



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:14 PM UTC

PDB ID : 4JT5 / pdb_00004jt5
Title : mTORdeltaN-mLST8-pp242 complex
Authors : Pavletich, N.P.; Yang, H.
Deposited on : 2013-03-22
Resolution : 3.45 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

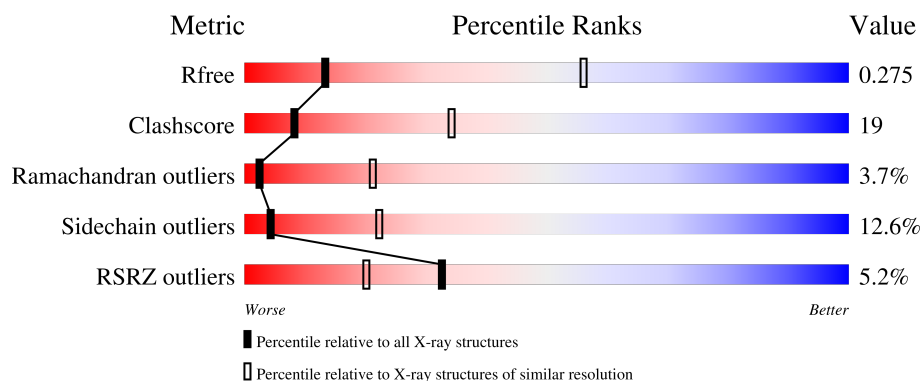
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	7% 54% 30% 6% • 10%
1	B	1174	3% 54% 30% 6% • 10%
2	C	326	4% 46% 40% 9% • •
2	D	326	4% 45% 41% 10% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22143 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 Serine/threonine-protein kinase 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			

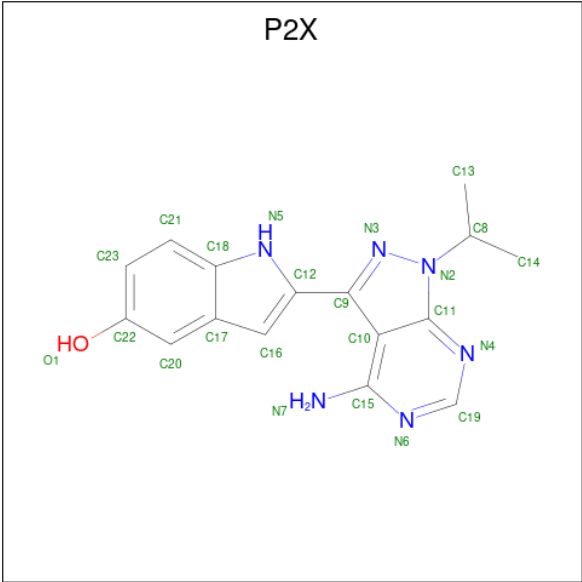
- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

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			

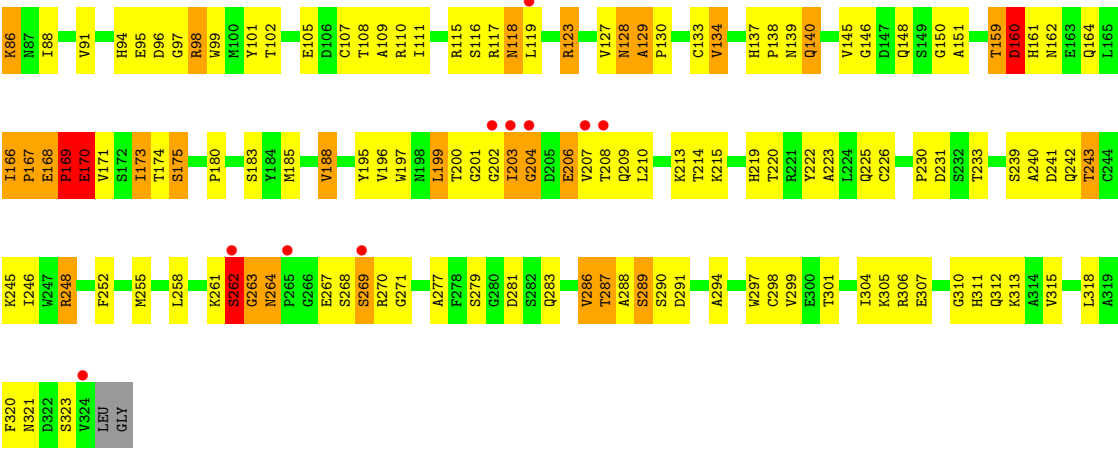
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	324	VAL	-	expression tag	UNP Q9BVC4
D	325	LEU	-	expression tag	UNP Q9BVC4
D	326	GLY	-	expression tag	UNP Q9BVC4
C	324	VAL	-	expression tag	UNP Q9BVC4
C	325	LEU	-	expression tag	UNP Q9BVC4
C	326	GLY	-	expression tag	UNP Q9BVC4

- Molecule 3 is 2-[4-amino-1-(propan-2-yl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-1H-indol-5-ol (CCD ID: P2X) (formula: C₁₆H₁₆N₆O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			23	16	6	1		
3	A	1	Total	C	N	O	0	0
			23	16	6	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	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 – 3.45 39.67 – 3.45	Depositor EDS
% Data completeness (in resolution range)	85.8 (39.67-3.45) 85.9 (39.67-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.233 , 0.271 0.235 , 0.275	Depositor DCC
R_{free} test set	1869 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.8	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	0.90	EDS
Total number of atoms	22143	wwPDB-VP
Average B, all atoms (Å ²)	68.0	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 41.10 % 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 2.4826e-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: P2X

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	0.45	0/8772	0.95	12/11872 (0.1%)
1	B	0.46	0/8805	0.96	15/11920 (0.1%)
2	C	0.52	0/2514	0.94	7/3426 (0.2%)
2	D	0.55	0/2514	0.97	5/3426 (0.1%)
All	All	0.48	0/22605	0.96	39/30644 (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	2
1	B	0	1
2	C	0	1
2	D	0	1
All	All	0	5

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1915	HIS	N-CA-C	11.76	126.08	109.15
1	B	1915	HIS	N-CA-C	11.40	125.57	109.15
1	B	1443	LEU	N-CA-C	-8.22	102.81	112.92
1	A	1443	LEU	N-CA-C	-7.35	103.88	112.92
1	B	1608	VAL	N-CA-C	7.17	114.08	107.56
1	B	2157	ALA	CA-C-N	7.00	126.63	119.56
1	B	2157	ALA	C-N-CA	7.00	126.63	119.56
1	B	1913	TYR	N-CA-C	6.75	120.80	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1913	TYR	N-CA-C	6.66	120.68	111.55
2	D	170	GLU	N-CA-C	-6.50	102.00	111.30
1	B	2422	VAL	N-CA-C	-6.43	104.58	110.82
1	A	2157	ALA	CA-C-N	6.36	125.98	119.56
1	A	2157	ALA	C-N-CA	6.36	125.98	119.56
2	D	321	ASN	N-CA-C	6.20	119.25	108.76
2	C	321	ASN	N-CA-C	6.00	118.91	108.76
1	A	1473	ASP	CA-C-N	5.99	127.32	119.84
1	A	1473	ASP	C-N-CA	5.99	127.32	119.84
1	B	1473	ASP	CA-C-N	5.96	127.29	119.84
1	B	1473	ASP	C-N-CA	5.96	127.29	119.84
1	A	1502	THR	N-CA-C	-5.86	104.58	110.97
1	B	1502	THR	N-CA-C	-5.80	104.65	110.97
1	A	2422	VAL	N-CA-C	-5.75	105.24	110.82
2	C	170	GLU	N-CA-C	-5.52	103.31	111.81
2	D	87	ASN	N-CA-C	5.48	117.61	110.43
2	C	74	ASN	N-CA-C	5.45	121.86	109.81
2	D	74	ASN	N-CA-C	5.42	121.80	109.81
1	A	1969	PRO	N-CA-C	-5.36	103.38	111.41
1	B	1442	GLU	N-CA-C	5.24	120.82	113.02
1	A	2307	SER	CA-C-N	5.21	124.90	119.64
1	A	2307	SER	C-N-CA	5.21	124.90	119.64
2	C	206	GLU	N-CA-C	5.20	117.57	110.55
1	B	1968	HIS	CA-C-N	-5.17	114.92	120.03
1	B	1968	HIS	C-N-CA	-5.17	114.92	120.03
2	C	169	PRO	N-CA-C	5.16	123.11	112.47
1	B	2307	SER	CA-C-N	5.13	124.82	119.64
1	B	2307	SER	C-N-CA	5.13	124.82	119.64
2	D	239	SER	N-CA-C	5.02	116.44	108.96
2	C	76	ASN	CA-C-N	-5.00	114.43	119.83
2	C	76	ASN	C-N-CA	-5.00	114.43	119.83

