



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:26 AM UTC

PDB ID : 4JT6 / pdb_00004jt6
Title : structure of mTORDeltaN-mLST8-PI-103 complex
Authors : Pavletich, N.P.; Yang, H.
Deposited on : 2013-03-22
Resolution : 3.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

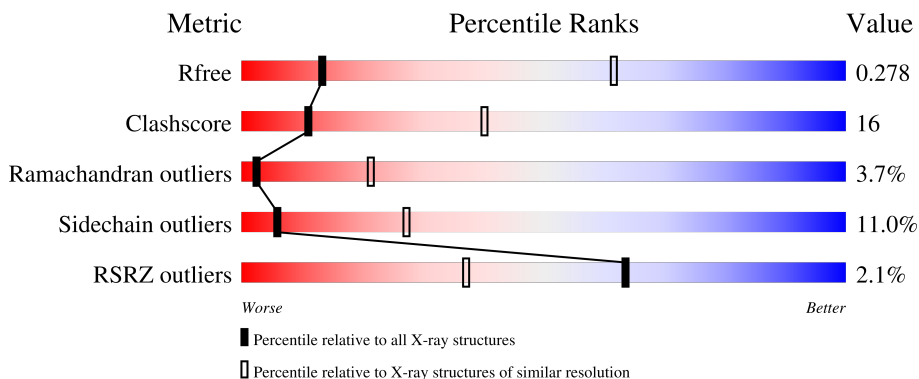
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	1174	2% 58% 26% 6% 10%
1	B	1174	2% 57% 27% 5% 10%
2	C	326	% 54% 33% 10% .
2	D	326	% 54% 34% 9% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 22149 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.

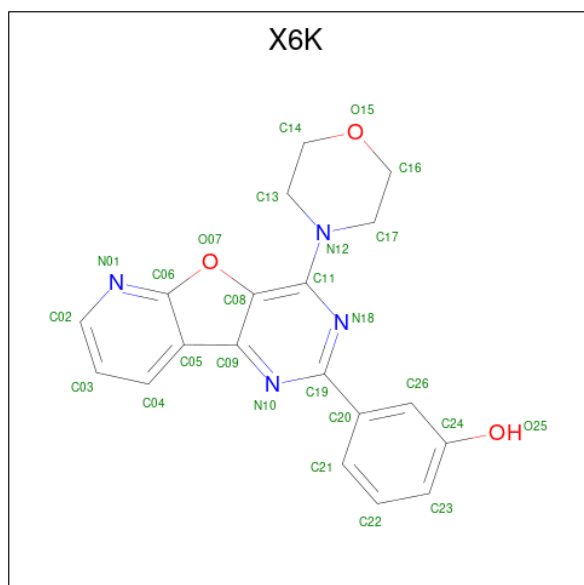
- Molecule 1 is a protein called mTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1058	Total	C	N	O	S	0	0	0
			8608	5472	1521	1552	63			
1	A	1054	Total	C	N	O	S	0	0	0
			8577	5451	1517	1546	63			

- Molecule 2 is a protein called mLST8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	317	Total	C	N	O	S	0	0	0
			2456	1526	436	476	18			
2	C	317	Total	C	N	O	S	0	0	0
			2456	1526	436	476	18			

- Molecule 3 is 3-(4-MORPHOLIN-4-YLPYRIDO[3',2':4,5]FURO[3,2-D]PYRIMIDIN-2-YL)PHENOL (CCD ID: X6K) (formula: C₁₉H₁₆N₄O₃).

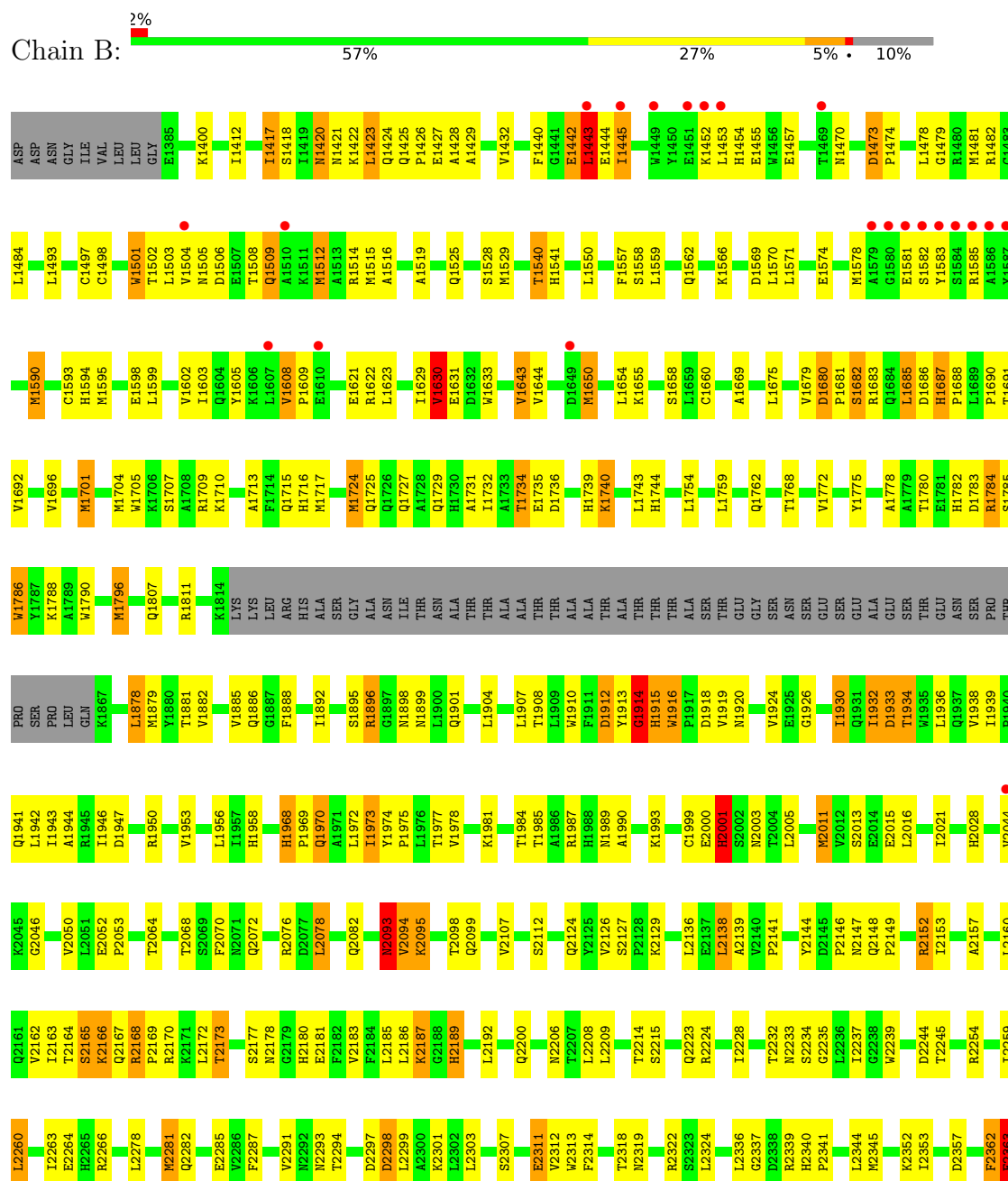


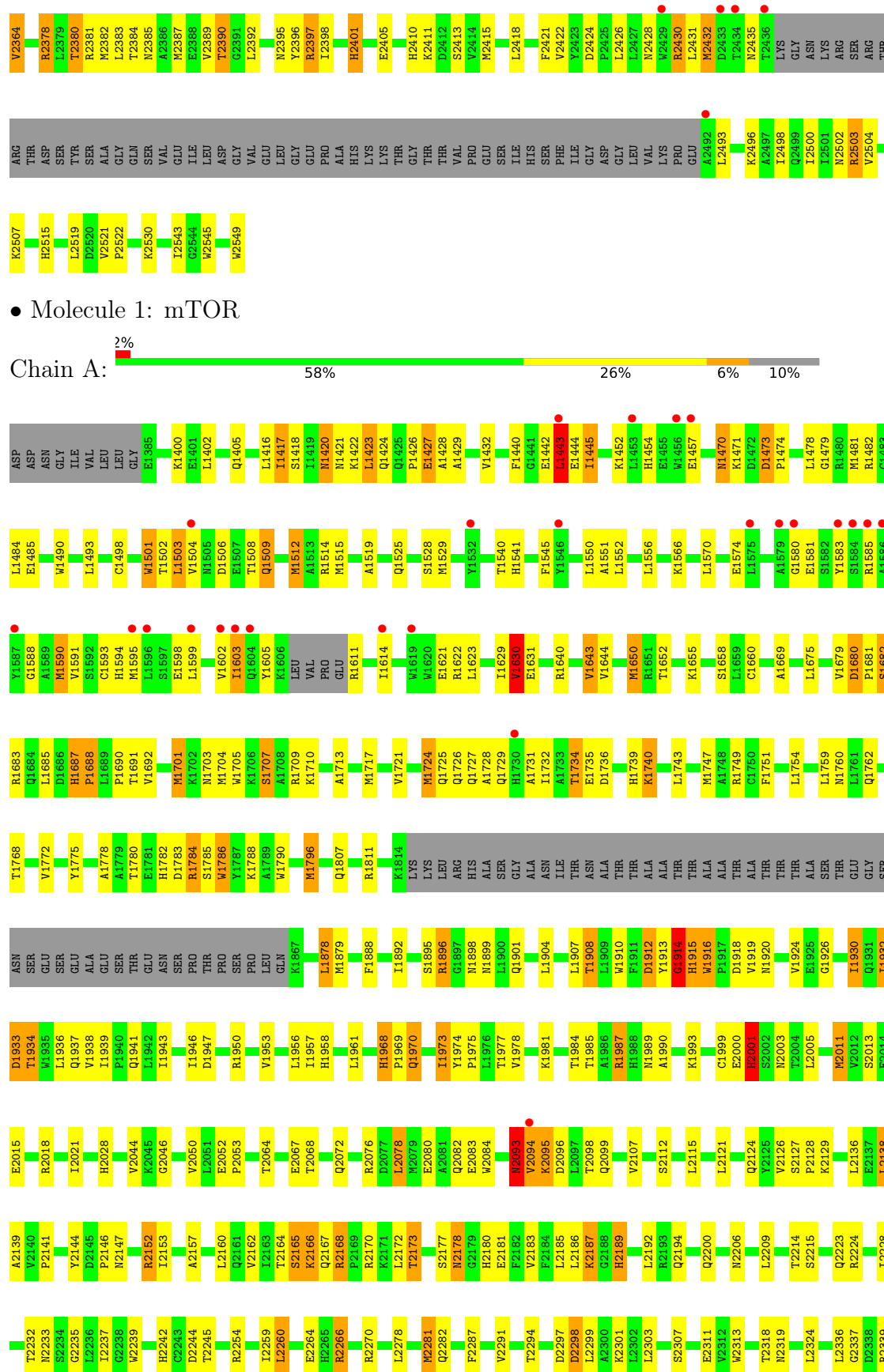
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			26	19	4	3		
3	A	1	Total	C	N	O	0	0
			26	19	4	3		

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.

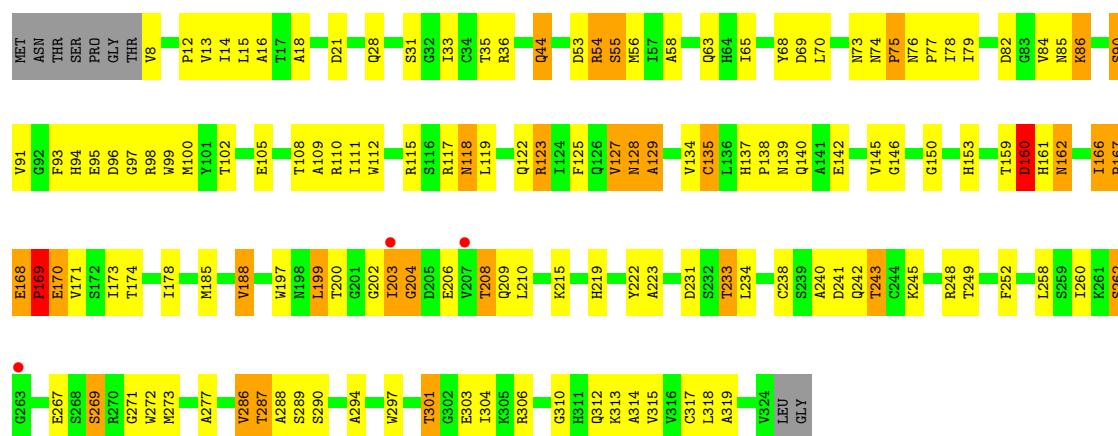
• Molecule 1: mTOR



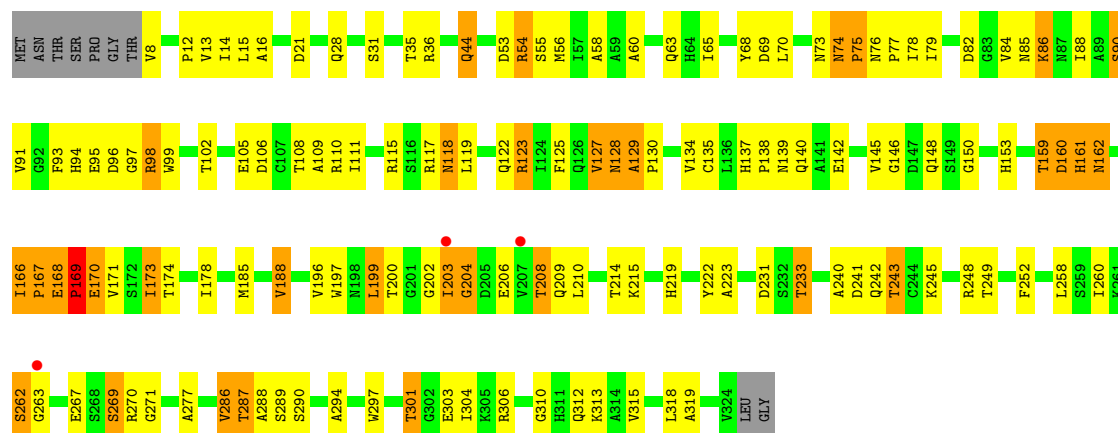




Chain D: 54% 34% 9% ...



