



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:02 PM UTC

PDB ID : 9U8C / pdb_00009u8c
Title : Crystal structure of EGFR exon20 insertion mutant in complex with enozertinib (ORIC-114)
Authors : Kim, H.; Park, Y.; Cho, H.
Deposited on : 2025-03-26
Resolution : 3.50 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

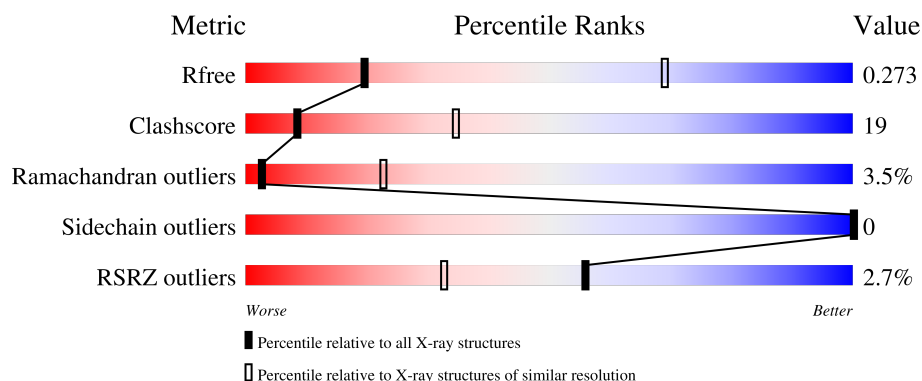
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	338	0% 53% 33% • 13%
1	B	338	2% 53% 32% • 14%
1	C	338	0% 53% 30% • 16%
1	D	338	4% 52% 33% • 15%
1	E	338	4% 45% 38% • 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11086 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	A	295	Total	C	N	O	S	0	0	0
			2192	1412	362	404	14			
1	B	291	Total	C	N	O	S	0	0	0
			2169	1402	362	390	15			
1	C	284	Total	C	N	O	S	0	0	0
			2176	1402	368	391	15			
1	D	288	Total	C	N	O	S	0	0	0
			2213	1424	373	402	14			
1	E	290	Total	C	N	O	S	0	0	0
			2144	1378	358	394	14			

There are 55 discrepancies between the modelled and reference sequences:

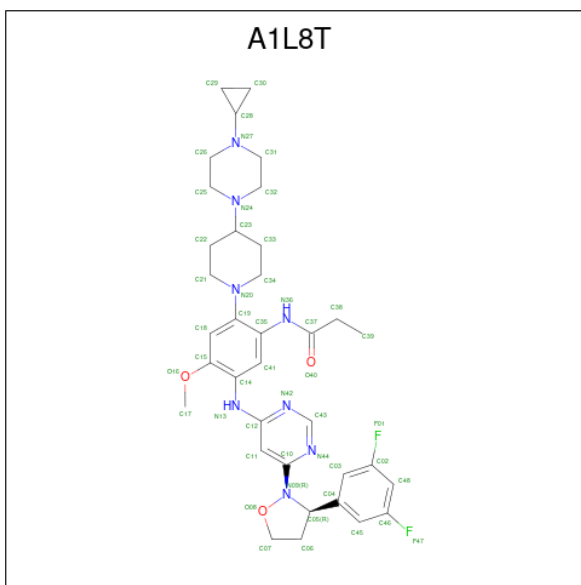
Chain	Residue	Modelled	Actual	Comment	Reference
A	688	GLY	-	expression tag	UNP P00533
A	689	ALA	-	expression tag	UNP P00533
A	690	MET	-	expression tag	UNP P00533
A	691	ASP	-	expression tag	UNP P00533
A	692	PRO	-	expression tag	UNP P00533
A	693	GLU	-	expression tag	UNP P00533
A	694	PHE	-	expression tag	UNP P00533
A	695	MET	-	expression tag	UNP P00533
A	771	ASN	-	insertion	UNP P00533
A	772	PRO	-	insertion	UNP P00533
A	773	GLY	-	insertion	UNP P00533
B	688	GLY	-	expression tag	UNP P00533
B	689	ALA	-	expression tag	UNP P00533
B	690	MET	-	expression tag	UNP P00533
B	691	ASP	-	expression tag	UNP P00533
B	692	PRO	-	expression tag	UNP P00533
B	693	GLU	-	expression tag	UNP P00533
B	694	PHE	-	expression tag	UNP P00533
B	695	MET	-	expression tag	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
B	771	ASN	-	insertion	UNP P00533
B	772	PRO	-	insertion	UNP P00533
B	773	GLY	-	insertion	UNP P00533
C	688	GLY	-	expression tag	UNP P00533
C	689	ALA	-	expression tag	UNP P00533
C	690	MET	-	expression tag	UNP P00533
C	691	ASP	-	expression tag	UNP P00533
C	692	PRO	-	expression tag	UNP P00533
C	693	GLU	-	expression tag	UNP P00533
C	694	PHE	-	expression tag	UNP P00533
C	695	MET	-	expression tag	UNP P00533
C	771	ASN	-	insertion	UNP P00533
C	772	PRO	-	insertion	UNP P00533
C	773	GLY	-	insertion	UNP P00533
D	688	GLY	-	expression tag	UNP P00533
D	689	ALA	-	expression tag	UNP P00533
D	690	MET	-	expression tag	UNP P00533
D	691	ASP	-	expression tag	UNP P00533
D	692	PRO	-	expression tag	UNP P00533
D	693	GLU	-	expression tag	UNP P00533
D	694	PHE	-	expression tag	UNP P00533
D	695	MET	-	expression tag	UNP P00533
D	771	ASN	-	insertion	UNP P00533
D	772	PRO	-	insertion	UNP P00533
D	773	GLY	-	insertion	UNP P00533
E	688	GLY	-	expression tag	UNP P00533
E	689	ALA	-	expression tag	UNP P00533
E	690	MET	-	expression tag	UNP P00533
E	691	ASP	-	expression tag	UNP P00533
E	692	PRO	-	expression tag	UNP P00533
E	693	GLU	-	expression tag	UNP P00533
E	694	PHE	-	expression tag	UNP P00533
E	695	MET	-	expression tag	UNP P00533
E	771	ASN	-	insertion	UNP P00533
E	772	PRO	-	insertion	UNP P00533
E	773	GLY	-	insertion	UNP P00533

- Molecule 2 is {N}-[5-[6-[(3 {R})-3-[3,5-bis(fluoranyl)phenyl]-1,2-oxazolidin-2-yl]pyrimidin-4-yl]amino]-2-[4-(4-cyclopropylpiperazin-1-yl)piperidin-1-yl]-4-methoxy-phenyl]propanamide (CCD ID: A1L8T) (formula: C₃₅H₄₄F₂N₈O₃).

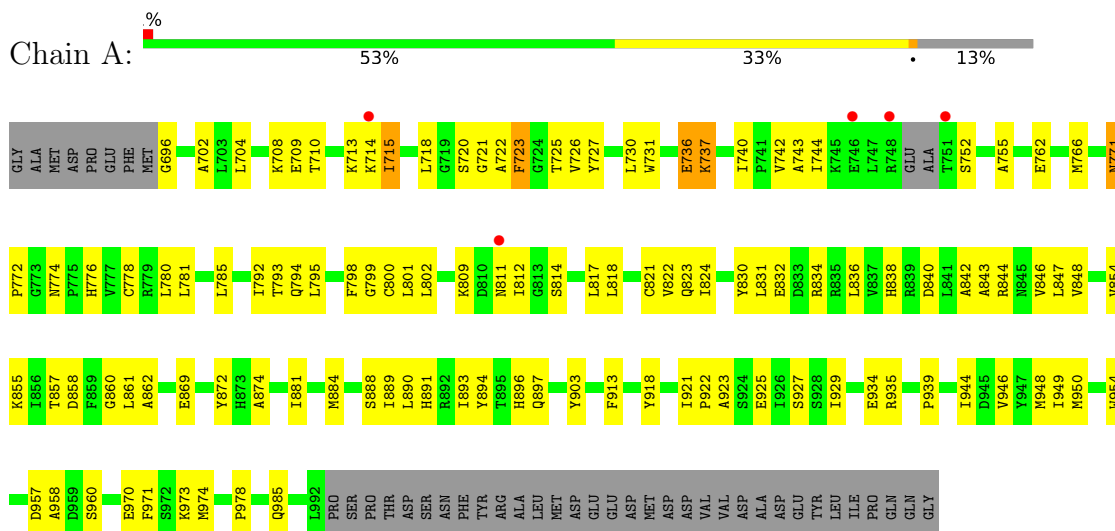


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 35	F 2	N 8	O 3	0	0
2	B	1	Total 48	C 35	F 2	N 8	O 3	0	0
2	C	1	Total 48	C 35	F 2	N 8	O 3	0	0
2	D	1	Total 48	C 35	F 2	N 8	O 3	0	0

