



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:26 PM UTC

PDB ID : 4JSP / pdb_00004jsp
Title : structure of mTORDeltaN-mLST8-ATPgammaS-Mg complex
Authors : Pavletich, N.P.; Yang, H.
Deposited on : 2013-03-22
Resolution : 3.30 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

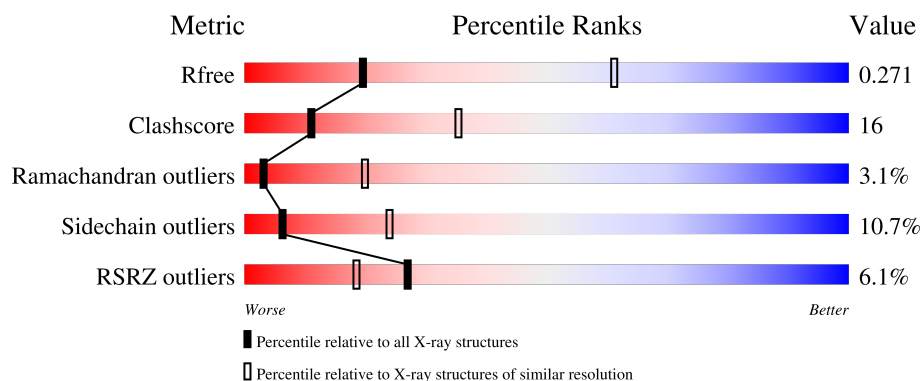
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	
1	B	1174	
2	C	326	
2	D	326	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 22194 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.

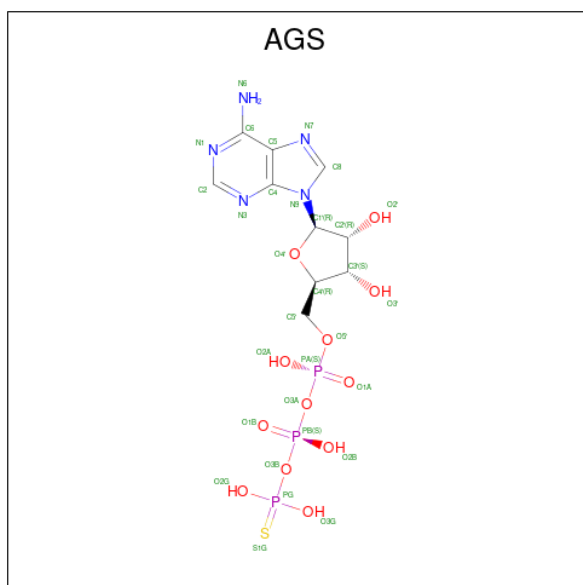
- Molecule 1 is a protein called Serine/threonine-protein kinase mTOR.

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	1058	Total	C	N	O	S	0	0	0
			8608	5472	1521	1552	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 PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).

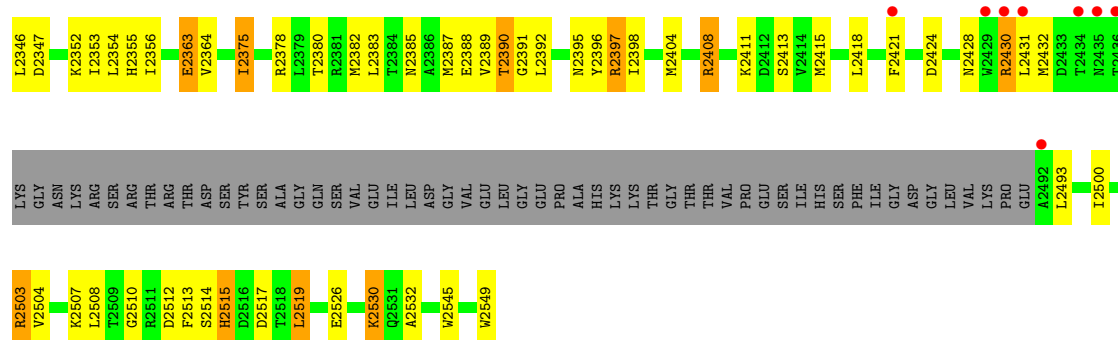


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
3	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

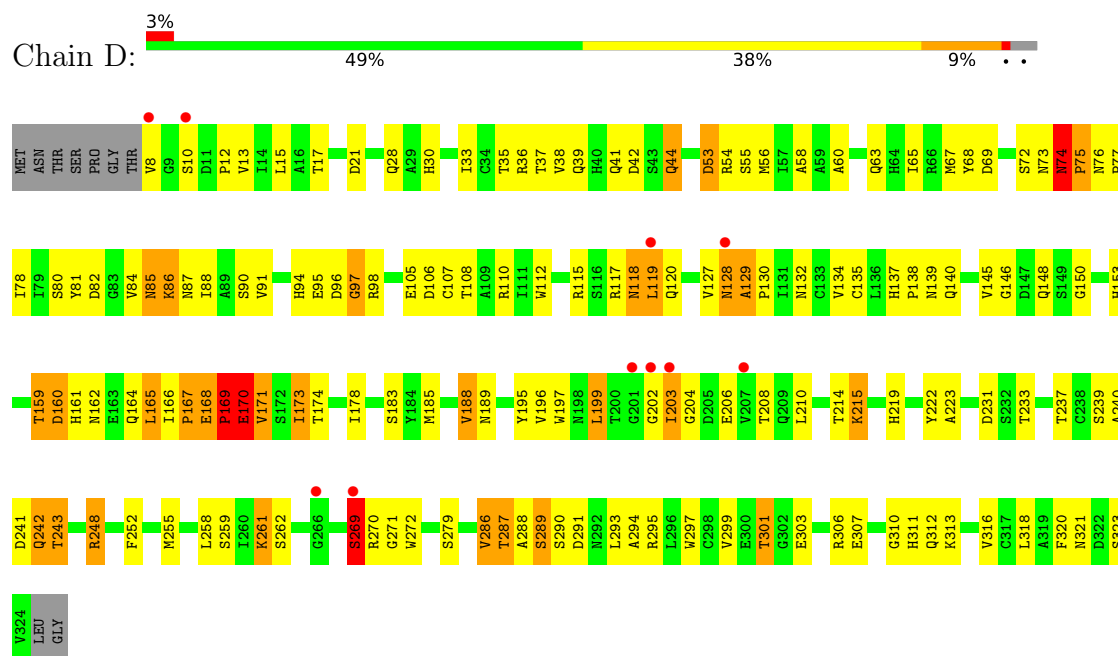
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		

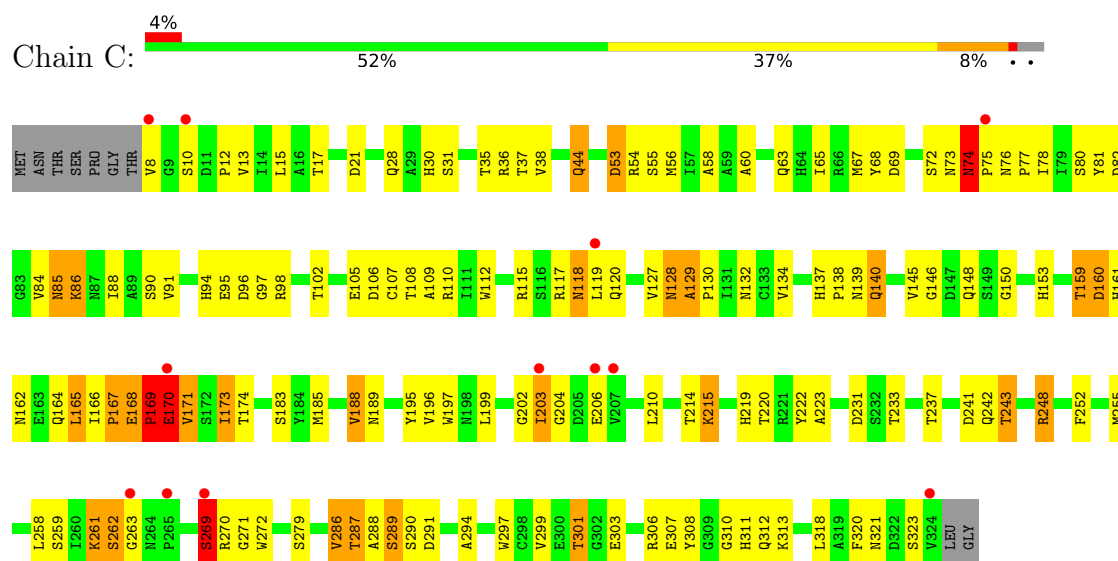




• Molecule 2: Target of rapamycin complex subunit LST8



• 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)	100.00 – 3.30 100.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	89.9 (100.00-3.30) 89.9 (100.00-3.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.233 , 0.268 0.234 , 0.271	Depositor DCC
R_{free} test set	1919 reflections (2.42%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.2	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	0.91	EDS
Total number of atoms	22194	wwPDB-VP
Average B, all atoms (Å ²)	70.0	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 40.83 % 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 2.5835e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, MG

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	0.49	3/8805 (0.0%)	0.96	15/11920 (0.1%)
1	B	0.48	1/8805 (0.0%)	0.95	15/11920 (0.1%)
2	C	0.51	0/2514	0.90	4/3426 (0.1%)
2	D	0.57	0/2514	0.95	8/3426 (0.2%)
All	All	0.50	4/22638 (0.0%)	0.95	42/30692 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
2	C	0	1
2	D	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1607	LEU	CA-C	9.29	1.61	1.52
1	B	1968	HIS	N-CA	5.95	1.50	1.46
1	A	1610	GLU	CA-C	5.52	1.58	1.53
1	A	1968	HIS	N-CA	5.13	1.50	1.46

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1915	HIS	N-CA-C	12.46	127.09	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1915	HIS	N-CA-C	12.32	126.89	109.15
1	A	1610	GLU	N-CA-C	12.30	126.58	109.11
2	D	170	GLU	N-CA-C	-9.78	99.70	112.41
2	C	170	GLU	N-CA-C	-9.00	100.71	112.41
1	B	1610	GLU	N-CA-C	8.73	120.85	108.54
1	B	1968	HIS	CA-C-N	-7.45	113.01	120.31
1	B	1968	HIS	C-N-CA	-7.45	113.01	120.31
1	A	1968	HIS	CA-C-N	-7.18	113.27	120.31
1	A	1968	HIS	C-N-CA	-7.18	113.27	120.31
1	B	1443	LEU	N-CA-C	-6.93	104.71	113.02
1	A	1443	LEU	N-CA-C	-6.59	105.12	113.02
1	B	1710	LYS	N-CA-C	6.05	120.94	113.50
1	A	2307	SER	CA-C-N	5.93	125.63	119.64
1	A	2307	SER	C-N-CA	5.93	125.63	119.64
1	B	2307	SER	CA-C-N	5.93	125.55	119.56
1	B	2307	SER	C-N-CA	5.93	125.55	119.56
1	B	1913	TYR	N-CA-C	5.88	119.61	111.55
1	A	1916	TRP	CA-C-N	5.87	127.17	119.84
1	A	1916	TRP	C-N-CA	5.87	127.17	119.84
1	A	1913	TYR	N-CA-C	5.83	119.54	111.55
1	B	1916	TRP	CA-C-N	5.70	126.97	119.84
1	B	1916	TRP	C-N-CA	5.70	126.97	119.84
2	D	87	ASN	N-CA-C	5.70	117.89	110.43
1	A	1710	LYS	N-CA-C	5.67	120.48	113.50
2	D	321	ASN	N-CA-C	5.46	118.00	108.76
1	A	1968	HIS	CB-CA-C	-5.40	106.30	111.00
2	C	321	ASN	N-CA-C	5.39	117.86	108.76
1	B	1973	ILE	N-CA-CB	5.38	116.73	110.65
1	B	2422	VAL	N-CA-C	-5.34	105.33	110.72
2	D	74	ASN	N-CA-C	5.31	121.55	109.81
2	C	169	PRO	N-CA-C	5.31	123.41	112.47
1	B	2381	ARG	N-CA-C	5.28	117.03	111.28
2	D	169	PRO	N-CA-C	5.15	123.08	112.47
2	C	74	ASN	N-CA-C	5.13	121.15	109.81
1	B	1968	HIS	CB-CA-C	-5.12	106.55	111.00
1	A	1898	ASN	N-CA-C	5.11	116.92	108.49
2	D	97	GLY	N-CA-C	5.10	125.26	113.18
1	A	1973	ILE	N-CA-CB	5.06	116.14	110.62
2	D	189	ASN	N-CA-C	5.01	116.30	109.18
1	A	1969	PRO	N-CA-C	-5.01	103.95	111.57
2	D	119	LEU	N-CA-C	-5.01	107.00	113.01