Chain C: 54% 33% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	139.40Å 163.20Å 207.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.67 – 3.60 39.67 – 3.60	Depositor EDS
% Data completeness (in resolution range)	75.7 (39.67-3.60) 75.7 (39.67-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.239 , 0.275 0.241 , 0.278	Depositor DCC
R_{free} test set	1530 reflections (2.70%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	22149	wwPDB-VP
Average B, all atoms (Å ²)	65.0	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 42.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0214e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: X6K

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	0.44	0/8772	0.93	7/11872 (0.1%)
1	B	0.44	0/8805	0.93	10/11920 (0.1%)
2	C	0.45	0/2514	0.88	2/3426 (0.1%)
2	D	0.49	0/2514	0.89	1/3426 (0.0%)
All	All	0.45	0/22605	0.92	20/30644 (0.1%)

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	B	0	1
2	C	0	1
2	D	0	1
All	All	0	4

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1915	HIS	N-CA-C	10.80	125.47	109.59
1	B	1915	HIS	N-CA-C	10.69	125.30	109.59
1	A	2003	ASN	N-CA-C	7.40	120.04	111.02
2	C	170	GLU	N-CA-C	-7.29	103.47	112.88
2	D	170	GLU	N-CA-C	-6.93	103.95	112.88
1	B	1443	LEU	N-CA-C	-6.91	104.73	113.02
1	B	2003	ASN	N-CA-C	6.84	119.37	111.02
1	A	1443	LEU	N-CA-C	-6.23	105.25	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1473	ASP	CA-C-N	5.39	126.57	119.84
1	A	1473	ASP	C-N-CA	5.39	126.57	119.84
2	C	98	ARG	N-CA-C	5.38	118.96	112.93
1	B	1473	ASP	CA-C-N	5.31	126.48	119.84
1	B	1473	ASP	C-N-CA	5.31	126.48	119.84
1	B	1557	PHE	N-CA-C	5.14	116.69	111.14
1	B	1442	GLU	N-CA-C	5.13	121.26	114.12
1	A	1687	HIS	CA-C-N	5.10	126.21	119.84
1	A	1687	HIS	C-N-CA	5.10	126.21	119.84
1	B	1687	HIS	CA-C-N	5.05	126.15	119.84
1	B	1687	HIS	C-N-CA	5.05	126.15	119.84
1	B	2381	ARG	N-CA-C	5.04	116.77	111.28

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1914	GLY	Peptide
1	B	1914	GLY	Peptide
2	C	169	PRO	Peptide
2	D	169	PRO	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	8577	0	8559	256	0
1	B	8608	0	8593	260	0
2	C	2456	0	2341	108	0
2	D	2456	0	2341	110	0
3	A	26	0	16	1	0
3	B	26	0	16	1	0
All	All	22149	0	21866	721	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 16.