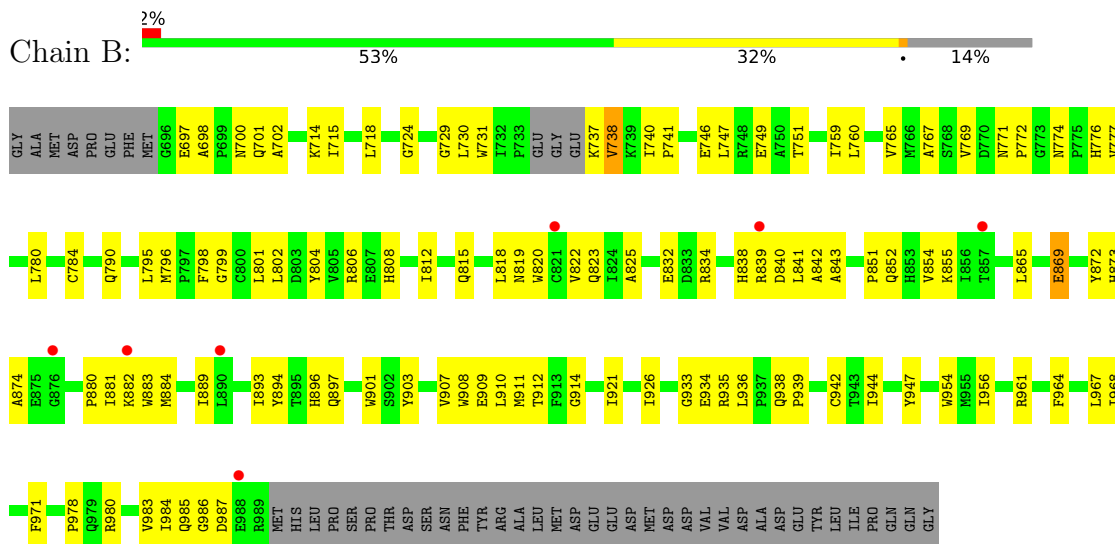
3 Residue-property plots

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

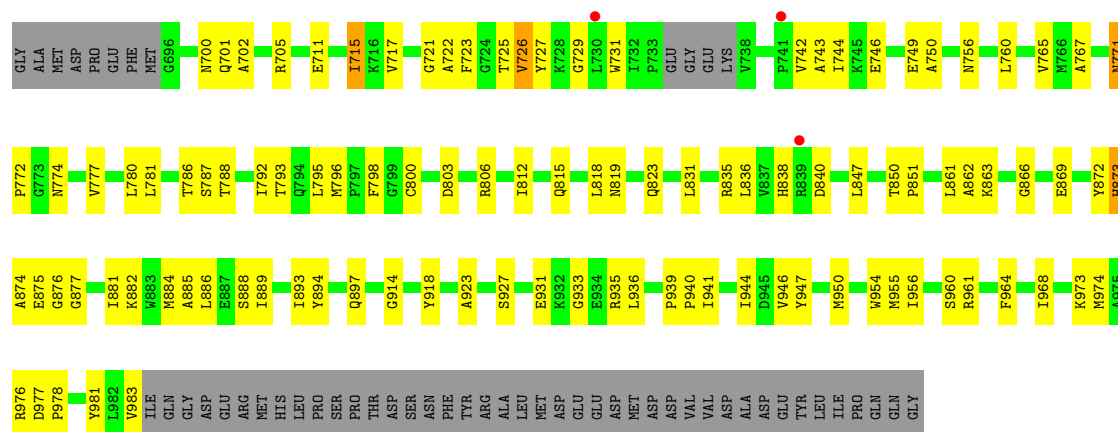


- Molecule 1: Epidermal growth factor receptor



- Molecule 1: Epidermal growth factor receptor

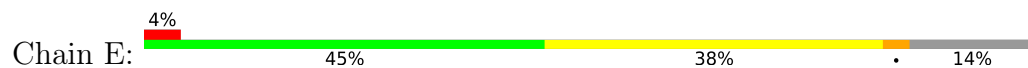




• Molecule 1: Epidermal growth factor receptor



• Molecule 1: Epidermal growth factor receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.23Å 102.16Å 414.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.60 – 3.50 49.60 – 3.50	Depositor EDS
% Data completeness (in resolution range)	92.8 (49.60-3.50) 92.8 (49.60-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.273 , 0.300 (Not available) , 0.273	Depositor DCC
R_{free} test set	2232 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	109.0	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 87.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11086	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: A1L8T

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	0.20	0/2242	0.51	0/3065
1	B	0.21	0/2219	0.51	1/3034 (0.0%)
1	C	0.20	0/2226	0.53	0/3032
1	D	0.21	0/2263	0.47	0/3082
1	E	0.24	0/2193	0.56	0/3001
All	All	0.21	0/11143	0.52	1/15214 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	718	LEU	CB-CA-C	-6.38	109.20	116.54

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	2192	0	2084	80	0
1	B	2169	0	2089	86	0
1	C	2176	0	2137	75	0
1	D	2213	0	2158	87	0
1	E	2144	0	2030	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	48	0	0	2	0
2	B	48	0	0	3	0
2	C	48	0	0	1	0
2	D	48	0	0	3	0
All	All	11086	0	10498	410	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 19.