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1442	GLU	Peptide
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	295	0
1	B	8608	0	8593	289	0
2	C	2456	0	2341	135	0
2	D	2456	0	2341	138	0
3	A	23	0	16	3	0
3	B	23	0	16	4	0
All	All	22143	0	21866	847	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (847) 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:76:ASN:HB3	2:C:77:PRO:HD2	1.35	1.09
1:A:1418:SER:HB2	1:A:1581:GLU:HG2	1.35	1.05
2:D:76:ASN:HB3	2:D:77:PRO:HD2	1.36	1.04
2:D:170:GLU:HA	2:D:170:GLU:OE2	1.61	0.98
2:C:170:GLU:OE2	2:C:170:GLU:HA	1.62	0.96
1:B:2380:THR:HG22	1:B:2383:LEU:HG	1.50	0.94
1:A:2380:THR:HG22	1:A:2383:LEU:HG	1.50	0.94
2:D:69:ASP:HB2	2:D:78:ILE:HD11	1.48	0.93
2:C:95:GLU:HB2	2:C:140:GLN:NE2	1.85	0.91
2:D:95:GLU:HB2	2:D:140:GLN:NE2	1.86	0.90
2:D:117:ARG:O	2:D:118:ASN:HB2	1.73	0.89
2:C:231:ASP:HB3	2:C:233:THR:OG1	1.74	0.87
2:C:69:ASP:HB2	2:C:78:ILE:HD11	1.54	0.86
2:C:95:GLU:HB2	2:C:140:GLN:HE22	1.37	0.86
2:C:117:ARG:O	2:C:118:ASN:HB2	1.74	0.86
1:B:1623:LEU:HG	1:B:1633:TRP:CH2	2.11	0.85
2:C:76:ASN:HB3	2:C:77:PRO:CD	2.06	0.85
1:A:2064:THR:HG22	1:A:2128:PRO:HD3	1.58	0.84
1:A:1969:PRO:O	1:A:1970:GLN:HB2	1.77	0.83
2:D:231:ASP:HB3	2:D:233:THR:OG1	1.78	0.83
2:D:95:GLU:HB2	2:D:140:GLN:HE22	1.41	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2192:LEU:HD12	1:A:2235:GLY:HA3	1.61	0.82
1:A:2415:MET:HE1	1:A:2501:ILE:HG23	1.61	0.82
2:D:76:ASN:HB3	2:D:77:PRO:CD	2.08	0.82
2:D:146:GLY:HA3	2:D:173:ILE:HD11	1.61	0.82
1:A:2390:THR:HG23	1:A:2390:THR:O	1.80	0.81
1:B:2192:LEU:HD12	1:B:2235:GLY:HA3	1.61	0.80
2:C:146:GLY:HA3	2:C:173:ILE:HD11	1.61	0.80
2:C:63:GLN:HE21	2:C:86:LYS:H	1.27	0.80
1:B:1958:HIS:CE1	1:B:1990:ALA:HB1	2.17	0.80
1:A:1422:LYS:HD3	1:A:1580:GLY:HA3	1.61	0.80
1:B:1969:PRO:O	1:B:1970:GLN:HB2	1.82	0.79
3:B:2601:P2X:H15	3:B:2601:P2X:C16	1.96	0.79
1:A:1908:THR:O	1:A:1912:ASP:HB2	1.83	0.79
1:A:2397:ARG:NH2	1:A:2526:GLU:OE1	2.15	0.78
1:A:2387:MET:CE	1:A:2396:TYR:HB2	2.13	0.78
1:B:2387:MET:CE	1:B:2396:TYR:HB2	2.14	0.78
2:D:63:GLN:HE21	2:D:86:LYS:H	1.29	0.77
1:A:2387:MET:HE3	1:A:2396:TYR:HB2	1.68	0.76
1:B:2390:THR:HG23	1:B:2390:THR:O	1.84	0.76
1:A:1704:MET:HG2	1:A:1713:ALA:HB2	1.66	0.76
1:A:1943:ILE:HA	1:A:1946:ILE:HG13	1.67	0.76
1:B:2415:MET:HE1	1:B:2501:ILE:HG23	1.67	0.76
1:A:2421:PHE:HA	1:A:2424:ASP:HB2	1.66	0.76
1:B:2387:MET:HE3	1:B:2396:TYR:HB2	1.69	0.75
1:A:1968:HIS:HB3	1:A:2144:TYR:OH	1.87	0.75
2:D:8:VAL:HG21	2:D:36:ARG:HD3	1.67	0.75
2:C:8:VAL:HG21	2:C:36:ARG:HD3	1.66	0.74
1:B:2397:ARG:NH2	1:B:2526:GLU:OE1	2.19	0.74
1:B:1422:LYS:HE2	1:B:1581:GLU:HG3	1.68	0.74
2:C:150:GLY:HA3	2:C:169:PRO:HB3	1.70	0.74
1:B:2421:PHE:HA	1:B:2424:ASP:HB2	1.68	0.74
3:B:2601:P2X:H15	3:B:2601:P2X:H5	1.52	0.73
1:A:1958:HIS:CE1	1:A:1990:ALA:HB1	2.23	0.73
2:D:167:PRO:HD2	2:D:169:PRO:HG2	1.71	0.73
2:D:150:GLY:HA3	2:D:169:PRO:HB3	1.70	0.73
1:B:2064:THR:HG22	1:B:2128:PRO:HD3	1.70	0.72
1:A:2298:ASP:HB2	1:A:2382:MET:CE	2.19	0.72
1:B:1701:MET:HE1	1:B:1717:MET:N	2.04	0.72
1:A:2281:MET:HE1	2:C:222:TYR:CD2	2.24	0.72
1:B:1943:ILE:HA	1:B:1946:ILE:HG13	1.72	0.72
1:A:2022:LEU:HD21	1:A:2126:VAL:HG13	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1958:HIS:HE1	1:B:1990:ALA:HB1	1.53	0.71
1:B:1908:THR:O	1:B:1912:ASP:HB2	1.91	0.70
1:B:1941:GLN:HE22	1:B:2200:GLN:HE22	1.37	0.70
1:B:1704:MET:HG2	1:B:1713:ALA:HB2	1.73	0.70
1:B:2298:ASP:HB2	1:B:2382:MET:CE	2.21	0.70
2:C:98:ARG:HD2	2:C:115:ARG:HB2	1.73	0.70
1:A:1670:HIS:HE1	1:A:1681:PRO:HB3	1.56	0.70
2:D:17:THR:HB	2:D:311:HIS:HE1	1.56	0.70
1:A:1701:MET:HE1	1:A:1717:MET:N	2.07	0.70
1:A:1493:LEU:HD23	1:A:1519:ALA:HB2	1.74	0.69
1:A:1529:MET:HE3	1:A:1550:LEU:HG	1.73	0.69
2:C:167:PRO:HD2	2:C:169:PRO:HG2	1.74	0.69
2:D:137:HIS:CD2	2:D:138:PRO:HD2	2.27	0.69
1:A:1415:SER:O	1:A:1419:ILE:HG22	1.93	0.69
1:B:2298:ASP:HB2	1:B:2382:MET:HE2	1.73	0.69
2:D:98:ARG:HD2	2:D:115:ARG:HB2	1.74	0.69
2:D:123:ARG:NH2	2:D:160:ASP:OD1	2.26	0.69
1:A:1732:ILE:HD13	1:A:1740:LYS:HB2	1.76	0.68
2:D:241:ASP:OD2	2:D:243:THR:HB	1.94	0.68
1:B:1415:SER:O	1:B:1419:ILE:HG22	1.94	0.68
2:C:231:ASP:CB	2:C:233:THR:OG1	2.41	0.67
1:B:2281:MET:HE1	2:D:222:TYR:CD2	2.30	0.67
1:A:1920:ASN:O	1:A:1924:VAL:HG23	1.94	0.67
1:B:1901:GLN:HG3	1:B:2413:SER:HA	1.76	0.67
1:B:1913:TYR:O	1:B:1915:HIS:HA	1.93	0.67
1:A:1508:THR:O	1:A:1512:MET:HB2	1.94	0.67
1:A:1759:LEU:HD11	1:A:1796:MET:HE3	1.77	0.67
1:B:1920:ASN:O	1:B:1924:VAL:HG23	1.93	0.67
1:B:2093:ASN:O	1:B:2094:VAL:HB	1.95	0.67
2:D:17:THR:HB	2:D:311:HIS:CE1	2.30	0.67
1:B:2249:LEU:HD13	1:B:2346:LEU:HD12	1.77	0.67
1:B:1433:LEU:HD23	1:B:1453:LEU:HD23	1.76	0.67
1:B:1508:THR:O	1:B:1512:MET:HB2	1.93	0.67
1:A:1691:THR:HG23	1:A:1724:MET:HE1	1.77	0.67
1:A:2160:LEU:HD22	1:A:2172:LEU:HA	1.77	0.67
1:B:2278:LEU:HD23	2:D:44:GLN:HG2	1.75	0.66
1:A:2298:ASP:HB2	1:A:2382:MET:HE2	1.75	0.66
1:B:2022:LEU:HD21	1:B:2126:VAL:HG13	1.78	0.66
1:B:1680:ASP:O	1:B:1682:SER:N	2.28	0.66
1:B:2514:SER:OG	1:B:2517:ASP:HB2	1.96	0.66
1:B:2363:GLU:OE2	1:B:2503:ARG:HD2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:306:ARG:HG2	2:D:307:GLU:H	1.60	0.66
1:A:1759:LEU:HG	1:A:1772:VAL:HG11	1.77	0.66
1:B:1393:TYR:CZ	1:B:1422:LYS:HD2	2.30	0.66
2:D:69:ASP:CB	2:D:78:ILE:HD11	2.24	0.66
1:A:2278:LEU:HD23	2:C:44:GLN:HG2	1.76	0.65
2:D:108:THR:OG1	2:D:110:ARG:NH1	2.30	0.65
1:A:1393:TYR:CZ	1:A:1422:LYS:HD2	2.32	0.65
1:A:2093:ASN:O	1:A:2094:VAL:HB	1.96	0.65
1:A:1874:SER:O	1:A:1878:LEU:HB2	1.96	0.65
1:A:1680:ASP:O	1:A:1682:SER:N	2.29	0.65
1:B:1691:THR:HG23	1:B:1724:MET:HE1	1.79	0.65
1:B:1968:HIS:HB3	1:B:2144:TYR:OH	1.97	0.64
2:D:231:ASP:CB	2:D:233:THR:OG1	2.45	0.64
1:A:1969:PRO:O	1:A:1970:GLN:CB	2.45	0.64
1:A:2249:LEU:HD13	1:A:2346:LEU:HD12	1.78	0.64
2:C:306:ARG:HG2	2:C:307:GLU:H	1.62	0.64
1:B:2389:VAL:O	1:B:2390:THR:HG22	1.97	0.64
1:B:1907:LEU:HD11	1:B:1938:VAL:CG1	2.28	0.64
2:D:55:SER:O	2:D:56:MET:HG2	1.97	0.64
1:A:1734:THR:O	1:A:1736:ASP:N	2.25	0.64
2:C:279:SER:HA	2:C:320:PHE:HE2	1.62	0.64
1:B:2167:GLN:O	1:B:2168:ARG:C	2.40	0.64
3:A:2601:P2X:H5	3:A:2601:P2X:H15	1.63	0.64
1:B:2167:GLN:HG2	1:B:2189:HIS:HD2	1.62	0.64
1:A:2130:LEU:HD22	1:A:2156:ILE:CD1	2.28	0.64
2:C:137:HIS:CD2	2:C:138:PRO:HD2	2.32	0.64
1:B:1422:LYS:HE2	1:B:1581:GLU:CG	2.28	0.63
2:C:17:THR:HB	2:C:311:HIS:HE1	1.63	0.63
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.31	0.63
1:A:1913:TYR:O	1:A:1915:HIS:HA	1.97	0.63
2:C:166:ILE:HG13	2:C:166:ILE:O	1.97	0.63
1:A:1680:ASP:C	1:A:1682:SER:N	2.56	0.63
2:C:94:HIS:CE1	2:C:96:ASP:HB2	2.34	0.63
1:B:1915:HIS:HE1	1:B:1919:VAL:HG11	1.63	0.63
1:A:1583:TYR:C	1:A:1585:ARG:H	2.06	0.63
2:D:279:SER:HA	2:D:320:PHE:HE2	1.63	0.63
1:A:1783:ASP:O	1:A:1785:SER:N	2.32	0.63
1:A:2363:GLU:OE2	1:A:2503:ARG:HD2	1.99	0.63
1:A:1958:HIS:HE1	1:A:1990:ALA:HB1	1.62	0.62
1:A:2194:GLN:HG2	1:A:2427:LEU:HD22	1.79	0.62
2:D:134:VAL:HG22	2:D:145:VAL:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:GLU:HA	2:C:130:PRO:HB3	1.81	0.62
1:B:2421:PHE:HD1	1:B:2430:ARG:NH2	1.97	0.62
1:A:2011:MET:HE2	1:A:2129:LYS:HB3	1.82	0.62
1:B:1969:PRO:O	1:B:1970:GLN:CB	2.47	0.62
1:A:2389:VAL:O	1:A:2390:THR:HG22	1.99	0.62
1:A:2503:ARG:HH11	1:A:2507:LYS:HE3	1.64	0.62
1:A:2167:GLN:HG2	1:A:2189:HIS:HD2	1.63	0.62
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.32	0.62
1:B:1646:PRO:HG3	1:B:1675:LEU:HD21	1.82	0.62
1:B:2418:LEU:HD23	1:B:2421:PHE:CZ	2.35	0.62
1:A:2390:THR:O	1:A:2390:THR:CG2	2.47	0.62
1:B:2160:LEU:HD22	1:B:2172:LEU:HA	1.82	0.62
2:C:17:THR:HB	2:C:311:HIS:CE1	2.35	0.62
2:C:108:THR:OG1	2:C:110:ARG:NH1	2.33	0.61
2:C:123:ARG:NH2	2:C:160:ASP:OD1	2.33	0.61
2:C:241:ASP:OD2	2:C:243:THR:HB	1.99	0.61
1:B:2167:GLN:HG2	1:B:2189:HIS:CD2	2.35	0.61
1:B:2515:HIS:N	1:B:2515:HIS:ND1	2.47	0.61
1:B:1680:ASP:C	1:B:1682:SER:N	2.57	0.61
1:B:1878:LEU:HD21	1:B:1918:ASP:HB2	1.81	0.61
1:B:2278:LEU:CD2	2:D:44:GLN:HG2	2.29	0.61
1:B:2194:GLN:HG2	1:B:2427:LEU:HD22	1.82	0.61
2:C:134:VAL:HG22	2:C:145:VAL:HG22	1.81	0.61
2:D:94:HIS:CE1	2:D:96:ASP:HB2	2.36	0.61
1:A:2167:GLN:HG2	1:A:2189:HIS:CD2	2.35	0.61
1:A:2278:LEU:CD2	2:C:44:GLN:HG2	2.30	0.61
1:A:2421:PHE:HD1	1:A:2430:ARG:NH2	1.97	0.61
2:C:69:ASP:CB	2:C:78:ILE:HD11	2.28	0.61
1:B:1759:LEU:HG	1:B:1772:VAL:HG11	1.82	0.61
1:B:2251:ARG:NH1	1:B:2252:ASP:OD1	2.34	0.61
1:B:2392:LEU:O	1:B:2397:ARG:HB2	2.01	0.61
1:A:2392:LEU:O	1:A:2397:ARG:HB2	2.01	0.61
1:A:1428:ALA:HB2	1:A:2395:ASN:ND2	2.16	0.60
1:A:1968:HIS:HB3	1:A:2144:TYR:HH	1.66	0.60
1:B:1583:TYR:C	1:B:1585:ARG:H	2.08	0.60
1:B:1874:SER:O	1:B:1878:LEU:HB2	2.01	0.60
1:A:2167:GLN:O	1:A:2168:ARG:C	2.43	0.60
1:B:2281:MET:HA	1:B:2281:MET:CE	2.31	0.60
1:B:1420:ASN:HB3	1:B:1429:ALA:HB2	1.83	0.60
1:B:1686:ASP:O	1:A:2266:ARG:HG3	2.02	0.60
1:B:1759:LEU:HD11	1:B:1796:MET:HE3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1701:MET:HE1	1:A:1716:HIS:C	2.27	0.60
2:C:248:ARG:HD2	2:C:255:MET:HB2	1.84	0.60
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.34	0.60
1:B:1783:ASP:O	1:B:1785:SER:N	2.35	0.59
1:A:2514:SER:OG	1:A:2517:ASP:HB2	2.02	0.59
2:D:128:ASN:H	2:D:128:ASN:ND2	1.99	0.59
1:A:2344:LEU:HD13	1:A:2353:ILE:HD11	1.83	0.59
1:B:2380:THR:HG23	1:B:2549:TRP:O	2.02	0.59
1:A:2415:MET:CE	1:A:2501:ILE:HG23	2.31	0.59
2:D:21:ASP:HB3	2:D:313:LYS:H	1.67	0.59
1:A:1878:LEU:HD21	1:A:1918:ASP:HB2	1.84	0.59
1:B:1785:SER:O	1:B:1786:TRP:CB	2.48	0.59
2:D:133:CYS:SG	2:D:175:SER:HA	2.42	0.59
1:A:1915:HIS:HE1	1:A:1919:VAL:HG11	1.67	0.59
3:B:2601:P2X:H5	3:B:2601:P2X:N7	2.17	0.59
2:C:271:GLY:HA2	2:C:290:SER:HB2	1.84	0.59
1:A:1890:ARG:O	1:A:1894:LEU:HG	2.01	0.59
1:A:1703:ASN:O	1:A:1707:SER:HB2	2.03	0.59
1:A:2515:HIS:ND1	1:A:2515:HIS:N	2.49	0.59
1:B:1422:LYS:CE	1:B:1581:GLU:HG3	2.33	0.58
2:D:105:GLU:HA	2:D:130:PRO:HB3	1.85	0.58
1:B:1930:ILE:HD11	1:B:1934:THR:HG21	1.85	0.58
1:B:2011:MET:HE2	1:B:2129:LYS:HB3	1.85	0.58
1:A:2254:ARG:HD3	1:A:2298:ASP:OD2	2.04	0.58
2:D:166:ILE:HG13	2:D:166:ILE:O	2.02	0.58
2:C:21:ASP:HB3	2:C:313:LYS:H	1.68	0.58
1:B:1907:LEU:HD11	1:B:1938:VAL:HG11	1.84	0.58
1:A:1785:SER:O	1:A:1786:TRP:CB	2.49	0.58
2:D:248:ARG:HD2	2:D:255:MET:HB2	1.86	0.58
1:A:1710:LYS:NZ	1:A:1760:ASN:HD21	2.01	0.58
1:A:1916:TRP:CD1	1:A:1916:TRP:H	2.20	0.58
1:A:2387:MET:HE1	1:A:2396:TYR:HB2	1.85	0.58
1:B:2154:GLN:HE21	1:B:2155:SER:HB3	1.68	0.58
2:C:55:SER:O	2:C:56:MET:HG2	2.03	0.58
1:B:2387:MET:HE1	1:B:2396:TYR:HB2	1.85	0.58
1:B:1701:MET:HE1	1:B:1716:HIS:C	2.29	0.58
1:B:2503:ARG:HH11	1:B:2507:LYS:HE3	1.69	0.58
1:A:1422:LYS:C	1:A:1424:GLN:H	2.12	0.58
2:C:199:LEU:HD22	2:C:210:LEU:HD22	1.85	0.58
1:A:1907:LEU:HD11	1:A:1938:VAL:CG1	2.34	0.57
1:B:1428:ALA:HB2	1:B:2395:ASN:ND2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2037:LEU:HD22	1:A:2043:ASN:HD22	1.69	0.57
2:C:133:CYS:SG	2:C:175:SER:HA	2.43	0.57
1:B:2390:THR:O	1:B:2390:THR:CG2	2.52	0.57
1:A:2240:VAL:HG23	3:A:2601:P2X:N6	2.20	0.57
1:A:2503:ARG:HH11	1:A:2507:LYS:CE	2.17	0.57
2:C:86:LYS:HE2	2:C:105:GLU:HB3	1.87	0.57
1:A:2521:VAL:HB	1:A:2522:PRO:HD3	1.86	0.57
1:B:1493:LEU:HD23	1:B:1519:ALA:HB2	1.86	0.57
2:D:199:LEU:HD22	2:D:210:LEU:HD22	1.86	0.57
2:C:128:ASN:ND2	2:C:128:ASN:H	2.01	0.57
1:B:1422:LYS:C	1:B:1424:GLN:H	2.13	0.57
3:A:2601:P2X:H15	3:A:2601:P2X:C16	2.17	0.57
1:A:1475:GLU:HA	1:A:1478:LEU:HD12	1.86	0.57
1:A:2251:ARG:HA	1:A:2261:LEU:CD1	2.35	0.57
1:B:1631:GLU:CD	1:B:1631:GLU:H	2.13	0.56
1:A:2408:ARG:HG2	1:A:2508:LEU:O	2.05	0.56
1:B:2130:LEU:HD22	1:B:2156:ILE:CD1	2.34	0.56
1:B:2281:MET:HE1	2:D:222:TYR:CG	2.39	0.56
1:A:1999:CYS:C	1:A:2001:HIS:H	2.12	0.56
1:A:2428:ASN:HB3	1:A:2493:LEU:HD13	1.86	0.56
1:B:1888:PHE:O	1:B:1892:ILE:HG13	2.05	0.56
1:B:2254:ARG:HD3	1:B:2298:ASP:OD2	2.06	0.56
1:A:1414:GLU:O	1:A:1417:ILE:HG13	2.05	0.56
1:A:1646:PRO:HG3	1:A:1675:LEU:HD21	1.88	0.56
2:D:86:LYS:HE2	2:D:105:GLU:HB3	1.88	0.56
1:A:2154:GLN:HE21	1:A:2155:SER:HB3	1.70	0.56
2:C:96:ASP:O	2:C:98:ARG:N	2.37	0.56
2:D:60:ALA:HB1	2:D:88:ILE:HG22	1.86	0.56
1:A:1888:PHE:O	1:A:1892:ILE:HG13	2.05	0.56
1:B:2503:ARG:HH11	1:B:2507:LYS:CE	2.19	0.56
2:D:107:CYS:HB3	2:D:127:VAL:O	2.05	0.56
1:A:1457:GLU:HG2	1:A:1487:LEU:HD21	1.88	0.56
1:A:1595:MET:HG2	1:A:1639:VAL:HG21	1.87	0.56
1:A:2152:ARG:HG2	1:A:2177:SER:OG	2.06	0.56
2:C:279:SER:HA	2:C:320:PHE:CE2	2.41	0.56
1:B:1457:GLU:HG2	1:B:1487:LEU:HD21	1.88	0.56
2:D:188:VAL:HG13	2:D:223:ALA:HB3	1.87	0.56
1:A:1631:GLU:CD	1:A:1631:GLU:H	2.14	0.56
1:B:1802:LEU:HD22	1:B:1806:HIS:NE2	2.20	0.56
1:A:1420:ASN:HB3	1:A:1429:ALA:HB2	1.88	0.55
1:B:2307:SER:CB	1:B:2313:TRP:HB2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2329:MET:HB3	1:B:2404:MET:HE2	1.87	0.55
1:A:1941:GLN:HE22	1:A:2200:GLN:HE22	1.53	0.55
1:B:2251:ARG:HA	1:B:2261:LEU:CD1	2.36	0.55
1:B:1703:ASN:O	1:B:1707:SER:HB2	2.05	0.55
2:D:268:SER:O	2:D:269:SER:HB3	2.07	0.55
1:A:1901:GLN:HG3	1:A:2413:SER:HA	1.89	0.55
2:C:36:ARG:NH2	2:C:69:ASP:O	2.39	0.55
1:B:1475:GLU:HA	1:B:1478:LEU:HD12	1.88	0.55
1:B:1916:TRP:H	1:B:1916:TRP:CD1	2.23	0.55
