



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:14 AM UTC

PDB ID : 3IKA / pdb_00003ika
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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

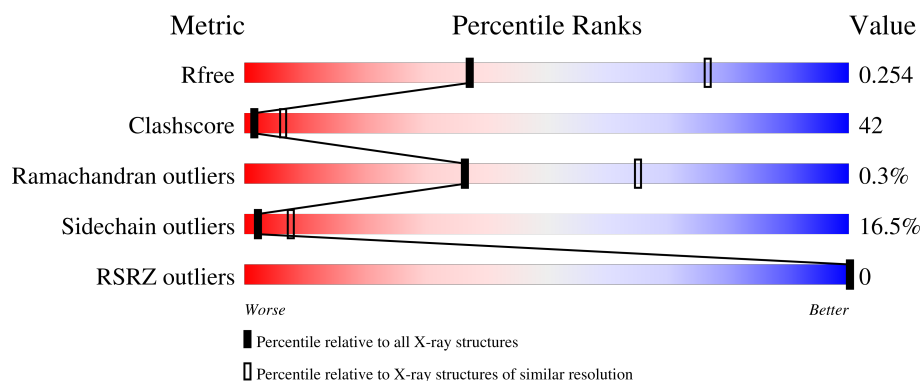
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 $\leq 5\%$. 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	

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.

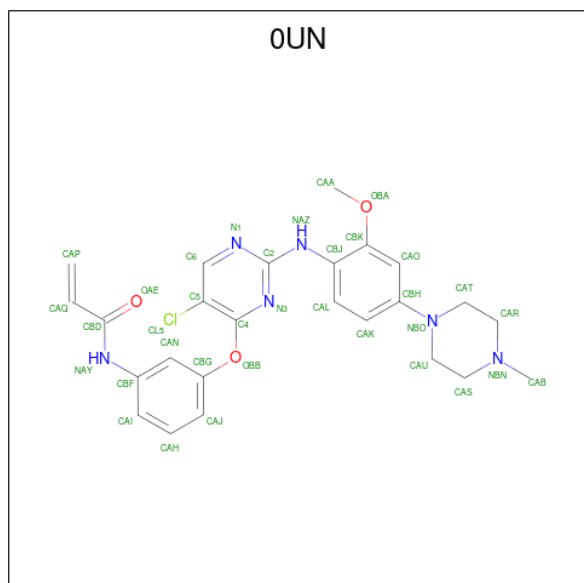
- Molecule 1 is a protein called Epidermal growth factor receptor.

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

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 (CCD ID: 0UN) (formula: C₂₅H₂₇ClN₆O₃).



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

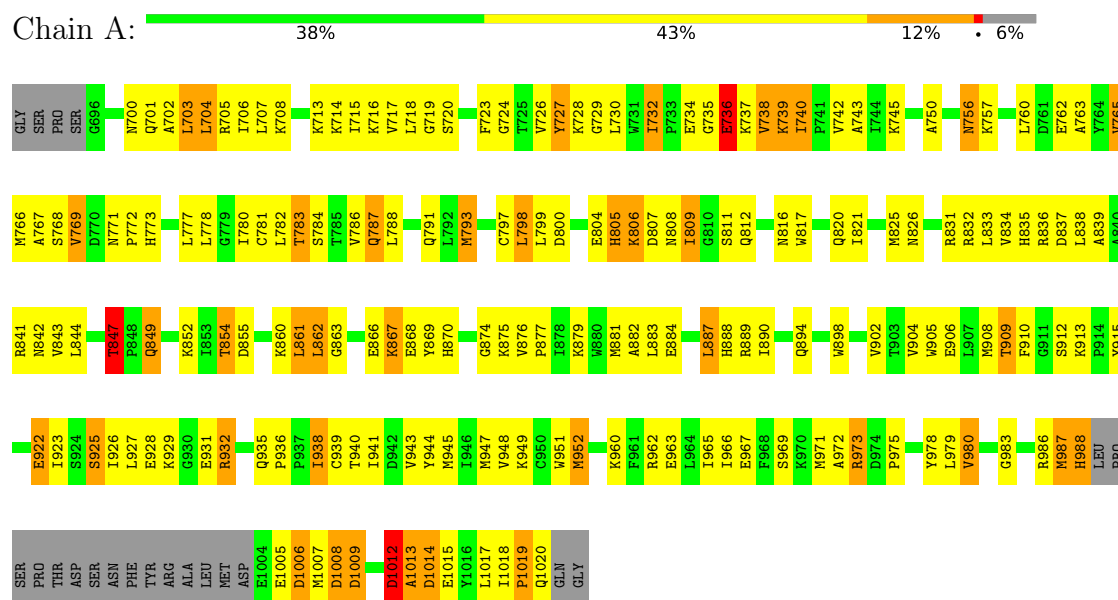
- Molecule 3 is water.