All (410) 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)
2:B:1101:A1L8T:O08	2:B:1101:A1L8T:N09	1.58	1.22
2:A:1101:A1L8T:N09	2:A:1101:A1L8T:O08	1.57	1.19
2:D:1101:A1L8T:O08	2:D:1101:A1L8T:N09	1.57	1.17
2:C:1101:A1L8T:N09	2:C:1101:A1L8T:O08	1.58	1.09
1:E:741:PRO:HG2	1:E:795:LEU:HD22	1.53	0.90
1:A:922:PRO:HG2	1:A:925:GLU:HG3	1.56	0.87
1:E:857:THR:HG22	1:E:858:ASP:H	1.40	0.84
1:C:815:GLN:HG2	1:C:978:PRO:HG3	1.63	0.80
1:B:815:GLN:HG2	1:B:978:PRO:HG3	1.65	0.78
1:A:857:THR:HG22	1:A:858:ASP:H	1.47	0.78
1:E:771:ASN:HB3	1:E:772:PRO:HD2	1.66	0.78
1:E:835:ARG:HG2	1:E:865:LEU:HB2	1.66	0.77
1:A:771:ASN:HB3	1:A:772:PRO:HD2	1.67	0.77
1:C:771:ASN:HB3	1:C:772:PRO:HD2	1.67	0.75
1:A:744:ILE:HG22	1:A:792:ILE:HG13	1.69	0.73
1:E:822:VAL:HG12	1:E:826:LYS:HD2	1.70	0.73
1:A:774:ASN:HB2	1:A:830:TYR:CD2	2.24	0.72
1:E:740:ILE:HD12	1:E:741:PRO:HD2	1.72	0.72
1:B:702:ALA:HB2	1:B:771:ASN:HB2	1.72	0.71
1:B:934:GLU:HB2	1:D:708:LYS:HG2	1.72	0.71
1:C:700:ASN:O	1:C:702:ALA:N	2.24	0.71
1:C:705:ARG:H	1:C:705:ARG:HD2	1.55	0.71
1:E:767:ALA:HB2	1:E:780:LEU:HD23	1.71	0.71
1:D:771:ASN:HB3	1:D:772:PRO:HD2	1.73	0.71
1:A:831:LEU:HG	1:A:836:LEU:HD23	1.72	0.71
1:B:822:VAL:HG22	1:B:971:PHE:HB3	1.73	0.70
1:B:881:ILE:HA	1:B:884:MET:HE2	1.74	0.69
1:E:747:LEU:HD11	1:E:755:ALA:HB1	1.73	0.69
1:E:836:LEU:HD11	1:E:862:ALA:HB1	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:742:VAL:HG11	1:C:792:ILE:HG23	1.75	0.69
1:E:766:MET:HG2	1:E:859:PHE:HD2	1.57	0.69
1:B:767:ALA:HB2	1:B:780:LEU:HD23	1.75	0.68
1:D:857:THR:HG22	1:D:858:ASP:H	1.57	0.68
1:E:840:ASP:HB2	1:E:861:LEU:HD12	1.76	0.67
1:E:769:VAL:HG11	1:E:836:LEU:HD22	1.77	0.67
1:A:781:LEU:HB3	1:A:792:ILE:HG22	1.77	0.67
1:C:836:LEU:HD11	1:C:862:ALA:HB1	1.75	0.67
1:D:977:ASP:OD2	1:E:696:GLY:N	2.27	0.67
1:A:802:LEU:HG	1:A:843:ALA:HB3	1.76	0.66
1:D:865:LEU:HD21	1:D:872:TYR:HB2	1.76	0.66
1:E:927:SER:O	1:E:931:GLU:HG2	1.95	0.66
1:E:747:LEU:HD22	1:E:749:GLU:H	1.61	0.66
1:E:880:PRO:O	1:E:882:LYS:N	2.29	0.66
1:B:700:ASN:O	1:B:702:ALA:N	2.29	0.66
1:C:743:ALA:HB2	1:C:795:LEU:HD13	1.78	0.66
1:D:980:ARG:O	1:E:699:PRO:HB3	1.95	0.66
1:D:763:ALA:HB2	1:D:791:LEU:HD21	1.79	0.65
1:D:912:THR:HG23	1:D:915:SER:H	1.61	0.65
1:A:696:GLY:N	1:C:977:ASP:OD2	2.29	0.65
1:C:767:ALA:HB2	1:C:780:LEU:HD23	1.78	0.65
1:E:928:SER:O	1:E:932:LYS:HG2	1.97	0.64
1:D:780:LEU:HA	1:D:793:THR:HG22	1.78	0.64
1:D:906:THR:O	1:D:910:LEU:HD12	1.97	0.64
1:E:720:SER:HA	1:E:725:THR:HA	1.79	0.64
1:E:766:MET:HG2	1:E:859:PHE:CD2	2.33	0.64
1:D:836:LEU:HD11	1:D:862:ALA:HB1	1.79	0.64
1:E:784:CYS:HB3	1:E:790:GLN:HB2	1.80	0.64
1:C:941:ILE:HG22	1:C:983:VAL:HB	1.79	0.63
1:B:934:GLU:HB2	1:D:708:LYS:CG	2.29	0.63
1:B:714:LYS:NZ	1:B:746:GLU:OE2	2.30	0.63
1:D:941:ILE:HG22	1:D:983:VAL:HB	1.81	0.63
1:E:786:THR:O	1:E:788:THR:N	2.31	0.63
1:E:848:VAL:HG22	1:E:854:VAL:HG12	1.81	0.62
1:B:774:ASN:HB3	1:B:777:VAL:HG12	1.80	0.61
1:A:881:ILE:HG21	1:A:923:ALA:HB1	1.82	0.61
1:C:715:ILE:HG13	1:C:729:GLY:HA2	1.81	0.61
1:D:958:ALA:HA	1:D:961:ARG:HG3	1.83	0.61
1:B:801:LEU:HD22	1:B:910:LEU:HD22	1.82	0.61
1:C:873:HIS:HB3	1:C:893:ILE:HG22	1.82	0.61
1:D:778:CYS:HA	1:D:855:LYS:HE2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:ASN:HB2	1:A:830:TYR:HD2	1.64	0.60
1:A:766:MET:HG2	1:A:780:LEU:HB2	1.82	0.60
1:A:771:ASN:HB3	1:A:772:PRO:CD	2.32	0.60
1:C:806:ARG:HG3	1:C:914:GLY:HA3	1.82	0.60
1:E:837:VAL:HG13	1:E:865:LEU:HD11	1.82	0.60
1:D:771:ASN:HB3	1:D:772:PRO:CD	2.32	0.60
1:B:746:GLU:HB3	1:B:790:GLN:HG2	1.84	0.59
1:C:955:MET:HG2	1:C:960:SER:HB2	1.82	0.59
1:E:798:PHE:CZ	1:E:851:PRO:HD3	2.37	0.59
1:D:951:VAL:HG13	1:E:785:LEU:HD21	1.83	0.59
1:B:980:ARG:O	1:D:699:PRO:HB3	2.02	0.59
1:E:706:ILE:HG13	1:E:707:LEU:H	1.67	0.59
1:A:881:ILE:HA	1:A:884:MET:HE3	1.83	0.59
1:A:704:LEU:HD23	1:C:944:ILE:HD11	1.85	0.59
1:C:831:LEU:HG	1:C:836:LEU:HD23	1.85	0.59
1:A:731:TRP:CZ3	1:A:781:LEU:HD11	2.38	0.59
1:C:711:GLU:O	1:C:731:TRP:HD1	1.86	0.58
1:D:786:THR:HG22	1:D:787:SER:H	1.67	0.58
1:D:831:LEU:HG	1:D:836:LEU:HD23	1.85	0.58
1:E:750:ALA:HB2	1:E:787:SER:O	2.03	0.58
1:C:742:VAL:HG13	1:C:793:THR:O	2.03	0.58
1:D:926:ILE:HG23	1:D:930:LEU:HD13	1.84	0.58
1:B:715:ILE:HG13	1:B:729:GLY:HA2	1.86	0.58
1:A:848:VAL:HG12	1:A:854:VAL:HG12	1.85	0.58
1:E:942:CYS:SG	1:E:946:VAL:HB	2.43	0.58
1:C:796:MET:HG3	1:C:847:LEU:HB3	1.85	0.58
1:B:812:ILE:HD11	1:B:820:TRP:HH2	1.69	0.57
1:D:956:ILE:HG21	1:E:787:SER:HB2	1.85	0.57
1:E:750:ALA:HB1	1:E:756:ASN:HD21	1.69	0.57
1:C:726:VAL:HA	1:C:744:ILE:O	2.05	0.57
1:A:785:LEU:O	1:C:933:GLY:HA2	2.06	0.56
1:B:884:MET:HE3	1:B:889:ILE:HG12	1.86	0.56
1:C:756:ASN:O	1:C:760:LEU:HG	2.05	0.56
1:E:983:VAL:HG22	1:E:984:ILE:H	1.70	0.56
1:D:886:LEU:HD21	1:D:931:GLU:HB3	1.88	0.56
1:A:714:LYS:HB3	1:A:727:TYR:HD2	1.70	0.56
1:B:819:ASN:O	1:B:823:GLN:HG3	2.06	0.56
1:B:939:PRO:HG2	1:B:942:CYS:HB2	1.88	0.56
1:D:761:ASP:O	1:D:765:VAL:HG12	2.06	0.56
1:A:840:ASP:HB2	1:A:861:LEU:HD12	1.88	0.56
1:E:761:ASP:HA	1:E:764:TYR:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:ALA:HB2	1:A:795:LEU:HD13	1.88	0.56
1:D:801:LEU:HD21	1:D:910:LEU:HD21	1.87	0.56
1:C:798:PHE:CE2	1:C:850:THR:HA	2.42	0.55
1:D:748:ARG:HH12	1:D:755:ALA:HB2	1.70	0.55
1:E:873:HIS:HA	1:E:892:ARG:O	2.06	0.55
1:E:907:VAL:O	1:E:911:MET:HG2	2.06	0.55
1:E:800:CYS:SG	1:E:803:ASP:HB2	2.45	0.55
1:A:918:TYR:HB3	1:A:921:ILE:HB	1.89	0.55
1:B:901:TRP:HE3	1:B:961:ARG:HH12	1.54	0.55
1:C:771:ASN:HB3	1:C:772:PRO:CD	2.32	0.55
1:D:796:MET:SD	1:D:855:LYS:HD3	2.46	0.55
1:D:795:LEU:HD23	1:D:795:LEU:O	2.07	0.54
1:A:742:VAL:HG21	1:A:792:ILE:HG23	1.88	0.54
1:E:730:LEU:HD13	1:E:731:TRP:N	2.22	0.54
1:B:749:GLU:HB3	1:B:751:THR:HG23	1.90	0.53
1:A:872:TYR:CE2	1:A:874:ALA:HB2	2.43	0.53
1:B:802:LEU:HD11	1:B:806:ARG:HH21	1.73	0.53
1:B:964:PHE:O	1:B:968:ILE:HG13	2.07	0.53
1:C:872:TYR:OH	1:C:874:ALA:HB2	2.08	0.53
1:D:832:GLU:HA	1:D:896:HIS:CE1	2.43	0.53
1:C:774:ASN:HB3	1:C:777:VAL:HB	1.89	0.53
1:E:771:ASN:HB3	1:E:772:PRO:CD	2.34	0.53
1:C:798:PHE:CE2	1:C:851:PRO:HD3	2.44	0.52
1:B:933:GLY:HA2	1:D:785:LEU:O	2.10	0.52
1:B:730:LEU:HA	1:B:741:PRO:HA	1.90	0.52
1:D:766:MET:HG2	1:D:780:LEU:HB2	1.92	0.52
1:E:742:VAL:HG11	1:E:792:ILE:HG23	1.90	0.52
1:E:822:VAL:O	1:E:826:LYS:HG3	2.09	0.52
1:E:857:THR:HG22	1:E:858:ASP:N	2.18	0.52
1:E:965:ARG:HA	1:E:968:ILE:HD12	1.91	0.52
1:B:897:GLN:HB3	1:B:961:ARG:HD2	1.92	0.52
1:A:872:TYR:CZ	1:A:874:ALA:HB2	2.45	0.51
1:B:944:ILE:HB	1:D:702:ALA:O	2.10	0.51
1:C:786:THR:HG22	1:C:787:SER:H	1.75	0.51
1:B:935:ARG:HH22	1:B:956:ILE:HD11	1.75	0.51
1:B:908:TRP:CZ3	1:B:912:THR:HG21	2.46	0.51
1:C:798:PHE:HE2	1:C:851:PRO:HD3	1.75	0.51
1:D:838:HIS:O	1:D:840:ASP:N	2.39	0.51
1:D:935:ARG:NH2	1:D:954:TRP:O	2.26	0.51
1:E:965:ARG:HG3	1:E:966:GLU:H	1.74	0.51
1:A:929:ILE:HG23	1:A:934:GLU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:GLY:HA2	2:A:1101:A1L8T:C41	2.40	0.51
1:A:832:GLU:HA	1:A:896:HIS:NE2	2.26	0.51
1:B:818:LEU:O	1:B:822:VAL:HG23	2.11	0.51
1:E:883:TRP:O	1:E:902:SER:OG	2.24	0.50
1:A:742:VAL:CG2	1:A:792:ILE:HG23	2.42	0.50
1:E:857:THR:CG2	1:E:858:ASP:H	2.19	0.50
1:A:811:ASN:HD21	1:B:741:PRO:HB3	1.76	0.50
1:E:944:ILE:HD12	1:E:944:ILE:H	1.76	0.50
1:E:818:LEU:O	1:E:822:VAL:HG23	2.11	0.50
1:A:897:GLN:HB2	1:A:958:ALA:HB1	1.94	0.50
1:A:842:ALA:O	1:A:846:VAL:HG23	2.12	0.50
1:E:762:GLU:O	1:E:766:MET:HG3	2.12	0.50
1:C:750:ALA:HB2	1:C:788:THR:HA	1.93	0.50
1:B:724:GLY:HA3	1:B:747:LEU:HA	1.93	0.49
1:D:784:CYS:HB3	1:D:790:GLN:HB2	1.94	0.49
1:E:935:ARG:NH2	1:E:954:TRP:O	2.45	0.49
1:B:771:ASN:HB3	1:B:772:PRO:HD3	1.93	0.49
1:E:936:LEU:HB2	1:E:954:TRP:CZ3	2.47	0.49
1:C:835:ARG:NH1	1:C:866:GLY:O	2.45	0.49
1:C:781:LEU:HB3	1:C:792:ILE:HG22	1.93	0.49
1:B:784:CYS:SG	1:B:790:GLN:HB2	2.52	0.49
1:B:825:ALA:HB2	1:B:903:TYR:OH	2.13	0.49
1:C:840:ASP:HB2	1:C:861:LEU:HD12	1.93	0.49
1:C:897:GLN:HB3	1:C:961:ARG:HD2	1.94	0.49
1:E:716:LYS:O	1:E:727:TYR:HB2	2.13	0.49
1:E:726:VAL:HB	1:E:745:LYS:HA	1.95	0.49
1:A:889:ILE:HG22	1:A:890:LEU:HD23	1.95	0.49
1:B:747:LEU:HD23	1:B:747:LEU:H	1.78	0.49
1:B:769:VAL:HA	1:B:834:ARG:NH1	2.29	0.48
1:A:742:VAL:HG23	1:A:793:THR:O	2.13	0.48
1:D:836:LEU:HD13	1:D:864:LEU:HD22	1.95	0.48
1:E:956:ILE:O	1:E:957:ASP:C	2.56	0.48
1:B:938:GLN:HA	1:B:947:TYR:CE1	2.48	0.48
1:E:901:TRP:HB2	1:E:961:ARG:NH1	2.29	0.48
1:A:812:ILE:HG23	1:A:817:LEU:HD11	1.96	0.48
1:C:705:ARG:HD2	1:C:705:ARG:N	2.27	0.48
1:A:776:HIS:CE1	1:A:823:GLN:HA	2.49	0.48
1:B:801:LEU:HD12	1:B:854:VAL:HG11	1.96	0.48
1:C:974:MET:HA	1:C:981:TYR:HE2	1.78	0.48
1:D:839:ARG:NH2	1:D:861:LEU:O	2.46	0.48
1:A:721:GLY:O	1:A:723:PHE:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:LEU:HD11	1:A:862:ALA:HB1	1.95	0.48
1:B:865:LEU:HD13	1:B:869:GLU:O	2.13	0.48
1:B:880:PRO:O	1:B:884:MET:HB2	2.14	0.48
1:C:796:MET:HG3	1:C:847:LEU:CB	2.44	0.48
1:D:774:ASN:HB2	1:D:830:TYR:CD2	2.48	0.48
1:D:909:GLU:HA	1:D:912:THR:HG22	1.96	0.48
1:D:748:ARG:HH22	1:D:752:SER:HB2	1.79	0.47
1:C:936:LEU:HB2	1:C:954:TRP:CH2	2.49	0.47
1:E:706:ILE:HA	1:E:783:ILE:O	2.14	0.47
1:B:765:VAL:O	1:B:769:VAL:HG22	2.14	0.47
1:B:832:GLU:HA	1:B:896:HIS:NE2	2.29	0.47
1:C:838:HIS:O	1:C:840:ASP:N	2.43	0.47
1:A:939:PRO:HG2	1:A:950:MET:HE1	1.96	0.47
1:C:927:SER:O	1:C:931:GLU:HG2	2.14	0.47
1:C:974:MET:HA	1:C:981:TYR:CE2	2.50	0.47
