Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2021 – 01:56 PM EDT

PDB ID	:	3IKA
Title	:	Crystal Structure of EGFR 696-1022 T790M Mutant Covalently Binding to WZ4002
Authors	:	Yun, C.-H.; Eck, M.J.
Deposited on	:	2009-08-05
Resolution	:	2.90 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 following versions of software and data (see references ⓘ) were used in the production of this report:

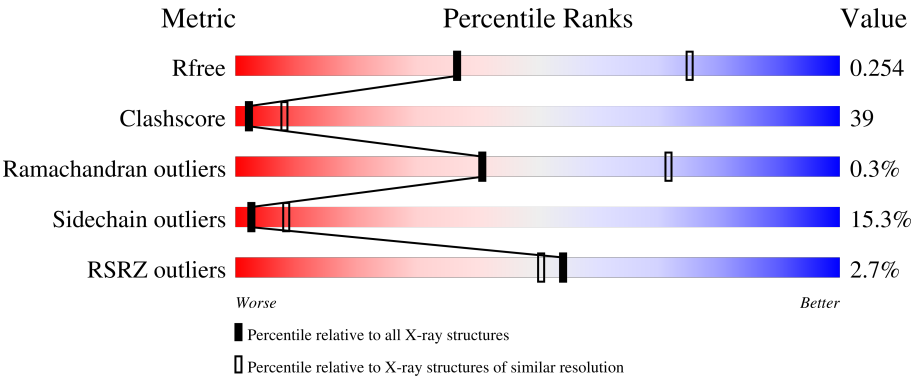
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	3% 43% 41% 10% 6%
1	B	331	2% 39% 48% 7% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5104 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.

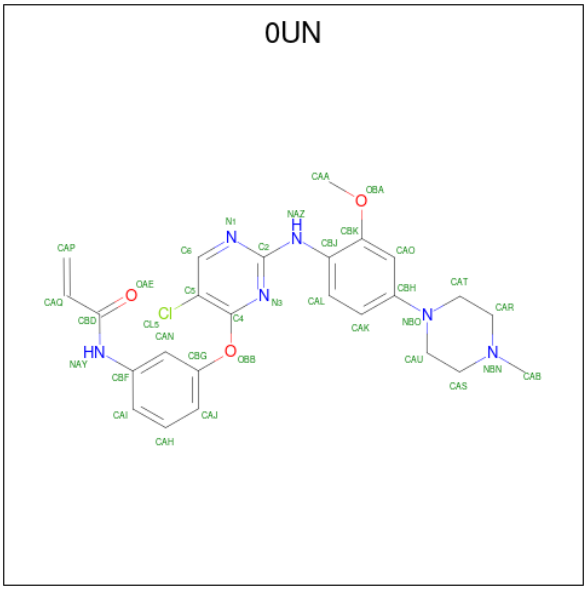
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2440	1567	411	444	18			
1	B	310	Total	C	N	O	S	0	1	0
			2481	1591	418	454	18			

There are 6 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	790	MET	THR	engineered mutation	UNP P00533
B	692	GLY	-	expression tag	UNP P00533
B	693	SER	-	expression tag	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533

- Molecule 2 is N-{3-[(5-chloro-2-{[2-methoxy-4-(4-methylpiperazin-1-yl)phenyl]amino}pyrimidin-4-yl)oxy]phenyl}prop-2-enamide (three-letter code: 0UN) (formula: $C_{25}H_{27}ClN_6O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			35	25	1	6	3		

- Molecule 3 is water.

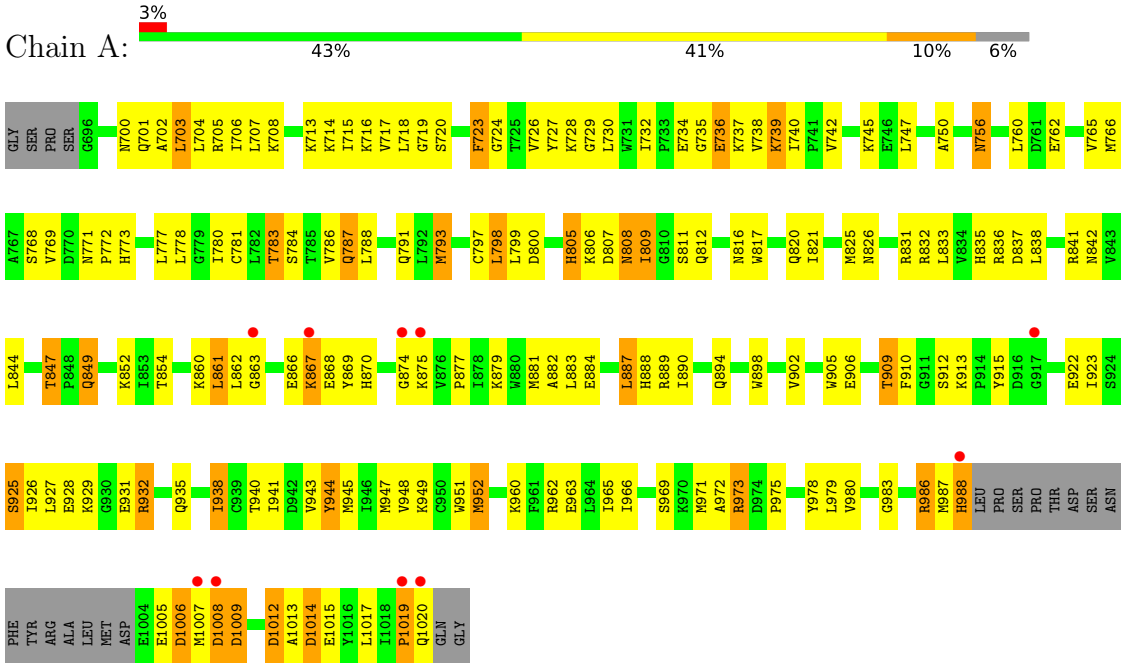
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total	O	0	0
			71	71		
3	B	77	Total	O	0	0
			77	77		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