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

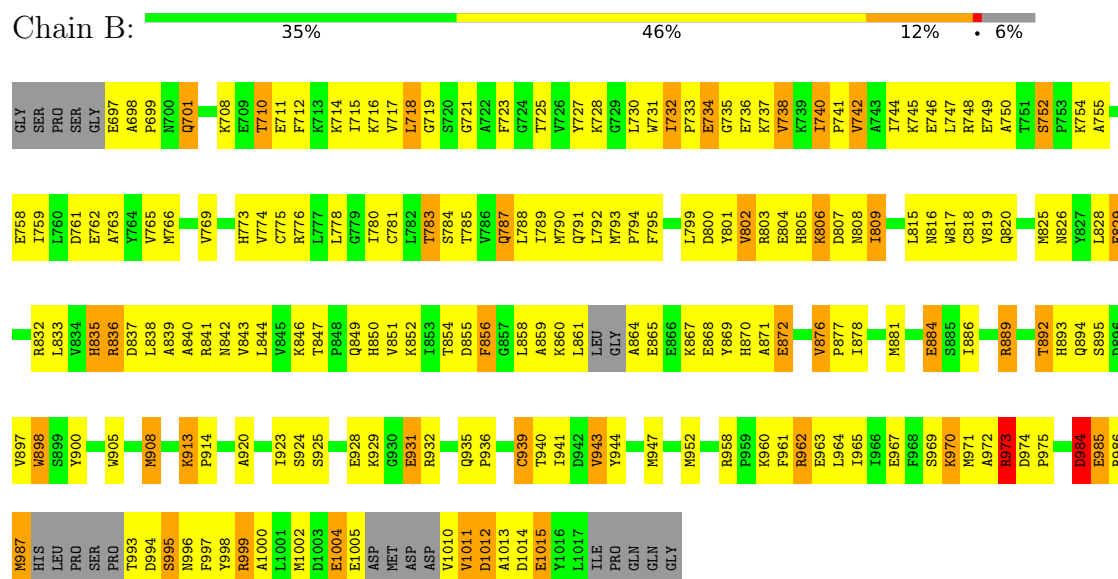
3 Residue-property plots

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



4 Data and refinement statistics

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 20.83 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.83-2.90) 96.7 (20.83-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.91%)	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 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