1:B:936:LEU:O	1:B:947:TYR:OH	2.30	0.47
1:C:721:GLY:O	1:C:723:PHE:N	2.48	0.47
1:C:881:ILE:HG21	1:C:923:ALA:HB1	1.95	0.47
1:D:765:VAL:HG11	1:D:862:ALA:HB3	1.95	0.47
1:D:824:ILE:HD11	1:D:846:VAL:HG11	1.96	0.47
1:E:717:VAL:HA	1:E:727:TYR:HB3	1.96	0.47
1:E:900:VAL:HG12	1:E:953:CYS:HB3	1.96	0.47
1:A:715:ILE:HD11	1:A:730:LEU:HD12	1.96	0.47
1:A:731:TRP:HB2	1:A:742:VAL:HG11	1.96	0.47
1:A:802:LEU:HG	1:A:843:ALA:CB	2.43	0.47
1:B:872:TYR:CZ	1:B:874:ALA:HB2	2.50	0.47
1:C:725:THR:HG22	1:C:746:GLU:O	2.15	0.47
1:C:964:PHE:O	1:C:968:ILE:HG13	2.14	0.47
1:A:731:TRP:HE3	1:A:740:ILE:HD11	1.80	0.47
1:A:935:ARG:HD2	1:A:954:TRP:HB3	1.97	0.47
1:A:713:LYS:HG3	1:A:714:LYS:H	1.80	0.47
1:B:908:TRP:CD2	1:B:936:LEU:HD13	2.50	0.47
1:D:706:ILE:HG13	1:D:783:ILE:HG23	1.96	0.46
1:E:844:ARG:NH1	1:E:845:ASN:OD1	2.48	0.46
1:D:947:TYR:HA	1:D:950:MET:HE3	1.96	0.46
1:E:742:VAL:HG13	1:E:793:THR:O	2.15	0.46
1:B:700:ASN:C	1:B:702:ALA:H	2.23	0.46
1:C:935:ARG:HH22	1:C:956:ILE:HG12	1.80	0.46
1:C:717:VAL:HA	1:C:727:TYR:HB3	1.96	0.46
1:C:946:VAL:HA	1:C:974:MET:HE1	1.98	0.46
1:D:769:VAL:HG11	1:D:836:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:PRO:C	1:B:795:LEU:HD22	2.41	0.46
1:B:815:GLN:HG2	1:B:978:PRO:CG	2.40	0.46
1:C:882:LYS:HD3	1:C:918:TYR:HB2	1.97	0.46
1:E:850:THR:HG23	1:E:852:GLN:HG2	1.98	0.46
1:C:946:VAL:HG22	1:C:974:MET:SD	2.56	0.46
1:A:858:ASP:C	1:A:860:GLY:H	2.23	0.46
1:D:795:LEU:HB2	2:D:1101:A1L8T:C17	2.46	0.46
1:E:846:VAL:HG22	1:E:856:ILE:HD13	1.98	0.46
1:A:838:HIS:O	1:A:840:ASP:N	2.43	0.46
1:B:798:PHE:CE2	1:B:851:PRO:HD3	2.51	0.46
1:C:881:ILE:HA	1:C:884:MET:HE2	1.97	0.46
1:B:903:TYR:HE2	1:B:967:LEU:HD22	1.81	0.45
1:D:806:ARG:HD3	1:D:914:GLY:O	2.16	0.45
1:D:776:HIS:O	1:D:856:ILE:HG12	2.17	0.45
1:E:709:GLU:HB2	1:E:711:GLU:HG3	1.97	0.45
1:E:817:LEU:HD12	1:E:982:LEU:HD13	1.98	0.45
1:E:905:VAL:HG13	1:E:936:LEU:HD11	1.97	0.45
1:B:907:VAL:O	1:B:911:MET:HG2	2.17	0.45
1:D:818:LEU:O	1:D:822:VAL:HG23	2.17	0.45
1:E:908:TRP:CD2	1:E:936:LEU:HD13	2.52	0.45
1:A:702:ALA:O	1:C:944:ILE:HD13	2.16	0.45
1:A:802:LEU:HD12	1:A:844:ARG:HG3	1.98	0.45
1:B:795:LEU:HA	2:B:1101:A1L8T:N42	2.32	0.45
1:E:881:ILE:HG12	1:E:923:ALA:HB1	1.98	0.45
1:B:812:ILE:HD11	1:B:820:TRP:CH2	2.50	0.45
1:B:873:HIS:HB3	1:B:893:ILE:HG22	1.98	0.45
1:D:708:LYS:HB3	1:D:708:LYS:HE3	1.71	0.45
1:D:756:ASN:O	1:D:760:LEU:HG	2.15	0.45
1:D:786:THR:HG22	1:D:787:SER:N	2.32	0.45
1:D:943:THR:HG21	1:D:981:TYR:HA	1.99	0.45
1:E:906:THR:O	1:E:910:LEU:HD12	2.17	0.45
1:A:888:SER:HB3	1:A:894:TYR:CE1	2.52	0.45
1:B:839:ARG:HD3	1:B:894:TYR:CZ	2.52	0.45
1:D:793:THR:HG23	2:D:1101:A1L8T:F47	2.07	0.45
1:D:806:ARG:HG2	1:D:914:GLY:HA3	1.99	0.45
1:D:944:ILE:HB	1:E:702:ALA:O	2.17	0.45
1:A:708:LYS:C	1:A:710:THR:N	2.75	0.45
1:A:720:SER:HA	1:A:725:THR:HA	1.98	0.45
1:A:821:CYS:O	1:A:903:TYR:OH	2.33	0.45
1:C:819:ASN:O	1:C:823:GLN:HG3	2.17	0.45
1:C:863:LYS:HG2	1:C:872:TYR:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:747:LEU:HD21	1:D:755:ALA:HB1	1.97	0.45
1:D:872:TYR:CG	1:D:873:HIS:N	2.85	0.45
1:A:822:VAL:HG22	1:A:971:PHE:HB3	1.99	0.44
1:E:964:PHE:HA	1:E:967:LEU:HD12	1.99	0.44
1:A:802:LEU:HD12	1:A:844:ARG:CG	2.46	0.44
1:C:700:ASN:C	1:C:702:ALA:H	2.22	0.44
1:D:800:CYS:SG	1:D:803:ASP:HB2	2.58	0.44
1:D:823:GLN:OE1	1:D:853:HIS:HA	2.17	0.44
1:E:775:PRO:O	1:E:853:HIS:NE2	2.50	0.44
1:B:921:ILE:HG22	1:B:926:ILE:HG13	1.99	0.44
1:C:765:VAL:HG11	1:C:862:ALA:HB3	1.99	0.44
1:E:765:VAL:O	1:E:769:VAL:HG22	2.16	0.44
1:E:938:GLN:HB2	1:E:947:TYR:CE2	2.52	0.44
1:D:731:TRP:HB3	1:D:740:ILE:HG23	1.99	0.44
1:E:766:MET:HE2	1:E:766:MET:HB3	1.76	0.44
1:E:843:ALA:N	1:E:906:THR:HG23	2.32	0.44
1:A:752:SER:HB3	1:A:755:ALA:HB3	2.00	0.44
1:B:799:GLY:HA2	2:B:1101:A1L8T:C35	2.47	0.44
1:D:953:CYS:O	1:D:961:ARG:HD3	2.18	0.44
1:E:832:GLU:OE2	1:E:964:PHE:HD2	2.01	0.44
1:C:725:THR:O	1:C:726:VAL:HG12	2.17	0.44
1:C:881:ILE:HG21	1:C:923:ALA:CB	2.47	0.44
1:D:908:TRP:CZ3	1:D:912:THR:HG21	2.53	0.44
1:E:965:ARG:HG3	1:E:966:GLU:N	2.33	0.44
1:A:814:SER:CB	1:A:978:PRO:HB2	2.48	0.44
1:B:841:LEU:HD12	1:B:842:ALA:N	2.33	0.44
1:C:973:LYS:HG3	1:C:976:ARG:HH21	1.83	0.44
1:A:834:ARG:HD2	1:A:834:ARG:HA	1.66	0.44
1:B:697:GLU:HG3	1:B:698:ALA:N	2.32	0.44
1:A:944:ILE:O	1:A:948:MET:HB2	2.18	0.43
1:B:700:ASN:C	1:B:702:ALA:N	2.75	0.43
1:B:882:LYS:HB2	1:B:883:TRP:CE3	2.53	0.43
1:B:908:TRP:NE1	1:B:936:LEU:HB3	2.33	0.43
1:C:744:ILE:HD12	1:C:792:ILE:HG13	1.99	0.43
1:E:784:CYS:SG	1:E:786:THR:HG23	2.58	0.43
1:E:918:TYR:HB3	1:E:921:ILE:HB	1.99	0.43
1:B:883:TRP:HE1	1:B:909:GLU:CD	2.25	0.43
1:B:944:ILE:HD11	1:D:704:LEU:HD23	2.00	0.43
1:C:884:MET:HE3	1:C:889:ILE:HG12	1.99	0.43
1:E:781:LEU:HB3	1:E:792:ILE:HG22	2.00	0.43
1:E:901:TRP:O	1:E:905:VAL:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:800:CYS:SG	1:C:803:ASP:HB2	2.58	0.43
1:B:967:LEU:HD23	1:B:967:LEU:O	2.19	0.43
1:D:749:GLU:HB3	1:D:750:ALA:H	1.57	0.43
1:D:822:VAL:O	1:D:826:LYS:HG3	2.19	0.43
1:E:798:PHE:CE2	1:E:851:PRO:HD3	2.53	0.43
1:B:967:LEU:HD23	1:B:971:PHE:HD2	1.84	0.43
1:A:946:VAL:HA	1:A:949:ILE:HD12	2.01	0.43
1:B:802:LEU:HB2	1:B:843:ALA:HB1	1.99	0.43
1:A:814:SER:HB2	1:A:978:PRO:HB2	2.00	0.43
1:B:802:LEU:HB2	1:B:843:ALA:CB	2.48	0.43
1:D:730:LEU:HA	1:D:741:PRO:HA	2.00	0.43
1:D:939:PRO:HA	1:D:940:PRO:HD3	1.94	0.43
1:A:793:THR:HG22	1:A:794:GLN:H	1.83	0.43
1:A:973:LYS:HE2	1:A:973:LYS:HB3	1.81	0.43
1:B:796:MET:CE	1:B:855:LYS:HD2	2.49	0.43
1:B:909:GLU:HA	1:B:912:THR:HG22	2.00	0.43
1:C:795:LEU:HD12	1:C:796:MET:H	1.83	0.43
1:A:824:ILE:HD11	1:A:846:VAL:HG11	2.01	0.43
1:D:955:MET:HE3	1:E:760:LEU:HD11	2.00	0.43
1:E:838:HIS:O	1:E:840:ASP:N	2.46	0.43
1:B:838:HIS:O	1:B:840:ASP:N	2.51	0.42
1:C:875:GLU:O	1:C:877:GLY:N	2.52	0.42
1:B:772:PRO:HD2	1:B:834:ARG:NH1	2.34	0.42
1:B:804:TYR:HD1	1:B:804:TYR:O	2.02	0.42
1:D:754:LYS:HB2	1:D:754:LYS:HE3	1.75	0.42
1:D:863:LYS:HG2	1:D:872:TYR:CD1	2.54	0.42
1:D:965:ARG:O	1:D:969:ILE:HG13	2.19	0.42
1:A:800:CYS:HA	1:A:847:LEU:HA	2.02	0.42
1:B:935:ARG:HG2	1:B:954:TRP:HE3	1.84	0.42
1:C:935:ARG:NH2	1:C:954:TRP:O	2.40	0.42
1:D:748:ARG:NH1	1:D:755:ALA:HB2	2.33	0.42
1:B:747:LEU:HD22	1:B:759:ILE:HD13	2.01	0.42
1:B:852:GLN:OE1	1:B:852:GLN:N	2.52	0.42
1:D:783:ILE:HG13	1:D:790:GLN:O	2.20	0.42
1:E:885:ALA:O	1:E:889:ILE:HG13	2.20	0.42
1:D:882:LYS:HG2	1:D:926:ILE:CD1	2.49	0.42
1:E:795:LEU:HD12	1:E:797:PRO:HD3	2.02	0.42
1:B:823:GLN:OE1	1:B:854:VAL:HG22	2.19	0.42
1:C:885:ALA:O	1:C:889:ILE:HG13	2.19	0.42
1:D:863:LYS:HG2	1:D:872:TYR:CE1	2.55	0.42
1:C:781:LEU:HB2	1:C:793:THR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:765:VAL:HG21	1:D:862:ALA:HB1	2.01	0.42
1:A:736:GLU:HB3	1:A:737:LYS:H	1.59	0.42
1:A:798:PHE:HB2	1:A:848:VAL:HG23	2.02	0.42
1:B:776:HIS:O	1:B:855:LYS:HA	2.20	0.42
1:C:947:TYR:HA	1:C:950:MET:HE3	2.02	0.42
1:B:731:TRP:CE3	1:B:740:ILE:HD11	2.55	0.41
1:D:926:ILE:O	1:D:930:LEU:HB2	2.19	0.41
1:E:712:PHE:O	1:E:712:PHE:HD1	2.03	0.41
1:E:801:LEU:HD21	1:E:910:LEU:HD21	2.02	0.41
1:A:970:GLU:O	1:A:974:MET:HG3	2.21	0.41
1:D:826:LYS:HA	1:D:968:ILE:HD11	2.02	0.41
1:B:901:TRP:HE3	1:B:961:ARG:NH1	2.17	0.41
1:C:818:LEU:HD12	1:C:978:PRO:HA	2.02	0.41
1:E:835:ARG:HD2	1:E:865:LEU:O	2.20	0.41
1:A:762:GLU:CD	1:A:860:GLY:HA2	2.45	0.41
1:B:760:LEU:HD23	1:B:760:LEU:HA	1.94	0.41
1:B:808:HIS:O	1:B:812:ILE:HB	2.20	0.41
1:A:890:LEU:HD21	1:A:927:SER:OG	2.20	0.41
1:B:936:LEU:HB2	1:B:954:TRP:CH2	2.54	0.41
1:D:785:LEU:HD23	1:D:785:LEU:HA	1.86	0.41
1:E:983:VAL:HG13	1:E:984:ILE:N	2.35	0.41
1:A:778:CYS:HA	1:A:855:LYS:HE2	2.03	0.41
1:A:801:LEU:HD12	1:A:846:VAL:CG1	2.51	0.41
1:C:944:ILE:HD12	1:C:944:ILE:HA	1.89	0.41
1:D:791:LEU:HA	1:D:791:LEU:HD23	1.89	0.41
1:E:842:ALA:C	1:E:906:THR:HG23	2.46	0.41
1:A:957:ASP:OD2	1:A:960:SER:N	2.52	0.41
1:B:746:GLU:CB	1:B:790:GLN:HG2	2.50	0.41
1:D:718:LEU:HD11	1:D:728:LYS:CB	2.51	0.41
1:E:945:ASP:OD1	1:E:945:ASP:N	2.54	0.41
1:B:741:PRO:HB2	1:B:795:LEU:HD21	2.02	0.41
1:C:798:PHE:HE2	1:C:850:THR:HA	1.86	0.41
1:E:722:ALA:C	1:E:724:GLY:H	2.28	0.41
1:E:828:MET:HA	1:E:831:LEU:HD13	2.03	0.41
1:C:812:ILE:HD12	1:C:812:ILE:HA	1.96	0.41
1:E:791:LEU:HD23	1:E:791:LEU:HA	1.90	0.41
1:A:708:LYS:C	1:A:710:THR:H	2.29	0.40
1:A:793:THR:HG22	1:A:794:GLN:N	2.35	0.40
1:C:886:LEU:HD12	1:C:889:ILE:HB	2.02	0.40
1:C:939:PRO:HA	1:C:940:PRO:HD3	1.99	0.40
1:E:885:ALA:HB1	1:E:961:ARG:HH22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:VAL:C	1:A:727:TYR:HD1	2.29	0.40
1:A:809:LYS:HG2	1:A:913:PHE:HB3	2.03	0.40
1:A:891:HIS:HB2	1:A:893:ILE:HG12	2.03	0.40
1:B:737:LYS:O	1:B:738:VAL:HG22	2.21	0.40
1:D:824:ILE:O	1:D:828:MET:HG2	2.22	0.40
1:D:950:MET:HG2	1:D:954:TRP:CZ2	2.55	0.40
1:D:709:GLU:OE2	1:D:790:GLN:NE2	2.55	0.40
1:A:818:LEU:O	1:A:822:VAL:HG23	2.21	0.40
1:A:897:GLN:CB	1:A:958:ALA:HB1	2.51	0.40
1:C:888:SER:HB3	1:C:894:TYR:CE2	2.56	0.40
1:D:741:PRO:HG2	1:D:795:LEU:HD21	2.03	0.40
1:D:842:ALA:O	1:D:846:VAL:HG23	2.21	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	291/338 (86%)	258 (89%)	23 (8%)	10 (3%)	3	23
1	B	287/338 (85%)	256 (89%)	22 (8%)	9 (3%)	3	25
1	C	280/338 (83%)	252 (90%)	19 (7%)	9 (3%)	3	24
1	D	282/338 (83%)	255 (90%)	22 (8%)	5 (2%)	6	34
1	E	288/338 (85%)	238 (83%)	33 (12%)	17 (6%)	1	12
All	All	1428/1690 (84%)	1259 (88%)	119 (8%)	50 (4%)	3	23

