



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:12 AM UTC

PDB ID : 4JSX / pdb_00004jsx
Title : structure of mTORDeltaN-mLST8-Torin2 complex
Authors : Pavletich, N.P.; Yang, H.
Deposited on : 2013-03-22
Resolution : 3.50 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

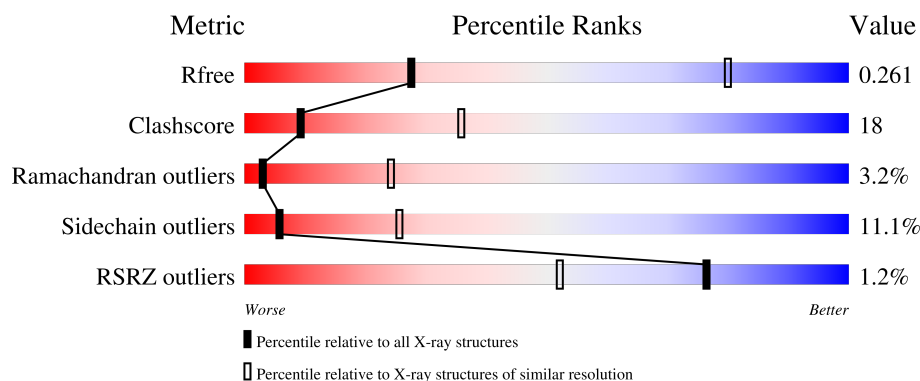
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	% 56% 29% 5% 10%
1	B	1174	% 56% 29% 5% 10%
2	C	326	% 50% 37% 9% ..
2	D	326	% 49% 38% 9% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	17G	A	2601	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 22160 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.

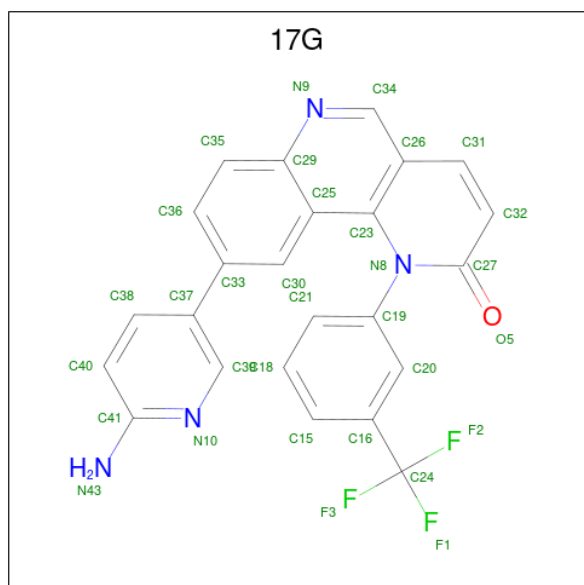
- Molecule 1 is a protein called Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1058	Total	C	N	O	S	0	0	0
			8607	5472	1520	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			

- Molecule 3 is 9-(6-aminopyridin-3-yl)-1-[3-(trifluoromethyl)phenyl]benzo[h][1,6]naphthyridine-2(1H)-one (CCD ID: 17G) (formula: C₂₄H₁₅F₃N₄O).

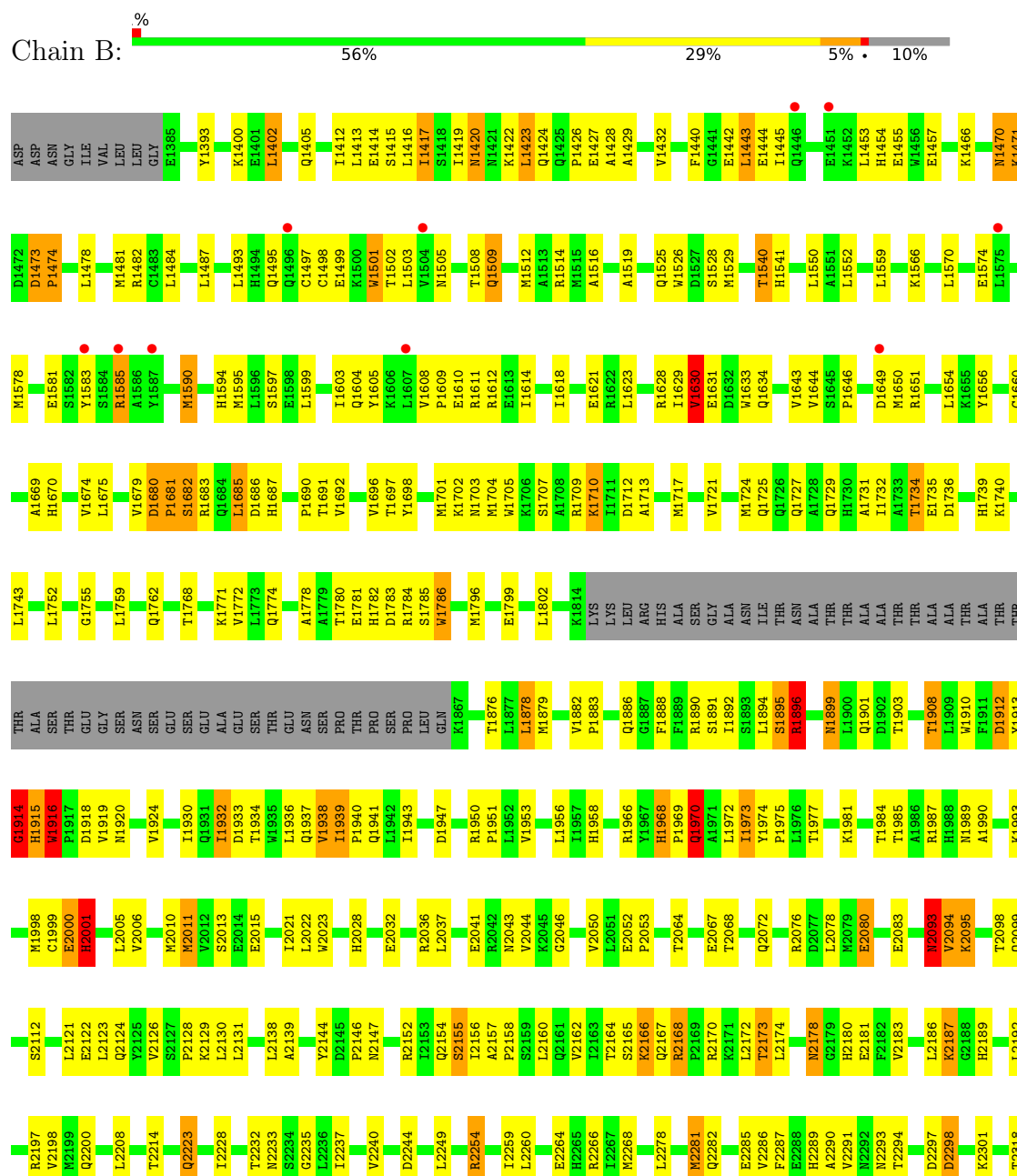


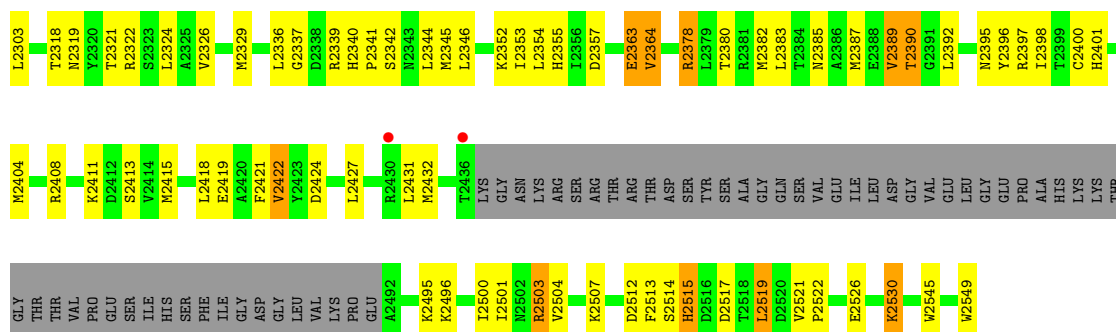
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			32	24	3	4	1		
3	A	1	Total	C	F	N	O	0	0
			32	24	3	4	1		

3 Residue-property plots

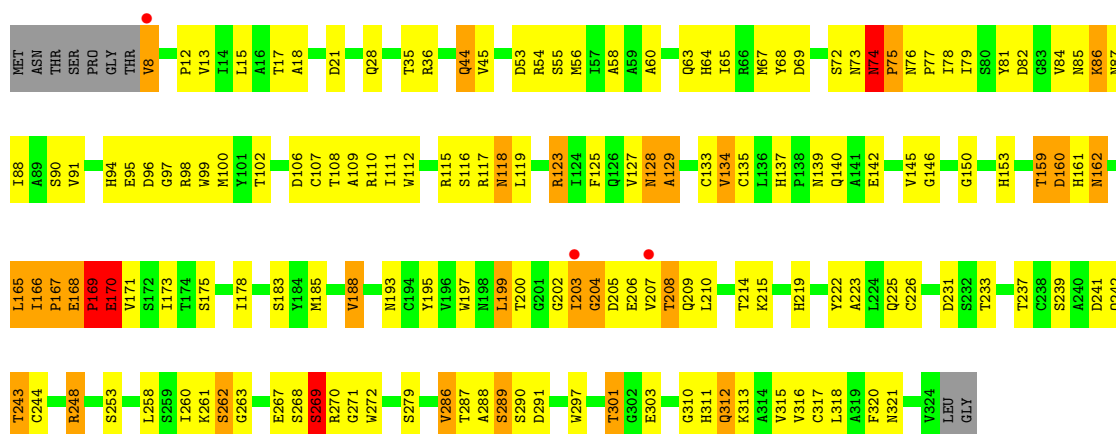
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Serine/threonine-protein kinase mTOR

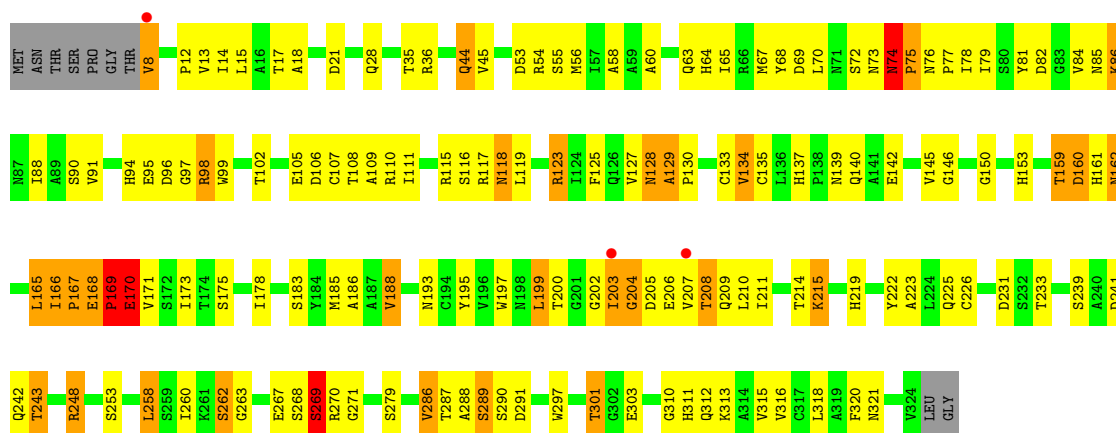




• Molecule 2: Target of rapamycin complex subunit LST8



• Molecule 2: Target of rapamycin complex subunit LST8



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 – 3.50 39.67 – 3.50	Depositor EDS
% Data completeness (in resolution range)	84.2 (39.67-3.50) 84.3 (39.67-3.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.224 , 0.257 0.227 , 0.261	Depositor DCC
R_{free} test set	1774 reflections (2.89%)	wwPDB-VP
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22160	wwPDB-VP
Average B, all atoms (Å ²)	75.0	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 44.36 % 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 1.5437e-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: 17G

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	0.46	0/8772	0.95	12/11872 (0.1%)
1	B	0.47	0/8804	0.96	10/11918 (0.1%)
2	C	0.49	0/2514	0.92	5/3426 (0.1%)
2	D	0.53	0/2514	0.95	6/3426 (0.2%)
All	All	0.48	0/22604	0.95	33/30642 (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	2
2	C	0	1
2	D	0	1
All	All	0	6

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1915	HIS	N-CA-C	11.06	126.32	108.63
1	A	1915	HIS	N-CA-C	11.02	126.26	108.63
2	D	170	GLU	N-CA-C	-9.06	101.19	112.88
1	B	1916	TRP	CA-C-N	8.69	130.70	119.84
1	B	1916	TRP	C-N-CA	8.69	130.70	119.84
1	A	1916	TRP	CA-C-N	8.21	130.11	119.84
1	A	1916	TRP	C-N-CA	8.21	130.11	119.84
2	C	170	GLU	N-CA-C	-8.02	102.54	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1443	LEU	N-CA-C	-7.21	104.37	113.02
1	A	1443	LEU	N-CA-C	-7.00	104.61	113.02
1	A	1473	ASP	CA-C-N	6.51	127.98	119.84
1	A	1473	ASP	C-N-CA	6.51	127.98	119.84
1	B	1473	ASP	CA-C-N	6.44	127.89	119.84
1	B	1473	ASP	C-N-CA	6.44	127.89	119.84
1	A	1687	HIS	CA-C-N	6.27	126.28	119.89
1	A	1687	HIS	C-N-CA	6.27	126.28	119.89
1	B	1687	HIS	CA-C-N	5.94	125.95	119.89
1	B	1687	HIS	C-N-CA	5.94	125.95	119.89
2	D	321	ASN	N-CA-C	5.76	118.50	108.76
2	C	321	ASN	N-CA-C	5.75	118.47	108.76
2	D	169	PRO	N-CA-C	5.64	124.09	112.47
2	C	169	PRO	N-CA-C	5.61	124.03	112.47
1	B	1502	THR	N-CA-C	-5.53	105.17	111.14
1	A	2422	VAL	N-CA-C	-5.46	105.05	111.00
2	C	206	GLU	N-CA-C	5.40	117.84	110.55
1	A	1935	TRP	N-CA-C	5.33	118.88	112.38
2	D	206	GLU	N-CA-C	5.31	117.72	110.55
1	A	1502	THR	N-CA-C	-5.21	105.51	111.14
1	A	1710	LYS	N-CA-C	5.21	119.79	113.38
2	D	317	CYS	N-CA-C	5.20	117.93	109.24
2	C	98	ARG	N-CA-C	5.06	119.54	113.17
2	D	87	ASN	N-CA-C	5.03	117.19	110.35
1	B	1710	LYS	N-CA-C	5.03	119.56	113.38

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1914	GLY	Peptide
1	A	2000	GLU	Peptide
1	B	1914	GLY	Peptide
1	B	2000	GLU	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	276	0
1	B	8607	0	8592	279	0
2	C	2456	0	2341	123	0
2	D	2456	0	2341	127	0
3	A	32	0	15	9	0
3	B	32	0	15	5	0
All	All	22160	0	21863	798	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 18.