All (721) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:231:ASP:HB3	2:C:233:THR:OG1	1.47	1.12
2:D:231:ASP:HB3	2:D:233:THR:OG1	1.47	1.12
1:A:1418:SER:HB2	1:A:1581:GLU:HG2	1.32	1.11
2:D:76:ASN:HB3	2:D:77:PRO:HD2	1.33	1.08
2:C:76:ASN:HB3	2:C:77:PRO:HD2	1.34	1.06
1:B:1422:LYS:HE2	1:B:1581:GLU:HG3	1.41	1.01
2:D:146:GLY:HA3	2:D:173:ILE:HD11	1.42	0.99
2:D:69:ASP:HB2	2:D:78:ILE:HD11	1.46	0.95
1:B:1908:THR:O	1:B:1912:ASP:HB2	1.64	0.95
2:C:146:GLY:HA3	2:C:173:ILE:HD11	1.47	0.93
1:A:1908:THR:O	1:A:1912:ASP:HB2	1.68	0.91
1:B:2281:MET:HE1	2:D:222:TYR:CD2	2.06	0.90
1:B:1901:GLN:HG3	1:B:2413:SER:HA	1.55	0.89
1:A:2281:MET:HE1	2:C:222:TYR:CD2	2.09	0.88
2:C:95:GLU:HB2	2:C:140:GLN:NE2	1.89	0.88
1:B:1428:ALA:HB2	1:B:2395:ASN:HD21	1.39	0.87
2:D:95:GLU:HB2	2:D:140:GLN:NE2	1.89	0.87
2:C:69:ASP:HB2	2:C:78:ILE:HD11	1.54	0.87
1:B:1643:VAL:HG12	1:B:1644:VAL:HG23	1.58	0.85
1:B:2380:THR:HG23	1:B:2549:TRP:O	1.77	0.85
1:A:2503:ARG:HH11	1:A:2507:LYS:HE2	1.43	0.83
1:A:1969:PRO:O	1:A:1970:GLN:HB2	1.80	0.81
1:A:1901:GLN:HG3	1:A:2413:SER:HA	1.63	0.81
1:A:2278:LEU:HD23	2:C:44:GLN:HG2	1.64	0.80
2:C:16:ALA:HB3	2:C:319:ALA:HB3	1.64	0.80
2:C:95:GLU:HB2	2:C:140:GLN:HE22	1.43	0.80
2:D:8:VAL:HG21	2:D:36:ARG:HD3	1.63	0.79
1:B:2503:ARG:HH11	1:B:2507:LYS:HE2	1.47	0.79
1:B:1566:LYS:O	1:B:1570:LEU:HG	1.81	0.79
1:A:2503:ARG:NH1	1:A:2507:LYS:HE2	1.98	0.79
1:B:1969:PRO:O	1:B:1970:GLN:HB2	1.83	0.79
2:D:76:ASN:HB3	2:D:77:PRO:CD	2.11	0.79
1:A:2380:THR:HG23	1:A:2549:TRP:O	1.84	0.78
1:A:1428:ALA:HB2	1:A:2395:ASN:HD21	1.47	0.78
2:D:95:GLU:HB2	2:D:140:GLN:HE22	1.46	0.78
1:A:2146:PRO:O	1:A:2147:ASN:HB2	1.84	0.78
1:A:1916:TRP:CD1	1:A:1916:TRP:H	2.02	0.78
1:B:2278:LEU:HD23	2:D:44:GLN:HG2	1.66	0.77
2:D:231:ASP:CB	2:D:233:THR:OG1	2.30	0.77
2:C:76:ASN:HB3	2:C:77:PRO:CD	2.13	0.77
2:C:117:ARG:O	2:C:118:ASN:HB2	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:117:ARG:O	2:D:118:ASN:HB2	1.82	0.77
1:B:2146:PRO:O	1:B:2147:ASN:HB2	1.85	0.76
1:B:2380:THR:HG22	1:B:2383:LEU:HG	1.66	0.76
2:D:16:ALA:HB3	2:D:319:ALA:HB3	1.68	0.76
1:A:2185:LEU:HD13	1:A:2239:TRP:HZ3	1.49	0.76
2:C:8:VAL:HG21	2:C:36:ARG:HD3	1.68	0.76
1:A:1643:VAL:HG12	1:A:1644:VAL:HG23	1.67	0.75
1:B:2298:ASP:HB2	1:B:2382:MET:HE2	1.66	0.75
1:B:1916:TRP:H	1:B:1916:TRP:CD1	2.03	0.75
1:B:1926:GLY:O	1:B:1930:ILE:HG22	1.86	0.75
2:C:137:HIS:CD2	2:C:139:ASN:H	2.05	0.74
1:A:2160:LEU:HD22	1:A:2172:LEU:HA	1.70	0.74
2:D:301:THR:HB	2:D:303:GLU:HG2	1.69	0.74
1:B:1623:LEU:HG	1:B:1633:TRP:CH2	2.23	0.74
1:A:2421:PHE:HA	1:A:2424:ASP:HB2	1.70	0.73
2:C:301:THR:HB	2:C:303:GLU:HG2	1.69	0.73
2:C:231:ASP:CB	2:C:233:THR:OG1	2.32	0.73
1:B:2421:PHE:HA	1:B:2424:ASP:HB2	1.71	0.73
1:A:2095:LYS:O	1:A:2099:GLN:HG2	1.87	0.73
1:A:2298:ASP:HB2	1:A:2382:MET:HE2	1.70	0.73
2:D:137:HIS:CD2	2:D:139:ASN:H	2.08	0.72
1:B:2160:LEU:HD22	1:B:2172:LEU:HA	1.72	0.72
1:B:2095:LYS:O	1:B:2099:GLN:HG2	1.89	0.72
1:A:2187:LYS:HB3	1:A:2187:LYS:HZ2	1.55	0.72
1:A:2380:THR:HG22	1:A:2383:LEU:HG	1.70	0.72
1:B:2503:ARG:NH1	1:B:2507:LYS:HE2	2.05	0.72
1:A:1422:LYS:HE2	1:A:1581:GLU:HG3	1.72	0.71
1:A:1732:ILE:HD13	1:A:1740:LYS:HB2	1.70	0.71
1:A:1691:THR:HG23	1:A:1724:MET:HE1	1.73	0.71
1:A:1508:THR:O	1:A:1512:MET:HB2	1.90	0.71
1:A:1926:GLY:O	1:A:1930:ILE:HG22	1.90	0.71
1:B:1691:THR:HG23	1:B:1724:MET:HE1	1.72	0.70
1:B:1508:THR:O	1:B:1512:MET:HB2	1.89	0.70
1:B:1422:LYS:HE2	1:B:1581:GLU:CG	2.20	0.70
1:A:1958:HIS:CE1	1:A:1990:ALA:HB1	2.27	0.70
1:B:1623:LEU:HG	1:B:1633:TRP:CZ3	2.27	0.69
1:A:2185:LEU:HD13	1:A:2239:TRP:CZ3	2.27	0.69
1:A:2390:THR:HG23	1:A:2390:THR:O	1.91	0.69
1:B:2192:LEU:HD12	1:B:2235:GLY:HA3	1.74	0.69
2:C:94:HIS:HB3	2:C:99:TRP:HB2	1.74	0.69
1:B:2187:LYS:HG3	1:B:2237:ILE:HD12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1734:THR:C	1:A:1736:ASP:H	2.00	0.68
1:A:1418:SER:CB	1:A:1581:GLU:HG2	2.19	0.68
1:A:2503:ARG:HH11	1:A:2507:LYS:CE	2.06	0.68
1:B:2390:THR:HG23	1:B:2390:THR:O	1.93	0.68
1:A:1566:LYS:O	1:A:1570:LEU:HG	1.94	0.68
1:B:2185:LEU:HD13	1:B:2239:TRP:HZ3	1.57	0.68
1:B:1958:HIS:CE1	1:B:1990:ALA:HB1	2.29	0.68
2:D:94:HIS:HB3	2:D:99:TRP:HB2	1.76	0.67
1:A:2378:ARG:NH1	1:A:2380:THR:HG21	2.09	0.67
1:B:1907:LEU:HD11	1:B:1938:VAL:HG11	1.76	0.67
1:B:1907:LEU:HD11	1:B:1938:VAL:CG1	2.24	0.67
2:C:108:THR:OG1	2:C:110:ARG:NH1	2.26	0.67
1:B:1501:TRP:HH2	1:B:1509:GLN:OE1	1.77	0.67
1:A:1784:ARG:O	1:A:1790:TRP:NE1	2.25	0.67
1:B:1913:TYR:O	1:B:1915:HIS:HA	1.95	0.66
1:B:1913:TYR:HB2	1:B:1915:HIS:CE1	2.31	0.66
1:A:1704:MET:HE3	1:A:1713:ALA:HA	1.76	0.66
1:B:2378:ARG:NH1	1:B:2380:THR:HG21	2.11	0.66
1:B:1784:ARG:O	1:B:1790:TRP:NE1	2.27	0.65
1:B:2167:GLN:HG2	1:B:2189:HIS:CD2	2.31	0.65
1:A:1913:TYR:HB2	1:A:1915:HIS:CE1	2.31	0.65
1:A:2192:LEU:HD12	1:A:2235:GLY:HA3	1.78	0.65
1:B:2387:MET:HE3	1:B:2396:TYR:HB2	1.78	0.65
2:C:166:ILE:HG13	2:C:166:ILE:O	1.96	0.65
1:A:1969:PRO:O	1:A:1970:GLN:CB	2.44	0.65
1:B:1704:MET:HE3	1:B:1713:ALA:HA	1.78	0.65
1:A:2392:LEU:O	1:A:2397:ARG:HB2	1.96	0.65
2:D:69:ASP:CB	2:D:78:ILE:HD11	2.24	0.65
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.29	0.64
1:A:1977:THR:HG21	1:A:2013:SER:OG	1.96	0.64
2:C:137:HIS:HD2	2:C:139:ASN:H	1.43	0.64
2:D:166:ILE:HG13	2:D:166:ILE:O	1.97	0.64
1:B:2380:THR:HG23	1:B:2549:TRP:C	2.22	0.64
1:A:2521:VAL:HB	1:A:2522:PRO:HD3	1.78	0.64
1:A:1913:TYR:O	1:A:1915:HIS:HA	1.97	0.64
1:A:1602:VAL:HG13	1:A:1643:VAL:HG23	1.80	0.64
1:A:1968:HIS:HB3	1:A:2144:TYR:OH	1.98	0.64
1:A:2411:LYS:O	1:A:2415:MET:HG3	1.97	0.64
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.31	0.64
1:B:1968:HIS:HB3	1:B:2144:TYR:OH	1.98	0.63
1:A:1732:ILE:CD1	1:A:1740:LYS:HB2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2389:VAL:O	1:A:2390:THR:HG22	1.98	0.63
1:A:1631:GLU:CD	1:A:1631:GLU:H	2.06	0.63
1:B:2169:PRO:HB3	1:B:2187:LYS:HE2	1.80	0.63
1:A:2167:GLN:HG2	1:A:2189:HIS:CD2	2.34	0.63
1:B:1969:PRO:O	1:B:1970:GLN:CB	2.47	0.63
1:B:2281:MET:CE	2:D:222:TYR:CD2	2.81	0.63
1:B:2245:THR:HA	1:B:2345:MET:HB3	1.81	0.63
1:A:1428:ALA:HB2	1:A:2395:ASN:ND2	2.13	0.62
1:A:2093:ASN:O	1:A:2094:VAL:HB	1.98	0.62
1:B:1428:ALA:HB2	1:B:2395:ASN:ND2	2.12	0.62
1:B:2093:ASN:O	1:B:2094:VAL:HB	1.98	0.62
1:B:2389:VAL:O	1:B:2390:THR:HG22	1.99	0.62
1:A:2278:LEU:CD2	2:C:44:GLN:HG2	2.29	0.62
1:A:2011:MET:HE2	1:A:2129:LYS:HB3	1.81	0.62
2:D:231:ASP:HB3	2:D:233:THR:HG1	1.61	0.62
1:B:2521:VAL:HB	1:B:2522:PRO:HD3	1.81	0.62
1:A:2187:LYS:HG3	1:A:2237:ILE:HD12	1.82	0.62
1:A:1796:MET:HE2	1:A:1796:MET:HA	1.81	0.62
1:A:1907:LEU:HD11	1:A:1938:VAL:CG1	2.30	0.62
1:B:2392:LEU:O	1:B:2397:ARG:HB2	1.99	0.62
1:B:2178:ASN:ND2	1:B:2180:HIS:H	1.97	0.61
1:A:1717:MET:HG3	1:A:1754:LEU:HG	1.83	0.61
1:A:2178:ASN:ND2	1:A:2180:HIS:H	1.97	0.61
1:A:2245:THR:HG22	1:A:2345:MET:HE2	1.82	0.61
2:C:127:VAL:HG11	2:C:153:HIS:CE1	2.35	0.61
1:B:1643:VAL:HG12	1:B:1644:VAL:CG2	2.30	0.61
2:D:127:VAL:HG11	2:D:153:HIS:CE1	2.36	0.61
2:D:134:VAL:HG22	2:D:145:VAL:HG22	1.82	0.61
2:D:137:HIS:HD2	2:D:139:ASN:H	1.47	0.61
1:B:2187:LYS:HB3	1:B:2187:LYS:HZ2	1.66	0.61
2:C:168:GLU:N	2:C:169:PRO:HD2	2.16	0.61
1:B:2187:LYS:HB3	1:B:2187:LYS:NZ	2.16	0.61
2:D:150:GLY:HA3	2:D:169:PRO:HB3	1.83	0.60
2:C:111:ILE:HD12	2:C:123:ARG:HD3	1.81	0.60
1:B:2254:ARG:HD3	1:B:2298:ASP:OD2	2.01	0.60
1:A:1907:LEU:HD11	1:A:1938:VAL:HG11	1.83	0.60
1:A:2387:MET:HE3	1:A:2396:TYR:HB2	1.82	0.60
1:B:1913:TYR:HB3	1:B:1916:TRP:HE1	1.65	0.60
1:A:2187:LYS:HB3	1:A:2187:LYS:NZ	2.16	0.60
1:A:1930:ILE:HD11	1:A:1934:THR:HG21	1.83	0.60
1:B:1660:CYS:HB2	1:B:1669:ALA:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1796:MET:HE2	1:B:1796:MET:HA	1.82	0.60
1:A:2380:THR:HG23	1:A:2549:TRP:C	2.27	0.60
1:A:2254:ARG:HD3	1:A:2298:ASP:OD2	2.02	0.60
1:B:1807:GLN:O	1:B:1811:ARG:HG2	2.02	0.60
1:B:2245:THR:HG22	1:B:2345:MET:HE2	1.83	0.59
1:B:1631:GLU:CD	1:B:1631:GLU:H	2.10	0.59
2:D:168:GLU:N	2:D:169:PRO:HD2	2.18	0.59
2:C:94:HIS:CE1	2:C:96:ASP:HB2	2.37	0.59
2:C:150:GLY:HA3	2:C:169:PRO:HB3	1.84	0.59
1:B:1701:MET:HE1	1:B:1717:MET:N	2.17	0.59
2:C:69:ASP:CB	2:C:78:ILE:HD11	2.30	0.59
2:D:108:THR:OG1	2:D:110:ARG:NH1	2.35	0.59
2:D:111:ILE:HD12	2:D:123:ARG:HD3	1.84	0.58
1:B:1739:HIS:O	1:B:1743:LEU:HB2	2.03	0.58
2:D:21:ASP:HB3	2:D:313:LYS:H	1.68	0.58
2:D:94:HIS:HE1	2:D:96:ASP:HB2	1.68	0.58
2:D:169:PRO:HA	2:D:171:VAL:HG22	1.85	0.58
1:A:2281:MET:CE	2:C:222:TYR:CD2	2.85	0.58
1:B:1734:THR:C	1:B:1736:ASP:H	2.09	0.58
1:B:1930:ILE:HD11	1:B:1934:THR:HG21	1.85	0.58
1:A:2382:MET:SD	1:A:2549:TRP:HA	2.44	0.58
1:B:2380:THR:CG2	1:B:2549:TRP:C	2.76	0.58
1:B:2503:ARG:HH11	1:B:2507:LYS:CE	2.13	0.58
2:C:94:HIS:HE1	2:C:96:ASP:HB2	1.69	0.58
1:B:1732:ILE:HD13	1:B:1740:LYS:HB2	1.86	0.58
1:A:2245:THR:HA	1:A:2345:MET:HB3	1.86	0.58
2:D:55:SER:O	2:D:56:MET:HG2	2.02	0.58
2:C:65:ILE:HD11	2:C:102:THR:HG21	1.85	0.58
2:D:94:HIS:CE1	2:D:96:ASP:HB2	2.38	0.57
1:A:2178:ASN:HD22	1:A:2180:HIS:H	1.52	0.57
2:C:288:ALA:HB2	2:C:318:LEU:HG	1.85	0.57
2:D:65:ILE:HD11	2:D:102:THR:HG21	1.85	0.57
1:A:1417:ILE:HG23	1:A:1432:VAL:HB	1.86	0.57
1:A:1913:TYR:HB3	1:A:1916:TRP:HE1	1.68	0.57
1:B:1914:GLY:HA3	1:B:1950:ARG:HE	1.68	0.57
1:B:1941:GLN:HE22	1:B:2200:GLN:HE22	1.52	0.57
1:B:2185:LEU:HD13	1:B:2239:TRP:CZ3	2.39	0.57
1:A:1807:GLN:O	1:A:1811:ARG:HG2	2.05	0.57
2:C:98:ARG:HD2	2:C:115:ARG:HB2	1.87	0.57
1:B:2281:MET:HE1	2:D:222:TYR:CG	2.40	0.57
1:A:1701:MET:HE1	1:A:1717:MET:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1739:HIS:O	1:A:1743:LEU:HB2	2.05	0.57
2:C:203:ILE:HA	2:C:206:GLU:HG2	1.87	0.57
1:B:1420:ASN:HB3	1:B:1429:ALA:HB2	1.86	0.56
1:A:1420:ASN:HB3	1:A:1429:ALA:HB2	1.86	0.56
1:A:2336:LEU:HG	1:A:2339:ARG:HD2	1.86	0.56
2:C:14:ILE:HD13	2:C:70:LEU:HD13	1.87	0.56
2:C:65:ILE:CD1	2:C:102:THR:HG21	2.35	0.56
2:C:169:PRO:HA	2:C:171:VAL:HG22	1.87	0.56
1:B:2015:GLU:OE2	1:B:2127:SER:OG	2.15	0.56
1:A:1892:ILE:HG21	1:A:1930:ILE:HD11	1.88	0.56
2:C:134:VAL:HG22	2:C:145:VAL:HG22	1.87	0.56
1:B:2278:LEU:CD2	2:D:44:GLN:HG2	2.35	0.56
2:C:21:ASP:HB3	2:C:313:LYS:H	1.70	0.56
2:C:271:GLY:HA2	2:C:290:SER:HB2	1.86	0.56
1:B:2515:HIS:N	1:B:2515:HIS:ND1	2.53	0.56
2:D:94:HIS:HD2	2:D:140:GLN:HB3	1.71	0.56
1:A:2387:MET:HE1	1:A:2392:LEU:HD23	1.87	0.56
2:D:200:THR:O	2:D:208:THR:HA	2.06	0.56
2:C:231:ASP:HB3	2:C:233:THR:HG1	1.67	0.56
1:B:1785:SER:O	1:B:1786:TRP:HB3	2.06	0.55
2:D:65:ILE:CD1	2:D:102:THR:HG21	2.36	0.55
2:C:63:GLN:HE21	2:C:86:LYS:H	1.53	0.55
1:B:2387:MET:HE1	1:B:2392:LEU:HD23	1.88	0.55
2:D:98:ARG:HD2	2:D:115:ARG:HB2	1.89	0.55
1:A:1910:TRP:O	1:A:1915:HIS:NE2	2.39	0.55
1:B:2382:MET:SD	1:B:2549:TRP:HA	2.46	0.55
1:A:1680:ASP:C	1:A:1682:SER:N	2.65	0.55
2:C:31:SER:C	2:C:306:ARG:HD3	2.31	0.55
1:B:1501:TRP:CH2	1:B:1509:GLN:OE1	2.60	0.55
1:A:1941:GLN:HE22	1:A:2200:GLN:HE22	1.55	0.55
1:A:1999:CYS:C	1:A:2001:HIS:H	2.15	0.55
1:A:2515:HIS:ND1	1:A:2515:HIS:N	2.54	0.55
1:A:1643:VAL:HG12	1:A:1644:VAL:CG2	2.36	0.55
1:B:1417:ILE:HG23	1:B:1432:VAL:HB	1.88	0.55
1:A:1493:LEU:HD23	1:A:1519:ALA:HB2	1.88	0.55
1:A:2095:LYS:HA	1:A:2098:THR:HG22	1.87	0.55