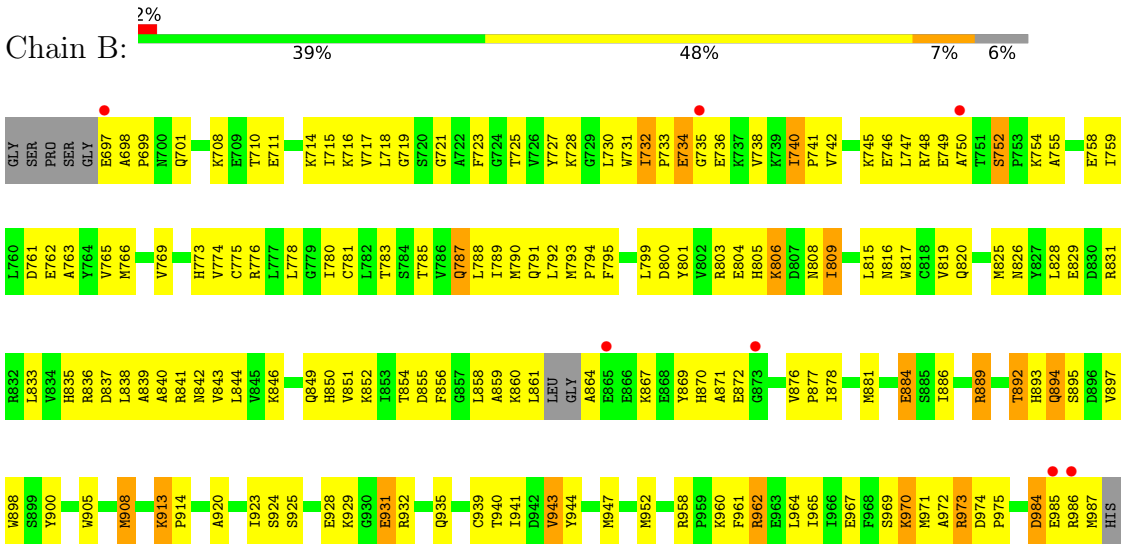
• Molecule 1: Epidermal growth factor receptor

Chain A:



• Molecule 1: Epidermal growth factor receptor

Chain B:




LEU
PRO
SER
PRO
T993
D994
S995
N996
F997
Y998
R999
A1000
L1001
M1002
D1003
E1004
E1005
ASP
MET
ASP
ASP
V1010
V1011
D1012
A1013
D1014
E1015
Y1016
L1017
ILE
PRO
GLN
GLN
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	48.23Å 89.13Å 165.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.83 – 2.90 20.65 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.83-2.90) 97.0 (20.65-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.5.0093	Depositor
R, R_{free}	0.208 , 0.257 0.204 , 0.254	Depositor DCC
R_{free} test set	806 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	64.2	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5104	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 0UN

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	1.22	1/2491 (0.0%)	0.85	0/3370
1	B	1.17	1/2534 (0.0%)	0.81	0/3422
All	All	1.20	2/5025 (0.0%)	0.83	0/6792

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	944	TYR	CE2-CZ	-5.23	1.31	1.38
1	B	817	TRP	CB-CG	-5.18	1.41	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2440	0	2444	183	0
1	B	2481	0	2499	205	0
2	A	35	0	26	9	0
3	A	71	0	0	9	0
3	B	77	0	0	22	0
All	All	5104	0	4969	389	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 39.

