



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 01:01 AM EDT

PDB ID : 5X2F
Title : Crystal structure of EGFR 696-1022 T790M/V948R in complex with SKLB(6)
Authors : Yun, C.H.
Deposited on : 2017-01-31
Resolution : 2.20 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

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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

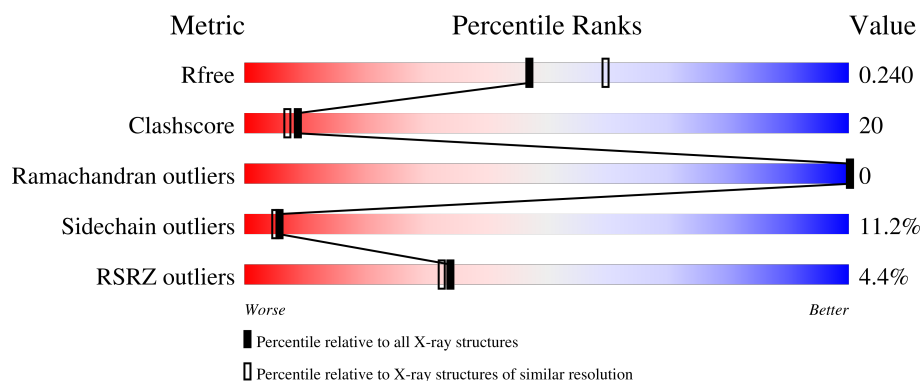
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 ≥ 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	
1	B	331	
1	C	331	
1	D	331	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10231 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	301	Total	C	N	O	S	0	2	0
			2412	1551	408	434	19			
1	B	312	Total	C	N	O	S	0	0	0
			2465	1584	419	443	19			
1	C	302	Total	C	N	O	S	0	0	0
			2395	1538	402	436	19			
1	D	309	Total	C	N	O	S	0	0	0
			2435	1568	410	439	18			

There are 24 discrepancies between the modelled and reference sequences:

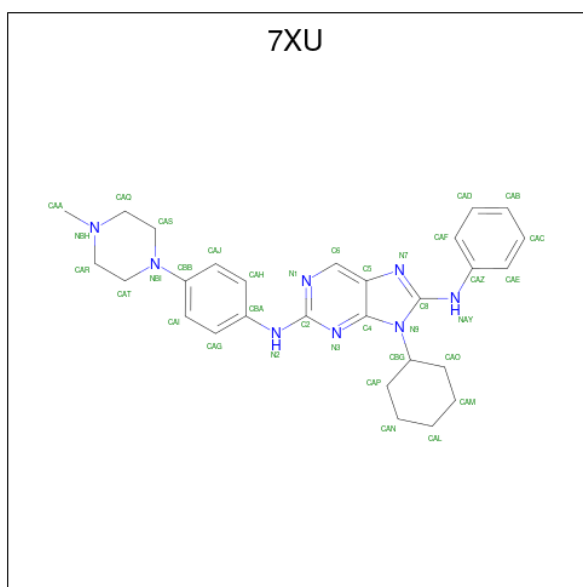
Chain	Residue	Modelled	Actual	Comment	Reference
A	692	GLY	-	expression tag	UNP P00533
A	693	SER	-	expression tag	UNP P00533
A	694	THR	-	expression tag	UNP P00533
A	695	SER	-	expression tag	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
B	692	GLY	-	expression tag	UNP P00533
B	693	SER	-	expression tag	UNP P00533
B	694	THR	-	expression tag	UNP P00533
B	695	SER	-	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	695	SER	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	695	SER	-	expression tag	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is 9-cyclohexyl-N2-[4-(4-methylpiperazin-1-yl)phenyl]-N8-phenyl-purine-2,8-diamine (three-letter code: 7XU) (formula: C₂₈H₃₄N₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 36	C 28	N 8	0	0
2	B	1	Total 36	C 28	N 8	0	0
2	C	1	Total 36	C 28	N 8	0	0
2	D	1	Total 36	C 28	N 8	0	0

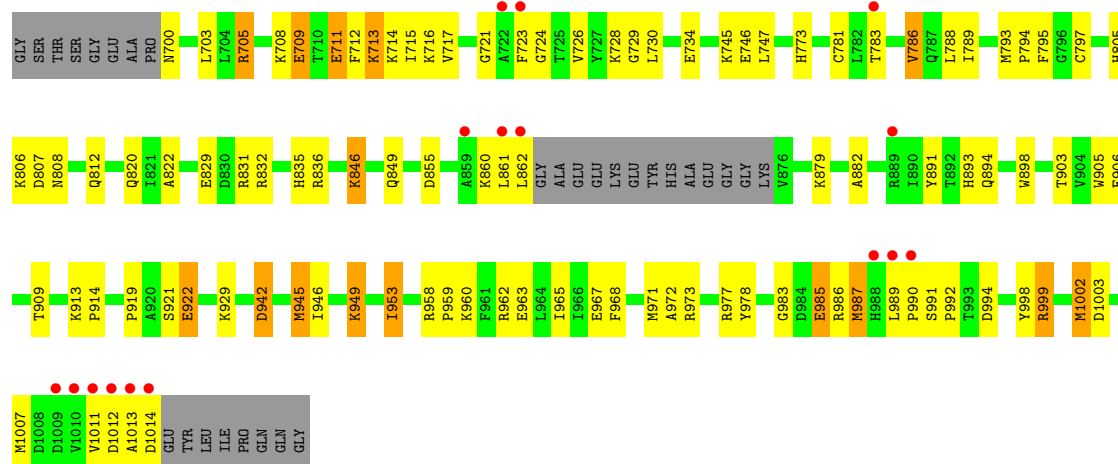
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	99	Total O 99 99	0	0
3	B	92	Total O 92 92	0	0
3	C	87	Total O 87 87	0	0

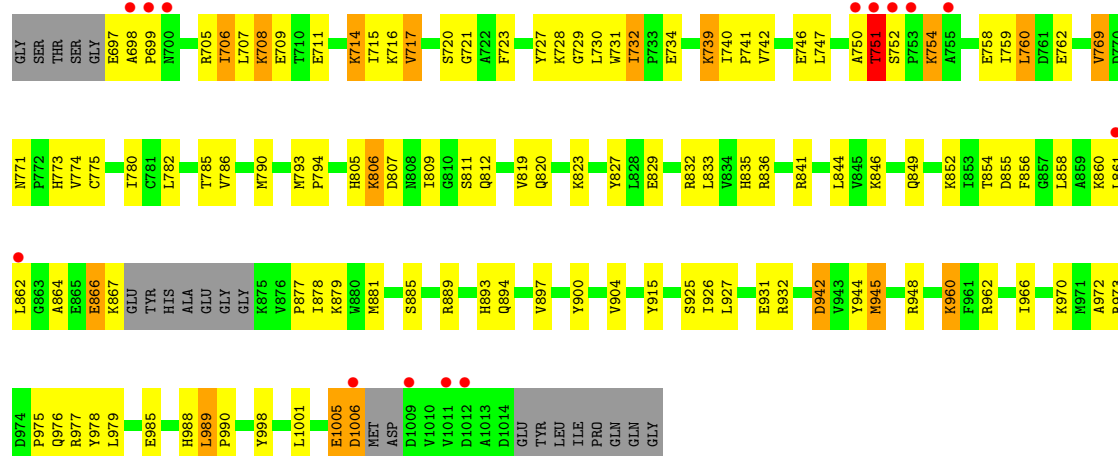
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	102	Total 102	O 102	0	0



• 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	71.50Å 102.59Å 87.03Å 90.00° 102.64° 90.00°	Depositor
Resolution (Å)	39.23 – 2.20 48.91 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.2 (39.23-2.20) 89.2 (48.91-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.203 , 0.240 0.210 , 0.240	Depositor DCC
R_{free} test set	2834 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10231	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 25.43 % 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 3.1772e-03.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7XU

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	0.77	0/2468	0.64	0/3339
1	B	0.76	0/2520	0.63	0/3412
1	C	0.77	0/2445	0.62	0/3311
1	D	0.71	0/2487	0.63	1/3368 (0.0%)
All	All	0.75	0/9920	0.63	1/13430 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	751	THR	N-CA-C	-5.49	96.17	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	749	GLU	Peptide
1	D	751	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2412	0	2447	104	0
1	B	2465	0	2467	99	0
1	C	2395	0	2409	89	0
1	D	2435	0	2445	105	0
2	A	36	0	0	3	0
2	B	36	0	0	3	0
2	C	36	0	0	3	0
2	D	36	0	0	4	0
3	A	99	0	0	9	0
3	B	92	0	0	11	0
3	C	87	0	0	7	0
3	D	102	0	0	10	0
All	All	10231	0	9768	400	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 20.