All (798) 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:D:76:ASN:HB3	2:D:77:PRO:HD2	1.30	1.13
2:C:76:ASN:HB3	2:C:77:PRO:HD2	1.29	1.13
2:D:146:GLY:HA3	2:D:173:ILE:HD11	1.33	1.06
2:C:146:GLY:HA3	2:C:173:ILE:HD11	1.33	1.04
1:A:1418:SER:HB2	1:A:1581:GLU:HG2	1.35	1.03
1:A:1908:THR:O	1:A:1912:ASP:HB2	1.65	0.97
2:D:231:ASP:HB3	2:D:233:THR:OG1	1.64	0.96
1:B:1908:THR:O	1:B:1912:ASP:HB2	1.65	0.96
2:C:231:ASP:HB3	2:C:233:THR:OG1	1.67	0.93
1:A:1969:PRO:O	1:A:1970:GLN:HB2	1.66	0.92
1:B:1422:LYS:HE2	1:B:1581:GLU:HG3	1.50	0.92
1:A:2380:THR:HG22	1:A:2383:LEU:HG	1.53	0.89
1:B:1969:PRO:O	1:B:1970:GLN:HB2	1.73	0.87
1:A:1892:ILE:HG21	1:A:1930:ILE:HD11	1.57	0.86
1:B:2380:THR:HG22	1:B:2383:LEU:HG	1.55	0.85
2:D:117:ARG:O	2:D:118:ASN:HB2	1.77	0.85
1:B:2281:MET:HE1	2:D:222:TYR:CD2	2.13	0.84
2:D:167:PRO:HD2	2:D:169:PRO:HG2	1.60	0.83
2:C:117:ARG:O	2:C:118:ASN:HB2	1.78	0.83
2:D:76:ASN:HB3	2:D:77:PRO:CD	2.07	0.83
2:C:76:ASN:HB3	2:C:77:PRO:CD	2.07	0.82
1:A:2344:LEU:HD13	1:A:2353:ILE:HD11	1.61	0.82
1:A:2160:LEU:HD22	1:A:2172:LEU:HA	1.63	0.81
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.13	0.80
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:167:PRO:HD2	2:C:169:PRO:HG2	1.63	0.79
1:A:1611:ARG:HH11	1:A:1614:ILE:HG21	1.47	0.79
1:B:1998:MET:HA	1:B:2001:HIS:HD2	1.47	0.79
1:A:2011:MET:HE2	1:A:2129:LYS:HB3	1.65	0.78
1:B:1892:ILE:HG21	1:B:1930:ILE:HD11	1.66	0.78
1:B:2390:THR:HG23	1:B:2390:THR:O	1.84	0.78
1:B:2160:LEU:HD22	1:B:2172:LEU:HA	1.66	0.78
1:A:1998:MET:HA	1:A:2001:HIS:HD2	1.46	0.78
1:B:1611:ARG:HH11	1:B:1614:ILE:HG21	1.48	0.77
1:B:2011:MET:HE2	1:B:2129:LYS:HB3	1.65	0.77
1:B:1428:ALA:HB2	1:B:2395:ASN:HD21	1.49	0.77
1:B:1901:GLN:HG3	1:B:2413:SER:HA	1.67	0.77
1:B:2095:LYS:O	1:B:2099:GLN:HG2	1.84	0.77
1:A:2095:LYS:O	1:A:2099:GLN:HG2	1.85	0.76
1:A:1670:HIS:HE1	1:A:1681:PRO:HB3	1.50	0.76
1:A:1958:HIS:CE1	1:A:1990:ALA:HB1	2.21	0.75
1:B:2344:LEU:HD13	1:B:2353:ILE:HD11	1.68	0.75
2:D:150:GLY:HA3	2:D:169:PRO:HB3	1.68	0.75
1:A:1427:GLU:HB2	1:A:2398:ILE:HD13	1.69	0.74
2:D:107:CYS:HB3	2:D:127:VAL:O	1.86	0.74
1:A:1422:LYS:HE2	1:A:1581:GLU:HG3	1.68	0.74
1:B:1941:GLN:HE22	1:B:2200:GLN:HE22	1.35	0.74
1:A:2421:PHE:HA	1:A:2424:ASP:HB2	1.69	0.74
1:B:2421:PHE:HA	1:B:2424:ASP:HB2	1.70	0.74
1:A:2281:MET:HE1	2:C:222:TYR:CD2	2.22	0.73
1:A:1892:ILE:CG2	1:A:1930:ILE:HD11	2.16	0.73
1:A:1901:GLN:HG3	1:A:2413:SER:HA	1.70	0.73
1:B:1427:GLU:HB2	1:B:2398:ILE:HD13	1.70	0.73
2:D:69:ASP:HB2	2:D:78:ILE:HD11	1.70	0.73
3:B:2601:17G:H8	3:B:2601:17G:C19	2.18	0.73
2:C:108:THR:OG1	2:C:110:ARG:NH1	2.21	0.73
2:D:123:ARG:NH2	2:D:160:ASP:OD1	2.20	0.73
2:C:150:GLY:HA3	2:C:169:PRO:HB3	1.70	0.73
1:A:2390:THR:HG23	1:A:2390:THR:O	1.89	0.73
2:D:95:GLU:HB2	2:D:140:GLN:NE2	2.02	0.73
2:C:107:CYS:HB3	2:C:127:VAL:O	1.87	0.73
2:D:108:THR:OG1	2:D:110:ARG:NH1	2.21	0.72
1:B:1958:HIS:CE1	1:B:1990:ALA:HB1	2.23	0.72
2:D:55:SER:O	2:D:56:MET:HG2	1.89	0.72
1:A:1734:THR:C	1:A:1736:ASP:H	1.95	0.72
3:A:2601:17G:H8	3:A:2601:17G:C19	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2093:ASN:O	1:A:2094:VAL:HB	1.91	0.71
1:B:2093:ASN:O	1:B:2094:VAL:HB	1.89	0.71
1:A:1428:ALA:HB2	1:A:2395:ASN:HD21	1.56	0.70
2:C:95:GLU:HB2	2:C:140:GLN:NE2	2.05	0.70
1:B:1422:LYS:HE2	1:B:1581:GLU:CG	2.21	0.70
2:C:69:ASP:HB2	2:C:78:ILE:HD11	1.72	0.70
1:B:2515:HIS:N	1:B:2515:HIS:ND1	2.39	0.69
1:A:2515:HIS:ND1	1:A:2515:HIS:N	2.39	0.69
1:A:2178:ASN:HD22	1:A:2180:HIS:H	1.39	0.69
2:D:289:SER:HB2	2:D:291:ASP:OD1	1.91	0.69
1:B:2178:ASN:HD22	1:B:2180:HIS:H	1.40	0.69
1:A:1916:TRP:CD1	1:A:1916:TRP:H	2.11	0.69
2:D:169:PRO:HA	2:D:171:VAL:H	1.56	0.69
1:B:1916:TRP:H	1:B:1916:TRP:CD1	2.11	0.69
1:A:1680:ASP:C	1:A:1682:SER:N	2.51	0.68
2:C:279:SER:HA	2:C:320:PHE:HE2	1.59	0.68
1:B:2336:LEU:HG	1:B:2339:ARG:HH11	1.60	0.67
1:A:1529:MET:HE3	1:A:1550:LEU:HG	1.76	0.67
1:A:1941:GLN:HE22	1:A:2200:GLN:HE22	1.41	0.67
2:C:123:ARG:NH2	2:C:160:ASP:OD1	2.26	0.67
2:C:95:GLU:H	2:C:140:GLN:HE22	1.41	0.67
1:B:1704:MET:HG2	1:B:1713:ALA:HB2	1.76	0.67
1:A:2387:MET:HE3	1:A:2396:TYR:HB2	1.76	0.66
1:B:1783:ASP:O	1:B:1785:SER:N	2.29	0.66
2:C:168:GLU:N	2:C:169:PRO:HD2	2.10	0.66
2:C:188:VAL:HG13	2:C:223:ALA:HB3	1.77	0.66
1:B:1680:ASP:C	1:B:1682:SER:N	2.53	0.66
2:D:168:GLU:N	2:D:169:PRO:HD2	2.11	0.66
1:A:1508:THR:O	1:A:1512:MET:HB2	1.94	0.66
1:B:1759:LEU:HG	1:B:1772:VAL:HG11	1.78	0.66
1:B:2192:LEU:HD12	1:B:2235:GLY:HA3	1.76	0.66
1:B:1508:THR:O	1:B:1512:MET:HB2	1.95	0.66
1:A:1422:LYS:HD3	1:A:1580:GLY:HA3	1.76	0.66
2:C:169:PRO:HA	2:C:171:VAL:H	1.60	0.65
1:A:1759:LEU:HG	1:A:1772:VAL:HG11	1.77	0.65
1:B:1734:THR:C	1:B:1736:ASP:H	2.04	0.65
1:B:1892:ILE:CG2	1:B:1930:ILE:HD11	2.26	0.65
1:A:1704:MET:HG2	1:A:1713:ALA:HB2	1.77	0.65
2:D:95:GLU:H	2:D:140:GLN:HE22	1.43	0.64
1:A:1418:SER:CB	1:A:1581:GLU:HG2	2.21	0.64
1:B:1428:ALA:HB2	1:B:2395:ASN:ND2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:188:VAL:HG13	2:D:223:ALA:HB3	1.78	0.64
2:D:134:VAL:HG22	2:D:145:VAL:HG22	1.79	0.64
1:A:1969:PRO:O	1:A:1970:GLN:CB	2.44	0.64
1:A:2192:LEU:HD12	1:A:2235:GLY:HA3	1.78	0.64
1:A:1680:ASP:C	1:A:1682:SER:H	2.04	0.63
2:C:134:VAL:HG22	2:C:145:VAL:HG22	1.79	0.63
1:A:1783:ASP:O	1:A:1785:SER:N	2.31	0.63
2:C:55:SER:O	2:C:56:MET:HG2	1.99	0.63
1:A:1732:ILE:HD13	1:A:1740:LYS:HD2	1.80	0.63
1:B:1660:CYS:HB2	1:B:1669:ALA:HB2	1.79	0.63
2:D:279:SER:HA	2:D:320:PHE:HE2	1.63	0.63
1:A:1690:PRO:HB2	1:A:1692:VAL:HG22	1.79	0.63
1:B:1691:THR:HG23	1:B:1724:MET:HE1	1.81	0.63
1:A:1691:THR:HG23	1:A:1724:MET:HE1	1.81	0.63
1:A:1977:THR:HG21	1:A:2013:SER:OG	1.99	0.62
1:A:2064:THR:HG22	1:A:2128:PRO:HD3	1.79	0.62
1:B:1604:GLN:O	1:B:1608:VAL:HG23	1.98	0.62
1:A:1734:THR:O	1:A:1736:ASP:N	2.32	0.62
2:C:74:ASN:H	2:C:75:PRO:HD3	1.64	0.62
1:B:1654:LEU:HD21	1:B:1696:VAL:HG22	1.80	0.62
1:A:2037:LEU:HD22	1:A:2043:ASN:HD22	1.64	0.62
1:B:2363:GLU:OE2	1:B:2503:ARG:HD2	2.00	0.62
2:D:74:ASN:H	2:D:75:PRO:HD3	1.64	0.62
1:A:1958:HIS:HE1	1:A:1990:ALA:HB1	1.65	0.62
1:A:1732:ILE:HD13	1:A:1740:LYS:HB2	1.82	0.61
1:B:1690:PRO:HB2	1:B:1692:VAL:HG22	1.82	0.61
1:B:1914:GLY:HA3	1:B:1950:ARG:HE	1.65	0.61
1:A:1914:GLY:HA3	1:A:1950:ARG:HE	1.63	0.61
1:B:1958:HIS:HE1	1:B:1990:ALA:HB1	1.66	0.61
1:A:2278:LEU:HD23	2:C:44:GLN:HG2	1.80	0.61
2:D:241:ASP:OD2	2:D:243:THR:HB	2.00	0.61
2:D:170:GLU:HA	2:D:170:GLU:OE2	2.01	0.61
1:B:2387:MET:HE3	1:B:2396:TYR:HB2	1.83	0.61
1:A:2336:LEU:HG	1:A:2339:ARG:HH11	1.66	0.61
2:C:289:SER:HB2	2:C:291:ASP:OD1	2.01	0.61
1:B:1968:HIS:HB3	1:B:2144:TYR:OH	2.01	0.60
1:B:1623:LEU:HG	1:B:1633:TRP:CH2	2.36	0.60
2:D:199:LEU:HD22	2:D:210:LEU:HD22	1.83	0.60
2:C:199:LEU:HD22	2:C:210:LEU:HD22	1.84	0.60
2:D:56:MET:HB2	2:D:68:TYR:O	2.02	0.60
1:B:1920:ASN:O	1:B:1924:VAL:HG23	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1428:ALA:HB2	1:A:2395:ASN:ND2	2.17	0.60
1:A:2321:THR:HG23	1:A:2387:MET:HG2	1.83	0.60
1:B:1734:THR:O	1:B:1736:ASP:N	2.31	0.60
2:C:241:ASP:OD2	2:C:243:THR:HB	2.01	0.60
1:B:1915:HIS:HD2	1:B:1953:VAL:HG22	1.67	0.60
1:B:1680:ASP:C	1:B:1682:SER:H	2.07	0.59
1:A:2380:THR:CG2	1:A:2383:LEU:HG	2.31	0.59
1:A:2278:LEU:CD2	2:C:44:GLN:HG2	2.32	0.59
2:C:137:HIS:HD2	2:C:139:ASN:H	1.49	0.59
1:B:1701:MET:HE1	1:B:1717:MET:N	2.17	0.59
1:A:1611:ARG:NH1	1:A:1614:ILE:HG21	2.16	0.59
1:B:1739:HIS:O	1:B:1743:LEU:HB2	2.02	0.59
1:B:1705:TRP:CE3	1:B:1710:LYS:HB2	2.38	0.59
1:A:1968:HIS:HB3	1:A:2144:TYR:OH	2.03	0.59
1:B:1422:LYS:C	1:B:1424:GLN:H	2.11	0.59
1:B:1422:LYS:CE	1:B:1581:GLU:HG3	2.29	0.59
1:B:2281:MET:HE3	1:B:2281:MET:HA	1.83	0.59
1:A:1701:MET:HE1	1:A:1717:MET:N	2.18	0.59
1:B:1969:PRO:O	1:B:1970:GLN:CB	2.49	0.58
1:B:2037:LEU:HD22	1:B:2043:ASN:HD22	1.68	0.58
1:B:2336:LEU:HG	1:B:2339:ARG:NH1	2.17	0.58
1:B:2298:ASP:HB2	1:B:2382:MET:CE	2.34	0.58
1:A:1583:TYR:C	1:A:1585:ARG:H	2.12	0.58
1:A:2411:LYS:O	1:A:2415:MET:HG3	2.03	0.58
2:C:301:THR:HB	2:C:303:GLU:HG2	1.85	0.58
1:A:1920:ASN:O	1:A:1924:VAL:HG23	2.03	0.58
1:A:1493:LEU:HD23	1:A:1519:ALA:HB2	1.85	0.58
1:B:2390:THR:O	1:B:2390:THR:CG2	2.52	0.58
1:A:1999:CYS:C	1:A:2001:HIS:H	2.12	0.57
1:B:2329:MET:HB3	1:B:2404:MET:HE2	1.85	0.57
1:A:2237:ILE:HG21	3:A:2601:17G:H11	1.87	0.57
2:C:279:SER:HA	2:C:320:PHE:CE2	2.39	0.57
2:D:231:ASP:CB	2:D:233:THR:OG1	2.48	0.57
2:C:202:GLY:O	2:C:203:ILE:O	2.22	0.57
1:B:1611:ARG:NH1	1:B:1614:ILE:HG21	2.18	0.57
2:D:137:HIS:CD2	2:D:139:ASN:H	2.22	0.57
1:A:1481:MET:HA	1:A:1484:LEU:HD12	1.87	0.57
1:A:2496:LYS:HE3	1:A:2500:ILE:HD11	1.87	0.57
2:D:137:HIS:HD2	2:D:139:ASN:H	1.51	0.57
1:B:2281:MET:HA	1:B:2281:MET:CE	2.35	0.56
1:B:1583:TYR:C	1:B:1585:ARG:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:137:HIS:CD2	2:C:139:ASN:H	2.23	0.56
2:D:202:GLY:O	2:D:203:ILE:O	2.23	0.56
1:B:1686:ASP:O	1:A:2266:ARG:HG3	2.05	0.56
2:C:111:ILE:HD12	2:C:123:ARG:HD3	1.87	0.56
1:B:2237:ILE:HG21	3:B:2601:17G:H11	1.87	0.56
2:D:225:GLN:HG2	2:D:226:CYS:N	2.19	0.56
1:B:2297:ASP:HB3	1:B:2301:LYS:HD2	1.87	0.56
2:D:21:ASP:HB3	2:D:313:LYS:H	1.71	0.56
2:D:159:THR:HG22	2:D:161:HIS:HD2	1.70	0.56
1:A:1910:TRP:O	1:A:1915:HIS:NE2	2.39	0.56
2:C:127:VAL:HG11	2:C:153:HIS:CE1	2.41	0.56