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	771	ASN
1	B	701	GLN

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Mol	Chain	Res	Type
1	B	738	VAL
1	B	985	GLN
1	C	701	GLN
1	C	722	ALA
1	C	726	VAL
1	C	771	ASN
1	D	771	ASN
1	D	869	GLU
1	E	716	LYS
1	E	734	GLU
1	E	747	LEU
1	E	748	ARG
1	E	771	ASN
1	E	881	ILE
1	E	956	ILE
1	A	709	GLU
1	A	722	ALA
1	A	723	PHE
1	A	869	GLU
1	A	985	GLN
1	B	984	ILE
1	B	986	GLY
1	C	869	GLU
1	C	876	GLY
1	D	720	SER
1	D	984	ILE
1	E	720	SER
1	E	722	ALA
1	E	789	VAL
1	E	875	GLU
1	E	984	ILE
1	A	718	LEU
1	B	869	GLU
1	C	873	HIS
1	D	701	GLN
1	E	708	LYS
1	E	957	ASP
1	A	737	LYS
1	B	987	ASP
1	E	707	LEU
1	A	715	ILE
1	A	736	GLU

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Mol	Chain	Res	Type
1	B	914	GLY
1	C	749	GLU
1	E	869	GLU
1	E	879	VAL
1	B	983	VAL
1	C	715	ILE

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	220/295 (75%)	220 (100%)	0	100	100
1	B	218/295 (74%)	218 (100%)	0	100	100
1	C	226/295 (77%)	226 (100%)	0	100	100
1	D	230/295 (78%)	230 (100%)	0	100	100
1	E	212/295 (72%)	212 (100%)	0	100	100
All	All	1106/1475 (75%)	1106 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	701	GLN
1	A	790	GLN
1	A	838	HIS
1	A	873	HIS
1	A	891	HIS
1	B	756	ASN
1	B	873	HIS
1	C	838	HIS
1	D	819	ASN
1	D	873	HIS
1	D	979	GLN

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Mol	Chain	Res	Type
1	E	891	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](#)

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	A1L8T	D	1101	1	54,54,54	3.86	25 (46%)	71,77,77	3.52	23 (32%)
2	A1L8T	B	1101	1	54,54,54	3.91	26 (48%)	71,77,77	3.60	26 (36%)
2	A1L8T	C	1101	1	54,54,54	3.88	23 (42%)	71,77,77	3.67	26 (36%)
2	A1L8T	A	1101	1	54,54,54	3.95	26 (48%)	71,77,77	3.57	22 (30%)

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	A1L8T	D	1101	1	-	10/28/64/64	0/7/7/7
2	A1L8T	B	1101	1	-	9/28/64/64	0/7/7/7
2	A1L8T	C	1101	1	-	6/28/64/64	0/7/7/7
2	A1L8T	A	1101	1	-	7/28/64/64	0/7/7/7

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	A1L8T	C05-N09	-14.91	1.29	1.48
2	C	1101	A1L8T	C05-N09	-14.48	1.29	1.48
2	B	1101	A1L8T	C05-N09	-14.34	1.29	1.48
2	D	1101	A1L8T	C05-N09	-13.84	1.30	1.48
2	B	1101	A1L8T	O08-N09	10.80	1.58	1.44
2	C	1101	A1L8T	O08-N09	10.66	1.58	1.44
2	A	1101	A1L8T	O08-N09	10.61	1.57	1.44
2	D	1101	A1L8T	O08-N09	10.48	1.57	1.44
2	D	1101	A1L8T	C06-C07	-7.87	1.30	1.51
2	A	1101	A1L8T	C06-C07	-7.83	1.30	1.51
2	C	1101	A1L8T	C06-C07	-7.77	1.31	1.51
2	B	1101	A1L8T	C06-C07	-7.72	1.31	1.51
2	D	1101	A1L8T	C28-N27	-7.48	1.29	1.48
2	A	1101	A1L8T	C28-N27	-7.32	1.29	1.48
2	C	1101	A1L8T	C28-N27	-7.30	1.30	1.48
2	B	1101	A1L8T	C28-N27	-7.30	1.30	1.48
2	A	1101	A1L8T	C23-N24	-6.79	1.31	1.48
2	B	1101	A1L8T	C23-N24	-6.66	1.31	1.48
2	D	1101	A1L8T	C23-N24	-6.56	1.31	1.48
2	C	1101	A1L8T	C23-N24	-6.32	1.32	1.48
2	A	1101	A1L8T	C37-N36	6.11	1.48	1.35
2	B	1101	A1L8T	C37-N36	5.77	1.48	1.35
2	C	1101	A1L8T	C37-N36	5.64	1.47	1.35
2	D	1101	A1L8T	C37-N36	5.54	1.47	1.35
2	D	1101	A1L8T	C26-N27	-5.38	1.37	1.47
2	B	1101	A1L8T	C31-N27	-5.30	1.37	1.47
2	B	1101	A1L8T	C12-N13	5.17	1.47	1.38
2	C	1101	A1L8T	C12-N13	5.10	1.47	1.38
2	D	1101	A1L8T	C25-N24	-5.08	1.37	1.47
2	A	1101	A1L8T	O08-C07	5.00	1.53	1.43
2	B	1101	A1L8T	O08-C07	4.98	1.53	1.43
2	A	1101	A1L8T	C32-N24	-4.97	1.38	1.47
2	C	1101	A1L8T	C31-N27	-4.96	1.38	1.47
2	C	1101	A1L8T	C25-N24	-4.95	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	A1L8T	C31-N27	-4.94	1.38	1.47
2	B	1101	A1L8T	C26-N27	-4.90	1.38	1.47
2	C	1101	A1L8T	O08-C07	4.87	1.53	1.43
2	D	1101	A1L8T	C34-N20	4.86	1.55	1.46
2	A	1101	A1L8T	C34-N20	4.86	1.55	1.46
2	D	1101	A1L8T	O08-C07	4.86	1.53	1.43
2	C	1101	A1L8T	C32-N24	-4.85	1.38	1.47
2	A	1101	A1L8T	C25-N24	-4.79	1.38	1.47
2	B	1101	A1L8T	C34-N20	4.76	1.54	1.46
2	B	1101	A1L8T	C32-N24	-4.74	1.38	1.47
2	A	1101	A1L8T	C26-N27	-4.73	1.38	1.47
2	D	1101	A1L8T	C31-N27	-4.71	1.38	1.47
2	D	1101	A1L8T	C12-N13	4.68	1.46	1.38
2	A	1101	A1L8T	C12-N13	4.68	1.46	1.38
2	C	1101	A1L8T	C26-N27	-4.67	1.38	1.47
2	D	1101	A1L8T	C21-N20	4.60	1.54	1.46
2	C	1101	A1L8T	C34-N20	4.57	1.54	1.46
2	D	1101	A1L8T	C32-N24	-4.46	1.38	1.47
2	A	1101	A1L8T	C21-N20	4.45	1.54	1.46
2	B	1101	A1L8T	C25-N24	-4.42	1.39	1.47
2	A	1101	A1L8T	C35-N36	4.16	1.50	1.41
2	B	1101	A1L8T	C35-N36	4.01	1.49	1.41
2	B	1101	A1L8T	C21-N20	3.97	1.53	1.46
2	D	1101	A1L8T	C10-N09	3.97	1.48	1.42
2	C	1101	A1L8T	C21-N20	3.88	1.53	1.46
2	B	1101	A1L8T	C10-N09	3.79	1.48	1.42
2	D	1101	A1L8T	C35-N36	3.75	1.49	1.41
2	C	1101	A1L8T	C35-N36	3.72	1.49	1.41
2	B	1101	A1L8T	C06-C05	3.72	1.63	1.54
2	C	1101	A1L8T	C06-C05	3.69	1.63	1.54
2	D	1101	A1L8T	C06-C05	3.56	1.63	1.54
2	C	1101	A1L8T	C10-N09	3.52	1.48	1.42
2	C	1101	A1L8T	C19-N20	3.50	1.48	1.41
2	A	1101	A1L8T	C19-N20	3.49	1.48	1.41
2	D	1101	A1L8T	C19-N20	3.45	1.48	1.41
2	A	1101	A1L8T	C06-C05	3.39	1.62	1.54
2	C	1101	A1L8T	C14-N13	3.25	1.48	1.39
2	B	1101	A1L8T	C14-N13	3.19	1.48	1.39
2	A	1101	A1L8T	C10-N09	3.13	1.47	1.42
2	B	1101	A1L8T	C04-C05	3.13	1.56	1.51
2	B	1101	A1L8T	C19-N20	3.07	1.48	1.41
2	A	1101	A1L8T	C14-N13	3.07	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	A1L8T	O16-C15	3.04	1.42	1.37
2	A	1101	A1L8T	C04-C05	2.97	1.56	1.51
2	C	1101	A1L8T	C04-C05	2.95	1.56	1.51
2	B	1101	A1L8T	O16-C15	2.94	1.41	1.37
2	D	1101	A1L8T	C04-C05	2.89	1.56	1.51
2	D	1101	A1L8T	C14-N13	2.87	1.47	1.39
2	C	1101	A1L8T	O16-C15	2.83	1.41	1.37
2	A	1101	A1L8T	O16-C15	2.70	1.41	1.37
2	C	1101	A1L8T	C30-C28	2.52	1.54	1.48
2	C	1101	A1L8T	C29-C28	2.49	1.54	1.48
2	A	1101	A1L8T	C29-C28	2.48	1.54	1.48
2	D	1101	A1L8T	C30-C28	2.45	1.54	1.48
2	B	1101	A1L8T	C30-C28	2.43	1.54	1.48
2	A	1101	A1L8T	C30-C28	2.41	1.54	1.48
2	D	1101	A1L8T	C29-C28	2.37	1.54	1.48
2	B	1101	A1L8T	C29-C28	2.27	1.53	1.48
2	D	1101	A1L8T	O40-C37	-2.27	1.18	1.23
2	B	1101	A1L8T	O40-C37	-2.13	1.19	1.23
2	D	1101	A1L8T	C22-C23	-2.11	1.47	1.52
2	A	1101	A1L8T	C22-C23	-2.06	1.47	1.52
2	A	1101	A1L8T	O40-C37	-2.05	1.19	1.23
2	B	1101	A1L8T	C33-C23	-2.03	1.47	1.52
2	A	1101	A1L8T	C33-C23	-2.03	1.47	1.52
2	B	1101	A1L8T	C22-C23	-2.00	1.47	1.52