All (400) 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:C:989:LEU:CD1	1:C:990:PRO:HD3	1.48	1.43
1:B:855:ASP:OD1	1:B:858:LEU:HD12	1.39	1.20
1:A:989:LEU:N	1:A:989:LEU:HD23	1.56	1.19
1:A:749:GLU:OE1	1:A:750:ALA:HB3	1.40	1.19
1:C:794:PRO:HD2	3:C:1226:HOH:O	1.40	1.19
1:C:989:LEU:HG	1:C:990:PRO:CD	1.73	1.17
1:C:985:GLU:HB3	3:C:1220:HOH:O	1.44	1.16
1:C:723:PHE:CB	1:C:862:LEU:HD21	1.76	1.15
1:C:849:GLN:HG2	3:C:1233:HOH:O	1.48	1.13
1:A:941:ILE:CD1	1:A:945:MET:HG2	1.77	1.12
1:C:989:LEU:CG	1:C:990:PRO:CD	2.30	1.10
1:C:989:LEU:CD1	1:C:990:PRO:CD	2.30	1.08
1:C:989:LEU:CG	1:C:990:PRO:HD2	1.86	1.05
1:D:728:LYS:HD3	3:D:1232:HOH:O	1.59	1.02
1:B:783:THR:CG2	1:B:784:SER:H	1.71	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:989:LEU:HG	1:C:990:PRO:HD2	1.03	1.00
1:B:986:ARG:HH21	1:B:986:ARG:HG3	1.27	1.00
1:D:707:LEU:HD23	1:D:711:GLU:OE2	1.60	1.00
1:C:989:LEU:HD12	1:C:990:PRO:CD	1.92	0.99
1:A:989:LEU:HD23	1:A:989:LEU:H	1.07	0.98
1:C:812:GLN:HG2	1:C:989:LEU:HD22	1.44	0.98
1:C:989:LEU:HD12	1:C:990:PRO:HD3	0.96	0.95
1:A:941:ILE:HD13	1:A:941:ILE:O	1.67	0.94
1:D:697:GLU:CB	1:D:699:PRO:HD2	1.97	0.94
1:D:866:GLU:OE1	1:D:866:GLU:HA	1.64	0.93
1:A:989:LEU:N	1:A:989:LEU:CD2	2.30	0.93
1:B:783:THR:HG22	1:B:784:SER:N	1.84	0.93
1:C:723:PHE:CB	1:C:862:LEU:CD2	2.47	0.92
1:C:973:ARG:HG2	1:C:1014:ASP:OD1	1.70	0.90
1:A:836:ARG:HG2	1:A:891:TYR:CD2	2.06	0.90
1:B:807:ASP:HA	3:B:1210:HOH:O	1.73	0.88
1:B:783:THR:HG23	1:B:784:SER:H	1.38	0.87
1:C:989:LEU:CG	1:C:990:PRO:HD3	2.02	0.87
1:B:700:ASN:HD21	1:B:702:ALA:HB3	1.40	0.87
1:A:941:ILE:CD1	1:A:945:MET:CG	2.52	0.86
1:A:983:GLY:CA	1:A:986:ARG:HE	1.89	0.86
1:A:961:PHE:HA	1:A:964:LEU:HD12	1.58	0.85
1:A:983:GLY:HA3	1:A:986:ARG:HE	1.42	0.84
1:A:972:ALA:HB3	1:A:1011:VAL:HG11	1.61	0.83
1:B:783:THR:CG2	1:B:784:SER:N	2.29	0.82
1:A:941:ILE:CD1	1:A:941:ILE:O	2.30	0.80
1:B:701:GLN:HG2	1:B:764:TYR:CZ	2.17	0.80
1:A:941:ILE:HD11	1:A:945:MET:HG2	1.64	0.80
1:B:700:ASN:ND2	1:B:702:ALA:HB3	1.98	0.79
1:A:941:ILE:HD13	1:A:945:MET:HG2	1.62	0.78
1:D:747:LEU:HD13	1:D:862:LEU:HD21	1.65	0.78
1:B:938:ILE:HG22	3:B:1208:HOH:O	1.84	0.77
1:C:773:HIS:NE2	1:C:820:GLN:HG2	1.99	0.77
1:B:714:LYS:HE2	1:B:787:GLN:OE1	1.85	0.77
1:B:960:LYS:HE3	1:B:960:LYS:HA	1.68	0.76
1:C:715:ILE:HD11	1:C:728:LYS:HE2	1.67	0.75
1:D:812:GLN:HG2	1:D:989:LEU:HD22	1.69	0.75
1:B:869:TYR:CE2	1:B:876:VAL:HG21	2.22	0.74
1:A:989:LEU:H	1:A:989:LEU:CD2	1.88	0.74
1:D:866:GLU:OE1	1:D:866:GLU:CA	2.33	0.74
1:D:714:LYS:HG2	1:D:727:TYR:CG	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:988:HIS:HB3	3:D:1261:HOH:O	1.87	0.74
1:D:773:HIS:CE1	1:D:820:GLN:HG2	2.23	0.74
1:A:773:HIS:CE1	1:A:820:GLN:HG2	2.23	0.73
1:D:698:ALA:N	1:D:699:PRO:CD	2.52	0.73
1:B:855:ASP:OD1	1:B:858:LEU:CD1	2.30	0.73
1:A:938:ILE:HG23	3:A:3165:HOH:O	1.87	0.73
1:C:723:PHE:CB	1:C:747:LEU:HD22	2.18	0.73
1:B:986:ARG:HG3	1:B:986:ARG:NH2	2.02	0.72
1:B:711:GLU:O	1:B:732:ILE:HD12	1.89	0.72
1:D:812:GLN:HG2	1:D:989:LEU:CD2	2.19	0.72
1:B:876:VAL:HG12	1:B:878:ILE:HD12	1.71	0.71
1:D:812:GLN:CG	1:D:989:LEU:HD22	2.19	0.71
1:A:944:TYR:CE2	1:A:948:ARG:HD3	2.26	0.70
1:B:905:TRP:HB2	1:B:947:MET:CE	2.21	0.70
1:A:749:GLU:OE1	1:A:750:ALA:CB	2.30	0.70
1:A:905:TRP:HD1	1:A:947:MET:HE1	1.56	0.70
2:D:1101:7XU:N3	2:D:1101:7XU:CAG	2.53	0.70
1:A:941:ILE:HD11	1:A:945:MET:CG	2.20	0.70
1:D:841:ARG:HH12	1:D:877:PRO:HB3	1.56	0.70
1:D:714:LYS:HG2	1:D:727:TYR:CD2	2.27	0.69
1:B:829:GLU:HG3	1:B:893:HIS:CG	2.27	0.69
1:C:726:VAL:HG22	1:C:745:LYS:HB2	1.74	0.69
1:C:812:GLN:CG	1:C:989:LEU:HD22	2.23	0.69
1:D:775:CYS:HB3	1:D:790:MET:CE	2.22	0.69
1:C:836:ARG:HG2	1:C:891:TYR:CD2	2.28	0.69
1:D:827:TYR:HD1	3:D:1206:HOH:O	1.75	0.69
1:A:905:TRP:CD1	1:A:947:MET:HE1	2.28	0.68
1:A:984:ASP:HA	1:A:987:MET:HG3	1.76	0.68
1:A:962[A]:ARG:HG3	3:A:3132:HOH:O	1.94	0.68
1:D:827:TYR:CD1	3:D:1206:HOH:O	2.46	0.68
1:D:900:TYR:O	1:D:904:VAL:HG23	1.94	0.67
1:B:876:VAL:CG1	1:B:878:ILE:HD12	2.24	0.67
1:B:894:GLN:OE1	1:B:960:LYS:NZ	2.24	0.67
1:A:944:TYR:CZ	1:A:948:ARG:HD3	2.30	0.66
1:B:835:HIS:O	1:B:836:ARG:HB2	1.94	0.66
1:D:835:HIS:O	1:D:836:ARG:HB2	1.95	0.66
2:D:1101:7XU:CAE	2:D:1101:7XU:N7	2.53	0.65
1:D:728:LYS:CD	3:D:1232:HOH:O	2.29	0.65
1:B:992:PRO:HD2	3:B:1226:HOH:O	1.97	0.65
1:B:909:THR:OG1	1:B:912:SER:HB2	1.97	0.64
1:B:992:PRO:O	1:B:996:ASN:ND2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:ILE:HD12	1:A:789:ILE:N	2.13	0.63
1:A:972:ALA:HB3	1:A:1011:VAL:CG1	2.26	0.63
1:D:793:MET:O	2:D:1101:7XU:N2	2.31	0.63
1:B:879:LYS:HG2	1:B:915:TYR:HD1	1.64	0.63
1:C:716:LYS:HG3	1:C:717:VAL:N	2.12	0.63
1:D:811:SER:OG	1:D:975:PRO:HB2	1.98	0.63
1:A:879:LYS:HD3	1:A:915:TYR:HB2	1.81	0.63
1:B:924:SER:O	1:B:928:GLU:HG3	1.99	0.63
1:B:981:ILE:HA	3:B:1208:HOH:O	1.99	0.62
1:C:999:ARG:HG3	1:C:1003:ASP:O	2.00	0.62
1:D:970:LYS:HA	1:D:973:ARG:HH11	1.64	0.62
1:C:962:ARG:NE	3:C:1201:HOH:O	2.26	0.62
1:C:747:LEU:HD12	1:C:786:VAL:CG1	2.28	0.62
1:D:855:ASP:OD1	1:D:858:LEU:HD12	1.99	0.62
1:B:869:TYR:CD2	1:B:876:VAL:HG21	2.35	0.62
1:B:961:PHE:HA	1:B:964:LEU:HD12	1.82	0.61
1:A:801:TYR:CE1	1:A:805:HIS:CE1	2.88	0.61
1:D:760:LEU:HD13	1:D:782:LEU:CD1	2.30	0.61
1:A:986:ARG:HG2	1:A:987:MET:N	2.14	0.61
1:A:962[A]:ARG:HH11	1:A:962[A]:ARG:HG2	1.65	0.61
1:D:775:CYS:HB3	1:D:790:MET:HE1	1.82	0.61
1:A:972:ALA:O	1:A:975:PRO:HD3	2.01	0.61
1:B:714:LYS:CE	1:B:787:GLN:OE1	2.48	0.61
1:A:986:ARG:HB3	1:A:986:ARG:CZ	2.29	0.60
1:D:942:ASP:OD1	1:D:942:ASP:N	2.31	0.60
1:D:926:ILE:HG13	1:D:927:LEU:N	2.17	0.60
1:B:748:ARG:HG2	3:B:1247:HOH:O	2.00	0.60
2:B:1101:7XU:N7	2:B:1101:7XU:CAE	2.62	0.60
1:C:709:GLU:CG	1:C:783:THR:HG21	2.31	0.60
2:A:3001:7XU:CAG	2:A:3001:7XU:N3	2.62	0.60
1:A:954:ASP:O	1:A:957:SER:HB2	2.02	0.60
1:B:967:GLU:O	1:B:971:MET:HG3	2.02	0.59
1:B:986:ARG:NH2	1:B:986:ARG:CG	2.65	0.59
1:C:709:GLU:HG2	1:C:783:THR:HG21	1.83	0.59
1:D:972:ALA:O	1:D:975:PRO:HD3	2.01	0.59
1:D:1005:GLU:HG3	1:D:1006:ASP:HB3	1.83	0.59
1:D:709:GLU:HG3	3:D:1264:HOH:O	2.02	0.59
1:D:760:LEU:CD1	1:D:782:LEU:CD1	2.81	0.59
1:C:991:SER:HB2	1:C:992:PRO:HD2	1.84	0.59
1:D:754:LYS:HG3	1:D:759:ILE:CD1	2.32	0.59
1:D:771:ASN:ND2	3:D:1206:HOH:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:VAL:HG12	1:B:727:TYR:CE2	2.37	0.58
1:C:829:GLU:HG3	1:C:893:HIS:CD2	2.38	0.58
1:B:941:ILE:O	1:B:945:MET:HG2	2.02	0.58
1:C:829:GLU:HG3	1:C:893:HIS:CG	2.37	0.58
1:C:793:MET:SD	1:C:846:LYS:HG2	2.42	0.58
1:D:962:ARG:O	1:D:966:ILE:HD12	2.04	0.58
2:C:1101:7XU:N3	2:C:1101:7XU:CAG	2.60	0.58
1:A:929:LYS:HD3	1:A:929:LYS:N	2.18	0.58
1:A:905:TRP:HD1	1:A:947:MET:CE	2.18	0.57
1:B:783:THR:HG22	1:B:785:THR:H	1.69	0.57
1:B:723:PHE:HD2	1:B:862:LEU:HD12	1.67	0.57
1:B:846:LYS:HE2	1:B:1003:ASP:OD2	2.03	0.57
1:D:819:VAL:HG12	1:D:823:LYS:HD2	1.86	0.57
1:B:960:LYS:HG2	1:B:963:GLU:OE2	2.04	0.57
1:C:808:ASN:HA	1:C:987:MET:CE	2.34	0.57
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.40	0.57
1:A:983:GLY:HA2	1:A:986:ARG:HH21	1.69	0.57
1:B:723:PHE:HE1	1:B:837:ASP:OD2	1.88	0.56
1:B:905:TRP:CB	1:B:947:MET:HE1	2.35	0.56
1:A:835:HIS:O	1:A:836:ARG:HB2	2.04	0.56
1:D:715:ILE:HD11	1:D:728:LYS:HE2	1.85	0.56
1:D:729:GLY:O	1:D:742:VAL:HG22	2.05	0.56
1:D:723:PHE:CD1	1:D:862:LEU:HD12	2.41	0.56
1:B:905:TRP:CD1	1:B:947:MET:HE1	2.41	0.55
1:C:894:GLN:HG2	3:C:1254:HOH:O	2.06	0.55
1:D:751:THR:O	1:D:752:SER:C	2.45	0.55
1:A:805:HIS:O	1:A:809:ILE:HG13	2.06	0.55
1:C:919:PRO:HG2	1:C:922:GLU:OE1	2.06	0.55
1:B:947:MET:HE2	1:B:951:TRP:HH2	1.71	0.55
1:A:806:LYS:O	1:A:910:PHE:CD1	2.60	0.55
1:A:973:ARG:O	1:A:1013:ALA:HA	2.06	0.55
1:C:898:TRP:CD1	1:C:898:TRP:C	2.80	0.54
1:D:931:GLU:O	1:D:932:ARG:NH1	2.30	0.54
1:A:941:ILE:CD1	1:A:941:ILE:C	2.76	0.54
1:A:1013:ALA:O	1:A:1014:ASP:CB	2.54	0.54
1:C:973:ARG:O	1:C:1013:ALA:HA	2.07	0.54
1:D:945:MET:CE	1:D:948:ARG:HB2	2.37	0.54
1:B:793:MET:O	2:B:1101:7XU:N2	2.41	0.54
1:C:973:ARG:O	1:C:1014:ASP:N	2.36	0.54
1:A:723:PHE:O	1:A:748:ARG:HB2	2.08	0.53
1:C:705:ARG:NH1	1:C:711:GLU:OE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:945:MET:HE3	1:D:948:ARG:HB2	1.89	0.53
1:D:714:LYS:HG2	1:D:727:TYR:CB	2.38	0.53
1:C:808:ASN:HA	1:C:987:MET:HE2	1.91	0.53
1:D:854:THR:O	1:D:855:ASP:HB2	2.07	0.53
1:C:700:ASN:HB3	1:C:703:LEU:HD12	1.90	0.53
1:D:988:HIS:CB	3:D:1261:HOH:O	2.53	0.53
1:C:747:LEU:HD12	1:C:786:VAL:HG11	1.90	0.53
1:C:991:SER:HB2	1:C:992:PRO:CD	2.39	0.53
1:D:775:CYS:CB	1:D:790:MET:HE1	2.39	0.53
1:D:723:PHE:HD1	1:D:862:LEU:HD12	1.74	0.53
1:B:701:GLN:HG2	1:B:764:TYR:CE1	2.44	0.53
1:A:941:ILE:HD12	1:A:945:MET:CG	2.39	0.52
1:D:698:ALA:N	1:D:699:PRO:HD2	2.24	0.52
2:A:3001:7XU:CAE	2:A:3001:7XU:N7	2.71	0.52
1:C:747:LEU:HD12	1:C:786:VAL:HG13	1.89	0.52
1:B:770:ASP:HA	3:B:1227:HOH:O	2.09	0.52
1:D:780:ILE:HD13	1:D:782:LEU:HD11	1.92	0.52
1:C:919:PRO:CG	1:C:922:GLU:OE1	2.57	0.52
1:D:841:ARG:NH1	1:D:877:PRO:HB3	2.24	0.52
1:A:826:ASN:HD21	1:A:962[A]:ARG:HG2	1.74	0.51
1:A:934:PRO:O	1:A:936:PRO:HD3	2.11	0.51
1:A:841:ARG:HD3	3:A:3138:HOH:O	2.09	0.51
1:C:968:PHE:HA	1:C:971:MET:HE3	1.92	0.51
1:B:716:LYS:HG3	1:B:717:VAL:N	2.25	0.51