2:C:15:LEU:HD11	2:C:286:VAL:HG11	1.88	0.55
1:A:1999:CYS:C	1:A:2001:HIS:N	2.64	0.55
2:C:196:VAL:HG11	2:C:252:PHE:CZ	2.42	0.55
2:C:268:SER:O	2:C:269:SER:HB3	2.07	0.55
1:A:1951:PRO:HB2	1:A:1955:ARG:HH21	1.72	0.55
2:C:286:VAL:HB	2:C:318:LEU:HD13	1.89	0.55
1:B:1970:GLN:NE2	1:B:2139:ALA:H	2.05	0.54
2:D:196:VAL:HG11	2:D:252:PHE:CZ	2.42	0.54
2:D:279:SER:HA	2:D:320:PHE:CE2	2.43	0.54
1:B:2344:LEU:HD13	1:B:2353:ILE:HD11	1.89	0.54
1:A:1552:LEU:HD22	1:A:1602:VAL:HG12	1.89	0.54
2:C:65:ILE:HD11	2:C:88:ILE:HD13	1.89	0.54
1:B:2415:MET:CE	1:B:2501:ILE:HG23	2.36	0.54
1:A:1930:ILE:HD11	1:A:1934:THR:HG21	1.89	0.54
1:B:1890:ARG:O	1:B:1894:LEU:HG	2.07	0.54
2:D:96:ASP:O	2:D:98:ARG:N	2.35	0.54
2:D:65:ILE:HD11	2:D:88:ILE:HD13	1.89	0.54
2:C:246:ILE:HD13	2:C:299:VAL:HG13	1.88	0.54
1:B:1781:GLU:OE1	1:B:1781:GLU:HA	2.07	0.53
2:D:246:ILE:HD13	2:D:299:VAL:HG13	1.90	0.53
1:A:2380:THR:HG23	1:A:2549:TRP:O	2.07	0.53
1:B:1414:GLU:O	1:B:1417:ILE:HG13	2.07	0.53
1:B:1766:GLU:OE1	1:B:1766:GLU:N	2.42	0.53
1:B:1773:LEU:HG	1:B:1796:MET:HG3	1.91	0.53
1:B:2428:ASN:HB3	1:B:2493:LEU:HD13	1.89	0.53
1:A:2251:ARG:NH1	1:A:2252:ASP:OD1	2.42	0.53
2:D:128:ASN:O	2:D:129:ALA:HB3	2.08	0.53
1:A:2418:LEU:O	1:A:2422:VAL:HG23	2.09	0.53
2:C:168:GLU:N	2:C:169:PRO:HD2	2.24	0.53
1:A:2307:SER:CB	1:A:2313:TRP:HB2	2.38	0.53
2:C:94:HIS:HB3	2:C:99:TRP:HB2	1.89	0.53
2:C:288:ALA:HB2	2:C:318:LEU:HG	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1999:CYS:C	1:B:2001:HIS:H	2.16	0.53
1:B:2095:LYS:O	1:B:2099:GLN:HG2	2.09	0.53
1:A:1401:GLU:HG2	1:A:2389:VAL:HG22	1.90	0.53
1:A:1681:PRO:O	1:A:1682:SER:C	2.52	0.53
1:A:2281:MET:HE1	2:C:222:TYR:CG	2.44	0.53
2:D:267:GLU:O	2:D:267:GLU:HG3	2.09	0.53
2:D:271:GLY:HA2	2:D:290:SER:HB2	1.91	0.53
2:D:289:SER:HB2	2:D:291:ASP:OD1	2.09	0.53
1:A:1704:MET:HE3	1:A:1713:ALA:HA	1.92	0.52
1:A:1913:TYR:HB2	1:A:1915:HIS:CE1	2.44	0.52
1:A:2095:LYS:O	1:A:2099:GLN:HG2	2.09	0.52
1:B:1433:LEU:HD23	1:B:1453:LEU:CD2	2.38	0.52
2:D:286:VAL:HB	2:D:318:LEU:HD13	1.91	0.52
1:A:1732:ILE:CD1	1:A:1740:LYS:HB2	2.37	0.52
2:C:202:GLY:O	2:C:203:ILE:O	2.28	0.52
1:B:2037:LEU:HD22	1:B:2043:ASN:HD22	1.74	0.52
1:A:1691:THR:CG2	1:A:1724:MET:HE1	2.38	0.52
1:A:2192:LEU:HD12	1:A:2235:GLY:CA	2.37	0.52
1:A:2512:ASP:OD1	1:A:2512:ASP:N	2.43	0.52
2:C:128:ASN:O	2:C:129:ALA:HB3	2.09	0.52
1:B:1915:HIS:HD2	1:B:1953:VAL:HG22	1.74	0.52
1:B:1999:CYS:C	1:B:2001:HIS:N	2.67	0.52
1:B:2521:VAL:HB	1:B:2522:PRO:HD3	1.91	0.52
2:C:159:THR:C	2:C:161:HIS:H	2.16	0.52
1:B:1552:LEU:HD11	1:B:1603:ILE:HG13	1.90	0.52
1:B:2417:VAL:O	1:B:2420:ALA:HB3	2.09	0.52
2:D:111:ILE:HD12	2:D:123:ARG:HD3	1.92	0.52
2:C:267:GLU:HG3	2:C:267:GLU:O	2.10	0.52
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.43	0.52
2:C:60:ALA:HB1	2:C:88:ILE:HG22	1.91	0.52
2:C:137:HIS:CD2	2:C:139:ASN:H	2.28	0.52
2:C:74:ASN:H	2:C:75:PRO:HD3	1.75	0.52
1:B:2197:ARG:NH1	1:B:2424:ASP:OD2	2.26	0.52
2:D:288:ALA:HB2	2:D:318:LEU:HG	1.92	0.52
2:D:36:ARG:NH2	2:D:69:ASP:O	2.43	0.51
1:A:1725:GLN:HB3	1:A:1747:MET:HE1	1.91	0.51
1:A:1649:ASP:O	1:A:1651:ARG:N	2.44	0.51
1:B:1684:GLN:HB3	1:B:1687:HIS:CD2	2.45	0.51
1:B:2028:HIS:HE1	1:B:2112:SER:OG	1.93	0.51
1:A:2281:MET:HA	1:A:2281:MET:CE	2.40	0.51
2:C:188:VAL:HG13	2:C:223:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:200:THR:O	2:C:208:THR:HA	2.11	0.51
1:B:1704:MET:HE3	1:B:1713:ALA:HA	1.92	0.51
1:A:1754:LEU:HD13	1:A:1775:TYR:CE2	2.45	0.51
1:B:1478:LEU:O	1:B:1482:ARG:HG3	2.11	0.51
2:D:137:HIS:CD2	2:D:139:ASN:H	2.28	0.51
1:A:2152:ARG:HG2	1:A:2177:SER:CB	2.41	0.51
2:C:202:GLY:HA3	2:C:208:THR:H	1.76	0.51
2:D:159:THR:C	2:D:161:HIS:H	2.17	0.51
1:A:1422:LYS:HE2	1:A:1581:GLU:HG3	1.92	0.51
1:A:1802:LEU:HD22	1:A:1806:HIS:NE2	2.25	0.51
1:A:1947:ASP:CG	1:A:1987:ARG:HG2	2.36	0.51
1:A:2418:LEU:HD23	1:A:2421:PHE:CZ	2.46	0.51
2:C:95:GLU:CB	2:C:140:GLN:HE22	2.15	0.51
2:D:54:ARG:HD2	2:D:323:SER:HB2	1.93	0.51
2:C:128:ASN:O	2:C:129:ALA:CB	2.59	0.51
1:B:1501:TRP:HA	1:B:1503:LEU:HG	1.92	0.51
1:B:1680:ASP:C	1:B:1682:SER:H	2.14	0.51
1:B:2408:ARG:HG2	1:B:2508:LEU:O	2.10	0.51
2:D:82:ASP:H	2:D:119:LEU:HD22	1.76	0.51
1:A:2417:VAL:O	1:A:2420:ALA:HB3	2.11	0.51
2:C:54:ARG:HD2	2:C:323:SER:HB2	1.93	0.51
1:B:1972:LEU:O	1:B:1975:PRO:HG2	2.11	0.51
2:D:15:LEU:HD11	2:D:286:VAL:HG11	1.93	0.51
2:D:137:HIS:CD2	2:D:138:PRO:CD	2.94	0.51
2:D:168:GLU:N	2:D:169:PRO:HD2	2.26	0.51
2:D:202:GLY:O	2:D:203:ILE:O	2.29	0.51
1:A:1530:GLU:HA	1:A:1550:LEU:HD11	1.91	0.51
2:C:262:SER:OG	2:C:267:GLU:HG2	2.11	0.51
1:B:1951:PRO:HB2	1:B:1955:ARG:HH21	1.76	0.50
2:C:14:ILE:HD13	2:C:70:LEU:HD13	1.92	0.50
1:B:1440:PHE:HB3	1:B:1442:GLU:HB2	1.93	0.50
1:B:1526:TRP:HE3	1:B:1529:MET:HE2	1.76	0.50
1:A:1907:LEU:HD11	1:A:1938:VAL:HG11	1.93	0.50
1:B:1428:ALA:HB2	1:B:2395:ASN:HD21	1.75	0.50
1:B:1977:THR:HG21	1:B:2013:SER:OG	2.12	0.50
1:A:1564:ILE:HG23	1:A:1596:LEU:HD22	1.94	0.50
2:C:130:PRO:HD2	2:C:148:GLN:HB2	1.92	0.50
1:A:1501:TRP:HA	1:A:1503:LEU:HG	1.92	0.50
2:C:107:CYS:HB3	2:C:127:VAL:O	2.11	0.50
1:A:1781:GLU:OE1	1:A:1781:GLU:HA	2.11	0.50
1:A:1936:LEU:HA	1:A:1939:ILE:HG13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1977:THR:HG22	1:A:1981:LYS:HE2	1.94	0.50
2:C:72:SER:O	2:C:74:ASN:N	2.45	0.50
2:C:207:VAL:HG12	2:C:209:GLN:HG2	1.94	0.50
1:B:1936:LEU:HA	1:B:1939:ILE:HG13	1.93	0.50
2:D:94:HIS:HD2	2:D:140:GLN:HB3	1.76	0.50
2:D:207:VAL:HG12	2:D:209:GLN:HG2	1.94	0.50
1:A:1670:HIS:HE1	1:A:1681:PRO:CB	2.22	0.50
1:A:1910:TRP:CD1	1:A:1910:TRP:C	2.90	0.50
1:B:1720:PHE:CZ	1:B:1724:MET:HE3	2.46	0.50
1:B:2027:TRP:O	1:B:2031:LEU:HG	2.11	0.50
1:B:2512:ASP:OD1	1:B:2512:ASP:N	2.41	0.50
2:D:137:HIS:HD2	2:D:138:PRO:N	2.10	0.50
1:A:1564:ILE:HD13	1:A:1600:GLU:HG3	1.93	0.50
1:B:1932:ILE:O	1:B:1933:ASP:C	2.55	0.50
1:A:1766:GLU:OE1	1:A:1766:GLU:N	2.45	0.50
1:B:1605:TYR:CZ	1:B:1612:ARG:HG2	2.46	0.49
2:C:63:GLN:NE2	2:C:86:LYS:H	2.04	0.49
1:B:1623:LEU:HG	1:B:1633:TRP:CZ3	2.46	0.49
1:B:1947:ASP:CG	1:B:1987:ARG:HG2	2.37	0.49
2:D:200:THR:O	2:D:208:THR:HA	2.12	0.49
1:A:1432:VAL:HG22	1:A:2390:THR:HG21	1.92	0.49
2:D:277:ALA:O	2:D:286:VAL:HG23	2.12	0.49
1:B:1649:ASP:O	1:B:1651:ARG:N	2.45	0.49
2:D:74:ASN:H	2:D:75:PRO:HD3	1.78	0.49
2:C:255:MET:HE1	2:C:299:VAL:HG12	1.93	0.49
2:C:185:MET:HE2	2:C:197:TRP:CD1	2.48	0.49
2:C:277:ALA:O	2:C:286:VAL:HG23	2.12	0.49
2:D:202:GLY:HA3	2:D:208:THR:H	1.78	0.49
1:A:1629:ILE:O	1:A:1630:VAL:C	2.55	0.49
1:A:2006:VAL:O	1:A:2010:MET:HB2	2.12	0.49
2:C:159:THR:C	2:C:161:HIS:N	2.70	0.49
1:B:1629:ILE:O	1:B:1630:VAL:C	2.56	0.49
1:B:1681:PRO:O	1:B:1682:SER:C	2.56	0.49
2:D:63:GLN:NE2	2:D:86:LYS:H	2.05	0.49
1:A:1628:ARG:HB2	1:A:1633:TRP:CD1	2.48	0.49
1:A:1684:GLN:HB3	1:A:1687:HIS:CD2	2.47	0.49
1:A:2329:MET:HB3	1:A:2404:MET:HE2	1.94	0.49
1:B:1621:GLU:C	1:B:1623:LEU:H	2.20	0.49
1:B:1754:LEU:HD13	1:B:1775:TYR:CE2	2.47	0.49
1:A:1402:LEU:O	1:A:1405:GLN:HB2	2.13	0.49
1:A:1605:TYR:CZ	1:A:1612:ARG:HG2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:180:PRO:HG2	2:C:230:PRO:HA	1.95	0.49
2:C:248:ARG:O	2:C:252:PHE:N	2.44	0.49
1:B:1529:MET:HE3	1:B:1550:LEU:HG	1.94	0.49
1:B:2162:VAL:HG22	1:B:2170:ARG:HG3	1.94	0.49
1:A:1428:ALA:HB2	1:A:2395:ASN:HD21	1.78	0.49
1:A:1970:GLN:NE2	1:A:2139:ALA:H	2.10	0.49
1:A:1977:THR:HG21	1:A:2013:SER:OG	2.13	0.49
1:A:2281:MET:CE	2:C:222:TYR:CD2	2.96	0.49
2:D:72:SER:O	2:D:74:ASN:N	2.46	0.48
1:A:1526:TRP:HE3	1:A:1529:MET:HE2	1.78	0.48
1:A:1786:TRP:CE3	1:A:1789:ALA:HB2	2.48	0.48
1:B:1913:TYR:HB2	1:B:1915:HIS:CE1	2.48	0.48
1:B:2374:LYS:HE3	1:B:2540:GLN:OE1	2.13	0.48
1:A:1621:GLU:C	1:A:1623:LEU:H	2.20	0.48
1:A:1734:THR:C	1:A:1736:ASP:H	2.19	0.48
1:B:1691:THR:CG2	1:B:1724:MET:HE1	2.43	0.48
2:D:128:ASN:O	2:D:129:ALA:CB	2.62	0.48
1:A:1478:LEU:O	1:A:1482:ARG:HG3	2.13	0.48
1:A:2271:MET:HE2	1:A:2286:VAL:HG22	1.95	0.48
1:B:1543:GLY:O	1:B:1547:ARG:HD2	2.13	0.48
2:D:159:THR:C	2:D:161:HIS:N	2.71	0.48
2:D:258:LEU:HD22	2:D:297:TRP:CE3	2.48	0.48
1:A:1623:LEU:HD13	1:A:1640:ARG:NH1	2.28	0.48
1:A:1892:ILE:HG21	1:A:1930:ILE:HD11	1.95	0.48
1:A:2162:VAL:HG22	1:A:2170:ARG:HG3	1.94	0.48
2:C:82:ASP:H	2:C:119:LEU:HD22	1.79	0.48
1:B:2011:MET:HE1	1:B:2133:CYS:SG	2.54	0.48
2:D:94:HIS:CD2	2:D:140:GLN:HB3	2.48	0.48
2:C:287:THR:O	2:C:294:ALA:HA	2.14	0.48
1:B:1899:ASN:O	1:B:1900:LEU:C	2.55	0.48
1:B:2411:LYS:O	1:B:2415:MET:HG3	2.14	0.48
1:B:1958:HIS:HE1	1:B:1990:ALA:CB	2.26	0.48
1:B:2336:LEU:HG	1:B:2339:ARG:HH11	1.79	0.48
1:B:2520:ASP:OD2	1:B:2522:PRO:HD2	2.13	0.48
1:A:1972:LEU:O	1:A:1975:PRO:HG2	2.14	0.48
1:B:2152:ARG:HG2	1:B:2177:SER:OG	2.14	0.48
1:B:2281:MET:HA	1:B:2281:MET:HE3	1.95	0.48
1:A:1543:GLY:O	1:A:1547:ARG:HD2	2.13	0.48
1:B:1417:ILE:O	1:B:1421:ASN:ND2	2.47	0.47
1:B:1418:SER:HB2	1:B:1581:GLU:HG2	1.96	0.47
1:B:1907:LEU:HD11	1:B:1938:VAL:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2154:GLN:NE2	1:B:2155:SER:HB3	2.28	0.47
2:D:130:PRO:HD2	2:D:148:GLN:HB2	1.95	0.47
1:B:2382:MET:SD	1:B:2549:TRP:HA	2.54	0.47
2:D:168:GLU:HB3	2:D:195:TYR:OH	2.15	0.47
1:A:1440:PHE:HB3	1:A:1442:GLU:HB2	1.96	0.47
1:A:1773:LEU:HG	1:A:1796:MET:HG3	1.96	0.47
1:A:1791:HIS:O	1:A:1795:VAL:HG23	2.15	0.47
2:C:68:TYR:HE2	2:C:77:PRO:HD3	1.79	0.47
2:C:69:ASP:HB3	2:C:72:SER:OG	2.14	0.47
1:B:1969:PRO:HB3	1:B:1998:MET:HE3	1.96	0.47
1:B:1973:ILE:H	1:B:1973:ILE:HG13	1.47	0.47
1:B:2129:LYS:O	1:B:2132:MET:HE2	2.14	0.47
1:B:1416:LEU:O	1:B:1420:ASN:HB2	2.14	0.47
1:B:1670:HIS:HE1	1:B:1681:PRO:HB3	1.79	0.47
1:A:1502:THR:HG22	1:A:1504:VAL:HG23	1.97	0.47
1:A:2146:PRO:O	1:A:2147:ASN:HB2	2.14	0.47
2:C:288:ALA:HB1	2:C:315:VAL:HG12	1.96	0.47
1:B:2282:GLN:HE21	2:D:316:VAL:HG11	1.79	0.47
2:D:68:TYR:HE2	2:D:77:PRO:HD3	1.79	0.47
2:D:94:HIS:HE1	2:D:96:ASP:HB2	1.78	0.47
1:A:2154:GLN:NE2	1:A:2155:SER:HB3	2.29	0.47
1:B:1690:PRO:HB2	1:B:1692:VAL:HG22	1.97	0.47
1:B:1915:HIS:HE1	1:B:1919:VAL:CG1	2.28	0.47
2:D:180:PRO:HG2	2:D:230:PRO:HA	1.97	0.47
1:A:1691:THR:HG22	1:A:1691:THR:O	2.15	0.47
1:A:1980:SER:O	1:A:1988:HIS:HB2	2.15	0.47
1:B:1910:TRP:CD1	1:B:1910:TRP:C	2.93	0.47
1:B:2347:ASP:OD1	1:B:2350:SER:OG	2.27	0.47
1:A:2411:LYS:O	1:A:2415:MET:HG3	2.15	0.47
2:C:258:LEU:HD22	2:C:297:TRP:CE3	2.49	0.47
1:B:1932:ILE:HD12	1:B:1933:ASP:H	1.78	0.47
1:B:2281:MET:CE	2:D:222:TYR:CD2	2.97	0.47
1:A:1936:LEU:C	1:A:1938:VAL:H	2.23	0.47
2:C:139:ASN:HD22	2:C:203:ILE:HG12	1.79	0.47
1:A:1690:PRO:HB2	1:A:1692:VAL:HG22	1.97	0.46
2:C:111:ILE:HD12	2:C:123:ARG:HD3	1.97	0.46
1:B:1566:LYS:O	1:B:1570:LEU:HG	2.14	0.46
1:B:1574:GLU:HG2	1:B:1585:ARG:NH2	2.30	0.46
1:B:1605:TYR:CG	1:B:1643:VAL:HG11	2.50	0.46
2:D:94:HIS:HB3	2:D:99:TRP:HB2	1.96	0.46
2:D:139:ASN:HD22	2:D:203:ILE:HG12	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:154:ILE:HD11	2:D:210:LEU:HD11	1.97	0.46
1:A:2245:THR:O	1:A:2249:LEU:HD12	2.15	0.46
1:B:1691:THR:O	1:B:1691:THR:HG22	2.15	0.46
1:A:1932:ILE:O	1:A:1933:ASP:C	2.58	0.46
1:B:1786:TRP:CE3	1:B:1789:ALA:HB2	2.50	0.46
2:D:53:ASP:C	2:D:55:SER:H	2.23	0.46
2:D:167:PRO:HD2	2:D:169:PRO:CG	2.43	0.46
1:A:1401:GLU:HG2	1:A:2389:VAL:CG2	2.46	0.46
1:A:1720:PHE:CZ	1:A:1724:MET:HE3	2.51	0.46
1:A:2382:MET:SD	1:A:2549:TRP:HA	2.56	0.46
1:B:1533:THR:C	1:B:1535:MET:H	2.22	0.46
1:B:1734:THR:O	1:B:1736:ASP:N	2.40	0.46
2:D:255:MET:HE1	2:D:299:VAL:HG12	1.97	0.46
2:D:270:ARG:HD2	2:D:270:ARG:HA	1.77	0.46
2:D:288:ALA:HB1	2:D:315:VAL:HG12	1.97	0.46
1:A:1482:ARG:HA	1:A:1485:GLU:HG2	1.97	0.46
1:A:1876:THR:HA	1:A:1879:MET:HE2	1.98	0.46
1:A:2028:HIS:HE1	1:A:2112:SER:OG	1.98	0.46
2:D:58:ALA:HB2	2:D:67:MET:HE3	1.97	0.46
1:A:1915:HIS:HD2	1:A:1953:VAL:HG22	1.81	0.46
1:B:1537:PRO:O	1:B:1543:GLY:HA3	2.15	0.46
1:B:2006:VAL:O	1:B:2010:MET:HB2	2.15	0.46
1:A:1701:MET:HB3	1:A:1701:MET:HE2	1.44	0.46
1:A:2298:ASP:HB2	1:A:2382:MET:HE1	1.95	0.46
1:B:1497:CYS:SG	1:B:1516:ALA:HB2	2.56	0.46
1:B:1502:THR:HG22	1:B:1504:VAL:HG23	1.98	0.46
1:B:1680:ASP:HB3	1:B:1683:ARG:H	1.79	0.46
1:A:1899:ASN:O	1:A:1900:LEU:C	2.58	0.46
1:A:2214:THR:O	1:A:2217:ARG:HB3	2.16	0.46
1:A:2333:ILE:CD1	1:A:2407:LEU:HD13	2.46	0.46
1:A:1595:MET:O	1:A:1599:LEU:HB2	2.16	0.46
1:A:1907:LEU:HD11	1:A:1938:VAL:HG13	1.97	0.46
1:A:2011:MET:HE1	1:A:2133:CYS:SG	2.56	0.46
2:D:225:GLN:HG2	2:D:226:CYS:N	2.30	0.46
1:A:2201:LEU:O	1:A:2205:VAL:HG23	2.15	0.46
2:C:94:HIS:HE1	2:C:96:ASP:HB2	1.81	0.46
2:C:159:THR:HB	2:C:161:HIS:HB2	1.97	0.46
1:B:1482:ARG:HA	1:B:1485:GLU:HG2	1.97	0.45
1:B:1913:TYR:O	1:B:1915:HIS:CG	2.69	0.45
1:B:1936:LEU:C	1:B:1938:VAL:H	2.24	0.45
1:B:2152:ARG:HG2	1:B:2177:SER:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2152:ARG:HE	1:B:2152:ARG:HB3	1.61	0.45
2:D:95:GLU:CB	2:D:140:GLN:HE22	2.18	0.45
2:D:262:SER:OG	2:D:267:GLU:HG2	2.16	0.45
1:A:1433:LEU:HD23	1:A:1453:LEU:HD23	1.99	0.45
1:A:2184:PHE:HB3	1:A:2236:LEU:HD22	1.98	0.45
1:A:2378:ARG:NH1	1:A:2380:THR:HG21	2.31	0.45
1:B:1915:HIS:CE1	1:B:1919:VAL:CG1	2.99	0.45
1:B:1968:HIS:HB3	1:B:2144:TYR:HH	1.81	0.45
1:A:1697:THR:O	1:A:1701:MET:HG3	2.16	0.45
2:C:270:ARG:HD2	2:C:270:ARG:HA	1.79	0.45
1:B:2214:THR:O	1:B:2217:ARG:HB3	2.16	0.45