1:B:1682:SER:O	1:B:1685:LEU:HD12	2.06	0.56
2:D:188:VAL:HG13	2:D:223:ALA:CB	2.35	0.56
1:A:1422:LYS:C	1:A:1424:GLN:H	2.14	0.56
1:A:1680:ASP:HB3	1:A:1683:ARG:H	1.71	0.56
1:B:1999:CYS:C	1:B:2001:HIS:H	2.14	0.56
1:B:1481:MET:HA	1:B:1484:LEU:HD12	1.88	0.55
1:B:1623:LEU:HG	1:B:1633:TRP:CZ3	2.41	0.55
2:D:63:GLN:HE21	2:D:86:LYS:H	1.54	0.55
1:A:1759:LEU:HD11	1:A:1796:MET:HE3	1.87	0.55
2:C:225:GLN:HG2	2:C:226:CYS:N	2.20	0.55
1:B:1609:PRO:HB3	1:B:1612:ARG:NH1	2.22	0.55
2:D:301:THR:HB	2:D:303:GLU:HG2	1.88	0.55
2:C:63:GLN:HE21	2:C:86:LYS:H	1.54	0.55
1:B:1910:TRP:O	1:B:1915:HIS:NE2	2.40	0.55
1:A:1631:GLU:CD	1:A:1631:GLU:H	2.15	0.55
1:A:1674:VAL:HG11	1:A:1681:PRO:HD3	1.87	0.55
1:A:1781:GLU:OE1	1:A:1781:GLU:HA	2.07	0.55
1:B:1778:ALA:O	1:B:1782:HIS:HD2	1.90	0.55
1:B:2380:THR:HG23	1:B:2549:TRP:O	2.06	0.55
2:D:15:LEU:HD11	2:D:286:VAL:HG11	1.89	0.55
1:B:2282:GLN:HE21	2:D:316:VAL:HG11	1.72	0.55
1:A:1739:HIS:O	1:A:1743:LEU:HB2	2.06	0.55
1:A:1915:HIS:HD2	1:A:1953:VAL:HG22	1.70	0.55
1:A:2298:ASP:HB2	1:A:2382:MET:CE	2.37	0.55
2:C:94:HIS:HB3	2:C:99:TRP:HB2	1.87	0.55
1:B:1762:GLN:HB2	1:B:1768:THR:HG21	1.89	0.55
1:B:2496:LYS:HE3	1:B:2500:ILE:HD11	1.89	0.55
2:D:111:ILE:HD12	2:D:123:ARG:HD3	1.88	0.55
2:D:117:ARG:O	2:D:118:ASN:CB	2.54	0.55
1:B:1913:TYR:HB3	1:B:1916:TRP:HE1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2122:GLU:O	1:A:2126:VAL:HG23	2.07	0.55
2:C:21:ASP:HB3	2:C:313:LYS:H	1.72	0.55
2:C:258:LEU:HD22	2:C:297:TRP:CE3	2.42	0.55
1:B:1680:ASP:HB3	1:B:1683:ARG:H	1.72	0.55
2:C:15:LEU:HD11	2:C:286:VAL:HG11	1.89	0.55
2:C:36:ARG:NH2	2:C:69:ASP:O	2.40	0.55
2:D:94:HIS:HB3	2:D:99:TRP:HB2	1.87	0.54
2:C:159:THR:HG22	2:C:161:HIS:HD2	1.71	0.54
2:C:170:GLU:OE2	2:C:170:GLU:HA	2.07	0.54
2:D:279:SER:HA	2:D:320:PHE:CE2	2.41	0.54
1:A:1501:TRP:CE3	1:A:1503:LEU:HD12	2.42	0.54
1:A:1682:SER:O	1:A:1685:LEU:HD12	2.07	0.54
2:D:36:ARG:NH2	2:D:69:ASP:O	2.40	0.54
1:B:2411:LYS:O	1:B:2415:MET:HG3	2.08	0.54
2:C:202:GLY:HA3	2:C:208:THR:H	1.72	0.54
2:C:12:PRO:O	2:C:54:ARG:NH2	2.40	0.54
2:C:56:MET:HB2	2:C:68:TYR:O	2.08	0.54
1:A:2336:LEU:HG	1:A:2339:ARG:NH1	2.22	0.54
2:C:288:ALA:HB2	2:C:318:LEU:HG	1.90	0.54
1:B:1759:LEU:HD11	1:B:1796:MET:HE3	1.90	0.54
2:D:96:ASP:O	2:D:98:ARG:N	2.41	0.54
2:D:165:LEU:HD11	2:D:197:TRP:CH2	2.43	0.54
2:D:288:ALA:HB2	2:D:318:LEU:HG	1.90	0.54
1:A:2521:VAL:HB	1:A:2522:PRO:HD3	1.88	0.54
1:B:1670:HIS:HE1	1:B:1681:PRO:HB3	1.73	0.53
2:D:94:HIS:CE1	2:D:96:ASP:HB2	2.42	0.53
1:A:1977:THR:HG22	1:A:1981:LYS:HE2	1.88	0.53
2:C:94:HIS:CE1	2:C:96:ASP:HB2	2.42	0.53
1:B:1643:VAL:HG12	1:B:1644:VAL:HG23	1.90	0.53
1:B:2064:THR:HG22	1:B:2128:PRO:HD3	1.89	0.53
2:D:202:GLY:HA3	2:D:208:THR:H	1.73	0.53
2:C:17:THR:HB	2:C:311:HIS:HE1	1.73	0.53
1:A:1913:TYR:HB3	1:A:1916:TRP:HE1	1.74	0.53
1:B:1936:LEU:HA	1:B:1939:ILE:HG13	1.91	0.53
2:D:12:PRO:O	2:D:54:ARG:NH2	2.41	0.53
1:B:1970:GLN:NE2	1:B:2139:ALA:H	2.07	0.53
2:D:53:ASP:C	2:D:55:SER:H	2.16	0.53
2:D:60:ALA:HB1	2:D:88:ILE:HG22	1.91	0.53
1:A:1705:TRP:CE3	1:A:1710:LYS:HB2	2.44	0.53
2:C:17:THR:HB	2:C:311:HIS:CE1	2.43	0.53
2:C:188:VAL:HG13	2:C:223:ALA:CB	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2197:ARG:NH1	1:B:2424:ASP:OD2	2.39	0.53
2:D:69:ASP:CB	2:D:78:ILE:HD11	2.39	0.53
1:A:2297:ASP:HB3	1:A:2301:LYS:HD2	1.90	0.53
1:B:2168:ARG:CZ	1:B:2168:ARG:HB2	2.38	0.53
1:B:2278:LEU:HD23	2:D:44:GLN:HG2	1.90	0.53
1:A:1896:ARG:NH2	1:A:1933:ASP:OD2	2.42	0.53
1:A:1913:TYR:O	1:A:1915:HIS:HA	2.08	0.53
1:B:2298:ASP:HB2	1:B:2382:MET:HE2	1.89	0.53
1:B:1680:ASP:O	1:B:1682:SER:N	2.32	0.53
2:D:133:CYS:SG	2:D:175:SER:HA	2.49	0.53
1:B:1478:LEU:O	1:B:1482:ARG:HG3	2.09	0.52
1:B:1631:GLU:CD	1:B:1631:GLU:H	2.17	0.52
1:A:1595:MET:O	1:A:1599:LEU:HB2	2.09	0.52
1:A:1660:CYS:HB2	1:A:1669:ALA:HB2	1.90	0.52
1:A:1762:GLN:HB2	1:A:1768:THR:HG21	1.92	0.52
1:B:2165:SER:OG	1:B:2166:LYS:N	2.42	0.52
1:A:1725:GLN:O	1:A:1729:GLN:HG2	2.09	0.52
1:B:1913:TYR:O	1:B:1915:HIS:HA	2.08	0.52
3:B:2601:17G:H8	3:B:2601:17G:C20	2.40	0.52
1:A:1704:MET:HE3	1:A:1713:ALA:HA	1.91	0.52
2:D:82:ASP:HB2	2:D:119:LEU:HD13	1.92	0.52
2:D:135:CYS:SG	2:D:178:ILE:HG22	2.50	0.52
1:A:1778:ALA:O	1:A:1782:HIS:HD2	1.93	0.52
1:A:1416:LEU:HA	1:A:1419:ILE:HG22	1.91	0.52
1:A:2281:MET:HE3	1:A:2281:MET:HA	1.91	0.52
2:D:166:ILE:HD12	2:D:167:PRO:O	2.10	0.52
1:A:2363:GLU:OE2	1:A:2503:ARG:HD2	2.10	0.52
1:A:1878:LEU:HD21	1:A:1918:ASP:HB2	1.92	0.52
2:C:115:ARG:O	2:C:116:SER:HB3	2.10	0.52
1:B:1416:LEU:HA	1:B:1419:ILE:HG22	1.91	0.52
2:D:94:HIS:HE1	2:D:96:ASP:HB2	1.75	0.52
2:D:258:LEU:HD22	2:D:297:TRP:CE3	2.45	0.52
2:C:53:ASP:C	2:C:55:SER:H	2.18	0.52
2:D:98:ARG:HD2	2:D:115:ARG:HB2	1.92	0.51
1:A:1422:LYS:HG2	1:A:1580:GLY:C	2.35	0.51
1:A:1649:ASP:O	1:A:1651:ARG:N	2.43	0.51
1:B:1566:LYS:O	1:B:1570:LEU:HG	2.10	0.51
1:B:1629:ILE:HG22	1:B:1630:VAL:HG23	1.92	0.51
1:B:1947:ASP:CG	1:B:1987:ARG:HG2	2.35	0.51
2:D:17:THR:HB	2:D:311:HIS:HE1	1.75	0.51
1:A:1611:ARG:HG2	1:A:1614:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1680:ASP:O	1:A:1682:SER:N	2.31	0.51
1:A:2382:MET:HG3	1:A:2549:TRP:O	2.10	0.51
1:B:1781:GLU:OE1	1:B:1781:GLU:HA	2.10	0.51
2:D:115:ARG:O	2:D:116:SER:HB3	2.09	0.51
1:A:2298:ASP:HB2	1:A:2382:MET:HE2	1.91	0.51
2:D:200:THR:O	2:D:208:THR:HA	2.11	0.51
1:A:2281:MET:HA	1:A:2281:MET:CE	2.40	0.51
1:B:2321:THR:HG23	1:B:2387:MET:HG2	1.92	0.51
2:C:165:LEU:HD11	2:C:197:TRP:CH2	2.46	0.51
1:B:1497:CYS:SG	1:B:1516:ALA:HB2	2.51	0.51
1:B:2521:VAL:HB	1:B:2522:PRO:HD3	1.91	0.51
1:B:1785:SER:O	1:B:1786:TRP:HB3	2.10	0.51
2:D:17:THR:HB	2:D:311:HIS:CE1	2.45	0.51
1:A:2123:LEU:HB2	1:A:2158:PRO:O	2.11	0.51
1:A:2178:ASN:ND2	1:A:2180:HIS:H	2.07	0.51
2:C:185:MET:HE2	2:C:197:TRP:CD1	2.45	0.51
1:A:1785:SER:O	1:A:1786:TRP:HB3	2.10	0.51
2:C:128:ASN:O	2:C:129:ALA:HB3	2.11	0.51
2:C:142:GLU:OE2	2:C:208:THR:HB	2.10	0.51
1:B:2178:ASN:ND2	1:B:2180:HIS:H	2.07	0.51
1:A:1936:LEU:HA	1:A:1939:ILE:HG13	1.93	0.51
1:A:2154:GLN:NE2	1:A:2155:SER:HB3	2.25	0.51
1:B:1501:TRP:CE3	1:B:1503:LEU:HD12	2.46	0.50
1:B:1878:LEU:HD21	1:B:1918:ASP:HB2	1.93	0.50
2:C:117:ARG:O	2:C:118:ASN:CB	2.55	0.50
1:B:1595:MET:O	1:B:1599:LEU:HB2	2.11	0.50
1:B:1649:ASP:O	1:B:1651:ARG:N	2.44	0.50
1:B:2289:HIS:O	1:B:2293:ASN:ND2	2.44	0.50
1:A:2168:ARG:HB2	1:A:2168:ARG:CZ	2.42	0.50
2:C:159:THR:C	2:C:161:HIS:H	2.19	0.50
1:B:1697:THR:O	1:B:1701:MET:HG3	2.11	0.50
1:B:1732:ILE:HD13	1:B:1740:LYS:HD2	1.92	0.50
1:A:2289:HIS:O	1:A:2293:ASN:ND2	2.44	0.50
2:C:78:ILE:HG22	2:C:79:ILE:HG13	1.93	0.50
2:C:96:ASP:O	2:C:98:ARG:N	2.44	0.50
1:B:2389:VAL:O	1:B:2390:THR:HG22	2.12	0.50
1:A:1888:PHE:O	1:A:1892:ILE:HG13	2.11	0.50
2:C:200:THR:O	2:C:208:THR:HA	2.12	0.50
2:D:128:ASN:O	2:D:129:ALA:HB3	2.12	0.50
2:C:94:HIS:HE1	2:C:96:ASP:HB2	1.76	0.50
1:A:1495:GLN:O	1:A:1499:GLU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:135:CYS:SG	2:C:178:ILE:HG22	2.52	0.50
1:B:2154:GLN:NE2	1:B:2155:SER:HB3	2.26	0.50
2:D:268:SER:O	2:D:269:SER:HB3	2.10	0.50
1:A:2389:VAL:O	1:A:2390:THR:HG22	2.12	0.50
2:C:8:VAL:HG11	2:C:36:ARG:HG2	1.93	0.50
2:C:169:PRO:HA	2:C:171:VAL:HG22	1.93	0.50
2:C:271:GLY:HA2	2:C:290:SER:HB2	1.92	0.50
2:D:8:VAL:HG11	2:D:36:ARG:HG2	1.93	0.50
2:D:219:HIS:HE1	2:D:243:THR:HG22	1.75	0.50
1:A:1602:VAL:HG13	1:A:1643:VAL:HG23	1.93	0.50
1:A:1882:VAL:HG12	1:A:1886:GLN:HE21	1.76	0.50
1:A:1913:TYR:O	1:A:1915:HIS:CG	2.65	0.50
2:C:69:ASP:CB	2:C:78:ILE:HD11	2.42	0.50
2:D:94:HIS:CD2	2:D:140:GLN:HB3	2.47	0.49
2:D:185:MET:HE2	2:D:197:TRP:CD1	2.47	0.49
1:B:1552:LEU:HD11	1:B:1603:ILE:HG13	1.94	0.49
1:B:1732:ILE:HD13	1:B:1740:LYS:HB2	1.94	0.49
1:B:1915:HIS:HE1	1:B:1919:VAL:HG11	1.78	0.49
2:D:142:GLU:OE2	2:D:208:THR:HB	2.12	0.49
1:A:1564:ILE:HG23	1:A:1596:LEU:HD22	1.94	0.49
1:A:1915:HIS:HE1	1:A:1919:VAL:HG11	1.77	0.49
1:A:1947:ASP:CG	1:A:1987:ARG:HG2	2.36	0.49
1:B:2254:ARG:HD2	1:B:2259:ILE:HB	1.95	0.49
2:D:127:VAL:HG11	2:D:153:HIS:CE1	2.47	0.49
2:D:185:MET:HB2	2:D:199:LEU:HD21	1.94	0.49
2:C:133:CYS:SG	2:C:175:SER:HA	2.52	0.49
1:B:1420:ASN:HB3	1:B:1429:ALA:HB2	1.95	0.49
2:C:98:ARG:HD2	2:C:115:ARG:HB2	1.94	0.49
1:A:2329:MET:HB3	1:A:2404:MET:HE2	1.94	0.49
1:B:1629:ILE:O	1:B:1630:VAL:C	2.54	0.49
1:B:2380:THR:CG2	1:B:2383:LEU:HG	2.37	0.49
1:A:1420:ASN:HB3	1:A:1429:ALA:HB2	1.95	0.49
1:A:1732:ILE:CD1	1:A:1740:LYS:HB2	2.42	0.49
1:A:1966:ARG:HA	1:A:2001:HIS:CE1	2.46	0.49
1:B:1609:PRO:HA	1:B:1612:ARG:NH1	2.28	0.49
2:D:271:GLY:HA2	2:D:290:SER:HB2	1.94	0.49
1:A:1697:THR:O	1:A:1701:MET:HG3	2.13	0.49
2:C:64:HIS:HA	2:C:81:TYR:O	2.13	0.49
1:B:1529:MET:HE3	1:B:1550:LEU:HG	1.93	0.49
1:B:1882:VAL:HG12	1:B:1886:GLN:HE21	1.77	0.49
1:B:1977:THR:HG21	1:B:2013:SER:OG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2380:THR:HG23	1:A:2549:TRP:O	2.13	0.49
1:A:2390:THR:O	1:A:2390:THR:CG2	2.57	0.49
2:C:94:HIS:CD2	2:C:140:GLN:HB3	2.48	0.49
1:B:1771:LYS:O	1:B:1774:GLN:HB3	2.12	0.49
1:A:1705:TRP:CZ3	1:A:1757:TRP:HB3	2.47	0.49
1:A:2397:ARG:NH2	1:A:2526:GLU:OE1	2.44	0.49
1:A:2530:LYS:HE2	1:A:2530:LYS:HA	1.93	0.49
2:D:58:ALA:HB2	2:D:67:MET:HE3	1.94	0.49
1:A:2006:VAL:O	1:A:2010:MET:HB2	2.12	0.49
