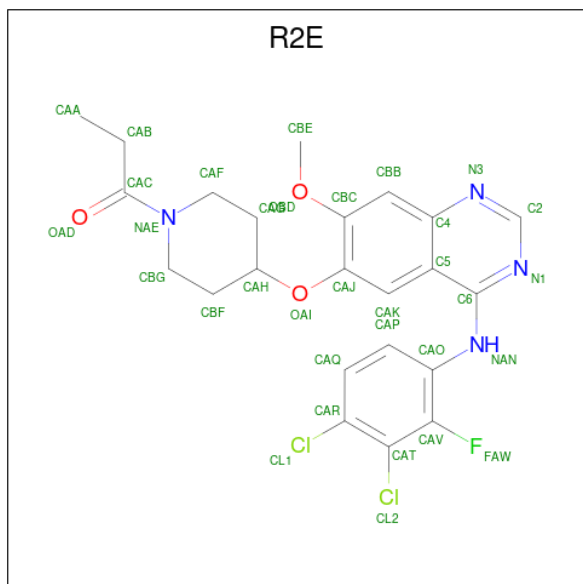
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	303	2430	1559	413	439	19	0	0	0
1	B	288	2322	1495	394	415	18	0	0	0
1	C	290	2336	1503	396	418	19	0	0	0
1	D	304	2438	1563	415	441	19	0	0	0

There are 20 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	THR	-	expression tag	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
B	692	GLY	-	expression tag	UNP P00533
B	693	SER	-	expression tag	UNP P00533
B	694	THR	-	expression tag	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
B	948	ARG	VAL	engineered mutation	UNP P00533
C	692	GLY	-	expression tag	UNP P00533
C	693	SER	-	expression tag	UNP P00533
C	694	THR	-	expression tag	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533
C	948	ARG	VAL	engineered mutation	UNP P00533
D	692	GLY	-	expression tag	UNP P00533
D	693	SER	-	expression tag	UNP P00533
D	694	THR	-	expression tag	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is 1-[4-[4-[[3,4-bis(chloranyl)-2-fluoranyl-phenyl]amino]-7-methoxy-quinazolin-6-yl]oxypiperidin-1-yl]propan-1-one (three-letter code: R2E) (formula:  $C_{23}H_{23}Cl_2FN_4O_3$ ) (labeled as "Ligand of Interest" by depositor).

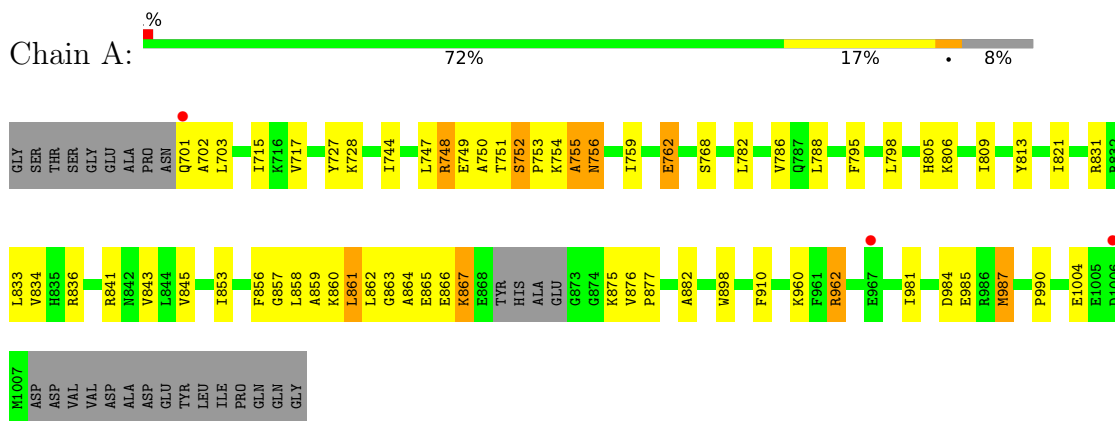


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	F	N			O
2	A	1	Total	C	Cl	F	N	O	0	0
			33	23	2	1	4	3		
2	B	1	Total	C	Cl	F	N	O	0	0
			33	23	2	1	4	3		
2	C	1	Total	C	Cl	F	N	O	0	0
			33	23	2	1	4	3		
2	D	1	Total	C	Cl	F	N	O	0	0
			33	23	2	1	4	3		

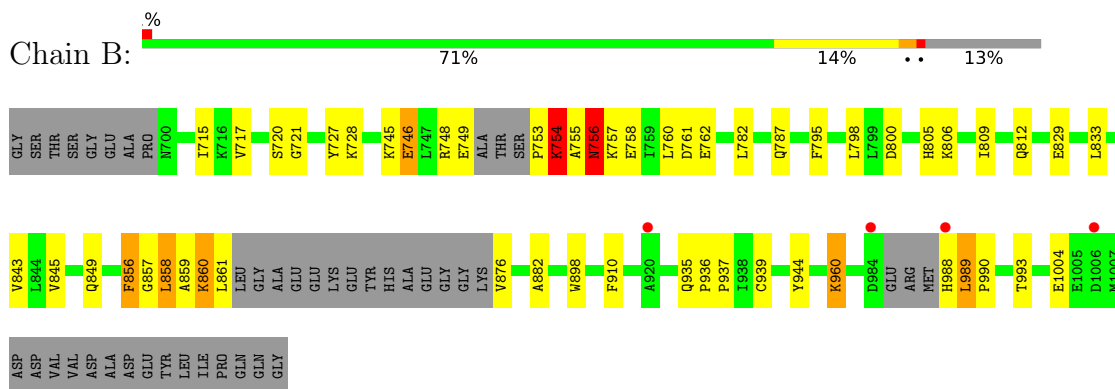
### 3 Residue-property plots [i](#)

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.

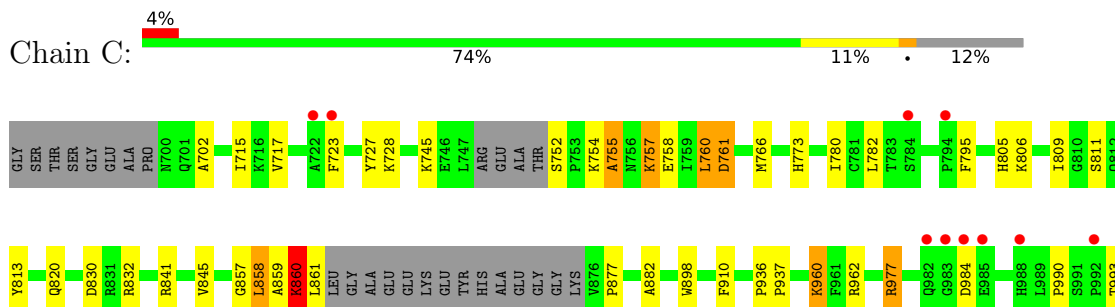
- Molecule 1: Epidermal growth factor receptor

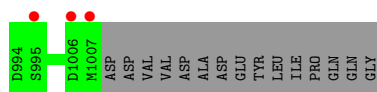


- Molecule 1: Epidermal growth factor receptor

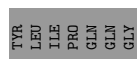
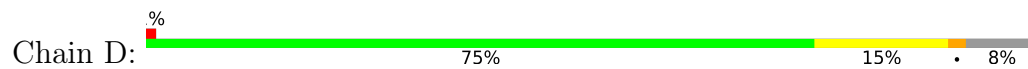


- Molecule 1: Epidermal growth factor receptor





- Molecule 1: Epidermal growth factor receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.79Å 102.53Å 87.33Å 90.00° 102.31° 90.00°	Depositor
Resolution (Å)	85.32 – 3.20 85.32 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (85.32-3.20) 97.1 (85.32-3.20)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.20.1	Depositor
R, $R_{free}$	0.231 , 0.274 0.236 , 0.235	Depositor DCC
$R_{free}$ test set	1033 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.8	Xtrriage
Anisotropy	0.552	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 35.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	9658	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.67 % 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 2.1094e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: R2E

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	0.29	0/2482	0.51	0/3353
1	B	0.27	0/2372	0.50	0/3205
1	C	0.28	0/2387	0.50	0/3227
1	D	0.30	0/2490	0.50	0/3364
All	All	0.28	0/9731	0.50	0/13149

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2430	0	2472	43	0
1	B	2322	0	2363	37	0
1	C	2336	0	2377	35	0
1	D	2438	0	2478	39	0
2	A	33	0	0	0	0
2	B	33	0	0	2	0
2	C	33	0	0	1	0
2	D	33	0	0	1	0
All	All	9658	0	9690	146	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 8.