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1914	GLY	Peptide
1	B	1914	GLY	Peptide
2	C	169	PRO	Peptide
2	D	169	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8608	0	8593	256	6
1	B	8608	0	8593	249	0
2	C	2456	0	2341	114	0
2	D	2456	0	2341	123	0
3	A	31	0	12	1	0
3	B	31	0	12	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	22194	0	21892	724	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (724) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2503:ARG:HH11	1:A:2507:LYS:HE2	1.11	1.13
1:B:2503:ARG:HH11	1:B:2507:LYS:HE2	1.10	1.07
2:C:76:ASN:HB3	2:C:77:PRO:HD2	1.38	1.06
2:C:231:ASP:HB3	2:C:233:THR:OG1	1.59	1.02
2:D:231:ASP:HB3	2:D:233:THR:OG1	1.61	1.00
1:A:2503:ARG:NH1	1:A:2507:LYS:HE2	1.80	0.95
1:B:1969:PRO:O	1:B:1970:GLN:HB2	1.66	0.95
2:D:76:ASN:HB3	2:D:77:PRO:HD2	1.46	0.95
2:D:167:PRO:HD2	2:D:169:PRO:HG2	1.49	0.94
1:B:2503:ARG:NH1	1:B:2507:LYS:HE2	1.83	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1969:PRO:O	1:A:1970:GLN:HB2	1.67	0.92
1:B:2278:LEU:HD23	2:D:44:GLN:HG2	1.57	0.86
2:C:167:PRO:HD2	2:C:169:PRO:HG2	1.55	0.86
1:A:2387:MET:HE3	1:A:2396:TYR:HB2	1.57	0.85
1:A:2278:LEU:HD23	2:C:44:GLN:HG2	1.58	0.85
1:A:1418:SER:HB2	1:A:1581:GLU:HG2	1.58	0.84
2:D:55:SER:O	2:D:56:MET:HG2	1.79	0.82
1:A:1493:LEU:HD23	1:A:1519:ALA:HB2	1.58	0.82
1:A:1704:MET:HG2	1:A:1713:ALA:HB2	1.62	0.82
1:A:2397:ARG:NH2	1:A:2526:GLU:OE1	2.13	0.81
2:D:69:ASP:HB2	2:D:78:ILE:HD11	1.62	0.81
1:B:2387:MET:HE3	1:B:2396:TYR:HB2	1.62	0.80
1:A:2421:PHE:HA	1:A:2424:ASP:HB2	1.64	0.80
1:B:2223:GLN:HE22	1:B:2352:LYS:CB	1.95	0.79
1:A:2344:LEU:HD13	1:A:2353:ILE:HD11	1.64	0.79
1:B:2421:PHE:HD1	1:B:2430:ARG:NH2	1.81	0.79
2:C:301:THR:HB	2:C:303:GLU:HG2	1.66	0.78
1:B:1623:LEU:HG	1:B:1633:TRP:CH2	2.19	0.78
1:B:2397:ARG:NH2	1:B:2526:GLU:OE1	2.15	0.78
1:A:2223:GLN:HE22	1:A:2352:LYS:CB	1.96	0.78
1:A:2421:PHE:HD1	1:A:2430:ARG:HH22	1.29	0.78
1:A:2278:LEU:CD2	2:C:44:GLN:HG2	2.13	0.78
1:B:2421:PHE:HD1	1:B:2430:ARG:HH22	1.32	0.78
1:B:2254:ARG:HD3	1:B:2298:ASP:OD2	1.83	0.78
1:B:2421:PHE:HA	1:B:2424:ASP:HB2	1.66	0.77
2:C:286:VAL:HB	2:C:318:LEU:HD13	1.66	0.77
1:A:2254:ARG:HD3	1:A:2298:ASP:OD2	1.84	0.77
1:A:2392:LEU:O	1:A:2397:ARG:HB2	1.84	0.77
1:A:2421:PHE:HD1	1:A:2430:ARG:NH2	1.83	0.76
3:B:3000:AGS:O2A	3:B:3000:AGS:H8	1.84	0.76
2:C:76:ASN:HB3	2:C:77:PRO:CD	2.14	0.76
2:D:286:VAL:HB	2:D:318:LEU:HD13	1.68	0.75
1:B:1704:MET:HG2	1:B:1713:ALA:HB2	1.67	0.75
2:C:95:GLU:HB2	2:C:140:GLN:NE2	2.01	0.75
2:C:117:ARG:O	2:C:118:ASN:HB2	1.86	0.75
2:D:301:THR:HB	2:D:303:GLU:HG2	1.69	0.74
2:C:146:GLY:HA3	2:C:173:ILE:HD11	1.68	0.74
1:B:2344:LEU:HD13	1:B:2353:ILE:HD11	1.68	0.73
1:A:1422:LYS:HD3	1:A:1580:GLY:HA3	1.69	0.73
2:D:95:GLU:HB2	2:D:140:GLN:NE2	2.04	0.72
3:A:3000:AGS:O2A	3:A:3000:AGS:H8	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:69:ASP:HB2	2:C:78:ILE:HD11	1.71	0.72
2:D:117:ARG:O	2:D:118:ASN:HB2	1.88	0.72
2:D:170:GLU:HA	2:D:170:GLU:OE2	1.87	0.72
1:A:2281:MET:HE1	2:C:222:TYR:CD2	2.24	0.72
2:C:168:GLU:N	2:C:169:PRO:HD2	2.05	0.72
1:B:1901:GLN:HG3	1:B:2413:SER:HA	1.72	0.72
1:B:1941:GLN:HE22	1:B:2200:GLN:HE22	1.36	0.72
2:D:168:GLU:N	2:D:169:PRO:HD2	2.05	0.72
1:B:1778:ALA:O	1:B:1782:HIS:HD2	1.72	0.71
2:D:63:GLN:HE21	2:D:86:LYS:H	1.38	0.71
1:B:2278:LEU:CD2	2:D:44:GLN:HG2	2.19	0.71
1:B:2392:LEU:O	1:B:2397:ARG:HB2	1.89	0.71
1:B:2022:LEU:HD21	1:B:2126:VAL:HG13	1.72	0.71
1:A:1759:LEU:HG	1:A:1772:VAL:HG11	1.73	0.71
2:D:76:ASN:HB3	2:D:77:PRO:CD	2.21	0.70
2:C:170:GLU:OE2	2:C:170:GLU:HA	1.89	0.70
1:B:2223:GLN:HE22	1:B:2352:LYS:HB3	1.55	0.70
1:B:2281:MET:HE1	2:D:222:TYR:CD2	2.26	0.70
1:A:1878:LEU:HD21	1:A:1918:ASP:HB2	1.72	0.70
2:D:146:GLY:HA3	2:D:173:ILE:HD11	1.72	0.70
2:C:279:SER:HA	2:C:320:PHE:HE2	1.56	0.70
1:A:1901:GLN:HG3	1:A:2413:SER:HA	1.73	0.69
1:A:2064:THR:HG22	1:A:2128:PRO:HD3	1.73	0.69
2:D:279:SER:HA	2:D:320:PHE:HE2	1.57	0.69
1:A:2223:GLN:HE22	1:A:2352:LYS:HB3	1.57	0.69
1:A:1705:TRP:HZ2	1:A:1760:ASN:HD22	1.39	0.69
1:B:1878:LEU:HD21	1:B:1918:ASP:HB2	1.74	0.68
1:B:1913:TYR:HB2	1:B:1915:HIS:CE1	2.28	0.68
1:A:1680:ASP:C	1:A:1682:SER:H	2.01	0.68
2:C:63:GLN:HE21	2:C:86:LYS:H	1.41	0.68
1:B:1680:ASP:C	1:B:1682:SER:H	2.02	0.68
1:B:1969:PRO:O	1:B:1970:GLN:CB	2.39	0.68
1:B:1493:LEU:HD23	1:B:1519:ALA:HB2	1.76	0.68
1:B:1701:MET:HE1	1:B:1717:MET:N	2.09	0.68
2:D:107:CYS:HB3	2:D:127:VAL:O	1.94	0.67
2:D:8:VAL:HG21	2:D:36:ARG:HD3	1.76	0.67
2:C:137:HIS:HD2	2:C:139:ASN:H	1.41	0.67
1:A:1778:ALA:O	1:A:1782:HIS:HD2	1.78	0.67
1:A:1913:TYR:HB2	1:A:1915:HIS:CE1	2.29	0.67
1:A:2022:LEU:HD21	1:A:2126:VAL:HG13	1.77	0.67
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:219:HIS:NE2	2:C:237:THR:HG22	2.09	0.66
2:D:150:GLY:HA3	2:D:169:PRO:HB3	1.77	0.66
1:A:2411:LYS:O	1:A:2415:MET:HG3	1.95	0.66
1:B:1680:ASP:C	1:B:1682:SER:N	2.53	0.66
2:C:150:GLY:HA3	2:C:169:PRO:HB3	1.77	0.66
1:A:1969:PRO:O	1:A:1970:GLN:CB	2.39	0.66
2:C:8:VAL:HG21	2:C:36:ARG:HD3	1.76	0.66
1:B:1964:ILE:O	1:B:1967:TYR:O	2.13	0.66
1:A:1964:ILE:O	1:A:1967:TYR:O	2.13	0.66
1:B:2064:THR:HG22	1:B:2128:PRO:HD3	1.77	0.66
1:A:1941:GLN:HE22	1:A:2200:GLN:HE22	1.43	0.66
1:A:1611:ARG:HG2	1:A:1614:ILE:HD12	1.79	0.65
1:B:2363:GLU:OE2	1:B:2503:ARG:HD2	1.95	0.65
2:D:188:VAL:HG13	2:D:223:ALA:HB3	1.79	0.65
1:A:1583:TYR:C	1:A:1585:ARG:H	2.05	0.65
2:C:55:SER:O	2:C:56:MET:HG2	1.97	0.65
2:D:137:HIS:HD2	2:D:139:ASN:H	1.42	0.65
1:A:1734:THR:C	1:A:1736:ASP:H	2.04	0.65
1:B:1907:LEU:HD11	1:B:1938:VAL:CG1	2.27	0.65
2:D:241:ASP:OD2	2:D:243:THR:HB	1.96	0.65
2:D:17:THR:HB	2:D:311:HIS:HE1	1.61	0.65
1:A:1701:MET:HE1	1:A:1717:MET:N	2.11	0.65
2:C:17:THR:HB	2:C:311:HIS:HE1	1.62	0.65
2:C:107:CYS:HB3	2:C:127:VAL:O	1.95	0.65
1:A:2192:LEU:HD12	1:A:2235:GLY:HA3	1.80	0.64
1:B:1907:LEU:HD11	1:B:1938:VAL:HG11	1.79	0.64
1:A:1926:GLY:O	1:A:1930:ILE:HG22	1.96	0.64
1:B:1583:TYR:C	1:B:1585:ARG:H	2.06	0.64
2:D:219:HIS:NE2	2:D:237:THR:HG22	2.13	0.64
1:A:1670:HIS:HE1	1:A:1681:PRO:HB3	1.62	0.64
1:A:2389:VAL:O	1:A:2390:THR:HG22	1.97	0.64
1:B:2390:THR:HG23	1:B:2390:THR:O	1.97	0.64
1:A:2363:GLU:OE2	1:A:2503:ARG:HD2	1.98	0.64
2:C:241:ASP:OD2	2:C:243:THR:HB	1.97	0.64
1:A:1680:ASP:C	1:A:1682:SER:N	2.53	0.63
1:A:2223:GLN:HE22	1:A:2352:LYS:HB2	1.62	0.63
1:B:1422:LYS:HE2	1:B:1581:GLU:HG2	1.78	0.63
2:D:60:ALA:HB1	2:D:88:ILE:HG22	1.80	0.63
1:B:2382:MET:HG3	1:B:2549:TRP:O	1.98	0.63
2:D:279:SER:HA	2:D:320:PHE:CE2	2.34	0.63
1:A:2382:MET:HG3	1:A:2549:TRP:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2387:MET:CE	1:A:2396:TYR:HB2	2.29	0.63
2:C:12:PRO:O	2:C:54:ARG:NH2	2.31	0.63
1:B:2223:GLN:HE22	1:B:2352:LYS:HB2	1.63	0.63
1:B:2380:THR:HG22	1:B:2383:LEU:HG	1.80	0.63
2:D:108:THR:OG1	2:D:110:ARG:NH1	2.32	0.63
2:C:108:THR:OG1	2:C:110:ARG:NH1	2.32	0.63
1:B:1759:LEU:HG	1:B:1772:VAL:HG11	1.80	0.62
1:B:2339:ARG:HH21	1:B:2343:ASN:HB3	1.64	0.62
2:D:118:ASN:HD22	2:D:120:GLN:HB2	1.63	0.62
1:A:1427:GLU:HB2	1:A:2398:ILE:HD13	1.81	0.62
2:C:36:ARG:NH2	2:C:69:ASP:O	2.32	0.62
1:A:1703:ASN:O	1:A:1707:SER:HB2	1.99	0.62
2:C:94:HIS:CD2	2:C:140:GLN:HB3	2.34	0.62
1:B:1703:ASN:O	1:B:1707:SER:HB2	1.99	0.62
2:C:279:SER:HA	2:C:320:PHE:CE2	2.35	0.62
1:B:2378:ARG:HH11	1:B:2380:THR:HG21	1.64	0.62
1:B:2389:VAL:O	1:B:2390:THR:HG22	1.99	0.62
1:B:2251:ARG:NH1	1:B:2252:ASP:OD1	2.32	0.62
2:D:169:PRO:HA	2:D:171:VAL:H	1.64	0.62
2:C:118:ASN:HD22	2:C:120:GLN:HB2	1.64	0.62
1:B:1705:TRP:HZ2	1:B:1760:ASN:HD22	1.48	0.62
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.32	0.62
2:D:36:ARG:NH2	2:D:69:ASP:O	2.33	0.62
1:B:1913:TYR:O	1:B:1915:HIS:HA	1.99	0.61
1:A:1607:LEU:O	1:A:1609:PRO:HD3	1.99	0.61
2:C:60:ALA:HB1	2:C:88:ILE:HG22	1.82	0.61
2:D:94:HIS:CD2	2:D:140:GLN:HB3	2.35	0.61
1:B:1691:THR:O	1:B:1691:THR:HG22	2.00	0.61
1:B:1422:LYS:HE2	1:B:1581:GLU:CG	2.30	0.61
1:A:1913:TYR:O	1:A:1915:HIS:HA	2.00	0.61
2:C:185:MET:HE2	2:C:197:TRP:CD1	2.35	0.61
1:B:2093:ASN:O	1:B:2094:VAL:HB	2.01	0.60
1:B:2380:THR:HG23	1:B:2549:TRP:O	2.01	0.60
1:B:2387:MET:CE	1:B:2396:TYR:HB2	2.31	0.60
1:B:2411:LYS:O	1:B:2415:MET:HG3	2.01	0.60
1:A:2380:THR:HG22	1:A:2383:LEU:HG	1.83	0.60
2:D:12:PRO:O	2:D:54:ARG:NH2	2.34	0.60
2:C:105:GLU:HA	2:C:130:PRO:HB3	1.84	0.60
1:B:2298:ASP:HB2	1:B:2382:MET:CE	2.31	0.60
2:D:132:ASN:HD21	2:D:148:GLN:HG2	1.66	0.60
1:A:2093:ASN:O	1:A:2094:VAL:HB	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2192:LEU:HD12	1:B:2235:GLY:HA3	1.84	0.59
1:A:1402:LEU:O	1:A:1405:GLN:HB2	2.03	0.59
1:A:2380:THR:HG23	1:A:2549:TRP:O	2.02	0.59
1:B:2281:MET:HE1	2:D:222:TYR:CG	2.37	0.59
2:C:169:PRO:HA	2:C:171:VAL:H	1.66	0.59
1:A:2339:ARG:HH21	1:A:2343:ASN:HB3	1.68	0.59
1:A:2390:THR:HG23	1:A:2390:THR:O	2.01	0.59
2:D:94:HIS:CE1	2:D:96:ASP:HB2	2.38	0.59
1:A:1691:THR:HG22	1:A:1691:THR:O	2.03	0.58
2:C:248:ARG:O	2:C:252:PHE:N	2.34	0.58
1:A:2287:PHE:O	1:A:2291:VAL:HG23	2.03	0.58
1:A:1732:ILE:CD1	1:A:1740:LYS:HB2	2.33	0.58
1:A:1734:THR:O	1:A:1736:ASP:N	2.31	0.58
1:A:2530:LYS:HE2	1:A:2530:LYS:HA	1.84	0.58
2:C:54:ARG:HD2	2:C:323:SER:HB2	1.85	0.58
1:B:1892:ILE:HD11	1:B:1903:THR:HA	1.85	0.58
2:D:137:HIS:CD2	2:D:138:PRO:HD2	2.38	0.58
2:C:21:ASP:HB3	2:C:313:LYS:H	1.68	0.58
1:B:1691:THR:HG23	1:B:1724:MET:HE1	1.86	0.58
1:B:2514:SER:OG	1:B:2517:ASP:HB2	2.04	0.58
1:A:2298:ASP:HB2	1:A:2382:MET:CE	2.33	0.58
1:A:2319:ASN:HB3	1:A:2352:LYS:HG2	1.85	0.58
2:D:105:GLU:HA	2:D:130:PRO:HB3	1.85	0.58
2:D:168:GLU:HB3	2:D:195:TYR:OH	2.04	0.58
1:B:1497:CYS:SG	1:B:1516:ALA:HB2	2.44	0.58
2:D:128:ASN:O	2:D:129:ALA:HB3	2.03	0.58
1:B:2287:PHE:O	1:B:2291:VAL:HG23	2.04	0.58
1:A:1907:LEU:HD11	1:A:1938:VAL:CG1	2.34	0.58
1:A:1725:GLN:HB3	1:A:1747:MET:HE1	1.86	0.57
1:A:1783:ASP:O	1:A:1785:SER:N	2.37	0.57
2:C:94:HIS:HD2	2:C:140:GLN:HB3	1.69	0.57
1:A:2378:ARG:HH11	1:A:2380:THR:HG21	1.70	0.57
2:C:168:GLU:HG2	2:C:169:PRO:N	2.19	0.57
1:B:1701:MET:HE1	1:B:1717:MET:CA	2.34	0.57
2:D:21:ASP:HB3	2:D:313:LYS:H	1.69	0.57
1:A:2515:HIS:ND1	1:A:2515:HIS:N	2.53	0.57
2:D:94:HIS:HD2	2:D:140:GLN:HB3	1.70	0.57
1:A:1943:ILE:O	1:A:1987:ARG:NH2	2.34	0.57
1:A:1785:SER:O	1:A:1786:TRP:CB	2.52	0.57
1:B:1785:SER:O	1:B:1786:TRP:CB	2.52	0.56
1:B:2515:HIS:ND1	1:B:2515:HIS:N	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:255:MET:HE1	2:D:299:VAL:HG12	1.87	0.56
1:A:1418:SER:HB2	1:A:1581:GLU:CG	2.33	0.56
1:A:2346:LEU:HD23	1:A:2353:ILE:HG13	1.85	0.56
2:C:132:ASN:HD21	2:C:148:GLN:HG2	1.70	0.56
2:D:168:GLU:HG2	2:D:169:PRO:N	2.21	0.56
1:A:1732:ILE:HD13	1:A:1740:LYS:HB2	1.87	0.56
1:A:2251:ARG:NH1	1:A:2252:ASP:OD1	2.38	0.56
1:B:1734:THR:O	1:B:1736:ASP:N	2.28	0.56
1:A:1422:LYS:HG2	1:A:1580:GLY:C	2.31	0.56
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.38	0.56
1:A:2339:ARG:NH2	1:A:2343:ASN:HB3	2.20	0.56
2:D:137:HIS:CD2	2:D:139:ASN:H	2.22	0.56
2:C:137:HIS:CD2	2:C:139:ASN:H	2.22	0.56
1:B:1926:GLY:O	1:B:1930:ILE:HG22	2.06	0.56
1:B:2530:LYS:HE2	1:B:2530:LYS:HA	1.87	0.56
1:A:2037:LEU:HD22	1:A:2043:ASN:HD22	1.71	0.55
2:C:128:ASN:O	2:C:129:ALA:HB3	2.05	0.55
1:A:1907:LEU:HD11	1:A:1938:VAL:HG11	1.87	0.55
1:A:2095:LYS:O	1:A:2099:GLN:HG2	2.06	0.55
2:C:76:ASN:CB	2:C:77:PRO:HD2	2.25	0.55
2:C:106:ASP:OD1	2:C:108:THR:OG1	2.18	0.55
1:B:1734:THR:C	1:B:1736:ASP:H	2.13	0.55