All (389) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861:LEU:HD12	1:A:862:LEU:N	1.43	1.30
1:A:825:MET:HE2	1:A:838:LEU:HD13	1.19	1.12
1:B:803:ARG:O	1:B:806:LYS:HE2	1.54	1.06
1:B:734:GLU:HG2	1:B:735:GLY:H	1.18	1.03
1:A:867:LYS:HE2	3:A:125:HOH:O	1.58	1.02
1:B:790:MET:CE	1:B:855:ASP:H	1.72	1.02
1:B:697:GLU:HG3	3:B:110:HOH:O	1.60	1.01
1:B:1002:MET:HE2	3:B:56:HOH:O	1.61	1.00
1:A:870:HIS:HB2	3:A:97:HOH:O	1.60	1.00
1:A:825:MET:CE	1:A:838:LEU:HD13	1.90	0.99
1:A:1013:ALA:O	1:A:1014:ASP:HB2	1.60	0.99
1:B:998:TYR:CE2	1:B:1002:MET:HE3	1.97	0.98
1:A:765:VAL:O	1:A:769:VAL:HG13	1.63	0.97
2:A:1797:0UN:HAL	2:A:1797:0UN:N3	1.76	0.96
1:A:887:LEU:HB3	1:A:888:HIS:CD2	2.00	0.94
1:B:708:LYS:HE3	3:B:98:HOH:O	1.66	0.92
1:A:938:ILE:N	1:A:938:ILE:CD1	2.32	0.92
1:A:861:LEU:HD12	1:A:862:LEU:H	0.97	0.92
1:B:1004:GLU:HA	3:B:122:HOH:O	1.68	0.91
1:A:905:TRP:O	1:A:909:THR:HG23	1.70	0.91
1:B:734:GLU:CG	1:B:735:GLY:H	1.83	0.90
1:A:988:HIS:H	1:A:988:HIS:CD2	1.84	0.90
1:B:836:ARG:HH11	1:B:859:ALA:HB2	1.36	0.90
1:B:973[B]:ARG:HH21	1:B:973[B]:ARG:HG3	1.36	0.89
1:A:887:LEU:HB3	1:A:888:HIS:HD2	1.36	0.86
1:B:835:HIS:O	1:B:836:ARG:HB2	1.75	0.86
1:B:835:HIS:CE1	1:B:837:ASP:O	2.28	0.85
1:A:771:ASN:ND2	1:A:773:HIS:H	1.72	0.85
1:B:800:ASP:O	1:B:804:GLU:HG3	1.75	0.85
1:A:771:ASN:HD22	1:A:773:HIS:H	1.23	0.85
1:A:740:ILE:HG13	1:A:1013:ALA:HB1	1.57	0.85
1:B:969:SER:O	1:B:972:ALA:HB3	1.77	0.84
2:A:1797:0UN:N3	2:A:1797:0UN:CAL	2.30	0.83
1:B:734:GLU:HG2	1:B:735:GLY:N	1.94	0.83
1:A:769:VAL:HG23	1:A:769:VAL:O	1.79	0.82
1:A:797:CYS:SG	1:A:797:CYS:O	2.36	0.82
1:A:833:LEU:HD23	1:A:861:LEU:HA	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:LYS:CE	3:A:125:HOH:O	2.22	0.82
1:B:924:SER:O	1:B:928:GLU:HG3	1.79	0.81
1:B:1002:MET:HE3	1:B:1010:VAL:N	1.94	0.81
1:B:999:ARG:HB3	1:B:999:ARG:CZ	2.12	0.80
1:A:861:LEU:CD1	1:A:862:LEU:H	1.89	0.80
1:B:793:MET:HB3	1:B:794:PRO:HD2	1.64	0.80
1:A:723:PHE:CD1	1:A:723:PHE:C	2.54	0.79
1:A:769:VAL:O	1:A:769:VAL:CG2	2.30	0.79
1:A:723:PHE:CD1	1:A:724:GLY:N	2.52	0.78
1:A:861:LEU:HD12	1:A:861:LEU:C	1.98	0.78
1:A:825:MET:HE2	1:A:838:LEU:CD1	2.07	0.78
1:B:973[B]:ARG:HH21	1:B:973[B]:ARG:CG	1.96	0.78
1:B:773:HIS:HD2	1:B:851:VAL:O	1.67	0.78
1:B:836:ARG:NH1	1:B:859:ALA:HB2	1.97	0.78
1:B:931:GLU:O	1:B:932:ARG:HD3	1.84	0.77
1:A:714:LYS:HD3	1:A:727:TYR:CD2	2.20	0.77
1:A:938:ILE:N	1:A:938:ILE:HD12	1.97	0.77
1:A:715:ILE:HD13	1:A:729:GLY:HA2	1.67	0.77
1:A:1013:ALA:O	1:A:1014:ASP:CB	2.33	0.76
1:A:905:TRP:HD1	1:A:947:MET:CE	1.99	0.76
1:B:815:LEU:O	1:B:819:VAL:HG23	1.86	0.76
1:A:931:GLU:O	1:A:932:ARG:HD3	1.87	0.75
1:A:938:ILE:HD13	1:A:938:ILE:H	1.51	0.75
1:B:790:MET:CE	1:B:855:ASP:N	2.49	0.75
1:B:1000:ALA:CB	3:B:143:HOH:O	2.33	0.75
1:B:1002:MET:CE	1:B:1010:VAL:N	2.49	0.75
1:A:765:VAL:HG23	1:A:766:MET:N	2.00	0.74
1:A:960:LYS:HZ3	1:A:962:ARG:HH22	1.34	0.74
1:A:960:LYS:NZ	1:A:962:ARG:HH22	1.85	0.74
1:B:835:HIS:HE1	1:B:837:ASP:O	1.70	0.74
1:B:710:THR:HG21	3:B:98:HOH:O	1.88	0.73
1:B:790:MET:HE3	1:B:855:ASP:OD2	1.88	0.73
1:B:776:ARG:HG2	1:B:791:GLN:OE1	1.87	0.73
1:B:1012:ASP:OD1	1:B:1015:GLU:HG2	1.89	0.73
1:B:790:MET:HE2	1:B:855:ASP:H	1.54	0.73
1:B:931:GLU:O	1:B:932:ARG:CD	2.36	0.73
1:B:984:ASP:HB3	3:B:146:HOH:O	1.87	0.73
1:B:986:ARG:O	1:B:987:MET:HB2	1.87	0.72
1:B:748:ARG:HB3	3:B:48:HOH:O	1.89	0.72
1:B:905:TRP:HB2	1:B:947:MET:CE	2.19	0.72
1:B:943:VAL:HG12	1:B:944:TYR:N	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:939:CYS:SG	1:B:943:VAL:HG11	2.29	0.72
1:A:988:HIS:H	1:A:988:HIS:HD2	1.36	0.72
1:B:987:MET:HB3	3:B:117:HOH:O	1.90	0.72
1:B:790:MET:HE1	1:B:855:ASP:H	1.54	0.71
1:B:998:TYR:CZ	1:B:1002:MET:HE3	2.24	0.71
1:B:1000:ALA:HB3	3:B:143:HOH:O	1.91	0.71
1:B:1012:ASP:OD1	1:B:1015:GLU:CG	2.38	0.71
1:A:730:LEU:HD23	1:A:739:LYS:HB3	1.73	0.70
1:A:1005:GLU:C	1:A:1006:ASP:OD1	2.29	0.70
1:B:790:MET:HE2	1:B:854:THR:HA	1.73	0.70
1:B:1011:VAL:HG13	1:B:1015:GLU:HG3	1.72	0.70
1:A:831:ARG:O	1:A:832:ARG:HB2	1.91	0.69
1:A:986:ARG:HH11	1:A:987:MET:CG	2.03	0.69
1:A:703:LEU:HA	1:B:935:GLN:HE22	1.57	0.69
1:A:835:HIS:O	1:A:836:ARG:HB2	1.91	0.69
1:A:909:THR:OG1	1:A:912:SER:HB2	1.93	0.69
1:A:707:LEU:O	1:A:781:CYS:SG	2.51	0.69
1:A:986:ARG:HH11	1:A:987:MET:HG3	1.56	0.68
1:B:794:PRO:HD3	1:B:1012:ASP:HB3	1.75	0.68
1:A:765:VAL:CG2	1:A:766:MET:N	2.57	0.68
1:A:805:HIS:O	1:A:806:LYS:C	2.31	0.68
1:A:938:ILE:CD1	1:A:938:ILE:H	2.06	0.68
1:B:1002:MET:CE	3:B:56:HOH:O	2.31	0.68
1:A:837:ASP:O	1:A:842:ASN:ND2	2.27	0.68
1:A:887:LEU:CB	1:A:888:HIS:HD2	2.06	0.67
1:A:816:ASN:O	1:A:820:GLN:HG3	1.94	0.67
1:B:1000:ALA:O	1:B:1004:GLU:HB2	1.94	0.67
1:A:1008:ASP:C	1:A:1009:ASP:OD2	2.33	0.67
1:A:861:LEU:CD1	1:A:862:LEU:N	2.39	0.67
1:B:762:GLU:HG2	1:B:766:MET:HE3	1.77	0.67
1:B:699:PRO:HB2	1:B:701:GLN:NE2	2.10	0.67
2:A:1797:0UN:OAE	2:A:1797:0UN:HAI	1.94	0.66
1:B:723:PHE:CE1	1:B:836:ARG:NH2	2.62	0.66
1:B:781:CYS:HB3	1:B:787:GLN:HG3	1.78	0.66
1:A:740:ILE:HG13	1:A:1013:ALA:CB	2.24	0.66
1:B:864:ALA:N	3:B:44:HOH:O	2.29	0.65
1:A:915:TYR:HE2	3:A:87:HOH:O	1.80	0.65
1:A:980:VAL:HG12	1:A:980:VAL:O	1.97	0.65
1:B:790:MET:HE1	1:B:855:ASP:N	2.10	0.65
1:B:905:TRP:HB2	1:B:947:MET:HE3	1.78	0.65
1:B:998:TYR:HE2	1:B:1002:MET:HE3	1.55	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:ASP:OD2	1:A:1009:ASP:N	2.30	0.64
1:B:708:LYS:CE	3:B:98:HOH:O	2.33	0.64
1:B:723:PHE:CD1	1:B:836:ARG:NH2	2.66	0.64
1:B:776:ARG:NH1	1:B:1014:ASP:OD1	2.31	0.64
1:B:877:PRO:O	1:B:881:MET:HG3	1.96	0.64
1:B:923:ILE:O	1:B:924:SER:C	2.35	0.64
1:B:794:PRO:HG2	1:B:795:PHE:H	1.63	0.64
1:A:944:TYR:O	1:A:948:VAL:HG23	1.98	0.63
1:B:762:GLU:O	1:B:766:MET:HG3	1.98	0.63
1:A:766:MET:HG2	1:A:777:LEU:HB2	1.79	0.63
1:A:706:ILE:HD12	1:B:944:TYR:OH	1.99	0.63
1:A:938:ILE:HG22	1:A:979:LEU:HD22	1.81	0.63
1:B:871:ALA:HB3	1:B:889:ARG:HG3	1.79	0.63