All (146) 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:755:ALA:HB1	1:A:759:ILE:HG12	1.43	0.97
1:B:753:PRO:O	1:B:754:LYS:HB3	1.77	0.82
1:D:747:LEU:HD11	1:D:788:LEU:HD11	1.65	0.79
1:A:747:LEU:HD11	1:A:788:LEU:HD11	1.65	0.77
1:D:782:LEU:HD23	1:D:786:VAL:HG13	1.69	0.75
1:D:759:ILE:HG21	1:D:782:LEU:HD21	1.74	0.69
1:B:756:ASN:H	1:B:756:ASN:HD22	1.40	0.68
1:A:751:THR:HG22	1:A:861:LEU:HA	1.76	0.68
1:C:766:MET:SD	1:C:857:GLY:HA3	2.36	0.66
1:B:936:PRO:HB2	1:B:939:CYS:SG	2.35	0.66
1:D:782:LEU:CD2	1:D:786:VAL:HG13	2.27	0.64
1:A:701:GLN:HG2	1:A:703:LEU:H	1.64	0.62
1:A:867:LYS:HD2	1:A:876:VAL:HG11	1.81	0.61
1:C:859:ALA:O	1:C:860:LYS:C	2.39	0.61
1:B:755:ALA:O	1:B:757:LYS:N	2.34	0.61
1:B:748:ARG:HH21	1:C:832:ARG:HH11	1.48	0.60
1:A:701:GLN:HE21	1:A:703:LEU:HB2	1.66	0.60
1:C:755:ALA:O	1:C:757:LYS:N	2.29	0.60
1:D:849:GLN:HG2	1:D:990:PRO:HG3	1.84	0.60
1:A:754:LYS:O	1:A:755:ALA:HB2	2.01	0.60
1:D:812:GLN:HG2	1:D:989:LEU:HG	1.83	0.59
1:A:981:ILE:HB	1:A:984:ASP:HB2	1.84	0.58
1:D:750:ALA:O	1:D:751:THR:C	2.42	0.58
1:D:780:ILE:HD11	1:D:782:LEU:HD21	1.86	0.58
1:B:833:LEU:HD13	1:B:856:PHE:CZ	2.38	0.57
1:B:746:GLU:HG2	1:B:787:GLN:HG2	1.88	0.56
1:A:701:GLN:NE2	1:A:703:LEU:HB2	2.21	0.55
1:A:782:LEU:HD23	1:A:786:VAL:HG22	1.87	0.55
1:A:756:ASN:H	1:A:759:ILE:HG12	1.72	0.55
1:A:703:LEU:HD12	1:A:768:SER:HA	1.89	0.55
1:C:760:LEU:HG	1:C:782:LEU:HD11	1.89	0.55
1:A:701:GLN:HE22	1:A:768:SER:HB3	1.71	0.55
1:C:723:PHE:HD1	1:C:861:LEU:HD12	1.73	0.52
1:D:821:ILE:HG23	1:D:853:ILE:HD11	1.90	0.52
1:D:806:LYS:HB2	1:D:910:PHE:HB3	1.92	0.52
1:C:806:LYS:HB2	1:C:910:PHE:HB3	1.92	0.52
1:B:805:HIS:O	1:B:809:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1004:GLU:HB2	1:B:1004:GLU:HB2	1.92	0.51
1:B:806:LYS:HB2	1:B:910:PHE:HB3	1.92	0.51
1:B:755:ALA:O	1:B:756:ASN:C	2.48	0.51
1:A:866:GLU:OE1	1:A:875:LYS:HE2	2.11	0.51
1:A:806:LYS:HB2	1:A:910:PHE:HB3	1.92	0.51
1:C:745:LYS:HG3	2:C:1101:R2E:CAT	2.41	0.51
1:C:760:LEU:HD21	1:C:780:ILE:HG21	1.93	0.50
1:C:758:GLU:HA	1:C:761:ASP:HB2	1.94	0.50
1:D:724:GLY:HA2	1:D:748:ARG:HG3	1.92	0.50
1:D:745:LYS:HG3	2:D:1101:R2E:CAT	2.42	0.50
1:D:757:LYS:O	1:D:761:ASP:HB2	2.12	0.50
1:A:754:LYS:O	1:A:754:LYS:HG3	2.10	0.50
1:B:753:PRO:O	1:B:754:LYS:CB	2.56	0.49
1:C:755:ALA:C	1:C:757:LYS:H	2.14	0.49
1:A:752:SER:O	1:A:754:LYS:N	2.46	0.49
1:A:865:GLU:H	1:A:865:GLU:CD	2.16	0.49
1:B:720:SER:HB3	1:C:830:ASP:HA	1.93	0.49
1:D:751:THR:HG23	1:D:752:SER:N	2.28	0.49
1:B:721:GLY:O	1:B:748:ARG:NH1	2.46	0.48
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.49	0.48
1:B:858:LEU:HD12	1:B:858:LEU:HA	1.69	0.48
1:D:782:LEU:CD2	1:D:786:VAL:HG22	2.42	0.48
1:C:757:LYS:O	1:C:761:ASP:HB2	2.13	0.48
1:D:782:LEU:HD22	1:D:786:VAL:HG22	1.95	0.48
1:D:763:ALA:HA	1:D:766:MET:HE2	1.96	0.48
1:B:745:LYS:HG3	2:B:1101:R2E:CAT	2.44	0.48
1:D:715:ILE:HG12	1:D:728:LYS:O	2.14	0.48
1:D:860:LYS:HA	1:D:860:LYS:HD2	1.48	0.47
1:C:960:LYS:HB3	1:C:960:LYS:HE3	1.36	0.47
1:B:755:ALA:O	1:B:758:GLU:N	2.46	0.46
1:B:812:GLN:HG2	1:B:989:LEU:HG	1.97	0.46
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.51	0.46
1:D:700:ASN:HA	1:D:703:LEU:HD12	1.98	0.46
1:A:862:LEU:HB3	1:A:863:GLY:H	1.48	0.46
1:A:755:ALA:HB1	1:A:759:ILE:CG1	2.30	0.46
1:B:800:ASP:OD2	1:C:962:ARG:NH1	2.46	0.46
1:A:715:ILE:HG12	1:A:728:LYS:O	2.16	0.46
1:B:717:VAL:HG22	1:B:727:TYR:CE2	2.50	0.46
1:D:962:ARG:HE	1:D:962:ARG:HB3	1.59	0.45
1:A:717:VAL:HG22	1:A:727:TYR:CE2	2.51	0.45
1:A:813:TYR:OH	1:A:990:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:ILE:HG23	1:A:853:ILE:HD11	1.98	0.45
1:C:715:ILE:HG12	1:C:728:LYS:O	2.17	0.45
1:D:717:VAL:HG22	1:D:727:TYR:CE2	2.51	0.45
1:A:857:GLY:C	1:A:859:ALA:H	2.20	0.45
1:A:863:GLY:O	1:A:864:ALA:HB3	2.17	0.45
1:B:849:GLN:HG2	1:B:990:PRO:HG3	1.98	0.45
1:A:751:THR:O	1:A:752:SER:C	2.55	0.45
1:B:829:GLU:OE2	1:B:960:LYS:NZ	2.48	0.45
1:B:860:LYS:HA	1:B:860:LYS:HD2	1.73	0.45
1:D:723:PHE:CD1	1:D:858:LEU:HB3	2.52	0.45
1:C:860:LYS:O	1:C:861:LEU:C	2.55	0.44
1:C:977:ARG:HE	1:C:977:ARG:HB3	1.35	0.44
1:D:751:THR:OG1	1:D:752:SER:N	2.50	0.44
1:C:795:PHE:HB2	1:C:845:VAL:O	2.17	0.44
1:A:702:ALA:O	1:B:993:THR:HA	2.17	0.44
1:B:715:ILE:HG12	1:B:728:LYS:O	2.17	0.44
1:C:858:LEU:HD12	1:C:860:LYS:HD2	1.98	0.44
1:B:795:PHE:HB2	1:B:845:VAL:O	2.18	0.43
1:B:935:GLN:HA	1:B:944:TYR:CE1	2.52	0.43
1:D:989:LEU:HD22	1:D:990:PRO:HD2	1.98	0.43
1:B:936:PRO:HA	1:B:937:PRO:HD3	1.89	0.43
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.53	0.43
1:B:758:GLU:HA	1:B:761:ASP:HB2	1.99	0.43
1:C:813:TYR:OH	1:C:990:PRO:HD3	2.18	0.43
1:D:759:ILE:HG21	1:D:782:LEU:CD2	2.45	0.43
1:A:987:MET:HE2	1:A:987:MET:HB2	1.83	0.43
1:A:795:PHE:HB2	1:A:845:VAL:O	2.19	0.42
1:C:755:ALA:C	1:C:757:LYS:N	2.71	0.42
1:D:750:ALA:HA	1:D:861:LEU:HG	2.01	0.42
1:A:744:ILE:HA	1:A:788:LEU:O	2.20	0.42
1:A:862:LEU:HD23	1:A:862:LEU:HA	1.78	0.42
1:B:756:ASN:HD22	1:B:756:ASN:N	2.10	0.42
1:D:849:GLN:CG	1:D:990:PRO:HG3	2.47	0.42
2:B:1101:R2E:CBG	1:C:962:ARG:NH2	2.82	0.42
1:C:858:LEU:HD12	1:C:858:LEU:HA	1.83	0.42
1:A:798:LEU:N	1:A:843:VAL:O	2.46	0.42
1:D:700:ASN:C	1:D:702:ALA:H	2.23	0.42
1:D:798:LEU:N	1:D:843:VAL:O	2.48	0.42
1:C:717:VAL:HG22	1:C:727:TYR:CE2	2.54	0.42
1:A:762:GLU:OE1	1:A:860:LYS:HB3	2.20	0.41
1:C:702:ALA:O	1:D:993:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:752:SER:O	1:C:755:ALA:N	2.53	0.41
1:D:857:GLY:C	1:D:859:ALA:H	2.23	0.41
1:B:760:LEU:HD23	1:B:760:LEU:HA	1.91	0.41
1:B:782:LEU:HD23	1:B:782:LEU:HA	1.87	0.41
1:C:773:HIS:CD2	1:C:820:GLN:HB3	2.56	0.41
1:D:783:THR:C	1:D:785:THR:N	2.72	0.41
1:A:833:LEU:HD13	1:A:856:PHE:CZ	2.54	0.41
1:A:833:LEU:HB3	1:A:856:PHE:CE1	2.55	0.41
1:B:989:LEU:HD22	1:B:989:LEU:HA	1.94	0.41
1:B:748:ARG:NE	1:C:832:ARG:HD3	2.36	0.41
1:D:795:PHE:HB2	1:D:845:VAL:O	2.21	0.41
1:A:841:ARG:HH22	1:A:877:PRO:HB3	1.85	0.41
1:C:841:ARG:HH22	1:C:877:PRO:HB3	1.85	0.41
1:D:882:ALA:HA	1:D:898:TRP:CD2	2.55	0.41
1:B:857:GLY:C	1:B:859:ALA:H	2.24	0.41
1:A:750:ALA:O	1:A:751:THR:C	2.58	0.41
1:A:962:ARG:H	1:A:962:ARG:HG2	1.37	0.41
1:B:798:LEU:N	1:B:843:VAL:O	2.47	0.41
1:D:780:ILE:HG13	1:D:788:LEU:HD23	2.03	0.41
1:A:834:VAL:HG12	1:A:836:ARG:HG3	2.03	0.41
1:C:805:HIS:O	1:C:809:ILE:HG13	2.21	0.40
1:C:811:SER:OG	1:C:984:ASP:OD2	2.35	0.40
1:C:936:PRO:HA	1:C:937:PRO:HD3	1.97	0.40
1:D:867:LYS:HE3	1:D:867:LYS:HB3	1.97	0.40
1:A:805:HIS:O	1:A:809:ILE:HG13	2.22	0.40
1:C:993:THR:HA	1:D:702:ALA:O	2.21	0.40
1:D:841:ARG:HH22	1:D:877:PRO:HB3	1.87	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	299/331 (90%)	275 (92%)	20 (7%)	4 (1%)	12	47
1	B	280/331 (85%)	267 (95%)	11 (4%)	2 (1%)	22	61
1	C	284/331 (86%)	271 (95%)	11 (4%)	2 (1%)	22	61
1	D	300/331 (91%)	275 (92%)	24 (8%)	1 (0%)	41	74
All	All	1163/1324 (88%)	1088 (94%)	66 (6%)	9 (1%)	19	58

