



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:48 am BST

PDB ID : 4JSV
Title : mTOR kinase structure, mechanism and regulation.
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

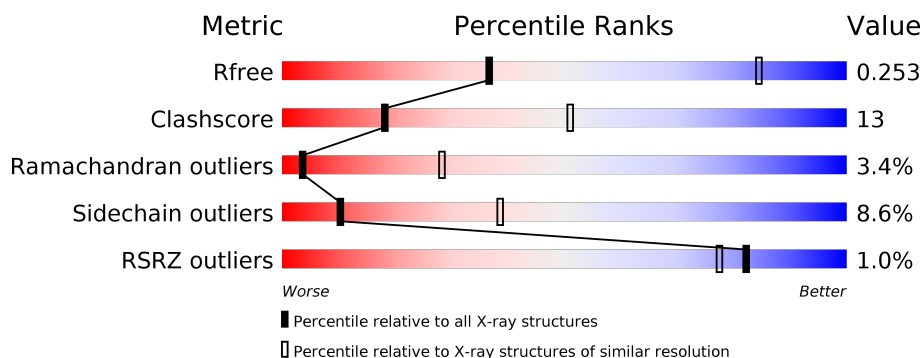
1 Overall quality at a glance ⓘ

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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on 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	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>24%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	1174	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>23%</div> <div>•</div> <div>10%</div> </div> </div>
2	C	326	<div> <div></div> <div> <div>54%</div> <div>37%</div> <div>6%</div> <div>• •</div> </div> </div>
2	D	326	<div> <div></div> <div> <div>53%</div> <div>37%</div> <div>6%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

There are 5 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.

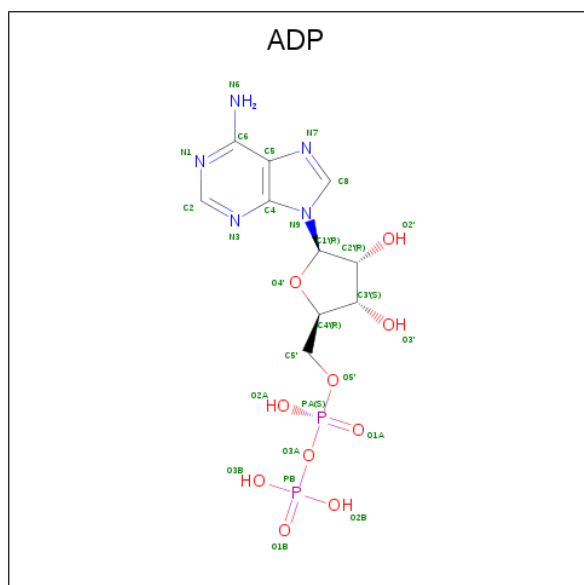
- Molecule 1 is a protein called Serine/threonine-protein kinase mTOR.

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 ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

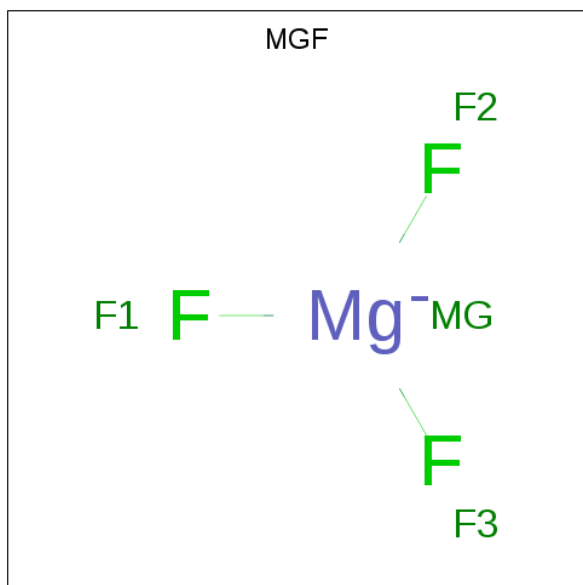


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: 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 5 is TRIFLUOROMAGNESATE (three-letter code: MGF) (formula: F₃Mg).

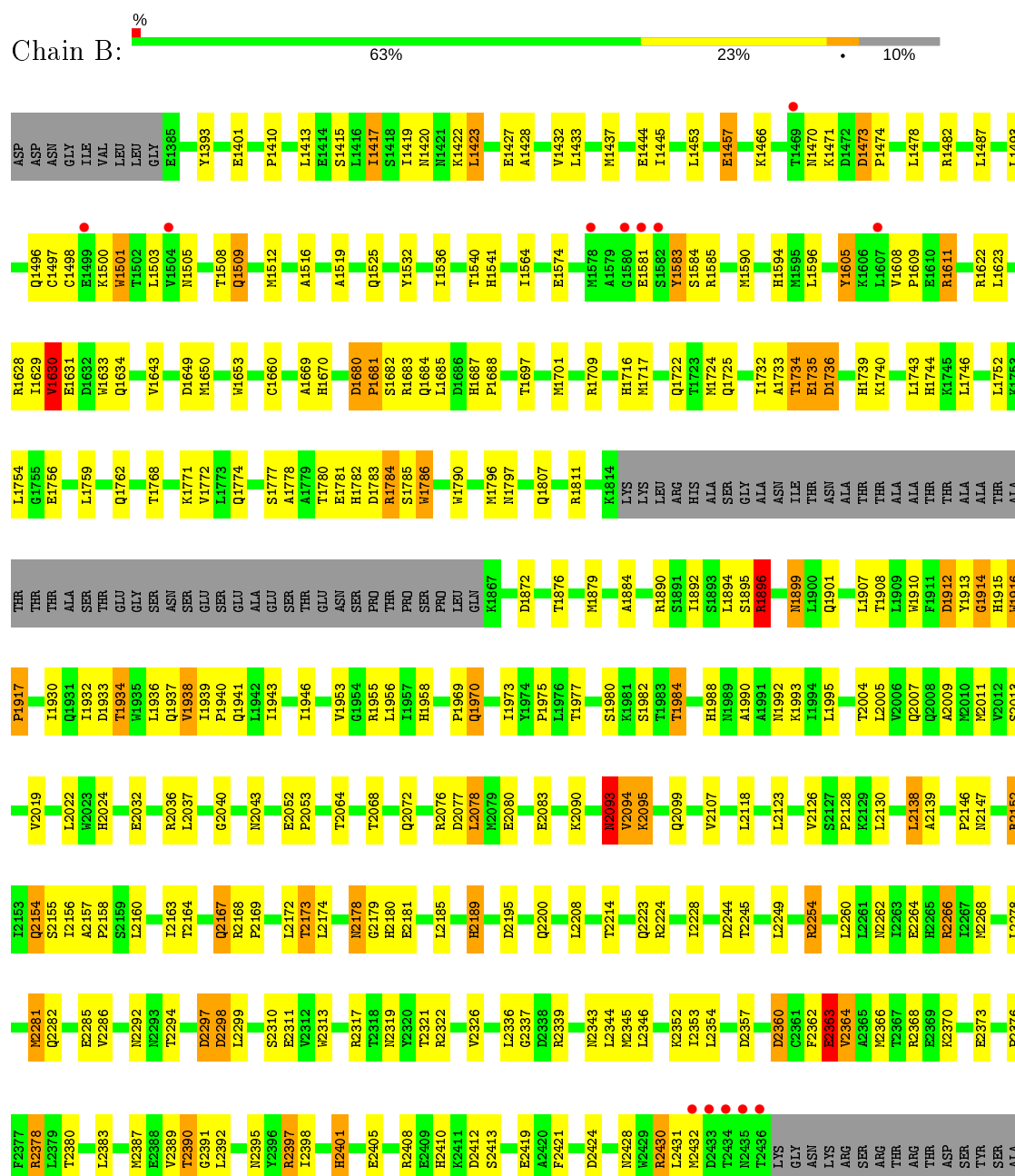


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	F	Mg	0	0
			4	3	1		
5	A	1	Total	F	Mg	0	0
			4	3	1		

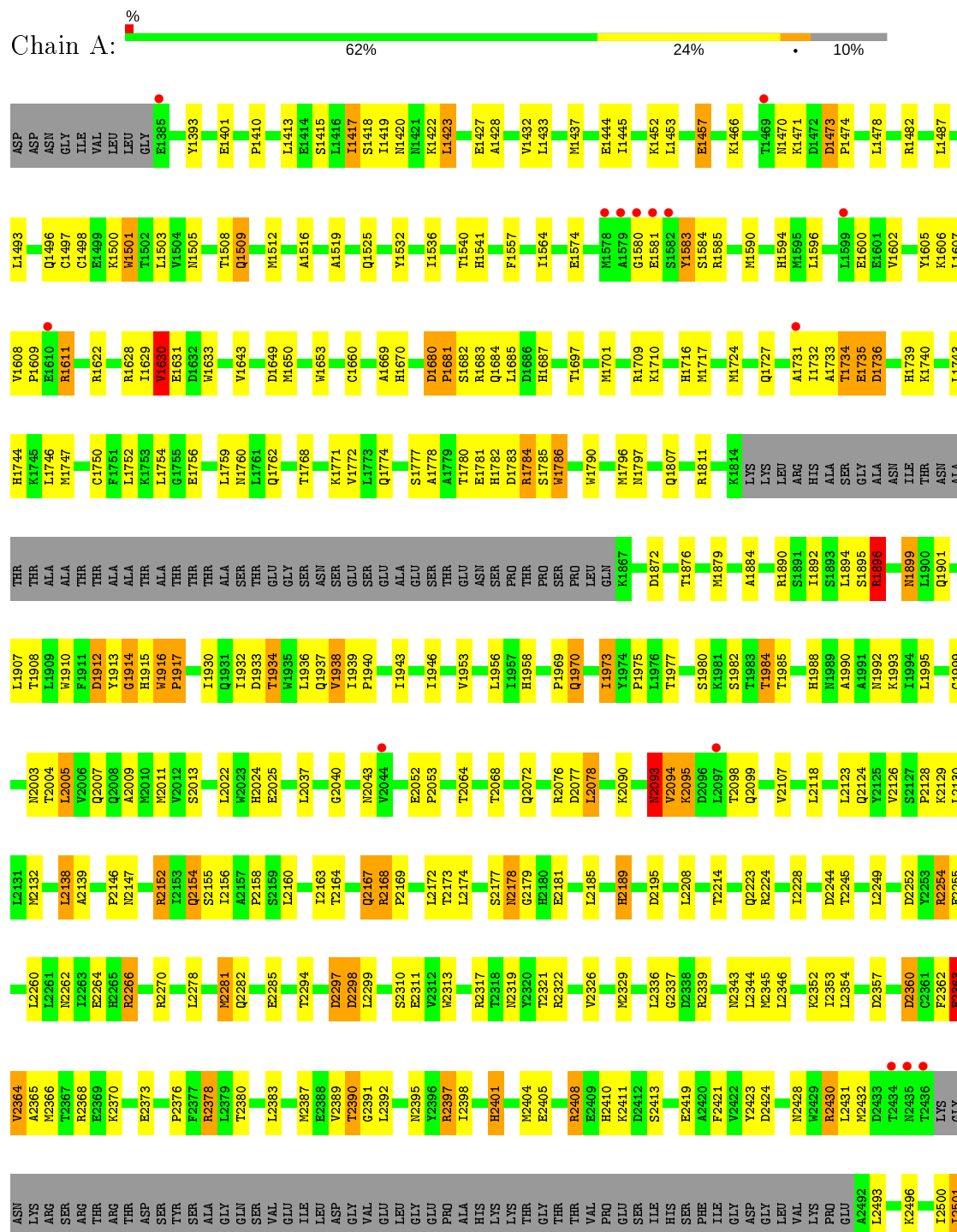
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