1:B:783:THR:HG22	1:B:784:SER:H	1.48	0.51
1:C:962:ARG:HA	1:C:965:ILE:HD12	1.92	0.51
1:D:750:ALA:C	1:D:751:THR:O	2.45	0.51
1:D:754:LYS:HG3	1:D:759:ILE:HD13	1.92	0.51
1:A:715:ILE:HD13	1:A:730:LEU:HG	1.91	0.51
1:A:962[A]:ARG:NH1	3:A:3106:HOH:O	2.44	0.51
1:C:945:MET:O	1:C:949:LYS:HG2	2.11	0.50
1:D:960:LYS:NZ	3:D:1216:HOH:O	2.44	0.50
1:D:1006:ASP:OD1	1:D:1006:ASP:O	2.29	0.50
1:B:933:LEU:HG	3:B:1202:HOH:O	2.11	0.50
1:D:769:VAL:HG21	1:D:774:VAL:HG12	1.93	0.50
1:C:962:ARG:HD3	3:C:1285:HOH:O	2.12	0.50
1:D:989:LEU:HD12	1:D:990:PRO:HD3	1.93	0.50
2:B:1101:7XU:CAG	2:B:1101:7XU:N3	2.74	0.50
1:D:706:ILE:HD13	1:D:706:ILE:N	2.26	0.50
1:D:970:LYS:HA	1:D:973:ARG:NH1	2.25	0.50
1:A:721:GLY:HA3	3:A:3112:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:834:VAL:HA	3:B:1203:HOH:O	2.11	0.50
1:B:854:THR:HA	3:B:1257:HOH:O	2.12	0.50
1:C:729:GLY:O	1:C:730:LEU:HD23	2.12	0.50
1:A:775:CYS:HB3	1:A:790:MET:CE	2.42	0.50
1:A:991:SER:HB2	1:A:992:PRO:CD	2.42	0.50
1:B:905:TRP:CB	1:B:947:MET:CE	2.90	0.50
1:D:805:HIS:O	1:D:809:ILE:HG13	2.12	0.50
1:A:760:LEU:HD11	1:A:782:LEU:HD21	1.94	0.49
1:B:898:TRP:CD1	1:B:898:TRP:C	2.86	0.49
1:A:716:LYS:HG3	1:A:717:VAL:N	2.26	0.49
1:A:808:ASN:OD1	1:A:808:ASN:O	2.30	0.49
1:B:723:PHE:CD2	1:B:862:LEU:HD12	2.46	0.49
1:B:701:GLN:CG	1:B:764:TYR:CZ	2.94	0.49
1:B:839:ALA:HB3	1:B:841:ARG:HD3	1.95	0.49
1:B:875:LYS:O	1:B:877:PRO:HD3	2.13	0.49
1:D:760:LEU:CD1	1:D:782:LEU:HD11	2.42	0.49
1:C:781:CYS:SG	1:C:783:THR:HG23	2.53	0.49
1:D:730:LEU:HD13	1:D:739:LYS:HB2	1.94	0.49
1:A:788:LEU:C	1:A:789:ILE:HD12	2.33	0.48
1:A:972:ALA:CB	1:A:1011:VAL:CG1	2.91	0.48
1:C:983:GLY:O	1:C:987:MET:HG3	2.14	0.48
1:C:985:GLU:HG2	1:C:986:ARG:N	2.27	0.48
1:D:754:LYS:NZ	1:D:762:GLU:OE1	2.47	0.48
1:C:789:ILE:HD12	1:C:789:ILE:N	2.28	0.48
1:D:846:LYS:NZ	1:D:1005:GLU:OE1	2.46	0.48
1:A:884:GLU:HG2	1:A:885:SER:N	2.26	0.48
1:A:986:ARG:CZ	1:A:986:ARG:CB	2.92	0.48
1:B:931:GLU:O	1:B:932:ARG:HD3	2.13	0.48
1:D:754:LYS:HB3	1:D:754:LYS:HE2	1.43	0.47
1:A:968:PHE:HA	1:A:971:MET:HE3	1.95	0.47
1:C:716:LYS:HG3	1:C:717:VAL:H	1.79	0.47
1:D:849:GLN:CD	1:D:849:GLN:H	2.17	0.47
1:C:977:ARG:NE	3:C:1206:HOH:O	2.47	0.47
1:D:833:LEU:HD13	1:D:856:PHE:CZ	2.49	0.47
1:A:775:CYS:HB3	1:A:790:MET:HE2	1.95	0.47
1:B:890:ILE:O	1:B:890:ILE:HG22	2.13	0.47
1:A:701:GLN:HG2	1:A:764:TYR:CE2	2.49	0.47
1:B:839:ALA:CB	1:B:841:ARG:HD3	2.44	0.47
1:D:751:THR:HG21	1:D:864:ALA:HA	1.97	0.47
1:D:754:LYS:HG3	1:D:759:ILE:HD11	1.96	0.47
1:B:935:GLN:HA	1:B:944:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.49	0.47
1:A:762:GLU:HB2	3:A:3166:HOH:O	2.14	0.47
1:A:769:VAL:HG11	1:A:774:VAL:CG1	2.45	0.47
1:A:801:TYR:CE1	1:A:805:HIS:HE1	2.31	0.47
1:B:960:LYS:HA	1:B:960:LYS:CE	2.42	0.47
1:C:972:ALA:HB3	1:C:1011:VAL:HG11	1.96	0.47
1:B:701:GLN:HG2	1:B:764:TYR:CE2	2.49	0.46
1:A:731:TRP:CE3	1:D:1001:LEU:HD12	2.50	0.46
1:A:962[A]:ARG:HG3	1:A:962[A]:ARG:H	1.51	0.46
1:D:945:MET:HE1	1:D:948:ARG:CB	2.46	0.46
1:A:981:ILE:O	1:A:984:ASP:HB2	2.16	0.46
1:B:738:VAL:HG21	1:C:795:PHE:CZ	2.51	0.46
1:C:879:LYS:HD3	1:C:914:PRO:O	2.15	0.46
1:A:988:HIS:C	1:A:989:LEU:HD23	2.28	0.46
1:B:718:LEU:HG	1:B:728:LYS:N	2.31	0.46
1:A:923:ILE:O	1:A:926:ILE:HG12	2.15	0.46
1:A:938:ILE:HD12	1:A:981:ILE:HD11	1.97	0.46
1:A:997:PHE:HE1	1:D:731:TRP:CD2	2.34	0.45
1:B:789:ILE:N	1:B:789:ILE:HD12	2.31	0.45
1:B:958:ARG:HB3	1:B:959:PRO:HD2	1.99	0.45
1:D:885:SER:O	1:D:889:ARG:HA	2.17	0.45
1:B:905:TRP:HA	1:B:947:MET:HE1	1.98	0.45
1:C:721:GLY:O	1:C:724:GLY:O	2.34	0.45
1:B:747:LEU:HD13	1:B:862:LEU:HD21	1.99	0.45
1:A:793:MET:O	2:A:3001:7XU:N2	2.50	0.45
1:B:905:TRP:HD1	1:B:947:MET:CE	2.29	0.45
1:B:960:LYS:HE3	3:B:1220:HOH:O	2.17	0.45
1:B:700:ASN:HB3	1:B:703:LEU:HD22	1.99	0.45
1:C:726:VAL:HG22	1:C:745:LYS:CB	2.43	0.45
1:C:919:PRO:HG2	1:C:922:GLU:HB2	1.99	0.44
1:A:977:ARG:NH2	1:A:978:TYR:OH	2.51	0.44
1:D:732:ILE:O	1:D:732:ILE:HG22	2.14	0.44
1:D:879:LYS:HB3	1:D:915:TYR:HD1	1.82	0.44
1:A:923:ILE:HD13	1:A:926:ILE:HD11	1.99	0.44
1:B:905:TRP:CD1	1:B:947:MET:CE	3.00	0.44
1:D:833:LEU:HB3	1:D:856:PHE:CE1	2.52	0.44
1:D:976:GLN:HE22	1:D:985:GLU:HG2	1.81	0.44
1:A:833:LEU:HD22	1:A:856:PHE:HZ	1.82	0.44
1:C:712:PHE:O	1:C:713:LYS:HE3	2.17	0.44
1:C:985:GLU:HG2	1:C:986:ARG:H	1.83	0.44
1:D:775:CYS:HB3	1:D:790:MET:HE2	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:924:SER:O	1:A:928:GLU:HG3	2.17	0.44
1:B:854:THR:O	1:B:855:ASP:HB2	2.17	0.44
1:C:971:MET:HG2	1:C:978:TYR:CG	2.53	0.44
1:A:760:LEU:HD12	1:A:760:LEU:HA	1.87	0.44
1:B:829:GLU:HG3	1:B:893:HIS:CD2	2.53	0.44
1:D:1006:ASP:OD1	1:D:1006:ASP:C	2.54	0.44
1:A:898:TRP:CD1	1:A:898:TRP:C	2.91	0.43
1:B:866:GLU:O	1:B:870:HIS:CD2	2.71	0.43
1:B:905:TRP:CA	1:B:947:MET:HE1	2.48	0.43
3:A:3158:HOH:O	1:D:705:ARG:HB2	2.18	0.43
2:C:1101:7XU:N7	2:C:1101:7XU:CAE	2.80	0.43
1:D:714:LYS:HB2	1:D:714:LYS:HE2	1.40	0.43
1:A:708:LYS:HG3	1:A:711:GLU:OE2	2.19	0.43
1:B:717:VAL:HG23	1:B:717:VAL:O	2.18	0.43
1:B:780:ILE:HG23	1:B:780:ILE:O	2.18	0.43
1:D:751:THR:HG21	1:D:864:ALA:CA	2.48	0.43
1:A:780:ILE:HG12	1:A:782:LEU:HD23	1.99	0.43
1:D:715:ILE:HG13	1:D:716:LYS:N	2.33	0.43
1:D:721:GLY:HA3	3:D:1260:HOH:O	2.18	0.43
1:D:760:LEU:HD13	1:D:782:LEU:HD13	1.98	0.43
1:A:861:LEU:HA	1:A:861:LEU:HD23	1.79	0.43
1:A:960:LYS:HA	3:A:3128:HOH:O	2.18	0.43
1:A:960:LYS:HB2	1:A:963:GLU:HG3	2.01	0.43
1:B:700:ASN:CG	1:B:702:ALA:HB3	2.38	0.43
1:D:708:LYS:HE3	1:D:708:LYS:HB2	1.65	0.43
1:B:782:LEU:HD23	1:B:786:VAL:HB	2.00	0.43
1:C:808:ASN:HA	1:C:987:MET:HE1	2.00	0.43
1:C:991:SER:CB	1:C:992:PRO:CD	2.97	0.43
1:D:978:TYR:O	1:D:979:LEU:HD23	2.19	0.43
1:A:838:LEU:HD12	1:A:839:ALA:N	2.34	0.43
1:A:944:TYR:O	1:A:948:ARG:HG2	2.19	0.43
1:B:825:MET:HB3	1:B:961:PHE:CZ	2.54	0.43
1:B:960:LYS:CE	3:B:1220:HOH:O	2.66	0.43
1:C:724:GLY:HA3	1:C:746:GLU:O	2.18	0.43
1:C:953:ILE:H	1:C:953:ILE:HG12	1.60	0.43
1:D:858:LEU:HD23	1:D:858:LEU:HA	1.70	0.43
1:C:715:ILE:HD11	1:C:728:LYS:CE	2.43	0.43
1:C:788:LEU:C	1:C:789:ILE:HD12	2.39	0.43
1:C:861:LEU:HD23	1:C:861:LEU:HA	1.85	0.43
1:D:793:MET:HA	1:D:794:PRO:HD2	1.86	0.43
1:C:942:ASP:O	1:C:946:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:ASN:O	1:A:808:ASN:CG	2.57	0.42
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.54	0.42
1:C:822:ALA:HB1	1:C:965:ILE:HG13	2.01	0.42
1:B:705:ARG:CZ	1:C:994:ASP:OD2	2.67	0.42
1:B:947:MET:HE2	1:B:951:TRP:CH2	2.54	0.42
1:D:716:LYS:HG2	1:D:717:VAL:N	2.34	0.42
1:C:773:HIS:CD2	1:C:820:GLN:HG2	2.53	0.42
1:C:960:LYS:HB2	1:C:963:GLU:HG3	2.02	0.42
1:B:905:TRP:HB2	1:B:947:MET:HE3	1.99	0.42
1:D:793:MET:CE	1:D:852:LYS:HD3	2.50	0.42
1:B:879:LYS:HG2	1:B:915:TYR:CD1	2.51	0.42
1:D:708:LYS:HB2	1:D:711:GLU:HG3	2.02	0.42
1:A:931:GLU:O	1:A:932:ARG:HD3	2.20	0.41
1:B:735:GLY:O	1:C:805:HIS:HE1	2.03	0.41
1:D:806:LYS:HG2	1:D:807:ASP:N	2.35	0.41
1:A:888:HIS:HB2	1:A:890:ILE:HG13	2.01	0.41
1:D:746:GLU:OE1	1:D:785:THR:HG21	2.20	0.41
1:A:789:ILE:N	1:A:789:ILE:CD1	2.82	0.41
1:C:905:TRP:CZ2	1:C:909:THR:HG21	2.56	0.41
1:D:819:VAL:CG1	1:D:823:LYS:HD2	2.49	0.41
1:A:829:GLU:HG3	1:A:893:HIS:CG	2.55	0.41
1:B:868:GLU:OE1	1:B:875:LYS:HB2	2.21	0.41
1:C:903:THR:O	1:C:906:GLU:HB2	2.19	0.41
1:B:754:LYS:HE3	1:B:861:LEU:O	2.21	0.41
1:B:935:GLN:HA	1:B:944:TYR:CD1	2.56	0.41
1:D:769:VAL:O	1:D:769:VAL:CG2	2.68	0.41
1:D:782:LEU:HD23	1:D:786:VAL:HG22	2.03	0.41
1:A:714:LYS:HD2	1:A:727:TYR:CG	2.56	0.41
1:A:962[B]:ARG:HD3	1:A:962[B]:ARG:HA	1.39	0.41
1:A:991:SER:HB2	1:A:992:PRO:HD2	2.02	0.41
1:B:876:VAL:HA	1:B:877:PRO:HD2	1.90	0.41
1:D:729:GLY:O	1:D:742:VAL:N	2.51	0.41
1:D:740:ILE:HA	1:D:741:PRO:HD3	1.94	0.41
1:D:894:GLN:O	1:D:897:VAL:HB	2.20	0.41
1:B:866:GLU:O	1:B:869:TYR:HB2	2.21	0.41
1:C:793:MET:O	2:C:1101:7XU:N2	2.54	0.41
1:C:835:HIS:O	1:C:836:ARG:HB2	2.20	0.40
1:C:958:ARG:HA	1:C:959:PRO:HD3	1.94	0.40
1:D:844:LEU:HD11	2:D:1101:7XU:C5	2.51	0.40
1:D:944:TYR:CZ	1:D:948:ARG:HD3	2.56	0.40
1:A:755:ALA:O	1:A:759:ILE:HD12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:LEU:HD12	1:A:839:ALA:H	1.87	0.40
1:B:832:ARG:HG3	1:B:832:ARG:HH11	1.85	0.40
1:C:723:PHE:CB	1:C:862:LEU:HD22	2.44	0.40
1:B:757:LYS:CD	1:B:757:LYS:O	2.68	0.40
1:B:757:LYS:HA	1:B:757:LYS:HD3	1.89	0.40
1:A:978:TYR:CD1	1:A:978:TYR:N	2.89	0.40
1:A:985:GLU:H	1:A:985:GLU:HG3	1.35	0.40
1:C:831:ARG:O	1:C:832:ARG:HB2	2.21	0.40
1:C:1002:MET:HE3	1:C:1002:MET:HB3	1.81	0.40
1:D:829:GLU:HG3	1:D:893:HIS:CG	2.56	0.40
1:A:785:THR:HG22	3:A:3129:HOH:O	2.21	0.40
1:C:793:MET:HA	1:C:794:PRO:HD3	1.88	0.40
1:C:985:GLU:H	1:C:985:GLU:CD	2.25	0.40
1:D:878:ILE:HA	1:D:881:MET:SD	2.60	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	297/331 (90%)	289 (97%)	8 (3%)	0	100	100
1	B	310/331 (94%)	302 (97%)	8 (3%)	0	100	100
1	C	298/331 (90%)	293 (98%)	5 (2%)	0	100	100
1	D	303/331 (92%)	297 (98%)	6 (2%)	0	100	100
All	All	1208/1324 (91%)	1181 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	264/290 (91%)	233 (88%)	31 (12%)	5	4
1	B	262/290 (90%)	233 (89%)	29 (11%)	6	5
1	C	260/290 (90%)	230 (88%)	30 (12%)	5	5
1	D	261/290 (90%)	233 (89%)	28 (11%)	6	6
All	All	1047/1160 (90%)	929 (89%)	118 (11%)	6	5