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	753	PRO
1	A	755	ALA
1	B	754	LYS
1	B	756	ASN
1	C	860	LYS
1	D	751	THR
1	A	861	LEU
1	C	755	ALA
1	A	748	ARG

### 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	267/290 (92%)	255 (96%)	12 (4%)	27	63
1	B	257/290 (89%)	244 (95%)	13 (5%)	24	60
1	C	259/290 (89%)	251 (97%)	8 (3%)	40	72
1	D	268/290 (92%)	257 (96%)	11 (4%)	30	66
All	All	1051/1160 (91%)	1007 (96%)	44 (4%)	30	65

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	748	ARG
1	A	749	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	752	SER
1	A	756	ASN
1	A	762	GLU
1	A	831	ARG
1	A	858	LEU
1	A	867	LYS
1	A	960	LYS
1	A	962	ARG
1	A	985	GLU
1	A	987	MET
1	B	746	GLU
1	B	749	GLU
1	B	754	LYS
1	B	756	ASN
1	B	762	GLU
1	B	856	PHE
1	B	858	LEU
1	B	860	LYS
1	B	861	LEU
1	B	876	VAL
1	B	960	LYS
1	B	988	HIS
1	B	989	LEU
1	C	754	LYS
1	C	757	LYS
1	C	760	LEU
1	C	761	ASP
1	C	858	LEU
1	C	860	LYS
1	C	960	LYS
1	C	977	ARG
1	D	752	SER
1	D	762	GLU
1	D	860	LYS
1	D	861	LEU
1	D	862	LEU
1	D	867	LYS
1	D	960	LYS
1	D	962	ARG
1	D	986	ARG
1	D	987	MET
1	D	989	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	701	GLN
1	A	816	ASN
1	B	756	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	R2E	B	1101	1	36,36,36	2.61	20 (55%)	50,51,51	2.28	17 (34%)
2	R2E	A	1101	1	36,36,36	2.63	20 (55%)	50,51,51	2.30	17 (34%)
2	R2E	C	1101	1	36,36,36	2.61	21 (58%)	50,51,51	2.30	17 (34%)
2	R2E	D	1101	1	36,36,36	2.58	19 (52%)	50,51,51	2.30	17 (34%)