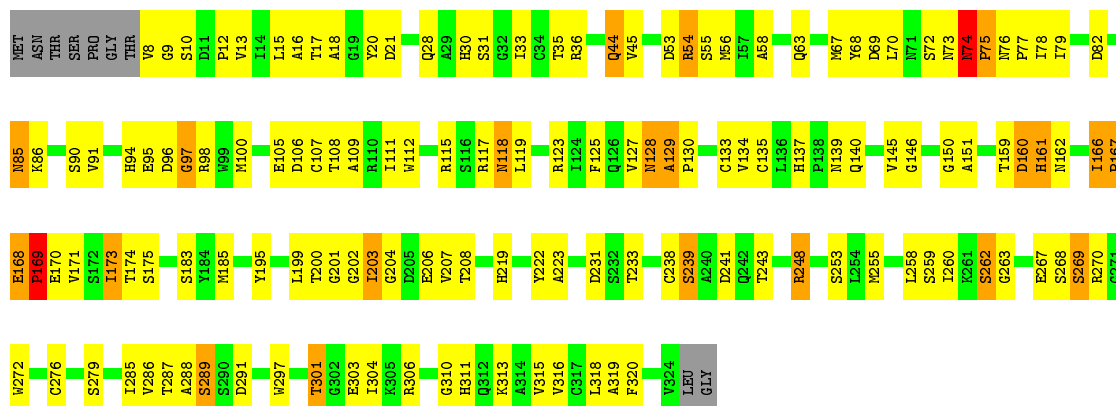
- Molecule 1: Serine/threonine-protein kinase mTOR





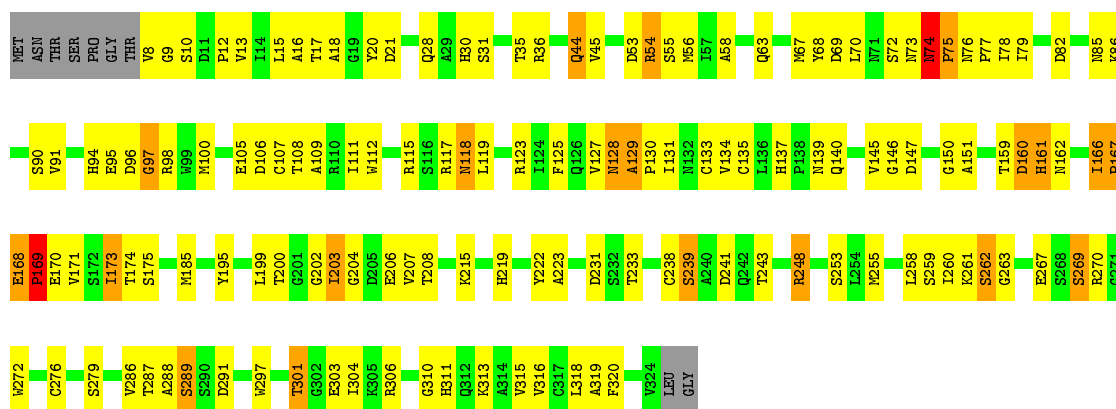
- Molecule 2: Target of rapamycin complex subunit LST8

Chain D: 53% 37% 6% ..



- Molecule 2: Target of rapamycin complex subunit LST8

Chain C: 54% 37% 6% ..



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	139.40 Å 163.20 Å 207.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.50 94.42 – 3.48	Depositor EDS
% Data completeness (in resolution range)	83.7 (100.00-3.50) 82.9 (94.42-3.48)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.49 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.231 , 0.251 0.232 , 0.253	Depositor DCC
R_{free} test set	1479 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22194	wwPDB-VP
Average B, all atoms (Å ²)	74.0	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 45.60 % 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 1.2913e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: MG, MGF, ADP

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	0.32	0/8805	0.56	0/11920
1	B	0.32	0/8805	0.56	0/11920
2	C	0.34	0/2514	0.61	0/3426
2	D	0.37	0/2514	0.62	0/3426
All	All	0.33	0/22638	0.57	0/30692

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

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

There are no bond length outliers.

There are no bond angle outliers.

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	215	5
1	B	8608	0	8593	203	0
2	C	2456	0	2341	91	0
2	D	2456	0	2341	94	0
3	A	27	0	12	1	0
3	B	27	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
All	All	22194	0	21892	589	5

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 13.