1:A:2329:MET:HE3	1:A:2400:CYS:SG	2.53	0.49
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.46	0.49
2:C:74:ASN:H	2:C:75:PRO:CD	2.26	0.49
2:D:64:HIS:HA	2:D:81:TYR:O	2.13	0.48
2:D:72:SER:O	2:D:74:ASN:N	2.45	0.48
2:D:159:THR:C	2:D:161:HIS:H	2.21	0.48
1:B:2278:LEU:CD2	2:D:44:GLN:HG2	2.43	0.48
1:A:1432:VAL:HG22	1:A:2390:THR:HG21	1.95	0.48
2:C:106:ASP:OD1	2:C:108:THR:OG1	2.24	0.48
1:B:1400:LYS:HG3	1:B:1416:LEU:HD13	1.94	0.48
1:B:1896:ARG:NH2	1:B:1933:ASP:OD2	2.46	0.48
1:B:2167:GLN:O	1:B:2168:ARG:C	2.55	0.48
1:B:2395:ASN:HA	1:B:2398:ILE:HD12	1.94	0.48
1:A:1691:THR:CG2	1:A:1724:MET:HE1	2.42	0.48
1:A:1400:LYS:HG3	1:A:1416:LEU:HD13	1.95	0.48
1:A:1629:ILE:HG22	1:A:1630:VAL:HG23	1.95	0.48
1:A:1943:ILE:HD13	1:A:1975:PRO:HB2	1.95	0.48
2:C:28:GLN:O	2:C:28:GLN:HG3	2.14	0.48
2:D:65:ILE:CD1	2:D:102:THR:HG21	2.43	0.48
1:A:1427:GLU:HB2	1:A:2398:ILE:CD1	2.40	0.48
1:A:1631:GLU:HA	1:A:1634:GLN:HE21	1.77	0.48
1:B:1913:TYR:O	1:B:1915:HIS:ND1	2.46	0.48
1:A:1999:CYS:C	1:A:2001:HIS:N	2.70	0.48
1:A:2187:LYS:HG3	1:A:2237:ILE:HD12	1.95	0.48
1:A:1892:ILE:HG21	1:A:1930:ILE:CD1	2.36	0.48
2:C:268:SER:O	2:C:269:SER:HB3	2.11	0.48
1:A:1654:LEU:HD21	1:A:1696:VAL:HG22	1.95	0.48
1:A:2249:LEU:CD1	1:A:2346:LEU:HD12	2.44	0.48
2:C:301:THR:CB	2:C:303:GLU:HG2	2.43	0.48
1:B:1643:VAL:HG12	1:B:1644:VAL:CG2	2.42	0.48
1:B:1704:MET:HE3	1:B:1713:ALA:HA	1.95	0.48
1:B:2006:VAL:O	1:B:2010:MET:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1478:LEU:O	1:A:1482:ARG:HG3	2.14	0.48
1:A:2052:GLU:HG2	1:A:2053:PRO:HD3	1.95	0.48
2:C:269:SER:OG	2:C:270:ARG:N	2.47	0.48
2:D:106:ASP:OD1	2:D:108:THR:OG1	2.24	0.47
1:A:1429:ALA:HA	1:A:1432:VAL:HG23	1.96	0.47
1:A:1913:TYR:HB2	1:A:1915:HIS:CE1	2.49	0.47
1:A:2162:VAL:CG1	1:A:2168:ARG:HG2	2.44	0.47
1:A:2165:SER:OG	1:A:2166:LYS:N	2.47	0.47
2:C:239:SER:HB3	2:C:241:ASP:OD2	2.14	0.47
1:B:1913:TYR:O	1:B:1915:HIS:CG	2.67	0.47
1:B:2514:SER:OG	1:B:2517:ASP:HB2	2.15	0.47
1:B:2530:LYS:HE2	1:B:2530:LYS:HA	1.94	0.47
1:B:1413:LEU:O	1:B:1417:ILE:HG12	2.13	0.47
1:B:1703:ASN:O	1:B:1707:SER:HB2	2.14	0.47
1:B:1734:THR:C	1:B:1736:ASP:N	2.71	0.47
2:D:204:GLY:O	2:D:205:ASP:HB2	2.13	0.47
1:A:2095:LYS:HA	1:A:2098:THR:HG22	1.95	0.47
1:A:2167:GLN:O	1:A:2168:ARG:C	2.57	0.47
1:B:1977:THR:HG22	1:B:1981:LYS:HE2	1.96	0.47
1:B:2123:LEU:HB2	1:B:2158:PRO:O	2.15	0.47
1:B:2249:LEU:CD1	1:B:2346:LEU:HD12	2.45	0.47
1:A:2339:ARG:HD3	1:A:2355:HIS:CE1	2.49	0.47
2:C:168:GLU:N	2:C:169:PRO:CD	2.76	0.47
1:B:2512:ASP:N	1:B:2512:ASP:OD1	2.47	0.47
1:A:1703:ASN:O	1:A:1707:SER:HB2	2.14	0.47
2:C:204:GLY:O	2:C:205:ASP:HB2	2.13	0.47
1:B:1400:LYS:HD2	1:B:1412:ILE:HG23	1.96	0.47
1:A:2146:PRO:O	1:A:2147:ASN:HB2	2.14	0.47
1:B:1493:LEU:HD23	1:B:1519:ALA:HB2	1.96	0.47
2:D:74:ASN:H	2:D:75:PRO:CD	2.28	0.47
1:A:1629:ILE:O	1:A:1630:VAL:C	2.57	0.47
1:A:2046:GLY:O	1:A:2050:VAL:HG23	2.15	0.47
1:A:2052:GLU:CG	1:A:2053:PRO:HD3	2.44	0.47
1:A:2401:HIS:CD2	1:A:2522:PRO:HA	2.50	0.47
2:C:17:THR:CG2	2:C:311:HIS:CE1	2.97	0.47
2:C:82:ASP:HB2	2:C:119:LEU:HD13	1.97	0.47
2:C:219:HIS:HE1	2:C:243:THR:HG22	1.78	0.47
1:B:1495:GLN:O	1:B:1499:GLU:HB2	2.15	0.47
1:B:1646:PRO:HG3	1:B:1675:LEU:HD21	1.96	0.47
1:A:1505:ASN:CB	1:A:1508:THR:HB	2.45	0.47
3:A:2601:17G:H8	3:A:2601:17G:C20	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1628:ARG:HB2	1:B:1633:TRP:CD1	2.50	0.47
1:B:2378:ARG:HH11	1:B:2380:THR:HG21	1.80	0.47
1:A:1933:ASP:O	1:A:1934:THR:C	2.58	0.47
2:C:207:VAL:HG12	2:C:209:GLN:HG2	1.96	0.47
1:B:2046:GLY:O	1:B:2050:VAL:HG23	2.15	0.46
1:B:2397:ARG:NH2	1:B:2526:GLU:OE1	2.46	0.46
1:A:1913:TYR:O	1:A:1915:HIS:ND1	2.48	0.46
1:A:2513:PHE:HB2	1:A:2519:LEU:HD11	1.97	0.46
1:B:1674:VAL:HG11	1:B:1681:PRO:HD3	1.97	0.46
1:B:2146:PRO:O	1:B:2147:ASN:HB2	2.15	0.46
2:C:91:VAL:HG12	2:C:102:THR:HG22	1.96	0.46
2:D:28:GLN:HG3	2:D:28:GLN:O	2.16	0.46
2:D:75:PRO:HB2	2:D:76:ASN:H	1.52	0.46
2:D:168:GLU:N	2:D:169:PRO:CD	2.77	0.46
1:A:1566:LYS:O	1:A:1570:LEU:HG	2.14	0.46
2:C:203:ILE:HG22	2:C:204:GLY:N	2.30	0.46
1:B:1611:ARG:HG2	1:B:1614:ILE:HD12	1.97	0.46
1:B:1785:SER:O	1:B:1786:TRP:CB	2.63	0.46
1:B:2419:GLU:HG2	1:B:2501:ILE:HD13	1.96	0.46
1:B:1621:GLU:C	1:B:1623:LEU:H	2.24	0.46
1:B:2095:LYS:HA	1:B:2098:THR:HG22	1.97	0.46
2:D:102:THR:O	2:D:109:ALA:HA	2.16	0.46
2:D:269:SER:OG	2:D:270:ARG:N	2.48	0.46
1:A:2392:LEU:O	1:A:2397:ARG:HB2	2.16	0.46
1:A:2395:ASN:HA	1:A:2398:ILE:HD12	1.97	0.46
1:A:2503:ARG:HH11	1:A:2507:LYS:CE	2.28	0.46
1:B:1505:ASN:CB	1:B:1508:THR:HB	2.46	0.46
1:B:2168:ARG:O	1:B:2170:ARG:NH1	2.49	0.46
2:D:168:GLU:HB3	2:D:195:TYR:OH	2.16	0.46
2:D:207:VAL:HG12	2:D:209:GLN:HG2	1.96	0.46
1:A:1498:CYS:HA	1:A:1501:TRP:HD1	1.80	0.46
1:A:1501:TRP:HA	1:A:1503:LEU:HG	1.97	0.46
2:C:65:ILE:CD1	2:C:102:THR:HG21	2.45	0.46
1:B:1725:GLN:O	1:B:1729:GLN:HG2	2.15	0.46
1:B:2162:VAL:CG1	1:B:2168:ARG:HG2	2.46	0.46
1:A:1413:LEU:O	1:A:1417:ILE:HG12	2.15	0.46
1:A:1466:LYS:O	1:A:1470:ASN:HB2	2.15	0.46
1:A:2022:LEU:HD21	1:A:2126:VAL:HG13	1.97	0.46
1:B:1427:GLU:HB2	1:B:2398:ILE:CD1	2.44	0.46
2:D:91:VAL:HG12	2:D:102:THR:HG22	1.96	0.46
1:A:1646:PRO:HG3	1:A:1675:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:203:ILE:HG22	2:D:204:GLY:N	2.31	0.46
1:A:1583:TYR:C	1:A:1585:ARG:N	2.75	0.46
1:A:2194:GLN:HG2	1:A:2427:LEU:HD22	1.97	0.46
2:C:125:PHE:CE1	2:C:162:ASN:HB2	2.51	0.46
1:B:1429:ALA:HA	1:B:1432:VAL:HG23	1.98	0.45
1:B:1466:LYS:O	1:B:1470:ASN:HB2	2.16	0.45
1:B:1968:HIS:HB3	1:B:2144:TYR:HH	1.81	0.45
2:D:288:ALA:HB1	2:D:315:VAL:HG12	1.97	0.45
1:A:1440:PHE:HB3	1:A:1442:GLU:HB2	1.98	0.45
1:A:1943:ILE:HA	1:A:1946:ILE:HG13	1.99	0.45
1:A:2093:ASN:HD22	1:A:2095:LYS:H	1.63	0.45
2:C:72:SER:O	2:C:74:ASN:N	2.48	0.45
1:B:1966:ARG:HA	1:B:2001:HIS:CE1	2.50	0.45
2:D:301:THR:CB	2:D:303:GLU:HG2	2.45	0.45
1:A:1643:VAL:HG12	1:A:1644:VAL:HG23	1.98	0.45
1:A:1970:GLN:NE2	1:A:2139:ALA:H	2.14	0.45
1:B:1470:ASN:HB3	1:B:1471:LYS:H	1.57	0.45
1:B:1970:GLN:C	1:B:1972:LEU:N	2.73	0.45
1:A:1621:GLU:C	1:A:1623:LEU:H	2.24	0.45
2:C:58:ALA:HB2	2:C:67:MET:HE3	1.98	0.45
1:B:2052:GLU:HG2	1:B:2053:PRO:HD3	1.97	0.45
2:D:17:THR:CG2	2:D:311:HIS:CE1	2.99	0.45
2:D:95:GLU:HB2	2:D:140:GLN:HE22	1.76	0.45
2:D:169:PRO:HA	2:D:171:VAL:HG22	1.98	0.45
1:A:1701:MET:HB3	1:A:1701:MET:HE2	1.55	0.45
1:B:1414:GLU:O	1:B:1417:ILE:HG13	2.17	0.45
1:B:2015:GLU:HB3	1:B:2130:LEU:CD1	2.46	0.45
2:D:242:GLN:NE2	2:D:261:LYS:HA	2.30	0.45
2:D:262:SER:OG	2:D:267:GLU:HG2	2.17	0.45
1:A:1882:VAL:N	1:A:1883:PRO:HD2	2.32	0.45
2:C:185:MET:HB2	2:C:199:LEU:HD21	1.99	0.45
1:B:1727:GLN:O	1:B:1731:ALA:HB3	2.17	0.45
2:D:125:PHE:CE1	2:D:162:ASN:HB2	2.52	0.45
1:A:2287:PHE:O	1:A:2291:VAL:HG23	2.17	0.45
1:A:2346:LEU:HD23	1:A:2353:ILE:HG13	1.98	0.45
1:A:2378:ARG:HH11	1:A:2380:THR:HG21	1.82	0.45
3:A:2601:17G:H11	3:A:2601:17G:H9	1.70	0.45
1:B:1432:VAL:HG22	1:B:2390:THR:HG21	1.99	0.45
1:B:1440:PHE:HB3	1:B:1442:GLU:HB2	1.98	0.45
1:B:1634:GLN:HG2	1:B:1656:TYR:OH	2.17	0.45
1:B:1989:ASN:HB3	1:B:1993:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2093:ASN:HD22	1:B:2095:LYS:H	1.63	0.45
1:A:1623:LEU:HD13	1:A:1640:ARG:NH1	2.32	0.45
1:A:1895:SER:HB2	1:A:1899:ASN:HB3	1.98	0.45
1:A:2514:SER:OG	1:A:2517:ASP:HB2	2.17	0.45
2:D:248:ARG:HG3	2:D:253:SER:OG	2.17	0.45
2:C:75:PRO:HB2	2:C:76:ASN:H	1.52	0.45
1:B:1590:MET:O	1:B:1594:HIS:HB2	2.17	0.45
1:B:1631:GLU:HA	1:B:1634:GLN:HE21	1.82	0.45
1:A:2223:GLN:HB3	1:A:2354:LEU:HD13	1.99	0.45
1:B:1691:THR:CG2	1:B:1724:MET:HE1	2.46	0.44
1:B:2036:ARG:HA	1:B:2036:ARG:HD3	1.73	0.44
1:B:2392:LEU:O	1:B:2397:ARG:HB2	2.17	0.44
1:A:2324:LEU:HA	1:A:2353:ILE:HG21	1.99	0.44
1:A:2418:LEU:O	1:A:2422:VAL:HG23	2.17	0.44
1:B:1913:TYR:HB2	1:B:1915:HIS:CE1	2.52	0.44
1:B:1999:CYS:C	1:B:2001:HIS:N	2.73	0.44
1:B:2052:GLU:CG	1:B:2053:PRO:HD3	2.46	0.44
1:B:2208:LEU:HD22	1:B:2410:HIS:CG	2.52	0.44
1:B:2297:ASP:O	1:B:2298:ASP:C	2.60	0.44
1:B:2513:PHE:HB2	1:B:2519:LEU:HD11	1.99	0.44
3:B:2601:17G:H11	3:B:2601:17G:H9	1.77	0.44
2:D:203:ILE:O	2:D:204:GLY:C	2.61	0.44
1:B:1583:TYR:C	1:B:1585:ARG:N	2.76	0.44
1:A:1974:TYR:O	1:A:1978:VAL:HG23	2.18	0.44
1:A:2209:LEU:O	1:A:2215:SER:HB2	2.17	0.44
2:C:248:ARG:HG3	2:C:253:SER:OG	2.18	0.44
1:B:1501:TRP:HH2	1:B:1509:GLN:OE1	2.01	0.44
1:B:2023:TRP:CD2	1:B:2067:GLU:HG2	2.53	0.44
1:B:2122:GLU:O	1:B:2126:VAL:HG23	2.17	0.44
1:B:1759:LEU:HD21	1:B:1772:VAL:HG21	1.99	0.44
1:B:2240:VAL:HG21	1:B:2354:LEU:HD21	1.99	0.44
1:B:2268:MET:HG2	1:B:2286:VAL:HG12	1.98	0.44
2:D:188:VAL:HA	2:D:193:ASN:O	2.17	0.44
2:D:242:GLN:HB2	2:D:260:ILE:HG13	1.99	0.44
1:A:1530:GLU:HA	1:A:1550:LEU:HD11	1.99	0.44
1:A:2322:ARG:O	1:A:2326:VAL:HG23	2.18	0.44
1:B:2278:LEU:HB3	1:B:2282:GLN:HB2	1.99	0.44
1:A:1416:LEU:HA	1:A:1419:ILE:CG2	2.48	0.44
1:A:1717:MET:O	1:A:1721:VAL:HG23	2.16	0.44
1:A:1759:LEU:HD21	1:A:1772:VAL:HG21	1.98	0.44
1:A:2344:LEU:CD1	1:A:2353:ILE:HD11	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2345:MET:CE	3:A:2601:17G:H1	2.47	0.44
2:C:15:LEU:HD13	2:C:320:PHE:HD1	1.83	0.44
2:C:102:THR:O	2:C:109:ALA:HA	2.18	0.44
2:C:188:VAL:HA	2:C:193:ASN:O	2.17	0.44