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	705	ARG
1	A	706	ILE
1	A	708	LYS
1	A	716	LYS
1	A	732	ILE
1	A	757	LYS
1	A	760	LEU
1	A	768	SER
1	A	782	LEU
1	A	785	THR
1	A	797	CYS
1	A	836	ARG
1	A	855	ASP
1	A	858	LEU
1	A	876	VAL
1	A	889	ARG
1	A	921	SER
1	A	929	LYS
1	A	941	ILE
1	A	954	ASP
1	A	962[A]	ARG
1	A	962[B]	ARG
1	A	967	GLU
1	A	977	ARG

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Mol	Chain	Res	Type
1	A	985	GLU
1	A	986	ARG
1	A	987	MET
1	A	989	LEU
1	A	998	TYR
1	A	1005	GLU
1	A	1006	ASP
1	B	703	LEU
1	B	705	ARG
1	B	707	LEU
1	B	732	ILE
1	B	756	ASN
1	B	759	ILE
1	B	768	SER
1	B	783	THR
1	B	784	SER
1	B	793	MET
1	B	804	GLU
1	B	841	ARG
1	B	846	LYS
1	B	855	ASP
1	B	866	GLU
1	B	872	GLU
1	B	878	ILE
1	B	889	ARG
1	B	929	LYS
1	B	942	ASP
1	B	960	LYS
1	B	962	ARG
1	B	977	ARG
1	B	991	SER
1	B	995	SER
1	B	1001	LEU
1	B	1005	GLU
1	B	1006	ASP
1	B	1007	MET
1	C	705	ARG
1	C	708	LYS
1	C	709	GLU
1	C	711	GLU
1	C	713	LYS
1	C	714	LYS