All (589) 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	1.23	1.14
2:C:76:ASN:HB3	2:C:77:PRO:HD2	1.21	1.14
2:C:76:ASN:HB3	2:C:77:PRO:CD	1.96	0.95
1:B:2380:THR:HG22	1:B:2383:LEU:HG	1.47	0.94
2:D:76:ASN:HB3	2:D:77:PRO:CD	1.98	0.94
1:A:1969:PRO:O	1:A:1970:GLN:HB2	1.69	0.93
1:B:1969:PRO:O	1:B:1970:GLN:HB2	1.70	0.91
1:A:2380:THR:HG22	1:A:2383:LEU:HG	1.50	0.90
2:D:167:PRO:HD2	2:D:169:PRO:HG2	1.55	0.88
1:A:1418:SER:HB2	1:A:1581:GLU:HG2	1.56	0.86
2:C:279:SER:HA	2:C:320:PHE:HE2	1.43	0.84
1:B:1908:THR:O	1:B:1912:ASP:HB2	1.77	0.83
1:A:1892:ILE:HG21	1:A:1930:ILE:HD11	1.59	0.82
2:D:279:SER:HA	2:D:320:PHE:HE2	1.45	0.82
2:C:167:PRO:HD2	2:C:169:PRO:HG2	1.62	0.82
1:A:1908:THR:O	1:A:1912:ASP:HB2	1.79	0.81
1:B:1892:ILE:HG21	1:B:1930:ILE:HD11	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1915:HIS:HD2	1:B:1953:VAL:HG22	1.47	0.79
1:B:2363:GLU:OE2	1:B:2503:ARG:HD2	1.83	0.79
2:C:137:HIS:HD2	2:C:139:ASN:H	1.31	0.78
2:C:146:GLY:HA3	2:C:173:ILE:HD11	1.64	0.78
1:A:2392:LEU:O	1:A:2397:ARG:HB2	1.84	0.78
2:D:69:ASP:HB2	2:D:78:ILE:HD11	1.63	0.77
2:D:107:CYS:HB3	2:D:127:VAL:O	1.83	0.77
1:B:2392:LEU:O	1:B:2397:ARG:HB2	1.84	0.77
2:D:137:HIS:HD2	2:D:139:ASN:H	1.34	0.76
1:A:2363:GLU:OE2	1:A:2503:ARG:HD2	1.86	0.76
1:A:2357:ASP:OD2	3:A:2601:ADP:O3B	2.04	0.76
2:C:69:ASP:HB2	2:C:78:ILE:HD11	1.65	0.76
2:C:107:CYS:HB3	2:C:127:VAL:O	1.84	0.76
1:A:1915:HIS:HD2	1:A:1953:VAL:HG22	1.51	0.76
1:A:2278:LEU:CD2	2:C:44:GLN:HG2	2.16	0.75
1:B:2401:HIS:O	1:B:2405:GLU:HB2	1.86	0.75
1:B:1778:ALA:O	1:B:1782:HIS:HD2	1.70	0.75
2:D:146:GLY:HA3	2:D:173:ILE:HD11	1.68	0.74
1:A:2064:THR:HG22	1:A:2128:PRO:HD3	1.68	0.74
1:B:1901:GLN:HG3	1:B:2413:SER:HA	1.69	0.74
1:A:1778:ALA:O	1:A:1782:HIS:HD2	1.71	0.74
1:A:1895:SER:HB2	1:A:1899:ASN:HB3	1.70	0.74
1:A:2278:LEU:HD23	2:C:44:GLN:HG2	1.69	0.74
1:B:2278:LEU:HD23	2:D:44:GLN:HG2	1.67	0.74
2:D:301:THR:HB	2:D:303:GLU:HG2	1.70	0.74
1:B:1895:SER:HB2	1:B:1899:ASN:HB3	1.70	0.73
1:A:2401:HIS:O	1:A:2405:GLU:HB2	1.86	0.73
1:B:2278:LEU:CD2	2:D:44:GLN:HG2	2.18	0.73
1:A:1493:LEU:HD23	1:A:1519:ALA:HB2	1.70	0.73
1:A:2266:ARG:HH11	1:A:2266:ARG:HB2	1.54	0.73
1:B:1915:HIS:CD2	1:B:1953:VAL:HG22	2.24	0.73
2:D:241:ASP:OD2	2:D:243:THR:HB	1.90	0.72
1:B:1497:CYS:SG	1:B:1516:ALA:HB2	2.30	0.72
1:A:1901:GLN:HG3	1:A:2413:SER:HA	1.72	0.71
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.23	0.71
2:C:117:ARG:O	2:C:118:ASN:HB2	1.90	0.71
2:C:301:THR:HB	2:C:303:GLU:HG2	1.73	0.71
1:A:1916:TRP:HD1	1:A:1916:TRP:H	1.38	0.71
1:B:2266:ARG:HB2	1:B:2266:ARG:HH11	1.56	0.70
2:C:279:SER:HA	2:C:320:PHE:CE2	2.27	0.70
1:A:2223:GLN:HE22	1:A:2352:LYS:HB2	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:VAL:HG21	2:D:36:ARG:HD3	1.72	0.70
2:D:117:ARG:O	2:D:118:ASN:HB2	1.91	0.69
2:C:8:VAL:HG21	2:C:36:ARG:HD3	1.73	0.69
1:B:2223:GLN:HE22	1:B:2352:LYS:HB2	1.56	0.69
2:C:241:ASP:OD2	2:C:243:THR:HB	1.92	0.69
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.24	0.69
1:B:1433:LEU:HD23	1:B:1453:LEU:HD23	1.74	0.69
2:D:279:SER:HA	2:D:320:PHE:CE2	2.28	0.69
2:C:200:THR:O	2:C:208:THR:HA	1.94	0.68
1:A:1990:ALA:HA	1:A:1993:LYS:HD2	1.74	0.68
1:A:2178:ASN:HD22	1:A:2179:GLY:N	1.91	0.68
1:B:2178:ASN:HD22	1:B:2179:GLY:N	1.91	0.68
1:A:1670:HIS:HE1	1:A:1681:PRO:HB3	1.58	0.68
2:D:200:THR:O	2:D:208:THR:HA	1.94	0.68
1:A:2167:GLN:HG2	1:A:2189:HIS:HD2	1.59	0.67
2:D:111:ILE:HD12	2:D:123:ARG:HD3	1.76	0.67
1:A:1915:HIS:CD2	1:A:1953:VAL:HG22	2.30	0.67
1:A:1680:ASP:C	1:A:1682:SER:H	1.97	0.66
1:A:2344:LEU:HD13	1:A:2353:ILE:HD11	1.78	0.66
2:C:137:HIS:CD2	2:C:139:ASN:H	2.12	0.66
1:A:1583:TYR:C	1:A:1585:ARG:H	1.99	0.66
2:D:15:LEU:HD11	2:D:286:VAL:HG11	1.77	0.66
1:A:1732:ILE:HD13	1:A:1740:LYS:HD2	1.78	0.66
1:A:1980:SER:O	1:A:1988:HIS:HB2	1.96	0.66
1:A:1422:LYS:HD3	1:A:1580:GLY:HA3	1.77	0.65
2:D:137:HIS:CD2	2:D:139:ASN:H	2.12	0.65
1:B:2167:GLN:HG2	1:B:2189:HIS:HD2	1.61	0.65
1:B:1583:TYR:C	1:B:1585:ARG:H	2.00	0.65
1:B:1680:ASP:C	1:B:1682:SER:H	1.99	0.65
2:C:134:VAL:HG22	2:C:145:VAL:HG22	1.79	0.65
2:C:15:LEU:HD11	2:C:286:VAL:HG11	1.78	0.65
2:D:134:VAL:HG22	2:D:145:VAL:HG22	1.79	0.65
1:B:1980:SER:O	1:B:1988:HIS:HB2	1.96	0.65
2:D:21:ASP:HB3	2:D:313:LYS:H	1.62	0.65
2:C:111:ILE:HD12	2:C:123:ARG:HD3	1.78	0.64
1:B:1958:HIS:CE1	1:B:1990:ALA:HB1	2.32	0.64
1:B:2281:MET:HE2	1:B:2281:MET:HA	1.79	0.64
1:B:1623:LEU:HG	1:B:1633:TRP:CH2	2.33	0.64
2:C:231:ASP:HB3	2:C:233:THR:OG1	1.98	0.64
2:C:133:CYS:SG	2:C:175:SER:HA	2.38	0.63
2:C:21:ASP:HB3	2:C:313:LYS:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:231:ASP:HB3	2:D:233:THR:OG1	1.98	0.63
1:A:2093:ASN:HD22	1:A:2094:VAL:H	1.46	0.63
1:A:1910:TRP:O	1:A:1915:HIS:NE2	2.31	0.63
1:B:2419:GLU:HA	1:B:2501:ILE:HD11	1.80	0.63
2:D:150:GLY:HA3	2:D:169:PRO:HB3	1.80	0.63
1:A:2421:PHE:HA	1:A:2424:ASP:HB2	1.81	0.63
1:B:2160:LEU:HD22	1:B:2172:LEU:HA	1.81	0.63
1:A:1417:ILE:HG23	1:A:1432:VAL:HB	1.79	0.62
1:B:1910:TRP:O	1:B:1915:HIS:NE2	2.31	0.62
1:B:2281:MET:HA	1:B:2281:MET:CE	2.29	0.62
1:B:1701:MET:HE1	1:B:1717:MET:N	2.14	0.62
1:B:2093:ASN:HD22	1:B:2094:VAL:H	1.47	0.62
1:A:2160:LEU:HD22	1:A:2172:LEU:HA	1.81	0.62
2:C:139:ASN:HD22	2:C:203:ILE:HG12	1.65	0.62
1:A:2037:LEU:HD22	1:A:2043:ASN:HD22	1.63	0.62
1:A:2022:LEU:HD21	1:A:2126:VAL:HG13	1.81	0.62
1:A:1958:HIS:CE1	1:A:1990:ALA:HB1	2.34	0.62
1:B:2421:PHE:HA	1:B:2424:ASP:HB2	1.82	0.62
2:C:150:GLY:HA3	2:C:169:PRO:HB3	1.81	0.61
2:D:185:MET:HB2	2:D:199:LEU:HD21	1.83	0.61
1:A:1701:MET:HE1	1:A:1717:MET:N	2.16	0.61
1:B:1422:LYS:HE2	1:B:1581:GLU:HG2	1.83	0.61
1:B:1417:ILE:HG23	1:B:1432:VAL:HB	1.80	0.61
1:B:2389:VAL:O	1:B:2390:THR:HG22	2.01	0.61
1:B:1401:GLU:OE1	1:B:2317:ARG:NH1	2.33	0.61
1:B:1990:ALA:HA	1:B:1993:LYS:HD2	1.82	0.61
1:A:1977:THR:HG21	1:A:2013:SER:OG	1.99	0.61
1:B:1732:ILE:HD13	1:B:1740:LYS:HD2	1.83	0.61
1:B:1970:GLN:NE2	1:B:2139:ALA:H	1.98	0.61
1:B:1916:TRP:HD1	1:B:1916:TRP:H	1.42	0.60
1:A:1771:LYS:O	1:A:1774:GLN:HB3	2.01	0.60
2:C:185:MET:HB2	2:C:199:LEU:HD21	1.84	0.60
1:B:2037:LEU:HD22	1:B:2043:ASN:HD22	1.66	0.60
1:A:2419:GLU:HA	1:A:2501:ILE:HD11	1.84	0.60
1:A:1680:ASP:C	1:A:1682:SER:N	2.55	0.60
1:B:1739:HIS:O	1:B:1743:LEU:HB2	2.02	0.60
2:D:168:GLU:HB3	2:D:195:TYR:OH	2.01	0.60
2:D:133:CYS:SG	2:D:175:SER:HA	2.41	0.60
1:B:1493:LEU:HD23	1:B:1519:ALA:HB2	1.84	0.60
1:A:2178:ASN:HD22	1:A:2179:GLY:H	1.50	0.60
1:A:2281:MET:CE	1:A:2281:MET:HA	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:139:ASN:HD22	2:D:203:ILE:HG12	1.68	0.59
1:B:1680:ASP:C	1:B:1682:SER:N	2.56	0.59
1:A:2389:VAL:O	1:A:2390:THR:HG22	2.03	0.59
1:A:1670:HIS:HE1	1:A:1681:PRO:CB	2.15	0.59
1:B:2064:THR:HG22	1:B:2128:PRO:HD3	1.83	0.59