1:B:1422:LYS:C	1:B:1424:GLN:H	2.14	0.54
1:A:1422:LYS:C	1:A:1424:GLN:H	2.15	0.54
1:B:1686:ASP:O	1:A:2266:ARG:HG3	2.07	0.54
1:A:2428:ASN:HB3	1:A:2493:LEU:HD13	1.89	0.54
2:D:63:GLN:HE21	2:D:86:LYS:H	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1583:TYR:C	1:A:1585:ARG:H	2.16	0.54
1:A:1623:LEU:HD13	1:A:1640:ARG:NH1	2.22	0.54
1:B:1691:THR:CG2	1:B:1724:MET:HE1	2.38	0.54
2:D:185:MET:HB2	2:D:199:LEU:HD21	1.89	0.54
1:A:2319:ASN:HD22	1:A:2352:LYS:HG3	1.72	0.54
1:B:1680:ASP:C	1:B:1682:SER:N	2.66	0.54
1:A:1914:GLY:HA3	1:A:1950:ARG:HE	1.73	0.54
1:B:2336:LEU:HG	1:B:2339:ARG:HD2	1.89	0.54
2:D:53:ASP:C	2:D:55:SER:H	2.16	0.54
2:D:288:ALA:HB2	2:D:318:LEU:HG	1.90	0.54
1:A:2264:GLU:HG3	1:A:2294:THR:HG21	1.90	0.54
1:B:1506:ASP:HA	1:B:1509:GLN:HB2	1.90	0.54
1:B:1574:GLU:HG2	1:B:1585:ARG:NH2	2.23	0.54
1:B:1583:TYR:C	1:B:1585:ARG:H	2.16	0.54
2:D:82:ASP:H	2:D:119:LEU:HD22	1.73	0.53
1:A:1660:CYS:HB2	1:A:1669:ALA:HB2	1.88	0.53
2:C:168:GLU:N	2:C:169:PRO:CD	2.72	0.53
1:A:2496:LYS:HE3	1:A:2500:ILE:HD11	1.90	0.53
1:B:2178:ASN:HD22	1:B:2180:HIS:H	1.55	0.53
2:D:123:ARG:NH2	2:D:160:ASP:OD1	2.41	0.53
1:A:1506:ASP:HA	1:A:1509:GLN:HB2	1.90	0.53
2:C:55:SER:O	2:C:56:MET:HG2	2.07	0.53
2:D:203:ILE:HA	2:D:206:GLU:HG2	1.91	0.53
2:D:262:SER:OG	2:D:267:GLU:HG2	2.09	0.53
2:C:200:THR:O	2:C:208:THR:HA	2.09	0.53
1:B:1629:ILE:HG22	1:B:1630:VAL:HG23	1.90	0.53
1:A:2418:LEU:O	1:A:2422:VAL:HG23	2.09	0.53
1:B:1759:LEU:HD11	1:B:1796:MET:HE3	1.89	0.53
1:B:1977:THR:HG21	1:B:2013:SER:OG	2.09	0.53
2:D:56:MET:HB2	2:D:68:TYR:O	2.08	0.53
2:D:297:TRP:CZ3	2:D:304:ILE:HG12	2.44	0.53
1:A:1943:ILE:HD13	1:A:1975:PRO:HB2	1.91	0.53
1:A:1785:SER:O	1:A:1786:TRP:HB3	2.08	0.52
1:A:2078:LEU:HD11	1:A:2107:VAL:HG21	1.90	0.52
1:A:2380:THR:CG2	1:A:2549:TRP:C	2.82	0.52
1:B:2028:HIS:HE1	1:B:2112:SER:OG	1.92	0.52
2:D:94:HIS:CD2	2:D:140:GLN:HB3	2.43	0.52
1:A:1759:LEU:HD11	1:A:1796:MET:HE3	1.90	0.52
2:C:185:MET:HB2	2:C:199:LEU:HD21	1.91	0.52
1:B:1654:LEU:HD21	1:B:1696:VAL:HG22	1.91	0.52
1:A:1501:TRP:HH2	1:A:1509:GLN:OE1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1734:THR:O	1:A:1736:ASP:N	2.36	0.52
1:A:2064:THR:HG22	1:A:2128:PRO:HD3	1.92	0.52
1:B:2011:MET:HE2	1:B:2129:LYS:HB3	1.92	0.52
2:D:14:ILE:HD13	2:D:70:LEU:HD13	1.92	0.52
2:D:248:ARG:O	2:D:252:PHE:HA	2.10	0.52
1:A:1479:GLY:HA2	1:A:1482:ARG:NH1	2.25	0.52
1:A:1888:PHE:O	1:A:1892:ILE:HG13	2.08	0.52
2:C:82:ASP:H	2:C:119:LEU:HD22	1.73	0.52
1:A:1947:ASP:CG	1:A:1987:ARG:HG2	2.34	0.52
1:B:1681:PRO:HG2	1:B:1683:ARG:HG3	1.92	0.52
1:B:1999:CYS:C	1:B:2001:HIS:H	2.18	0.52
1:B:2095:LYS:HA	1:B:2098:THR:HG22	1.91	0.52
2:C:53:ASP:C	2:C:55:SER:H	2.18	0.52
1:B:1910:TRP:O	1:B:1915:HIS:NE2	2.42	0.52
2:D:168:GLU:N	2:D:169:PRO:CD	2.73	0.52
1:A:2401:HIS:HB3	1:A:2521:VAL:HG12	1.91	0.52
2:C:94:HIS:HD2	2:C:140:GLN:HB3	1.75	0.52
1:B:1690:PRO:HB2	1:B:1692:VAL:HG22	1.93	0.51
1:B:2278:LEU:HB3	1:B:2282:GLN:HB2	1.91	0.51
1:A:1594:HIS:HE1	1:A:1622:ARG:HD2	1.75	0.51
1:B:2319:ASN:HD22	1:B:2352:LYS:HG3	1.75	0.51
1:A:1717:MET:CG	1:A:1754:LEU:HG	2.40	0.51
1:A:1785:SER:O	1:A:1786:TRP:CB	2.58	0.51
1:A:1913:TYR:O	1:A:1914:GLY:C	2.52	0.51
1:B:2254:ARG:NH1	1:B:2298:ASP:OD2	2.43	0.51
1:B:2428:ASN:HB3	1:B:2493:LEU:HD13	1.92	0.51
2:D:219:HIS:CE1	2:D:245:LYS:HD2	2.45	0.51
1:B:2264:GLU:HG3	1:B:2294:THR:HG21	1.93	0.51
1:B:2411:LYS:O	1:B:2415:MET:HG3	2.09	0.51
2:D:200:THR:HB	2:D:209:GLN:H	1.75	0.51
1:A:1502:THR:HG22	1:A:1504:VAL:HG23	1.93	0.51
1:A:1529:MET:HE3	1:A:1550:LEU:HG	1.92	0.51
1:A:2187:LYS:CG	1:A:2237:ILE:HD12	2.41	0.51
1:A:2281:MET:HE1	2:C:222:TYR:CG	2.46	0.51
2:C:262:SER:OG	2:C:267:GLU:HG2	2.10	0.51
1:B:1594:HIS:HE1	1:B:1622:ARG:HD2	1.76	0.51
1:B:1605:TYR:HD2	1:B:1605:TYR:O	1.93	0.51
1:B:1913:TYR:O	1:B:1914:GLY:C	2.53	0.51
1:B:1915:HIS:HD2	1:B:1953:VAL:HG22	1.75	0.51
1:B:2363:GLU:OE2	1:B:2503:ARG:HD2	2.10	0.51
1:B:2418:LEU:O	1:B:2422:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:203:ILE:HG22	2:D:204:GLY:H	1.76	0.51
1:B:1936:LEU:HA	1:B:1939:ILE:HG13	1.92	0.51
1:A:1786:TRP:NE1	1:A:1788:LYS:HB2	2.25	0.51
1:B:1783:ASP:O	1:B:1785:SER:N	2.44	0.51
2:D:167:PRO:HD2	2:D:169:PRO:HG2	1.92	0.51
1:B:1786:TRP:NE1	1:B:1788:LYS:HB2	2.25	0.50
2:D:287:THR:O	2:D:294:ALA:HA	2.10	0.50
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.44	0.50
2:C:203:ILE:HG22	2:C:204:GLY:H	1.76	0.50
1:B:1762:GLN:HB2	1:B:1768:THR:HG21	1.94	0.50
1:A:2064:THR:HG21	1:A:2126:VAL:O	2.10	0.50
1:B:2401:HIS:HB3	1:B:2521:VAL:HG12	1.92	0.50
1:A:2052:GLU:CG	1:A:2053:PRO:HD3	2.41	0.50
2:D:203:ILE:HG22	2:D:204:GLY:N	2.26	0.50
1:A:2278:LEU:HB3	1:A:2282:GLN:HB2	1.93	0.50
1:B:1892:ILE:HG21	1:B:1930:ILE:HD11	1.94	0.50
2:C:123:ARG:NH2	2:C:160:ASP:OD1	2.44	0.50
2:C:200:THR:HB	2:C:209:GLN:H	1.75	0.50
2:C:203:ILE:HG22	2:C:204:GLY:N	2.26	0.50
2:C:240:ALA:C	2:C:242:GLN:H	2.19	0.50
2:C:297:TRP:CZ3	2:C:304:ILE:HG12	2.46	0.50
1:B:2167:GLN:HG2	1:B:2189:HIS:HD2	1.77	0.50
1:B:2168:ARG:O	1:B:2170:ARG:NH1	2.43	0.50
1:B:2298:ASP:HB2	1:B:2382:MET:CE	2.38	0.50
1:A:1605:TYR:HD2	1:A:1605:TYR:O	1.94	0.50
1:A:2390:THR:O	1:A:2390:THR:CG2	2.60	0.50
1:B:2297:ASP:HB3	1:B:2301:LYS:HD2	1.94	0.50
1:A:1878:LEU:HD21	1:A:1918:ASP:HB2	1.92	0.50
1:A:1936:LEU:HA	1:A:1939:ILE:HG13	1.93	0.50
1:A:2297:ASP:HB3	1:A:2301:LYS:HD2	1.93	0.50
2:D:271:GLY:HA2	2:D:290:SER:HB2	1.93	0.50
1:A:1681:PRO:HG2	1:A:1683:ARG:HG3	1.94	0.50
1:B:1785:SER:O	1:B:1786:TRP:CB	2.60	0.49
1:B:1947:ASP:CG	1:B:1987:ARG:HG2	2.36	0.49
1:A:1783:ASP:O	1:A:1785:SER:N	2.45	0.49
1:B:1502:THR:HG22	1:B:1504:VAL:HG23	1.94	0.49
1:A:1551:ALA:HB1	1:A:1556:LEU:HB2	1.94	0.49
1:B:2078:LEU:HD11	1:B:2107:VAL:HG21	1.94	0.49
2:D:169:PRO:HA	2:D:171:VAL:H	1.77	0.49
1:A:1514:ARG:HH21	1:A:1540:THR:HG21	1.76	0.49
1:B:2170:ARG:HB2	1:B:2186:LEU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:248:ARG:O	2:D:252:PHE:N	2.45	0.49
2:D:288:ALA:HB1	2:D:315:VAL:HG12	1.95	0.49
2:C:169:PRO:HA	2:C:171:VAL:H	1.77	0.49
2:C:185:MET:HE2	2:C:197:TRP:CD1	2.48	0.49
1:B:1479:GLY:HA2	1:B:1482:ARG:NH1	2.28	0.49
2:C:94:HIS:CD2	2:C:140:GLN:HB3	2.47	0.49
2:C:287:THR:O	2:C:294:ALA:HA	2.11	0.49
2:C:167:PRO:HD2	2:C:169:PRO:HG2	1.93	0.49
2:D:199:LEU:HD22	2:D:210:LEU:CD2	2.43	0.49
1:B:1623:LEU:O	1:B:1633:TRP:HH2	1.96	0.49
1:B:2297:ASP:O	1:B:2298:ASP:C	2.55	0.49
2:C:241:ASP:OD2	2:C:243:THR:HB	2.12	0.49
1:B:1497:CYS:SG	1:B:1516:ALA:HB2	2.53	0.49
1:B:1655:LYS:O	1:B:1658:SER:HB3	2.13	0.49
1:B:1878:LEU:HD21	1:B:1918:ASP:HB2	1.93	0.49
1:B:2157:ALA:HB3	1:B:2173:THR:HG23	1.94	0.49
1:A:1915:HIS:HD2	1:A:1953:VAL:HG22	1.77	0.49
1:B:1958:HIS:HE1	1:B:1990:ALA:HB1	1.74	0.48
1:A:2170:ARG:HB2	1:A:2186:LEU:HB3	1.94	0.48
1:A:1443:LEU:CD2	1:A:1452:LYS:HZ3	2.27	0.48
1:A:1629:ILE:HG22	1:A:1630:VAL:HG23	1.94	0.48
1:A:1690:PRO:HB2	1:A:1692:VAL:HG22	1.95	0.48
1:B:1443:LEU:CD2	1:B:1452:LYS:HZ3	2.27	0.48
1:A:1514:ARG:NH2	1:A:1540:THR:HG21	2.28	0.48
1:B:1478:LEU:O	1:B:1482:ARG:HG3	2.13	0.48
2:D:31:SER:C	2:D:306:ARG:HD3	2.38	0.48
2:C:139:ASN:HD22	2:C:203:ILE:HG12	1.78	0.48
1:A:1958:HIS:HE1	1:A:1990:ALA:HB1	1.75	0.48
2:C:199:LEU:HD22	2:C:210:LEU:CD2	2.44	0.48
1:A:1427:GLU:HB2	1:A:2398:ILE:HD13	1.95	0.48
1:A:1443:LEU:HD23	1:A:1452:LYS:HZ3	1.78	0.48
1:B:2046:GLY:O	1:B:2050:VAL:HG23	2.13	0.48
1:A:2297:ASP:O	1:A:2298:ASP:C	2.56	0.48
2:C:28:GLN:O	2:C:28:GLN:HG3	2.13	0.48
1:B:2052:GLU:CG	1:B:2053:PRO:HD3	2.44	0.48
1:B:2307:SER:CB	1:B:2313:TRP:HB2	2.44	0.48
2:D:28:GLN:HE21	2:D:33:ILE:HD12	1.78	0.48
2:D:185:MET:HE2	2:D:197:TRP:CD1	2.49	0.48
1:B:1888:PHE:O	1:B:1892:ILE:HG13	2.13	0.48
2:C:288:ALA:HB1	2:C:315:VAL:HG12	1.96	0.48
1:B:1574:GLU:OE2	1:B:1585:ARG:NH1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2018:ARG:NH1	1:A:2067:GLU:OE2	2.37	0.47
2:C:138:PRO:HD2	2:C:178:ILE:HD13	1.96	0.47
2:C:188:VAL:HG13	2:C:223:ALA:HB3	1.96	0.47
1:B:1514:ARG:NH2	1:B:1540:THR:HG21	2.30	0.47
2:D:76:ASN:CB	2:D:77:PRO:HD2	2.23	0.47
1:A:2167:GLN:HG2	1:A:2189:HIS:HD2	1.79	0.47
1:A:2340:HIS:HB2	1:A:2341:PRO:CD	2.45	0.47
1:A:2498:ILE:HG22	1:A:2502:ASN:HD21	1.80	0.47
2:D:137:HIS:HD2	2:D:138:PRO:N	2.12	0.47
1:A:2046:GLY:O	1:A:2050:VAL:HG23	2.14	0.47
1:B:1920:ASN:O	1:B:1924:VAL:HG23	2.14	0.47
1:B:2390:THR:O	1:B:2390:THR:CG2	2.62	0.47
2:D:139:ASN:HD22	2:D:203:ILE:HG12	1.79	0.47
1:A:1655:LYS:O	1:A:1658:SER:HB3	2.15	0.47
1:B:1621:GLU:C	1:B:1623:LEU:H	2.21	0.47
1:B:1629:ILE:O	1:B:1630:VAL:C	2.57	0.47
1:A:1422:LYS:HD3	1:A:1580:GLY:HA3	1.97	0.47
1:A:1501:TRP:HA	1:A:1503:LEU:HG	1.97	0.47
1:A:1621:GLU:C	1:A:1623:LEU:H	2.22	0.47
1:A:2307:SER:CB	1:A:2313:TRP:HB2	2.45	0.47
2:C:63:GLN:NE2	2:C:86:LYS:H	2.12	0.47
2:C:248:ARG:O	2:C:252:PHE:N	2.47	0.47
1:B:1904:LEU:O	1:B:1907:LEU:HB2	2.14	0.47
2:D:56:MET:HA	2:D:70:LEU:HG	1.97	0.47
1:A:1701:MET:HB3	1:A:1701:MET:HE2	1.54	0.47
1:A:2015:GLU:OE2	1:A:2127:SER:OG	2.29	0.47
1:A:1481:MET:HA	1:A:1484:LEU:HD12	1.97	0.47
1:A:1796:MET:HA	1:A:1796:MET:CE	2.42	0.47
1:B:1705:TRP:CE3	1:B:1710:LYS:HB2	2.49	0.47
2:D:100:MET:HB3	2:D:112:TRP:HB2	1.97	0.47
2:D:233:THR:HB	2:D:234:LEU:HG	1.97	0.47
1:A:1762:GLN:HB2	1:A:1768:THR:HG21	1.97	0.47
1:B:1481:MET:HA	1:B:1484:LEU:HD12	1.97	0.47
1:B:1562:GLN:HB3	1:B:1566:LYS:NZ	2.29	0.47
1:A:2209:LEU:O	1:A:2215:SER:HB2	2.15	0.47
2:C:137:HIS:HD2	2:C:138:PRO:N	2.13	0.47
1:B:1939:ILE:HA	1:B:1942:LEU:HD12	1.96	0.46
1:B:1943:ILE:HD13	1:B:1975:PRO:HB2	1.98	0.46
1:B:1701:MET:HE2	1:B:1701:MET:HB3	1.58	0.46
1:A:1482:ARG:N	1:A:1515:MET:HE1	2.29	0.46
1:B:1440:PHE:HB3	1:B:1442:GLU:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1529:MET:HE3	1:B:1550:LEU:HG	1.97	0.46
1:B:1590:MET:HA	1:B:1593:CYS:SG	2.56	0.46
1:A:1440:PHE:HB3	1:A:1442:GLU:HB2	1.97	0.46
1:A:2363:GLU:OE2	1:A:2503:ARG:HD2	2.14	0.46
2:C:125:PHE:HE1	2:C:162:ASN:HB2	1.81	0.46
1:B:1778:ALA:O	1:B:1782:HIS:HD2	1.98	0.46
1:B:2138:LEU:HB3	1:B:2153:ILE:HD12	1.96	0.46
1:B:2340:HIS:HB2	1:B:2341:PRO:CD	2.46	0.46
2:D:240:ALA:C	2:D:242:GLN:H	2.23	0.46
1:A:1913:TYR:CB	1:A:1915:HIS:CE1	2.99	0.46
1:A:1727:GLN:O	1:A:1731:ALA:HB3	2.15	0.46
1:A:2298:ASP:HB2	1:A:2382:MET:CE	2.42	0.46
1:B:1972:LEU:O	1:B:1975:PRO:HG2	2.15	0.46
3:B:2601:X6K:O07	3:B:2601:X6K:H132	2.16	0.46
1:A:2344:LEU:HD13	1:A:2353:ILE:HD11	1.97	0.46
1:B:1501:TRP:CE3	1:B:1503:LEU:HD12	2.50	0.46
1:B:1717:MET:HG3	1:B:1754:LEU:HG	1.97	0.46
1:A:2194:GLN:HG2	1:A:2427:LEU:HD22	1.97	0.46
1:A:1680:ASP:C	1:A:1682:SER:H	2.23	0.46
2:D:135:CYS:SG	2:D:178:ILE:HG22	2.56	0.46
1:A:2139:ALA:HA	1:A:2152:ARG:HA	1.97	0.46
1:B:1427:GLU:OE2	1:B:2322:ARG:NH2	2.49	0.45
1:B:1482:ARG:N	1:B:1515:MET:HE1	2.31	0.45
2:D:286:VAL:HB	2:D:318:LEU:HD13	1.99	0.45
1:A:1691:THR:CG2	1:A:1724:MET:HE1	2.43	0.45
1:A:1977:THR:HG22	1:A:1981:LYS:HE2	1.97	0.45
1:A:2206:ASN:ND2	1:A:2224:ARG:HD2	2.31	0.45
2:C:68:TYR:HE2	2:C:77:PRO:HD3	1.82	0.45
1:B:1681:PRO:O	1:B:1682:SER:C	2.59	0.45
2:D:28:GLN:HG3	2:D:28:GLN:O	2.15	0.45
1:B:1501:TRP:HA	1:B:1503:LEU:HG	1.99	0.45
1:B:2496:LYS:HE3	1:B:2500:ILE:HD11	1.98	0.45
1:B:2167:GLN:O	1:B:2168:ARG:C	2.60	0.45