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Mol	Chain	Res	Type
1	C	734	GLU
1	C	786	VAL
1	C	797	CYS
1	C	806	LYS
1	C	807	ASP
1	C	846	LYS
1	C	855	ASP
1	C	860	LYS
1	C	913	LYS
1	C	921	SER
1	C	922	GLU
1	C	929	LYS
1	C	942	ASP
1	C	945	MET
1	C	949	LYS
1	C	953	ILE
1	C	967	GLU
1	C	985	GLU
1	C	987	MET
1	C	998	TYR
1	C	999	ARG
1	C	1002	MET
1	C	1007	MET
1	C	1012	ASP
1	D	706	ILE
1	D	708	LYS
1	D	714	LYS
1	D	717	VAL
1	D	720	SER
1	D	732	ILE
1	D	734	GLU
1	D	739	LYS
1	D	751	THR
1	D	754	LYS
1	D	758	GLU
1	D	760	LEU
1	D	769	VAL
1	D	806	LYS
1	D	832	ARG
1	D	860	LYS
1	D	861	LEU
1	D	866	GLU

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Mol	Chain	Res	Type
1	D	867	LYS
1	D	925	SER
1	D	942	ASP
1	D	945	MET
1	D	960	LYS
1	D	977	ARG
1	D	989	LEU
1	D	998	TYR
1	D	1005	GLU
1	D	1006	ASP

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	805	HIS
1	A	826	ASN
1	A	888	HIS
1	A	893	HIS
1	B	812	GLN
1	B	849	GLN
1	B	870	HIS
1	B	996	ASN
1	C	805	HIS
1	D	812	GLN
1	D	976	GLN
1	D	988	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	7XU	A	3001	-	36,41,41	1.42	5 (13%)	45,57,57	1.68	7 (15%)
2	7XU	B	1101	-	36,41,41	1.26	3 (8%)	45,57,57	1.74	6 (13%)
2	7XU	C	1101	-	36,41,41	1.24	4 (11%)	45,57,57	1.74	7 (15%)
2	7XU	D	1101	-	36,41,41	1.34	4 (11%)	45,57,57	1.69	9 (20%)