1:B:1783:ASP:O	1:B:1785:SER:N	2.39	0.55
2:D:38:VAL:HG11	2:D:68:TYR:CD2	2.41	0.55
1:B:2378:ARG:NH1	1:B:2380:THR:HG21	2.20	0.55
1:B:1415:SER:O	1:B:1419:ILE:HG22	2.07	0.55
1:B:2056:ALA:HA	1:B:2059:GLU:HB2	1.88	0.55
1:A:2387:MET:HE1	1:A:2392:LEU:HD23	1.89	0.55
2:D:53:ASP:HB2	2:D:55:SER:OG	2.07	0.55
2:C:188:VAL:HG13	2:C:223:ALA:HB3	1.89	0.55
1:B:2146:PRO:O	1:B:2147:ASN:HB2	2.07	0.55
1:A:2408:ARG:HG2	1:A:2508:LEU:O	2.06	0.55
1:A:2503:ARG:HH11	1:A:2507:LYS:CE	2.02	0.55
1:B:2346:LEU:HD23	1:B:2353:ILE:HG13	1.88	0.54
2:D:95:GLU:HB2	2:D:140:GLN:HE21	1.72	0.54
1:A:1691:THR:HG23	1:A:1724:MET:HE1	1.89	0.54
1:B:2095:LYS:O	1:B:2099:GLN:HG2	2.07	0.54
1:B:2282:GLN:HE21	2:D:316:VAL:HG11	1.72	0.54
2:D:82:ASP:HB2	2:D:119:LEU:HD13	1.90	0.54
2:D:117:ARG:O	2:D:118:ASN:CB	2.55	0.54
2:C:117:ARG:O	2:C:118:ASN:CB	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:269:SER:OG	2:C:270:ARG:N	2.41	0.54
1:B:1428:ALA:HB2	1:B:2395:ASN:HD21	1.72	0.54
1:A:2281:MET:HE1	2:C:222:TYR:CG	2.43	0.54
2:C:255:MET:HE1	2:C:299:VAL:HG12	1.90	0.54
1:B:1621:GLU:C	1:B:1623:LEU:H	2.15	0.54
1:A:1508:THR:O	1:A:1512:MET:HB2	2.08	0.54
1:A:2178:ASN:HD22	1:A:2180:HIS:H	1.56	0.54
1:B:2339:ARG:NH2	1:B:2343:ASN:HB3	2.22	0.54
2:D:54:ARG:HD2	2:D:323:SER:HB2	1.90	0.54
1:B:2082:GLN:HG2	1:B:2086:ARG:HD3	1.90	0.54
1:A:1621:GLU:C	1:A:1623:LEU:H	2.15	0.54
1:B:1402:LEU:O	1:B:1405:GLN:HB2	2.08	0.53
2:D:96:ASP:O	2:D:98:ARG:N	2.38	0.53
1:A:2298:ASP:HB2	1:A:2382:MET:HE1	1.90	0.53
2:C:96:ASP:O	2:C:98:ARG:N	2.37	0.53
1:B:1623:LEU:HG	1:B:1633:TRP:CZ3	2.43	0.53
1:A:1422:LYS:HE2	1:A:1581:GLU:HG3	1.90	0.53
1:A:1701:MET:HE1	1:A:1717:MET:CA	2.37	0.53
2:C:195:TYR:CE2	2:C:215:LYS:HG3	2.43	0.53
1:A:1590:MET:O	1:A:1594:HIS:HB2	2.09	0.53
1:A:1754:LEU:HD13	1:A:1775:TYR:CE2	2.43	0.53
1:A:1807:GLN:O	1:A:1810:ALA:HB3	2.08	0.53
1:B:2418:LEU:HD23	1:B:2421:PHE:CZ	2.43	0.53
1:A:1422:LYS:HE2	1:A:1581:GLU:CG	2.39	0.53
1:A:1892:ILE:HD11	1:A:1903:THR:HA	1.90	0.53
2:D:185:MET:HE2	2:D:197:TRP:CD1	2.44	0.53
1:A:1393:TYR:CZ	1:A:1422:LYS:HD2	2.44	0.53
1:B:1508:THR:O	1:B:1512:MET:HB2	2.09	0.52
1:B:2530:LYS:HA	1:B:2530:LYS:CE	2.39	0.52
2:D:127:VAL:HG11	2:D:153:HIS:CE1	2.44	0.52
1:B:1807:GLN:O	1:B:1810:ALA:HB3	2.08	0.52
1:B:2178:ASN:HD22	1:B:2180:HIS:H	1.57	0.52
1:A:1698:TYR:O	1:A:1702:LYS:HG2	2.09	0.52
1:A:2056:ALA:HA	1:A:2059:GLU:HB2	1.90	0.52
1:B:1590:MET:O	1:B:1594:HIS:HB2	2.10	0.52
1:B:1913:TYR:CB	1:B:1915:HIS:CE1	2.92	0.52
2:D:269:SER:OG	2:D:270:ARG:N	2.43	0.52
1:A:1393:TYR:O	1:A:1419:ILE:HD11	2.10	0.52
1:A:1415:SER:O	1:A:1419:ILE:HG22	2.10	0.52
2:C:130:PRO:HD2	2:C:148:GLN:HB2	1.91	0.52
1:A:1913:TYR:CB	1:A:1915:HIS:CE1	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:38:VAL:HG11	2:C:68:TYR:CD2	2.44	0.52
2:C:168:GLU:HB3	2:C:195:TYR:OH	2.10	0.52
2:C:259:SER:HB2	2:C:261:LYS:HE3	1.92	0.52
1:B:1698:TYR:O	1:B:1702:LYS:HG2	2.10	0.52
2:D:72:SER:O	2:D:74:ASN:N	2.42	0.52
1:A:2130:LEU:HD22	1:A:2156:ILE:HD13	1.91	0.52
1:A:1989:ASN:O	1:A:1993:LYS:HD2	2.09	0.52
1:A:2146:PRO:O	1:A:2147:ASN:HB2	2.10	0.52
1:B:2156:ILE:HG12	1:B:2174:LEU:HD22	1.92	0.51
1:B:1943:ILE:O	1:B:1987:ARG:NH2	2.39	0.51
1:A:1915:HIS:HE1	1:A:1919:VAL:HG11	1.75	0.51
1:B:1611:ARG:HG2	1:B:1614:ILE:HD12	1.93	0.51
1:A:2278:LEU:HD23	2:C:44:GLN:CG	2.35	0.51
2:C:137:HIS:CD2	2:C:138:PRO:HD2	2.46	0.51
1:B:1698:TYR:CE2	1:B:1702:LYS:HD3	2.45	0.51
1:B:2037:LEU:HD22	1:B:2043:ASN:HD22	1.75	0.51
1:A:2378:ARG:NH1	1:A:2380:THR:HG21	2.25	0.51
1:B:2298:ASP:HB2	1:B:2382:MET:HE1	1.92	0.51
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.44	0.51
2:D:259:SER:HB2	2:D:261:LYS:HE3	1.92	0.51
1:A:2082:GLN:HG2	1:A:2086:ARG:HD3	1.93	0.51
2:C:72:SER:O	2:C:74:ASN:N	2.43	0.51
2:D:76:ASN:CB	2:D:77:PRO:HD2	2.30	0.51
1:B:1643:VAL:HG12	1:B:1644:VAL:HG22	1.92	0.51
1:B:1938:VAL:CG1	1:B:1938:VAL:O	2.59	0.51
2:C:286:VAL:HB	2:C:318:LEU:CD1	2.40	0.50
1:B:1913:TYR:O	1:B:1915:HIS:CG	2.64	0.50
1:A:1698:TYR:CE2	1:A:1702:LYS:HD3	2.47	0.50
1:A:2530:LYS:HA	1:A:2530:LYS:CE	2.41	0.50
1:B:1660:CYS:HB2	1:B:1669:ALA:HB2	1.92	0.50
1:B:2428:ASN:HB3	1:B:2493:LEU:HD13	1.94	0.50
2:C:127:VAL:HG11	2:C:153:HIS:CE1	2.47	0.50
1:A:1717:MET:HG3	1:A:1754:LEU:HG	1.92	0.50
1:A:2340:HIS:HB2	1:A:2341:PRO:HD2	1.94	0.50
2:D:159:THR:C	2:D:161:HIS:H	2.20	0.50
2:C:271:GLY:HA2	2:C:290:SER:HB2	1.93	0.50
2:C:159:THR:C	2:C:161:HIS:H	2.20	0.50
2:D:128:ASN:O	2:D:129:ALA:CB	2.59	0.50
1:A:2514:SER:OG	1:A:2517:ASP:HB2	2.12	0.50
1:B:1393:TYR:CZ	1:B:1422:LYS:HD2	2.47	0.50
2:C:168:GLU:N	2:C:169:PRO:CD	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:248:ARG:O	2:D:252:PHE:N	2.43	0.49
1:B:1466:LYS:O	1:B:1470:ASN:HB2	2.12	0.49
1:B:2340:HIS:HB2	1:B:2341:PRO:HD2	1.94	0.49
1:A:1908:THR:O	1:A:1912:ASP:HB2	2.12	0.49
2:C:196:VAL:HG11	2:C:252:PHE:CZ	2.47	0.49
1:B:1686:ASP:O	1:A:2266:ARG:HG3	2.12	0.49
1:B:2278:LEU:HD23	2:D:44:GLN:CG	2.37	0.49
2:D:196:VAL:HG11	2:D:252:PHE:CZ	2.47	0.49
1:A:1916:TRP:CD1	1:A:1916:TRP:H	2.29	0.49
1:B:1930:ILE:HD11	1:B:1934:THR:HG21	1.95	0.49
1:B:2345:MET:HE1	3:B:3000:AGS:H2'	1.93	0.49
1:B:2421:PHE:CD1	1:B:2430:ARG:NH2	2.71	0.49
2:C:53:ASP:HB2	2:C:55:SER:OG	2.12	0.49
1:B:1629:ILE:HG22	1:B:1630:VAL:HG23	1.94	0.49
1:B:2285:GLU:HB2	2:D:272:TRP:CZ3	2.46	0.49
1:A:1784:ARG:O	1:A:1790:TRP:NE1	2.37	0.49
2:C:202:GLY:O	2:C:203:ILE:O	2.31	0.49
1:A:1529:MET:HE3	1:A:1550:LEU:HG	1.94	0.49
1:A:1913:TYR:O	1:A:1915:HIS:CG	2.65	0.49
2:C:94:HIS:CE1	2:C:96:ASP:HB2	2.48	0.49
1:B:2130:LEU:HD22	1:B:2156:ILE:HD13	1.94	0.49
2:C:219:HIS:NE2	2:C:237:THR:CG2	2.76	0.49
1:A:1466:LYS:O	1:A:1470:ASN:HB2	2.12	0.49
2:C:134:VAL:HG22	2:C:145:VAL:HG22	1.94	0.49
1:B:1930:ILE:HG12	1:B:1931:GLN:N	2.28	0.49
1:B:2319:ASN:HB3	1:B:2352:LYS:HG2	1.94	0.49
2:D:168:GLU:N	2:D:169:PRO:CD	2.74	0.49
1:A:1878:LEU:HD21	1:A:1918:ASP:CB	2.42	0.49
1:B:2298:ASP:HB2	1:B:2382:MET:HE2	1.93	0.48
2:D:231:ASP:CB	2:D:233:THR:OG1	2.50	0.48
2:C:128:ASN:O	2:C:129:ALA:CB	2.60	0.48
1:B:1628:ARG:HB2	1:B:1633:TRP:CD1	2.48	0.48
1:B:1980:SER:O	1:B:1988:HIS:HB2	2.13	0.48
1:B:1989:ASN:O	1:B:1993:LYS:HD2	2.13	0.48
2:C:95:GLU:HB2	2:C:140:GLN:HE21	1.73	0.48
1:B:1916:TRP:H	1:B:1916:TRP:CD1	2.30	0.48
2:D:41:GLN:O	2:D:42:ASP:HB2	2.13	0.48
2:D:58:ALA:HB2	2:D:67:MET:HE3	1.95	0.48
2:D:306:ARG:HG2	2:D:307:GLU:H	1.78	0.48
2:C:98:ARG:HD2	2:C:115:ARG:HB2	1.96	0.48
1:A:1530:GLU:HA	1:A:1550:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1393:TYR:O	1:B:1419:ILE:HD11	2.13	0.48
1:B:1943:ILE:O	1:B:1946:ILE:HG13	2.14	0.48
1:B:2512:ASP:OD1	1:B:2512:ASP:N	2.36	0.48
2:D:202:GLY:O	2:D:203:ILE:O	2.32	0.48
2:D:219:HIS:HE1	2:D:243:THR:HG22	1.77	0.48
1:A:1980:SER:O	1:A:1988:HIS:HB2	2.14	0.48
1:A:2185:LEU:CD1	1:A:2239:TRP:HZ3	2.27	0.48
1:B:1428:ALA:HB2	1:B:2395:ASN:ND2	2.29	0.48
1:A:1608:VAL:O	1:A:1610:GLU:N	2.46	0.48
1:A:1628:ARG:HB2	1:A:1633:TRP:CD1	2.49	0.48
1:A:2428:ASN:HB3	1:A:2493:LEU:HD13	1.96	0.48
2:C:306:ARG:HG2	2:C:307:GLU:H	1.79	0.48
1:B:1649:ASP:HB2	1:B:1653:TRP:CD1	2.49	0.48
1:B:2281:MET:HA	1:B:2281:MET:CE	2.44	0.48
1:B:2387:MET:HE1	1:B:2392:LEU:HD23	1.96	0.48
1:A:1970:GLN:NE2	1:A:2139:ALA:H	2.12	0.48
1:A:1999:CYS:C	1:A:2001:HIS:H	2.22	0.48
1:B:2208:LEU:HD22	1:B:2410:HIS:CG	2.49	0.47
2:D:98:ARG:HD2	2:D:115:ARG:HB2	1.96	0.47
1:A:2421:PHE:CD1	1:A:2430:ARG:NH2	2.73	0.47
1:A:2019:VAL:HG22	1:A:2126:VAL:HG12	1.96	0.47
1:B:2297:ASP:O	1:B:2298:ASP:C	2.57	0.47
1:A:2418:LEU:HD23	1:A:2421:PHE:CZ	2.48	0.47
2:C:219:HIS:HE1	2:C:243:THR:HG22	1.78	0.47
1:B:1938:VAL:O	1:B:1938:VAL:HG13	2.13	0.47
1:B:2146:PRO:O	1:B:2147:ASN:CB	2.62	0.47
1:A:1649:ASP:HB2	1:A:1653:TRP:CD1	2.49	0.47
2:C:185:MET:HE2	2:C:197:TRP:HD1	1.78	0.47
1:B:1725:GLN:HB3	1:B:1747:MET:HE1	1.96	0.47
1:B:1754:LEU:HD13	1:B:1775:TYR:CE2	2.49	0.47
1:B:1908:THR:O	1:B:1912:ASP:HB2	2.14	0.47
2:D:134:VAL:HG22	2:D:145:VAL:HG22	1.95	0.47
2:D:289:SER:HB2	2:D:291:ASP:OD1	2.14	0.47
1:A:2513:PHE:HB2	1:A:2519:LEU:HD11	1.97	0.47
1:B:1878:LEU:HD21	1:B:1918:ASP:CB	2.42	0.47
1:A:1643:VAL:HG12	1:A:1644:VAL:HG22	1.96	0.47
1:B:1684:GLN:HB3	1:B:1687:HIS:CD2	2.50	0.47
1:B:1705:TRP:HZ2	1:B:1760:ASN:ND2	2.10	0.47
2:D:167:PRO:HD2	2:D:169:PRO:CG	2.33	0.47
1:A:1943:ILE:O	1:A:1946:ILE:HG13	2.15	0.47
1:A:2297:ASP:O	1:A:2300:ALA:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2297:ASP:O	1:A:2298:ASP:C	2.57	0.47
1:A:2408:ARG:NH2	1:A:2510:GLY:HA3	2.30	0.47
1:A:1428:ALA:HB2	1:A:2395:ASN:ND2	2.30	0.47
1:B:2166:LYS:O	1:B:2166:LYS:HE2	2.15	0.47
2:D:69:ASP:CB	2:D:78:ILE:HD11	2.38	0.47
1:A:1498:CYS:HA	1:A:1501:TRP:HD1	1.80	0.47
1:A:2130:LEU:HD22	1:A:2156:ILE:CD1	2.45	0.47
1:B:1498:CYS:HA	1:B:1501:TRP:HD1	1.79	0.47
1:B:2036:ARG:HA	1:B:2036:ARG:HD3	1.70	0.47
1:A:1660:CYS:HB2	1:A:1669:ALA:HB2	1.97	0.47
1:A:1724:MET:CA	1:A:1724:MET:HE2	2.45	0.47
1:A:1791:HIS:O	1:A:1795:VAL:HG23	2.15	0.47
1:B:1594:HIS:HE1	1:B:1622:ARG:HD2	1.80	0.46
1:B:1920:ASN:O	1:B:1924:VAL:HG23	2.14	0.46
1:A:1670:HIS:HE1	1:A:1681:PRO:CB	2.27	0.46
1:A:2134:ARG:O	1:A:2135:ASP:C	2.58	0.46
2:C:15:LEU:HD11	2:C:286:VAL:HG11	1.98	0.46
2:C:95:GLU:HB2	2:C:140:GLN:HE22	1.76	0.46
1:B:1691:THR:CG2	1:B:1724:MET:HE1	2.46	0.46
2:D:165:LEU:HD23	2:D:210:LEU:HD12	1.97	0.46
2:D:219:HIS:NE2	2:D:237:THR:CG2	2.78	0.46
2:C:289:SER:HB2	2:C:291:ASP:OD1	2.15	0.46
1:B:1970:GLN:NE2	1:B:2139:ALA:H	2.12	0.46
1:A:1938:VAL:CG1	1:A:1938:VAL:O	2.63	0.46
2:C:159:THR:HB	2:C:161:HIS:HB2	1.96	0.46
1:B:1705:TRP:CE3	1:B:1710:LYS:HB2	2.51	0.46
1:B:2324:LEU:HA	1:B:2353:ILE:HG21	1.98	0.46
1:B:2390:THR:O	1:B:2390:THR:CG2	2.64	0.46
1:A:1440:PHE:HB3	1:A:1442:GLU:HB2	1.97	0.46
2:C:159:THR:C	2:C:161:HIS:N	2.72	0.46
1:B:1607:LEU:O	1:B:1609:PRO:HD3	2.15	0.46
1:B:1943:ILE:HD13	1:B:1975:PRO:HB2	1.98	0.46
1:B:1881:THR:HG23	1:B:1909:LEU:HD22	1.98	0.46
1:B:2245:THR:HA	1:B:2345:MET:HB3	1.96	0.46
1:B:2513:PHE:HB2	1:B:2519:LEU:HD11	1.98	0.46
1:A:1564:ILE:HD13	1:A:1600:GLU:HG3	1.97	0.46
1:A:1684:GLN:HB3	1:A:1687:HIS:CD2	2.50	0.46
1:B:1501:TRP:HA	1:B:1503:LEU:HG	1.98	0.46
1:B:1910:TRP:CD1	1:B:1910:TRP:C	2.94	0.46
1:B:2208:LEU:HD22	1:B:2410:HIS:CD2	2.51	0.46
2:D:86:LYS:HE2	2:D:105:GLU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:159:THR:C	2:D:161:HIS:N	2.72	0.46
1:A:1490:TRP:CE3	1:A:1519:ALA:HA	2.50	0.46
1:A:2339:ARG:HD3	1:A:2355:HIS:CE1	2.51	0.46
1:A:2345:MET:HG3	1:A:2354:LEU:HD23	1.98	0.46
1:B:1999:CYS:C	1:B:2001:HIS:H	2.24	0.46
1:A:1505:ASN:HB2	1:A:1508:THR:HB	1.97	0.46
1:A:1701:MET:HB3	1:A:1701:MET:HE2	1.49	0.46
1:A:2028:HIS:HE1	1:A:2112:SER:OG	1.99	0.46
2:C:287:THR:O	2:C:294:ALA:HA	2.16	0.46
1:B:1958:HIS:CE1	1:B:1990:ALA:HB1	2.51	0.46
1:B:2408:ARG:NH2	1:B:2510:GLY:HA3	2.31	0.46
2:D:159:THR:HB	2:D:161:HIS:HB2	1.97	0.46
1:B:1629:ILE:O	1:B:1630:VAL:C	2.59	0.45
1:A:1595:MET:HG2	1:A:1639:VAL:HG21	1.97	0.45
1:A:1973:ILE:H	1:A:1973:ILE:HG13	1.57	0.45
1:B:1915:HIS:HE1	1:B:1919:VAL:HG11	1.81	0.45
1:B:2028:HIS:HE1	1:B:2112:SER:OG	1.99	0.45
1:A:1473:ASP:HA	1:A:1474:PRO:HD2	1.83	0.45
2:C:86:LYS:HE2	2:C:105:GLU:HB3	1.97	0.45
1:B:2375:ILE:HD13	1:B:2375:ILE:HA	1.74	0.45
1:A:1594:HIS:HE1	1:A:1622:ARG:HD2	1.81	0.45
1:A:1943:ILE:HD13	1:A:1975:PRO:HB2	1.98	0.45