2:C:106:ASP:OD1	2:C:108:THR:OG1	2.20	0.59
2:C:166:ILE:HG13	2:C:166:ILE:O	2.02	0.59
1:B:1958:HIS:HE1	1:B:1990:ALA:HB1	1.66	0.58
1:A:2167:GLN:HG2	1:A:2189:HIS:CD2	2.38	0.58
1:B:1783:ASP:O	1:B:1785:SER:N	2.37	0.58
1:A:1733:ALA:O	1:A:1735:GLU:N	2.36	0.58
1:B:2380:THR:CG2	1:B:2383:LEU:HG	2.28	0.58
1:A:1783:ASP:O	1:A:1785:SER:N	2.37	0.58
2:C:95:GLU:H	2:C:140:GLN:HE22	1.50	0.58
2:C:151:ALA:HA	2:C:166:ILE:HG22	1.84	0.58
1:A:2281:MET:HE2	1:A:2281:MET:HA	1.85	0.58
1:B:2022:LEU:HD21	1:B:2126:VAL:HG13	1.85	0.58
1:B:2167:GLN:HG2	1:B:2189:HIS:CD2	2.39	0.58
1:B:1771:LYS:O	1:B:1774:GLN:HB3	2.03	0.58
1:B:2344:LEU:HD13	1:B:2353:ILE:HD11	1.86	0.58
2:C:168:GLU:HB3	2:C:195:TYR:OH	2.04	0.58
2:D:166:ILE:O	2:D:166:ILE:HG13	2.03	0.57
2:D:151:ALA:HA	2:D:166:ILE:HG22	1.85	0.57
1:A:1701:MET:HE1	1:A:1717:MET:CA	2.35	0.57
1:B:1574:GLU:HG2	1:B:1585:ARG:NH2	2.20	0.57
2:D:106:ASP:OD1	2:D:108:THR:OG1	2.22	0.57
1:A:1759:LEU:HG	1:A:1772:VAL:HG11	1.87	0.57
1:B:1505:ASN:HB2	1:B:1508:THR:HB	1.86	0.56
1:B:2178:ASN:HD22	1:B:2179:GLY:H	1.52	0.56
2:D:219:HIS:HE1	2:D:243:THR:HG22	1.71	0.56
1:A:1505:ASN:HB2	1:A:1508:THR:HB	1.87	0.56
2:C:219:HIS:HE1	2:C:243:THR:HG22	1.71	0.56
2:D:95:GLU:H	2:D:140:GLN:HE22	1.51	0.56
1:A:2521:VAL:HB	1:A:2522:PRO:HD3	1.87	0.56
1:B:1913:TYR:O	1:B:1915:HIS:ND1	2.38	0.56
2:C:17:THR:HB	2:C:311:HIS:HE1	1.70	0.56
1:A:1466:LYS:O	1:A:1470:ASN:HB2	2.06	0.56
1:A:1739:HIS:O	1:A:1743:LEU:HB2	2.06	0.56
1:A:2163:ILE:HB	1:A:2169:PRO:HG2	1.87	0.56
2:C:18:ALA:HB1	2:C:45:VAL:HG21	1.88	0.56
1:A:1930:ILE:HD11	1:A:1934:THR:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1759:LEU:HG	1:B:1772:VAL:HG11	1.87	0.56
1:B:1498:CYS:HA	1:B:1501:TRP:HD1	1.70	0.55
1:B:2390:THR:HG23	1:B:2390:THR:O	2.06	0.55
1:A:2336:LEU:HG	1:A:2339:ARG:HH11	1.72	0.55
2:D:168:GLU:N	2:D:169:PRO:HD2	2.20	0.55
1:A:2390:THR:O	1:A:2390:THR:HG23	2.06	0.55
1:B:1623:LEU:HG	1:B:1633:TRP:CZ3	2.41	0.55
1:B:1680:ASP:OD2	1:B:1683:ARG:HB2	2.06	0.55
1:B:1701:MET:HE1	1:B:1717:MET:CA	2.37	0.55
2:C:168:GLU:N	2:C:169:PRO:HD2	2.21	0.55
2:C:167:PRO:HB2	2:C:169:PRO:HD2	1.89	0.55
1:A:1498:CYS:HA	1:A:1501:TRP:HD1	1.71	0.55
1:A:1784:ARG:O	1:A:1790:TRP:NE1	2.38	0.55
1:B:1466:LYS:O	1:B:1470:ASN:HB2	2.07	0.55
1:A:1680:ASP:OD2	1:A:1683:ARG:HB2	2.07	0.55
1:A:2380:THR:CG2	1:A:2383:LEU:HG	2.32	0.54
2:D:167:PRO:HB2	2:D:169:PRO:HD2	1.89	0.54
2:D:18:ALA:HB1	2:D:45:VAL:HG21	1.89	0.54
1:A:1710:LYS:NZ	1:A:1760:ASN:HD21	2.04	0.54
1:B:2336:LEU:HG	1:B:2339:ARG:HH11	1.72	0.54
1:A:2278:LEU:HD21	2:C:44:GLN:HG2	1.90	0.54
2:D:17:THR:HB	2:D:311:HIS:HE1	1.72	0.54
1:A:1958:HIS:HE1	1:A:1990:ALA:HB1	1.71	0.54
2:D:288:ALA:HB2	2:D:318:LEU:HG	1.89	0.54
1:B:2163:ILE:HB	1:B:2169:PRO:HG2	1.90	0.54
2:D:288:ALA:HB1	2:D:315:VAL:HG12	1.90	0.54
2:D:53:ASP:C	2:D:55:SER:H	2.11	0.54
1:A:1970:GLN:NE2	1:A:2139:ALA:H	2.05	0.54
1:B:1930:ILE:HD11	1:B:1934:THR:HG21	1.89	0.54
1:B:1933:ASP:O	1:B:1934:THR:C	2.47	0.54
1:B:1943:ILE:O	1:B:1946:ILE:HG13	2.08	0.54
2:C:288:ALA:HB2	2:C:318:LEU:HG	1.89	0.53
2:C:36:ARG:NH2	2:C:69:ASP:O	2.41	0.53
1:B:2368:ARG:HD2	1:B:2370:LYS:O	2.08	0.53
1:B:1684:GLN:HB3	1:B:1687:HIS:CD2	2.43	0.53
2:C:8:VAL:HG11	2:C:36:ARG:HE	1.73	0.53
1:A:1916:TRP:CD1	1:A:1916:TRP:N	2.64	0.53
2:C:12:PRO:O	2:C:54:ARG:NH2	2.42	0.53
1:B:1762:GLN:HB2	1:B:1768:THR:HG21	1.91	0.53
1:A:1913:TYR:O	1:A:1915:HIS:ND1	2.41	0.53
1:B:1457:GLU:HG2	1:B:1487:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1660:CYS:HB2	1:B:1669:ALA:HB2	1.90	0.53
2:D:55:SER:O	2:D:56:MET:HG2	2.09	0.53
1:B:1969:PRO:O	1:B:1970:GLN:CB	2.50	0.53
1:B:2357:ASP:OD2	3:B:2601:ADP:O3B	2.27	0.53
2:C:269:SER:OG	2:C:270:ARG:N	2.42	0.53
2:D:128:ASN:O	2:D:129:ALA:HB3	2.09	0.53
1:B:2282:GLN:HE21	2:D:316:VAL:HG11	1.74	0.53
2:D:36:ARG:NH2	2:D:69:ASP:O	2.42	0.53
2:C:105:GLU:HA	2:C:130:PRO:HB3	1.90	0.52
2:D:169:PRO:HA	2:D:171:VAL:H	1.74	0.52
2:D:223:ALA:HA	2:D:239:SER:HB2	1.92	0.52
1:A:1969:PRO:O	1:A:1970:GLN:CB	2.50	0.52
2:C:223:ALA:HA	2:C:239:SER:HB2	1.91	0.52
1:A:1732:ILE:HD13	1:A:1740:LYS:HB2	1.91	0.52
1:A:1684:GLN:HB3	1:A:1687:HIS:CD2	2.45	0.52
1:B:2521:VAL:HB	1:B:2522:PRO:HD3	1.91	0.52
1:A:1557:PHE:CE2	1:A:1606:LYS:HB3	2.44	0.52
1:B:1629:ILE:HG22	1:B:1630:VAL:HG23	1.91	0.52
1:A:2139:ALA:HA	1:A:2152:ARG:HA	1.92	0.52
1:A:2368:ARG:HD2	1:A:2370:LYS:O	2.10	0.52
2:C:28:GLN:O	2:C:28:GLN:HG3	2.10	0.52
2:C:288:ALA:HB1	2:C:315:VAL:HG12	1.92	0.52
1:B:1701:MET:HE1	1:B:1716:HIS:C	2.30	0.51
2:D:12:PRO:O	2:D:54:ARG:NH2	2.44	0.51
2:C:9:GLY:HA3	2:C:70:LEU:HB3	1.93	0.51
2:D:69:ASP:CB	2:D:78:ILE:HD11	2.38	0.51
2:D:8:VAL:HG11	2:D:36:ARG:HE	1.74	0.51
1:A:1401:GLU:OE1	1:A:2317:ARG:NH1	2.40	0.51
1:A:1457:GLU:HG2	1:A:1487:LEU:HD21	1.92	0.51
1:A:1999:CYS:HA	1:A:2003:ASN:HA	1.92	0.51
2:C:28:GLN:OE1	2:C:30:HIS:CE1	2.64	0.51
2:C:31:SER:C	2:C:306:ARG:HD3	2.30	0.51
1:B:1605:TYR:CD2	1:B:1643:VAL:HG11	2.46	0.51
1:A:1427:GLU:HB2	1:A:2398:ILE:HD13	1.91	0.51
2:C:97:GLY:HA3	2:C:115:ARG:NH2	2.25	0.51
2:C:169:PRO:HA	2:C:171:VAL:H	1.76	0.51
2:C:53:ASP:C	2:C:55:SER:H	2.14	0.51
2:D:105:GLU:HA	2:D:130:PRO:HB3	1.92	0.51
2:D:28:GLN:OE1	2:D:30:HIS:CE1	2.64	0.51
2:D:9:GLY:HA3	2:D:70:LEU:HB3	1.93	0.51
1:A:2052:GLU:HG2	1:A:2053:PRO:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2264:GLU:HG3	1:B:2294:THR:HG21	1.93	0.50
1:A:1437:MET:SD	1:A:1453:LEU:HD11	2.52	0.50
2:C:238:CYS:SG	2:C:276:CYS:HB3	2.52	0.50
2:C:128:ASN:O	2:C:129:ALA:HB3	2.11	0.50
1:A:1762:GLN:HB2	1:A:1768:THR:HG21	1.93	0.50
1:A:1933:ASP:O	1:A:1934:THR:C	2.50	0.50
1:B:2156:ILE:HG12	1:B:2174:LEU:HD22	1.94	0.50
1:A:1660:CYS:HB2	1:A:1669:ALA:HB2	1.93	0.50
1:A:1943:ILE:O	1:A:1946:ILE:HG13	2.12	0.50
1:A:1785:SER:O	1:A:1786:TRP:HB3	2.12	0.50
1:A:1943:ILE:CD1	1:A:1975:PRO:HB2	2.41	0.50
2:D:31:SER:C	2:D:306:ARG:HD3	2.32	0.50
1:B:1752:LEU:O	1:B:1756:GLU:HB2	2.12	0.50
1:B:1784:ARG:O	1:B:1790:TRP:NE1	2.42	0.50
1:B:1936:LEU:HD23	1:B:1939:ILE:HD11	1.94	0.50
2:C:17:THR:HB	2:C:311:HIS:CE1	2.47	0.50
1:A:2245:THR:HA	1:A:2345:MET:HB3	1.94	0.49
1:A:2345:MET:HG3	1:A:2354:LEU:HD23	1.93	0.49
1:B:2245:THR:HA	1:B:2345:MET:HB3	1.94	0.49
1:A:1497:CYS:SG	1:A:1516:ALA:HB2	2.52	0.49
1:B:1697:THR:O	1:B:1701:MET:HG3	2.12	0.49
1:B:2052:GLU:HG2	1:B:2053:PRO:HD3	1.93	0.49
1:A:1393:TYR:CE2	1:A:1422:LYS:HD2	2.47	0.49
1:B:1797:ASN:HB3	1:B:1884:ALA:HB2	1.93	0.49
2:D:97:GLY:HA3	2:D:115:ARG:NH2	2.27	0.49
2:D:203:ILE:HA	2:D:206:GLU:HG2	1.95	0.49
1:B:2139:ALA:HA	1:B:2152:ARG:HA	1.94	0.49
1:A:1807:GLN:O	1:A:1811:ARG:HG2	2.13	0.49
1:A:2321:THR:HG23	1:A:2387:MET:HG2	1.94	0.49
1:A:2366:MET:HG2	1:A:2373:GLU:O	2.13	0.49
1:B:1916:TRP:N	1:B:1916:TRP:CD1	2.66	0.49