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	7XU	A	3001	-	-	0/10/34/34	0/6/6/6
2	7XU	B	1101	-	-	0/10/34/34	0/6/6/6
2	7XU	C	1101	-	-	0/10/34/34	0/6/6/6
2	7XU	D	1101	-	-	2/10/34/34	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	7XU	CAZ-NAY	-4.58	1.30	1.40
2	B	1101	7XU	CAZ-NAY	-4.50	1.30	1.40
2	D	1101	7XU	CBA-N2	-4.32	1.31	1.40
2	D	1101	7XU	CAZ-NAY	-4.32	1.31	1.40
2	C	1101	7XU	CBA-N2	-4.08	1.31	1.40
2	A	3001	7XU	CBA-N2	-4.03	1.31	1.40
2	C	1101	7XU	CAZ-NAY	-3.86	1.32	1.40
2	B	1101	7XU	CBA-N2	-3.34	1.33	1.40
2	A	3001	7XU	C5-N7	-2.60	1.30	1.38
2	D	1101	7XU	C2-N2	-2.47	1.31	1.36
2	A	3001	7XU	C2-N2	-2.42	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	7XU	C4-N3	-2.35	1.32	1.35
2	C	1101	7XU	C5-N7	-2.30	1.31	1.38
2	C	1101	7XU	C2-N2	-2.29	1.31	1.36
2	B	1101	7XU	C5-N7	-2.18	1.31	1.38
2	D	1101	7XU	C5-N7	-2.03	1.32	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	7XU	N1-C2-N3	-6.84	119.91	126.52
2	C	1101	7XU	N1-C2-N3	-5.85	120.87	126.52
2	D	1101	7XU	N1-C2-N3	-5.22	121.48	126.52
2	A	3001	7XU	N1-C2-N3	-4.86	121.82	126.52
2	C	1101	7XU	CAT-NBI-CAS	4.77	122.05	111.52
2	A	3001	7XU	CAT-NBI-CAS	4.75	122.01	111.52
2	D	1101	7XU	CAT-NBI-CAS	4.75	121.99	111.52
2	B	1101	7XU	C2-N3-C4	4.45	120.33	115.28
2	B	1101	7XU	C6-N1-C2	4.41	122.42	115.88
2	B	1101	7XU	CAT-NBI-CAS	4.37	121.17	111.52
2	C	1101	7XU	C6-N1-C2	4.22	122.14	115.88
2	D	1101	7XU	C6-N1-C2	4.03	121.85	115.88
2	A	3001	7XU	C2-N3-C4	4.00	119.81	115.28
2	A	3001	7XU	CAS-CAQ-NBH	-3.67	106.66	110.80
2	A	3001	7XU	CAR-NBH-CAQ	-3.64	104.43	109.52
2	C	1101	7XU	C2-N3-C4	3.54	119.29	115.28
2	D	1101	7XU	C2-N3-C4	3.38	119.12	115.28
2	A	3001	7XU	C6-N1-C2	3.27	120.73	115.88
2	B	1101	7XU	CAZ-NAY-C8	-2.98	119.65	128.00
2	C	1101	7XU	CAS-CAQ-NBH	-2.87	107.56	110.80
2	D	1101	7XU	CAR-NBH-CAQ	-2.87	105.52	109.52
2	C	1101	7XU	CAA-NBH-CAQ	-2.84	106.41	110.66
2	C	1101	7XU	CAI-CBB-NBI	-2.78	117.54	121.38
2	A	3001	7XU	CAZ-NAY-C8	-2.72	120.37	128.00
2	D	1101	7XU	CAS-CAQ-NBH	-2.57	107.90	110.80
2	D	1101	7XU	CAZ-NAY-C8	-2.52	120.94	128.00
2	D	1101	7XU	CBA-N2-C2	-2.34	122.46	129.23
2	B	1101	7XU	CAR-NBH-CAQ	-2.33	106.27	109.52
2	D	1101	7XU	CAN-CAP-CBG	-2.03	108.57	111.57

There are no chirality outliers.

All (2) torsion outliers are listed below:

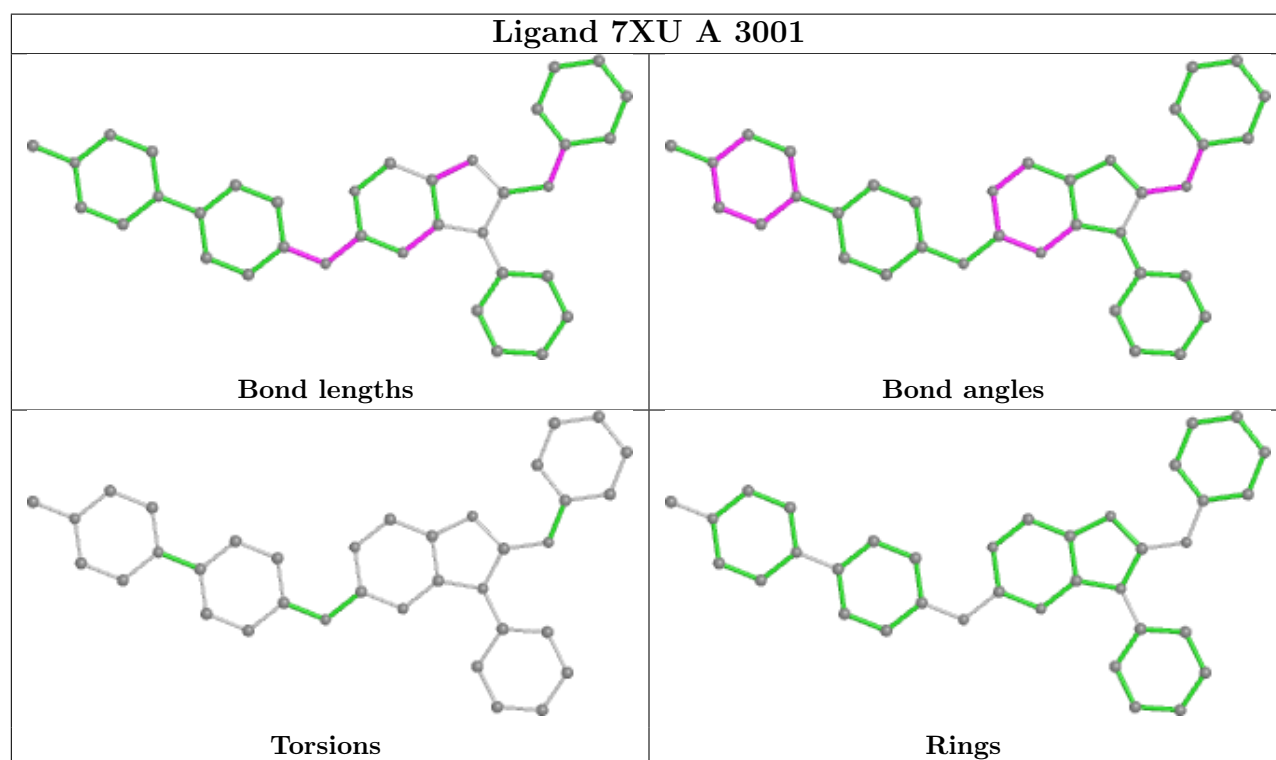
Mol	Chain	Res	Type	Atoms
2	D	1101	7XU	N1-C2-N2-CBA
2	D	1101	7XU	N3-C2-N2-CBA

There are no ring outliers.

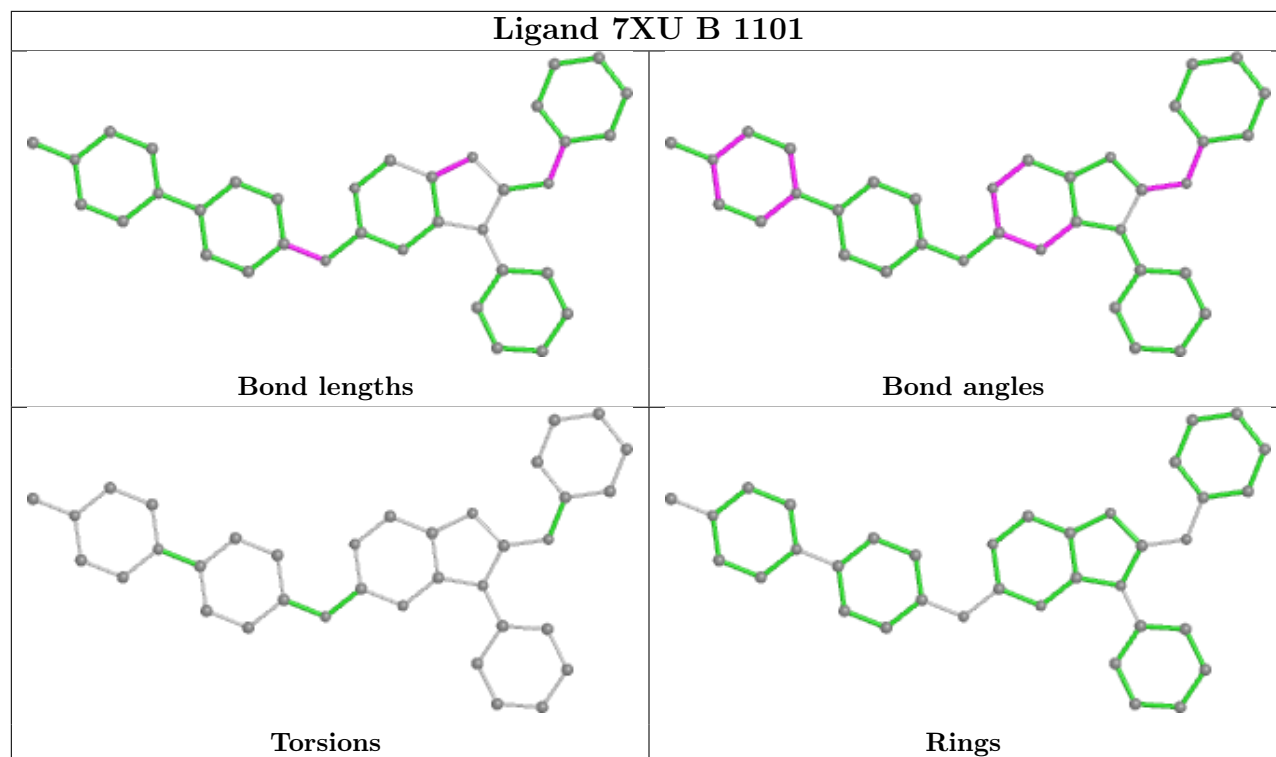
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	7XU	3	0
2	B	1101	7XU	3	0
2	C	1101	7XU	3	0
2	D	1101	7XU	4	0