2:C:82:ASP:HB2	2:C:119:LEU:HD13	1.99	0.45
1:B:1478:LEU:O	1:B:1482:ARG:HG3	2.16	0.45
1:B:1722:GLN:HA	1:B:1725:GLN:NE2	2.30	0.45
1:B:1784:ARG:O	1:B:1790:TRP:NE1	2.39	0.45
2:D:288:ALA:HB2	2:D:318:LEU:HG	1.98	0.45
1:B:1473:ASP:HA	1:B:1474:PRO:HD2	1.83	0.45
1:B:1697:THR:O	1:B:1701:MET:HG3	2.16	0.45
1:B:2339:ARG:NH2	1:B:2356:ILE:O	2.49	0.45
2:C:28:GLN:O	2:C:28:GLN:HG3	2.16	0.45
1:B:1400:LYS:HG3	1:B:1416:LEU:HD13	1.99	0.45
1:B:2134:ARG:O	1:B:2135:ASP:C	2.60	0.45
1:A:1910:TRP:CD1	1:A:1910:TRP:C	2.95	0.45
1:A:1920:ASN:O	1:A:1924:VAL:HG23	2.15	0.45
2:C:258:LEU:HD22	2:C:297:TRP:CE3	2.51	0.45
1:B:1710:LYS:NZ	1:B:1760:ASN:HD21	2.14	0.45
2:D:86:LYS:HB2	2:D:105:GLU:HB2	1.97	0.45
2:D:169:PRO:CA	2:D:171:VAL:H	2.30	0.45
1:A:1545:PHE:CZ	1:A:1595:MET:HE2	2.52	0.45
1:A:1977:THR:HG21	1:A:2013:SER:OG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1680:ASP:O	1:B:1682:SER:N	2.30	0.45
1:B:1759:LEU:HD11	1:B:1796:MET:HE3	1.98	0.45
1:B:1907:LEU:HD11	1:B:1938:VAL:HG13	1.99	0.45
1:B:1705:TRP:CZ2	1:B:1760:ASN:ND2	2.81	0.45
1:B:1973:ILE:H	1:B:1973:ILE:HG13	1.60	0.45
2:D:53:ASP:C	2:D:55:SER:H	2.25	0.45
1:A:1432:VAL:HG22	1:A:2390:THR:HG21	1.98	0.45
1:A:1915:HIS:CE1	1:A:1919:VAL:HG11	2.52	0.45
1:A:2223:GLN:NE2	1:A:2352:LYS:HB2	2.30	0.45
2:C:288:ALA:HB2	2:C:318:LEU:HG	1.99	0.45
1:B:2223:GLN:NE2	1:B:2352:LYS:HB2	2.30	0.45
2:D:130:PRO:HD2	2:D:148:GLN:HB2	1.99	0.45
2:D:195:TYR:CE2	2:D:215:LYS:HG3	2.52	0.45
1:A:1501:TRP:HA	1:A:1503:LEU:HG	1.99	0.45
1:B:2281:MET:CE	2:D:222:TYR:CD2	3.00	0.44
2:D:240:ALA:HB1	2:D:272:TRP:CE2	2.52	0.44
1:B:1643:VAL:HG12	1:B:1644:VAL:CG2	2.47	0.44
2:D:242:GLN:NE2	2:D:261:LYS:HB3	2.33	0.44
1:B:1913:TYR:O	1:B:1915:HIS:ND1	2.50	0.44
2:D:271:GLY:HA2	2:D:290:SER:HB2	1.99	0.44
1:A:1629:ILE:HG22	1:A:1630:VAL:HG23	2.00	0.44
1:A:2260:LEU:HD21	1:A:2266:ARG:NH1	2.32	0.44
1:A:2260:LEU:HD12	1:A:2261:LEU:N	2.33	0.44
1:B:2408:ARG:HG2	1:B:2508:LEU:O	2.17	0.44
2:C:165:LEU:HD23	2:C:210:LEU:HD12	1.99	0.44
1:B:2185:LEU:CD1	1:B:2239:TRP:HZ3	2.31	0.44
2:D:85:ASN:ND2	2:D:85:ASN:H	2.15	0.44
1:A:2298:ASP:HB2	1:A:2382:MET:HE2	1.98	0.44
2:C:21:ASP:HB3	2:C:313:LYS:HB2	2.00	0.44
2:C:169:PRO:CA	2:C:171:VAL:H	2.31	0.44
1:B:2345:MET:HG3	1:B:2354:LEU:HD23	1.99	0.44
1:A:1930:ILE:HD11	1:A:1934:THR:HG21	2.00	0.44
1:A:2156:ILE:HG12	1:A:2174:LEU:HD22	2.00	0.44
1:A:2245:THR:HA	1:A:2345:MET:HB3	1.99	0.44
1:A:2430:ARG:H	1:A:2430:ARG:HG3	1.71	0.44
2:C:58:ALA:HB2	2:C:67:MET:HE3	2.00	0.44
1:B:2297:ASP:O	1:B:2300:ALA:N	2.51	0.44
2:D:106:ASP:OD1	2:D:108:THR:OG1	2.18	0.44
1:A:1629:ILE:O	1:A:1630:VAL:C	2.61	0.44
1:B:2198:VAL:HG11	1:B:2358:PHE:CD2	2.53	0.44
1:A:1970:GLN:C	1:A:1972:LEU:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1910:TRP:HD1	1:B:1910:TRP:O	2.01	0.43
2:D:94:HIS:HE1	2:D:96:ASP:HB2	1.79	0.43
1:A:2375:ILE:HD12	1:A:2532:ALA:HA	2.00	0.43
1:B:2130:LEU:HD22	1:B:2156:ILE:CD1	2.49	0.43
1:B:2329:MET:HB3	1:B:2404:MET:HE2	1.98	0.43
1:B:1802:LEU:HD22	1:B:1806:HIS:NE2	2.33	0.43
1:A:1681:PRO:HG2	1:A:1683:ARG:HE	1.84	0.43
1:B:1670:HIS:HE1	1:B:1681:PRO:HB3	1.82	0.43
1:B:2019:VAL:HG22	1:B:2126:VAL:HG12	1.99	0.43
2:D:81:TYR:CD2	2:D:112:TRP:CE3	3.07	0.43
2:D:82:ASP:H	2:D:119:LEU:HD22	1.84	0.43
1:A:2036:ARG:HA	1:A:2036:ARG:HD3	1.71	0.43
1:A:2095:LYS:HA	1:A:2098:THR:HG22	1.99	0.43
2:D:203:ILE:HA	2:D:206:GLU:HG2	2.01	0.43
1:A:1478:LEU:O	1:A:1482:ARG:HG3	2.18	0.43
1:A:1938:VAL:O	1:A:1938:VAL:HG13	2.16	0.43
1:A:2146:PRO:O	1:A:2147:ASN:CB	2.66	0.43
1:A:2324:LEU:HA	1:A:2353:ILE:HG21	2.01	0.43
1:B:2281:MET:HE1	2:D:222:TYR:CE2	2.54	0.43
1:B:2307:SER:CB	1:B:2313:TRP:HB2	2.49	0.43
2:D:86:LYS:CB	2:D:105:GLU:HB2	2.48	0.43
1:A:1666:LEU:HD13	1:A:1707:SER:HA	2.00	0.43
1:A:1691:THR:CG2	1:A:1724:MET:HE1	2.49	0.43
1:A:2302:LEU:C	1:A:2302:LEU:HD12	2.44	0.43
1:B:1932:ILE:O	1:B:1933:ASP:C	2.61	0.43
2:D:21:ASP:HB3	2:D:313:LYS:HB2	2.01	0.43
2:D:293:LEU:HD12	2:D:295:ARG:NH2	2.34	0.43
1:A:1759:LEU:HD11	1:A:1796:MET:HE3	2.00	0.43
1:A:1932:ILE:O	1:A:1933:ASP:C	2.62	0.43
1:A:2254:ARG:HH22	1:A:2264:GLU:CD	2.27	0.43
1:A:2281:MET:HE1	2:C:222:TYR:CE2	2.54	0.43
1:A:2285:GLU:HB2	2:C:272:TRP:CZ3	2.54	0.43
1:B:2168:ARG:CZ	1:B:2168:ARG:HB2	2.48	0.43
2:D:270:ARG:HA	2:D:270:ARG:HD2	1.76	0.43
1:A:1734:THR:C	1:A:1736:ASP:N	2.71	0.43
2:C:53:ASP:C	2:C:55:SER:H	2.27	0.43
2:C:203:ILE:HA	2:C:206:GLU:HG2	2.01	0.43
1:A:1705:TRP:HZ2	1:A:1760:ASN:ND2	2.10	0.43
1:A:1705:TRP:CE3	1:A:1710:LYS:HB2	2.54	0.43
1:A:1916:TRP:HA	1:A:1917:PRO:HD2	1.73	0.43
1:B:1605:TYR:CG	1:B:1643:VAL:HG11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1807:GLN:O	1:B:1811:ARG:HG2	2.19	0.42
1:B:1773:LEU:HG	1:B:1796:MET:HG3	2.01	0.42
1:B:1973:ILE:O	1:B:1974:TYR:C	2.63	0.42
2:D:68:TYR:CE2	2:D:77:PRO:HD3	2.54	0.42
1:A:2270:ARG:O	2:C:313:LYS:NZ	2.43	0.42
1:B:1505:ASN:HB2	1:B:1508:THR:HB	2.00	0.42
1:B:2093:ASN:HB3	1:B:2094:VAL:H	1.62	0.42
1:A:1518:ALA:HB2	1:A:1546:TYR:OH	2.19	0.42
1:A:2140:VAL:HG11	1:A:2182:PHE:CG	2.55	0.42
1:B:1453:LEU:C	1:B:1455:GLU:H	2.28	0.42
1:B:1914:GLY:HA3	1:B:1950:ARG:HE	1.84	0.42
2:D:95:GLU:HB2	2:D:140:GLN:HE22	1.83	0.42
1:A:2168:ARG:CZ	1:A:2168:ARG:HB2	2.49	0.42
1:B:1905:ARG:HD3	1:B:1905:ARG:HA	1.75	0.42
1:A:1722:GLN:HA	1:A:1725:GLN:NE2	2.34	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	1.56	0.42
1:B:1440:PHE:HB3	1:B:1442:GLU:HB2	2.00	0.42
1:B:2340:HIS:HB2	1:B:2341:PRO:CD	2.49	0.42
2:D:287:THR:O	2:D:294:ALA:HA	2.19	0.42
1:A:2281:MET:CE	2:C:222:TYR:CE2	3.03	0.42
1:B:1433:LEU:HD23	1:B:1453:LEU:CD2	2.50	0.42
1:B:1734:THR:C	1:B:1736:ASP:N	2.77	0.42
1:B:2095:LYS:HA	1:B:2098:THR:HG22	2.00	0.42
2:D:44:GLN:H	2:D:44:GLN:HG3	1.42	0.42
1:A:1428:ALA:HB2	1:A:2395:ASN:HD21	1.83	0.42
1:A:1595:MET:O	1:A:1599:LEU:HB2	2.19	0.42
1:A:2187:LYS:HD2	1:A:2237:ILE:CD1	2.50	0.42
2:C:17:THR:HB	2:C:311:HIS:CE1	2.47	0.42
2:C:82:ASP:H	2:C:119:LEU:HD22	1.85	0.42
1:B:1529:MET:HE3	1:B:1550:LEU:HG	2.02	0.42
1:B:1724:MET:HE2	1:B:1724:MET:CA	2.49	0.42
2:D:17:THR:HB	2:D:311:HIS:CE1	2.47	0.42
2:D:28:GLN:OE1	2:D:30:HIS:CE1	2.72	0.42
1:A:1400:LYS:HG3	1:A:1416:LEU:HD13	2.02	0.42
1:A:1495:GLN:O	1:A:1499:GLU:HB2	2.20	0.42
1:A:2192:LEU:HD12	1:A:2235:GLY:CA	2.49	0.42
1:A:2307:SER:CB	1:A:2313:TRP:HB2	2.50	0.42
1:B:1591:VAL:HG21	1:B:1632:ASP:OD1	2.20	0.42
1:B:1943:ILE:HG12	1:B:1946:ILE:HD11	2.02	0.42
2:D:15:LEU:HD11	2:D:286:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1393:TYR:CE2	1:A:1422:LYS:HD2	2.55	0.42
1:A:1726:GLN:HA	1:A:1729:GLN:HG2	2.01	0.42
1:B:1778:ALA:O	1:B:1782:HIS:CD2	2.62	0.42
1:B:1938:VAL:HG22	1:B:1941:GLN:HE21	1.85	0.42
1:B:2336:LEU:HG	1:B:2339:ARG:HH11	1.85	0.42
2:D:135:CYS:SG	2:D:178:ILE:HG22	2.60	0.42
1:A:1502:THR:HG22	1:A:1504:VAL:HG23	2.01	0.42
1:A:1618:ILE:H	1:A:1618:ILE:HG13	1.73	0.42
1:A:1762:GLN:HB2	1:A:1768:THR:HG21	2.01	0.42
2:C:294:ALA:HB3	2:C:308:TYR:HB2	2.02	0.42
1:B:2368:ARG:HD2	1:B:2370:LYS:O	2.20	0.41
2:D:258:LEU:HD22	2:D:297:TRP:CE3	2.54	0.41
1:A:1422:LYS:C	1:A:1424:GLN:H	2.29	0.41
1:A:1552:LEU:HD22	1:A:1602:VAL:HG12	2.02	0.41
1:A:1621:GLU:C	1:A:1623:LEU:N	2.78	0.41
1:A:2160:LEU:HD22	1:A:2172:LEU:HA	2.02	0.41
2:C:86:LYS:HB2	2:C:105:GLU:HB2	2.00	0.41
1:A:1943:ILE:HG12	1:A:1946:ILE:HD11	2.02	0.41
1:A:2503:ARG:O	1:A:2507:LYS:HG3	2.20	0.41
2:C:69:ASP:CB	2:C:78:ILE:HD11	2.43	0.41
1:B:2260:LEU:HD21	1:B:2266:ARG:NH1	2.35	0.41
1:A:2281:MET:CE	2:C:222:TYR:CD2	2.98	0.41
1:A:2380:THR:HG22	1:A:2383:LEU:CG	2.49	0.41
2:C:255:MET:CE	2:C:299:VAL:HG12	2.50	0.41
1:B:1621:GLU:C	1:B:1623:LEU:N	2.79	0.41
1:B:2254:ARG:HH22	1:B:2264:GLU:CD	2.28	0.41
1:A:1905:ARG:HD3	1:A:1905:ARG:HA	1.77	0.41
1:A:2329:MET:SD	1:A:2404:MET:HE2	2.60	0.41
1:A:2344:LEU:CD1	1:A:2353:ILE:HD11	2.44	0.41
2:C:28:GLN:OE1	2:C:30:HIS:CE1	2.73	0.41
1:B:1583:TYR:C	1:B:1585:ARG:N	2.73	0.41
1:B:1916:TRP:HA	1:B:1917:PRO:HD2	1.74	0.41
1:B:2053:PRO:O	1:B:2057:MET:HB2	2.20	0.41
1:B:2268:MET:HG3	1:B:2290:ALA:HB2	2.01	0.41
1:B:2380:THR:CG2	1:B:2383:LEU:HG	2.48	0.41
1:A:1881:THR:HG23	1:A:1909:LEU:HD22	2.02	0.41
1:A:1910:TRP:HD1	1:A:1910:TRP:O	2.04	0.41
1:A:1914:GLY:HA3	1:A:1950:ARG:HE	1.85	0.41
2:C:28:GLN:NE2	2:C:31:SER:OG	2.54	0.41
2:C:102:THR:O	2:C:109:ALA:HA	2.20	0.41
2:C:168:GLU:OE1	2:C:189:ASN:ND2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1948:THR:HG22	1:B:1950:ARG:H	1.86	0.41
1:B:1977:THR:HG21	1:B:2013:SER:OG	2.21	0.41
1:B:2297:ASP:O	1:B:2299:LEU:N	2.53	0.41
1:B:2307:SER:OG	1:B:2313:TRP:HB2	2.21	0.41
1:B:2339:ARG:HD3	1:B:2355:HIS:CE1	2.55	0.41
2:D:28:GLN:HE21	2:D:33:ILE:HD12	1.85	0.41
2:D:75:PRO:HB2	2:D:76:ASN:H	1.63	0.41
1:A:1907:LEU:HD11	1:A:1938:VAL:HG13	2.03	0.41
1:A:2251:ARG:HG2	1:A:2251:ARG:HH11	1.86	0.41
1:A:2268:MET:HG3	1:A:2290:ALA:HB2	2.02	0.41
2:C:85:ASN:H	2:C:85:ASN:ND2	2.19	0.41
1:B:2302:LEU:C	1:B:2302:LEU:HD12	2.46	0.41
2:D:188:VAL:HG13	2:D:223:ALA:CB	2.48	0.41
1:A:1453:LEU:C	1:A:1455:GLU:H	2.29	0.41
1:A:1892:ILE:HG21	1:A:1930:ILE:HD11	2.03	0.41
1:A:1999:CYS:C	1:A:2001:HIS:N	2.79	0.41
1:A:2339:ARG:NH2	1:A:2356:ILE:O	2.53	0.41
1:B:1874:SER:O	1:B:1878:LEU:HB2	2.21	0.41
1:B:2160:LEU:HD22	1:B:2172:LEU:HA	2.02	0.41
2:D:39:GLN:HB3	2:D:41:GLN:NE2	2.36	0.41
2:D:68:TYR:HE2	2:D:77:PRO:HD3	1.86	0.41
2:D:165:LEU:HD11	2:D:197:TRP:CH2	2.56	0.41
2:D:255:MET:CE	2:D:299:VAL:HG12	2.50	0.41
1:A:1488:GLY:HA3	1:A:1634:GLN:OE1	2.21	0.41
1:A:1631:GLU:CD	1:A:1631:GLU:H	2.29	0.41
1:A:1807:GLN:O	1:A:1811:ARG:HG2	2.21	0.41
1:A:1874:SER:O	1:A:1878:LEU:HB2	2.21	0.41
1:A:2500:ILE:O	1:A:2504:VAL:HG23	2.20	0.41
2:C:81:TYR:CD2	2:C:112:TRP:CE3	3.09	0.41
1:B:1717:MET:O	1:B:1718:GLN:C	2.64	0.41
1:B:2268:MET:HG2	1:B:2286:VAL:HG12	2.03	0.41
1:B:2332:TYR:CZ	1:B:2507:LYS:HD3	2.56	0.41
1:A:1583:TYR:C	1:A:1585:ARG:N	2.72	0.41
2:C:270:ARG:HA	2:C:270:ARG:HD2	1.77	0.41
1:B:1502:THR:HG22	1:B:1504:VAL:HG23	2.03	0.40
1:B:1681:PRO:HG2	1:B:1683:ARG:HE	1.86	0.40
1:A:2053:PRO:O	1:A:2057:MET:HB2	2.21	0.40
1:A:2363:GLU:OE1	1:A:2363:GLU:HA	2.21	0.40
1:B:1450:TYR:HB2	1:B:1459:ALA:HB2	2.02	0.40
1:B:1595:MET:O	1:B:1599:LEU:HB2	2.21	0.40
1:B:2011:MET:HE2	1:B:2129:LYS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2363:GLU:OE1	1:B:2363:GLU:HA	2.21	0.40
2:D:239:SER:OG	2:D:240:ALA:N	2.54	0.40
2:C:98:ARG:O	2:C:98:ARG:HG3	2.20	0.40
1:B:1470:ASN:HB3	1:B:1471:LYS:H	1.59	0.40
1:B:1497:CYS:SG	1:B:1516:ALA:CB	3.09	0.40
2:D:28:GLN:HG3	2:D:28:GLN:O	2.21	0.40
2:D:185:MET:HB2	2:D:199:LEU:HD21	2.03	0.40
1:A:1423:LEU:HD12	1:A:1423:LEU:HA	1.96	0.40
1:A:1895:SER:HB2	1:A:1899:ASN:HB3	2.02	0.40
1:B:1574:GLU:HG2	1:B:1585:ARG:HH22	1.86	0.40
1:B:2121:LEU:HD23	1:B:2121:LEU:HA	1.88	0.40
1:A:1691:THR:O	1:A:1691:THR:CG2	2.70	0.40
1:A:1710:LYS:NZ	1:A:1760:ASN:HD21	2.19	0.40
1:A:2166:LYS:HE2	1:A:2166:LYS:O	2.21	0.40
2:C:86:LYS:CB	2:C:105:GLU:HB2	2.51	0.40
1:B:1732:ILE:HD13	1:B:1740:LYS:HB2	2.02	0.40
1:A:2408:ARG:CG	1:A:2508:LEU:O	2.67	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1607:LEU:N	1:A:1609:PRO:O[2_554]	1.39	0.81
1:A:1607:LEU:CA	1:A:1609:PRO:O[2_554]	1.77	0.43
1:A:1608:VAL:O	1:A:1608:VAL:O[2_554]	1.84	0.36
1:A:1606:LYS:C	1:A:1609:PRO:O[2_554]	1.92	0.28
1:A:1607:LEU:N	1:A:1609:PRO:C[2_554]	2.13	0.07
1:A:1607:LEU:C	1:A:1609:PRO:O[2_554]	2.14	0.06