2:D:115:ARG:O	2:D:116:SER:HB3	2.17	0.45
1:A:1964:ILE:O	1:A:1967:TYR:O	2.35	0.45
1:A:2333:ILE:HD12	1:A:2407:LEU:HD13	1.98	0.45
2:C:137:HIS:CD2	2:C:138:PRO:CD	2.99	0.45
2:C:225:GLN:HG2	2:C:226:CYS:N	2.30	0.45
1:B:1970:GLN:C	1:B:1972:LEU:N	2.73	0.45
2:D:132:ASN:HD21	2:D:148:GLN:HG2	1.81	0.45
1:A:1477:MET:HE2	1:A:1477:MET:HB3	1.88	0.45
1:A:1913:TYR:O	1:A:1915:HIS:CG	2.70	0.45
2:C:63:GLN:HE21	2:C:86:LYS:N	2.05	0.45
1:B:2387:MET:HE1	1:B:2396:TYR:CB	2.46	0.45
1:A:1413:LEU:O	1:A:1417:ILE:HG12	2.16	0.45
1:A:1533:THR:C	1:A:1535:MET:H	2.23	0.45
1:B:2378:ARG:NH1	1:B:2380:THR:HG21	2.32	0.45
1:B:2418:LEU:O	1:B:2422:VAL:HG23	2.17	0.45
2:D:248:ARG:O	2:D:252:PHE:HA	2.17	0.45
1:A:2027:TRP:O	1:A:2031:LEU:HG	2.16	0.45
2:D:306:ARG:HG2	2:D:307:GLU:N	2.29	0.45
2:C:168:GLU:HB3	2:C:195:TYR:OH	2.17	0.45
2:D:287:THR:O	2:D:294:ALA:HA	2.17	0.45
1:A:1989:ASN:O	1:A:1993:LYS:HD2	2.17	0.45
2:D:16:ALA:O	2:D:318:LEU:HA	2.17	0.45
1:A:1913:TYR:CB	1:A:1915:HIS:CE1	3.00	0.45
2:C:16:ALA:O	2:C:318:LEU:HA	2.17	0.45
1:B:1697:THR:O	1:B:1701:MET:HG3	2.17	0.45
2:D:188:VAL:HG13	2:D:223:ALA:CB	2.47	0.45
1:B:1506:ASP:HA	1:B:1509:GLN:HB2	1.99	0.44
1:B:1698:TYR:O	1:B:1702:LYS:HG2	2.17	0.44
2:D:231:ASP:HB2	2:D:233:THR:H	1.82	0.44
1:A:1422:LYS:HG2	1:A:1580:GLY:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1631:GLU:HA	1:A:1634:GLN:HE21	1.81	0.44
1:A:1785:SER:O	1:A:1786:TRP:HB3	2.17	0.44
1:A:2210:ALA:O	1:A:2216:LEU:HD22	2.17	0.44
2:C:137:HIS:HD2	2:C:138:PRO:N	2.16	0.44
1:B:2316:ARG:NH2	1:B:2349:LEU:HD23	2.32	0.44
2:D:69:ASP:HB3	2:D:72:SER:OG	2.17	0.44
1:A:2513:PHE:HB2	1:A:2519:LEU:HD11	1.99	0.44
1:B:1605:TYR:CE2	1:B:1612:ARG:HG2	2.53	0.44
1:B:1881:THR:HG23	1:B:1909:LEU:HD22	2.00	0.44
2:D:239:SER:OG	2:D:240:ALA:N	2.50	0.44
1:A:1674:VAL:HG11	1:A:1681:PRO:HD3	1.99	0.44
1:A:2192:LEU:HD21	1:A:2237:ILE:HD11	1.99	0.44
1:A:2260:LEU:HD12	1:A:2261:LEU:N	2.32	0.44
1:B:2339:ARG:NH2	1:B:2356:ILE:O	2.50	0.44
2:D:21:ASP:HB3	2:D:313:LYS:HB2	1.99	0.44
2:D:82:ASP:HB2	2:D:119:LEU:HD13	1.99	0.44
2:D:135:CYS:SG	2:D:178:ILE:HG22	2.57	0.44
1:A:2321:THR:HG23	1:A:2387:MET:HE3	2.00	0.44
1:A:2363:GLU:HA	1:A:2363:GLU:OE1	2.18	0.44
2:C:28:GLN:O	2:C:28:GLN:HG3	2.17	0.44
1:B:1628:ARG:HB2	1:B:1633:TRP:CD1	2.53	0.44
1:A:1393:TYR:CE2	1:A:1422:LYS:HD2	2.52	0.44
1:A:1506:ASP:HA	1:A:1509:GLN:HB2	1.99	0.44
1:A:1970:GLN:HA	1:A:1973:ILE:HD11	2.00	0.44
1:A:2261:LEU:HD23	1:A:2262:ASN:ND2	2.32	0.44
1:A:2401:HIS:CD2	1:A:2522:PRO:HA	2.52	0.44
2:C:169:PRO:HA	2:C:171:VAL:HG22	1.98	0.44
1:B:1712:ASP:OD1	1:A:2266:ARG:NH2	2.50	0.44
2:D:159:THR:HB	2:D:161:HIS:HB2	1.99	0.44
1:A:1427:GLU:HB2	1:A:2398:ILE:HD13	1.98	0.44
1:A:2021:ILE:HG22	1:A:2025:GLU:HB2	1.99	0.44
1:B:1964:ILE:O	1:B:1967:TYR:O	2.35	0.44
1:B:2254:ARG:HH22	1:B:2264:GLU:CD	2.25	0.44
2:D:69:ASP:HB2	2:D:78:ILE:CD1	2.34	0.44
2:D:102:THR:O	2:D:109:ALA:HA	2.17	0.44
1:B:1481:MET:HA	1:B:1484:LEU:HD12	1.99	0.44
1:B:2316:ARG:HH21	1:B:2349:LEU:HD23	1.83	0.44
1:B:1413:LEU:O	1:B:1417:ILE:HG12	2.17	0.43
1:B:2271:MET:HE2	1:B:2286:VAL:HG22	2.00	0.43
2:D:14:ILE:HD13	2:D:70:LEU:HD13	1.99	0.43
1:A:1739:HIS:O	1:A:1743:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2129:LYS:O	1:A:2132:MET:HE2	2.18	0.43
1:A:2538:LEU:C	1:A:2540:GLN:H	2.26	0.43
2:C:263:GLY:O	2:C:264:ASN:HB3	2.18	0.43
2:D:219:HIS:CE1	2:D:245:LYS:HD2	2.53	0.43
1:A:1505:ASN:CB	1:A:1508:THR:HB	2.49	0.43
1:A:2319:ASN:HB3	1:A:2352:LYS:HG2	1.99	0.43
1:A:2496:LYS:HE3	1:A:2500:ILE:HD11	1.99	0.43
1:B:1970:GLN:C	1:B:1972:LEU:H	2.26	0.43
1:A:1680:ASP:HB3	1:A:1683:ARG:H	1.82	0.43
1:B:1453:LEU:O	1:B:1455:GLU:N	2.52	0.43
1:B:1605:TYR:HD2	1:B:1605:TYR:O	2.01	0.43
1:B:2380:THR:CG2	1:B:2549:TRP:C	2.91	0.43
1:B:1973:ILE:O	1:B:1974:TYR:C	2.61	0.43
1:B:2281:MET:HA	1:B:2281:MET:HE2	2.00	0.43
1:A:1416:LEU:O	1:A:1420:ASN:HB2	2.18	0.43
1:A:1701:MET:HE1	1:A:1717:MET:CA	2.49	0.43
2:C:58:ALA:HB2	2:C:67:MET:HE3	2.00	0.43
1:A:2332:TYR:O	1:A:2507:LYS:NZ	2.36	0.43
1:B:1701:MET:HE1	1:B:1717:MET:CA	2.49	0.43
1:B:1705:TRP:CZ2	1:B:1710:LYS:HD2	2.54	0.43
1:A:1682:SER:O	1:A:1685:LEU:HD12	2.19	0.43
2:C:115:ARG:O	2:C:116:SER:HB3	2.19	0.43
1:A:1913:TYR:O	1:A:1914:GLY:C	2.62	0.43
1:A:2042:ARG:HA	1:A:2042:ARG:HD3	1.87	0.43
2:C:231:ASP:HB2	2:C:233:THR:H	1.84	0.43
1:B:1732:ILE:HD13	1:B:1740:LYS:HB2	2.01	0.43
1:B:1739:HIS:O	1:B:1743:LEU:HB2	2.18	0.43
1:B:1878:LEU:HD21	1:B:1918:ASP:CB	2.47	0.43
1:B:2036:ARG:HA	1:B:2036:ARG:HD3	1.62	0.43
1:B:2401:HIS:CD2	1:B:2522:PRO:HA	2.53	0.43
1:A:2380:THR:CG2	1:A:2549:TRP:C	2.92	0.43
2:C:151:ALA:HA	2:C:166:ILE:HG22	2.01	0.43
1:B:1470:ASN:HB3	1:B:1471:LYS:H	1.60	0.43
1:B:1682:SER:O	1:B:1685:LEU:HD12	2.19	0.43
1:A:1415:SER:O	1:A:1419:ILE:CG2	2.65	0.43
1:A:1470:ASN:HB3	1:A:1471:LYS:H	1.60	0.43
1:A:1705:TRP:CZ3	1:A:1757:TRP:HB3	2.54	0.43
1:A:2374:LYS:HE3	1:A:2540:GLN:OE1	2.19	0.43
2:C:53:ASP:C	2:C:55:SER:H	2.27	0.43
2:C:94:HIS:CD2	2:C:140:GLN:HB3	2.53	0.43
2:C:94:HIS:HD2	2:C:140:GLN:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:185:MET:HE2	2:C:197:TRP:HD1	1.81	0.43
2:C:262:SER:HB2	2:C:263:GLY:H	1.65	0.43
1:B:2424:ASP:O	1:B:2428:ASN:ND2	2.52	0.42
1:A:1970:GLN:C	1:A:1972:LEU:N	2.76	0.42
2:C:102:THR:O	2:C:109:ALA:HA	2.18	0.42
1:B:1505:ASN:CB	1:B:1508:THR:HB	2.50	0.42
1:B:1892:ILE:HG21	1:B:1930:ILE:HD11	2.01	0.42
1:B:1910:TRP:CZ2	1:B:1956:LEU:HB3	2.54	0.42
1:B:2021:ILE:HG22	1:B:2025:GLU:HB2	2.01	0.42
1:B:2184:PHE:HB3	1:B:2236:LEU:HD22	2.01	0.42
1:B:2538:LEU:C	1:B:2540:GLN:H	2.27	0.42
1:A:1900:LEU:HD23	1:A:2204:LEU:HD22	2.00	0.42
1:A:2036:ARG:HA	1:A:2036:ARG:HD3	1.61	0.42
1:A:2064:THR:CG2	1:A:2128:PRO:HD3	2.40	0.42
1:B:1473:ASP:HA	1:B:1474:PRO:HD2	1.83	0.42
1:B:2321:THR:HG23	1:B:2387:MET:HE3	2.02	0.42
2:D:169:PRO:HA	2:D:171:VAL:HG22	2.00	0.42
2:D:213:LYS:HD3	2:D:252:PHE:HE1	1.84	0.42
1:A:1514:ARG:HE	1:A:1542:ASP:CG	2.27	0.42
2:C:306:ARG:HG2	2:C:307:GLU:N	2.31	0.42
1:B:1631:GLU:HA	1:B:1634:GLN:HE21	1.84	0.42
1:B:1710:LYS:NZ	1:B:1760:ASN:HD21	2.17	0.42
1:B:1778:ALA:O	1:B:1782:HIS:HD2	2.01	0.42
2:D:248:ARG:O	2:D:252:PHE:N	2.50	0.42
1:A:1453:LEU:O	1:A:1455:GLU:N	2.53	0.42
2:C:150:GLY:HA3	2:C:169:PRO:CB	2.44	0.42
2:C:168:GLU:HG2	2:C:169:PRO:N	2.30	0.42
2:C:248:ARG:O	2:C:252:PHE:HA	2.20	0.42
1:B:2042:ARG:HA	1:B:2042:ARG:HD3	1.87	0.42
1:B:2165:SER:OG	1:B:2166:LYS:N	2.52	0.42
2:D:150:GLY:HA3	2:D:169:PRO:CB	2.43	0.42
1:A:1734:THR:C	1:A:1736:ASP:N	2.77	0.42
1:A:1910:TRP:HD1	1:A:1910:TRP:O	2.03	0.42
1:A:2037:LEU:HD22	1:A:2043:ASN:ND2	2.33	0.42
1:A:2503:ARG:NH1	1:A:2507:LYS:CE	2.82	0.42
2:C:203:ILE:HG22	2:C:204:GLY:N	2.34	0.42
2:C:219:HIS:CE1	2:C:245:LYS:HD2	2.55	0.42
2:C:298:CYS:HB2	2:C:305:LYS:HE3	2.02	0.42
1:B:1701:MET:HE2	1:B:1701:MET:HB3	1.45	0.42
2:D:203:ILE:O	2:D:204:GLY:C	2.63	0.42
2:D:297:TRP:CZ3	2:D:304:ILE:HG12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1915:HIS:HE1	1:A:1919:VAL:CG1	2.33	0.42
1:A:2530:LYS:HE2	1:A:2530:LYS:HA	2.00	0.42
2:C:21:ASP:HB3	2:C:313:LYS:HB2	2.02	0.42
1:B:1595:MET:O	1:B:1599:LEU:HB2	2.20	0.42
1:B:2123:LEU:HD12	1:B:2123:LEU:HA	1.97	0.42
1:B:2368:ARG:HD2	1:B:2370:LYS:O	2.20	0.42
2:D:28:GLN:HG2	2:D:31:SER:OG	2.20	0.42
1:B:1614:ILE:O	1:B:1618:ILE:HG13	2.19	0.42
1:B:1725:GLN:HB3	1:B:1747:MET:HE1	2.01	0.42
1:B:2333:ILE:HD12	1:B:2407:LEU:HD13	2.01	0.42
1:B:2513:PHE:HB2	1:B:2519:LEU:HD11	2.01	0.42
1:A:2101:TRP:HA	1:A:2104:TYR:HB2	2.01	0.42
1:B:2022:LEU:HD23	1:B:2022:LEU:HA	1.91	0.42
2:D:63:GLN:HE21	2:D:86:LYS:N	2.07	0.42
1:A:1974:TYR:O	1:A:1978:VAL:HG23	2.20	0.42
1:A:2281:MET:HA	1:A:2281:MET:HE3	2.01	0.42
1:A:2421:PHE:HD1	1:A:2430:ARG:HH22	1.65	0.42
1:B:2298:ASP:HB2	1:B:2382:MET:HE1	2.00	0.42
1:B:2364:VAL:HG12	1:B:2365:ALA:N	2.33	0.42
2:D:75:PRO:HB2	2:D:76:ASN:H	1.48	0.42
2:D:203:ILE:HG22	2:D:204:GLY:N	2.35	0.42
1:A:2281:MET:CE	2:C:222:TYR:CE2	3.03	0.42
1:A:2424:ASP:O	1:A:2428:ASN:ND2	2.53	0.42
1:B:1400:LYS:HG3	1:B:1416:LEU:HD13	2.01	0.41
1:B:1903:THR:HG22	1:B:1938:VAL:HG21	2.02	0.41
1:B:2376:PRO:HG2	1:B:2532:ALA:HB2	2.02	0.41
1:A:1493:LEU:CD2	1:A:1519:ALA:HB2	2.46	0.41
1:A:1623:LEU:HD13	1:A:1640:ARG:HH12	1.84	0.41
1:A:2128:PRO:HD2	1:A:2129:LYS:H	1.85	0.41
1:A:2184:PHE:CB	1:A:2236:LEU:HD22	2.50	0.41
2:C:213:LYS:HD3	2:C:252:PHE:HE1	1.85	0.41
2:C:281:ASP:OD1	2:C:283:GLN:HG3	2.20	0.41
2:C:289:SER:HB2	2:C:291:ASP:OD1	2.20	0.41
1:B:1415:SER:O	1:B:1419:ILE:CG2	2.66	0.41
1:B:2004:THR:HA	1:B:2007:GLN:HB2	2.01	0.41
1:B:2146:PRO:O	1:B:2147:ASN:HB2	2.20	0.41
1:B:2261:LEU:HD23	1:B:2262:ASN:ND2	2.35	0.41
1:A:1481:MET:HA	1:A:1484:LEU:HD12	2.01	0.41
1:A:2418:LEU:HD13	1:A:2504:VAL:HG11	2.01	0.41
1:B:1497:CYS:SG	1:B:1516:ALA:CB	3.08	0.41
1:A:1566:LYS:O	1:A:1570:LEU:HG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1605:TYR:HD2	1:A:1605:TYR:O	2.03	0.41
1:A:1915:HIS:CE1	1:A:1919:VAL:CG1	3.03	0.41
1:A:2082:GLN:HE21	1:A:2082:GLN:HB3	1.64	0.41
1:B:1422:LYS:C	1:B:1424:GLN:N	2.78	0.41
1:B:2529:ILE:O	1:B:2533:THR:HB	2.20	0.41
2:D:137:HIS:CD2	2:D:138:PRO:N	2.87	0.41
1:A:1473:ASP:HA	1:A:1474:PRO:HD2	1.83	0.41
1:A:1970:GLN:C	1:A:1972:LEU:H	2.29	0.41
1:A:2382:MET:HG3	1:A:2549:TRP:O	2.19	0.41
2:C:127:VAL:HG12	2:C:128:ASN:N	2.34	0.41
2:C:203:ILE:HA	2:C:206:GLU:HG2	2.02	0.41
1:B:2250:ILE:O	1:B:2251:ARG:C	2.64	0.41
2:D:298:CYS:HB2	2:D:305:LYS:HE3	2.03	0.41
1:A:2500:ILE:O	1:A:2504:VAL:HG23	2.20	0.41
2:C:137:HIS:HD2	2:C:139:ASN:H	1.67	0.41
1:B:1629:ILE:HG22	1:B:1630:VAL:HG23	2.03	0.41
1:B:1895:SER:HB3	1:B:1898:ASN:O	2.20	0.41
1:B:2225:TYR:CD1	3:B:2601:P2X:H2	2.55	0.41
2:D:28:GLN:O	2:D:28:GLN:HG3	2.20	0.41
2:D:281:ASP:OD1	2:D:283:GLN:HG3	2.20	0.41
1:A:2339:ARG:NH2	1:A:2343:ASN:HB3	2.36	0.41
1:A:2347:ASP:OD1	1:A:2350:SER:OG	2.25	0.41
2:C:18:ALA:HB1	2:C:45:VAL:HG21	2.03	0.41
1:B:1453:LEU:C	1:B:1455:GLU:H	2.29	0.41
1:B:2496:LYS:HE3	1:B:2500:ILE:HD11	2.02	0.41
1:A:1422:LYS:C	1:A:1424:GLN:N	2.78	0.41
1:A:1733:ALA:O	1:A:1734:THR:C	2.64	0.41
1:A:2127:SER:HA	1:A:2128:PRO:HD3	1.93	0.41
1:A:2281:MET:HE1	2:C:222:TYR:CE2	2.56	0.41
2:C:297:TRP:CZ3	2:C:304:ILE:HG12	2.55	0.41
1:B:1425:GLN:HG2	1:B:2314:PHE:HZ	1.84	0.41
1:B:1514:ARG:HE	1:B:1542:ASP:CG	2.29	0.41
1:B:1526:TRP:CE3	1:B:1529:MET:HE2	2.55	0.41
1:B:1989:ASN:O	1:B:1993:LYS:HD2	2.21	0.41
1:A:1518:ALA:HB2	1:A:1546:TYR:OH	2.20	0.41
1:A:2023:TRP:CD2	1:A:2067:GLU:HG2	2.56	0.41
1:A:2538:LEU:C	1:A:2540:GLN:N	2.78	0.41
2:C:85:ASN:H	2:C:85:ASN:ND2	2.18	0.41
1:B:1514:ARG:HH21	1:B:1540:THR:HG21	1.86	0.41
1:B:1807:GLN:NE2	1:B:1811:ARG:HH21	2.19	0.41
1:B:1910:TRP:HZ2	1:B:1956:LEU:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2046:GLY:O	1:B:2050:VAL:HG23	2.20	0.41
1:B:2128:PRO:HD2	1:B:2129:LYS:H	1.86	0.41
1:B:2268:MET:HG3	1:B:2290:ALA:HB2	2.03	0.41
1:B:2278:LEU:HB3	1:B:2282:GLN:HB2	2.03	0.41
2:D:150:GLY:HA2	2:D:173:ILE:HG23	2.03	0.41
2:D:151:ALA:HA	2:D:166:ILE:HG22	2.03	0.41
2:D:248:ARG:CZ	2:D:248:ARG:HB3	2.51	0.41
1:A:1526:TRP:CE3	1:A:1529:MET:HE2	2.56	0.41
1:A:2275:TYR:HE1	1:A:2286:VAL:HB	1.85	0.41
1:A:2387:MET:HE1	1:A:2396:TYR:CB	2.49	0.41
2:C:82:ASP:HB2	2:C:119:LEU:HD13	2.02	0.41
2:D:263:GLY:O	2:D:264:ASN:HB3	2.21	0.41
1:B:1913:TYR:CB	1:B:1915:HIS:CE1	3.05	0.40
1:B:2189:HIS:CD2	1:B:2189:HIS:N	2.89	0.40
1:B:2530:LYS:HE2	1:B:2530:LYS:HA	2.02	0.40
2:D:127:VAL:HG12	2:D:128:ASN:N	2.35	0.40
1:A:1400:LYS:HG3	1:A:1416:LEU:HD13	2.02	0.40
1:A:1417:ILE:O	1:A:1421:ASN:ND2	2.54	0.40
1:A:1605:TYR:CE2	1:A:1612:ARG:HG2	2.57	0.40
1:A:1681:PRO:HG2	1:A:1683:ARG:HG3	2.03	0.40
1:B:2101:TRP:HA	1:B:2104:TYR:HB2	2.03	0.40
2:D:258:LEU:HD11	2:D:285:ILE:HG21	2.02	0.40
1:A:1903:THR:HG22	1:A:1938:VAL:HG21	2.02	0.40
1:B:1722:GLN:HA	1:B:1725:GLN:HE21	1.86	0.40
1:B:2297:ASP:O	1:B:2299:LEU:N	2.54	0.40
1:B:2421:PHE:HD1	1:B:2430:ARG:HH22	1.68	0.40
2:D:68:TYR:CE2	2:D:77:PRO:HD3	2.57	0.40
1:A:1670:HIS:CE1	1:A:1681:PRO:HB3	2.47	0.40
2:C:168:GLU:N	2:C:169:PRO:CD	2.84	0.40
2:C:200:THR:HB	2:C:209:GLN:HB2	2.02	0.40
2:C:239:SER:OG	2:C:240:ALA:N	2.54	0.40
1:B:1618:ILE:HG13	1:B:1618:ILE:H	1.71	0.40
1:B:1905:ARG:HD3	1:B:1905:ARG:HA	1.80	0.40
1:B:1980:SER:O	1:B:1988:HIS:HB2	2.22	0.40
2:D:85:ASN:ND2	2:D:85:ASN:H	2.19	0.40
1:A:2368:ARG:HD2	1:A:2370:LYS:O	2.21	0.40
1:A:2378:ARG:HH11	1:A:2380:THR:HG21	1.86	0.40
2:C:12:PRO:O	2:C:54:ARG:NH2	2.54	0.40
2:C:68:TYR:CE2	2:C:77:PRO:HD3	2.57	0.40
1:B:1954:GLY:O	1:B:1955:ARG:C	2.64	0.40
1:B:2332:TYR:O	1:B:2507:LYS:NZ	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:18:ALA:HB1	2:D:45:VAL:HG21	2.04	0.40
2:D:313:LYS:HA	2:D:313:LYS:HD3	1.86	0.40
1:A:1401:GLU:CG	1:A:2389:VAL:HG22	2.51	0.40
1:A:1440:PHE:C	1:A:1442:GLU:N	2.78	0.40
1:A:2332:TYR:CE1	1:A:2507:LYS:HE2	2.56	0.40
2:C:101:TYR:HA	2:C:110:ARG:O	2.20	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%)	904 (86%)	111 (11%)	31 (3%)	3	25
1	B	1052/1174 (90%)	913 (87%)	108 (10%)	31 (3%)	3	26
2	C	315/326 (97%)	266 (84%)	30 (10%)	19 (6%)	1	12
2	D	315/326 (97%)	266 (84%)	30 (10%)	19 (6%)	1	12
All	All	2728/3000 (91%)	2349 (86%)	279 (10%)	100 (4%)	2	21