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: 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	1.62	13/2491 (0.5%)	1.25	20/3370 (0.6%)
1	B	1.52	7/2534 (0.3%)	1.23	24/3422 (0.7%)
All	All	1.57	20/5025 (0.4%)	1.24	44/6792 (0.6%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	738	VAL	CA-CB	-9.18	1.49	1.55
1	A	743	ALA	CA-CB	-6.94	1.43	1.53
1	B	742	VAL	CA-CB	-6.55	1.45	1.54
1	A	1018	ILE	CA-CB	-6.44	1.49	1.53
1	A	727	TYR	CA-C	-5.95	1.45	1.52
1	A	738	VAL	CA-C	-5.91	1.46	1.52
1	A	843	VAL	CA-CB	-5.91	1.47	1.54
1	A	834	VAL	CA-CB	-5.89	1.47	1.54
1	A	765	VAL	CA-CB	-5.85	1.46	1.54
1	B	829	GLU	CA-C	-5.72	1.45	1.52
1	B	742	VAL	CA-C	-5.55	1.45	1.52
1	B	802	VAL	CA-CB	-5.40	1.47	1.54
1	A	763	ALA	CA-CB	-5.39	1.44	1.53
1	A	876	VAL	CA-CB	-5.38	1.47	1.54
1	A	839	ALA	CA-CB	-5.27	1.44	1.53
1	A	767	ALA	CA-CB	-5.18	1.44	1.53
1	B	817	TRP	C-O	-5.15	1.18	1.24
1	A	834	VAL	C-O	-5.11	1.18	1.24
1	B	744	ILE	CA-CB	-5.05	1.48	1.54
1	B	818	CYS	C-O	-5.01	1.18	1.24

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	872	GLU	N-CA-C	-8.28	99.84	110.53
1	B	984	ASP	N-CA-C	7.99	119.61	111.07
1	A	1013	ALA	N-CA-C	7.85	120.06	108.14
1	B	738	VAL	N-CA-C	7.71	120.54	109.51
1	A	987	MET	N-CA-C	7.71	120.96	110.55
1	A	1018	ILE	CB-CA-C	-7.55	106.35	114.35
1	B	718	LEU	N-CA-C	-7.25	104.03	113.17
1	B	865	GLU	N-CA-C	-6.96	103.97	113.30
1	A	806	LYS	N-CA-C	-6.89	102.99	111.33
1	B	973[A]	ARG	N-CA-C	6.83	119.74	111.82
1	B	973[B]	ARG	N-CA-C	6.83	119.74	111.82
1	A	738	VAL	CB-CA-C	-6.60	105.54	111.74
1	B	835	HIS	N-CA-C	6.46	118.20	111.03
1	A	804	GLU	N-CA-C	6.31	118.24	111.36
1	B	876	VAL	N-CA-C	6.24	114.31	109.19
1	B	836	ARG	N-CA-CB	-6.15	107.16	114.17
1	A	782	LEU	N-CA-C	6.12	119.19	110.68
1	A	738	VAL	N-CA-C	-6.08	100.28	107.70
1	A	736	GLU	N-CA-C	-6.06	101.07	110.10
1	B	1012	ASP	N-CA-C	-5.98	102.48	110.55
1	A	862	LEU	N-CA-C	5.77	118.88	109.59
1	B	783	THR	N-CA-C	-5.76	100.99	109.18
1	A	704	LEU	CA-C-N	-5.72	112.92	122.64
1	A	704	LEU	C-N-CA	-5.72	112.92	122.64
1	B	1004	GLU	N-CA-C	-5.64	105.13	111.28
1	B	847	THR	N-CA-C	-5.63	101.72	108.25
1	B	710	THR	CB-CA-C	-5.55	101.57	110.79
1	A	854	THR	CA-C-N	-5.52	115.42	122.77
1	A	854	THR	C-N-CA	-5.52	115.42	122.77
1	B	936	PRO	O-C-N	5.52	123.74	121.15
1	B	939	CYS	N-CA-C	5.50	119.20	109.96
1	B	737	LYS	CA-C-N	5.50	128.07	120.49
1	B	737	LYS	C-N-CA	5.50	128.07	120.49
1	B	963	GLU	N-CA-C	-5.47	105.32	111.28
1	B	898	TRP	N-CA-C	-5.44	105.25	111.07
1	A	967	GLU	N-CA-C	5.42	116.99	111.14
1	A	939	CYS	N-CA-C	5.41	118.06	109.24
1	B	712	PHE	N-CA-C	5.37	117.99	109.50
1	A	855	ASP	N-CA-C	5.18	117.17	108.73
1	A	1012	ASP	CA-C-N	-5.14	112.54	122.09
1	A	1012	ASP	C-N-CA	-5.14	112.54	122.09
1	B	1011	VAL	N-CA-C	5.10	115.92	108.53
1	B	985	GLU	N-CA-C	5.06	116.49	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	847	THR	N-CA-C	-5.05	100.28	108.82

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	201	0
1	B	2481	0	2499	214	0
2	A	35	0	26	9	0
3	A	71	0	0	9	0
3	B	77	0	0	21	0
All	All	5104	0	4969	414	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 42.