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	A1L8T	C30-C28-N27	22.08	142.18	117.84
2	B	1101	A1L8T	C30-C28-N27	21.97	142.05	117.84
2	C	1101	A1L8T	C30-C28-N27	21.74	141.80	117.84
2	D	1101	A1L8T	C30-C28-N27	20.78	140.74	117.84
2	A	1101	A1L8T	O08-N09-C10	9.91	127.63	110.88
2	D	1101	A1L8T	O08-N09-C10	9.38	126.74	110.88
2	C	1101	A1L8T	O08-N09-C10	8.81	125.79	110.88
2	D	1101	A1L8T	C43-N44-C10	8.56	122.14	114.95
2	B	1101	A1L8T	O08-N09-C10	8.42	125.12	110.88
2	B	1101	A1L8T	C43-N44-C10	7.61	121.34	114.95
2	C	1101	A1L8T	C43-N44-C10	7.30	121.07	114.95
2	A	1101	A1L8T	C43-N44-C10	7.29	121.07	114.95
2	C	1101	A1L8T	C29-C28-N27	-6.70	110.45	117.84
2	D	1101	A1L8T	C29-C28-N27	-6.61	110.55	117.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	A1L8T	C29-C28-N27	-6.30	110.89	117.84
2	B	1101	A1L8T	C29-C28-N27	-5.91	111.33	117.84
2	A	1101	A1L8T	C22-C23-N24	-5.34	98.97	112.66
2	A	1101	A1L8T	N44-C43-N42	-5.23	120.67	128.58
2	D	1101	A1L8T	N44-C43-N42	-5.13	120.82	128.58
2	C	1101	A1L8T	C25-C26-N27	5.01	119.42	110.61
2	B	1101	A1L8T	N44-C43-N42	-4.89	121.18	128.58
2	C	1101	A1L8T	N44-C43-N42	-4.82	121.29	128.58
2	C	1101	A1L8T	C34-C33-C23	4.75	119.48	110.78
2	B	1101	A1L8T	C22-C23-N24	-4.66	100.72	112.66
2	B	1101	A1L8T	C26-C25-N24	4.51	118.55	110.61
2	C	1101	A1L8T	O16-C15-C14	4.46	120.37	114.81
2	B	1101	A1L8T	C32-N24-C25	4.45	117.61	109.13
2	C	1101	A1L8T	C31-N27-C26	4.39	117.49	109.13
2	D	1101	A1L8T	C31-C32-N24	4.34	118.24	110.61
2	D	1101	A1L8T	C10-N09-C05	4.31	126.78	117.34
2	C	1101	A1L8T	C10-N09-C05	4.28	126.73	117.34
2	D	1101	A1L8T	O16-C15-C14	4.26	120.12	114.81
2	B	1101	A1L8T	C10-N09-C05	4.14	126.42	117.34
2	D	1101	A1L8T	C32-C31-N27	3.86	117.41	110.61
2	A	1101	A1L8T	O16-C15-C14	3.85	119.60	114.81
2	C	1101	A1L8T	C26-C25-N24	3.79	117.28	110.61
2	A	1101	A1L8T	C10-N09-C05	3.78	125.63	117.34
2	B	1101	A1L8T	O16-C15-C14	3.75	119.49	114.81
2	A	1101	A1L8T	C48-C02-C03	-3.64	119.08	123.50
2	C	1101	A1L8T	C06-C05-N09	3.62	108.70	103.49
2	B	1101	A1L8T	C11-C12-N42	-3.60	118.19	122.92
2	D	1101	A1L8T	C06-C05-N09	3.48	108.51	103.49
2	C	1101	A1L8T	C22-C23-N24	-3.47	103.76	112.66
2	C	1101	A1L8T	C11-C12-N42	-3.47	118.37	122.92
2	B	1101	A1L8T	C25-C26-N27	3.40	116.59	110.61
2	B	1101	A1L8T	C48-C02-C03	-3.39	119.38	123.50
2	B	1101	A1L8T	C12-C11-C10	3.33	119.30	116.64
2	A	1101	A1L8T	C17-O16-C15	-3.24	112.77	117.51
2	A	1101	A1L8T	C06-C05-C04	-3.22	107.27	113.69
2	C	1101	A1L8T	C12-C11-C10	3.16	119.17	116.64
2	D	1101	A1L8T	C22-C23-N24	-3.07	104.78	112.66
2	A	1101	A1L8T	C11-C12-N42	-2.92	119.09	122.92
2	D	1101	A1L8T	C31-N27-C26	2.91	114.68	109.13
2	A	1101	A1L8T	C32-N24-C25	2.90	114.65	109.13
2	C	1101	A1L8T	C48-C02-C03	-2.88	120.00	123.50
2	D	1101	A1L8T	C48-C02-C03	-2.87	120.01	123.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	A1L8T	C33-C23-N24	2.76	119.73	112.66
2	C	1101	A1L8T	C17-O16-C15	-2.72	113.53	117.51
2	A	1101	A1L8T	C33-C23-N24	2.71	119.61	112.66
2	D	1101	A1L8T	C11-C12-N42	-2.61	119.50	122.92
2	C	1101	A1L8T	C34-N20-C21	-2.60	105.71	111.57
2	B	1101	A1L8T	C11-C10-N44	-2.58	118.53	122.82
2	C	1101	A1L8T	O16-C15-C18	-2.55	119.68	124.08
2	A	1101	A1L8T	C25-C26-N27	2.54	115.08	110.61
2	B	1101	A1L8T	C17-O16-C15	-2.53	113.80	117.51
2	D	1101	A1L8T	C34-C33-C23	2.52	115.39	110.78
2	A	1101	A1L8T	C34-N20-C19	2.51	122.14	116.19
2	D	1101	A1L8T	C11-C10-N44	-2.51	118.65	122.82
2	C	1101	A1L8T	C46-C48-C02	2.49	119.71	116.08
2	B	1101	A1L8T	C06-C05-N09	2.48	107.06	103.49
2	A	1101	A1L8T	C31-N27-C26	2.45	113.81	109.13
2	C	1101	A1L8T	C11-C10-N44	-2.45	118.74	122.82
2	B	1101	A1L8T	F01-C02-C48	2.44	121.75	118.28
2	D	1101	A1L8T	C04-C05-N09	-2.44	108.24	111.57
2	A	1101	A1L8T	C04-C03-C02	2.42	121.35	118.74
2	A	1101	A1L8T	F01-C02-C03	2.41	121.70	118.28
2	B	1101	A1L8T	C46-C48-C02	2.39	119.56	116.08
2	C	1101	A1L8T	C34-N20-C19	2.37	121.82	116.19
2	D	1101	A1L8T	C18-C19-N20	-2.34	119.19	122.59
2	D	1101	A1L8T	C33-C34-N20	2.30	116.15	110.92
2	C	1101	A1L8T	C32-C31-N27	2.30	114.66	110.61
2	A	1101	A1L8T	C46-C48-C02	2.29	119.42	116.08
2	C	1101	A1L8T	C48-C46-C45	-2.28	120.73	123.50
2	C	1101	A1L8T	C33-C34-N20	2.28	116.08	110.92
2	B	1101	A1L8T	C48-C46-C45	-2.24	120.78	123.50
2	C	1101	A1L8T	C04-C05-N09	-2.20	108.57	111.57
2	D	1101	A1L8T	C32-N24-C25	2.20	113.32	109.13
2	D	1101	A1L8T	C46-C48-C02	2.19	119.27	116.08
2	B	1101	A1L8T	C04-C03-C02	2.13	121.03	118.74
2	A	1101	A1L8T	C43-N42-C12	2.12	122.19	115.25
2	B	1101	A1L8T	C38-C37-N36	2.08	120.01	114.65
2	A	1101	A1L8T	O16-C15-C18	-2.07	120.52	124.08
2	B	1101	A1L8T	O40-C37-N36	-2.06	119.94	123.64
2	B	1101	A1L8T	C34-N20-C19	2.05	121.06	116.19
2	D	1101	A1L8T	F01-C02-C48	2.05	121.19	118.28
2	D	1101	A1L8T	O16-C15-C18	-2.03	120.58	124.08
2	B	1101	A1L8T	C31-C32-N24	2.02	114.16	110.61

There are no chirality outliers.