1:B:2278:LEU:HD21	2:D:44:GLN:HG2	1.95	0.49
1:B:1734:THR:O	1:B:1736:ASP:N	2.46	0.48
1:B:2009:ALA:HA	1:B:2138:LEU:HD11	1.94	0.48
1:B:2345:MET:HG3	1:B:2354:LEU:HD23	1.95	0.48
2:C:203:ILE:HA	2:C:206:GLU:HG2	1.95	0.48
1:A:2078:LEU:HD11	1:A:2107:VAL:HG21	1.95	0.48
1:A:2254:ARG:HD3	1:A:2298:ASP:OD2	2.13	0.48
1:B:2281:MET:HE2	1:B:2281:MET:CA	2.41	0.48
1:A:1629:ILE:HG22	1:A:1630:VAL:HG23	1.94	0.48
1:A:2310:SER:HA	1:A:2313:TRP:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1433:LEU:HD23	1:B:1453:LEU:CD2	2.43	0.48
1:A:1701:MET:HE1	1:A:1716:HIS:C	2.33	0.48
1:A:1943:ILE:HD13	1:A:1975:PRO:HB2	1.94	0.48
1:A:2428:ASN:HB3	1:A:2493:LEU:HD13	1.94	0.48
1:A:1496:GLN:NE2	1:A:1500:LYS:HG3	2.29	0.48
1:A:2024:HIS:NE2	1:A:2118:LEU:HD11	2.29	0.48
1:A:1895:SER:CB	1:A:1899:ASN:HB3	2.41	0.48
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.47	0.48
1:B:1916:TRP:HA	1:B:1917:PRO:HD2	1.62	0.48
1:B:1992:ASN:HA	1:B:1995:LEU:HD12	1.96	0.48
1:B:2310:SER:HA	1:B:2313:TRP:HB3	1.96	0.48
1:A:2282:GLN:HE21	2:C:316:VAL:HG11	1.79	0.48
1:B:1478:LEU:O	1:B:1482:ARG:HG3	2.14	0.48
1:B:1807:GLN:O	1:B:1811:ARG:HG2	2.14	0.48
2:D:28:GLN:O	2:D:28:GLN:HG3	2.14	0.48
1:A:1717:MET:HG3	1:A:1754:LEU:HG	1.94	0.48
1:B:1733:ALA:O	1:B:1735:GLU:N	2.47	0.48
1:B:2095:LYS:O	1:B:2099:GLN:HG2	2.14	0.48
1:A:1670:HIS:CE1	1:A:1681:PRO:HB3	2.46	0.47
1:A:1734:THR:O	1:A:1736:ASP:N	2.47	0.47
1:A:1876:THR:O	1:A:1879:MET:HB3	2.14	0.47
1:A:2264:GLU:HG3	1:A:2294:THR:HG21	1.96	0.47
1:A:1428:ALA:HB2	1:A:2395:ASN:HD21	1.78	0.47
1:B:1785:SER:O	1:B:1786:TRP:HB3	2.14	0.47
1:A:1752:LEU:O	1:A:1756:GLU:HB2	2.14	0.47
2:C:69:ASP:CB	2:C:78:ILE:HD11	2.39	0.47
1:B:1496:GLN:NE2	1:B:1500:LYS:HG3	2.29	0.47
1:B:1564:ILE:HG23	1:B:1596:LEU:HD22	1.95	0.47
1:B:1907:LEU:HD11	1:B:1938:VAL:CG1	2.45	0.47
2:C:289:SER:HB2	2:C:291:ASP:OD1	2.15	0.47
1:B:1428:ALA:HB2	1:B:2395:ASN:HD21	1.80	0.47
2:C:55:SER:O	2:C:56:MET:HG2	2.14	0.47
2:D:269:SER:OG	2:D:270:ARG:N	2.47	0.47
1:A:1982:SER:OG	1:A:1984:THR:HG23	2.14	0.47
1:B:1734:THR:C	1:B:1736:ASP:H	2.18	0.47
2:D:63:GLN:HE21	2:D:86:LYS:H	1.62	0.47
1:A:1608:VAL:O	1:A:1608:VAL:HG23	2.15	0.47
1:A:2025:GLU:HG2	1:A:2168:ARG:HH21	1.80	0.47
2:D:109:ALA:HB3	2:D:125:PHE:HB3	1.97	0.47
2:C:159:THR:C	2:C:161:HIS:H	2.18	0.47
1:B:1393:TYR:CE2	1:B:1422:LYS:HD2	2.49	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	2.49	0.47
1:B:1744:HIS:O	1:B:1782:HIS:HB3	2.15	0.47
1:A:1508:THR:O	1:A:1512:MET:HB2	2.14	0.47
1:A:1734:THR:C	1:A:1736:ASP:H	2.18	0.47
1:A:2154:GLN:NE2	1:A:2155:SER:HB2	2.30	0.47
2:D:58:ALA:HA	2:D:67:MET:HG2	1.97	0.47
1:B:1508:THR:O	1:B:1512:MET:HB2	2.13	0.47
1:B:2428:ASN:HB3	1:B:2493:LEU:HD13	1.95	0.47
2:C:16:ALA:HB3	2:C:319:ALA:HB3	1.97	0.47
2:C:63:GLN:NE2	2:C:86:LYS:H	2.13	0.47
2:D:82:ASP:HB2	2:D:119:LEU:HD13	1.97	0.47
1:A:2156:ILE:HG12	1:A:2174:LEU:HD22	1.97	0.46
2:D:202:GLY:HA3	2:D:207:VAL:H	1.80	0.46
1:A:1747:MET:O	1:A:1750:CYS:HB2	2.14	0.46
1:B:2421:PHE:CD1	1:B:2430:ARG:NH2	2.84	0.46
2:D:248:ARG:HG3	2:D:253:SER:OG	2.16	0.46
2:D:238:CYS:SG	2:D:276:CYS:HB3	2.56	0.46
1:A:1602:VAL:HG13	1:A:1643:VAL:HG23	1.97	0.46
1:A:1797:ASN:HB3	1:A:1884:ALA:HB2	1.96	0.46
1:A:2095:LYS:O	1:A:2099:GLN:HG2	2.14	0.46
1:A:2336:LEU:HG	1:A:2339:ARG:NH1	2.30	0.46
2:D:159:THR:C	2:D:161:HIS:H	2.17	0.46
1:B:2339:ARG:HH21	1:B:2343:ASN:HB3	1.79	0.46
2:D:117:ARG:O	2:D:118:ASN:CB	2.62	0.46
2:D:63:GLN:NE2	2:D:86:LYS:H	2.14	0.46
1:A:2281:MET:HE2	1:A:2281:MET:CA	2.45	0.46
1:B:2360:ASP:N	1:B:2360:ASP:OD1	2.49	0.46
1:B:1594:HIS:HE1	1:B:1622:ARG:HD2	1.81	0.46
1:B:1939:ILE:N	1:B:1940:PRO:HD2	2.31	0.46
1:A:1564:ILE:HD13	1:A:1600:GLU:HG3	1.98	0.46
1:B:1895:SER:O	1:B:1896:ARG:C	2.54	0.46
1:B:1415:SER:O	1:B:1419:ILE:HG22	2.15	0.46
1:B:1977:THR:HG21	1:B:2013:SER:OG	2.15	0.46
1:B:2019:VAL:HG22	1:B:2126:VAL:HG12	1.98	0.46
1:B:2154:GLN:NE2	1:B:2155:SER:HB2	2.31	0.46
1:B:2363:GLU:O	1:B:2366:MET:N	2.45	0.46
2:C:117:ARG:O	2:C:118:ASN:CB	2.62	0.46
2:D:56:MET:HB2	2:D:68:TYR:O	2.15	0.46
1:A:2322:ARG:O	1:A:2326:VAL:HG23	2.17	0.45
1:B:2254:ARG:HD3	1:B:2298:ASP:OD2	2.16	0.45
1:A:1433:LEU:HD23	1:A:1453:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1649:ASP:HB3	1:A:1653:TRP:HD1	1.81	0.45
1:A:2208:LEU:HD22	1:A:2410:HIS:CD2	2.51	0.45
1:A:2363:GLU:OE2	1:A:2503:ARG:NH1	2.49	0.45
1:A:1594:HIS:HE1	1:A:1622:ARG:HD2	1.81	0.45
1:A:2123:LEU:HB2	1:A:2158:PRO:O	2.17	0.45
1:A:2329:MET:HB3	1:A:2404:MET:HE2	1.99	0.45
1:A:2421:PHE:CD1	1:A:2430:ARG:NH2	2.85	0.45
1:B:2078:LEU:HD11	1:B:2107:VAL:HG21	1.98	0.45
1:B:2336:LEU:HG	1:B:2339:ARG:NH1	2.31	0.45
2:C:20:TYR:HD2	2:C:44:GLN:HB3	1.81	0.45
1:A:1433:LEU:HD21	1:A:1452:LYS:HB3	1.98	0.45
1:A:2363:GLU:O	1:A:2366:MET:N	2.47	0.45
1:A:1428:ALA:HB2	1:A:2395:ASN:ND2	2.32	0.45
1:B:1943:ILE:CD1	1:B:1975:PRO:HB2	2.46	0.45
1:B:2004:THR:HA	1:B:2007:GLN:HB2	1.99	0.45
1:A:1478:LEU:O	1:A:1482:ARG:HG3	2.17	0.45
1:A:1916:TRP:HA	1:A:1917:PRO:HD2	1.65	0.45
1:B:1437:MET:SD	1:B:1453:LEU:HD11	2.57	0.45
1:B:2208:LEU:HD22	1:B:2410:HIS:CD2	2.52	0.45
2:D:86:LYS:HE2	2:D:105:GLU:HB3	1.97	0.45
2:D:248:ARG:HD2	2:D:255:MET:HB2	1.99	0.45
1:A:1415:SER:O	1:A:1419:ILE:HG22	2.16	0.45
1:A:1936:LEU:HD23	1:A:1939:ILE:HD11	1.98	0.45
2:D:289:SER:HB2	2:D:291:ASP:OD1	2.17	0.45
2:D:17:THR:HB	2:D:311:HIS:CE1	2.49	0.45
1:B:1982:SER:OG	1:B:1984:THR:HG23	2.16	0.45
2:C:86:LYS:HE2	2:C:105:GLU:HB3	1.98	0.45
1:A:2496:LYS:HE3	1:A:2500:ILE:HD11	1.99	0.45
1:B:1732:ILE:HD13	1:B:1740:LYS:HB2	1.99	0.45
1:A:1631:GLU:H	1:A:1631:GLU:CD	2.20	0.45
1:A:1701:MET:HE1	1:A:1717:MET:HA	1.98	0.45
2:D:72:SER:O	2:D:74:ASN:N	2.50	0.45
1:B:1895:SER:CB	1:B:1899:ASN:HB3	2.44	0.44
1:B:1574:GLU:HG2	1:B:1585:ARG:HH22	1.81	0.44
1:B:1876:THR:O	1:B:1879:MET:HB3	2.17	0.44
1:A:1473:ASP:HA	1:A:1474:PRO:HD2	1.82	0.44
1:A:1574:GLU:HG2	1:A:1585:ARG:NH2	2.32	0.44
1:A:1744:HIS:O	1:A:1782:HIS:HB3	2.18	0.44
1:A:2004:THR:HA	1:A:2007:GLN:HB2	1.99	0.44
1:A:2167:GLN:CG	1:A:2189:HIS:CD2	3.00	0.44
1:A:2281:MET:HE1	2:C:222:TYR:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1649:ASP:HB3	1:B:1653:TRP:HD1	1.83	0.44
1:B:2167:GLN:CG	1:B:2189:HIS:CD2	3.00	0.44
1:B:1501:TRP:CE3	1:B:1503:LEU:HD12	2.52	0.44
1:B:1583:TYR:C	1:B:1585:ARG:N	2.68	0.44
1:B:1796:MET:HA	1:B:1796:MET:CE	2.48	0.44
2:C:94:HIS:CD2	2:C:140:GLN:HB3	2.52	0.44
2:C:202:GLY:HA3	2:C:207:VAL:H	1.82	0.44
2:C:258:LEU:HD22	2:C:297:TRP:CE3	2.52	0.44
1:B:2268:MET:HG2	1:B:2286:VAL:HG12	2.00	0.44
1:B:2366:MET:HG2	1:B:2373:GLU:O	2.17	0.44
1:A:1796:MET:HA	1:A:1796:MET:CE	2.48	0.44
1:B:1890:ARG:O	1:B:1894:LEU:HG	2.17	0.44
2:C:72:SER:O	2:C:74:ASN:N	2.51	0.44
1:A:1427:GLU:HB2	1:A:2398:ILE:CD1	2.48	0.44