1:B:1933:ASP:O	1:B:1934:THR:C	2.60	0.44
1:A:1710:LYS:NZ	1:A:1760:ASN:HD21	2.16	0.44
1:A:1785:SER:O	1:A:1786:TRP:CB	2.65	0.44
1:A:2023:TRP:CD2	1:A:2067:GLU:HG2	2.53	0.44
1:A:2170:ARG:HB2	1:A:2186:LEU:HB3	2.00	0.44
3:A:2601:17G:C19	3:A:2601:17G:C30	2.90	0.44
2:C:195:TYR:CE2	2:C:215:LYS:HG3	2.53	0.44
2:C:231:ASP:CB	2:C:233:THR:OG1	2.53	0.44
1:B:1895:SER:HB2	1:B:1899:ASN:HB3	2.00	0.44
1:B:2418:LEU:HD13	1:B:2504:VAL:HG11	1.99	0.44
1:B:1498:CYS:HA	1:B:1501:TRP:HD1	1.82	0.43
1:B:1698:TYR:O	1:B:1702:LYS:HG2	2.17	0.43
1:B:1755:GLY:HA2	1:B:1772:VAL:HG12	2.00	0.43
1:B:2322:ARG:O	1:B:2326:VAL:HG23	2.18	0.43
1:B:2380:THR:CG2	1:B:2549:TRP:C	2.90	0.43
2:D:239:SER:HB3	2:D:241:ASP:OD2	2.18	0.43
2:C:270:ARG:HD2	2:C:270:ARG:HA	1.87	0.43
1:B:1892:ILE:HD11	1:B:1903:THR:HA	2.00	0.43
1:B:2281:MET:HE1	2:D:222:TYR:CG	2.53	0.43
2:D:237:THR:O	2:D:244:CYS:HA	2.18	0.43
1:A:1755:GLY:HA2	1:A:1772:VAL:HG12	2.00	0.43
1:A:2512:ASP:OD1	1:A:2512:ASP:N	2.50	0.43
1:B:1422:LYS:C	1:B:1424:GLN:N	2.76	0.43
1:B:1936:LEU:C	1:B:1938:VAL:H	2.26	0.43
1:A:1595:MET:HG2	1:A:1639:VAL:HG21	2.00	0.43
1:A:2028:HIS:HE1	1:A:2112:SER:OG	2.00	0.43
2:C:128:ASN:O	2:C:129:ALA:CB	2.66	0.43
1:B:1393:TYR:CZ	1:B:1422:LYS:HD2	2.53	0.43
1:B:2170:ARG:HB2	1:B:2186:LEU:HB3	2.00	0.43
1:B:2378:ARG:NH1	1:B:2380:THR:HG21	2.33	0.43
2:D:267:GLU:O	2:D:267:GLU:HG3	2.18	0.43
1:A:1594:HIS:HE1	1:A:1622:ARG:HD2	1.82	0.43
1:A:2297:ASP:O	1:A:2298:ASP:C	2.61	0.43
1:B:2022:LEU:HD21	1:B:2126:VAL:HG13	2.00	0.43
1:B:2093:ASN:ND2	1:B:2095:LYS:H	2.16	0.43
1:A:1564:ILE:HD13	1:A:1600:GLU:HG3	2.00	0.43
2:C:166:ILE:HD12	2:C:167:PRO:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1416:LEU:HA	1:B:1419:ILE:CG2	2.49	0.43
1:B:1402:LEU:O	1:B:1405:GLN:HB2	2.19	0.43
1:B:1623:LEU:O	1:B:1633:TRP:HH2	2.01	0.43
1:B:2324:LEU:HA	1:B:2353:ILE:HG21	2.00	0.43
1:A:1400:LYS:HD2	1:A:1412:ILE:HG23	2.00	0.43
1:A:1771:LYS:O	1:A:1774:GLN:HB3	2.18	0.43
1:B:1423:LEU:HD12	1:B:1423:LEU:HA	1.92	0.43
1:B:1950:ARG:HA	1:B:1951:PRO:HD3	1.90	0.43
2:D:262:SER:HB2	2:D:263:GLY:H	1.60	0.43
1:A:1414:GLU:O	1:A:1417:ILE:HG13	2.19	0.43
1:A:1970:GLN:C	1:A:1972:LEU:N	2.76	0.43
1:A:1470:ASN:HB3	1:A:1471:LYS:H	1.59	0.43
1:A:1701:MET:HE1	1:A:1716:HIS:C	2.44	0.43
1:A:1936:LEU:C	1:A:1938:VAL:H	2.27	0.43
1:A:1972:LEU:O	1:A:1975:PRO:HG2	2.19	0.43
1:A:2254:ARG:HD2	1:A:2259:ILE:HB	2.01	0.43
1:B:1501:TRP:HA	1:B:1503:LEU:HG	2.00	0.43
1:B:1514:ARG:HH21	1:B:1540:THR:HG21	1.84	0.43
1:B:1892:ILE:HG21	1:B:1930:ILE:CD1	2.42	0.43
2:D:15:LEU:HD13	2:D:320:PHE:HD1	1.84	0.43
1:A:1473:ASP:HA	1:A:1474:PRO:HD2	1.71	0.43
1:A:1900:LEU:HD23	1:A:2204:LEU:HD22	2.01	0.42
1:A:2036:ARG:HA	1:A:2036:ARG:HD3	1.74	0.42
1:A:2282:GLN:HE21	2:C:316:VAL:HG11	1.84	0.42
1:B:1890:ARG:O	1:B:1894:LEU:HG	2.19	0.42
2:D:78:ILE:HG22	2:D:79:ILE:HG13	2.01	0.42
2:D:166:ILE:HG13	2:D:166:ILE:O	2.19	0.42
1:A:1590:MET:O	1:A:1594:HIS:HB2	2.20	0.42
1:A:2240:VAL:O	3:A:2601:17G:H7	2.19	0.42
1:A:2378:ARG:NH1	1:A:2380:THR:HG21	2.34	0.42
1:A:2380:THR:CG2	1:A:2549:TRP:C	2.92	0.42
2:C:127:VAL:HG11	2:C:153:HIS:HE1	1.81	0.42
1:B:1574:GLU:HG2	1:B:1585:ARG:NH2	2.34	0.42
2:D:270:ARG:HD2	2:D:270:ARG:HA	1.87	0.42
1:A:1721:VAL:HG11	1:A:1751:PHE:CZ	2.54	0.42
1:A:2080:GLU:O	1:A:2083:GLU:HB3	2.19	0.42
2:C:203:ILE:O	2:C:204:GLY:C	2.63	0.42
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.53	0.42
1:A:2345:MET:HE1	3:A:2601:17G:H1	2.01	0.42
1:B:2198:VAL:HG11	1:B:2358:PHE:CD2	2.54	0.42
1:A:1453:LEU:C	1:A:1455:GLU:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1602:VAL:HG13	1:A:1643:VAL:CG2	2.48	0.42
1:A:2093:ASN:ND2	1:A:2095:LYS:H	2.17	0.42
1:A:2319:ASN:HB3	1:A:2352:LYS:HG2	2.00	0.42
1:A:2340:HIS:HB2	1:A:2341:PRO:CD	2.49	0.42
2:C:262:SER:HB2	2:C:263:GLY:H	1.57	0.42
1:B:2156:ILE:HG12	1:B:2174:LEU:HD22	2.01	0.42
1:A:1882:VAL:HG12	1:A:1886:GLN:NE2	2.35	0.42
2:C:95:GLU:HB2	2:C:140:GLN:HE22	1.80	0.42
2:C:242:GLN:HB2	2:C:260:ILE:HG13	2.01	0.42
1:B:1972:LEU:O	1:B:1975:PRO:HG2	2.19	0.42
1:B:2281:MET:CE	2:D:222:TYR:CD2	2.94	0.42
1:B:1604:GLN:O	1:B:1608:VAL:CG2	2.65	0.42
2:D:95:GLU:HB2	2:D:140:GLN:HE21	1.80	0.42
1:A:1437:MET:SD	1:A:1453:LEU:HD11	2.59	0.42
2:C:168:GLU:HB3	2:C:195:TYR:OH	2.20	0.42
2:C:288:ALA:HB1	2:C:315:VAL:HG12	2.01	0.42
1:B:1414:GLU:C	1:B:1416:LEU:H	2.27	0.42
1:B:1717:MET:O	1:B:1721:VAL:HG23	2.18	0.42
1:B:1882:VAL:HG12	1:B:1886:GLN:NE2	2.35	0.42
2:D:128:ASN:O	2:D:129:ALA:CB	2.67	0.42
1:A:1643:VAL:HG12	1:A:1644:VAL:CG2	2.48	0.42
2:C:60:ALA:HB1	2:C:88:ILE:HG22	2.02	0.42
1:A:1423:LEU:HD12	1:A:1423:LEU:HA	1.94	0.42
1:A:1681:PRO:O	1:A:1682:SER:C	2.62	0.42
1:B:2285:GLU:HG3	2:D:272:TRP:CE2	2.55	0.41
2:D:18:ALA:HB1	2:D:45:VAL:HG21	2.02	0.41
1:A:1791:HIS:O	1:A:1795:VAL:HG23	2.20	0.41
1:A:2140:VAL:O	1:A:2141:PRO:C	2.63	0.41
2:C:262:SER:OG	2:C:267:GLU:HG2	2.20	0.41
1:B:1497:CYS:SG	1:B:1516:ALA:CB	3.09	0.41
1:B:1680:ASP:OD2	1:B:1683:ARG:HB2	2.20	0.41
1:B:1932:ILE:O	1:B:1933:ASP:C	2.60	0.41
1:B:1939:ILE:N	1:B:1940:PRO:HD2	2.36	0.41
1:B:2187:LYS:HG3	1:B:2237:ILE:HD12	2.02	0.41
1:B:2240:VAL:O	3:B:2601:17G:H7	2.20	0.41
1:B:2346:LEU:HD23	1:B:2353:ILE:HG13	2.01	0.41
1:A:1422:LYS:C	1:A:1424:GLN:N	2.78	0.41
1:A:2199:MET:SD	1:A:2224:ARG:HB2	2.60	0.41
2:C:44:GLN:H	2:C:44:GLN:HG3	1.56	0.41
1:B:1473:ASP:HA	1:B:1474:PRO:HD2	1.72	0.41
1:B:1712:ASP:OD1	1:A:2266:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1759:LEU:CD1	1:B:1796:MET:HE3	2.51	0.41
1:B:1882:VAL:N	1:B:1883:PRO:HD2	2.36	0.41
1:B:1882:VAL:CG1	1:B:1886:GLN:HE21	2.33	0.41
1:B:2339:ARG:HH21	1:B:2343:ASN:HB3	1.85	0.41
2:D:69:ASP:HB2	2:D:78:ILE:CD1	2.47	0.41
1:A:1402:LEU:O	1:A:1405:GLN:HB2	2.21	0.41
1:A:1414:GLU:C	1:A:1416:LEU:H	2.27	0.41
1:A:1680:ASP:OD2	1:A:1683:ARG:HB2	2.20	0.41
1:A:1807:GLN:O	1:A:1810:ALA:HB3	2.20	0.41
2:C:166:ILE:O	2:C:166:ILE:HG13	2.20	0.41
2:D:44:GLN:H	2:D:44:GLN:HG3	1.53	0.41
2:C:105:GLU:HA	2:C:130:PRO:HB3	2.01	0.41
2:C:186:ALA:HA	2:C:195:TYR:O	2.20	0.41
1:B:2281:MET:HE1	2:D:222:TYR:CE2	2.53	0.41
1:B:2382:MET:HG3	1:B:2549:TRP:O	2.21	0.41
2:D:167:PRO:HB2	2:D:168:GLU:H	1.64	0.41
1:A:1628:ARG:HB2	1:A:1633:TRP:CD1	2.55	0.41
1:A:2139:ALA:HA	1:A:2151:ILE:O	2.21	0.41
1:B:2028:HIS:HE1	1:B:2112:SER:OG	2.03	0.41
1:B:2401:HIS:CD2	1:B:2522:PRO:HA	2.56	0.41
2:D:286:VAL:HB	2:D:318:LEU:HD13	2.03	0.41
2:D:312:GLN:H	2:D:312:GLN:HG2	1.64	0.41
1:A:2503:ARG:HH11	1:A:2507:LYS:HE3	1.86	0.41
2:C:8:VAL:HG21	2:C:36:ARG:HD3	2.03	0.41
1:B:1453:LEU:C	1:B:1455:GLU:H	2.29	0.41
1:B:1526:TRP:HE3	1:B:1529:MET:HE2	1.85	0.41
2:D:100:MET:HB3	2:D:112:TRP:HB2	2.02	0.41
1:A:1634:GLN:HG2	1:A:1656:TYR:OH	2.21	0.41
1:A:1890:ARG:O	1:A:1894:LEU:HG	2.20	0.41
1:B:2080:GLU:O	1:B:2083:GLU:HB3	2.21	0.41
2:D:65:ILE:HD13	2:D:102:THR:HG21	2.02	0.41
2:C:267:GLU:O	2:C:267:GLU:HG3	2.20	0.41
1:B:1916:TRP:CD1	1:B:1916:TRP:N	2.80	0.41
1:B:1943:ILE:CD1	1:B:1975:PRO:HB2	2.51	0.41
1:B:2121:LEU:HD23	1:B:2121:LEU:HA	1.86	0.41
1:B:2287:PHE:O	1:B:2291:VAL:HG23	2.21	0.41
1:A:1734:THR:C	1:A:1736:ASP:N	2.64	0.41
1:A:1915:HIS:CE1	1:A:1919:VAL:HG11	2.55	0.41
2:C:76:ASN:CB	2:C:77:PRO:HD2	2.21	0.41
2:C:178:ILE:HD11	2:C:199:LEU:HD11	2.02	0.41
1:B:1701:MET:HE1	1:B:1717:MET:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2197:ARG:HB3	1:B:2421:PHE:CD2	2.56	0.41
1:B:2297:ASP:HB2	1:B:2298:ASP:H	1.67	0.41
1:A:1493:LEU:CD2	1:A:1519:ALA:HB2	2.51	0.41
1:A:1717:MET:HG3	1:A:1754:LEU:HG	2.02	0.41
2:C:14:ILE:HD13	2:C:70:LEU:HD13	2.03	0.41
1:B:1605:TYR:CG	1:B:1643:VAL:HG11	2.56	0.40
1:B:1609:PRO:HB3	1:B:1612:ARG:HH11	1.86	0.40
1:A:1916:TRP:CD1	1:A:1916:TRP:N	2.80	0.40
1:A:2418:LEU:HD13	1:A:2504:VAL:HG11	2.02	0.40
1:A:2419:GLU:HG2	1:A:2501:ILE:HD13	2.02	0.40
1:B:1915:HIS:CE1	1:B:1919:VAL:HG11	2.56	0.40
1:B:1970:GLN:C	1:B:1972:LEU:H	2.29	0.40
1:B:1973:ILE:O	1:B:1974:TYR:C	2.64	0.40
1:A:1892:ILE:HD11	1:A:1903:THR:HA	2.03	0.40
1:A:2299:LEU:O	1:A:2303:LEU:HG	2.22	0.40
1:B:2032:GLU:O	1:B:2036:ARG:HG2	2.21	0.40
1:B:2530:LYS:HA	1:B:2530:LYS:CE	2.50	0.40
2:D:262:SER:CB	2:D:267:GLU:HG2	2.51	0.40
1:A:2064:THR:HG21	1:A:2126:VAL:O	2.22	0.40
1:A:2173:THR:HB	1:A:2183:VAL:HG13	2.04	0.40
2:C:95:GLU:HB2	2:C:140:GLN:HE21	1.81	0.40
1:B:1888:PHE:O	1:B:1892:ILE:HG13	2.20	0.40
1:B:2268:MET:HG3	1:B:2290:ALA:HB2	2.04	0.40
1:A:1481:MET:C	1:A:1515:MET:HE1	2.47	0.40
1:A:1880:TYR:O	1:A:1883:PRO:HG2	2.22	0.40
1:A:1980:SER:O	1:A:1988:HIS:HB2	2.22	0.40
1:A:2415:MET:O	1:A:2419:GLU:HB2	2.21	0.40
2:C:65:ILE:HD13	2:C:102:THR:HG21	2.02	0.40
1:B:1608:VAL:HA	1:B:1609:PRO:HD3	1.81	0.40
1:B:2157:ALA:HB3	1:B:2173:THR:HG23	2.04	0.40
1:B:2223:GLN:HB3	1:B:2354:LEU:HD13	2.04	0.40
1:B:2264:GLU:HG3	1:B:2294:THR:HG21	2.03	0.40
1:A:1445:ILE:C	1:A:1447:ALA:H	2.30	0.40
1:A:2345:MET:HE1	3:A:2601:17G:C21	2.52	0.40
2:C:18:ALA:HB1	2:C:45:VAL:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1046/1174 (89%)	922 (88%)	96 (9%)	28 (3%)	4	27
1	B	1052/1174 (90%)	925 (88%)	97 (9%)	30 (3%)	3	26
2	C	315/326 (97%)	275 (87%)	26 (8%)	14 (4%)	2	17
2	D	315/326 (97%)	272 (86%)	29 (9%)	14 (4%)	2	17
All	All	2728/3000 (91%)	2394 (88%)	248 (9%)	86 (3%)	3	24