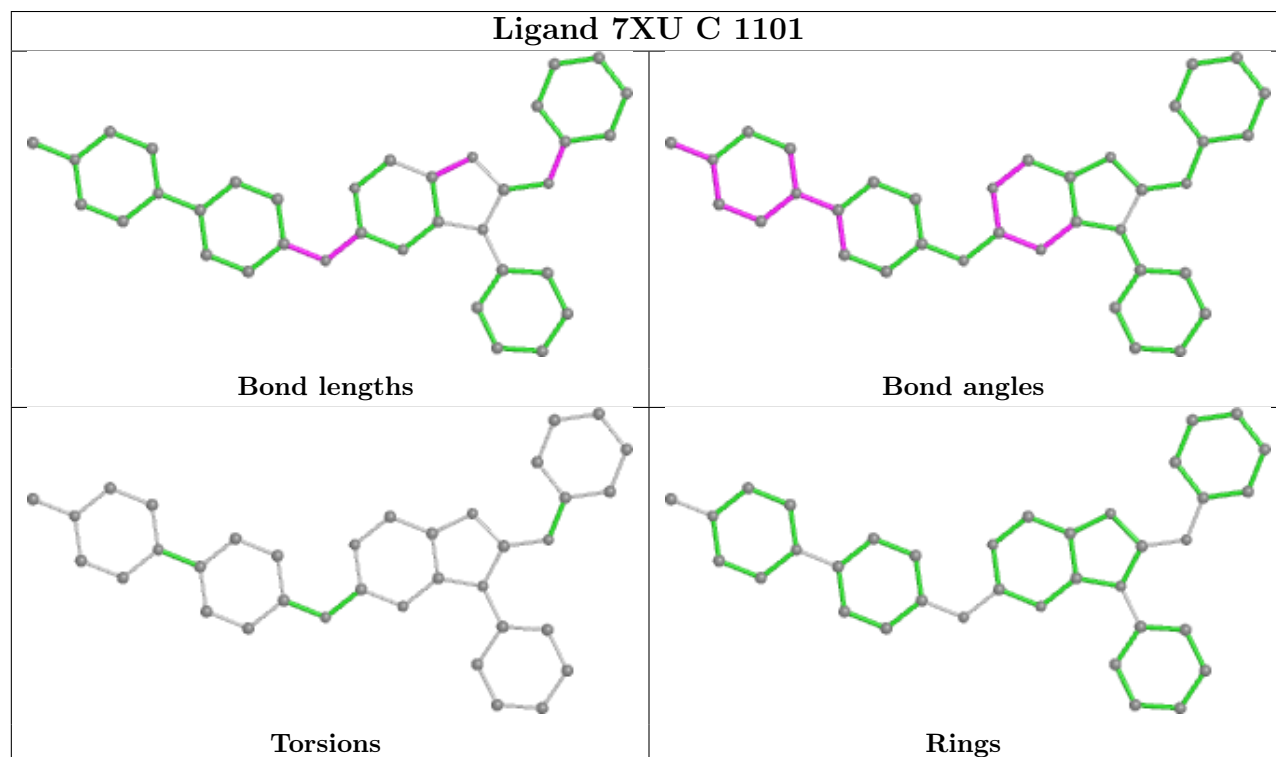
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

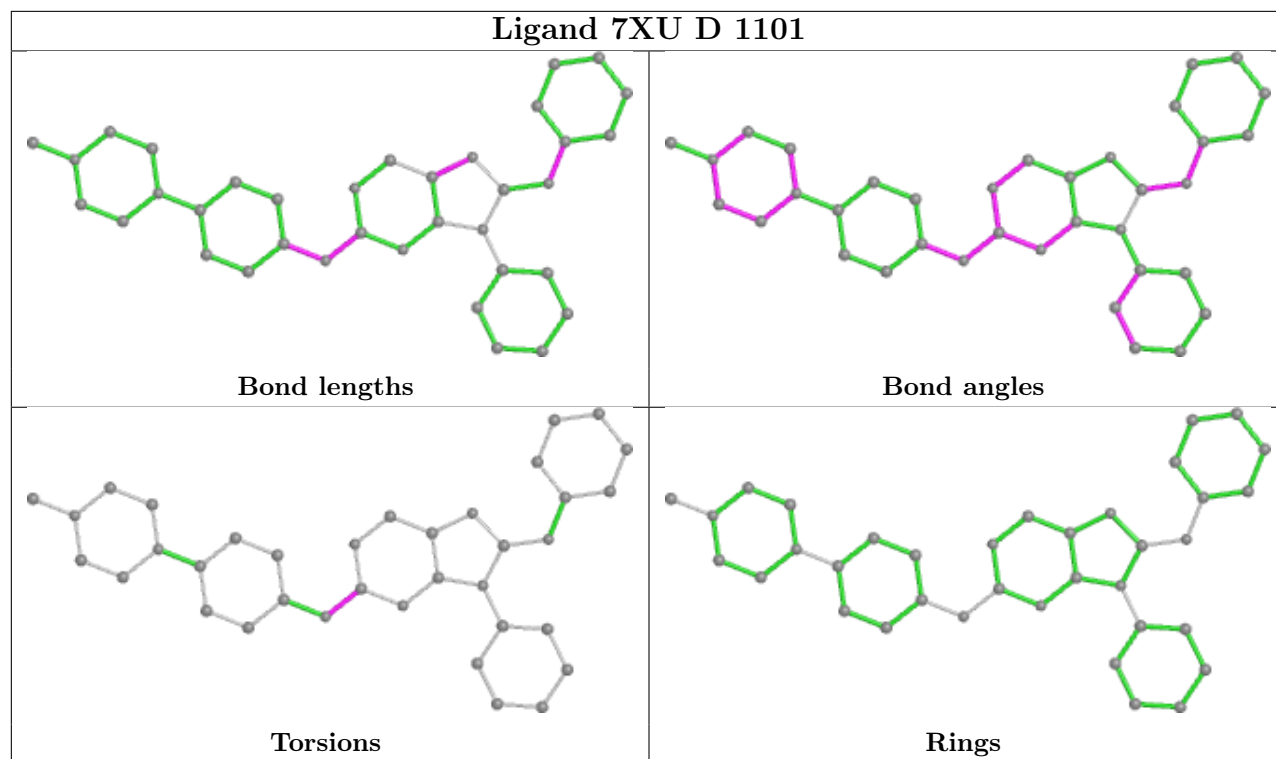


Ligand 7XU B 1101



Ligand 7XU 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	301/331 (90%)	-0.06	7 (2%) 60 58	17, 31, 58, 79	3 (0%)
1	B	312/331 (94%)	-0.01	17 (5%) 25 24	17, 35, 60, 82	11 (3%)
1	C	302/331 (91%)	-0.07	16 (5%) 26 25	16, 33, 58, 74	7 (2%)
1	D	309/331 (93%)	0.13	14 (4%) 33 32	24, 38, 63, 76	5 (1%)
All	All	1224/1324 (92%)	-0.00	54 (4%) 34 32	16, 35, 61, 82	26 (2%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1013	ALA	7.9
1	A	751	THR	7.8
1	D	699	PRO	7.5
1	C	988	HIS	6.0
1	D	698	ALA	5.9
1	B	871	ALA	5.4
1	A	750	ALA	5.1
1	D	752	SER	4.7
1	B	1010	VAL	4.7
1	C	722	ALA	4.4
1	C	1011	VAL	4.4
1	B	866	GLU	4.0
1	D	753	PRO	3.9
1	C	1012	ASP	3.6
1	C	1009	ASP	3.4
1	B	869	TYR	3.4
1	B	870	HIS	3.3
1	B	863	GLY	3.3
1	B	1008	ASP	3.2
1	C	859	ALA	3.2
1	C	783	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	990	PRO	3.1
1	B	988	HIS	3.0
1	D	1009	ASP	3.0
1	B	864	ALA	2.9
1	C	1014	ASP	2.9
1	A	985	GLU	2.8
1	A	988	HIS	2.8
1	D	700	ASN	2.8
1	B	699	PRO	2.8
1	C	1010	VAL	2.8
1	D	861	LEU	2.7
1	D	751	THR	2.6
1	C	862	LEU	2.6
1	B	868	GLU	2.5
1	A	1013	ALA	2.5
1	C	723	PHE	2.5
1	D	1006	ASP	2.4
1	B	753	PRO	2.4
1	B	701	GLN	2.3
1	A	752	SER	2.3
1	B	752	SER	2.3
1	D	750	ALA	2.2
1	D	755	ALA	2.2
1	A	989	LEU	2.2
1	C	861	LEU	2.2
1	C	989	LEU	2.1
1	D	862	LEU	2.1
1	D	1011	VAL	2.1
1	B	700	ASN	2.1
1	B	987	MET	2.1
1	C	889	ARG	2.1
1	B	875	LYS	2.1
1	D	1012	ASP	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 ⓘ