1:A:1785:SER:O	1:A:1786:TRP:CB	2.65	0.44
1:A:2319:ASN:HD22	1:A:2352:LYS:HG3	1.82	0.44
1:B:1470:ASN:HB3	1:B:1471:LYS:H	1.61	0.44
2:D:270:ARG:HA	2:D:270:ARG:HD2	1.85	0.44
2:C:248:ARG:HD2	2:C:255:MET:HB2	2.00	0.44
1:A:1973:ILE:HD13	1:A:2005:LEU:HD22	1.99	0.43
1:B:2130:LEU:HD22	1:B:2156:ILE:HD13	2.00	0.43
2:D:16:ALA:HB3	2:D:319:ALA:HB3	2.00	0.43
1:A:2146:PRO:O	1:A:2147:ASN:HB2	2.18	0.43
1:A:1890:ARG:O	1:A:1894:LEU:HG	2.17	0.43
1:A:2249:LEU:HD13	1:A:2346:LEU:HD12	2.00	0.43
1:A:2514:SER:OG	1:A:2517:ASP:HB2	2.18	0.43
1:B:1473:ASP:HA	1:B:1474:PRO:HD2	1.83	0.43
1:B:2123:LEU:HB2	1:B:2158:PRO:O	2.18	0.43
1:A:1896:ARG:NH2	1:A:1933:ASP:OD2	2.52	0.43
1:A:1899:ASN:ND2	1:A:1937:GLN:HE22	2.17	0.43
1:B:1427:GLU:HB2	1:B:2398:ILE:HD13	2.01	0.43
2:C:109:ALA:HB3	2:C:125:PHE:HB3	2.01	0.43
1:A:1501:TRP:CE3	1:A:1503:LEU:HD12	2.53	0.43
1:A:1992:ASN:HA	1:A:1995:LEU:HD12	2.00	0.43
2:D:100:MET:HB3	2:D:112:TRP:HB2	2.01	0.43
1:A:1710:LYS:HZ1	1:A:1760:ASN:HD21	1.65	0.43
1:B:1785:SER:O	1:B:1786:TRP:CB	2.65	0.43
1:B:1913:TYR:O	1:B:1915:HIS:HA	2.18	0.43
1:B:2363:GLU:OE2	1:B:2503:ARG:NH1	2.51	0.43
2:C:270:ARG:HA	2:C:270:ARG:HD2	1.87	0.43
2:C:56:MET:HB2	2:C:68:TYR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:ASN:H	2:D:75:PRO:HD3	1.83	0.43
1:B:1423:LEU:HA	1:B:1423:LEU:HD12	1.88	0.43
2:D:20:TYR:HD2	2:D:44:GLN:HB3	1.83	0.43
1:B:1907:LEU:HD11	1:B:1938:VAL:HG13	2.00	0.43
1:B:2024:HIS:NE2	1:B:2118:LEU:HD11	2.34	0.43
1:A:1697:THR:O	1:A:1701:MET:HG3	2.18	0.43
1:A:1759:LEU:HD21	1:A:1772:VAL:HG21	2.00	0.43
1:A:1892:ILE:CG2	1:A:1930:ILE:HD11	2.39	0.43
1:A:2297:ASP:O	1:A:2299:LEU:N	2.51	0.43
2:C:159:THR:C	2:C:161:HIS:N	2.71	0.43
2:D:159:THR:C	2:D:161:HIS:N	2.72	0.43
1:B:2285:GLU:HB2	2:D:272:TRP:CZ3	2.54	0.43
1:A:1505:ASN:O	1:A:1509:GLN:HB2	2.19	0.43
1:A:2009:ALA:HA	1:A:2138:LEU:HD11	2.01	0.43
1:B:1943:ILE:HD13	1:B:1975:PRO:HB2	2.00	0.43
1:B:2322:ARG:O	1:B:2326:VAL:HG23	2.19	0.43
1:A:2129:LYS:O	1:A:2132:MET:HB3	2.19	0.42
1:A:2339:ARG:HH21	1:A:2343:ASN:HB3	1.83	0.42
1:B:1505:ASN:O	1:B:1509:GLN:HB2	2.19	0.42
1:B:2297:ASP:O	1:B:2299:LEU:N	2.52	0.42
1:A:1939:ILE:N	1:A:1940:PRO:HD2	2.35	0.42
1:A:2052:GLU:CG	1:A:2053:PRO:HD3	2.49	0.42
1:B:1717:MET:HG3	1:B:1754:LEU:HG	2.00	0.42
1:A:1418:SER:HB2	1:A:1581:GLU:CG	2.39	0.42
1:B:2157:ALA:HB3	1:B:2173:THR:HG23	2.02	0.42
1:B:2321:THR:HG23	1:B:2387:MET:HG2	2.01	0.42
2:D:28:GLN:HE21	2:D:31:SER:HG	1.66	0.42
2:D:258:LEU:HD22	2:D:297:TRP:CE3	2.53	0.42
1:A:1628:ARG:HB2	1:A:1633:TRP:CD1	2.55	0.42
1:A:1717:MET:CG	1:A:1754:LEU:HG	2.49	0.42
1:B:1913:TYR:O	1:B:1915:HIS:CG	2.72	0.42
2:C:231:ASP:HB3	2:C:233:THR:H	1.84	0.42
2:C:248:ARG:HG3	2:C:253:SER:OG	2.20	0.42
2:D:96:ASP:O	2:D:98:ARG:N	2.52	0.42
1:A:1727:GLN:O	1:A:1731:ALA:HB3	2.19	0.42
1:A:1777:SER:O	1:A:1781:GLU:HG2	2.20	0.42
1:A:1913:TYR:O	1:A:1915:HIS:CG	2.72	0.42
1:A:2362:PHE:O	1:A:2364:VAL:N	2.52	0.42
1:B:2249:LEU:HD13	1:B:2346:LEU:HD12	2.02	0.42
1:B:2397:ARG:NH2	1:B:2526:GLU:OE1	2.48	0.42
2:C:63:GLN:HE21	2:C:86:LYS:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:74:ASN:H	2:C:75:PRO:CD	2.32	0.42
2:D:231:ASP:HB3	2:D:233:THR:H	1.84	0.42
2:D:85:ASN:HD22	2:D:85:ASN:H	1.66	0.42
1:B:1608:VAL:HA	1:B:1609:PRO:HD3	1.89	0.42
2:C:82:ASP:HB2	2:C:119:LEU:HD13	2.00	0.42
2:C:74:ASN:H	2:C:75:PRO:HD3	1.84	0.42
1:A:1532:TYR:O	1:A:1536:ILE:HG13	2.20	0.42
1:A:1913:TYR:O	1:A:1915:HIS:HA	2.20	0.42
1:A:1564:ILE:HG23	1:A:1596:LEU:HD22	2.01	0.42
1:A:2130:LEU:HD22	1:A:2156:ILE:HD13	2.01	0.42
1:B:1631:GLU:CD	1:B:1631:GLU:H	2.23	0.42
1:B:1701:MET:HE1	1:B:1717:MET:HA	2.02	0.42
1:B:1722:GLN:HA	1:B:1725:GLN:NE2	2.35	0.42
1:B:1899:ASN:ND2	1:B:1937:GLN:HE22	2.18	0.42
2:D:74:ASN:H	2:D:75:PRO:CD	2.33	0.42
1:B:2319:ASN:HD22	1:B:2352:LYS:HG3	1.85	0.41
2:C:96:ASP:O	2:C:98:ARG:N	2.53	0.41
1:A:2064:THR:HG21	1:A:2126:VAL:O	2.21	0.41
1:A:2360:ASP:OD1	1:A:2360:ASP:N	2.54	0.41
1:B:2052:GLU:CG	1:B:2053:PRO:HD3	2.49	0.41
1:B:2223:GLN:HE22	1:B:2352:LYS:CB	2.28	0.41
1:A:1410:PRO:HA	1:A:1413:LEU:HB2	2.02	0.41
1:A:2319:ASN:ND2	1:A:2352:LYS:HE3	2.35	0.41
1:B:1680:ASP:HB3	1:B:1683:ARG:H	1.85	0.41
1:B:1941:GLN:HE22	1:B:2200:GLN:HE22	1.68	0.41
1:A:1470:ASN:HB3	1:A:1471:LYS:H	1.60	0.41
1:A:1680:ASP:HB3	1:A:1683:ARG:H	1.85	0.41
1:B:1410:PRO:HA	1:B:1413:LEU:HB2	2.02	0.41
1:B:1631:GLU:HA	1:B:1634:GLN:HE21	1.84	0.41
2:C:262:SER:OG	2:C:267:GLU:HG2	2.20	0.41
2:D:248:ARG:H	2:D:248:ARG:HG2	1.67	0.41
1:A:1895:SER:O	1:A:1896:ARG:C	2.59	0.41
1:A:2154:GLN:HE21	1:A:2155:SER:HB2	1.85	0.41
1:B:1938:VAL:O	1:B:1938:VAL:HG13	2.21	0.41
1:B:2362:PHE:O	1:B:2364:VAL:N	2.53	0.41
2:C:75:PRO:HB2	2:C:76:ASN:H	1.62	0.41
1:B:2281:MET:HE1	2:D:222:TYR:CG	2.56	0.41
2:D:31:SER:HG	2:D:33:ILE:HG13	1.86	0.41
1:A:2363:GLU:O	1:A:2365:ALA:N	2.53	0.41
1:B:2080:GLU:O	1:B:2083:GLU:HB3	2.21	0.41
1:B:2146:PRO:O	1:B:2147:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:195:TYR:CE2	2:C:215:LYS:HG3	2.56	0.41
1:A:1423:LEU:HD12	1:A:1423:LEU:HA	1.89	0.41
1:A:2093:ASN:HD22	1:A:2094:VAL:N	2.13	0.41
1:B:1892:ILE:CG2	1:B:1930:ILE:HD11	2.42	0.41
1:B:2496:LYS:HE3	1:B:2500:ILE:HD11	2.03	0.41
1:B:1670:HIS:HE1	1:B:1681:PRO:HB3	1.85	0.41
1:A:2285:GLU:HB2	2:C:272:TRP:CZ3	2.56	0.41
2:D:262:SER:OG	2:D:267:GLU:HG2	2.21	0.41
2:D:285:ILE:HG23	2:D:297:TRP:HB2	2.02	0.41
1:A:1427:GLU:HG2	1:A:1427:GLU:H	1.64	0.41
1:A:2423:TYR:CE1	1:A:2501:ILE:HD13	2.56	0.41
1:B:2178:ASN:ND2	1:B:2180:HIS:H	2.18	0.41
2:C:100:MET:HB3	2:C:112:TRP:HB2	2.03	0.41
1:A:1734:THR:C	1:A:1736:ASP:N	2.74	0.41
1:A:2254:ARG:HH22	1:A:2264:GLU:CD	2.24	0.41
1:B:1532:TYR:O	1:B:1536:ILE:HG13	2.20	0.41
1:B:1955:ARG:HE	1:B:1955:ARG:HB2	1.77	0.41
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.54	0.41
2:D:94:HIS:CE1	2:D:96:ASP:HB2	2.56	0.41
1:B:1759:LEU:HD21	1:B:1772:VAL:HG21	2.03	0.40
1:B:2154:GLN:HE21	1:B:2155:SER:HB2	1.86	0.40
2:C:202:GLY:HA3	2:C:208:THR:H	1.86	0.40
1:A:2252:ASP:O	1:A:2255:GLU:HG2	2.21	0.40
1:A:2408:ARG:O	1:A:2411:LYS:HG2	2.21	0.40
1:B:1777:SER:O	1:B:1781:GLU:HG2	2.22	0.40
1:B:2032:GLU:O	1:B:2036:ARG:HG2	2.19	0.40
1:B:2292:ASN:HB3	2:D:268:SER:HB2	2.02	0.40
1:A:1907:LEU:HD11	1:A:1938:VAL:CG1	2.51	0.40
1:A:2095:LYS:HA	1:A:2098:THR:HG22	2.03	0.40
1:A:2152:ARG:HG2	1:A:2177:SER:HB3	2.03	0.40
1:A:2378:ARG:HB2	1:A:2378:ARG:HE	1.67	0.40
1:A:2512:ASP:OD1	1:A:2512:ASP:N	2.49	0.40
1:B:2093:ASN:HD22	1:B:2094:VAL:N	2.14	0.40
1:B:1688:PRO:HB3	1:A:2270:ARG:NH2	2.37	0.40
1:B:2514:SER:OG	1:B:2517:ASP:HB2	2.21	0.40
2:C:131:ILE:HA	2:C:147:ASP:HA	2.03	0.40
1:B:2254:ARG:HH22	1:B:2264:GLU:CD	2.25	0.40
2:C:58:ALA:HA	2:C:67:MET:HG2	2.04	0.40
2:D:202:GLY:HA3	2:D:208:THR:H	1.86	0.40