All (86) 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	73	ASN
2	D	74	ASN
2	D	97	GLY
2	D	118	ASN
2	D	203	ILE
2	D	269	SER
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

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Mol	Chain	Res	Type
2	C	73	ASN
2	C	74	ASN
2	C	97	GLY
2	C	118	ASN
2	C	203	ILE
2	C	269	SER
1	B	1445	ILE
1	B	1470	ASN
1	B	1735	GLU
1	B	1914	GLY
1	B	1937	GLN
1	B	2093	ASN
1	B	2364	VAL
2	D	35	THR
2	D	75	PRO
2	D	167	PRO
2	D	169	PRO
2	D	204	GLY
1	A	1445	ILE
1	A	1734	THR
1	A	1735	GLU
1	A	1914	GLY
1	A	1937	GLN
1	A	2093	ASN
1	A	2364	VAL
2	C	35	THR
2	C	75	PRO
2	C	167	PRO
2	C	169	PRO
2	C	204	GLY
1	B	1444	GLU
1	B	1681	PRO
1	B	1682	SER
1	B	1784	ARG
1	B	2000	GLU
1	B	2357	ASP
1	B	2368	ARG
2	D	129	ALA
1	A	1444	GLU
1	A	1454	HIS
1	A	1470	ASN
1	A	1681	PRO