All (32) torsion outliers are listed below:

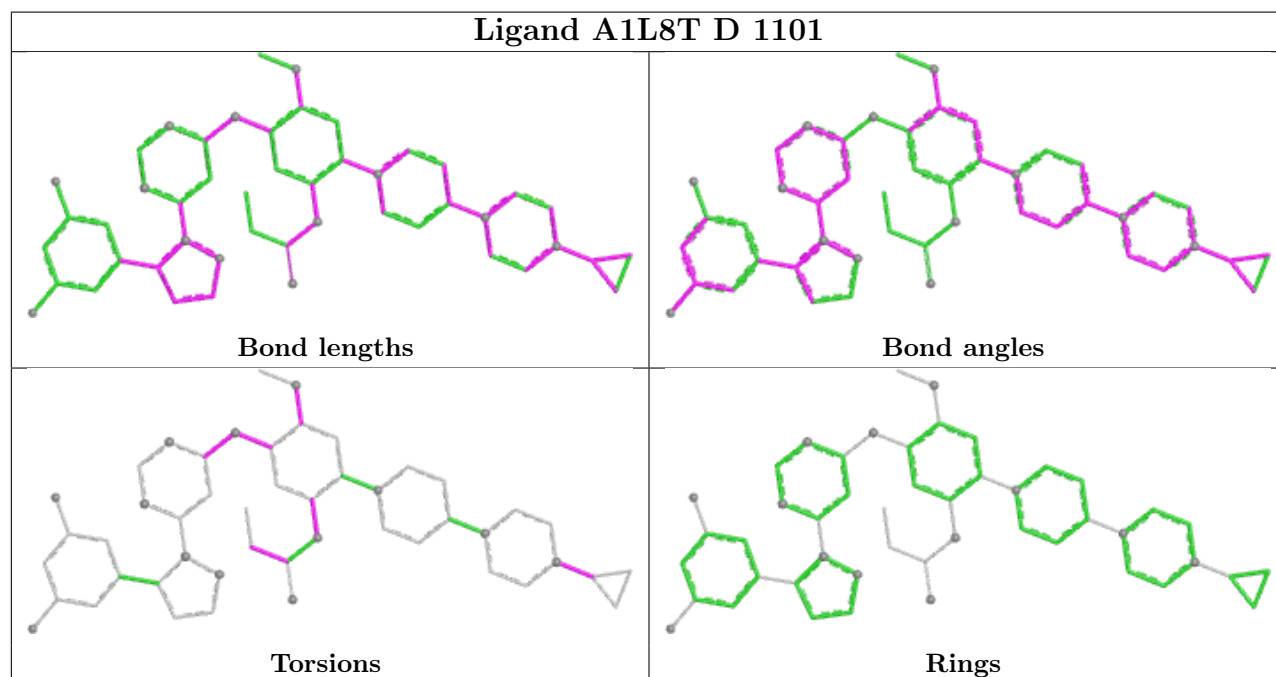
Mol	Chain	Res	Type	Atoms
2	A	1101	A1L8T	C33-C23-N24-C25
2	B	1101	A1L8T	C33-C23-N24-C25
2	B	1101	A1L8T	C30-C28-N27-C26
2	D	1101	A1L8T	C30-C28-N27-C26
2	C	1101	A1L8T	C14-C15-O16-C17
2	A	1101	A1L8T	C14-C15-O16-C17
2	D	1101	A1L8T	C14-C15-O16-C17
2	B	1101	A1L8T	C14-C15-O16-C17
2	B	1101	A1L8T	C18-C15-O16-C17
2	C	1101	A1L8T	C18-C15-O16-C17
2	A	1101	A1L8T	C18-C15-O16-C17
2	A	1101	A1L8T	C22-C23-N24-C25
2	D	1101	A1L8T	C18-C15-O16-C17
2	B	1101	A1L8T	C19-C35-N36-C37
2	B	1101	A1L8T	C41-C35-N36-C37
2	C	1101	A1L8T	C19-C35-N36-C37
2	C	1101	A1L8T	C41-C35-N36-C37
2	D	1101	A1L8T	C41-C35-N36-C37
2	D	1101	A1L8T	C19-C35-N36-C37
2	A	1101	A1L8T	C22-C23-N24-C32
2	A	1101	A1L8T	C33-C23-N24-C32
2	B	1101	A1L8T	C22-C23-N24-C25
2	B	1101	A1L8T	N36-C37-C38-C39
2	D	1101	A1L8T	N36-C37-C38-C39
2	B	1101	A1L8T	O40-C37-C38-C39
2	D	1101	A1L8T	O40-C37-C38-C39
2	D	1101	A1L8T	C41-C14-N13-C12
2	A	1101	A1L8T	C29-C28-N27-C26
2	D	1101	A1L8T	N42-C12-N13-C14
2	C	1101	A1L8T	O40-C37-C38-C39
2	C	1101	A1L8T	N36-C37-C38-C39
2	D	1101	A1L8T	C11-C12-N13-C14

There are no ring outliers.

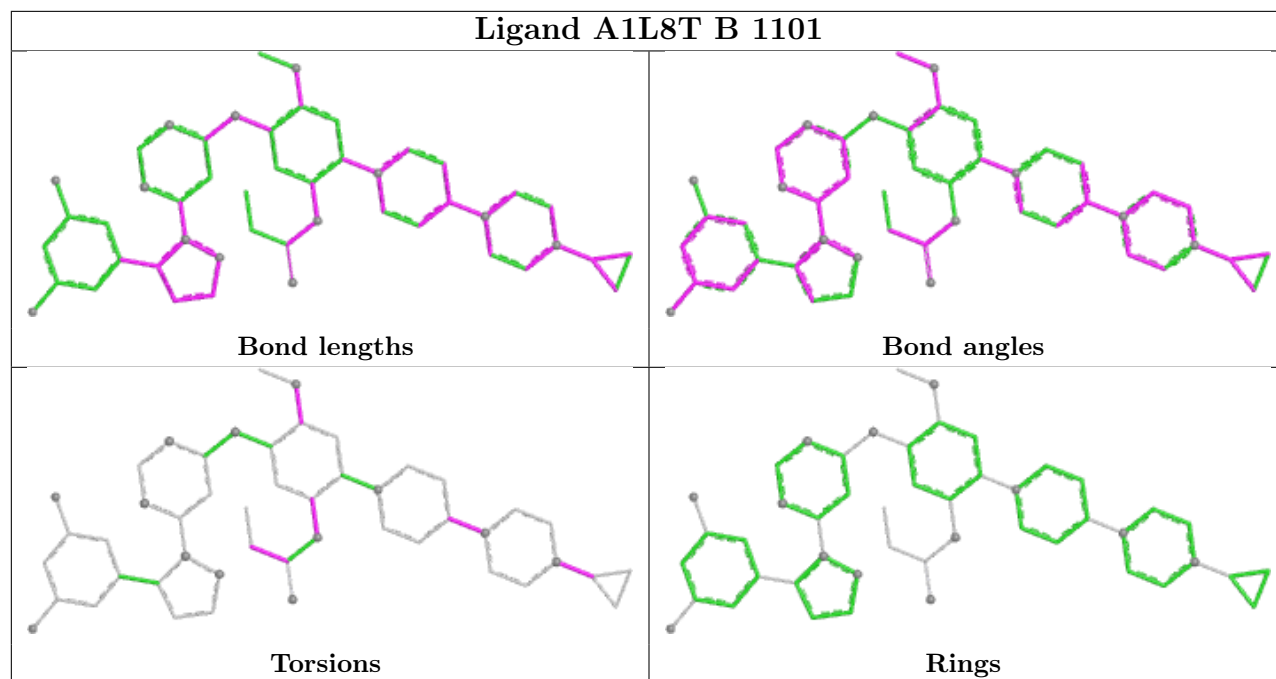
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1101	A1L8T	3	0
2	B	1101	A1L8T	3	0
2	C	1101	A1L8T	1	0
2	A	1101	A1L8T	2	0

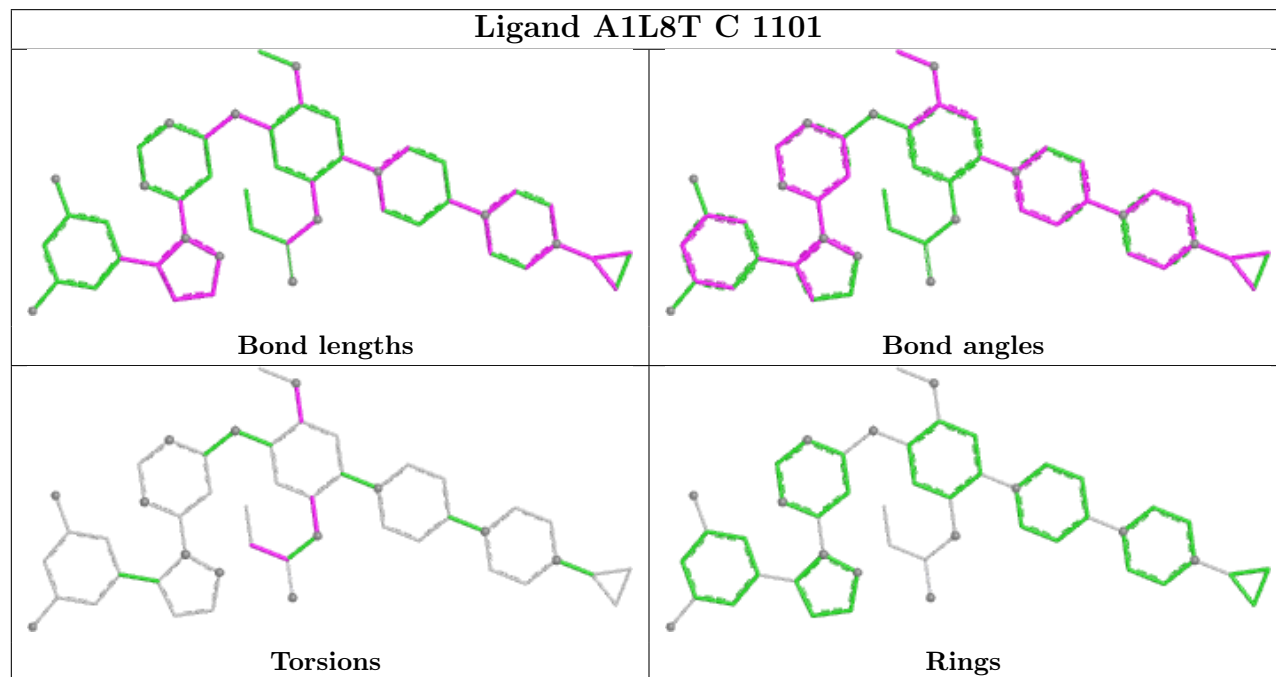
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