1:A:909:THR:OG1	1:A:912:SER:CB	2.47	0.62
1:B:924:SER:O	1:B:928:GLU:CG	2.47	0.62
1:A:793:MET:HG3	1:A:844:LEU:HB3	1.80	0.62
1:B:925:SER:O	1:B:929:LYS:HG3	1.98	0.62
1:A:715:ILE:CD1	1:A:729:GLY:HA2	2.29	0.62
1:A:972:ALA:O	1:A:975:PRO:HD3	2.00	0.62
1:B:793:MET:HE3	1:B:852:LYS:HD3	1.80	0.62
1:A:938:ILE:N	1:A:938:ILE:HD13	2.08	0.61
1:B:803:ARG:O	1:B:806:LYS:HG2	2.00	0.61
1:B:935:GLN:HG3	1:B:944:TYR:CG	2.35	0.61
1:A:938:ILE:HG22	1:A:938:ILE:O	1.99	0.61
1:B:734:GLU:CG	1:B:735:GLY:N	2.58	0.61
1:A:740:ILE:HG22	1:A:742:VAL:HG13	1.82	0.60
1:A:988:HIS:CD2	1:A:988:HIS:N	2.60	0.60
1:A:706:ILE:C	1:A:707:LEU:HD23	2.22	0.60
1:B:973[B]:ARG:CG	1:B:973[B]:ARG:NH2	2.59	0.60
1:A:714:LYS:HD3	1:A:727:TYR:CG	2.35	0.60
1:A:1012:ASP:O	1:A:1013:ALA:HB2	2.01	0.60
1:A:777:LEU:HD11	1:A:788:LEU:HB3	1.84	0.59
1:A:805:HIS:ND1	1:A:805:HIS:N	2.50	0.59
1:B:778:LEU:HD21	1:B:791:GLN:HB3	1.84	0.59
1:B:803:ARG:O	1:B:806:LYS:CE	2.42	0.59
1:A:723:PHE:CG	1:A:724:GLY:N	2.70	0.59
1:B:877:PRO:O	1:B:881:MET:CG	2.51	0.59
1:A:793:MET:HG3	1:A:844:LEU:CB	2.32	0.59
1:A:963:GLU:O	1:A:966:ILE:HG12	2.03	0.59
1:B:773:HIS:CD2	1:B:851:VAL:O	2.54	0.59
1:A:888:HIS:CD2	1:A:888:HIS:N	2.71	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:MET:HE3	1:A:838:LEU:HB2	1.85	0.58
1:B:754:LYS:O	1:B:758:GLU:HG3	2.03	0.58
1:B:833:LEU:HD23	1:B:860:LYS:HA	1.84	0.58
1:A:863:GLY:HA3	1:A:866:GLU:HG3	1.85	0.58
1:B:998:TYR:HE2	1:B:1010:VAL:N	2.01	0.58
1:B:974:ASP:N	1:B:975:PRO:CD	2.67	0.57
1:A:833:LEU:HD23	1:A:861:LEU:HD13	1.86	0.57
1:A:700:ASN:HD21	1:A:768:SER:HB2	1.69	0.57
1:A:1006:ASP:HB2	1:A:1009:ASP:OD2	2.05	0.57
1:B:775:CYS:SG	1:B:844:LEU:HD12	2.45	0.57
1:B:805:HIS:O	1:B:809:ILE:HG13	2.05	0.57
1:B:1000:ALA:HB1	3:B:143:HOH:O	2.01	0.57
1:A:762:GLU:O	1:A:765:VAL:HG22	2.05	0.57
1:B:962:ARG:HG2	3:B:29:HOH:O	2.03	0.56
1:A:704:LEU:H	1:B:935:GLN:NE2	2.02	0.56
1:A:938:ILE:O	1:A:938:ILE:CG2	2.53	0.56
1:A:941:ILE:O	1:A:945:MET:HB2	2.05	0.56
1:B:740:ILE:CD1	1:B:1013:ALA:HA	2.35	0.56
1:B:711:GLU:OE2	1:B:733:PRO:HA	2.05	0.56
1:B:801:TYR:O	1:B:805:HIS:HD2	1.89	0.55
1:B:931:GLU:O	1:B:932:ARG:HD2	2.06	0.55
1:B:998:TYR:OH	1:B:1002:MET:CE	2.55	0.54
1:A:737:LYS:O	1:A:738:VAL:HG13	2.08	0.54
1:B:725:THR:HG22	1:B:727:TYR:CE2	2.42	0.54
1:B:842:ASN:O	1:B:854:THR:HG23	2.08	0.54
1:B:749:GLU:N	3:B:48:HOH:O	2.41	0.54
1:B:731:TRP:CZ2	1:B:733:PRO:HB3	2.43	0.54
1:A:887:LEU:C	1:A:888:HIS:CD2	2.82	0.53
1:B:793:MET:CB	1:B:794:PRO:HD2	2.37	0.53
1:A:842:ASN:O	1:A:854:THR:HG22	2.09	0.53
1:A:943:VAL:HG22	1:A:971:MET:SD	2.48	0.53
1:B:892:THR:HG23	1:B:895:SER:H	1.71	0.53
1:A:925:SER:O	1:A:929:LYS:HG2	2.08	0.53
1:B:894:GLN:HA	1:B:894:GLN:OE1	2.07	0.53
1:A:708:LYS:NZ	1:A:734:GLU:CD	2.63	0.52
1:B:717:VAL:HG12	1:B:719:GLY:H	1.74	0.52
1:A:817:TRP:O	1:A:821:ILE:HG13	2.09	0.52
1:B:776:ARG:NE	1:B:1014:ASP:OD1	2.39	0.52
1:B:716:LYS:HE2	3:B:64:HOH:O	2.09	0.52
1:A:806:LYS:NZ	1:A:910:PHE:O	2.42	0.52
1:B:1011:VAL:HG12	1:B:1012:ASP:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:PRO:O	1:A:881:MET:HG3	2.10	0.52
1:B:793:MET:HE3	1:B:852:LYS:CD	2.39	0.52
1:A:806:LYS:HA	1:A:809:ILE:HG13	1.91	0.52
1:A:706:ILE:O	1:A:707:LEU:HD23	2.10	0.51
1:A:1006:ASP:OD1	1:A:1006:ASP:N	2.43	0.51
1:B:986:ARG:O	1:B:987:MET:CB	2.56	0.51
1:B:998:TYR:CZ	1:B:1002:MET:CE	2.92	0.51
1:B:1002:MET:HE2	1:B:1010:VAL:N	2.25	0.51
1:A:718:LEU:HD21	1:A:728:LYS:HB2	1.93	0.51
1:A:760:LEU:HD11	1:B:952:MET:CE	2.41	0.51
1:B:721:GLY:O	1:B:748:ARG:HD3	2.10	0.51
1:B:769:VAL:HG11	1:B:774:VAL:CG1	2.41	0.51
1:A:986:ARG:NH1	1:A:987:MET:CG	2.73	0.51
1:A:883:LEU:HD21	1:A:928:GLU:HG2	1.92	0.51
1:B:714:LYS:HD3	1:B:727:TYR:CD1	2.46	0.51
1:B:939:CYS:SG	1:B:943:VAL:CG1	2.97	0.51
1:A:837:ASP:O	1:A:837:ASP:OD1	2.29	0.50
1:B:708:LYS:HG3	1:B:710:THR:HB	1.94	0.50
1:A:926:ILE:HA	1:A:929:LYS:HG3	1.93	0.50
1:B:790:MET:HE2	1:B:854:THR:CA	2.39	0.50
1:B:931:GLU:C	1:B:932:ARG:HD3	2.31	0.50
1:B:741:PRO:C	1:B:742:VAL:CG1	2.80	0.50
1:B:820:GLN:OE1	1:B:851:VAL:HG22	2.11	0.50
1:A:780:ILE:HG12	1:A:781:CYS:N	2.27	0.50
1:B:994:ASP:OD1	1:B:994:ASP:O	2.30	0.50
1:B:750:ALA:O	1:B:752:SER:OG	2.30	0.50
1:B:723:PHE:HE1	1:B:836:ARG:HH21	1.50	0.50
1:A:932:ARG:NH1	1:A:951:TRP:O	2.44	0.49
1:B:1012:ASP:OD1	1:B:1012:ASP:O	2.30	0.49
1:A:986:ARG:NH1	1:A:987:MET:HG2	2.28	0.49
1:A:1019:PRO:O	1:A:1020:GLN:O	2.30	0.49
1:A:719:GLY:HA3	2:A:1797:0UN:HAH	1.94	0.49
1:B:758:GLU:O	1:B:759:ILE:C	2.50	0.49
1:B:825:MET:CE	1:B:838:LEU:HD22	2.43	0.49
1:B:715:ILE:HD11	1:B:730:LEU:CD1	2.41	0.49
1:A:765:VAL:O	1:A:769:VAL:CG1	2.49	0.49
1:A:826:ASN:HB2	1:A:965:ILE:HD11	1.94	0.49
1:B:715:ILE:HD11	1:B:730:LEU:HG	1.94	0.48
1:B:762:GLU:HG2	1:B:766:MET:CE	2.43	0.48
1:B:1011:VAL:CG1	1:B:1012:ASP:O	2.61	0.48
1:B:886:ILE:HG21	1:B:924:SER:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:VAL:HG11	1:B:774:VAL:HG11	1.94	0.48
1:B:776:ARG:HH11	1:B:1014:ASP:HA	1.78	0.48
1:B:801:TYR:C	1:B:801:TYR:CD2	2.87	0.48
1:B:998:TYR:CE2	1:B:1010:VAL:N	2.80	0.48
1:A:771:ASN:HD22	1:A:773:HIS:N	2.00	0.48
1:B:741:PRO:C	1:B:742:VAL:HG13	2.33	0.48
1:A:962:ARG:HA	1:A:965:ILE:HD12	1.95	0.48
1:B:998:TYR:HH	1:B:1010:VAL:N	2.11	0.48
1:A:863:GLY:CA	1:A:866:GLU:HG3	2.44	0.48
1:A:888:HIS:O	1:A:889:ARG:C	2.49	0.48
1:A:923:ILE:O	1:A:927:LEU:HB2	2.13	0.48
1:A:805:HIS:O	1:A:809:ILE:HG12	2.14	0.48
1:B:748:ARG:CB	3:B:48:HOH:O	2.54	0.48
1:A:909:THR:HG1	1:A:912:SER:CB	2.26	0.48
1:A:960:LYS:NZ	1:A:962:ARG:NH2	2.58	0.48
1:B:894:GLN:NE2	1:B:960:LYS:HE2	2.29	0.48
1:A:783:THR:O	1:A:784:SER:C	2.49	0.47
1:B:816:ASN:O	1:B:820:GLN:HG3	2.14	0.47
1:B:962:ARG:CG	3:B:29:HOH:O	2.62	0.47
1:B:790:MET:HE2	1:B:855:ASP:N	2.23	0.47
1:B:835:HIS:O	1:B:836:ARG:CB	2.50	0.47
1:A:888:HIS:HB2	1:A:890:ILE:HD12	1.96	0.47
1:A:932:ARG:HG3	1:A:951:TRP:CE3	2.50	0.47
1:B:718:LEU:HD13	1:B:728:LYS:HB2	1.96	0.47