All (414) 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: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:B:998:TYR:CE2	1:B:1002:MET:HE3	1.93	1.02
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: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: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:825:MET:HE3	1:A:838:LEU:HD13	1.48	0.95
1:A:887:LEU:HB3	1:A:888:HIS:CD2	2.00	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1002:MET:HE2	3:B:56:HOH:O	1.73	0.88
1:B:790:MET:HE1	1:B:855:ASP:H	1.39	0.87
1:B:825:MET:HE2	1:B:838:LEU:HD22	1.53	0.87
1:B:998:TYR:CZ	1:B:1002:MET:HE3	2.10	0.87
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:B:790:MET:HE1	1:B:855:ASP:N	1.91	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
1:A:723:PHE:CD1	1:A:723:PHE:C	2.54	0.84
2:A:1797:OUN:N3	2:A:1797:OUN:CAL	2.30	0.83
1:A:825:MET:HE3	1:A:838:LEU:HD22	1.60	0.83
1:B:734:GLU:HG2	1:B:735:GLY:N	1.94	0.83
1:A:861:LEU:HD12	1:A:861:LEU:C	1.98	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
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: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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1002:MET:CE	1:B:1010:VAL:N	2.49	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:A:1005:GLU:C	1:A:1006:ASP:OD1	2.29	0.75
1:B:1000:ALA:CB	3:B:143:HOH:O	2.33	0.75
1:A:825:MET:HE2	1:A:838:LEU:HD13	1.69	0.74
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: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:A:805:HIS:O	1:A:806:LYS:C	2.31	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:1002:MET:CE	3:B:56:HOH:O	2.31	0.72
1:A:760:LEU:HD11	1:B:952:MET:HE2	1.72	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:A:1008:ASP:C	1:A:1009:ASP:OD2	2.33	0.72
1:B:943:VAL:HG12	1:B:944:TYR:N	2.04	0.72
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:986:ARG:O	1:B:987:MET:HB2	1.87	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:B:905:TRP:HB2	1:B:947:MET:HE3	1.73	0.70
1:A:730:LEU:HD23	1:A:739:LYS:HB3	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:923:ILE:O	1:B:924:SER:C	2.35	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:790:MET:CE	1:B:855:ASP:N	2.49	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:938:ILE:CD1	1:A:938:ILE:H	2.06	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:B:1002:MET:HE3	1:B:1010:VAL:N	2.09	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:861:LEU:CD1	1:A:862:LEU:N	2.39	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:1002:MET:HE2	1:B:1010:VAL:N	2.10	0.66
1:B:723:PHE:CE1	1:B:836:ARG:NH2	2.62	0.66
1:B:775:CYS:HB2	1:B:790:MET:HE2	1.76	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:A:825:MET:HE3	1:A:838:LEU:CD1	2.23	0.66
1:A:807:ASP:O	1:A:987:MET:HE2	1.96	0.65
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:B:793:MET:HE3	1:B:852:LYS:HD3	1.78	0.65
1:A:706:ILE:C	1:A:707:LEU:HD23	2.22	0.65
1:A:980:VAL:HG12	1:A:980:VAL:O	1.97	0.65
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:793:MET:HE3	1:B:852:LYS:CD	2.28	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: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:B:905:TRP:HD1	1:B:947:MET:HE1	1.64	0.61
1:B:998:TYR:OH	1:B:1002:MET:HE3	2.01	0.61
1:A:825:MET:HE3	1:A:838:LEU:CD2	2.31	0.61
1:A:938:ILE:HG22	1:A:938:ILE:O	1.99	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: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:B:905:TRP:CD1	1:B:947:MET:HE1	2.36	0.60
1:A:941:ILE:CG2	1:A:945:MET:HE2	2.32	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:A:971:MET:HE2	1:A:978:TYR:CD1	2.38	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:A:905:TRP:HD1	1:A:947:MET:HE3	1.67	0.59
1:B:790:MET:HE3	1:B:855:ASP:OD2	2.02	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
1:A:887:LEU:C	1:A:888:HIS:CD2	2.82	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:708:LYS:NZ	1:A:734:GLU:CD	2.63	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:998:TYR:HE2	1:B:1002:MET:HE3	1.61	0.55
1:B:931:GLU:C	1:B:932:ARG:HD3	2.31	0.55
1:B:766:MET:HE1	1:B:856:PHE:CD2	2.42	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:905:TRP:CD1	1:A:947:MET:HE3	2.43	0.54
1:A:737:LYS:O	1:A:738:VAL:HG13	2.08	0.54
1:B:741:PRO:C	1:B:742:VAL:CG1	2.80	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:758:GLU:O	1:B:759:ILE:C	2.50	0.54
1:B:731:TRP:CZ2	1:B:733:PRO:HB3	2.43	0.54