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	1052/1174 (90%)	938 (89%)	85 (8%)	29 (3%)	4	21
1	B	1052/1174 (90%)	940 (89%)	84 (8%)	28 (3%)	4	22
2	C	315/326 (97%)	270 (86%)	31 (10%)	14 (4%)	2	13
2	D	315/326 (97%)	273 (87%)	27 (9%)	15 (5%)	2	12
All	All	2734/3000 (91%)	2421 (89%)	227 (8%)	86 (3%)	3	20

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1630	VAL
1	B	1650	MET
1	B	1937	GLN
1	B	1970	GLN
1	B	2094	VAL
1	B	2298	ASP
1	B	2364	VAL
2	D	73	ASN
2	D	74	ASN
2	D	97	GLY
2	D	118	ASN
2	D	169	PRO
2	D	203	ILE
2	D	269	SER
1	A	1630	VAL
1	A	1650	MET
1	A	1937	GLN
1	A	1970	GLN
1	A	2094	VAL
1	A	2298	ASP
1	A	2364	VAL
2	C	73	ASN
2	C	74	ASN
2	C	97	GLY
2	C	118	ASN
2	C	169	PRO
2	C	203	ILE
2	C	269	SER
1	B	1444	GLU
1	B	1735	GLU
1	B	1786	TRP
1	B	1914	GLY
1	B	2093	ASN