1:B:961:PHE:O	1:B:965:ILE:HG13	2.15	0.47
1:A:860:LYS:HE2	1:A:869:TYR:OH	2.15	0.47
1:B:998:TYR:OH	1:B:1002:MET:HE1	2.15	0.47
1:B:783:THR:OG1	1:B:785:THR:O	2.33	0.47
1:B:994:ASP:OD1	1:B:999:ARG:HD3	2.15	0.46
1:A:905:TRP:CD1	1:A:947:MET:CE	2.89	0.46
1:B:780:ILE:HG22	1:B:788:LEU:HD23	1.98	0.46
1:B:920:ALA:HA	1:B:923:ILE:HD13	1.95	0.46
1:B:898:TRP:CE3	1:B:958:ARG:NH1	2.83	0.46
1:A:1007:MET:HB3	3:A:19:HOH:O	2.16	0.46
1:A:844:LEU:HD11	1:A:854:THR:OG1	2.15	0.46
2:A:1797:0UN:OAE	2:A:1797:0UN:CAI	2.57	0.46
1:B:763:ALA:HB2	1:B:788:LEU:HD21	1.96	0.46
1:B:998:TYR:OH	1:B:1002:MET:HE3	2.15	0.46
1:B:736:GLU:HB3	1:B:738:VAL:HG12	1.97	0.46
1:B:826:ASN:ND2	3:B:29:HOH:O	2.49	0.46
1:B:969:SER:O	1:B:972:ALA:CB	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:SER:OG	1:A:975:PRO:HB2	2.15	0.46
1:A:874:GLY:HA3	3:A:95:HOH:O	2.16	0.46
1:A:704:LEU:H	1:B:935:GLN:HE22	1.63	0.46
1:A:808:ASN:OD1	1:A:808:ASN:N	2.47	0.46
1:A:702:ALA:CB	1:A:768:SER:HA	2.46	0.45
1:A:1014:ASP:HB3	1:A:1015:GLU:H	1.52	0.45
1:B:790:MET:CE	1:B:855:ASP:OD2	2.61	0.45
1:A:800:ASP:HB2	3:A:147:HOH:O	2.17	0.45
1:B:905:TRP:CB	1:B:947:MET:CE	2.93	0.45
1:A:800:ASP:CB	3:A:147:HOH:O	2.64	0.45
1:A:949:LYS:O	1:A:952:MET:HB2	2.16	0.45
1:A:732:ILE:HG23	1:A:738:VAL:O	2.16	0.45
1:A:793:MET:CG	1:A:844:LEU:HB3	2.47	0.45
1:A:905:TRP:CD1	1:A:947:MET:HE3	2.51	0.45
1:B:725:THR:CG2	1:B:727:TYR:CE2	2.99	0.45
1:B:897:VAL:O	1:B:900:TYR:HB3	2.17	0.45
1:B:697:GLU:HB3	1:B:698:ALA:H	1.49	0.45
1:B:805:HIS:O	1:B:809:ILE:CG1	2.64	0.45
1:B:855:ASP:HB2	1:B:858:LEU:HD11	1.99	0.45
1:B:861:LEU:HD23	1:B:861:LEU:HA	1.63	0.45
1:B:905:TRP:CD1	1:B:947:MET:HE1	2.52	0.45
1:A:983:GLY:O	1:A:986:ARG:HB3	2.17	0.45
1:B:1012:ASP:OD1	1:B:1012:ASP:N	2.47	0.45
1:A:812:GLN:O	1:A:816:ASN:ND2	2.50	0.45
1:A:798:LEU:O	1:A:799:LEU:C	2.54	0.44
1:A:969:SER:O	1:A:972:ALA:HB3	2.16	0.44
1:B:967:GLU:O	1:B:971:MET:HG3	2.18	0.44
1:B:717:VAL:HG12	1:B:719:GLY:N	2.32	0.44
1:B:898:TRP:CZ3	1:B:958:ARG:NH1	2.84	0.44
1:B:970:LYS:HB2	1:B:970:LYS:HE2	1.50	0.44
1:A:883:LEU:HG	1:A:887:LEU:HD22	1.99	0.44
1:B:869:TYR:CE2	1:B:870:HIS:O	2.70	0.44
1:B:799:LEU:HB2	1:B:840:ALA:HB3	1.98	0.44
1:B:974:ASP:N	1:B:975:PRO:HD3	2.33	0.44
1:A:766:MET:HE2	1:A:766:MET:HB2	1.87	0.44
1:B:1000:ALA:O	1:B:1004:GLU:CB	2.64	0.44
2:A:1797:0UN:HAUA	2:A:1797:0UN:HAK	1.67	0.44
1:A:708:LYS:HZ3	1:A:734:GLU:CD	2.21	0.44
1:A:879:LYS:HD3	1:A:915:TYR:HB2	1.99	0.44
1:B:765:VAL:O	1:B:769:VAL:HG23	2.17	0.44
1:A:833:LEU:CD2	1:A:861:LEU:HD13	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:728:LYS:HE3	1:B:997:PHE:CE2	2.53	0.43
1:A:797:CYS:O	1:A:798:LEU:C	2.57	0.43
1:A:940:THR:HG23	1:A:978:TYR:O	2.18	0.43
1:B:735:GLY:O	1:B:736:GLU:HG2	2.19	0.43
1:B:960:LYS:O	1:B:961:PHE:C	2.53	0.43
1:A:841:ARG:CG	1:A:842:ASN:N	2.82	0.43
1:B:846:LYS:HD2	1:B:850:HIS:ND1	2.34	0.43
1:B:884:GLU:H	1:B:884:GLU:HG3	1.33	0.43
1:A:847:THR:OG1	1:A:849:GLN:NE2	2.51	0.43
1:B:1012:ASP:OD1	1:B:1015:GLU:HG3	2.17	0.43
1:A:719:GLY:CA	2:A:1797:0UN:HAH	2.48	0.43
1:B:803:ARG:O	1:B:806:LYS:CG	2.65	0.43
1:A:805:HIS:O	1:A:809:ILE:CG1	2.67	0.43
1:A:812:GLN:HG3	1:A:816:ASN:HD21	1.83	0.43
1:A:935:GLN:HG3	1:A:944:TYR:CD2	2.54	0.43
2:A:1797:0UN:HAO	2:A:1797:0UN:HAT	1.74	0.43
1:B:839:ALA:O	1:B:843:VAL:HG23	2.19	0.43
1:B:913:LYS:HA	1:B:914:PRO:HD3	1.82	0.43
1:A:973:ARG:H	1:A:973:ARG:HG3	1.56	0.42
1:B:908:MET:CG	1:B:939:CYS:SG	3.07	0.42
1:B:960:LYS:NZ	3:B:8:HOH:O	2.52	0.42
1:A:805:HIS:C	1:A:807:ASP:N	2.69	0.42
1:B:747:LEU:HG	1:B:759:ILE:HD13	2.01	0.42
1:A:745:LYS:O	1:A:787:GLN:HA	2.19	0.42
1:A:793:MET:CE	1:A:852:LYS:HD2	2.49	0.42
1:A:833:LEU:CD2	1:A:861:LEU:HA	2.41	0.42
1:A:902:VAL:O	1:A:906:GLU:HG3	2.20	0.42
1:B:745:LYS:HG2	1:B:746:GLU:N	2.33	0.42
1:B:717:VAL:CG1	1:B:719:GLY:H	2.32	0.42
1:A:714:LYS:HD3	1:A:727:TYR:CE2	2.54	0.42
1:A:922:GLU:O	1:A:923:ILE:C	2.58	0.42
1:B:790:MET:HG2	1:B:791:GLN:N	2.34	0.42
1:B:829:GLU:HA	1:B:893:HIS:CE1	2.55	0.42
1:A:700:ASN:OD1	1:A:700:ASN:C	2.57	0.42
1:A:715:ILE:HD12	1:A:715:ILE:N	2.35	0.42
1:A:745:LYS:NZ	3:A:14:HOH:O	2.48	0.42
1:B:964:LEU:HD12	1:B:964:LEU:HA	1.86	0.42
1:A:706:ILE:HG21	1:B:932:ARG:HB2	2.02	0.42
1:A:771:ASN:CG	1:A:772:PRO:HD2	2.40	0.42
1:A:860:LYS:HE2	1:A:869:TYR:CZ	2.55	0.42
1:A:1014:ASP:O	1:A:1015:GLU:C	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:ASP:O	1:B:765:VAL:HG23	2.20	0.41
1:B:825:MET:HA	1:B:828:LEU:HD12	2.01	0.41
1:B:995:SER:O	1:B:998:TYR:N	2.53	0.41
1:A:831:ARG:HE	1:A:831:ARG:HB3	1.71	0.41
2:A:1797:0UN:HAO	2:A:1797:0UN:HAAB	1.55	0.41
1:B:892:THR:HG23	1:B:895:SER:N	2.34	0.41
1:A:905:TRP:HD1	1:A:947:MET:HE2	1.81	0.41
1:A:1005:GLU:O	1:A:1006:ASP:OD1	2.38	0.41
1:A:894:GLN:HE22	1:A:960:LYS:HG2	1.86	0.41
1:B:869:TYR:CD2	1:B:870:HIS:N	2.89	0.41
1:B:878:ILE:HA	1:B:881:MET:HG3	2.02	0.41
1:B:898:TRP:HE3	1:B:958:ARG:CZ	2.34	0.41
1:A:740:ILE:HD11	1:A:1017:LEU:HD22	2.03	0.41
1:B:789:ILE:N	1:B:789:ILE:HD12	2.35	0.41
1:A:735:GLY:O	1:A:736:GLU:C	2.57	0.40
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.56	0.40
1:B:775:CYS:HB2	1:B:790:MET:HE2	2.04	0.40
1:A:723:PHE:CD1	1:A:724:GLY:CA	3.04	0.40
1:A:750:ALA:HB3	1:A:756:ASN:OD1	2.21	0.40
1:A:1017:LEU:O	1:A:1017:LEU:HG	2.19	0.40
1:B:747:LEU:CD1	1:B:755:ALA:HB1	2.52	0.40
1:A:809:ILE:HG23	1:A:809:ILE:HD13	1.83	0.40
1:B:732:ILE:CG1	3:B:71:HOH:O	2.69	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	306/331 (92%)	293 (96%)	11 (4%)	2 (1%)	22 54
1	B	303/331 (92%)	294 (97%)	9 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	609/662 (92%)	587 (96%)	20 (3%)	2 (0%)	41 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1014	ASP
1	A	1019	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	260/290 (90%)	216 (83%)	44 (17%)	2 6
1	B	269/290 (93%)	231 (86%)	38 (14%)	3 10
All	All	529/580 (91%)	447 (84%)	82 (16%)	2 8