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1525	GLN
1	B	1630	VAL
1	B	1650	MET
1	B	1680	ASP
1	B	1970	GLN
1	B	2094	VAL
1	B	2298	ASP
1	B	2364	VAL
2	D	74	ASN

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Mol	Chain	Res	Type
2	D	97	GLY
2	D	203	ILE
2	D	269	SER
1	A	1454	HIS
1	A	1525	GLN
1	A	1630	VAL
1	A	1650	MET
1	A	1680	ASP
1	A	1970	GLN
1	A	2094	VAL
1	A	2298	ASP
1	A	2364	VAL
2	C	35	THR
2	C	73	ASN
2	C	74	ASN
2	C	97	GLY
2	C	203	ILE
2	C	269	SER
1	B	1444	GLU
1	B	1454	HIS
1	B	1682	SER
1	B	1709	ARG
1	B	1735	GLU
1	B	1786	TRP
1	B	1914	GLY
1	B	1937	GLN
1	B	2000	GLU
2	D	35	THR
2	D	73	ASN
2	D	75	PRO
2	D	118	ASN
2	D	160	ASP
2	D	167	PRO
2	D	204	GLY
1	A	1444	GLU
1	A	1445	ILE
1	A	1682	SER
1	A	1709	ARG
1	A	1735	GLU
1	A	1786	TRP
1	A	1914	GLY
1	A	1937	GLN