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Mol	Chain	Res	Type
1	A	1682	SER
1	A	1784	ARG
1	A	2000	GLU
1	A	2357	ASP
2	C	129	ALA
1	B	1426	PRO
1	B	1734	THR
1	B	2001	HIS
2	D	208	THR
1	A	1426	PRO
1	A	2001	HIS
1	B	1454	HIS
1	B	1786	TRP
1	A	1786	TRP
2	C	208	THR
2	C	310	GLY
1	B	1415	SER
2	D	310	GLY
1	A	2072	GLN
1	B	1474	PRO
1	A	1474	PRO
1	B	1680	ASP

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%)	828 (89%)	99 (11%)	6	27
1	B	930/1024 (91%)	832 (90%)	98 (10%)	6	27
2	C	269/276 (98%)	234 (87%)	35 (13%)	4	21
2	D	269/276 (98%)	236 (88%)	33 (12%)	4	22
All	All	2395/2600 (92%)	2130 (89%)	265 (11%)	6	25

All (265) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1402	LEU
1	B	1417	ILE
1	B	1420	ASN
1	B	1423	LEU
1	B	1443	LEU
1	B	1457	GLU
1	B	1471	LYS
1	B	1487	LEU
1	B	1501	TRP
1	B	1509	GLN
1	B	1528	SER
1	B	1540	THR
1	B	1541	HIS
1	B	1559	LEU
1	B	1578	MET
1	B	1585	ARG
1	B	1590	MET
1	B	1597	SER
1	B	1610	GLU
1	B	1618	ILE
1	B	1630	VAL
1	B	1679	VAL
1	B	1685	LEU
1	B	1752	LEU
1	B	1780	THR
1	B	1799	GLU
1	B	1802	LEU
1	B	1876	THR
1	B	1878	LEU
1	B	1879	MET
1	B	1891	SER
1	B	1895	SER
1	B	1896	ARG
1	B	1899	ASN
1	B	1908	THR
1	B	1912	ASP
1	B	1916	TRP
1	B	1932	ILE
1	B	1938	VAL
1	B	1939	ILE
1	B	1956	LEU
1	B	1968	HIS
1	B	1970	GLN

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Mol	Chain	Res	Type
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	2041	GLU
1	B	2044	VAL
1	B	2068	THR
1	B	2072	GLN
1	B	2076	ARG
1	B	2078	LEU
1	B	2080	GLU
1	B	2093	ASN
1	B	2095	LYS
1	B	2124	GLN
1	B	2131	LEU
1	B	2138	LEU
1	B	2152	ARG
1	B	2155	SER
1	B	2164	THR
1	B	2166	LYS
1	B	2168	ARG
1	B	2173	THR
1	B	2178	ASN
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	2254	ARG
1	B	2260	LEU
1	B	2266	ARG
1	B	2281	MET
1	B	2318	THR
1	B	2342	SER

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Mol	Chain	Res	Type
1	B	2363	GLU
1	B	2364	VAL
1	B	2378	ARG
1	B	2385	ASN
1	B	2390	THR
1	B	2408	ARG
1	B	2431	LEU
1	B	2432	MET
1	B	2495	LYS
1	B	2503	ARG
1	B	2515	HIS
1	B	2519	LEU
1	B	2530	LYS
2	D	8	VAL
2	D	13	VAL
2	D	44	GLN
2	D	74	ASN
2	D	84	VAL
2	D	85	ASN
2	D	86	LYS
2	D	90	SER
2	D	123	ARG
2	D	128	ASN
2	D	134	VAL
2	D	159	THR
2	D	160	ASP
2	D	162	ASN
2	D	165	LEU
2	D	166	ILE
2	D	168	GLU
2	D	169	PRO
2	D	170	GLU
2	D	183	SER
2	D	188	VAL
2	D	199	LEU
2	D	214	THR
2	D	215	LYS
2	D	243	THR
2	D	248	ARG
2	D	262	SER
2	D	269	SER
2	D	286	VAL

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Mol	Chain	Res	Type
2	D	287	THR
2	D	289	SER
2	D	301	THR
2	D	312	GLN
1	A	1385	GLU
1	A	1402	LEU
1	A	1417	ILE
1	A	1420	ASN
1	A	1423	LEU
1	A	1443	LEU
1	A	1457	GLU
1	A	1471	LYS
1	A	1487	LEU
1	A	1501	TRP
1	A	1509	GLN
1	A	1528	SER
1	A	1540	THR
1	A	1541	HIS
1	A	1559	LEU
1	A	1578	MET
1	A	1585	ARG
1	A	1590	MET
1	A	1618	ILE
1	A	1630	VAL
1	A	1644	VAL
1	A	1679	VAL
1	A	1685	LEU
1	A	1752	LEU
1	A	1780	THR
1	A	1799	GLU
1	A	1802	LEU
1	A	1878	LEU
1	A	1879	MET
1	A	1891	SER
1	A	1895	SER
1	A	1896	ARG
1	A	1899	ASN
1	A	1908	THR
1	A	1912	ASP
1	A	1916	TRP
1	A	1932	ILE
1	A	1938	VAL

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Mol	Chain	Res	Type
1	A	1939	ILE
1	A	1956	LEU
1	A	1968	HIS
1	A	1970	GLN
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	2041	GLU
1	A	2044	VAL
1	A	2068	THR
1	A	2072	GLN
1	A	2076	ARG
1	A	2078	LEU
1	A	2080	GLU
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	2155	SER
1	A	2164	THR
1	A	2166	LYS
1	A	2168	ARG
1	A	2172	LEU
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	2244	ASP
1	A	2254	ARG

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Mol	Chain	Res	Type
1	A	2260	LEU
1	A	2266	ARG
1	A	2281	MET
1	A	2318	THR
1	A	2342	SER
1	A	2363	GLU
1	A	2364	VAL
1	A	2378	ARG
1	A	2385	ASN
1	A	2389	VAL
1	A	2390	THR
1	A	2408	ARG
1	A	2431	LEU
1	A	2432	MET
1	A	2495	LYS
1	A	2503	ARG
1	A	2515	HIS
1	A	2519	LEU
1	A	2530	LYS
2	C	8	VAL
2	C	13	VAL
2	C	44	GLN
2	C	74	ASN
2	C	84	VAL
2	C	85	ASN
2	C	86	LYS
2	C	90	SER
2	C	123	ARG
2	C	128	ASN
2	C	134	VAL
2	C	159	THR
2	C	160	ASP
2	C	162	ASN
2	C	165	LEU
2	C	166	ILE
2	C	168	GLU
2	C	169	PRO
2	C	170	GLU
2	C	183	SER
2	C	188	VAL
2	C	199	LEU
2	C	211	ILE

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Mol	Chain	Res	Type
2	C	214	THR
2	C	215	LYS
2	C	243	THR
2	C	248	ARG
2	C	258	LEU
2	C	262	SER
2	C	269	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 (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1421	ASN
1	B	1496	GLN
1	B	1505	ASN
1	B	1541	HIS
1	B	1594	HIS
1	B	1604	GLN
1	B	1624	GLN
1	B	1670	HIS
1	B	1687	HIS
1	B	1727	GLN
1	B	1741	GLN
1	B	1760	ASN
1	B	1782	HIS
1	B	1886	GLN
1	B	1898	ASN
1	B	1937	GLN
1	B	1941	GLN
1	B	1958	HIS
1	B	1970	GLN
1	B	1992	ASN
1	B	2001	HIS
1	B	2028	HIS
1	B	2082	GLN
1	B	2093	ASN
1	B	2167	GLN
1	B	2178	ASN

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Mol	Chain	Res	Type
1	B	2189	HIS
1	B	2223	GLN
1	B	2247	HIS
1	B	2262	ASN
1	B	2277	HIS
1	B	2319	ASN
1	B	2355	HIS
1	B	2395	ASN
1	B	2401	HIS
2	D	30	HIS
2	D	63	GLN
2	D	73	ASN
2	D	85	ASN
2	D	94	HIS
2	D	122	GLN
2	D	137	HIS
2	D	140	GLN
2	D	153	HIS
2	D	161	HIS
2	D	283	GLN
2	D	311	HIS
2	D	312	GLN
1	A	1496	GLN
1	A	1505	ASN
1	A	1541	HIS
1	A	1594	HIS
1	A	1604	GLN
1	A	1624	GLN
1	A	1670	HIS
1	A	1687	HIS
1	A	1703	ASN
1	A	1716	HIS
1	A	1727	GLN
1	A	1760	ASN
1	A	1782	HIS
1	A	1808	ASN
1	A	1886	GLN
1	A	1898	ASN
1	A	1941	GLN
1	A	1958	HIS
1	A	1959	GLN
1	A	1970	GLN

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Mol	Chain	Res	Type
1	A	1992	ASN
1	A	2001	HIS
1	A	2028	HIS
1	A	2082	GLN
1	A	2093	ASN
1	A	2154	GLN
1	A	2167	GLN
1	A	2178	ASN
1	A	2189	HIS
1	A	2223	GLN
1	A	2247	HIS
1	A	2262	ASN
1	A	2265	HIS
1	A	2319	ASN
1	A	2395	ASN
1	A	2401	HIS
2	C	30	HIS
2	C	63	GLN
2	C	73	ASN
2	C	85	ASN
2	C	94	HIS
2	C	122	GLN
2	C	137	HIS
2	C	140	GLN
2	C	161	HIS
2	C	164	GLN
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	17G	B	2601	-	35,36,36	1.20	3 (8%)	50,54,54	1.89	11 (22%)
3	17G	A	2601	-	35,36,36	1.22	4 (11%)	50,54,54	1.75	9 (18%)

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	17G	B	2601	-	-	2/14/14/14	0/5/5/5
3	17G	A	2601	-	-	2/14/14/14	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	17G	C37-C33	-4.05	1.39	1.49
3	B	2601	17G	C37-C33	-3.77	1.40	1.49
3	B	2601	17G	C26-C31	-2.44	1.39	1.44
3	A	2601	17G	C32-C31	2.44	1.38	1.34
3	B	2601	17G	C32-C31	2.34	1.38	1.34
3	A	2601	17G	C26-C31	-2.27	1.39	1.44
3	A	2601	17G	C23-N8	2.21	1.44	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2601	17G	C21-C19-N8	5.07	125.54	119.72
3	B	2601	17G	C19-N8-C23	4.35	124.92	118.14
3	A	2601	17G	C19-N8-C23	4.21	124.70	118.14
3	B	2601	17G	C32-C27-N8	4.00	121.81	114.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2601	17G	C34-C26-C31	-3.89	116.64	122.91
3	A	2601	17G	C32-C27-N8	3.82	121.47	114.02
3	A	2601	17G	C21-C19-N8	3.79	124.08	119.72
3	B	2601	17G	C34-N9-C29	3.71	121.25	116.96
3	A	2601	17G	C26-C23-C25	-3.61	117.18	121.06
3	A	2601	17G	C34-C26-C31	-3.59	117.13	122.91
3	B	2601	17G	C20-C19-N8	-3.52	115.78	119.42
3	A	2601	17G	C34-N9-C29	3.43	120.93	116.96
3	B	2601	17G	C26-C23-C25	-3.41	117.40	121.06
3	A	2601	17G	C20-C19-N8	-3.21	116.10	119.42
3	B	2601	17G	C26-C34-N9	-2.98	120.27	124.14
3	A	2601	17G	C26-C34-N9	-2.55	120.82	124.14
3	A	2601	17G	C25-C23-N8	2.46	125.66	120.73
3	B	2601	17G	C37-C39-N10	-2.37	120.51	124.28
3	B	2601	17G	C25-C23-N8	2.37	125.47	120.73
3	B	2601	17G	C23-C26-C31	2.16	122.58	117.93