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	R2E	B	1101	1	-	6/16/26/26	0/4/4/4
2	R2E	A	1101	1	-	6/16/26/26	0/4/4/4
2	R2E	C	1101	1	-	6/16/26/26	0/4/4/4
2	R2E	D	1101	1	-	6/16/26/26	0/4/4/4

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	R2E	C6-NAN	5.32	1.44	1.36
2	C	1101	R2E	C6-NAN	5.18	1.44	1.36
2	A	1101	R2E	CAC-NAE	5.17	1.45	1.35
2	D	1101	R2E	CAC-NAE	5.17	1.45	1.35
2	C	1101	R2E	CAC-NAE	5.08	1.45	1.35
2	B	1101	R2E	C6-NAN	5.06	1.43	1.36
2	B	1101	R2E	CAC-NAE	5.05	1.45	1.35
2	D	1101	R2E	C6-NAN	5.01	1.43	1.36
2	B	1101	R2E	C6-C5	4.45	1.50	1.44
2	C	1101	R2E	C6-C5	4.43	1.50	1.44
2	A	1101	R2E	C6-C5	4.39	1.50	1.44
2	D	1101	R2E	C6-C5	4.12	1.49	1.44
2	A	1101	R2E	FAW-CAV	-3.89	1.29	1.35
2	D	1101	R2E	FAW-CAV	-3.87	1.29	1.35
2	B	1101	R2E	FAW-CAV	-3.84	1.29	1.35
2	C	1101	R2E	FAW-CAV	-3.82	1.29	1.35
2	D	1101	R2E	CAA-CAB	-3.81	1.34	1.51
2	A	1101	R2E	CAA-CAB	-3.80	1.34	1.51
2	B	1101	R2E	CAA-CAB	-3.79	1.34	1.51
2	C	1101	R2E	CAA-CAB	-3.78	1.34	1.51
2	D	1101	R2E	CBB-C4	3.71	1.47	1.41
2	B	1101	R2E	CAT-CAV	3.67	1.43	1.38
2	D	1101	R2E	CAT-CAV	3.65	1.43	1.38
2	B	1101	R2E	CAO-CAV	3.63	1.44	1.38
2	C	1101	R2E	C2-N1	3.57	1.40	1.33
2	C	1101	R2E	CAT-CAV	3.55	1.43	1.38
2	A	1101	R2E	CAT-CAV	3.55	1.43	1.38
2	C	1101	R2E	CAO-CAV	3.54	1.44	1.38
2	D	1101	R2E	CAO-CAV	3.54	1.44	1.38
2	B	1101	R2E	CBB-C4	3.53	1.47	1.41
2	A	1101	R2E	CBB-C4	3.51	1.47	1.41
2	A	1101	R2E	CAO-CAV	3.51	1.44	1.38
2	A	1101	R2E	C2-N1	3.51	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	R2E	CBB-C4	3.48	1.47	1.41
2	B	1101	R2E	C2-N1	3.47	1.40	1.33
2	D	1101	R2E	C2-N1	3.47	1.40	1.33
2	B	1101	R2E	CBC-CAJ	3.23	1.47	1.40
2	C	1101	R2E	CBC-CAJ	3.23	1.47	1.40
2	D	1101	R2E	CBC-CAJ	3.14	1.47	1.40
2	A	1101	R2E	CBC-CAJ	3.13	1.47	1.40
2	B	1101	R2E	CAR-CL1	2.92	1.80	1.73
2	D	1101	R2E	CAR-CL1	2.86	1.80	1.73
2	B	1101	R2E	CAG-CAH	2.82	1.58	1.51
2	A	1101	R2E	CAR-CL1	2.81	1.80	1.73
2	A	1101	R2E	C4-N3	2.81	1.42	1.37
2	C	1101	R2E	CAG-CAH	2.81	1.58	1.51
2	A	1101	R2E	CAG-CAH	2.76	1.58	1.51
2	D	1101	R2E	CAG-CAH	2.75	1.58	1.51
2	D	1101	R2E	C4-N3	2.73	1.42	1.37
2	C	1101	R2E	CAR-CL1	2.72	1.80	1.73
2	C	1101	R2E	C4-N3	2.72	1.42	1.37
2	B	1101	R2E	C4-N3	2.68	1.42	1.37
2	A	1101	R2E	CAB-CAC	2.66	1.55	1.51
2	A	1101	R2E	CAO-NAN	2.60	1.47	1.39
2	B	1101	R2E	CAB-CAC	2.57	1.55	1.51
2	C	1101	R2E	CAO-NAN	2.56	1.47	1.39
2	B	1101	R2E	CAO-NAN	2.56	1.47	1.39
2	D	1101	R2E	CAB-CAC	2.51	1.55	1.51
2	B	1101	R2E	CAT-CL2	2.48	1.78	1.72
2	D	1101	R2E	CAO-NAN	2.48	1.46	1.39
2	A	1101	R2E	CAT-CL2	2.46	1.78	1.72
2	C	1101	R2E	CAB-CAC	2.46	1.55	1.51
2	D	1101	R2E	CAT-CL2	2.39	1.78	1.72
2	C	1101	R2E	CAT-CL2	2.35	1.77	1.72
2	C	1101	R2E	CBF-CAH	2.34	1.57	1.51
2	A	1101	R2E	CBF-CAH	2.32	1.57	1.51
2	D	1101	R2E	CBF-CAH	2.27	1.57	1.51
2	B	1101	R2E	CBF-CAH	2.25	1.57	1.51
2	C	1101	R2E	CAG-CAF	2.24	1.58	1.52
2	B	1101	R2E	CAG-CAF	2.22	1.58	1.52
2	B	1101	R2E	CAF-NAE	2.20	1.50	1.47
2	A	1101	R2E	CAF-NAE	2.18	1.50	1.47
2	A	1101	R2E	CAG-CAF	2.12	1.58	1.52
2	C	1101	R2E	CAF-NAE	2.11	1.50	1.47
2	D	1101	R2E	CAF-NAE	2.08	1.50	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	R2E	CAK-CAJ	2.08	1.40	1.36
2	A	1101	R2E	CAK-CAJ	2.08	1.40	1.36
2	B	1101	R2E	CAK-CAJ	2.07	1.40	1.36
2	D	1101	R2E	CAG-CAF	2.04	1.58	1.52
2	C	1101	R2E	CAQ-CAP	2.00	1.42	1.38