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Mol	Chain	Res	Type
1	A	2000	GLU
2	C	75	PRO
2	C	118	ASN
2	C	160	ASP
2	C	167	PRO
2	C	204	GLY
1	B	1445	ILE
1	B	1896	ARG
1	B	1933	ASP
1	B	2001	HIS
1	B	2093	ASN
1	B	2135	ASP
2	D	169	PRO
2	D	264	ASN
1	A	1896	ARG
1	A	1933	ASP
1	A	2093	ASN
2	C	129	ALA
2	C	169	PRO
2	C	264	ASN
1	B	2357	ASP
1	B	2387	MET
2	D	129	ALA
1	A	2001	HIS
1	A	2135	ASP
1	A	2357	ASP
2	C	263	GLY
1	B	1583	TYR
1	B	1681	PRO
1	B	2515	HIS
2	D	140	GLN
2	D	263	GLY
1	A	1681	PRO
1	A	1784	ARG
1	A	2191	ASP
1	A	2515	HIS
2	C	262	SER
1	B	1474	PRO
1	B	2191	ASP
1	A	1474	PRO
1	A	2168	ARG
1	A	2387	MET

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Mol	Chain	Res	Type
1	B	2168	ARG
2	D	201	GLY
2	C	76	ASN
2	C	201	GLY
2	C	310	GLY
2	D	76	ASN
2	D	310	GLY

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%)	818 (88%)	109 (12%)	5	24
1	B	931/1024 (91%)	818 (88%)	113 (12%)	5	23
2	C	269/276 (98%)	229 (85%)	40 (15%)	3	17
2	D	269/276 (98%)	229 (85%)	40 (15%)	3	17
All	All	2396/2600 (92%)	2094 (87%)	302 (13%)	4	22

All (302) 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	1473	ASP
1	B	1475	GLU
1	B	1501	TRP
1	B	1509	GLN
1	B	1528	SER
1	B	1540	THR
1	B	1541	HIS
1	B	1559	LEU

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Mol	Chain	Res	Type
1	B	1576	THR
1	B	1590	MET
1	B	1598	GLU
1	B	1611	ARG
1	B	1630	VAL
1	B	1643	VAL
1	B	1644	VAL
1	B	1650	MET
1	B	1685	LEU
1	B	1709	ARG
1	B	1740	LYS
1	B	1767	SER
1	B	1768	THR
1	B	1780	THR
1	B	1781	GLU
1	B	1799	GLU
1	B	1870	THR
1	B	1876	THR
1	B	1878	LEU
1	B	1891	SER
1	B	1895	SER
1	B	1896	ARG
1	B	1898	ASN
1	B	1899	ASN
1	B	1908	THR
1	B	1916	TRP
1	B	1930	ILE
1	B	1932	ILE
1	B	1938	VAL
1	B	1956	LEU
1	B	1968	HIS
1	B	1973	ILE
1	B	1984	THR
1	B	1985	THR
1	B	2005	LEU
1	B	2011	MET
1	B	2021	ILE
1	B	2035	SER
1	B	2068	THR
1	B	2072	GLN
1	B	2076	ARG
1	B	2077	ASP

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Mol	Chain	Res	Type
1	B	2078	LEU
1	B	2080	GLU
1	B	2093	ASN
1	B	2095	LYS
1	B	2098	THR
1	B	2102	ASP
1	B	2123	LEU
1	B	2124	GLN
1	B	2136	LEU
1	B	2138	LEU
1	B	2152	ARG
1	B	2154	GLN
1	B	2155	SER
1	B	2164	THR
1	B	2165	SER
1	B	2167	GLN
1	B	2168	ARG
1	B	2173	THR
1	B	2181	GLU
1	B	2183	VAL
1	B	2185	LEU
1	B	2189	HIS
1	B	2190	GLU
1	B	2228	ILE
1	B	2232	THR
1	B	2240	VAL
1	B	2244	ASP
1	B	2245	THR
1	B	2254	ARG
1	B	2259	ILE
1	B	2260	LEU
1	B	2263	ILE
1	B	2266	ARG
1	B	2281	MET
1	B	2294	THR
1	B	2301	LYS
1	B	2318	THR
1	B	2342	SER
1	B	2354	LEU
1	B	2363	GLU
1	B	2367	THR
1	B	2378	ARG

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Mol	Chain	Res	Type
1	B	2383	LEU
1	B	2384	THR
1	B	2390	THR
1	B	2397	ARG
1	B	2408	ARG
1	B	2430	ARG
1	B	2431	LEU
1	B	2432	MET
1	B	2503	ARG
1	B	2512	ASP
1	B	2515	HIS
1	B	2519	LEU
1	B	2530	LYS
1	B	2533	THR
1	B	2538	LEU
2	D	10	SER
2	D	13	VAL
2	D	37	THR
2	D	44	GLN
2	D	84	VAL
2	D	85	ASN
2	D	86	LYS
2	D	91	VAL
2	D	98	ARG
2	D	123	ARG
2	D	128	ASN
2	D	134	VAL
2	D	140	GLN
2	D	159	THR
2	D	160	ASP
2	D	162	ASN
2	D	164	GLN
2	D	166	ILE
2	D	168	GLU
2	D	169	PRO
2	D	170	GLU
2	D	173	ILE
2	D	174	THR
2	D	175	SER
2	D	183	SER
2	D	188	VAL
2	D	199	LEU

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Mol	Chain	Res	Type
2	D	214	THR
2	D	215	LYS
2	D	220	THR
2	D	242	GLN
2	D	243	THR
2	D	248	ARG
2	D	261	LYS
2	D	262	SER
2	D	286	VAL
2	D	287	THR
2	D	289	SER
2	D	301	THR
2	D	312	GLN
1	A	1417	ILE
1	A	1420	ASN
1	A	1423	LEU
1	A	1443	LEU
1	A	1445	ILE
1	A	1457	GLU
1	A	1473	ASP
1	A	1475	GLU
1	A	1501	TRP
1	A	1509	GLN
1	A	1540	THR
1	A	1541	HIS
1	A	1559	LEU
1	A	1576	THR
1	A	1590	MET
1	A	1598	GLU
1	A	1611	ARG
1	A	1630	VAL
1	A	1643	VAL
1	A	1644	VAL
1	A	1650	MET
1	A	1685	LEU
1	A	1709	ARG
1	A	1740	LYS
1	A	1767	SER
1	A	1768	THR
1	A	1780	THR
1	A	1781	GLU
1	A	1799	GLU