2:C:102:THR:O	2:C:109:ALA:HA	2.15	0.45
1:B:1913:TYR:CB	1:B:1915:HIS:CE1	2.99	0.45
1:A:1705:TRP:HZ2	1:A:1760:ASN:ND2	2.15	0.45
1:A:2028:HIS:HE1	1:A:2112:SER:OG	1.98	0.45
1:A:1473:ASP:HA	1:A:1474:PRO:HD2	1.75	0.45
1:A:2138:LEU:HB3	1:A:2153:ILE:HD12	1.98	0.45
1:B:1734:THR:O	1:B:1736:ASP:N	2.34	0.45
1:B:1943:ILE:HA	1:B:1946:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:258:LEU:HD22	2:D:297:TRP:CE3	2.52	0.45
1:B:2148:GLN:HA	1:B:2149:PRO:HD2	1.85	0.45
1:A:1743:LEU:O	1:A:1747:MET:HG3	2.17	0.45
2:C:219:HIS:CE1	2:C:245:LYS:HD2	2.51	0.45
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.50	0.45
1:A:1999:CYS:C	1:A:2001:HIS:N	2.75	0.45
2:C:258:LEU:HD22	2:C:297:TRP:CE3	2.52	0.45
1:B:1578:MET:HB2	1:B:1582:SER:HB3	1.98	0.45
1:B:1602:VAL:HG13	1:B:1643:VAL:HG23	1.99	0.45
1:B:1944:ALA:HA	1:B:2426:LEU:HD11	1.98	0.45
2:D:137:HIS:CD2	2:D:137:HIS:C	2.94	0.45
1:B:1796:MET:HA	1:B:1796:MET:CE	2.43	0.44
1:B:1881:THR:O	1:B:1885:VAL:HG23	2.17	0.44
1:B:2344:LEU:HD13	1:B:2353:ILE:HD11	1.97	0.44
2:D:58:ALA:HB2	2:D:93:PHE:HZ	1.82	0.44
2:D:68:TYR:HE2	2:D:77:PRO:HD3	1.83	0.44
1:A:1957:ILE:HG22	1:A:1961:LEU:HD12	1.99	0.44
2:C:58:ALA:HB2	2:C:93:PHE:HZ	1.82	0.44
2:C:277:ALA:O	2:C:286:VAL:HG23	2.16	0.44
1:B:1608:VAL:HA	1:B:1609:PRO:HD3	1.84	0.44
1:B:1725:GLN:O	1:B:1729:GLN:HG2	2.17	0.44
1:A:1501:TRP:CE3	1:A:1503:LEU:HD12	2.51	0.44
1:A:1943:ILE:CD1	1:A:1975:PRO:HB2	2.47	0.44
1:A:2324:LEU:HA	1:A:2353:ILE:HG21	1.99	0.44
2:D:241:ASP:OD2	2:D:243:THR:HB	2.17	0.44
1:A:1892:ILE:HG21	1:A:1930:ILE:CD1	2.47	0.44
2:C:56:MET:HB2	2:C:68:TYR:O	2.16	0.44
2:D:238:CYS:HB3	2:D:273:MET:O	2.17	0.44
1:A:1623:LEU:HD13	1:A:1640:ARG:HH12	1.82	0.44
2:C:130:PRO:HD2	2:C:148:GLN:HB2	1.99	0.44
2:C:248:ARG:O	2:C:252:PHE:HA	2.17	0.44
1:B:1882:VAL:HG12	1:B:1886:GLN:NE2	2.33	0.44
1:B:2362:PHE:O	1:B:2364:VAL:N	2.50	0.44
1:A:1590:MET:HA	1:A:1593:CYS:SG	2.57	0.44
1:A:1623:LEU:HD22	1:A:1652:THR:HG23	1.99	0.44
1:A:1932:ILE:O	1:A:1933:ASP:C	2.60	0.44
1:A:2157:ALA:HB3	1:A:2173:THR:HG23	1.99	0.44
2:C:28:GLN:HG3	2:C:31:SER:HG	1.83	0.44
1:A:1478:LEU:O	1:A:1482:ARG:HG3	2.17	0.44
1:A:1778:ALA:O	1:A:1782:HIS:HD2	2.01	0.44
1:B:1974:TYR:O	1:B:1978:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:GLN:NE2	2:D:86:LYS:H	2.15	0.44
1:A:1629:ILE:O	1:A:1630:VAL:C	2.60	0.44
1:A:1681:PRO:O	1:A:1682:SER:C	2.61	0.44
1:A:1705:TRP:CZ2	1:A:1760:ASN:ND2	2.85	0.44
1:A:1725:GLN:O	1:A:1729:GLN:HG2	2.17	0.44
1:A:2418:LEU:HD13	1:A:2504:VAL:HG11	2.00	0.44
1:A:2401:HIS:HB3	1:A:2521:VAL:CG1	2.47	0.44
1:B:1571:LEU:HA	1:B:1574:GLU:HB3	2.00	0.43
2:D:203:ILE:O	2:D:204:GLY:C	2.62	0.43
1:A:1943:ILE:HA	1:A:1946:ILE:HG13	1.99	0.43
2:C:137:HIS:CD2	2:C:137:HIS:C	2.95	0.43
1:B:2418:LEU:HD13	1:B:2504:VAL:HG11	1.99	0.43
1:B:2421:PHE:HD1	1:B:2430:ARG:NH2	2.15	0.43
1:A:1915:HIS:CE1	1:A:1919:VAL:HG11	2.53	0.43
1:B:1915:HIS:CE1	1:B:1919:VAL:HG11	2.53	0.43
1:B:2187:LYS:O	1:B:2234:SER:HA	2.18	0.43
2:D:102:THR:O	2:D:109:ALA:HA	2.17	0.43
1:A:1485:GLU:OE2	1:A:1515:MET:HE3	2.18	0.43
1:A:1595:MET:O	1:A:1599:LEU:HB2	2.19	0.43
1:A:1759:LEU:HD21	1:A:1772:VAL:HG21	1.99	0.43
1:B:1443:LEU:HD23	1:B:1452:LYS:HZ3	1.82	0.43
1:B:2208:LEU:HD22	1:B:2410:HIS:CD2	2.54	0.43
2:D:28:GLN:HG3	2:D:31:SER:HG	1.84	0.43
2:D:117:ARG:O	2:D:118:ASN:CB	2.60	0.43
2:C:15:LEU:HD11	2:C:286:VAL:HG11	2.00	0.43
2:D:12:PRO:O	2:D:54:ARG:NH2	2.51	0.43
1:A:1974:TYR:O	1:A:1978:VAL:HG23	2.19	0.43
1:A:2187:LYS:NZ	1:A:2187:LYS:CB	2.81	0.43
1:A:1490:TRP:CE3	1:A:1519:ALA:HA	2.53	0.43
1:A:1502:THR:O	1:A:1503:LEU:C	2.61	0.43
1:A:2115:LEU:HD23	1:A:2115:LEU:HA	1.94	0.43
1:B:1605:TYR:O	1:B:1605:TYR:CD2	2.70	0.43
1:B:2324:LEU:HA	1:B:2353:ILE:HG21	2.00	0.43
1:B:2430:ARG:H	1:B:2430:ARG:HG3	1.65	0.43
1:A:1583:TYR:C	1:A:1585:ARG:N	2.77	0.43
1:A:1687:HIS:HA	1:A:1688:PRO:HD2	1.80	0.43
2:C:86:LYS:HB3	2:C:105:GLU:HB2	2.01	0.43
2:C:202:GLY:O	2:C:203:ILE:O	2.37	0.43
1:B:1493:LEU:HD23	1:B:1519:ALA:HB2	2.01	0.43
1:B:1691:THR:O	1:B:1691:THR:HG22	2.19	0.43
1:B:1727:GLN:O	1:B:1731:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1915:HIS:HE1	1:B:1919:VAL:HG11	1.83	0.43
1:B:2336:LEU:HG	1:B:2339:ARG:HH11	1.83	0.43
2:C:117:ARG:O	2:C:118:ASN:CB	2.61	0.43
1:B:1973:ILE:H	1:B:1973:ILE:HG13	1.52	0.43
1:B:2187:LYS:NZ	1:B:2187:LYS:CB	2.82	0.43
2:D:127:VAL:HG11	2:D:153:HIS:HE1	1.81	0.43
1:A:2162:VAL:CG1	1:A:2168:ARG:HG2	2.49	0.43
1:A:2167:GLN:O	1:A:2168:ARG:C	2.62	0.43
2:C:36:ARG:NH2	2:C:69:ASP:O	2.52	0.43
2:C:74:ASN:H	2:C:75:PRO:CD	2.32	0.43
1:B:1473:ASP:HA	1:B:1474:PRO:HD2	1.77	0.42
1:B:2162:VAL:CG1	1:B:2168:ARG:HG2	2.50	0.42
1:B:2260:LEU:HB3	1:B:2263:ILE:HD12	2.01	0.42
2:C:12:PRO:O	2:C:54:ARG:NH2	2.52	0.42
1:B:1427:GLU:HB2	1:B:2398:ILE:HD13	2.01	0.42
1:B:2209:LEU:O	1:B:2215:SER:HB2	2.19	0.42
2:D:128:ASN:O	2:D:129:ALA:HB3	2.18	0.42
2:D:202:GLY:HA3	2:D:208:THR:H	1.84	0.42
2:D:277:ALA:O	2:D:286:VAL:HG23	2.19	0.42
1:A:2187:LYS:HG3	1:A:2237:ILE:CD1	2.49	0.42
1:B:1425:GLN:HG2	1:B:2314:PHE:HZ	1.84	0.42
1:B:1970:GLN:HA	1:B:1973:ILE:HD11	2.01	0.42
1:B:1977:THR:HG22	1:B:1981:LYS:HE2	2.00	0.42
1:B:2165:SER:OG	1:B:2166:LYS:N	2.52	0.42
1:B:2418:LEU:HD23	1:B:2421:PHE:CZ	2.55	0.42
2:D:69:ASP:HB2	2:D:78:ILE:CD1	2.33	0.42
1:A:1726:GLN:HG2	1:A:1729:GLN:HE21	1.84	0.42
1:A:1915:HIS:HE1	1:A:1919:VAL:HG11	1.83	0.42
1:A:1933:ASP:O	1:A:1934:THR:C	2.62	0.42
1:A:1989:ASN:O	1:A:1993:LYS:HD2	2.19	0.42
2:C:137:HIS:CD2	2:C:138:PRO:N	2.88	0.42
1:B:1418:SER:O	1:B:1421:ASN:HB2	2.19	0.42
1:B:1784:ARG:HA	1:B:1784:ARG:HD3	1.85	0.42
2:D:188:VAL:HG13	2:D:223:ALA:HB3	2.00	0.42
1:A:1605:TYR:O	1:A:1605:TYR:CD2	2.71	0.42
1:B:1422:LYS:CE	1:B:1581:GLU:HG3	2.29	0.42
1:B:1595:MET:O	1:B:1599:LEU:HB2	2.20	0.42
1:B:2206:ASN:ND2	1:B:2224:ARG:HD2	2.34	0.42
1:B:2432:MET:HE3	1:B:2435:ASN:ND2	2.34	0.42
2:D:137:HIS:CD2	2:D:138:PRO:N	2.88	0.42
1:A:2287:PHE:O	1:A:2291:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:ASP:OD1	2:C:108:THR:OG1	2.29	0.42
1:B:1744:HIS:O	1:B:1782:HIS:HB3	2.19	0.42
1:B:2208:LEU:HD22	1:B:2410:HIS:CG	2.54	0.42
1:B:2299:LEU:O	1:B:2303:LEU:HG	2.19	0.42
1:A:1920:ASN:O	1:A:1924:VAL:HG23	2.19	0.42
1:A:2084:TRP:HB3	1:A:2096:ASP:O	2.20	0.42
1:A:2254:ARG:HH22	1:A:2264:GLU:CD	2.27	0.42
2:C:202:GLY:HA3	2:C:208:THR:H	1.84	0.42
1:B:1498:CYS:HA	1:B:1501:TRP:HD1	1.85	0.42
1:B:2401:HIS:HB3	1:B:2521:VAL:CG1	2.49	0.42
1:A:1418:SER:O	1:A:1421:ASN:HB2	2.19	0.42
1:A:2165:SER:OG	1:A:2166:LYS:N	2.53	0.42
1:B:1400:LYS:HD2	1:B:1412:ILE:HG23	2.01	0.42
2:D:138:PRO:HD2	2:D:178:ILE:HD13	2.02	0.42
1:A:2421:PHE:HD1	1:A:2430:ARG:NH2	2.17	0.42
2:C:90:SER:O	2:C:102:THR:HA	2.20	0.42
1:B:1892:ILE:HG21	1:B:1930:ILE:CD1	2.50	0.41
2:C:289:SER:O	2:C:315:VAL:HB	2.20	0.41
1:B:1999:CYS:C	1:B:2001:HIS:N	2.78	0.41
1:B:2064:THR:HG21	1:B:2126:VAL:O	2.20	0.41
1:B:2152:ARG:HG2	1:B:2177:SER:OG	2.20	0.41
1:B:2254:ARG:HH22	1:B:2264:GLU:CD	2.28	0.41
2:D:15:LEU:HD11	2:D:286:VAL:HG11	2.02	0.41
1:A:1725:GLN:HB3	1:A:1747:MET:HE1	2.02	0.41
1:A:2432:MET:HE3	1:A:2435:ASN:ND2	2.35	0.41
1:B:1474:PRO:HB3	1:B:1505:ASN:HD22	1.85	0.41
1:B:2293:ASN:O	1:B:2294:THR:HG23	2.20	0.41
1:A:2152:ARG:HG2	1:A:2177:SER:OG	2.20	0.41
2:C:56:MET:HA	2:C:70:LEU:HG	2.02	0.41
1:B:1716:HIS:CE1	1:A:2266:ARG:HE	2.38	0.41
2:D:90:SER:O	2:D:102:THR:HA	2.20	0.41
2:D:142:GLU:OE2	2:D:208:THR:HB	2.20	0.41
2:D:262:SER:CB	2:D:267:GLU:HG2	2.51	0.41
1:A:1574:GLU:HG2	1:A:1585:ARG:NH2	2.35	0.41
2:C:128:ASN:O	2:C:129:ALA:HB3	2.19	0.41
1:B:1732:ILE:CD1	1:B:1740:LYS:HB2	2.50	0.41
1:B:1734:THR:C	1:B:1736:ASP:N	2.74	0.41
1:B:2070:PHE:CD2	1:B:2070:PHE:C	2.98	0.41
1:B:2498:ILE:HG22	1:B:2502:ASN:HD21	1.86	0.41
1:B:1989:ASN:O	1:B:1993:LYS:HD2	2.20	0.41
1:B:2285:GLU:HB2	2:D:272:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:LYS:HB3	2:D:105:GLU:HB2	2.03	0.41
2:D:289:SER:O	2:D:315:VAL:HB	2.20	0.41
2:D:290:SER:HA	2:D:314:ALA:HB1	2.03	0.41
1:A:1705:TRP:CE3	1:A:1710:LYS:HB2	2.55	0.41
2:C:60:ALA:HB1	2:C:88:ILE:HG22	2.02	0.41
2:C:127:VAL:HG11	2:C:153:HIS:HE1	1.82	0.41
1:B:1901:GLN:HG3	1:B:2413:SER:CA	2.39	0.41
1:B:2016:LEU:O	1:B:2186:LEU:HD21	2.20	0.41
1:A:1400:LYS:HG3	1:A:1416:LEU:HD13	2.03	0.41
1:A:1482:ARG:HA	1:A:1515:MET:HE1	2.02	0.41
1:A:2080:GLU:O	1:A:2083:GLU:HB3	2.21	0.41
2:C:196:VAL:HG11	2:C:252:PHE:CZ	2.56	0.41
2:C:203:ILE:O	2:C:204:GLY:C	2.64	0.41
1:B:1514:ARG:HH21	1:B:1540:THR:HG21	1.85	0.41
1:B:2082:GLN:HE21	1:B:2082:GLN:HB3	1.62	0.41
2:D:75:PRO:HB2	2:D:76:ASN:H	1.63	0.41
2:D:82:ASP:HB2	2:D:119:LEU:HD13	2.01	0.41
2:D:125:PHE:HE1	2:D:162:ASN:HB2	1.86	0.41
1:A:1772:VAL:HA	1:A:1775:TYR:HD1	1.86	0.41
1:A:1904:LEU:O	1:A:1907:LEU:HB2	2.21	0.41
1:A:1973:ILE:H	1:A:1973:ILE:HG13	1.56	0.41
1:A:2401:HIS:O	1:A:2405:GLU:HB2	2.21	0.41
3:A:2601:X6K:O07	3:A:2601:X6K:H132	2.20	0.41
2:C:159:THR:C	2:C:161:HIS:N	2.78	0.41
2:C:286:VAL:HB	2:C:318:LEU:HD13	2.03	0.41
1:B:1502:THR:O	1:B:1503:LEU:C	2.63	0.41
1:B:1562:GLN:HB3	1:B:1566:LYS:HZ2	1.86	0.41
1:B:1715:GLN:HG3	1:A:2260:LEU:HD23	2.02	0.41
1:B:1932:ILE:O	1:B:1933:ASP:C	2.64	0.41
1:A:1498:CYS:HA	1:A:1501:TRP:HD1	1.86	0.41
1:A:1552:LEU:HD11	1:A:1603:ILE:HG13	2.02	0.41
2:C:82:ASP:HB2	2:C:119:LEU:HD13	2.01	0.41
2:D:248:ARG:O	2:D:252:PHE:CA	2.69	0.40
2:C:262:SER:HB2	2:C:263:GLY:H	1.58	0.40
1:B:1772:VAL:HA	1:B:1775:TYR:HD1	1.86	0.40
1:B:2401:HIS:O	1:B:2405:GLU:HB2	2.21	0.40
1:A:1402:LEU:O	1:A:1405:GLN:HB2	2.22	0.40
1:A:1470:ASN:HB3	1:A:1471:LYS:H	1.60	0.40
1:A:1545:PHE:CE1	1:A:1599:LEU:HD22	2.57	0.40
1:A:1623:LEU:CD2	1:A:1652:THR:HG23	2.51	0.40
1:A:2121:LEU:HD23	1:A:2121:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2378:ARG:HH11	1:A:2380:THR:HG21	1.83	0.40
2:C:95:GLU:CB	2:C:140:GLN:HE22	2.24	0.40
1:B:1453:LEU:C	1:B:1455:GLU:H	2.29	0.40
1:B:1501:TRP:HE3	1:B:1501:TRP:O	2.05	0.40
1:B:1682:SER:O	1:B:1685:LEU:HD12	2.21	0.40
1:B:1687:HIS:HA	1:B:1688:PRO:HD2	1.81	0.40
1:B:2287:PHE:O	1:B:2291:VAL:HG23	2.21	0.40
1:A:1588:GLY:O	1:A:1591:VAL:HB	2.22	0.40
1:A:1611:ARG:HH11	1:A:1614:ILE:HG21	1.86	0.40
1:A:1728:ALA:HB2	1:A:1743:LEU:HD23	2.03	0.40
1:B:1973:ILE:O	1:B:1974:TYR:C	2.65	0.40
1:A:1973:ILE:O	1:A:1974:TYR:C	2.65	0.40
1:A:2344:LEU:HD12	1:A:2344:LEU:C	2.47	0.40
2:C:68:TYR:CE2	2:C:77:PRO:HD3	2.57	0.40
2:C:142:GLU:OE2	2:C:208:THR:HB	2.21	0.40
1:B:1688:PRO:HG3	1:A:2270:ARG:HA	2.03	0.40
1:B:1970:GLN:NE2	1:B:2139:ALA:H	2.20	0.40
1:B:2311:GLU:HG2	1:B:2312:VAL:N	2.37	0.40
2:D:18:ALA:HB3	2:D:317:CYS:HB2	2.04	0.40
1:A:1422:LYS:HG2	1:A:1580:GLY:C	2.46	0.40
1:A:1703:ASN:O	1:A:1707:SER:HB2	2.22	0.40
1:A:1721:VAL:HG11	1:A:1751:PHE:CE2	2.57	0.40
1:A:2082:GLN:HE21	1:A:2082:GLN:HB3	1.63	0.40
1:A:2299:LEU:O	1:A:2303:LEU:HG	2.21	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	1046/1174 (89%)	936 (90%)	74 (7%)	36 (3%)	3 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1052/1174 (90%)	941 (89%)	77 (7%)	34 (3%)	3	24
2	C	315/326 (97%)	271 (86%)	28 (9%)	16 (5%)	1	15
2	D	315/326 (97%)	272 (86%)	27 (9%)	16 (5%)	1	15
All	All	2728/3000 (91%)	2420 (89%)	206 (8%)	102 (4%)	2	21