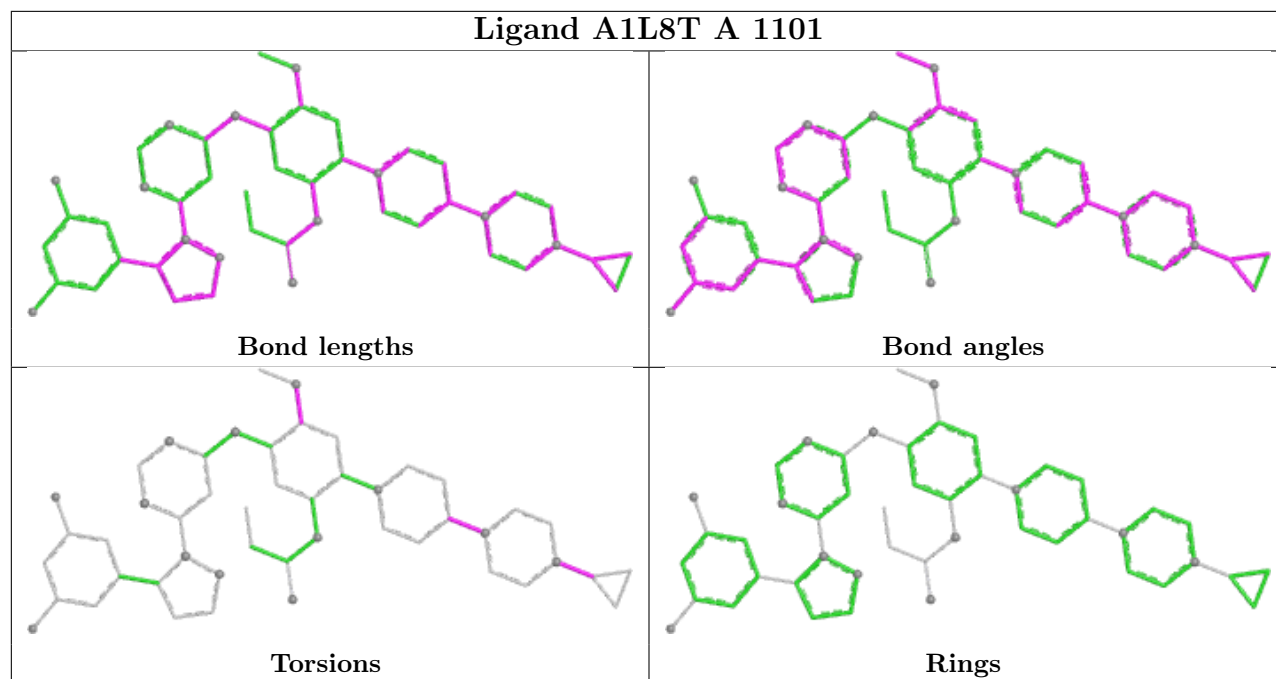


Ligand A1L8T B 1101



Ligand A1L8T C 1101





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	295/338 (87%)	0.21	5 (1%) 69 43	59, 84, 130, 153	0
1	B	291/338 (86%)	0.20	7 (2%) 59 35	52, 85, 121, 147	0
1	C	284/338 (84%)	0.25	3 (1%) 78 54	68, 102, 138, 153	0
1	D	288/338 (85%)	0.34	12 (4%) 40 22	70, 100, 132, 144	0
1	E	290/338 (85%)	0.41	12 (4%) 41 22	83, 125, 157, 168	0
All	All	1448/1690 (85%)	0.28	39 (2%) 56 33	52, 99, 143, 168	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	887	GLU	3.7
1	B	988	GLU	3.6
1	E	917	PRO	2.9
1	E	747	LEU	2.9
1	D	898	SER	2.9
1	A	748	ARG	2.8
1	E	845	ASN	2.8
1	A	714	LYS	2.8
1	D	734	GLU	2.7
1	D	874	ALA	2.6
1	B	857	THR	2.6
1	A	811	ASN	2.6
1	C	839	ARG	2.6
1	D	715	ILE	2.5
1	E	942	CYS	2.5
1	D	982	LEU	2.4
1	B	882	LYS	2.4
1	B	839	ARG	2.4
1	D	814	SER	2.4
1	C	741	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	840	ASP	2.4
1	D	723	PHE	2.3
1	D	722	ALA	2.3
1	E	745	LYS	2.2
1	D	813	GLY	2.2
1	E	706	ILE	2.2
1	C	730	LEU	2.2
1	B	876	GLY	2.2
1	E	844	ARG	2.1
1	B	821	CYS	2.1
1	A	746	GLU	2.1
1	D	990	MET	2.1
1	E	985	GLN	2.1
1	E	890	LEU	2.1
1	A	751	THR	2.1
1	E	709	GLU	2.0
1	E	832	GLU	2.0
1	D	897	GLN	2.0
1	B	890	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

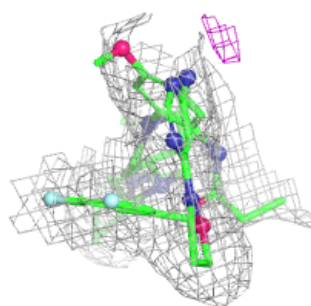
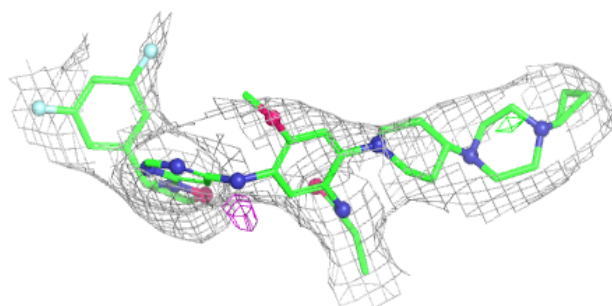
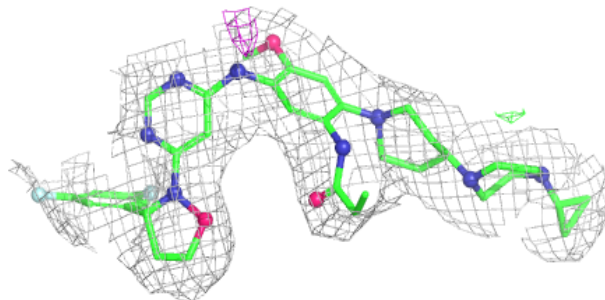
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1L8T	D	1101	48/48	0.87	0.13	80,96,103,105	0
2	A1L8T	C	1101	48/48	0.89	0.14	80,96,112,116	0
2	A1L8T	B	1101	48/48	0.90	0.13	53,76,96,103	0
2	A1L8T	A	1101	48/48	0.91	0.12	54,68,84,105	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.

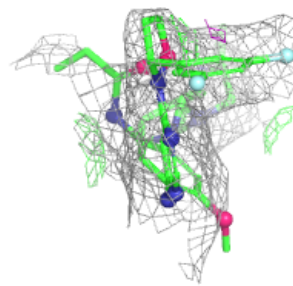
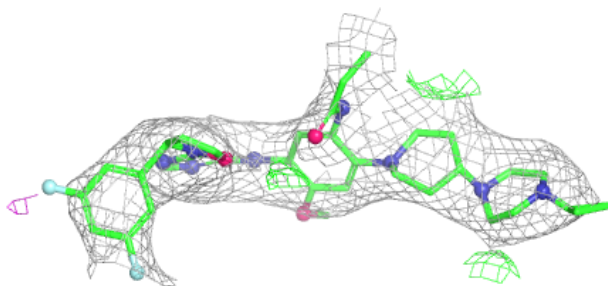
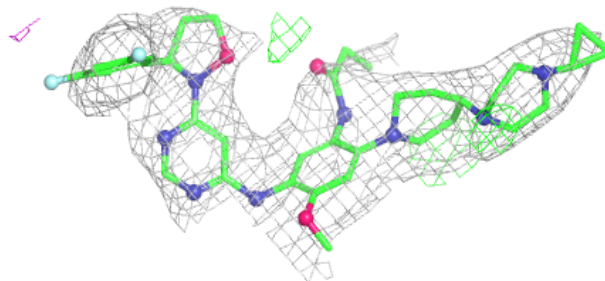
Electron density around A1L8T D 1101:

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

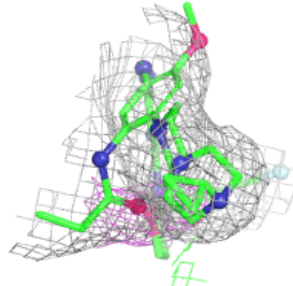
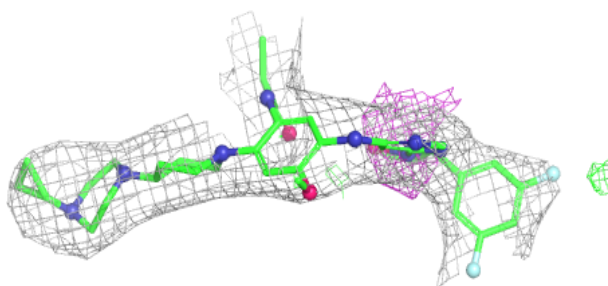
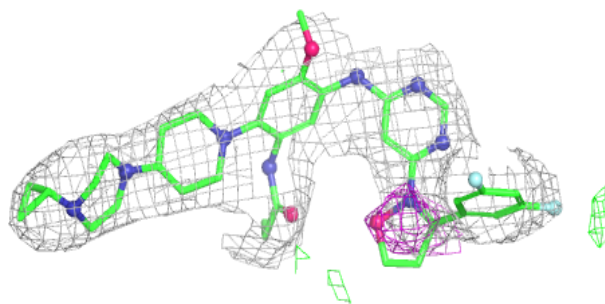


Electron density around A1L8T C 1101:

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

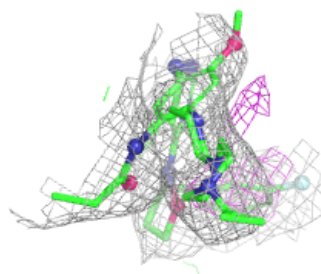
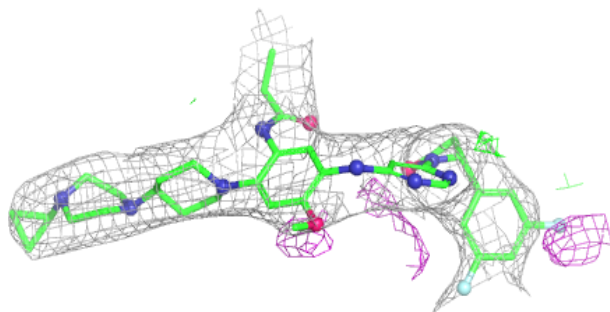
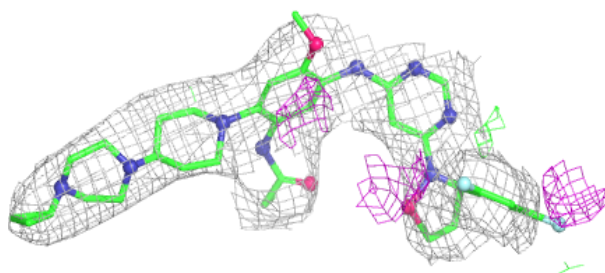
**Electron density around A1L8T B 1101:**

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



Electron density around A1L8T A 1101:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.