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:801:TYR:C	1:B:801:TYR:CD2	2.87	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:741:PRO:C	1:B:742:VAL:HG13	2.33	0.53
1:B:894:GLN:HA	1:B:894:GLN:OE1	2.07	0.53
1:A:888:HIS:O	1:A:889:ARG:C	2.49	0.53
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:B:766:MET:HE1	1:B:856:PHE:CE2	2.45	0.52
1:A:783:THR:O	1:A:784:SER:C	2.49	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:877:PRO:O	1:A:881:MET:HG3	2.10	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:A:718:LEU:HD21	1:A:728:LYS:HB2	1.93	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: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:A:941:ILE:HG22	1:A:945:MET:HE2	1.94	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:998:TYR:HH	1:B:1010:VAL:N	2.10	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:OUN:HAH	1.94	0.49
1:B:715:ILE:HD11	1:B:730:LEU:CD1	2.41	0.49
1:A:936:PRO:CG	1:A:947:MET:HE1	2.43	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:A:798:LEU:O	1:A:799:LEU:C	2.54	0.48
1:A:936:PRO:HG2	1:A:947:MET:HE1	1.95	0.48
1:B:886:ILE:HG21	1:B:924:SER:HB3	1.94	0.48
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:797:CYS:O	1:A:798:LEU:C	2.57	0.48
1:A:962:ARG:HA	1:A:965:ILE:HD12	1.95	0.48
1:B:790:MET:CE	1:B:855:ASP:OD2	2.61	0.48
1:A:760:LEU:HD11	1:B:952:MET:CE	2.41	0.48
1:A:863:GLY:CA	1:A:866:GLU:HG3	2.44	0.48
1:B:960:LYS:O	1:B:961:PHE:C	2.53	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:908:MET:HE1	1:A:979:LEU:HD11	1.95	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:708:LYS:HZ3	1:A:734:GLU:CD	2.21	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:A:805:HIS:C	1:A:807:ASP:N	2.69	0.47
1:A:825:MET:HE3	1:A:838:LEU:CG	2.44	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:A:922:GLU:O	1:A:923:ILE:C	2.58	0.47
1:B:790:MET:HE1	1:B:854:THR:CA	2.45	0.47
1:B:783:THR:OG1	1:B:785:THR:O	2.33	0.47
1:A:700:ASN:OD1	1:A:700:ASN:C	2.57	0.46
1:A:771:ASN:CG	1:A:772:PRO:HD2	2.40	0.46
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:A:1014:ASP:O	1:A:1015:GLU:C	2.55	0.46
1:B:734:GLU:CG	1:B:735:GLY:N	2.58	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:735:GLY:O	1:A:736:GLU:C	2.57	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: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: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: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:1012:ASP:OD1	1:B:1012:ASP:C	2.60	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:904:VAL:O	1:A:905:TRP:C	2.60	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:793:MET:HE2	1:A:852:LYS:HD2	1.99	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:793:MET:HE3	1:B:852:LYS:HD2	1.98	0.44
1:A:833:LEU:CD2	1:A:861:LEU:HD13	2.48	0.43
1:B:728:LYS:HE3	1:B:997:PHE:CE2	2.53	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:A:708:LYS:HZ1	1:A:734:GLU:CD	2.26	0.43
1:A:898:TRP:CD1	1:A:898:TRP:C	2.95	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:783:THR:O	1:B:784:SER:C	2.60	0.43
1:B:807:ASP:O	1:B:987:MET:HE2	2.19	0.43
1:B:839:ALA:O	1:B:843:VAL:HG23	2.19	0.43
1:A:737:LYS:C	1:A:738:VAL:HG13	2.44	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: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:A:729:GLY:C	1:A:730:LEU:HD12	2.45	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:1019:PRO:C	1:A:1020:GLN:O	2.61	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:B:967:GLU:OE1	1:B:971:MET:HE3	2.19	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:LYS:HE2	1:A:869:TYR:CZ	2.55	0.42
1:A:887:LEU:C	1:A:888:HIS:HD2	2.27	0.42
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:825:MET:HE1	1:B:835:HIS:CB	2.50	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:762:GLU:HG2	1:B:766:MET:HE3	2.00	0.41
1:B:892:THR:HG23	1:B:895:SER:N	2.34	0.41
1:A:842:ASN:C	1:A:854:THR:HG22	2.45	0.41
1:A:1005:GLU:O	1:A:1006:ASP:OD1	2.38	0.41
1:B:905:TRP:CB	1:B:947:MET:HE3	2.46	0.41
1:A:760:LEU:CD1	1:B:952:MET:HE2	2.45	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:766:MET:HE3	1:B:788:LEU:HD13	2.02	0.41
1:B:878:ILE:HA	1:B:881:MET:HG3	2.02	0.41
1:B:897:VAL:O	1:B:898:TRP:C	2.62	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:B:790:MET:HE1	1:B:854:THR:C	2.44	0.40
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.56	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 ⓘ