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	701	GLN
1	A	703	LEU
1	A	705	ARG
1	A	713	LYS
1	A	716	LYS
1	A	717	VAL
1	A	720	SER
1	A	723	PHE
1	A	726	VAL
1	A	736	GLU
1	A	739	LYS
1	A	747	LEU
1	A	756	ASN
1	A	778	LEU
1	A	783	THR
1	A	786	VAL

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Mol	Chain	Res	Type
1	A	787	GLN
1	A	791	GLN
1	A	793	MET
1	A	798	LEU
1	A	805	HIS
1	A	808	ASN
1	A	809	ILE
1	A	847	THR
1	A	849	GLN
1	A	861	LEU
1	A	867	LYS
1	A	868	GLU
1	A	875	LYS
1	A	884	GLU
1	A	887	LEU
1	A	909	THR
1	A	913	LYS
1	A	925	SER
1	A	932	ARG
1	A	938	ILE
1	A	952	MET
1	A	973	ARG
1	A	986	ARG
1	A	988	HIS
1	A	1006	ASP
1	A	1008	ASP
1	A	1009	ASP
1	A	1012	ASP
1	B	732	ILE
1	B	734	GLU
1	B	740	ILE
1	B	752	SER
1	B	787	GLN
1	B	792	LEU
1	B	806	LYS
1	B	808	ASN
1	B	809	ILE
1	B	831	ARG
1	B	841	ARG
1	B	849	GLN
1	B	856	PHE
1	B	867	LYS