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	R2E	CAF-CAG-CAH	7.40	118.46	110.32
2	B	1101	R2E	CAF-CAG-CAH	7.32	118.37	110.32
2	C	1101	R2E	CAF-CAG-CAH	7.16	118.20	110.32
2	A	1101	R2E	CAF-CAG-CAH	7.16	118.20	110.32
2	D	1101	R2E	CAA-CAB-CAC	6.91	125.49	112.72
2	B	1101	R2E	CAA-CAB-CAC	6.88	125.44	112.72
2	C	1101	R2E	CAA-CAB-CAC	6.87	125.41	112.72
2	A	1101	R2E	CAA-CAB-CAC	6.84	125.36	112.72
2	B	1101	R2E	CBG-CBF-CAH	4.63	115.41	110.32
2	C	1101	R2E	CBG-CBF-CAH	4.59	115.37	110.32
2	D	1101	R2E	CBG-CBF-CAH	4.50	115.27	110.32
2	A	1101	R2E	CBG-CBF-CAH	4.49	115.25	110.32
2	D	1101	R2E	CAB-CAC-NAE	3.65	123.84	117.95
2	C	1101	R2E	CAB-CAC-NAE	3.57	123.72	117.95
2	A	1101	R2E	CAB-CAC-NAE	3.53	123.65	117.95
2	B	1101	R2E	CAB-CAC-NAE	3.47	123.55	117.95
2	D	1101	R2E	CBB-C4-N3	3.41	121.86	117.97
2	C	1101	R2E	CBC-CBB-C4	3.41	123.95	120.12
2	A	1101	R2E	CBC-CBB-C4	3.39	123.94	120.12
2	B	1101	R2E	CBC-CBB-C4	3.38	123.92	120.12
2	D	1101	R2E	CBC-CBB-C4	3.34	123.88	120.12
2	C	1101	R2E	CBB-C4-N3	3.31	121.74	117.97
2	A	1101	R2E	CBB-C4-N3	3.29	121.72	117.97
2	B	1101	R2E	CBB-C4-N3	3.28	121.71	117.97
2	A	1101	R2E	CAV-CAT-CL2	-2.73	117.65	120.94
2	A	1101	R2E	C5-C6-NAN	2.70	122.70	119.73
2	C	1101	R2E	CAV-CAT-CAR	2.66	120.19	117.92
2	B	1101	R2E	CAV-CAT-CAR	2.62	120.16	117.92
2	C	1101	R2E	CAV-CAT-CL2	-2.59	117.81	120.94
2	C	1101	R2E	C5-C6-NAN	2.57	122.55	119.73
2	D	1101	R2E	CAV-CAT-CL2	-2.56	117.85	120.94
2	B	1101	R2E	CAV-CAT-CL2	-2.52	117.89	120.94
2	A	1101	R2E	CAV-CAT-CAR	2.52	120.07	117.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	R2E	C2-N3-C4	2.50	118.84	115.40
2	D	1101	R2E	CAV-CAT-CAR	2.49	120.04	117.92
2	C	1101	R2E	C2-N3-C4	2.48	118.82	115.40
2	D	1101	R2E	C2-N3-C4	2.47	118.80	115.40
2	B	1101	R2E	C5-C6-NAN	2.45	122.43	119.73
2	A	1101	R2E	C2-N3-C4	2.43	118.75	115.40
2	B	1101	R2E	CBG-NAE-CAF	-2.43	107.94	112.62
2	D	1101	R2E	CBG-NAE-CAF	-2.43	107.94	112.62
2	C	1101	R2E	CBG-NAE-CAF	-2.42	107.96	112.62
2	A	1101	R2E	CBG-NAE-CAF	-2.42	107.96	112.62
2	D	1101	R2E	CBB-CBC-CAJ	-2.39	117.70	120.07
2	D	1101	R2E	C5-C6-NAN	2.36	122.33	119.73
2	D	1101	R2E	C5-C4-N3	-2.30	120.38	122.83
2	C	1101	R2E	CBB-CBC-CAJ	-2.29	117.80	120.07
2	A	1101	R2E	CBB-CBC-CAJ	-2.28	117.81	120.07
2	C	1101	R2E	C5-C4-N3	-2.28	120.41	122.83
2	B	1101	R2E	C5-C4-N3	-2.26	120.43	122.83
2	B	1101	R2E	CBB-CBC-CAJ	-2.24	117.85	120.07
2	A	1101	R2E	C5-C4-N3	-2.22	120.47	122.83
2	D	1101	R2E	CAJ-CAK-C5	2.22	124.70	120.58
2	D	1101	R2E	CAG-CAF-NAE	2.21	114.18	110.82
2	D	1101	R2E	OAD-CAC-CAB	-2.20	116.74	121.42
2	C	1101	R2E	OAD-CAC-CAB	-2.18	116.76	121.42
2	D	1101	R2E	N3-C2-N1	-2.17	125.28	128.68
2	A	1101	R2E	N3-C2-N1	-2.17	125.28	128.68
2	C	1101	R2E	CAJ-CAK-C5	2.16	124.60	120.58
2	B	1101	R2E	N3-C2-N1	-2.15	125.31	128.68
2	C	1101	R2E	CAG-CAF-NAE	2.15	114.09	110.82
2	A	1101	R2E	CAJ-CAK-C5	2.14	124.55	120.58
2	B	1101	R2E	CAJ-CAK-C5	2.14	124.55	120.58
2	B	1101	R2E	OAD-CAC-CAB	-2.14	116.86	121.42
2	C	1101	R2E	N3-C2-N1	-2.14	125.34	128.68
2	A	1101	R2E	CAG-CAF-NAE	2.14	114.07	110.82
2	A	1101	R2E	OAD-CAC-CAB	-2.13	116.88	121.42
2	B	1101	R2E	CAG-CAF-NAE	2.07	113.97	110.82

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	R2E	CAA-CAB-CAC-NAE
2	B	1101	R2E	CAA-CAB-CAC-NAE

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Mol	Chain	Res	Type	Atoms
2	C	1101	R2E	CAA-CAB-CAC-NAE
2	D	1101	R2E	CAA-CAB-CAC-NAE
2	B	1101	R2E	CBF-CAH-OAI-CAJ
2	D	1101	R2E	CBF-CAH-OAI-CAJ
2	A	1101	R2E	CAA-CAB-CAC-OAD
2	B	1101	R2E	CAA-CAB-CAC-OAD
2	C	1101	R2E	CAA-CAB-CAC-OAD
2	D	1101	R2E	CAA-CAB-CAC-OAD
2	A	1101	R2E	CAG-CAH-OAI-CAJ
2	A	1101	R2E	CBF-CAH-OAI-CAJ
2	B	1101	R2E	CAG-CAH-OAI-CAJ
2	C	1101	R2E	CAG-CAH-OAI-CAJ
2	C	1101	R2E	CBF-CAH-OAI-CAJ
2	D	1101	R2E	CAG-CAH-OAI-CAJ
2	B	1101	R2E	CAK-CAJ-OAI-CAH
2	B	1101	R2E	CBC-CAJ-OAI-CAH
2	A	1101	R2E	CAK-CAJ-OAI-CAH
2	C	1101	R2E	CAK-CAJ-OAI-CAH
2	D	1101	R2E	CAK-CAJ-OAI-CAH
2	A	1101	R2E	CAV-CAO-NAN-C6
2	C	1101	R2E	CAV-CAO-NAN-C6
2	D	1101	R2E	CAV-CAO-NAN-C6