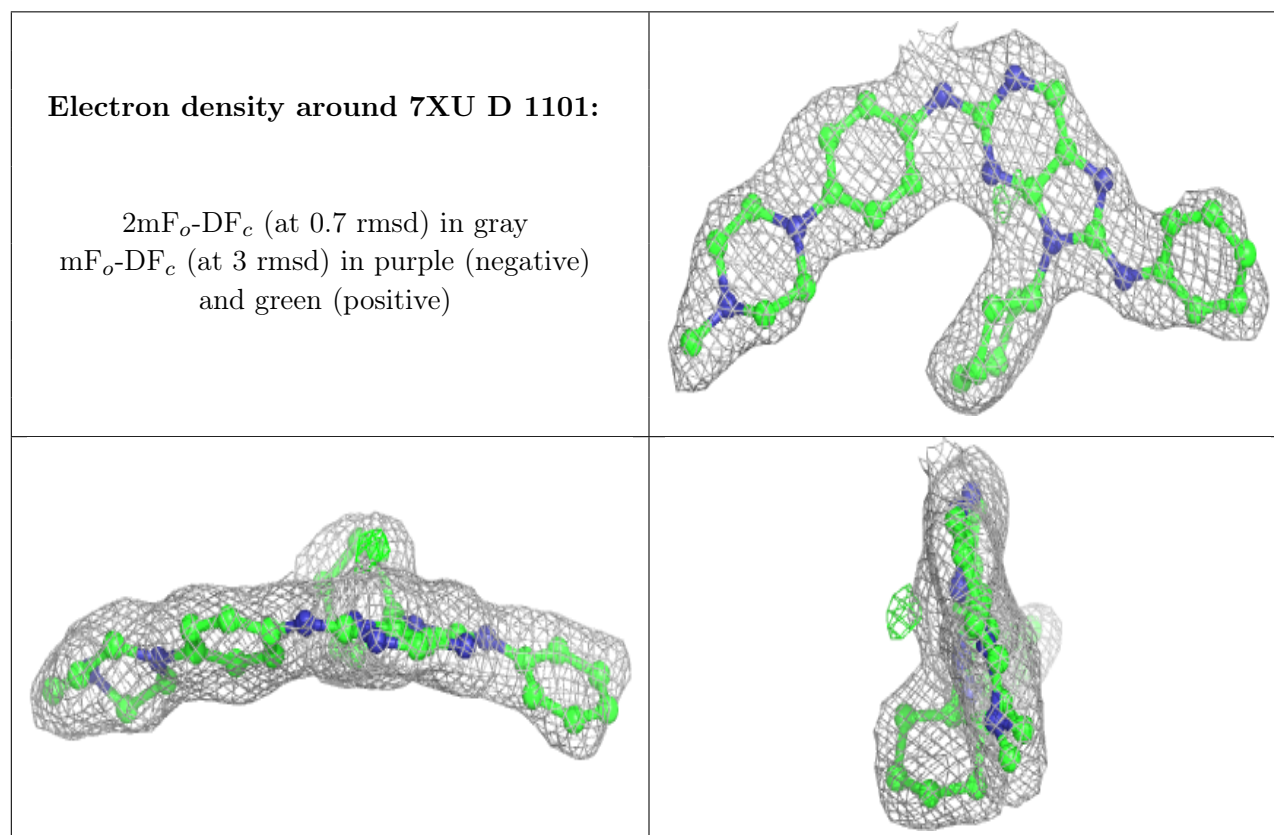
There are no monosaccharides in this entry.

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, 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.

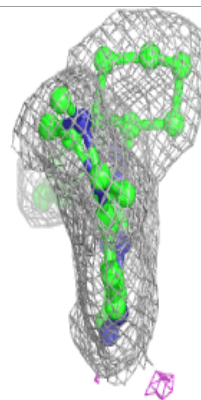
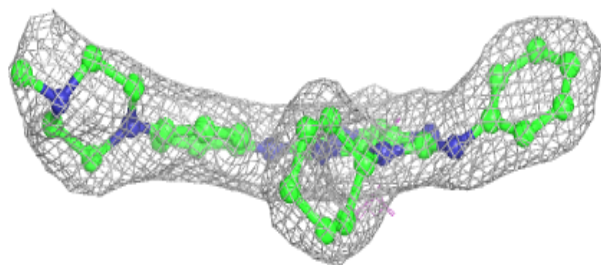
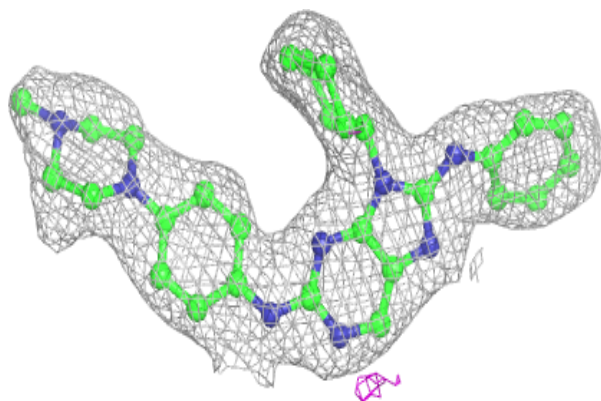
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	7XU	D	1101	36/36	0.90	0.15	33,38,50,55	0
2	7XU	C	1101	36/36	0.95	0.10	18,29,46,47	0
2	7XU	A	3001	36/36	0.96	0.14	15,22,49,53	0
2	7XU	B	1101	36/36	0.96	0.11	20,29,46,49	0

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.

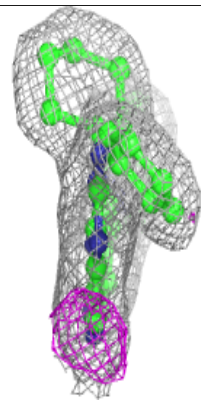
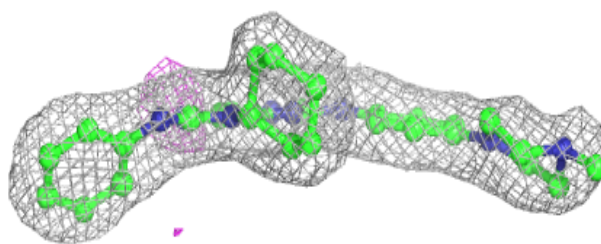
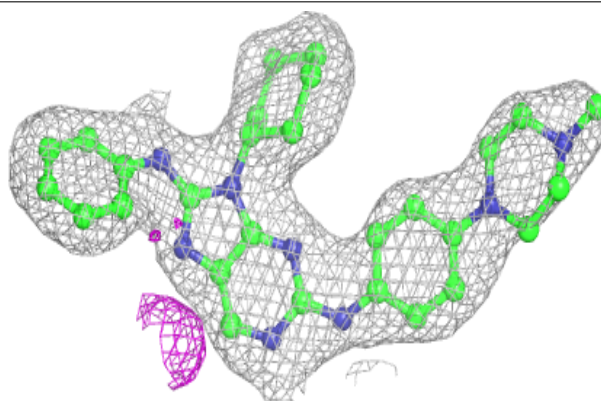


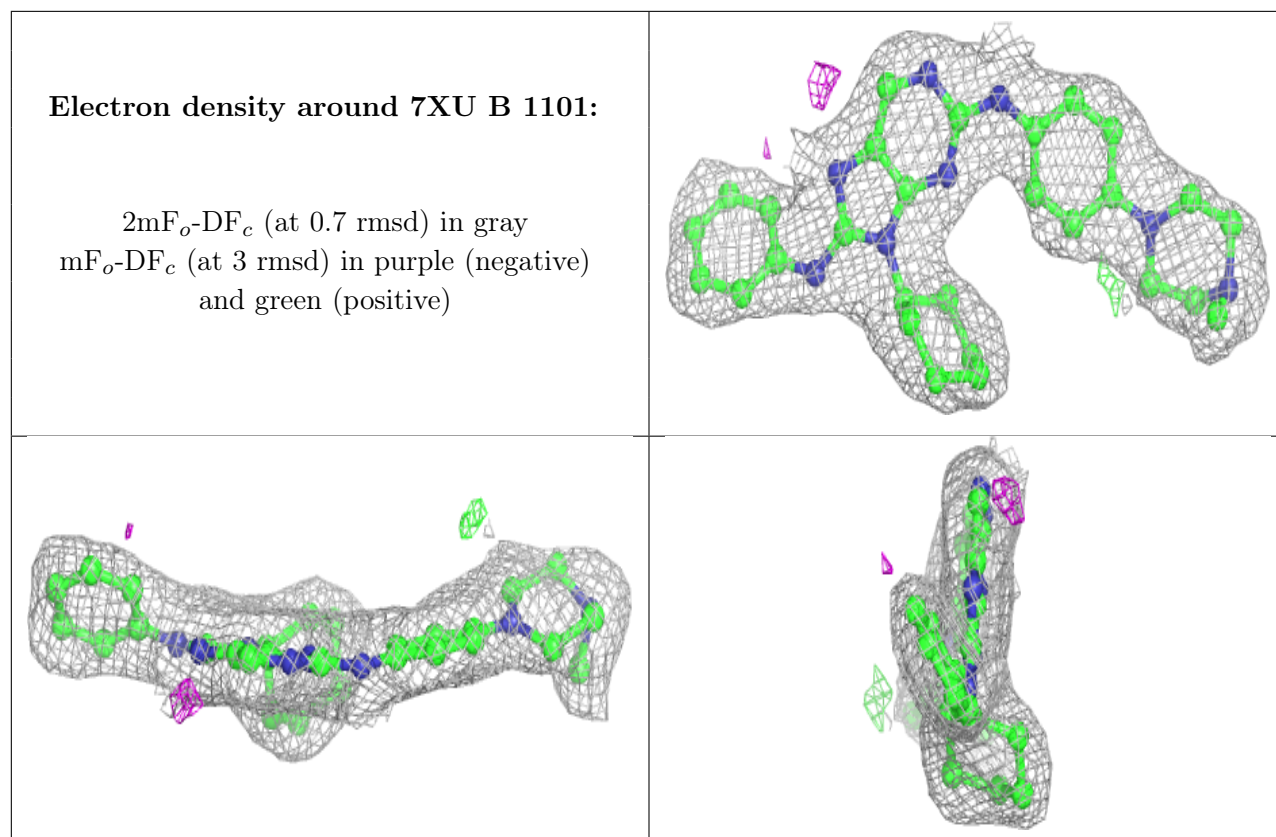
Electron density around 7XU C 1101:

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

**Electron density around 7XU A 3001:**

$2mF_o-DF_c$ (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.