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1525	GLN
1	B	1630	VAL
1	B	1650	MET
1	B	1709	ARG
1	B	1896	ARG
1	B	1970	GLN
1	B	2094	VAL
1	B	2298	ASP
2	D	75	PRO
2	D	97	GLY
2	D	203	ILE
1	A	1525	GLN
1	A	1630	VAL
1	A	1650	MET
1	A	1709	ARG
1	A	1896	ARG
1	A	1970	GLN
1	A	2094	VAL
1	A	2298	ASP
2	C	97	GLY
2	C	203	ILE
1	B	1444	GLU
1	B	1445	ILE
1	B	1682	SER
1	B	1735	GLU
1	B	1784	ARG
1	B	1914	GLY
1	B	2357	ASP
2	D	35	THR
2	D	74	ASN
2	D	118	ASN
2	D	167	PRO
2	D	204	GLY

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Mol	Chain	Res	Type
1	A	1444	GLU
1	A	1445	ILE
1	A	1682	SER
1	A	1735	GLU
1	A	1784	ARG
1	A	1914	GLY
1	A	2357	ASP
1	A	2364	VAL
2	C	35	THR
2	C	74	ASN
2	C	75	PRO
2	C	118	ASN
2	C	167	PRO
2	C	204	GLY
1	B	1707	SER
1	B	1734	THR
1	B	2000	GLU
1	B	2001	HIS
1	B	2093	ASN
1	B	2364	VAL
2	D	54	ARG
2	D	208	THR
1	A	1707	SER
1	A	1734	THR
1	A	1786	TRP
1	A	2000	GLU
1	A	2001	HIS
1	A	2093	ASN
2	C	208	THR
1	B	1423	LEU
1	B	1786	TRP
1	B	1934	THR
1	B	2362	PHE
2	D	169	PRO
2	D	269	SER
1	A	1423	LEU
1	A	1934	THR
1	A	1937	GLN
2	C	54	ARG
2	C	73	ASN
2	C	169	PRO
2	C	269	SER