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	306/331 (92%)	293 (96%)	11 (4%)	2 (1%)	18	48
1	B	303/331 (92%)	294 (97%)	9 (3%)	0	100	100
All	All	609/662 (92%)	587 (96%)	20 (3%)	2 (0%)	36	65

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	260/290 (90%)	213 (82%)	47 (18%)	2	6
1	B	269/290 (93%)	228 (85%)	41 (15%)	3	9
All	All	529/580 (91%)	441 (83%)	88 (17%)	2	7

All (88) 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	726	VAL
1	A	732	ILE
1	A	736	GLU
1	A	739	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	740	ILE
1	A	756	ASN
1	A	757	LYS
1	A	769	VAL
1	A	778	LEU
1	A	783	THR
1	A	786	VAL
1	A	787	GLN
1	A	791	GLN
1	A	793	MET
1	A	798	LEU
1	A	805	HIS
1	A	809	ILE
1	A	841	ARG
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	922	GLU
1	A	925	SER
1	A	932	ARG
1	A	938	ILE
1	A	952	MET
1	A	973	ARG
1	A	980	VAL
1	A	988	HIS
1	A	1006	ASP
1	A	1008	ASP
1	A	1009	ASP
1	A	1012	ASP
1	B	701	GLN
1	B	732	ILE
1	B	734	GLU
1	B	740	ILE
1	B	752	SER
1	B	787	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	792	LEU
1	B	802	VAL
1	B	806	LYS
1	B	808	ASN
1	B	809	ILE
1	B	832	ARG
1	B	841	ARG
1	B	849	GLN
1	B	856	PHE
1	B	867	LYS
1	B	868	GLU
1	B	872	GLU
1	B	876	VAL
1	B	884	GLU
1	B	889	ARG
1	B	892	THR
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	987	MET
1	B	993	THR
1	B	995	SER
1	B	996	ASN
1	B	999	ARG
1	B	1005	GLU
1	B	1015	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	771	ASN
1	A	791	GLN
1	A	816	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	805	HIS
1	B	888	HIS
1	B	893	HIS
1	B	935	GLN