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Mol	Chain	Res	Type
2	D	35	THR
2	D	75	PRO
2	D	160	ASP
2	D	167	PRO
2	D	204	GLY
1	A	1444	GLU
1	A	1735	GLU
1	A	1786	TRP
1	A	1914	GLY
1	A	2093	ASN
2	C	35	THR
2	C	75	PRO
2	C	167	PRO
2	C	204	GLY
1	B	1445	ILE
1	B	1470	ASN
1	B	1525	GLN
1	B	1682	SER
1	B	1707	SER
1	A	1445	ILE
1	A	1525	GLN
1	A	1609	PRO
1	A	1682	SER
1	A	1707	SER
1	A	2000	GLU
1	A	2135	ASP
2	C	160	ASP
1	B	1680	ASP
1	B	2000	GLU
1	B	2135	ASP
1	B	2147	ASN
1	B	2391	GLY
2	D	129	ALA
1	A	1470	ASN
1	A	1680	ASP
1	A	2147	ASN
1	A	2391	GLY
2	C	129	ALA
1	B	1681	PRO
1	B	2362	PHE
2	D	208	THR
1	A	1454	HIS

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Mol	Chain	Res	Type
1	A	1681	PRO
1	B	1454	HIS
1	B	1609	PRO
1	A	1784	ARG
1	B	1473	ASP
1	A	1473	ASP
1	B	1426	PRO
1	A	1426	PRO
1	A	1608	VAL
2	C	310	GLY
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	931/1024 (91%)	846 (91%)	85 (9%)	9	31
1	B	931/1024 (91%)	846 (91%)	85 (9%)	9	31
2	C	269/276 (98%)	225 (84%)	44 (16%)	2	11
2	D	269/276 (98%)	227 (84%)	42 (16%)	2	12
All	All	2400/2600 (92%)	2144 (89%)	256 (11%)	6	24

All (256) 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	1501	TRP
1	B	1509	GLN
1	B	1540	THR
1	B	1541	HIS

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Mol	Chain	Res	Type
1	B	1590	MET
1	B	1598	GLU
1	B	1603	ILE
1	B	1608	VAL
1	B	1610	GLU
1	B	1630	VAL
1	B	1643	VAL
1	B	1644	VAL
1	B	1650	MET
1	B	1685	LEU
1	B	1724	MET
1	B	1740	LYS
1	B	1768	THR
1	B	1780	THR
1	B	1878	LEU
1	B	1896	ARG
1	B	1898	ASN
1	B	1899	ASN
1	B	1916	TRP
1	B	1930	ILE
1	B	1932	ILE
1	B	1938	VAL
1	B	1939	ILE
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	2068	THR
1	B	2072	GLN
1	B	2076	ARG
1	B	2078	LEU
1	B	2093	ASN
1	B	2095	LYS
1	B	2123	LEU
1	B	2138	LEU
1	B	2152	ARG
1	B	2154	GLN
1	B	2164	THR
1	B	2166	LYS

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Mol	Chain	Res	Type
1	B	2168	ARG
1	B	2173	THR
1	B	2178	ASN
1	B	2181	GLU
1	B	2185	LEU
1	B	2189	HIS
1	B	2195	ASP
1	B	2214	THR
1	B	2223	GLN
1	B	2224	ARG
1	B	2228	ILE
1	B	2244	ASP
1	B	2260	LEU
1	B	2266	ARG
1	B	2281	MET
1	B	2297	ASP
1	B	2318	THR
1	B	2342	SER
1	B	2347	ASP
1	B	2363	GLU
1	B	2375	ILE
1	B	2385	ASN
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
2	D	10	SER
2	D	13	VAL
2	D	37	THR
2	D	44	GLN
2	D	53	ASP
2	D	65	ILE
2	D	74	ASN
2	D	80	SER
2	D	84	VAL

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Mol	Chain	Res	Type
2	D	85	ASN
2	D	86	LYS
2	D	90	SER
2	D	91	VAL
2	D	128	ASN
2	D	159	THR
2	D	160	ASP
2	D	162	ASN
2	D	164	GLN
2	D	165	LEU
2	D	166	ILE
2	D	168	GLU
2	D	169	PRO
2	D	170	GLU
2	D	171	VAL
2	D	173	ILE
2	D	174	THR
2	D	183	SER
2	D	188	VAL
2	D	199	LEU
2	D	214	THR
2	D	215	LYS
2	D	242	GLN
2	D	243	THR
2	D	248	ARG
2	D	261	LYS
2	D	262	SER
2	D	269	SER
2	D	286	VAL
2	D	287	THR
2	D	289	SER
2	D	301	THR
2	D	312	GLN
1	A	1402	LEU
1	A	1417	ILE
1	A	1420	ASN
1	A	1443	LEU
1	A	1457	GLU
1	A	1501	TRP
1	A	1509	GLN
1	A	1540	THR
1	A	1541	HIS

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Mol	Chain	Res	Type
1	A	1590	MET
1	A	1598	GLU
1	A	1603	ILE
1	A	1608	VAL
1	A	1610	GLU
1	A	1630	VAL
1	A	1643	VAL
1	A	1644	VAL
1	A	1650	MET
1	A	1685	LEU
1	A	1724	MET
1	A	1740	LYS
1	A	1768	THR
1	A	1780	THR
1	A	1878	LEU
1	A	1896	ARG
1	A	1898	ASN
1	A	1899	ASN
1	A	1916	TRP
1	A	1930	ILE
1	A	1932	ILE
1	A	1938	VAL
1	A	1939	ILE
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	2068	THR
1	A	2072	GLN
1	A	2076	ARG
1	A	2078	LEU
1	A	2093	ASN
1	A	2095	LYS
1	A	2123	LEU
1	A	2138	LEU
1	A	2152	ARG
1	A	2154	GLN
1	A	2164	THR
1	A	2166	LYS