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Mol	Chain	Res	Type
1	B	1454	HIS
1	B	1470	ASN
1	B	1512	MET
1	B	2363	GLU
2	D	73	ASN
2	D	160	ASP
1	A	1470	ASN
1	A	1512	MET
1	A	1933	ASP
1	A	1987	ARG
1	A	2362	PHE
2	C	270	ARG
1	B	1680	ASP
1	B	1933	ASP
1	A	1454	HIS
1	A	1503	LEU
1	A	1680	ASP
2	D	129	ALA
2	D	310	GLY
1	A	1688	PRO
2	C	129	ALA
1	A	2141	PRO
2	C	310	GLY
1	B	1426	PRO
1	B	2141	PRO
1	B	2163	ILE
1	A	1426	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	927/1024 (90%)	831 (90%)	96 (10%)	7	29
1	B	931/1024 (91%)	836 (90%)	95 (10%)	7	30
2	C	269/276 (98%)	232 (86%)	37 (14%)	3	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	269/276 (98%)	233 (87%)	36 (13%)	4	21
All	All	2396/2600 (92%)	2132 (89%)	264 (11%)	6	27

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1417	ILE
1	B	1420	ASN
1	B	1423	LEU
1	B	1443	LEU
1	B	1445	ILE
1	B	1457	GLU
1	B	1501	TRP
1	B	1509	GLN
1	B	1528	SER
1	B	1540	THR
1	B	1541	HIS
1	B	1558	SER
1	B	1559	LEU
1	B	1569	ASP
1	B	1590	MET
1	B	1598	GLU
1	B	1603	ILE
1	B	1608	VAL
1	B	1630	VAL
1	B	1643	VAL
1	B	1650	MET
1	B	1675	LEU
1	B	1679	VAL
1	B	1685	LEU
1	B	1701	MET
1	B	1724	MET
1	B	1740	LYS
1	B	1780	THR
1	B	1796	MET
1	B	1878	LEU
1	B	1879	MET
1	B	1895	SER
1	B	1896	ARG
1	B	1898	ASN
1	B	1899	ASN
1	B	1912	ASP

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Mol	Chain	Res	Type
1	B	1916	TRP
1	B	1930	ILE
1	B	1932	ILE
1	B	1956	LEU
1	B	1968	HIS
1	B	1973	ILE
1	B	1984	THR
1	B	1985	THR
1	B	2001	HIS
1	B	2005	LEU
1	B	2011	MET
1	B	2021	ILE
1	B	2044	VAL
1	B	2068	THR
1	B	2072	GLN
1	B	2076	ARG
1	B	2078	LEU
1	B	2093	ASN
1	B	2095	LYS
1	B	2124	GLN
1	B	2136	LEU
1	B	2138	LEU
1	B	2152	ARG
1	B	2164	THR
1	B	2165	SER
1	B	2166	LYS
1	B	2168	ARG
1	B	2173	THR
1	B	2181	GLU
1	B	2183	VAL
1	B	2187	LYS
1	B	2189	HIS
1	B	2214	THR
1	B	2223	GLN
1	B	2228	ILE
1	B	2232	THR
1	B	2233	ASN
1	B	2244	ASP
1	B	2259	ILE
1	B	2260	LEU
1	B	2266	ARG
1	B	2281	MET

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Mol	Chain	Res	Type
1	B	2311	GLU
1	B	2318	THR
1	B	2363	GLU
1	B	2378	ARG
1	B	2380	THR
1	B	2384	THR
1	B	2385	ASN
1	B	2390	THR
1	B	2397	ARG
1	B	2401	HIS
1	B	2430	ARG
1	B	2431	LEU
1	B	2432	MET
1	B	2503	ARG
1	B	2519	LEU
1	B	2530	LYS
1	B	2543	ILE
2	D	13	VAL
2	D	44	GLN
2	D	55	SER
2	D	79	ILE
2	D	84	VAL
2	D	85	ASN
2	D	86	LYS
2	D	90	SER
2	D	91	VAL
2	D	122	GLN
2	D	123	ARG
2	D	127	VAL
2	D	128	ASN
2	D	135	CYS
2	D	159	THR
2	D	160	ASP
2	D	161	HIS
2	D	162	ASN
2	D	166	ILE
2	D	168	GLU
2	D	169	PRO
2	D	170	GLU
2	D	174	THR
2	D	188	VAL
2	D	199	LEU

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Mol	Chain	Res	Type
2	D	215	LYS
2	D	233	THR
2	D	243	THR
2	D	249	THR
2	D	260	ILE
2	D	262	SER
2	D	269	SER
2	D	286	VAL
2	D	287	THR
2	D	301	THR
2	D	312	GLN
1	A	1417	ILE
1	A	1420	ASN
1	A	1423	LEU
1	A	1427	GLU
1	A	1443	LEU
1	A	1445	ILE
1	A	1457	GLU
1	A	1501	TRP
1	A	1509	GLN
1	A	1528	SER
1	A	1541	HIS
1	A	1590	MET
1	A	1598	GLU
1	A	1603	ILE
1	A	1630	VAL
1	A	1643	VAL
1	A	1650	MET
1	A	1675	LEU
1	A	1679	VAL
1	A	1685	LEU
1	A	1701	MET
1	A	1724	MET
1	A	1740	LYS
1	A	1749	ARG
1	A	1780	THR
1	A	1796	MET
1	A	1878	LEU
1	A	1879	MET
1	A	1895	SER
1	A	1896	ARG
1	A	1898	ASN

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Mol	Chain	Res	Type
1	A	1899	ASN
1	A	1908	THR
1	A	1912	ASP
1	A	1916	TRP
1	A	1930	ILE
1	A	1932	ILE
1	A	1956	LEU
1	A	1968	HIS
1	A	1973	ILE
1	A	1984	THR
1	A	1985	THR
1	A	2001	HIS
1	A	2005	LEU
1	A	2011	MET
1	A	2021	ILE
1	A	2044	VAL
1	A	2068	THR
1	A	2072	GLN
1	A	2076	ARG
1	A	2078	LEU
1	A	2093	ASN
1	A	2095	LYS
1	A	2124	GLN
1	A	2136	LEU
1	A	2138	LEU
1	A	2152	ARG
1	A	2164	THR
1	A	2165	SER
1	A	2166	LYS
1	A	2168	ARG
1	A	2173	THR
1	A	2178	ASN
1	A	2181	GLU
1	A	2183	VAL
1	A	2187	LYS
1	A	2189	HIS
1	A	2214	THR
1	A	2223	GLN
1	A	2228	ILE
1	A	2232	THR
1	A	2233	ASN
1	A	2242	HIS

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Mol	Chain	Res	Type
1	A	2244	ASP
1	A	2259	ILE
1	A	2260	LEU
1	A	2266	ARG
1	A	2281	MET
1	A	2311	GLU
1	A	2318	THR
1	A	2363	GLU
1	A	2378	ARG
1	A	2384	THR
1	A	2385	ASN
1	A	2390	THR
1	A	2397	ARG
1	A	2401	HIS
1	A	2408	ARG
1	A	2430	ARG
1	A	2431	LEU
1	A	2432	MET
1	A	2503	ARG
1	A	2519	LEU
1	A	2527	LEU
1	A	2530	LYS
1	A	2543	ILE
2	C	13	VAL
2	C	44	GLN
2	C	79	ILE
2	C	84	VAL
2	C	85	ASN
2	C	86	LYS
2	C	90	SER
2	C	91	VAL
2	C	122	GLN
2	C	123	ARG
2	C	127	VAL
2	C	128	ASN
2	C	135	CYS
2	C	159	THR
2	C	160	ASP
2	C	161	HIS
2	C	162	ASN
2	C	166	ILE
2	C	168	GLU

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Mol	Chain	Res	Type
2	C	169	PRO
2	C	170	GLU
2	C	173	ILE
2	C	174	THR
2	C	188	VAL
2	C	199	LEU
2	C	214	THR
2	C	215	LYS
2	C	233	THR
2	C	243	THR
2	C	249	THR
2	C	260	ILE
2	C	262	SER
2	C	269	SER
2	C	286	VAL
2	C	287	THR
2	C	301	THR
2	C	312	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1425	GLN
1	B	1496	GLN
1	B	1505	ASN
1	B	1525	GLN
1	B	1624	GLN
1	B	1693	HIS
1	B	1695	GLN
1	B	1741	GLN
1	B	1760	ASN
1	B	1782	HIS
1	B	1797	ASN
1	B	1803	HIS
1	B	1807	GLN
1	B	1886	GLN
1	B	1898	ASN
1	B	1901	GLN
1	B	1920	ASN
1	B	1941	GLN
1	B	1958	HIS
1	B	1968	HIS

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Mol	Chain	Res	Type
1	B	1970	GLN
1	B	2028	HIS
1	B	2082	GLN
1	B	2093	ASN
1	B	2167	GLN
1	B	2178	ASN
1	B	2247	HIS
1	B	2262	ASN
1	B	2319	ASN
1	B	2395	ASN
1	B	2401	HIS
1	B	2428	ASN
2	D	30	HIS
2	D	63	GLN
2	D	64	HIS
2	D	94	HIS
2	D	118	ASN
2	D	122	GLN
2	D	137	HIS
2	D	140	GLN
2	D	148	GLN
2	D	153	HIS
2	D	242	GLN
2	D	311	HIS
2	D	312	GLN
1	A	1496	GLN
1	A	1594	HIS
1	A	1624	GLN
1	A	1670	HIS
1	A	1693	HIS
1	A	1695	GLN
1	A	1715	GLN
1	A	1741	GLN
1	A	1760	ASN
1	A	1782	HIS
1	A	1797	ASN
1	A	1803	HIS
1	A	1808	ASN
1	A	1886	GLN
1	A	1898	ASN
1	A	1899	ASN
1	A	1901	GLN

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Mol	Chain	Res	Type
1	A	1920	ASN
1	A	1941	GLN
1	A	1958	HIS
1	A	1968	HIS
1	A	1970	GLN
1	A	2028	HIS
1	A	2082	GLN
1	A	2167	GLN
1	A	2178	ASN
1	A	2262	ASN
1	A	2319	ASN
1	A	2395	ASN
1	A	2401	HIS
1	A	2428	ASN
1	A	2502	ASN
2	C	30	HIS
2	C	63	GLN
2	C	71	ASN
2	C	74	ASN
2	C	85	ASN
2	C	94	HIS
2	C	118	ASN
2	C	137	HIS
2	C	140	GLN
2	C	153	HIS
2	C	311	HIS
2	C	312	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 oligosaccharides in this entry.

5.6 Ligand geometry

2 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
3	X6K	B	2601	-	29,30,30	1.39	3 (10%)	35,43,43	1.61	8 (22%)
3	X6K	A	2601	-	29,30,30	1.46	4 (13%)	35,43,43	1.61	7 (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
3	X6K	B	2601	-	-	0/8/16/16	0/5/5/5
3	X6K	A	2601	-	-	0/8/16/16	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2601	X6K	C05-C09	-5.51	1.37	1.46
3	B	2601	X6K	C05-C09	-5.02	1.38	1.46
3	B	2601	X6K	O07-C08	-2.77	1.34	1.38
3	A	2601	X6K	O07-C08	-2.60	1.34	1.38
3	A	2601	X6K	O07-C06	-2.25	1.35	1.38
3	A	2601	X6K	C06-N01	2.05	1.36	1.32
3	B	2601	X6K	O07-C06	-2.04	1.35	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2601	X6K	C03-C04-C05	-3.67	114.15	120.23
3	B	2601	X6K	O07-C08-C11	3.57	130.04	126.48
3	B	2601	X6K	C08-C11-N18	-3.55	116.19	123.81
3	A	2601	X6K	O07-C08-C11	3.52	129.99	126.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2601	X6K	C08-C11-N18	-3.34	116.65	123.81
3	B	2601	X6K	C14-C13-N12	-3.06	104.14	109.93
3	B	2601	X6K	C03-C04-C05	-3.05	115.17	120.23
3	B	2601	X6K	C11-N18-C19	3.04	123.05	115.92
3	A	2601	X6K	C14-C13-N12	-2.54	105.12	109.93
3	A	2601	X6K	C11-N18-C19	2.44	121.65	115.92
3	A	2601	X6K	N18-C11-N12	2.27	121.05	116.77
3	B	2601	X6K	N18-C19-N10	-2.21	121.49	125.13
3	B	2601	X6K	C16-O15-C14	2.09	116.63	109.88
3	A	2601	X6K	C20-C19-N18	2.06	120.80	117.40
3	B	2601	X6K	C16-C17-N12	-2.06	106.04	109.93

There are no chirality outliers.

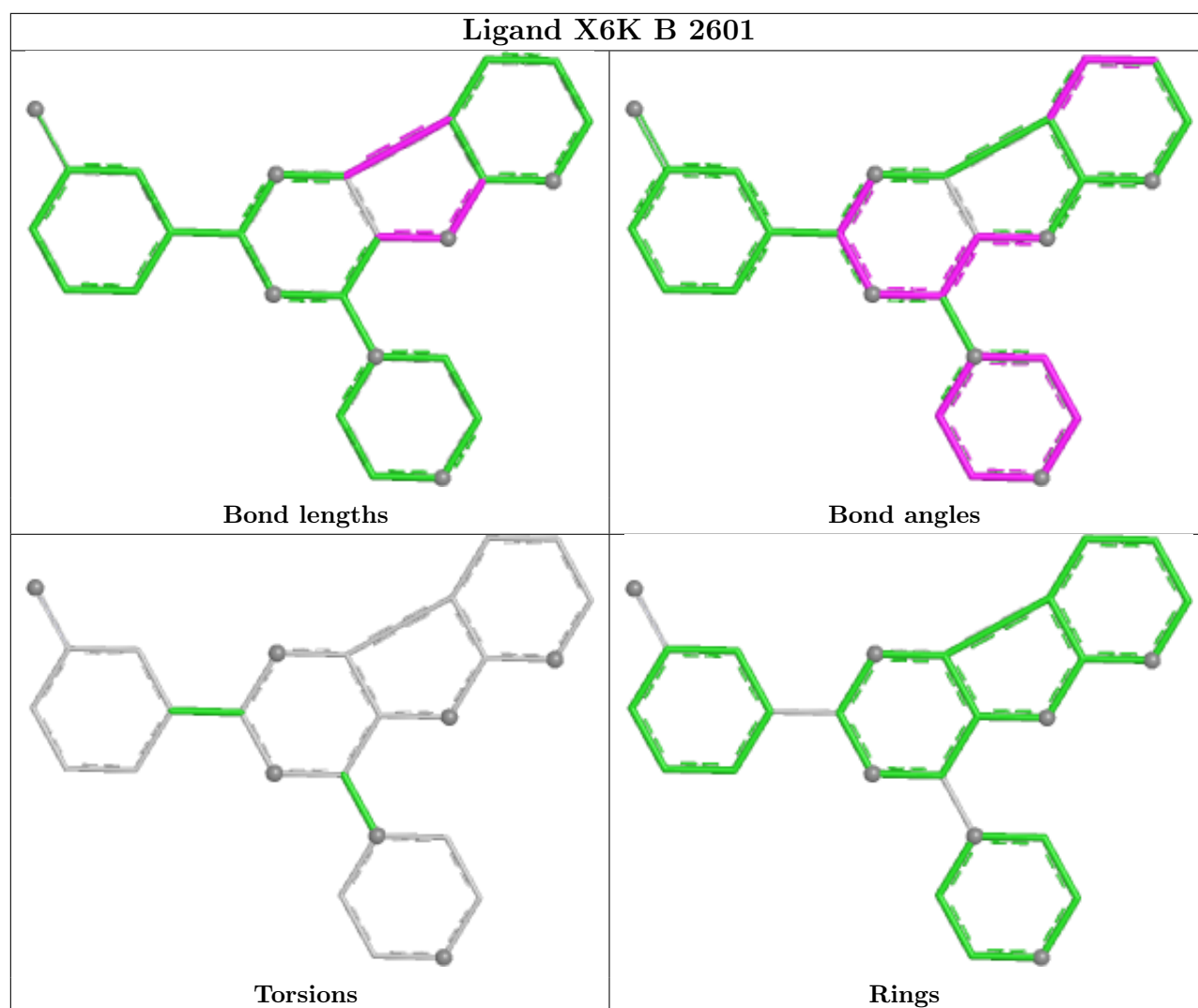
There are no torsion outliers.