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Mol	Chain	Res	Type
1	B	872	GLU
1	B	876	VAL
1	B	884	GLU
1	B	889	ARG
1	B	892	THR
1	B	894	GLN
1	B	908	MET
1	B	913	LYS
1	B	931	GLU
1	B	940	THR
1	B	941	ILE
1	B	943	VAL
1	B	962	ARG
1	B	970	LYS
1	B	973[A]	ARG
1	B	973[B]	ARG
1	B	984	ASP
1	B	985	GLU
1	B	993	THR
1	B	995	SER
1	B	999	ARG
1	B	1003	ASP
1	B	1005	GLU
1	B	1015	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	771	ASN
1	A	787	GLN
1	A	791	GLN
1	A	816	ASN
1	A	849	GLN
1	A	888	HIS
1	A	894	GLN
1	A	935	GLN
1	A	988	HIS
1	B	701	GLN
1	B	756	ASN
1	B	773	HIS
1	B	787	GLN
1	B	805	HIS

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Mol	Chain	Res	Type
1	B	888	HIS
1	B	935	GLN

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

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	0UN	A	1797	1	37,38,38	2.21	14 (37%)	48,52,52	2.69	13 (27%)

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	0UN	A	1797	1	-	4/20/30/30	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1797	0UN	CBF-NAY	-5.17	1.31	1.41
2	A	1797	0UN	CAP-CAQ	4.57	1.52	1.30
2	A	1797	0UN	CBJ-NAZ	-4.30	1.27	1.39
2	A	1797	0UN	OBA-CBK	-3.56	1.31	1.37
2	A	1797	0UN	CBJ-CBK	-3.41	1.33	1.40
2	A	1797	0UN	C2-NAZ	-3.30	1.29	1.36
2	A	1797	0UN	C6-C5	-3.30	1.35	1.39
2	A	1797	0UN	CAQ-CBD	2.90	1.53	1.48
2	A	1797	0UN	OBB-CBG	-2.71	1.33	1.39
2	A	1797	0UN	CBD-NAY	-2.58	1.31	1.35
2	A	1797	0UN	CAL-CBJ	-2.51	1.35	1.39
2	A	1797	0UN	C6-N1	-2.50	1.29	1.34
2	A	1797	0UN	C5-CL5	-2.15	1.68	1.73
2	A	1797	0UN	C2-N1	-2.01	1.31	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1797	0UN	CAA-OBA-CBK	-10.64	101.48	117.53
2	A	1797	0UN	CAP-CAQ-CBD	-7.71	113.45	122.27
2	A	1797	0UN	C5-C6-N1	-5.55	118.08	122.84
2	A	1797	0UN	CAU-NBO-CAT	4.82	122.16	111.52
2	A	1797	0UN	CBJ-NAZ-C2	-4.12	117.19	129.60
2	A	1797	0UN	N1-C2-N3	-3.54	123.19	126.55
2	A	1797	0UN	CAU-CAS-NBN	-3.34	107.03	110.80
2	A	1797	0UN	CBF-NAY-CBD	-3.28	123.30	128.26
2	A	1797	0UN	C6-N1-C2	2.95	120.34	115.88
2	A	1797	0UN	CAS-NBN-CAR	-2.66	105.81	109.52
2	A	1797	0UN	CAT-CAR-NBN	-2.60	107.86	110.80
2	A	1797	0UN	CAB-NBN-CAS	-2.54	106.86	110.66
2	A	1797	0UN	CAL-CBJ-CBK	2.22	121.91	119.05

There are no chirality outliers.