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Mol	Chain	Res	Type
1	A	2168	ARG
1	A	2173	THR
1	A	2178	ASN
1	A	2181	GLU
1	A	2185	LEU
1	A	2189	HIS
1	A	2195	ASP
1	A	2214	THR
1	A	2223	GLN
1	A	2224	ARG
1	A	2228	ILE
1	A	2244	ASP
1	A	2260	LEU
1	A	2266	ARG
1	A	2281	MET
1	A	2297	ASP
1	A	2318	THR
1	A	2342	SER
1	A	2347	ASP
1	A	2363	GLU
1	A	2375	ILE
1	A	2385	ASN
1	A	2388	GLU
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	2512	ASP
1	A	2515	HIS
1	A	2519	LEU
1	A	2530	LYS
2	C	10	SER
2	C	13	VAL
2	C	37	THR
2	C	44	GLN
2	C	53	ASP
2	C	65	ILE
2	C	74	ASN
2	C	80	SER

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Mol	Chain	Res	Type
2	C	84	VAL
2	C	85	ASN
2	C	86	LYS
2	C	90	SER
2	C	91	VAL
2	C	128	ASN
2	C	140	GLN
2	C	159	THR
2	C	160	ASP
2	C	162	ASN
2	C	164	GLN
2	C	165	LEU
2	C	166	ILE
2	C	168	GLU
2	C	169	PRO
2	C	170	GLU
2	C	171	VAL
2	C	173	ILE
2	C	174	THR
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	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 (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1496	GLN
1	B	1525	GLN

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Mol	Chain	Res	Type
1	B	1541	HIS
1	B	1594	HIS
1	B	1670	HIS
1	B	1687	HIS
1	B	1695	GLN
1	B	1719	HIS
1	B	1730	HIS
1	B	1741	GLN
1	B	1760	ASN
1	B	1782	HIS
1	B	1803	HIS
1	B	1898	ASN
1	B	1915	HIS
1	B	1941	GLN
1	B	1970	GLN
1	B	2001	HIS
1	B	2028	HIS
1	B	2082	GLN
1	B	2093	ASN
1	B	2147	ASN
1	B	2154	GLN
1	B	2161	GLN
1	B	2189	HIS
1	B	2223	GLN
1	B	2247	HIS
1	B	2289	HIS
1	B	2293	ASN
1	B	2395	ASN
1	B	2401	HIS
1	B	2428	ASN
2	D	22	HIS
2	D	30	HIS
2	D	40	HIS
2	D	41	GLN
2	D	63	GLN
2	D	73	ASN
2	D	85	ASN
2	D	94	HIS
2	D	118	ASN
2	D	128	ASN
2	D	132	ASN
2	D	137	HIS

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Mol	Chain	Res	Type
2	D	161	HIS
2	D	162	ASN
2	D	198	ASN
2	D	311	HIS
2	D	312	GLN
1	A	1496	GLN
1	A	1541	HIS
1	A	1561	GLN
1	A	1594	HIS
1	A	1624	GLN
1	A	1670	HIS
1	A	1687	HIS
1	A	1695	GLN
1	A	1719	HIS
1	A	1741	GLN
1	A	1760	ASN
1	A	1782	HIS
1	A	1803	HIS
1	A	1808	ASN
1	A	1898	ASN
1	A	1915	HIS
1	A	1941	GLN
1	A	1958	HIS
1	A	1970	GLN
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	2161	GLN
1	A	2189	HIS
1	A	2223	GLN
1	A	2247	HIS
1	A	2289	HIS
1	A	2293	ASN
1	A	2395	ASN
1	A	2401	HIS
1	A	2499	GLN
2	C	22	HIS
2	C	30	HIS
2	C	39	GLN

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Mol	Chain	Res	Type
2	C	40	HIS
2	C	41	GLN
2	C	63	GLN
2	C	73	ASN
2	C	85	ASN
2	C	94	HIS
2	C	118	ASN
2	C	128	ASN
2	C	132	ASN
2	C	137	HIS
2	C	153	HIS
2	C	162	ASN
2	C	198	ASN
2	C	242	GLN
2	C	283	GLN
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](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	AGS	B	3000	4	32,33,33	2.27	10 (31%)	45,52,52	1.68	9 (20%)
3	AGS	A	3000	4	32,33,33	2.19	7 (21%)	45,52,52	1.94	11 (24%)

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	AGS	B	3000	4	-	5/21/38/38	0/3/3/3
3	AGS	A	3000	4	-	5/21/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3000	AGS	PG-S1G	8.89	2.09	1.90
3	B	3000	AGS	PG-S1G	8.86	2.09	1.90
3	B	3000	AGS	C5-C4	4.61	1.47	1.39
3	A	3000	AGS	C5-C4	4.54	1.47	1.39
3	B	3000	AGS	PB-O3B	3.41	1.63	1.59
3	A	3000	AGS	PB-O3B	2.98	1.62	1.59
3	A	3000	AGS	C5-C6	2.86	1.49	1.41
3	B	3000	AGS	C5-N7	-2.79	1.34	1.39
3	A	3000	AGS	PG-O2G	2.58	1.63	1.54
3	B	3000	AGS	PB-O3A	2.58	1.62	1.59
3	B	3000	AGS	PG-O2G	2.56	1.63	1.54
3	B	3000	AGS	C5-C6	2.40	1.47	1.41
3	A	3000	AGS	C5-N7	-2.37	1.34	1.39
3	A	3000	AGS	C8-N7	2.34	1.36	1.31
3	B	3000	AGS	C4-N9	-2.32	1.32	1.37
3	B	3000	AGS	PA-O3A	2.19	1.61	1.59
3	B	3000	AGS	C8-N7	2.17	1.35	1.31

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3000	AGS	C5-C4-N3	-5.63	118.96	126.72
3	B	3000	AGS	C5-C4-N3	-4.99	119.85	126.72
3	A	3000	AGS	N3-C4-N9	4.48	134.78	127.17
3	B	3000	AGS	N3-C4-N9	3.96	133.90	127.17
3	A	3000	AGS	C2-N3-C4	3.95	121.47	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3000	AGS	N3-C2-N1	-3.73	122.94	128.58
3	A	3000	AGS	C4-C5-N7	-3.52	106.55	110.58
3	A	3000	AGS	PB-O3B-PG	-3.40	120.73	133.17
3	B	3000	AGS	C2-N3-C4	3.40	120.12	111.83
3	B	3000	AGS	N3-C2-N1	-3.38	123.46	128.58
3	A	3000	AGS	C4-N9-C8	2.83	108.71	105.74
3	B	3000	AGS	C4-C5-N7	-2.82	107.36	110.58
3	B	3000	AGS	PB-O3B-PG	-2.67	123.40	133.17
3	A	3000	AGS	C5-N7-C8	2.67	107.64	103.45
3	A	3000	AGS	C6-C5-N7	2.39	136.69	132.09
3	A	3000	AGS	N9-C8-N7	-2.18	110.84	113.94
3	B	3000	AGS	C2-N1-C6	2.17	122.29	118.73
3	B	3000	AGS	C4-N9-C8	2.15	107.99	105.74
3	B	3000	AGS	O4'-C1'-N9	2.14	112.20	108.09
3	A	3000	AGS	C3'-C2'-C1'	2.02	105.29	101.46

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3000	AGS	PB-O3B-PG-O2G
3	A	3000	AGS	PB-O3B-PG-O3G
3	B	3000	AGS	C3'-C4'-C5'-O5'
3	B	3000	AGS	O4'-C4'-C5'-O5'
3	B	3000	AGS	PA-O3A-PB-O3B
3	A	3000	AGS	PB-O3A-PA-O1A
3	A	3000	AGS	C3'-C4'-C5'-O5'
3	B	3000	AGS	PA-O3A-PB-O1B
3	A	3000	AGS	PB-O3A-PA-O2A
3	B	3000	AGS	PA-O3A-PB-O2B

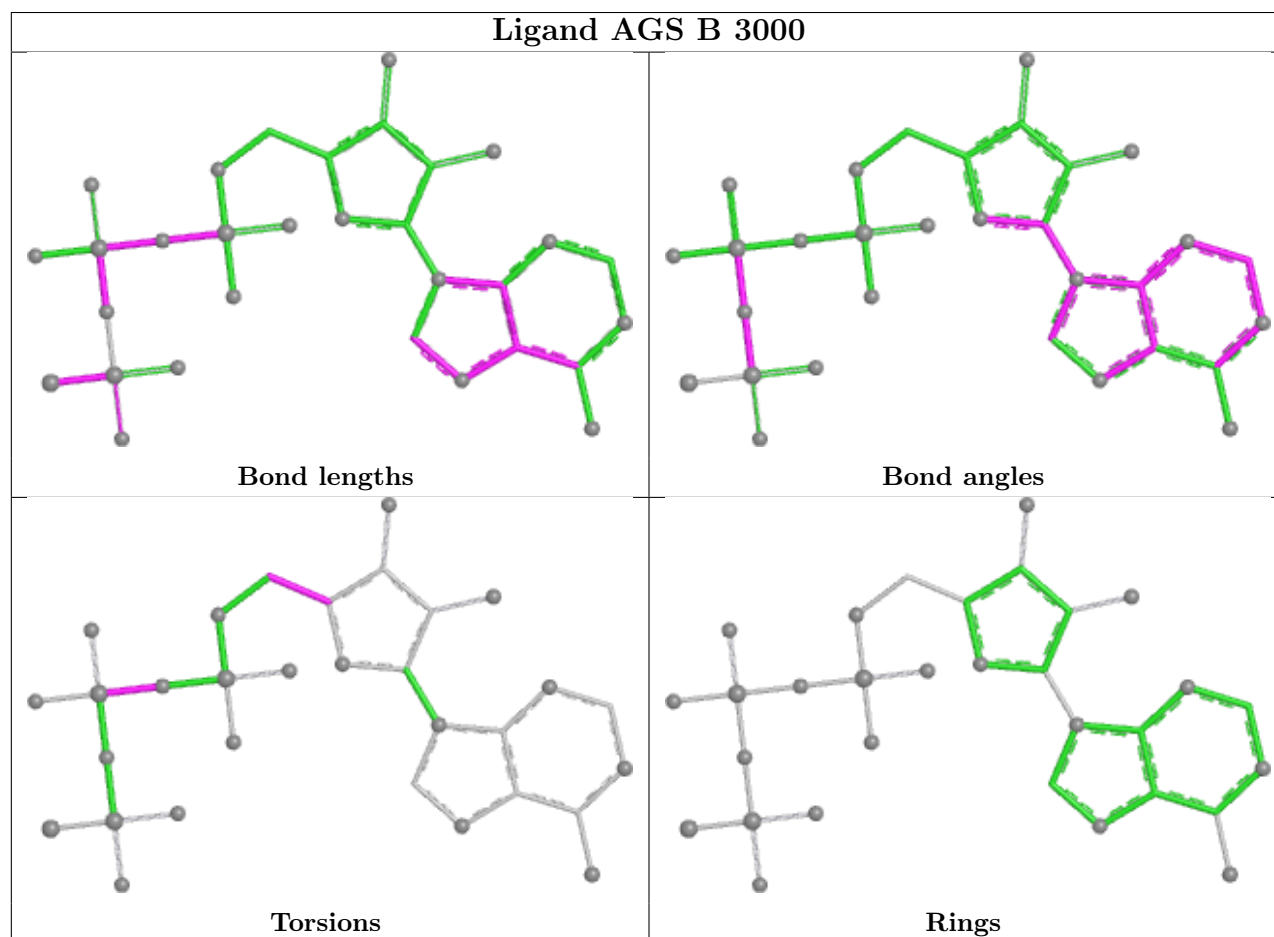
There are no ring outliers.