All (5) 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]	1.45	0.75
1:A:1608:VAL:O	1:A:1608:VAL:O[2_554]	1.62	0.58
1:A:1607:LEU:CA	1:A:1609:PRO:O[2_554]	1.83	0.37
1:A:1606:LYS:C	1:A:1609:PRO:O[2_554]	1.99	0.21
1:A:1607:LEU:C	1:A:1609:PRO:O[2_554]	2.01	0.19

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1052/1174 (90%)	939 (89%)	84 (8%)	29 (3%)	5	32
1	B	1052/1174 (90%)	938 (89%)	85 (8%)	29 (3%)	5	32
2	C	315/326 (97%)	265 (84%)	32 (10%)	18 (6%)	1	16
2	D	315/326 (97%)	264 (84%)	33 (10%)	18 (6%)	1	16
All	All	2734/3000 (91%)	2406 (88%)	234 (9%)	94 (3%)	3	28

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1525	GLN
1	B	1611	ARG
1	B	1630	VAL
1	B	1650	MET
1	B	1734	THR
1	B	2298	ASP
1	B	2364	VAL
2	D	74	ASN
2	D	97	GLY
2	D	169	PRO
2	D	269	SER
1	A	1525	GLN
1	A	1611	ARG

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Mol	Chain	Res	Type
1	A	1630	VAL
1	A	1650	MET
1	A	1734	THR
1	A	1970	GLN
1	A	2298	ASP
1	A	2364	VAL
2	C	74	ASN
2	C	97	GLY
2	C	169	PRO
2	C	269	SER
1	B	1444	GLU
1	B	1445	ILE
1	B	1735	GLU
1	B	1896	ARG
1	B	1914	GLY
1	B	1970	GLN
1	B	2094	VAL
2	D	35	THR
2	D	54	ARG
2	D	73	ASN
2	D	75	PRO
2	D	160	ASP
2	D	203	ILE
1	A	1445	ILE
1	A	1735	GLU
1	A	1896	ARG
1	A	1914	GLY
1	A	2094	VAL
2	C	35	THR
2	C	73	ASN
2	C	75	PRO
2	C	167	PRO
2	C	203	ILE
1	B	1709	ARG
1	B	1917	PRO
2	D	118	ASN
2	D	167	PRO
1	A	1444	GLU
1	A	1784	ARG
1	A	1917	PRO
1	A	2363	GLU
2	C	54	ARG