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Mol	Chain	Res	Type
1	A	1870	THR
1	A	1878	LEU
1	A	1891	SER
1	A	1895	SER
1	A	1896	ARG
1	A	1899	ASN
1	A	1901	GLN
1	A	1908	THR
1	A	1916	TRP
1	A	1930	ILE
1	A	1932	ILE
1	A	1938	VAL
1	A	1956	LEU
1	A	1968	HIS
1	A	1973	ILE
1	A	1984	THR
1	A	1985	THR
1	A	2005	LEU
1	A	2011	MET
1	A	2021	ILE
1	A	2035	SER
1	A	2068	THR
1	A	2072	GLN
1	A	2076	ARG
1	A	2077	ASP
1	A	2078	LEU
1	A	2080	GLU
1	A	2093	ASN
1	A	2095	LYS
1	A	2098	THR
1	A	2102	ASP
1	A	2123	LEU
1	A	2124	GLN
1	A	2138	LEU
1	A	2152	ARG
1	A	2154	GLN
1	A	2155	SER
1	A	2164	THR
1	A	2165	SER
1	A	2167	GLN
1	A	2168	ARG
1	A	2173	THR

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Mol	Chain	Res	Type
1	A	2181	GLU
1	A	2183	VAL
1	A	2185	LEU
1	A	2189	HIS
1	A	2190	GLU
1	A	2228	ILE
1	A	2232	THR
1	A	2240	VAL
1	A	2244	ASP
1	A	2245	THR
1	A	2254	ARG
1	A	2259	ILE
1	A	2260	LEU
1	A	2263	ILE
1	A	2266	ARG
1	A	2281	MET
1	A	2301	LYS
1	A	2318	THR
1	A	2342	SER
1	A	2354	LEU
1	A	2363	GLU
1	A	2367	THR
1	A	2378	ARG
1	A	2383	LEU
1	A	2384	THR
1	A	2390	THR
1	A	2397	ARG
1	A	2408	ARG
1	A	2430	ARG
1	A	2431	LEU
1	A	2432	MET
1	A	2503	ARG
1	A	2515	HIS
1	A	2519	LEU
1	A	2527	LEU
1	A	2530	LYS
1	A	2533	THR
1	A	2538	LEU
2	C	10	SER
2	C	13	VAL
2	C	37	THR
2	C	44	GLN

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Mol	Chain	Res	Type
2	C	84	VAL
2	C	85	ASN
2	C	86	LYS
2	C	91	VAL
2	C	98	ARG
2	C	123	ARG
2	C	128	ASN
2	C	134	VAL
2	C	140	GLN
2	C	159	THR
2	C	160	ASP
2	C	162	ASN
2	C	164	GLN
2	C	166	ILE
2	C	168	GLU
2	C	169	PRO
2	C	170	GLU
2	C	173	ILE
2	C	174	THR
2	C	175	SER
2	C	183	SER
2	C	188	VAL
2	C	199	LEU
2	C	214	THR
2	C	215	LYS
2	C	220	THR
2	C	242	GLN
2	C	243	THR
2	C	248	ARG
2	C	261	LYS
2	C	262	SER
2	C	286	VAL
2	C	287	THR
2	C	289	SER
2	C	301	THR
2	C	312	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1398	HIS
1	B	1496	GLN

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Mol	Chain	Res	Type
1	B	1541	HIS
1	B	1624	GLN
1	B	1670	HIS
1	B	1687	HIS
1	B	1695	GLN
1	B	1727	GLN
1	B	1730	HIS
1	B	1739	HIS
1	B	1744	HIS
1	B	1760	ASN
1	B	1807	GLN
1	B	1898	ASN
1	B	1915	HIS
1	B	1920	ASN
1	B	1941	GLN
1	B	1958	HIS
1	B	1970	GLN
1	B	2028	HIS
1	B	2082	GLN
1	B	2093	ASN
1	B	2154	GLN
1	B	2161	GLN
1	B	2167	GLN
1	B	2189	HIS
1	B	2262	ASN
1	B	2277	HIS
1	B	2292	ASN
1	B	2293	ASN
1	B	2385	ASN
1	B	2395	ASN
1	B	2401	HIS
1	B	2428	ASN
1	B	2499	GLN
1	B	2502	ASN
2	D	22	HIS
2	D	30	HIS
2	D	41	GLN
2	D	63	GLN
2	D	74	ASN
2	D	85	ASN
2	D	94	HIS
2	D	118	ASN

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Mol	Chain	Res	Type
2	D	128	ASN
2	D	132	ASN
2	D	137	HIS
2	D	140	GLN
2	D	161	HIS
2	D	242	GLN
2	D	311	HIS
2	D	312	GLN
1	A	1398	HIS
1	A	1421	ASN
1	A	1496	GLN
1	A	1541	HIS
1	A	1561	GLN
1	A	1562	GLN
1	A	1594	HIS
1	A	1624	GLN
1	A	1670	HIS
1	A	1687	HIS
1	A	1719	HIS
1	A	1725	GLN
1	A	1727	GLN
1	A	1739	HIS
1	A	1744	HIS
1	A	1760	ASN
1	A	1898	ASN
1	A	1920	ASN
1	A	1941	GLN
1	A	1958	HIS
1	A	1970	GLN
1	A	2028	HIS
1	A	2082	GLN
1	A	2093	ASN
1	A	2154	GLN
1	A	2161	GLN
1	A	2167	GLN
1	A	2189	HIS
1	A	2262	ASN
1	A	2277	HIS
1	A	2292	ASN
1	A	2385	ASN
1	A	2395	ASN
1	A	2401	HIS

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Mol	Chain	Res	Type
1	A	2428	ASN
1	A	2499	GLN
1	A	2502	ASN
2	C	22	HIS
2	C	30	HIS
2	C	41	GLN
2	C	63	GLN
2	C	73	ASN
2	C	74	ASN
2	C	85	ASN
2	C	94	HIS
2	C	118	ASN
2	C	128	ASN
2	C	137	HIS
2	C	140	GLN
2	C	153	HIS
2	C	161	HIS
2	C	311	HIS
2	C	312	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](#)

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	P2X	A	2601	-	26,26,26	1.73	2 (7%)	37,39,39	3.06	20 (54%)
3	P2X	B	2601	-	26,26,26	1.73	4 (15%)	37,39,39	3.15	20 (54%)

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	P2X	A	2601	-	-	3/8/8/8	0/4/4/4
3	P2X	B	2601	-	-	4/8/8/8	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2601	P2X	C11-N2	5.46	1.42	1.36
3	B	2601	P2X	C17-C18	4.81	1.48	1.41
3	A	2601	P2X	C17-C18	4.78	1.48	1.41
3	B	2601	P2X	C11-N2	4.66	1.41	1.36
3	B	2601	P2X	C10-C15	-2.98	1.39	1.42
3	B	2601	P2X	C23-C21	2.00	1.42	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2601	P2X	C10-C11-N4	-7.56	118.95	126.97
3	B	2601	P2X	C10-C11-N4	-7.15	119.39	126.97
3	B	2601	P2X	C20-C17-C18	5.57	122.58	119.13
3	B	2601	P2X	N6-C19-N4	-5.32	120.52	128.58
3	A	2601	P2X	C9-N3-N2	5.27	109.73	106.95
3	B	2601	P2X	C9-N3-N2	5.13	109.65	106.95
3	B	2601	P2X	N4-C11-N2	4.92	132.46	126.05
3	A	2601	P2X	N4-C11-N2	4.89	132.42	126.05
3	A	2601	P2X	C20-C17-C18	4.79	122.09	119.13
3	A	2601	P2X	N6-C19-N4	-4.77	121.36	128.58
3	B	2601	P2X	C15-C10-C9	-4.62	134.46	139.09
3	A	2601	P2X	C17-C16-C12	-4.58	103.31	107.41
3	B	2601	P2X	C21-C18-C17	-4.54	118.02	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2601	P2X	C10-C9-N3	-4.53	107.10	110.19
3	A	2601	P2X	C11-N2-N3	-4.14	108.25	110.90
3	B	2601	P2X	C15-C10-C11	4.13	118.83	115.74
3	A	2601	P2X	C18-C17-C16	4.00	110.08	106.80
3	B	2601	P2X	C11-N2-N3	-3.94	108.38	110.90
3	A	2601	P2X	C15-C10-C11	3.79	118.58	115.74
3	A	2601	P2X	C19-N4-C11	3.72	120.92	111.83
3	B	2601	P2X	C19-N4-C11	3.64	120.72	111.83
3	B	2601	P2X	C17-C16-C12	-3.58	104.21	107.41
3	A	2601	P2X	C21-C18-C17	-3.56	118.91	122.13
3	B	2601	P2X	C21-C23-C22	3.42	123.49	119.88
3	A	2601	P2X	C10-C9-N3	-3.39	107.88	110.19
3	A	2601	P2X	C21-C23-C22	3.25	123.31	119.88
3	A	2601	P2X	C15-C10-C9	-3.17	135.91	139.09
3	A	2601	P2X	C17-C18-N5	-3.15	104.37	107.65
3	A	2601	P2X	C17-C20-C22	-3.05	117.74	120.92
3	B	2601	P2X	C16-C12-C9	-3.03	119.47	131.53
3	B	2601	P2X	C18-C17-C16	2.98	109.25	106.80
3	A	2601	P2X	C16-C12-N5	2.93	112.06	109.15
3	B	2601	P2X	C21-C18-N5	2.93	136.75	130.83
3	A	2601	P2X	C21-C18-N5	2.91	136.72	130.83
3	B	2601	P2X	C16-C12-N5	2.86	111.98	109.15
3	B	2601	P2X	C11-C10-C9	2.86	106.71	104.73
3	A	2601	P2X	C16-C12-C9	-2.77	120.48	131.53
3	B	2601	P2X	C17-C20-C22	-2.72	118.08	120.92
3	B	2601	P2X	C17-C18-N5	-2.32	105.23	107.65
3	A	2601	P2X	C10-C11-N2	2.27	108.63	107.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

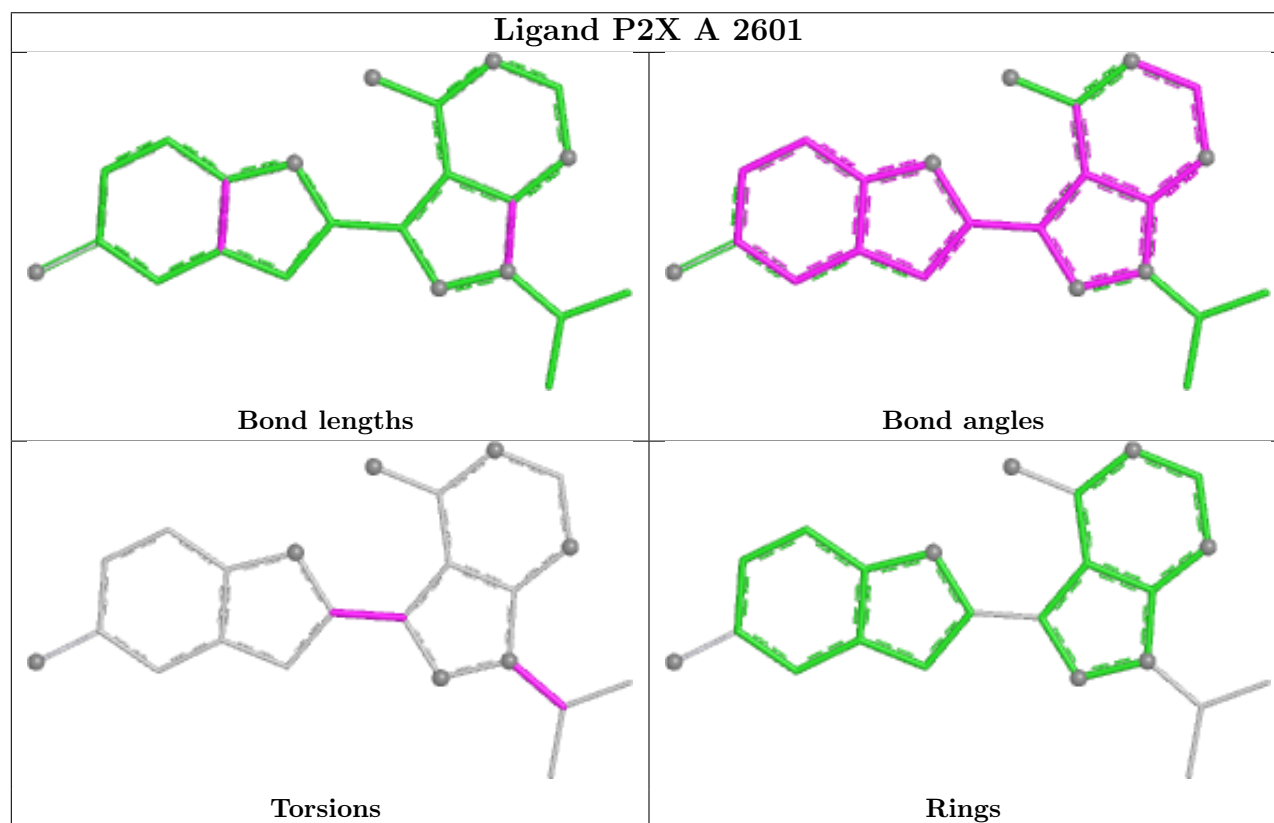
Mol	Chain	Res	Type	Atoms
3	B	2601	P2X	N5-C12-C9-N3
3	B	2601	P2X	C13-C8-N2-C11
3	B	2601	P2X	C13-C8-N2-N3
3	A	2601	P2X	C13-C8-N2-C11
3	A	2601	P2X	C13-C8-N2-N3
3	A	2601	P2X	N5-C12-C9-N3
3	B	2601	P2X	C16-C12-C9-N3