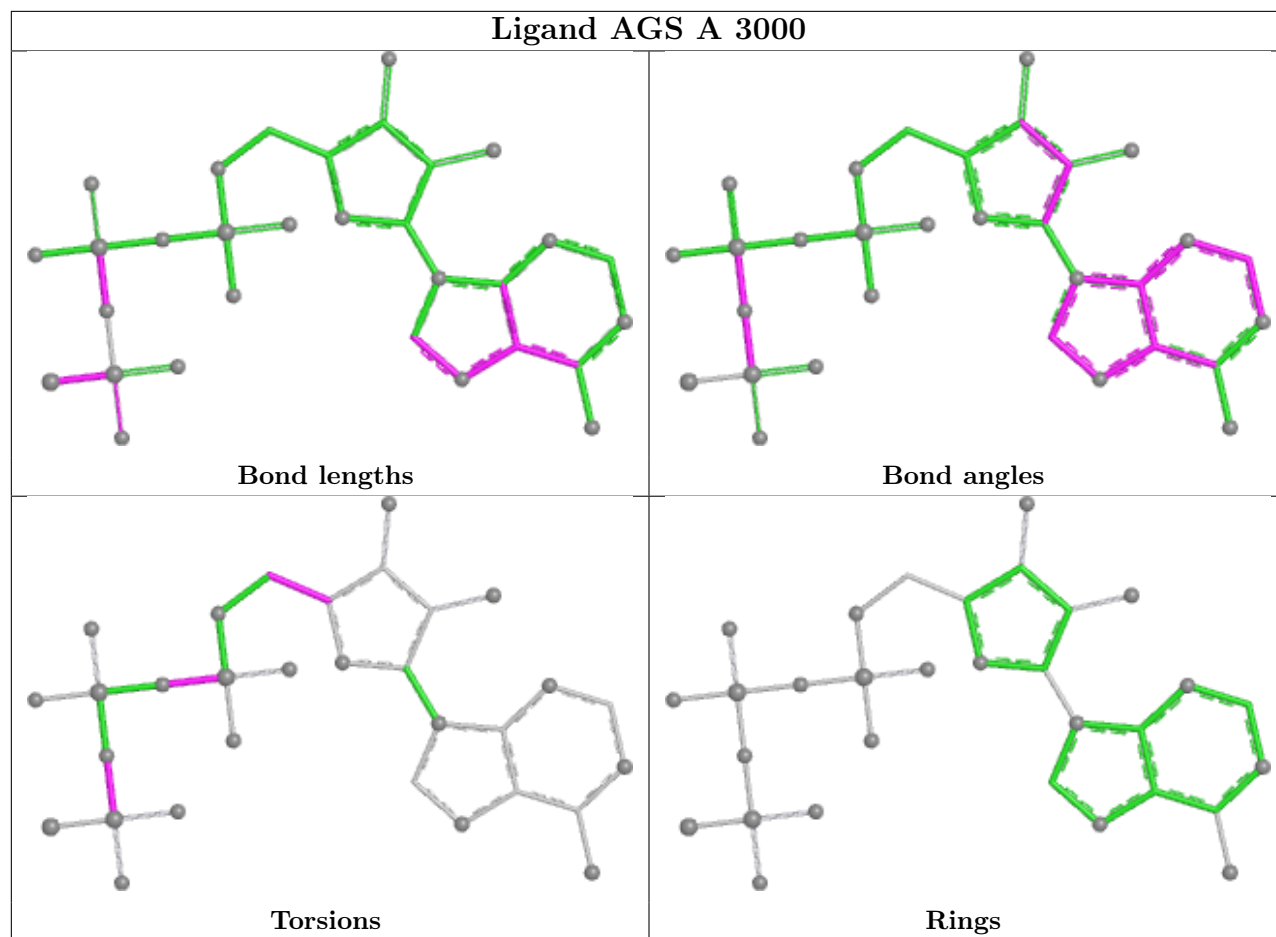
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3000	AGS	2	0
3	A	3000	AGS	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	1058/1174 (90%)	0.49	89 (8%)	17 13	30, 64, 156, 230	0
1	B	1058/1174 (90%)	0.26	58 (5%)	30 21	25, 54, 134, 177	0
2	C	317/326 (97%)	0.26	12 (3%)	44 30	36, 63, 113, 157	0
2	D	317/326 (97%)	0.09	10 (3%)	50 34	27, 43, 94, 127	0
All	All	2750/3000 (91%)	0.33	169 (6%)	27 18	25, 57, 143, 230	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1599	LEU	5.4
1	A	1610	GLU	5.3
1	B	2434	THR	5.2
1	A	1619	TRP	5.2
1	A	1614	ILE	5.1
1	B	1504	VAL	4.9
1	A	1603	ILE	4.7
1	B	1608	VAL	4.7
1	A	1608	VAL	4.6
1	A	1443	LEU	4.5
1	A	1604	GLN	4.4
1	A	1504	VAL	4.4
2	C	203	ILE	4.3
1	A	1575	LEU	4.3
1	A	1580	GLY	4.2
1	B	1607	LEU	4.0
1	B	1649	ASP	3.9
1	B	2436	THR	3.9
1	A	1469	THR	3.8
1	B	1609	PRO	3.7
2	D	203	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
2	C	324	VAL	3.5
1	B	1445	ILE	3.5
1	B	1469	THR	3.4
2	C	119	LEU	3.4
1	A	1623	LEU	3.4
1	B	1731	ALA	3.4
1	A	2436	THR	3.4
1	A	1444	GLU	3.4
1	A	1595	MET	3.4
1	A	1549	VAL	3.3
1	B	2492	ALA	3.3
1	A	1586	ALA	3.3
2	C	8	VAL	3.2
2	D	119	LEU	3.2
1	A	1730	HIS	3.2
1	A	2492	ALA	3.2
2	D	207	VAL	3.2
1	A	1579	ALA	3.2
1	B	1736	ASP	3.1
1	A	1627	GLN	3.1
1	A	2164	THR	3.1
2	D	8	VAL	3.1
1	A	2434	THR	3.0
1	A	2118	LEU	3.0
1	B	1579	ALA	3.0
1	B	1680	ASP	2.9
1	B	1443	LEU	2.9
1	B	1732	ILE	2.8
1	A	1615	ILE	2.8
1	B	1387	ALA	2.8
1	A	1596	LEU	2.8
1	B	1605	TYR	2.8
1	B	1442	GLU	2.8
1	B	1575	LEU	2.8
1	A	1585	ARG	2.8
1	B	1473	ASP	2.7
2	C	207	VAL	2.7
1	A	1559	LEU	2.7
1	B	1584	SER	2.7
1	B	1682	SER	2.7
2	D	269	SER	2.7
1	A	1602	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	75	PRO	2.7
1	A	1635	LYS	2.7
1	A	2430	ARG	2.7
1	A	1653	TRP	2.7
1	A	1573	ALA	2.7
1	A	1583	TYR	2.7
1	B	1444	GLU	2.6
1	A	1475	GLU	2.6
1	A	1582	SER	2.6
1	A	1646	PRO	2.6
1	A	1581	GLU	2.6
1	A	1622	ARG	2.6
1	B	1587	TYR	2.6
1	A	1629	ILE	2.6
1	B	1583	TYR	2.6
1	B	1451	GLU	2.6
1	A	1587	TYR	2.5
1	A	2431	LEU	2.5
1	B	1475	GLU	2.5
1	B	2429	TRP	2.5
1	B	1914	GLY	2.5
1	A	2044	VAL	2.5
1	A	1731	ALA	2.5
1	B	1578	MET	2.5
2	D	128	ASN	2.5
1	A	1566	LYS	2.5
1	B	2089	MET	2.4
1	A	1501	TRP	2.4
1	A	1618	ILE	2.4
1	A	1503	LEU	2.4
1	A	1642	LEU	2.4
1	A	1472	ASP	2.4
1	B	1867	LYS	2.4
1	A	1528	SER	2.4
1	A	1558	SER	2.4
2	D	202	GLY	2.4
1	A	1611	ARG	2.3
1	B	1446	GLN	2.3
1	B	1496	GLN	2.3
2	C	269	SER	2.3
1	B	1576	THR	2.3
1	B	2431	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	265	PRO	2.3
1	A	1526	TRP	2.3
2	D	266	GLY	2.3
1	A	1546	TYR	2.3
1	B	1632	ASP	2.3
1	B	2433	ASP	2.3
1	A	2095	LYS	2.3
1	A	1576	THR	2.3
2	C	10	SER	2.3
1	A	1550	LEU	2.3
1	A	1552	LEU	2.3
1	A	1626	CYS	2.3
2	C	170	GLU	2.3
1	B	1573	ALA	2.3
1	A	1620	TRP	2.3
1	A	1418	SER	2.3
1	A	1471	LYS	2.3
1	A	1442	GLU	2.2
1	A	2429	TRP	2.2
1	A	2050	VAL	2.2
1	A	1578	MET	2.2
1	B	1501	TRP	2.2
1	A	2421	PHE	2.2
1	A	1613	GLU	2.2
1	B	1586	ALA	2.2
2	C	263	GLY	2.2
1	B	2430	ARG	2.2
1	B	1581	GLU	2.2
2	D	201	GLY	2.2
1	B	2045	LYS	2.2
1	A	1732	ILE	2.2
1	A	1606	LYS	2.2
1	A	1810	ALA	2.2
1	A	1682	SER	2.1
1	A	1733	ALA	2.1
1	B	1630	VAL	2.1
1	B	2044	VAL	2.1
1	A	1562	GLN	2.1
1	B	1577	ALA	2.1
1	B	2514	SER	2.1
1	A	1473	ASP	2.1
1	A	2119	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2079	MET	2.1
1	A	2089	MET	2.1
1	B	1457	GLU	2.1
1	A	1584	SER	2.1
1	A	1633	TRP	2.1
1	B	1535	MET	2.1
2	C	206	GLU	2.1
1	A	2435	ASN	2.1
1	A	1535	MET	2.1
1	B	1869	VAL	2.0
1	A	2090	LYS	2.0
2	D	10	SER	2.0
1	B	1453	LEU	2.0
1	A	1607	LEU	2.0
1	A	1565	ASP	2.0
1	B	1627	GLN	2.0
1	B	1742	GLU	2.0
1	A	2094	VAL	2.0
1	B	1500	LYS	2.0
1	B	1414	GLU	2.0
1	B	1610	GLU	2.0
1	A	1598	GLU	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
4	MG	A	3002	1/1	0.80	0.19	72,72,72,72	0

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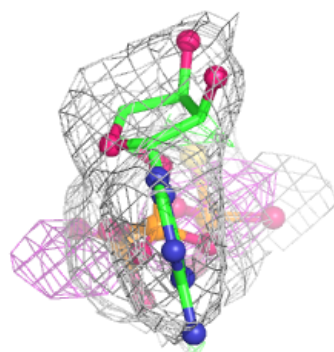
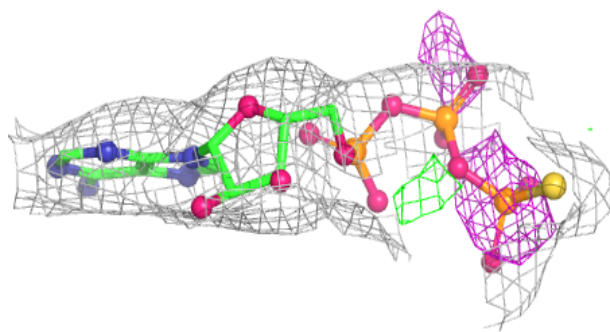
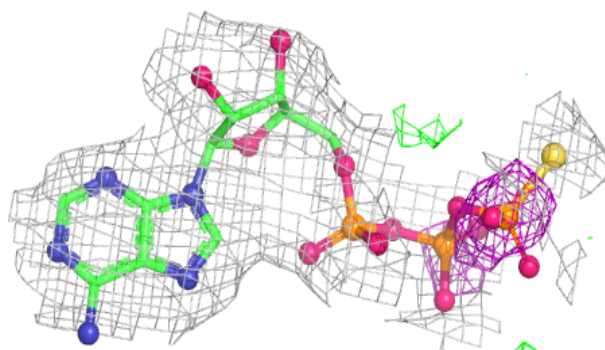
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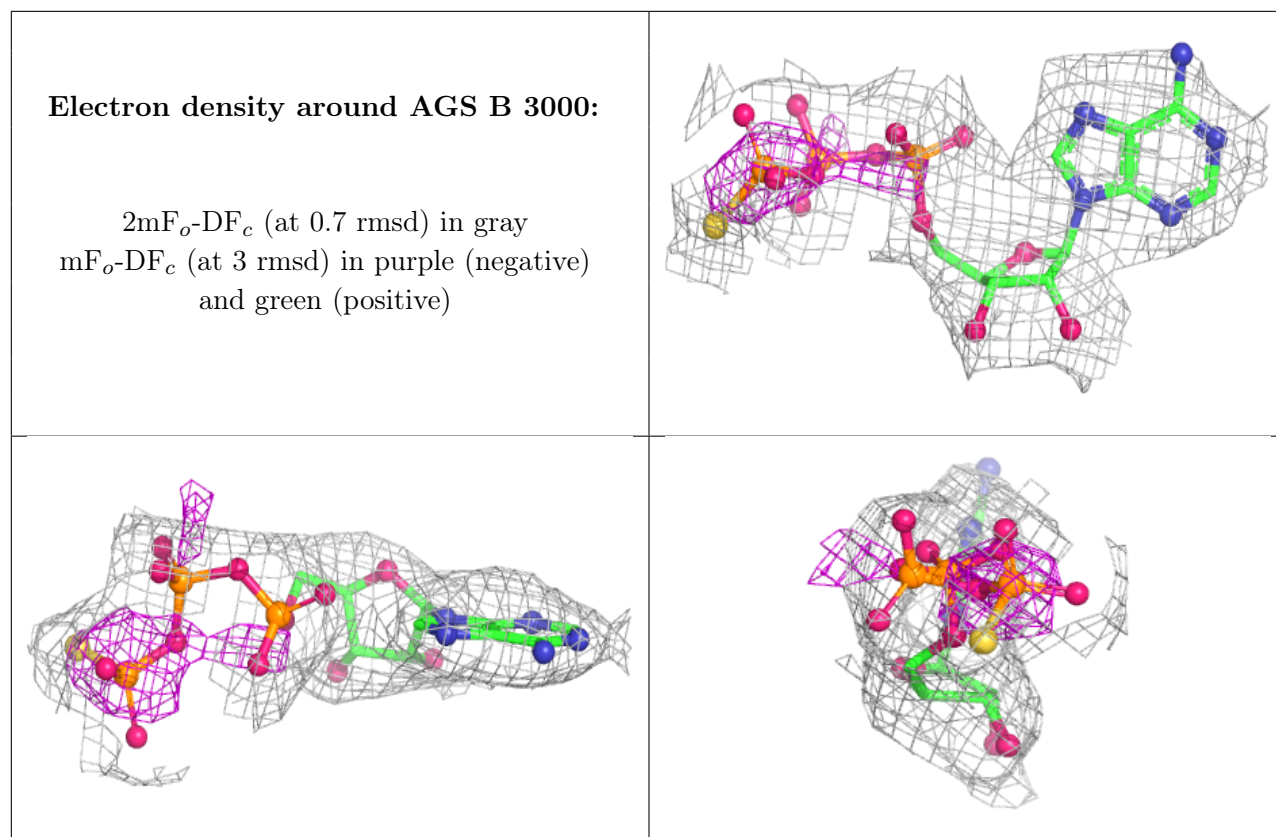
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	3001	1/1	0.82	0.12	66,66,66,66	0
3	AGS	A	3000	31/31	0.90	0.11	51,60,81,85	0
4	MG	B	3002	1/1	0.90	0.13	69,69,69,69	0
4	MG	B	3001	1/1	0.91	0.09	63,63,63,63	0
3	AGS	B	3000	31/31	0.91	0.11	50,56,79,84	0

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 AGS A 3000:

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.