All (4) torsion outliers are listed below:

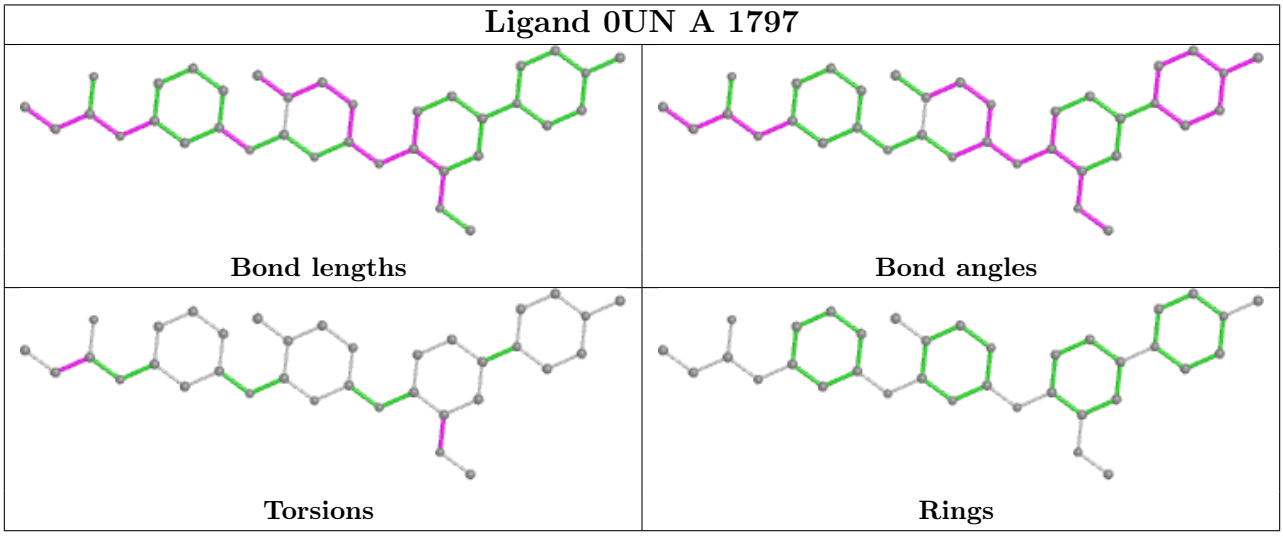
Mol	Chain	Res	Type	Atoms
2	A	1797	0UN	CAP-CAQ-CBD-NAY
2	A	1797	0UN	CAP-CAQ-CBD-OAE
2	A	1797	0UN	CBJ-CBK-OBA-CAA
2	A	1797	0UN	CAO-CBK-OBA-CAA

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1797	0UN	9	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	310/331 (93%)	-0.18	10 (3%) 47 43	34, 59, 97, 118	0
1	B	310/331 (93%)	-0.09	7 (2%) 60 58	31, 58, 103, 120	0
All	All	620/662 (93%)	-0.13	17 (2%) 54 50	31, 59, 101, 120	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	873	GLY	5.9
1	B	865	GLU	3.2
1	B	697	GLU	3.1
1	A	1020	GLN	2.9
1	B	986	ARG	2.8
1	B	985	GLU	2.8
1	A	874	GLY	2.8
1	A	1008	ASP	2.7
1	A	1007	MET	2.6
1	B	735	GLY	2.6
1	A	867	LYS	2.3
1	A	875	LYS	2.3
1	A	988	HIS	2.2
1	B	750	ALA	2.1
1	A	1019	PRO	2.1
1	A	863	GLY	2.1
1	A	917	GLY	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

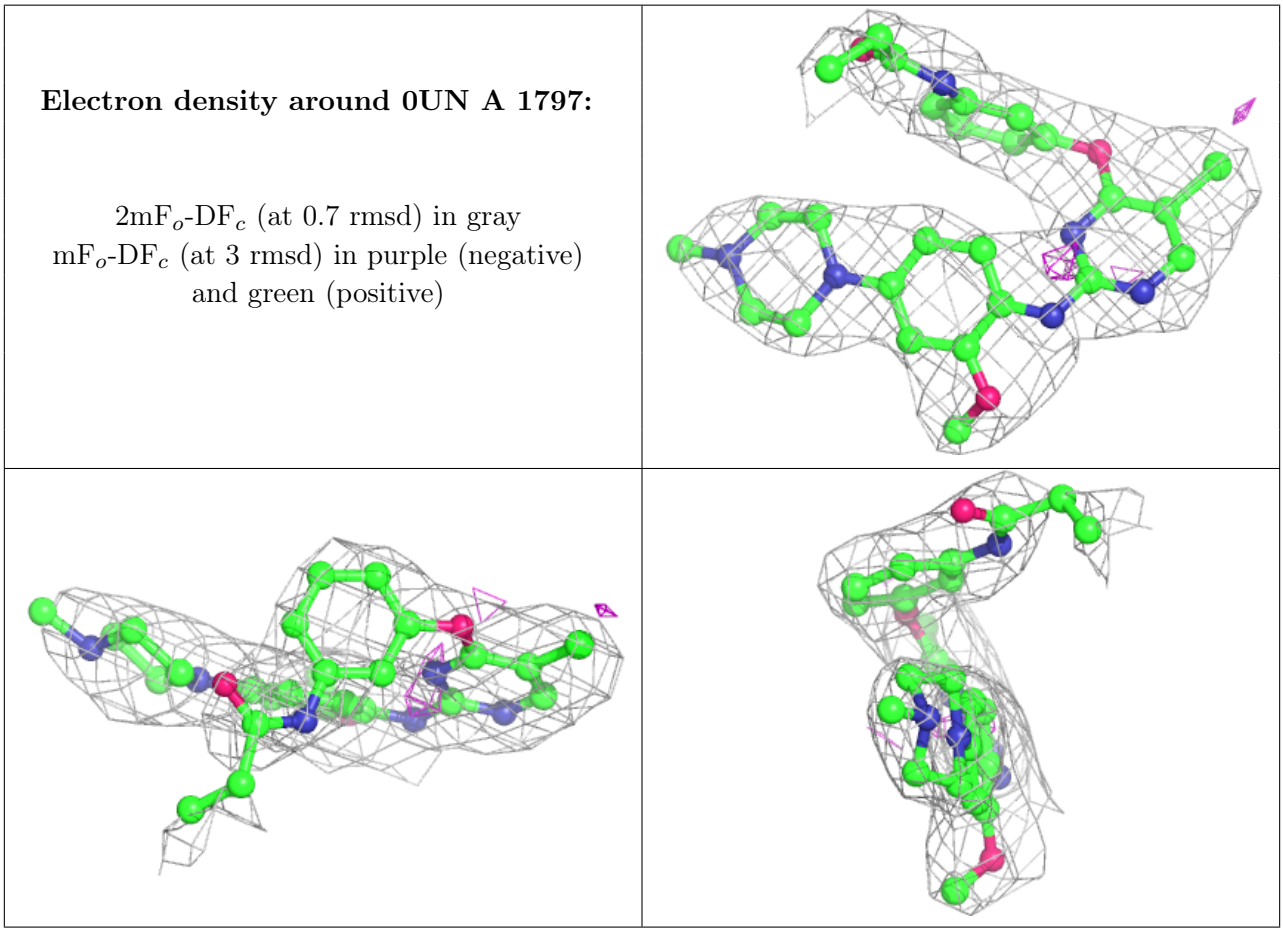
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	0UN	A	1797	35/35	0.90	0.21	67,69,72,76	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 0UN A 1797:

$2mF_o$-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.