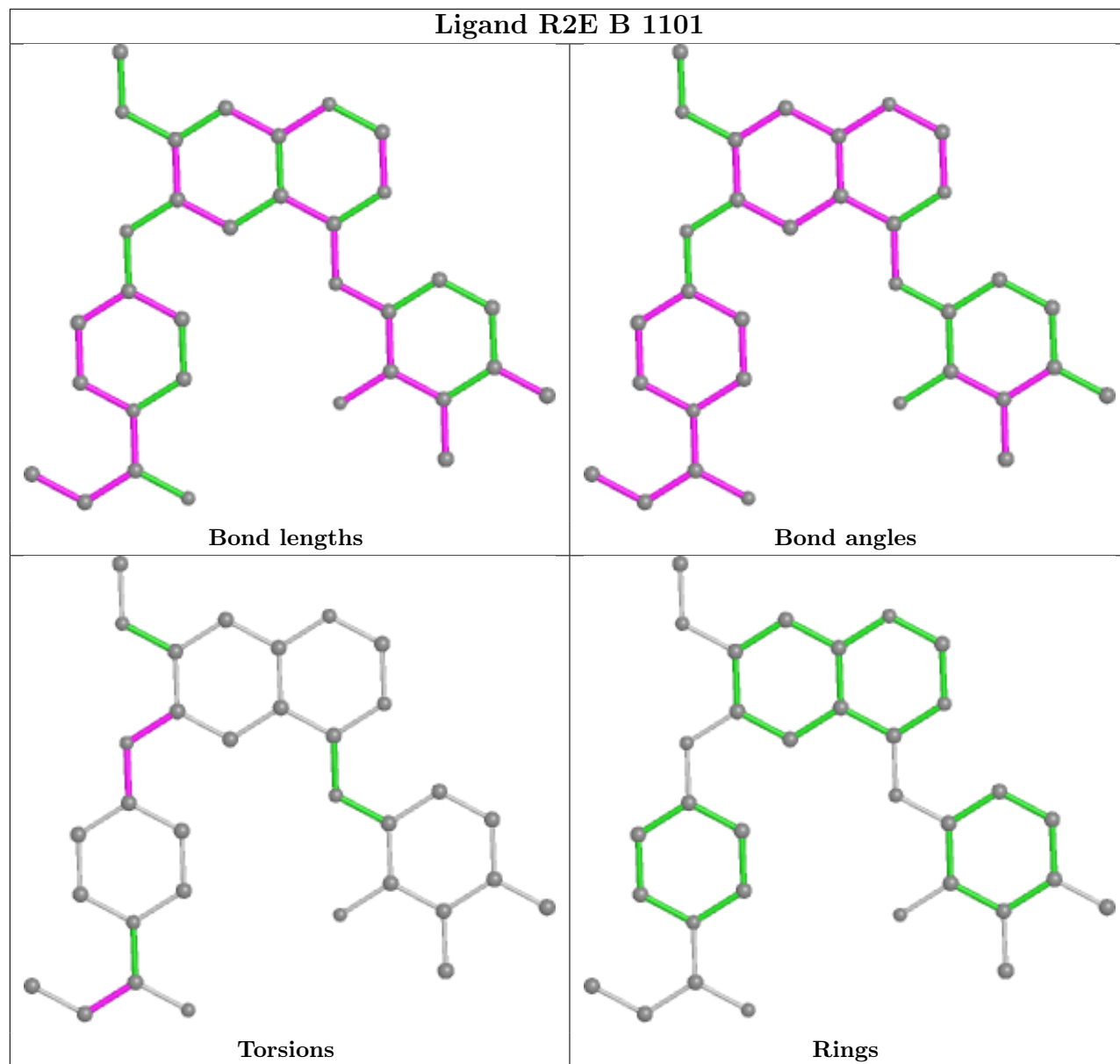
There are no ring outliers.

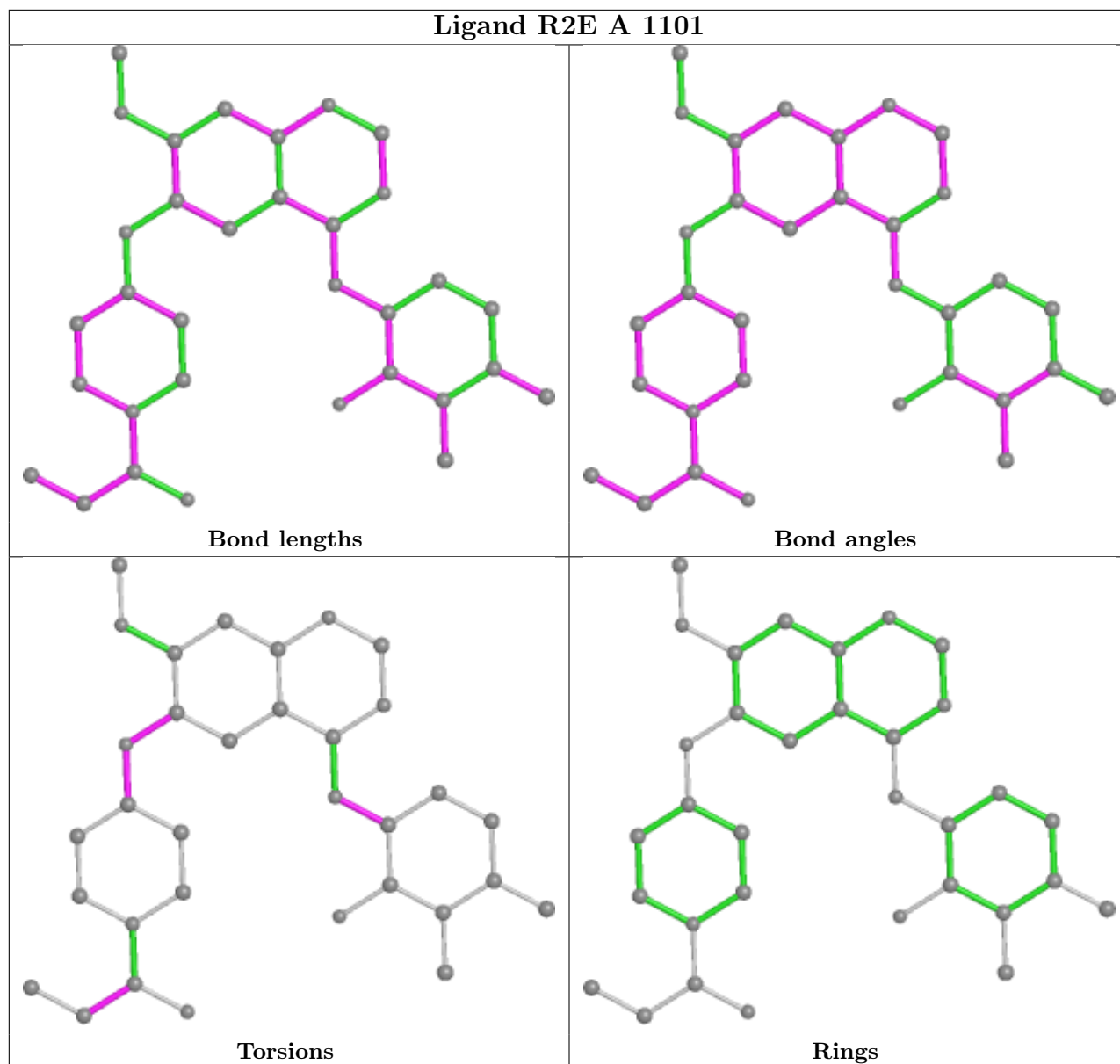
3 monomers are involved in 4 short contacts:

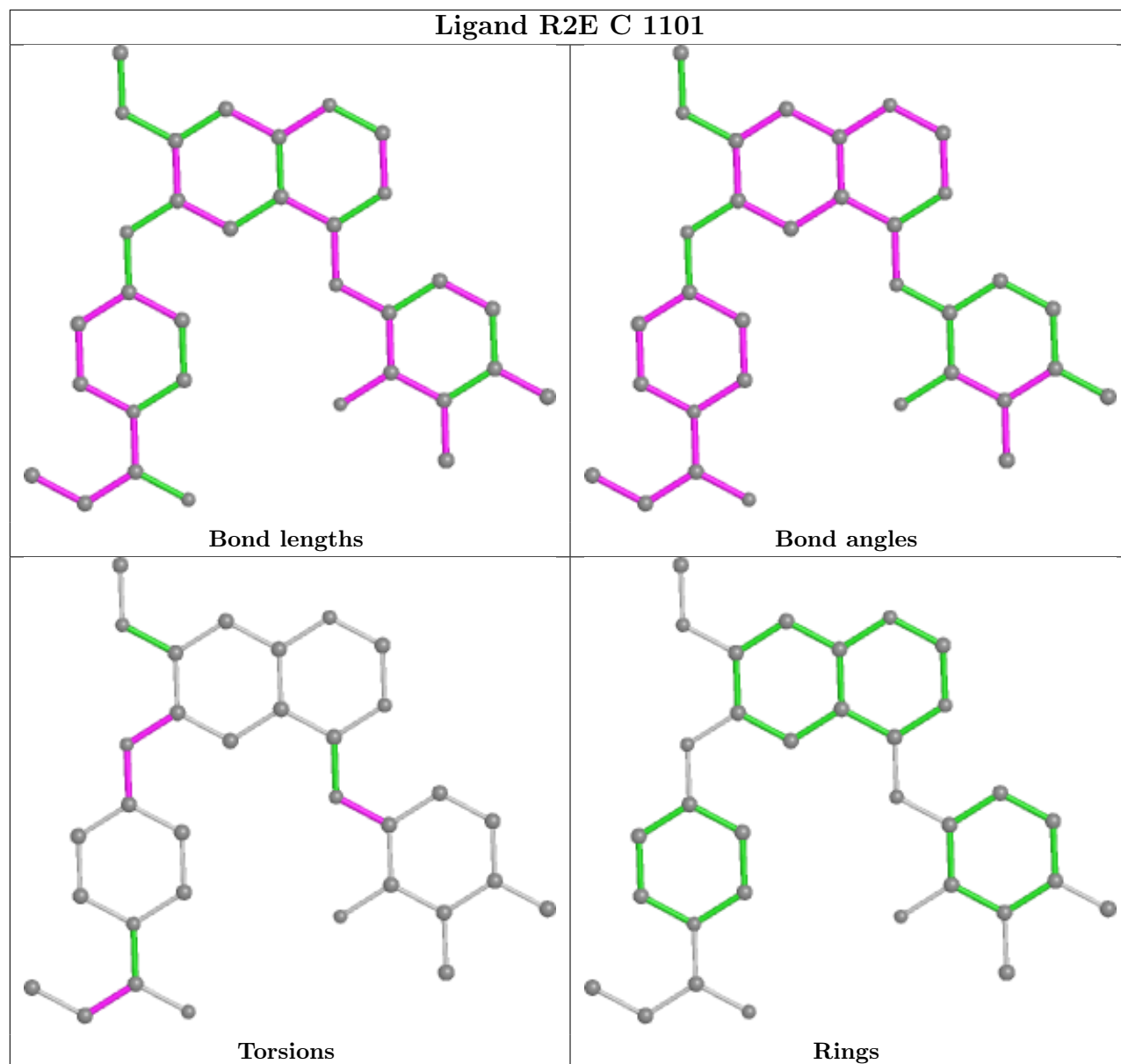
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	R2E	2	0
2	C	1101	R2E	1	0
2	D	1101	R2E	1	0

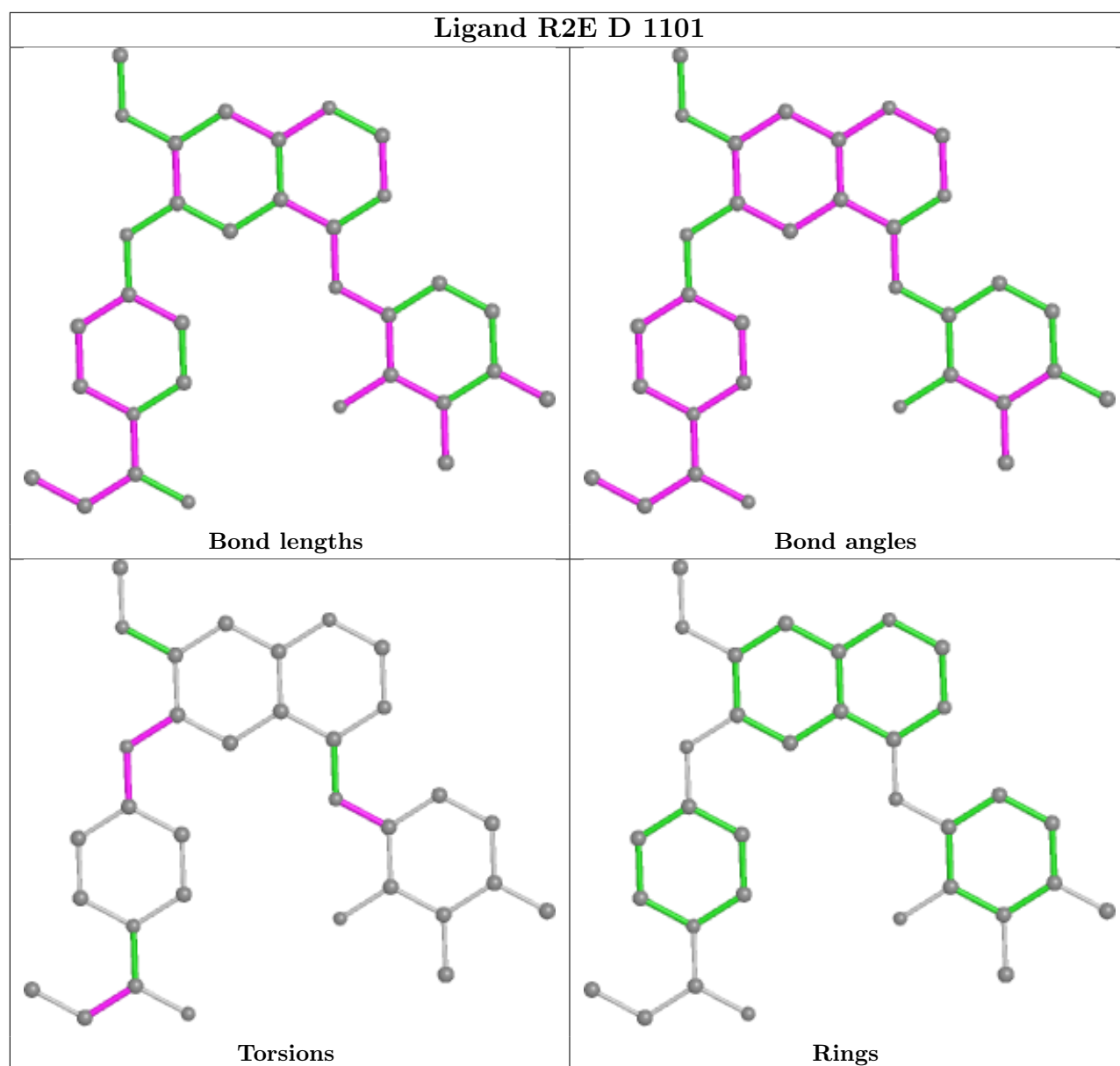
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	303/331 (91%)	0.03	3 (0%) 82 72	27, 51, 88, 116	0
1	B	288/331 (87%)	0.04	4 (1%) 75 63	30, 51, 87, 119	0
1	C	290/331 (87%)	0.10	13 (4%) 33 21	27, 56, 100, 133	0
1	D	304/331 (91%)	0.04	4 (1%) 77 65	28, 53, 91, 124	0
All	All	1185/1324 (89%)	0.05	24 (2%) 65 51	27, 53, 92, 133	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	988	HIS	4.4
1	B	984	ASP	4.0
1	C	988	HIS	3.9
1	C	984	ASP	3.6
1	C	1006	ASP	3.2
1	C	723	PHE	2.9
1	D	742	VAL	2.7
1	C	1007	MET	2.7
1	C	985	GLU	2.7
1	C	784	SER	2.7
1	D	988	HIS	2.7
1	D	876	VAL	2.7
1	C	722	ALA	2.6
1	C	982	GLN	2.6
1	C	995	SER	2.5
1	C	992	PRO	2.4
1	C	794	PRO	2.3
1	A	701	GLN	2.2
1	A	1006	ASP	2.2
1	A	967	GLU	2.2
1	B	1006	ASP	2.2