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2601	17G	C30-C33-C37-C39
3	A	2601	17G	C30-C33-C37-C39
3	B	2601	17G	C36-C33-C37-C39
3	A	2601	17G	C36-C33-C37-C39

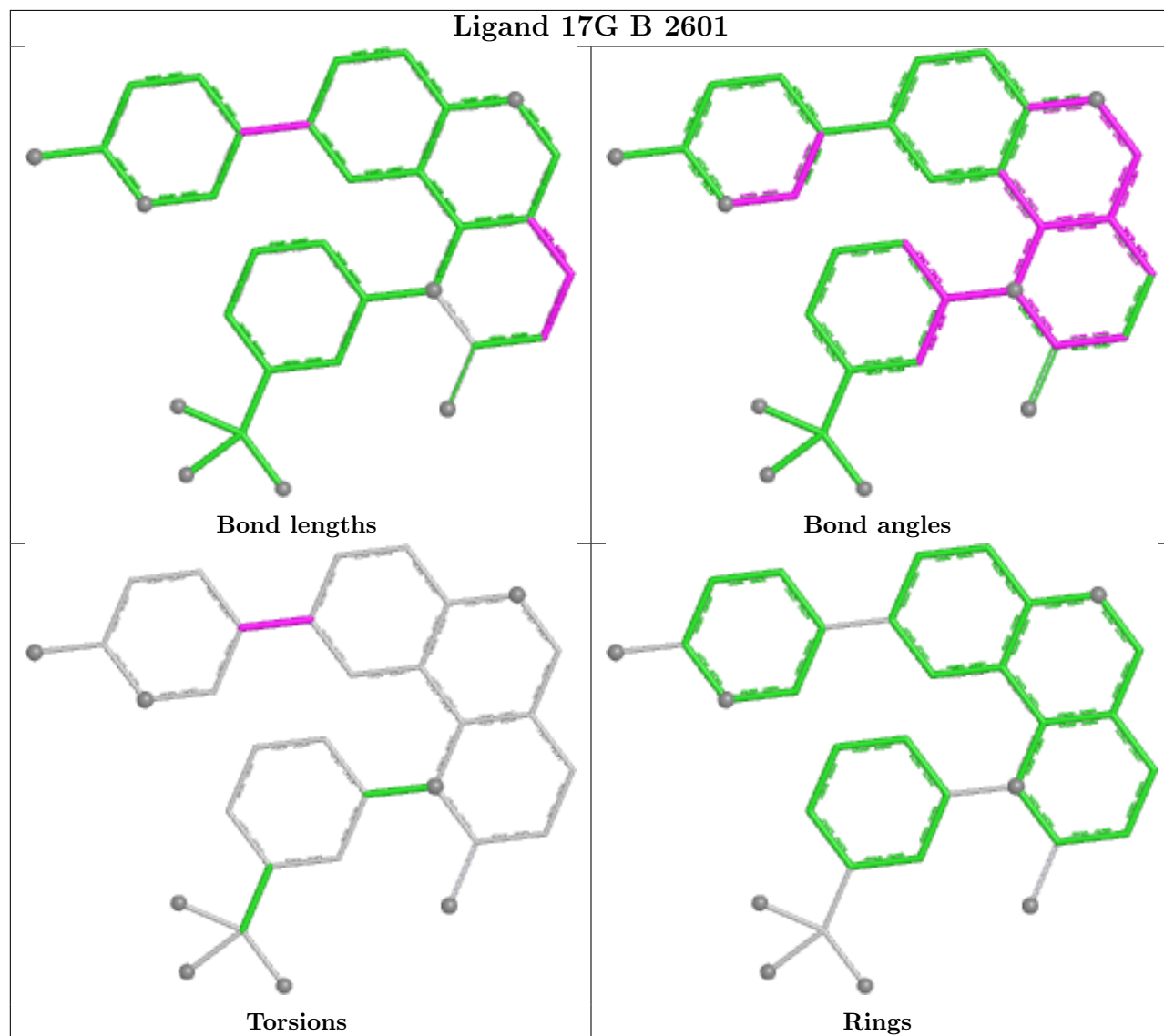
There are no ring outliers.

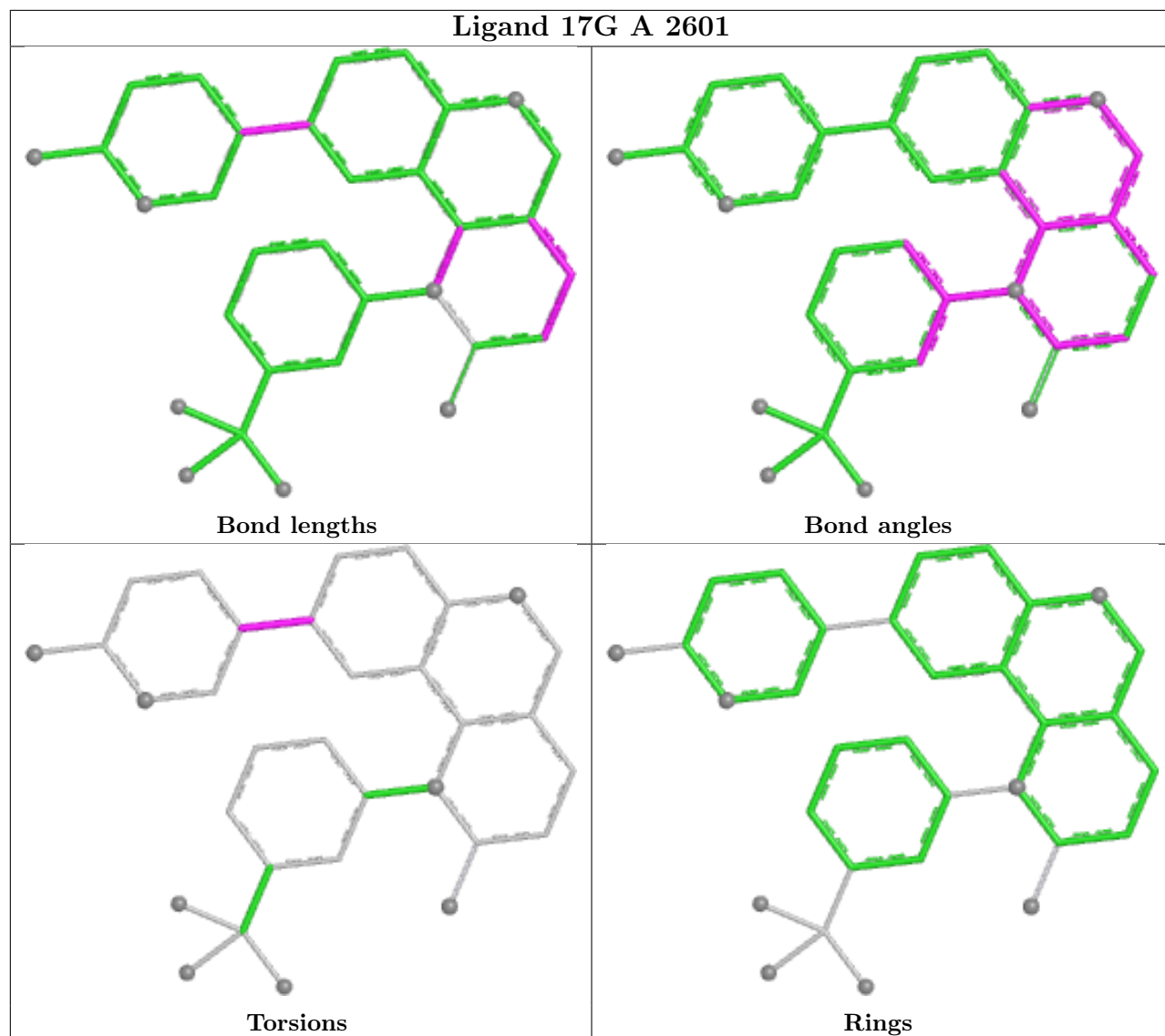
2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2601	17G	5	0
3	A	2601	17G	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [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%)	0.01	15 (1%)	73 48	37, 70, 153, 188	0
1	B	1058/1174 (90%)	-0.10	11 (1%)	79 56	32, 61, 135, 180	0
2	C	317/326 (97%)	-0.01	3 (0%)	81 58	38, 70, 118, 156	0
2	D	317/326 (97%)	-0.23	3 (0%)	81 58	29, 49, 97, 141	0
All	All	2746/3000 (91%)	-0.06	32 (1%)	76 52	29, 63, 144, 188	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1504	VAL	4.8
2	D	203	ILE	3.8
1	B	1607	LEU	3.5
2	C	203	ILE	3.2
1	B	1587	TYR	3.2
2	C	8	VAL	3.1
1	A	1595	MET	3.1
1	A	1504	VAL	3.0
1	A	1619	TRP	2.8
1	B	1575	LEU	2.7
1	A	1586	ALA	2.7
1	B	1649	ASP	2.5
1	B	1585	ARG	2.4
1	A	1603	ILE	2.4
1	A	1604	GLN	2.4
1	B	1446	GLN	2.4
1	B	1451	GLU	2.4
2	D	207	VAL	2.3
1	A	1579	ALA	2.3
1	A	1496	GLN	2.3
1	A	1585	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1496	GLN	2.2
1	A	2430	ARG	2.1
1	A	1615	ILE	2.1
2	C	207	VAL	2.1
1	A	1587	TYR	2.1
1	A	2436	THR	2.1
1	A	1614	ILE	2.1
1	B	1583	TYR	2.1
2	D	8	VAL	2.0
1	A	1583	TYR	2.0
1	B	2429	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

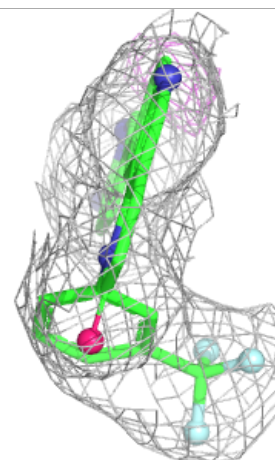
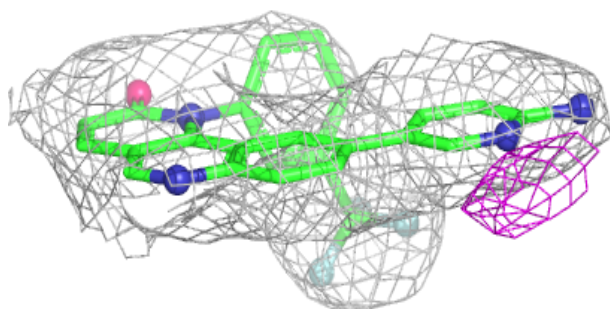
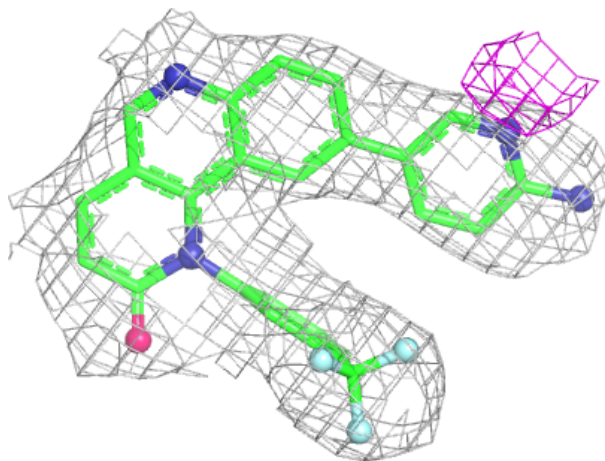
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	17G	A	2601	32/32	0.95	0.08	38,40,44,44	0
3	17G	B	2601	32/32	0.97	0.07	36,37,38,38	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.

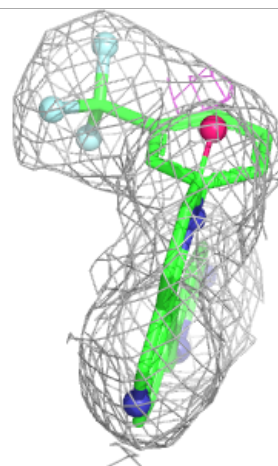
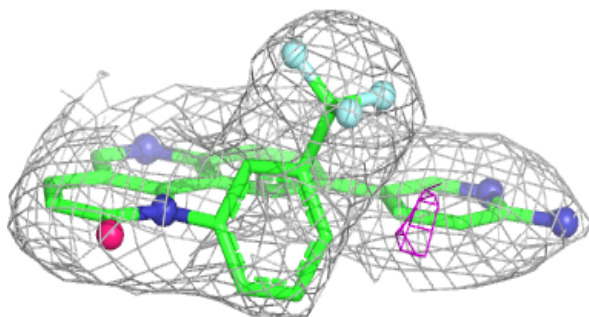
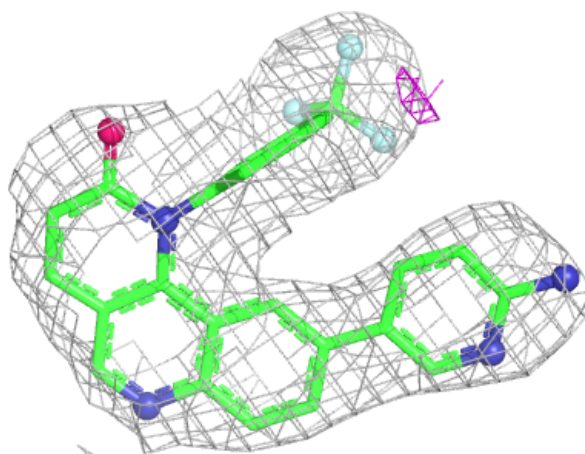
Electron density around 17G A 2601:

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



Electron density around 17G B 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.