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](#)

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	38,38,38	2.25	15 (39%)	51,52,52	2.68	12 (23%)

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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1797	0UN	CBF-NAY	-5.18	1.31	1.41
2	A	1797	0UN	CAP-CAQ	4.69	1.52	1.30
2	A	1797	0UN	CBJ-NAZ	-4.39	1.27	1.39
2	A	1797	0UN	OBA-CBK	-3.51	1.31	1.37
2	A	1797	0UN	CBJ-CBK	-3.46	1.33	1.40
2	A	1797	0UN	C6-C5	-3.30	1.35	1.39
2	A	1797	0UN	C2-NAZ	-3.18	1.29	1.36
2	A	1797	0UN	CAQ-CBD	3.04	1.53	1.48
2	A	1797	0UN	C5-C4	-2.82	1.36	1.39
2	A	1797	0UN	OBB-CBG	-2.70	1.33	1.39
2	A	1797	0UN	CAL-CBJ	-2.64	1.35	1.39
2	A	1797	0UN	C6-N1	-2.57	1.29	1.34
2	A	1797	0UN	CBD-NAY	-2.37	1.31	1.35
2	A	1797	0UN	C5-CL5	-2.14	1.68	1.73
2	A	1797	0UN	C2-N1	-2.07	1.31	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1797	0UN	CAA-OBA-CBK	-10.93	101.48	117.51
2	A	1797	0UN	CAP-CAQ-CBD	-7.98	113.45	122.22
2	A	1797	0UN	C5-C6-N1	-6.12	118.08	122.78
2	A	1797	0UN	CAU-NBO-CAT	4.71	122.16	111.57
2	A	1797	0UN	C5-C4-N3	-4.65	118.41	122.63
2	A	1797	0UN	CBJ-NAZ-C2	-3.94	117.19	129.22
2	A	1797	0UN	N1-C2-N3	-3.34	123.19	126.42
2	A	1797	0UN	C6-N1-C2	3.30	120.34	115.81
2	A	1797	0UN	CBF-NAY-CBD	-2.54	123.30	128.07
2	A	1797	0UN	CAU-CAS-NBN	-2.38	107.03	110.86
2	A	1797	0UN	CAS-NBN-CAR	-2.34	105.81	109.54
2	A	1797	0UN	CAL-CBJ-CBK	2.23	121.91	119.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

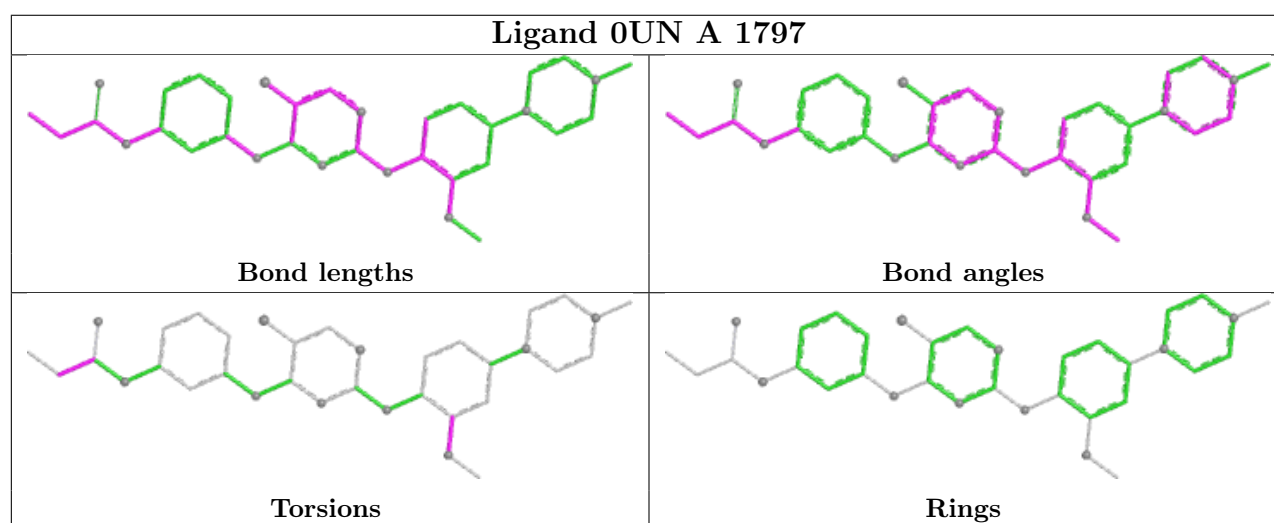
Mol	Chain	Res	Type	Atoms
2	A	1797	0UN	CAP-CAQ-CBD-NAY
2	A	1797	0UN	CAP-CAQ-CBD-OAE
2	A	1797	0UN	CBJ-CBK-OBA-CAA
2	A	1797	0UN	CAO-CBK-OBA-CAA