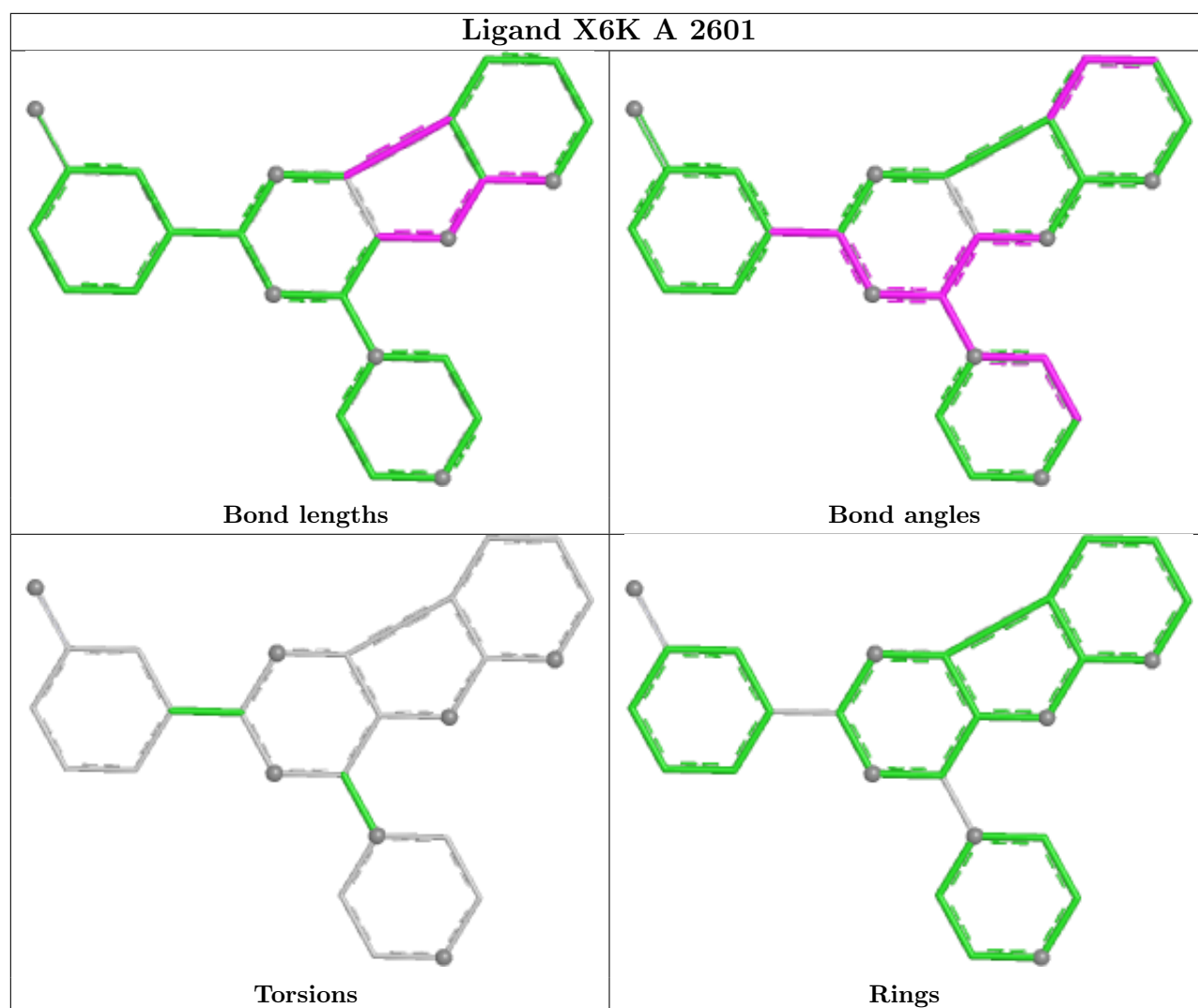
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2601	X6K	1	0
3	A	2601	X6K	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1054/1174 (89%)	0.25	25 (2%) 59 34	26, 57, 146, 187	0
1	B	1058/1174 (90%)	0.09	27 (2%) 57 33	21, 48, 126, 166	0
2	C	317/326 (97%)	0.20	3 (0%) 81 56	30, 58, 102, 126	0
2	D	317/326 (97%)	-0.01	3 (0%) 81 56	23, 40, 83, 138	0
All	All	2746/3000 (91%)	0.16	58 (2%) 63 37	21, 51, 137, 187	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1504	VAL	4.0
1	A	1619	TRP	3.6
1	A	1730	HIS	3.5
1	A	1614	ILE	3.4
1	B	1607	LEU	3.3
1	A	1586	ALA	3.2
2	D	203	ILE	3.2
1	A	1580	GLY	3.1
1	B	1580	GLY	3.1
2	D	207	VAL	3.1
1	A	1457	GLU	3.0
1	A	1504	VAL	2.9
1	A	1585	ARG	2.9
1	A	1596	LEU	2.9
1	A	1603	ILE	2.8
1	A	1584	SER	2.7
1	B	1587	TYR	2.7
2	C	203	ILE	2.7
1	B	1453	LEU	2.7
1	B	1582	SER	2.7
1	B	1586	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1649	ASP	2.6
1	A	1587	TYR	2.6
1	B	1443	LEU	2.5
1	A	1599	LEU	2.5
1	A	1443	LEU	2.5
1	A	1583	TYR	2.5
1	B	1451	GLU	2.5
1	A	1579	ALA	2.5
1	B	2044	VAL	2.5
1	B	1469	THR	2.5
1	B	1584	SER	2.4
1	B	1585	ARG	2.4
1	B	1452	LYS	2.4
1	B	2436	THR	2.3
2	C	207	VAL	2.3
1	B	2434	THR	2.3
2	D	263	GLY	2.3
1	A	1595	MET	2.3
1	B	2433	ASP	2.3
1	A	1532	TYR	2.2
1	B	1581	GLU	2.2
1	B	2492	ALA	2.2
1	A	1546	TYR	2.2
1	A	2094	VAL	2.2
1	B	1610	GLU	2.2
1	B	1579	ALA	2.1
1	A	1602	VAL	2.1
1	B	1583	TYR	2.1
1	B	2429	TRP	2.1
1	A	1604	GLN	2.1
1	A	1575	LEU	2.1
2	C	263	GLY	2.1
1	B	1449	TRP	2.1
1	B	1445	ILE	2.1
1	A	1453	LEU	2.0
1	A	1456	TRP	2.0
1	B	1510	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

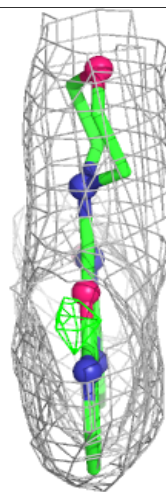
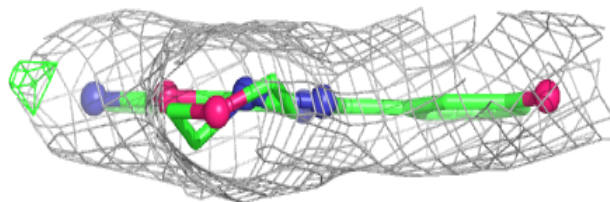
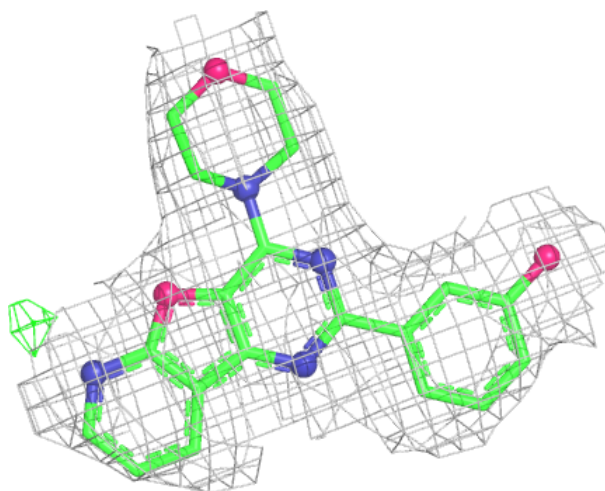
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

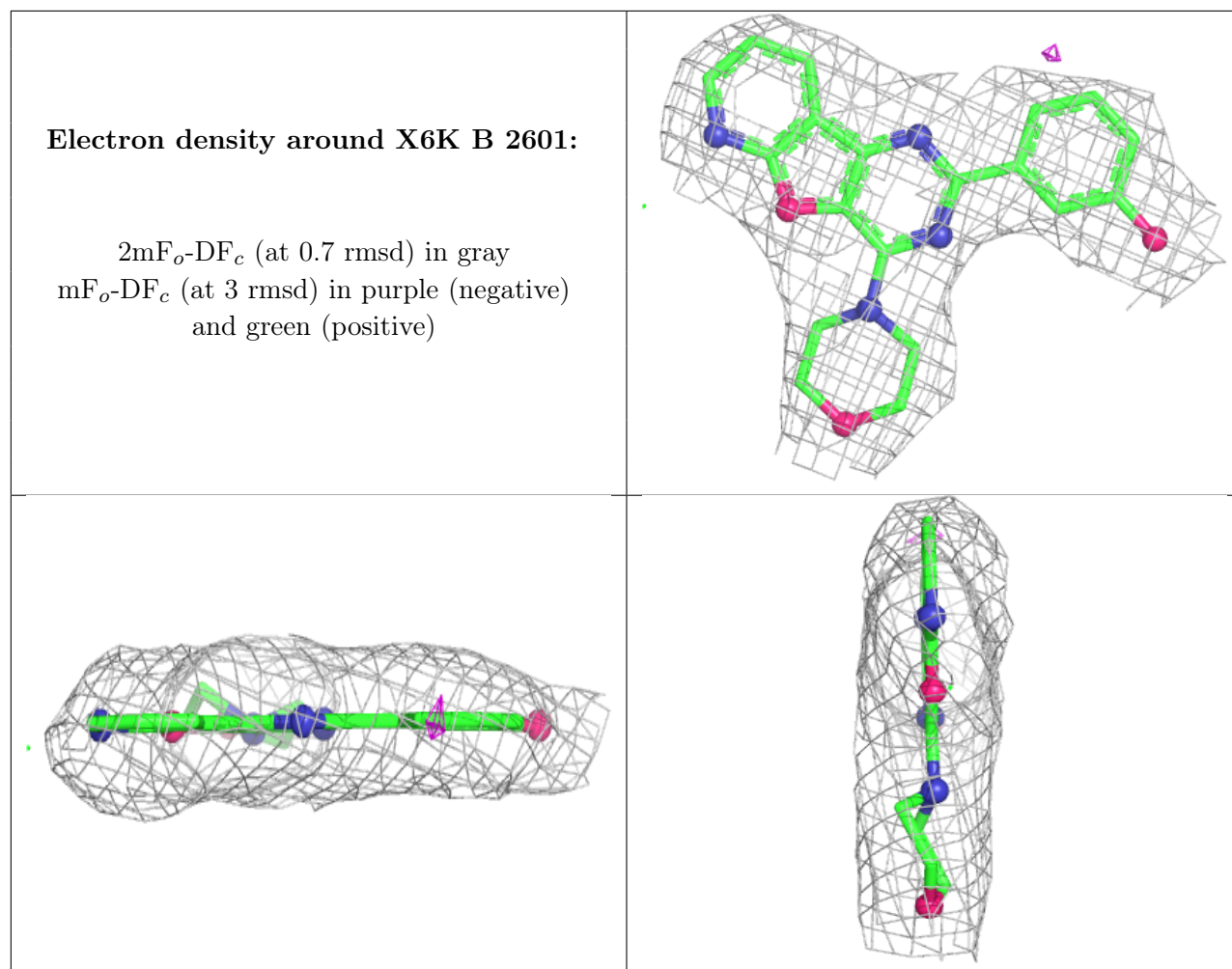
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	X6K	A	2601	26/26	0.94	0.10	32,35,35,36	0
3	X6K	B	2601	26/26	0.96	0.09	24,25,25,25	0

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 X6K A 2601:

$2mF_o-DF_c$ (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.