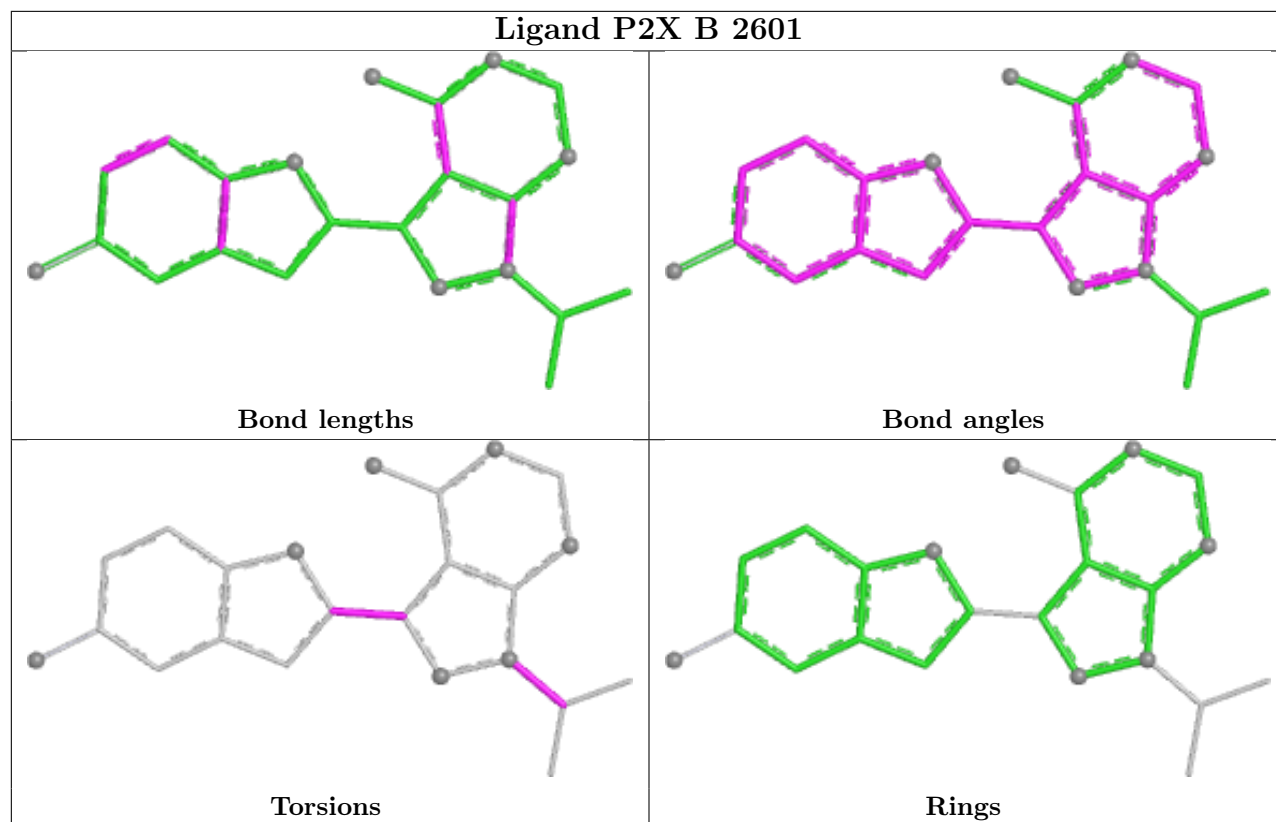
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2601	P2X	3	0
3	B	2601	P2X	4	0

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





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%)	0.51	78 (7%) 20 14	26, 62, 152, 178	0
1	B	1058/1174 (90%)	0.26	38 (3%) 46 27	23, 53, 128, 168	0
2	C	317/326 (97%)	0.43	14 (4%) 39 23	29, 61, 115, 156	0
2	D	317/326 (97%)	0.09	12 (3%) 44 26	23, 40, 91, 142	0
All	All	2746/3000 (91%)	0.35	142 (5%) 33 20	23, 56, 140, 178	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1504	VAL	5.8
1	A	1619	TRP	5.8
2	C	8	VAL	5.2
1	A	1599	LEU	5.0
2	D	203	ILE	4.8
2	C	203	ILE	4.8
1	A	1603	ILE	4.5
1	B	1578	MET	4.3
1	A	1586	ALA	4.1
1	B	2434	THR	4.0
1	A	1504	VAL	3.8
1	A	1595	MET	3.8
1	B	1583	TYR	3.8
1	A	1443	LEU	3.7
1	A	1584	SER	3.6
1	A	1604	GLN	3.6
1	A	2434	THR	3.6
1	B	1587	TYR	3.5
1	A	2436	THR	3.5
1	A	1602	VAL	3.5
2	C	119	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	1584	SER	3.5
1	B	1575	LEU	3.4
1	A	1585	ARG	3.4
1	A	1587	TYR	3.3
2	D	207	VAL	3.3
1	B	1585	ARG	3.2
1	B	1607	LEU	3.2
1	A	2048	PHE	3.2
1	A	1583	TYR	3.2
1	A	1546	TYR	3.2
1	B	1586	ALA	3.2
1	A	1614	ILE	3.2
1	A	1549	VAL	3.1
2	C	207	VAL	3.1
1	A	1629	ILE	3.1
1	A	1472	ASP	3.1
2	D	8	VAL	3.0
1	A	1575	LEU	3.0
1	A	1502	THR	3.0
1	A	1469	THR	2.9
1	A	1552	LEU	2.9
1	B	1546	TYR	2.9
1	B	1475	GLU	2.9
1	A	1639	VAL	2.9
1	B	1469	THR	2.8
2	C	9	GLY	2.7
2	C	324	VAL	2.7
1	B	2429	TRP	2.7
1	A	1630	VAL	2.7
1	A	1503	LEU	2.7
1	A	1682	SER	2.7
1	A	1611	ARG	2.7
1	A	1615	ILE	2.7
1	A	1633	TRP	2.7
1	A	1559	LEU	2.7
1	B	1472	ASP	2.7
1	A	1730	HIS	2.7
2	C	202	GLY	2.6
1	B	1649	ASP	2.6
1	A	2079	MET	2.6
1	B	1443	LEU	2.6
1	A	1461	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1548	ALA	2.6
2	C	269	SER	2.6
1	A	1606	LYS	2.6
1	A	2053	PRO	2.5
1	B	1682	SER	2.5
1	A	2063	GLN	2.5
1	B	1581	GLU	2.5
1	A	1733	ALA	2.5
1	A	1582	SER	2.5
1	A	1566	LYS	2.5
1	A	2038	TYR	2.5
2	C	265	PRO	2.5
2	D	119	LEU	2.5
2	D	265	PRO	2.4
1	B	1580	GLY	2.4
1	A	2044	VAL	2.4
1	A	2494	ASN	2.4
2	C	204	GLY	2.4
1	A	2032	GLU	2.4
1	B	2492	ALA	2.4
1	B	1576	THR	2.4
2	D	208	THR	2.4
1	A	1580	GLY	2.4
1	A	2428	ASN	2.4
1	A	1810	ALA	2.4
1	B	1632	ASP	2.3
1	B	1630	VAL	2.3
1	A	1468	ASP	2.3
1	B	1500	LYS	2.3
1	A	1646	PRO	2.3
1	A	1578	MET	2.3
2	D	200	THR	2.3
1	A	1539	ASP	2.3
2	D	324	VAL	2.3
1	B	1445	ILE	2.2
1	B	1732	ILE	2.2
1	A	1576	THR	2.2
2	C	10	SER	2.2
1	A	1457	GLU	2.2
1	A	1601	GLU	2.2
1	A	2103	LEU	2.2
1	A	1653	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	2429	TRP	2.2
1	A	1544	ALA	2.2
1	A	1628	ARG	2.2
2	D	269	SER	2.2
1	A	2435	ASN	2.2
2	C	208	THR	2.1
1	B	1614	ILE	2.1
1	A	1623	LEU	2.1
1	A	1640	ARG	2.1
1	A	2039	PHE	2.1
1	B	2044	VAL	2.1
1	A	1656	TYR	2.1
1	A	1600	GLU	2.1
1	B	1501	TRP	2.1
1	B	2103	LEU	2.1
1	B	2436	THR	2.1
2	C	68	TYR	2.1
2	D	202	GLY	2.1
1	B	1582	SER	2.1
2	C	262	SER	2.1
1	B	1629	ILE	2.1
1	B	1814	LYS	2.1
1	A	2118	LEU	2.1
2	D	204	GLY	2.1
1	A	1496	GLN	2.0
1	A	1475	GLU	2.0
1	A	2095	LYS	2.0
1	A	1564	ILE	2.0
1	A	1535	MET	2.0
1	B	1579	ALA	2.0
1	A	1388	ALA	2.0
1	A	1734	THR	2.0
1	A	2492	ALA	2.0
2	D	263	GLY	2.0
1	B	1457	GLU	2.0
1	B	1453	LEU	2.0
1	A	2431	LEU	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](#)

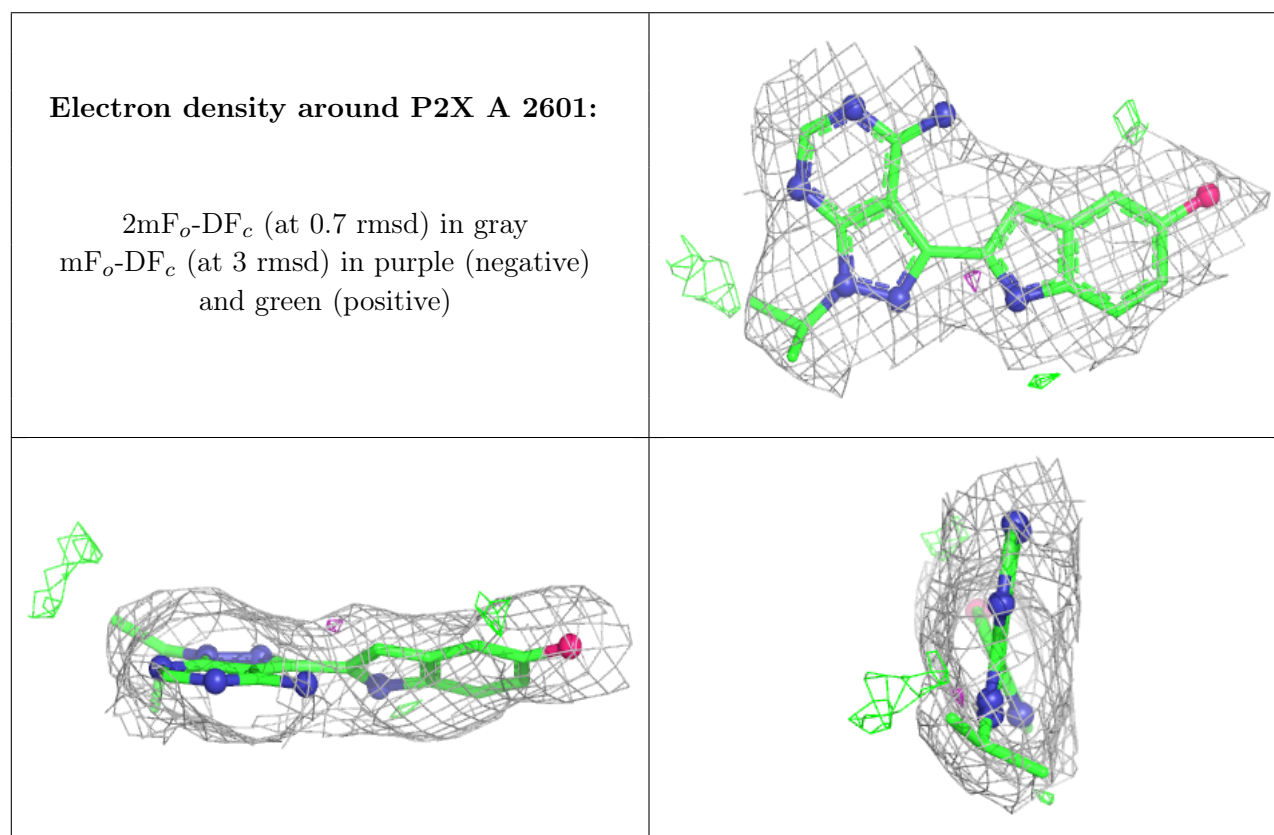
There are no oligosaccharides in this entry.

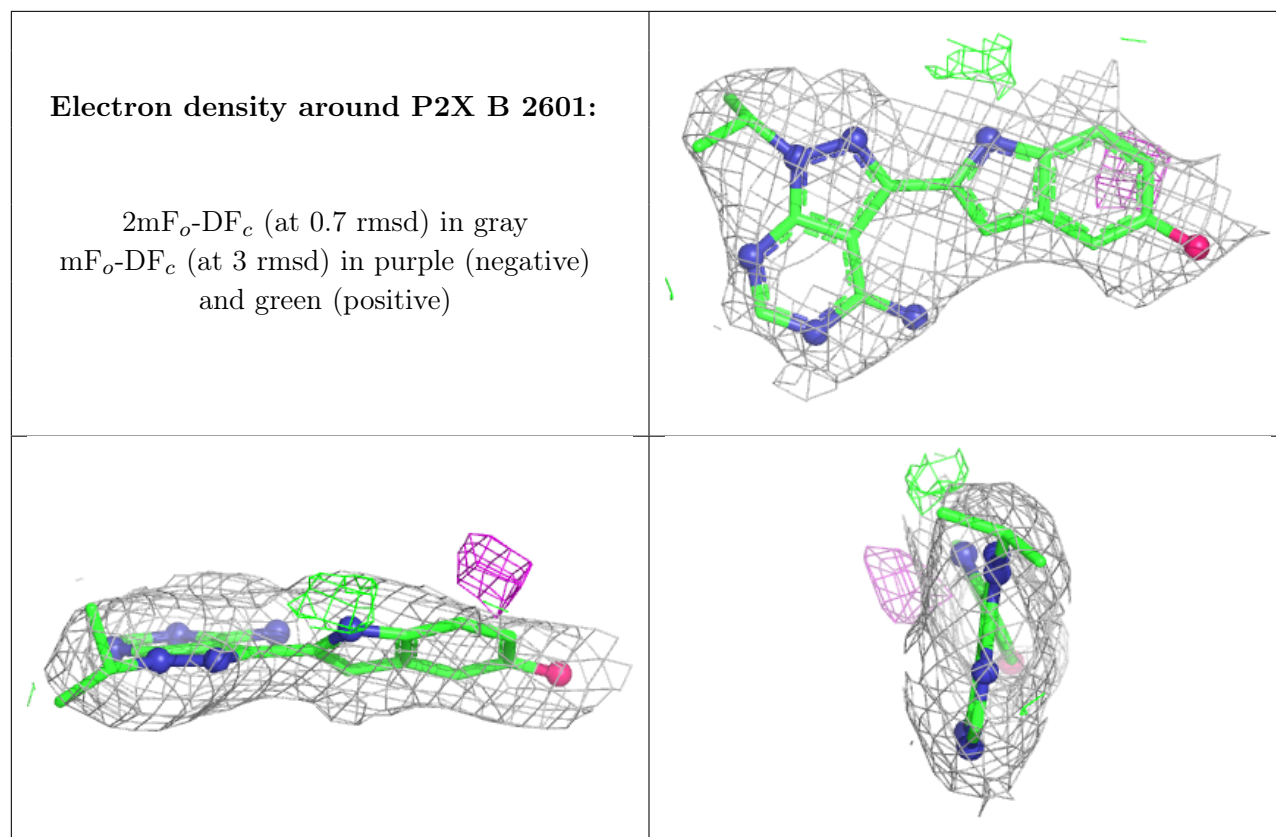
6.4 Ligands [i](#)

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	P2X	A	2601	23/23	0.93	0.11	37,37,38,38	0
3	P2X	B	2601	23/23	0.95	0.10	33,34,35,35	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.