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	310/331 (93%)	-0.41	0 100 100	34, 59, 97, 118	0
1	B	310/331 (93%)	-0.37	0 100 100	31, 58, 103, 120	1 (0%)
All	All	620/662 (93%)	-0.39	0 100 100	31, 59, 101, 120	1 (0%)

There are no RSRZ outliers to report.

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](#)

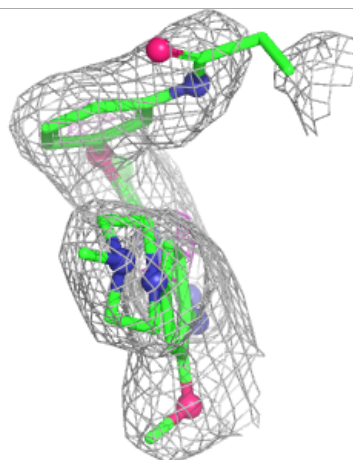
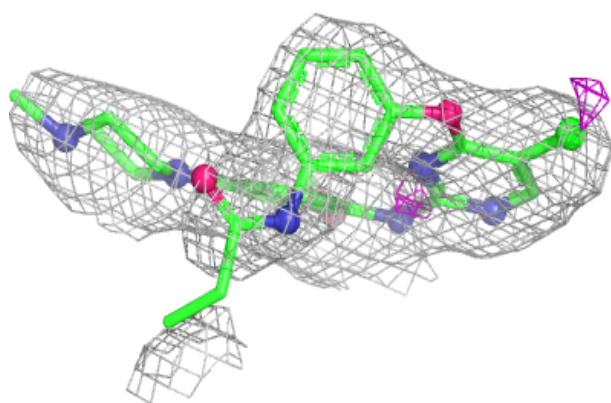
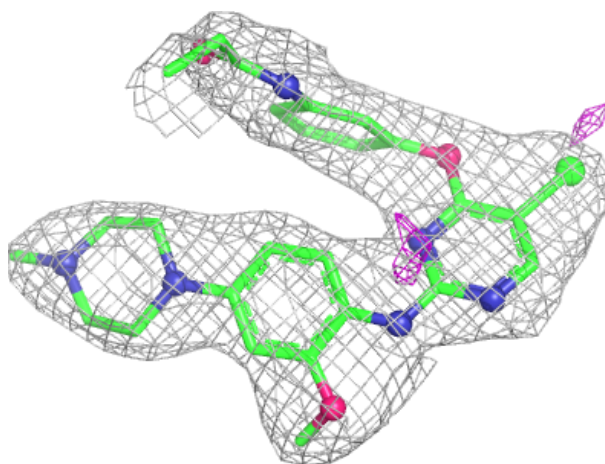
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	0UN	A	1797	35/35	0.89	0.10	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.