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	C	983	GLY	2.1
1	D	722	ALA	2.1
1	B	920	ALA	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](#)

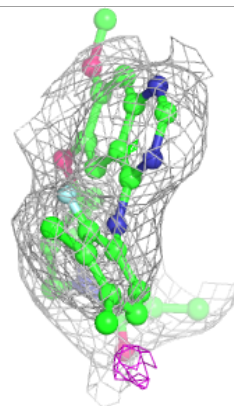
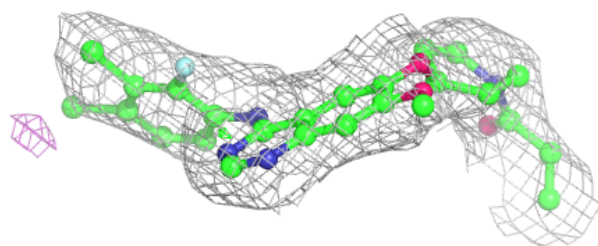
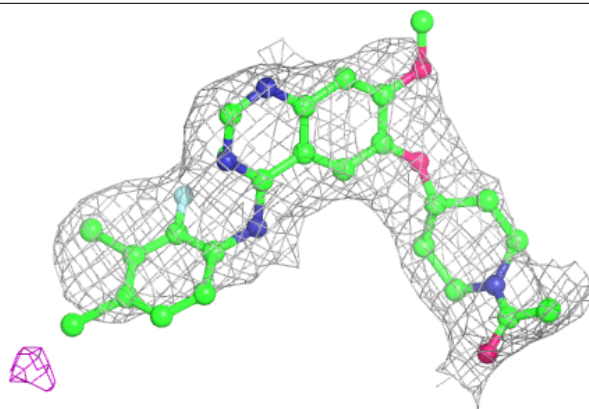
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	R2E	A	1101	33/33	0.89	0.24	29,47,71,104	0
2	R2E	C	1101	33/33	0.89	0.24	40,52,67,77	0
2	R2E	B	1101	33/33	0.92	0.23	30,44,64,96	0
2	R2E	D	1101	33/33	0.92	0.21	21,46,67,113	0

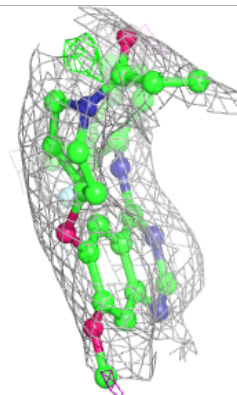
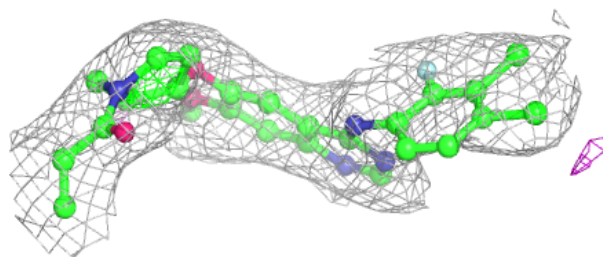
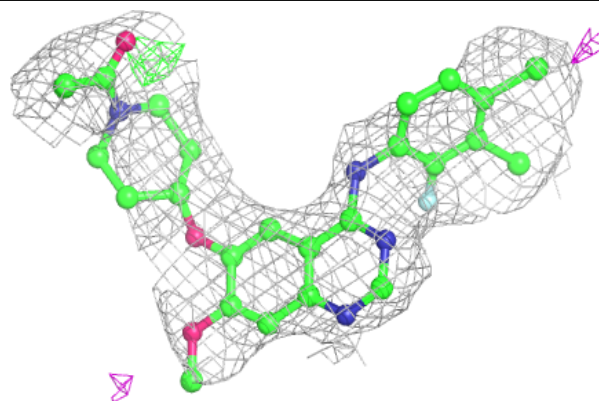
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around R2E A 1101:**

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

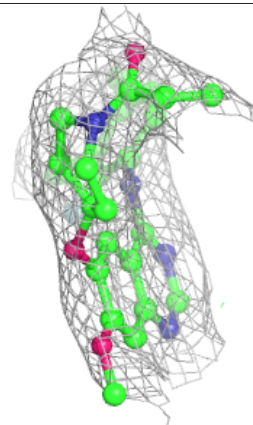
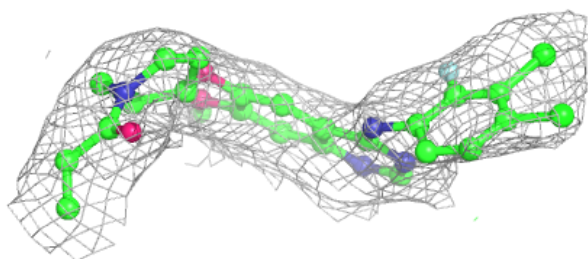
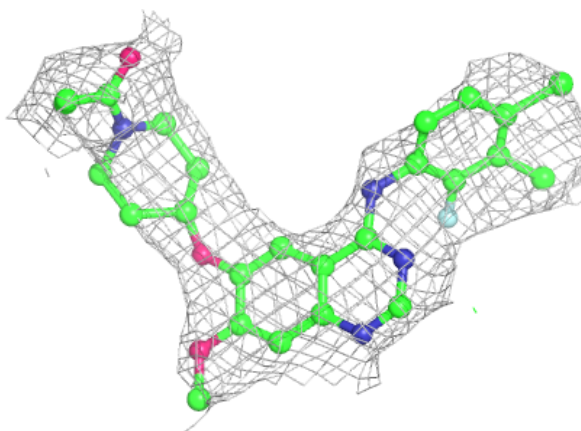
**Electron density around R2E C 1101:**

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

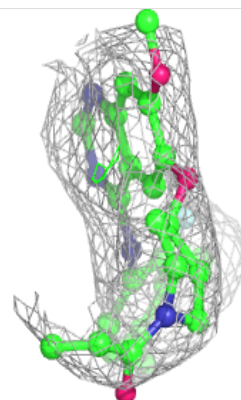
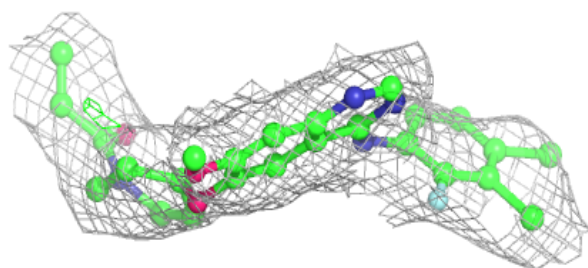
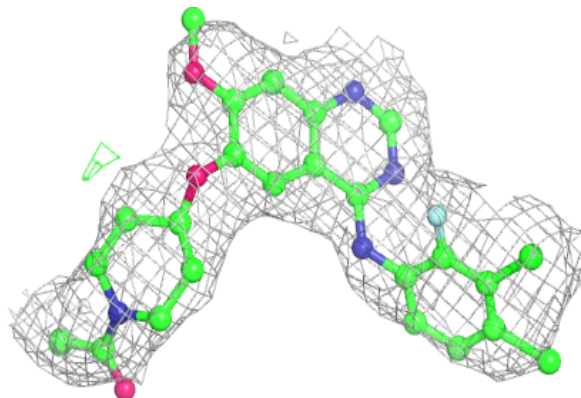


**Electron density around R2E B 1101:**

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

**Electron density around R2E D 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.