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Mol	Chain	Res	Type
2	C	118	ASN
2	C	160	ASP
1	B	1583	TYR
1	B	1784	ARG
1	B	1786	TRP
1	B	1934	THR
1	B	2093	ASN
1	B	2363	GLU
1	A	1583	TYR
1	A	1709	ARG
1	A	1786	TRP
1	A	1934	THR
1	A	2093	ASN
1	B	1584	SER
2	D	129	ALA
1	A	1584	SER
2	C	129	ALA
1	B	1681	PRO
2	D	262	SER
1	A	1681	PRO
2	C	261	LYS
2	C	262	SER
1	B	1473	ASP
1	B	2040	GLY
2	D	263	GLY
1	A	1473	ASP
1	A	2040	GLY
2	C	263	GLY
1	B	1680	ASP
1	B	2391	GLY
2	D	204	GLY
2	D	310	GLY
2	C	204	GLY
1	A	1680	ASP
2	D	201	GLY
1	A	2391	GLY
2	C	310	GLY
1	B	2376	PRO
1	A	2376	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	931/1024 (91%)	855 (92%)	76 (8%)	11	40
1	B	931/1024 (91%)	856 (92%)	75 (8%)	11	41
2	C	269/276 (98%)	242 (90%)	27 (10%)	7	32
2	D	269/276 (98%)	241 (90%)	28 (10%)	7	31
All	All	2400/2600 (92%)	2194 (91%)	206 (9%)	10	38

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1417	ILE
1	B	1420	ASN
1	B	1423	LEU
1	B	1457	GLU
1	B	1501	TRP
1	B	1509	GLN
1	B	1540	THR
1	B	1541	HIS
1	B	1590	MET
1	B	1605	TYR
1	B	1611	ARG
1	B	1630	VAL
1	B	1685	LEU
1	B	1724	MET
1	B	1736	ASP
1	B	1746	LEU
1	B	1780	THR
1	B	1872	ASP
1	B	1896	ARG
1	B	1899	ASN
1	B	1912	ASP
1	B	1916	TRP
1	B	1932	ILE
1	B	1938	VAL

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Mol	Chain	Res	Type
1	B	1956	LEU
1	B	1973	ILE
1	B	1984	THR
1	B	2005	LEU
1	B	2011	MET
1	B	2068	THR
1	B	2072	GLN
1	B	2076	ARG
1	B	2077	ASP
1	B	2078	LEU
1	B	2090	LYS
1	B	2093	ASN
1	B	2095	LYS
1	B	2138	LEU
1	B	2152	ARG
1	B	2154	GLN
1	B	2164	THR
1	B	2167	GLN
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	2224	ARG
1	B	2228	ILE
1	B	2244	ASP
1	B	2254	ARG
1	B	2260	LEU
1	B	2262	ASN
1	B	2266	ARG
1	B	2281	MET
1	B	2297	ASP
1	B	2311	GLU
1	B	2360	ASP
1	B	2363	GLU
1	B	2378	ARG
1	B	2390	THR
1	B	2397	ARG
1	B	2401	HIS

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Mol	Chain	Res	Type
1	B	2408	ARG
1	B	2412	ASP
1	B	2430	ARG
1	B	2431	LEU
1	B	2432	MET
1	B	2501	ILE
1	B	2503	ARG
1	B	2515	HIS
1	B	2530	LYS
2	D	10	SER
2	D	13	VAL
2	D	44	GLN
2	D	74	ASN
2	D	79	ILE
2	D	85	ASN
2	D	90	SER
2	D	91	VAL
2	D	128	ASN
2	D	135	CYS
2	D	160	ASP
2	D	161	HIS
2	D	162	ASN
2	D	166	ILE
2	D	168	GLU
2	D	169	PRO
2	D	170	GLU
2	D	173	ILE
2	D	174	THR
2	D	183	SER
2	D	239	SER
2	D	248	ARG
2	D	259	SER
2	D	260	ILE
2	D	287	THR
2	D	289	SER
2	D	301	THR
2	D	304	ILE
1	A	1417	ILE
1	A	1420	ASN
1	A	1423	LEU
1	A	1457	GLU
1	A	1501	TRP

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Mol	Chain	Res	Type
1	A	1509	GLN
1	A	1540	THR
1	A	1541	HIS
1	A	1590	MET
1	A	1605	TYR
1	A	1611	ARG
1	A	1630	VAL
1	A	1685	LEU
1	A	1724	MET
1	A	1736	ASP
1	A	1746	LEU
1	A	1780	THR
1	A	1872	ASP
1	A	1896	ARG
1	A	1899	ASN
1	A	1912	ASP
1	A	1916	TRP
1	A	1932	ILE
1	A	1938	VAL
1	A	1956	LEU
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	2077	ASP
1	A	2078	LEU
1	A	2090	LYS
1	A	2093	ASN
1	A	2095	LYS
1	A	2124	GLN
1	A	2138	LEU
1	A	2152	ARG
1	A	2154	GLN
1	A	2164	THR
1	A	2167	GLN
1	A	2168	ARG
1	A	2173	THR
1	A	2178	ASN

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Mol	Chain	Res	Type
1	A	2181	GLU
1	A	2185	LEU
1	A	2189	HIS
1	A	2195	ASP
1	A	2214	THR
1	A	2224	ARG
1	A	2228	ILE
1	A	2244	ASP
1	A	2254	ARG
1	A	2260	LEU
1	A	2262	ASN
1	A	2266	ARG
1	A	2281	MET
1	A	2297	ASP
1	A	2311	GLU
1	A	2360	ASP
1	A	2363	GLU
1	A	2378	ARG
1	A	2390	THR
1	A	2397	ARG
1	A	2401	HIS
1	A	2408	ARG
1	A	2430	ARG
1	A	2431	LEU
1	A	2432	MET
1	A	2501	ILE
1	A	2503	ARG
1	A	2519	LEU
1	A	2530	LYS
2	C	10	SER
2	C	13	VAL
2	C	44	GLN
2	C	74	ASN
2	C	79	ILE
2	C	85	ASN
2	C	90	SER
2	C	91	VAL
2	C	128	ASN
2	C	135	CYS
2	C	160	ASP
2	C	161	HIS
2	C	162	ASN

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Mol	Chain	Res	Type
2	C	166	ILE
2	C	168	GLU
2	C	169	PRO
2	C	170	GLU
2	C	173	ILE
2	C	174	THR
2	C	239	SER
2	C	248	ARG
2	C	259	SER
2	C	260	ILE
2	C	287	THR
2	C	289	SER
2	C	301	THR
2	C	304	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1496	GLN
1	B	1594	HIS
1	B	1687	HIS
1	B	1695	GLN
1	B	1760	ASN
1	B	1782	HIS
1	B	1898	ASN
1	B	1899	ASN
1	B	1941	GLN
1	B	1958	HIS
1	B	1970	GLN
1	B	2028	HIS
1	B	2043	ASN
1	B	2082	GLN
1	B	2093	ASN
1	B	2154	GLN
1	B	2178	ASN
1	B	2189	HIS
1	B	2211	ASN
1	B	2223	GLN
1	B	2277	HIS
1	B	2319	ASN
1	B	2385	ASN
1	B	2395	ASN

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Mol	Chain	Res	Type
1	B	2410	HIS
1	B	2502	ASN
2	D	28	GLN
2	D	30	HIS
2	D	63	GLN
2	D	71	ASN
2	D	85	ASN
2	D	118	ASN
2	D	137	HIS
2	D	140	GLN
2	D	153	HIS
2	D	161	HIS
2	D	311	HIS
2	D	312	GLN
1	A	1496	GLN
1	A	1594	HIS
1	A	1670	HIS
1	A	1687	HIS
1	A	1695	GLN
1	A	1760	ASN
1	A	1782	HIS
1	A	1898	ASN
1	A	1899	ASN
1	A	1941	GLN
1	A	1958	HIS
1	A	1970	GLN
1	A	2028	HIS
1	A	2043	ASN
1	A	2082	GLN
1	A	2093	ASN
1	A	2154	GLN
1	A	2178	ASN
1	A	2189	HIS
1	A	2211	ASN
1	A	2223	GLN
1	A	2277	HIS
1	A	2319	ASN
1	A	2340	HIS
1	A	2385	ASN
1	A	2395	ASN
1	A	2410	HIS
1	A	2502	ASN

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Mol	Chain	Res	Type
2	C	28	GLN
2	C	30	HIS
2	C	44	GLN
2	C	63	GLN
2	C	71	ASN
2	C	85	ASN
2	C	118	ASN
2	C	137	HIS
2	C	140	GLN
2	C	153	HIS
2	C	161	HIS
2	C	311	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	ADP	A	2601	5,4	24,29,29	1.15	3 (12%)	29,45,45	1.20	3 (10%)
5	MGF	B	2604	3	0,3,3	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MGF	A	2604	3	0,3,3	0.00	-	-		
3	ADP	B	2601	5,4	24,29,29	1.13	3 (12%)	29,45,45	1.18	2 (6%)

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	ADP	A	2601	5,4	-	8/12/32/32	0/3/3/3
3	ADP	B	2601	5,4	-	2/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2601	ADP	O4'-C1'	2.95	1.45	1.41
3	A	2601	ADP	C5-C4	2.81	1.48	1.40
3	A	2601	ADP	O4'-C1'	2.73	1.44	1.41
3	B	2601	ADP	C5-C4	2.62	1.47	1.40
3	A	2601	ADP	C2-N3	2.26	1.35	1.32
3	B	2601	ADP	C2-N3	2.06	1.35	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2601	ADP	N3-C2-N1	-3.64	122.99	128.68
3	B	2601	ADP	N3-C2-N1	-3.26	123.59	128.68
3	B	2601	ADP	C4-C5-N7	-2.35	106.95	109.40
3	A	2601	ADP	C4-C5-N7	-2.19	107.11	109.40
3	A	2601	ADP	O3B-PB-O2B	2.08	115.57	107.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2601	ADP	C5'-O5'-PA-O1A
3	A	2601	ADP	O4'-C4'-C5'-O5'
3	A	2601	ADP	C3'-C4'-C5'-O5'
3	A	2601	ADP	C4'-C5'-O5'-PA
3	A	2601	ADP	C5'-O5'-PA-O3A

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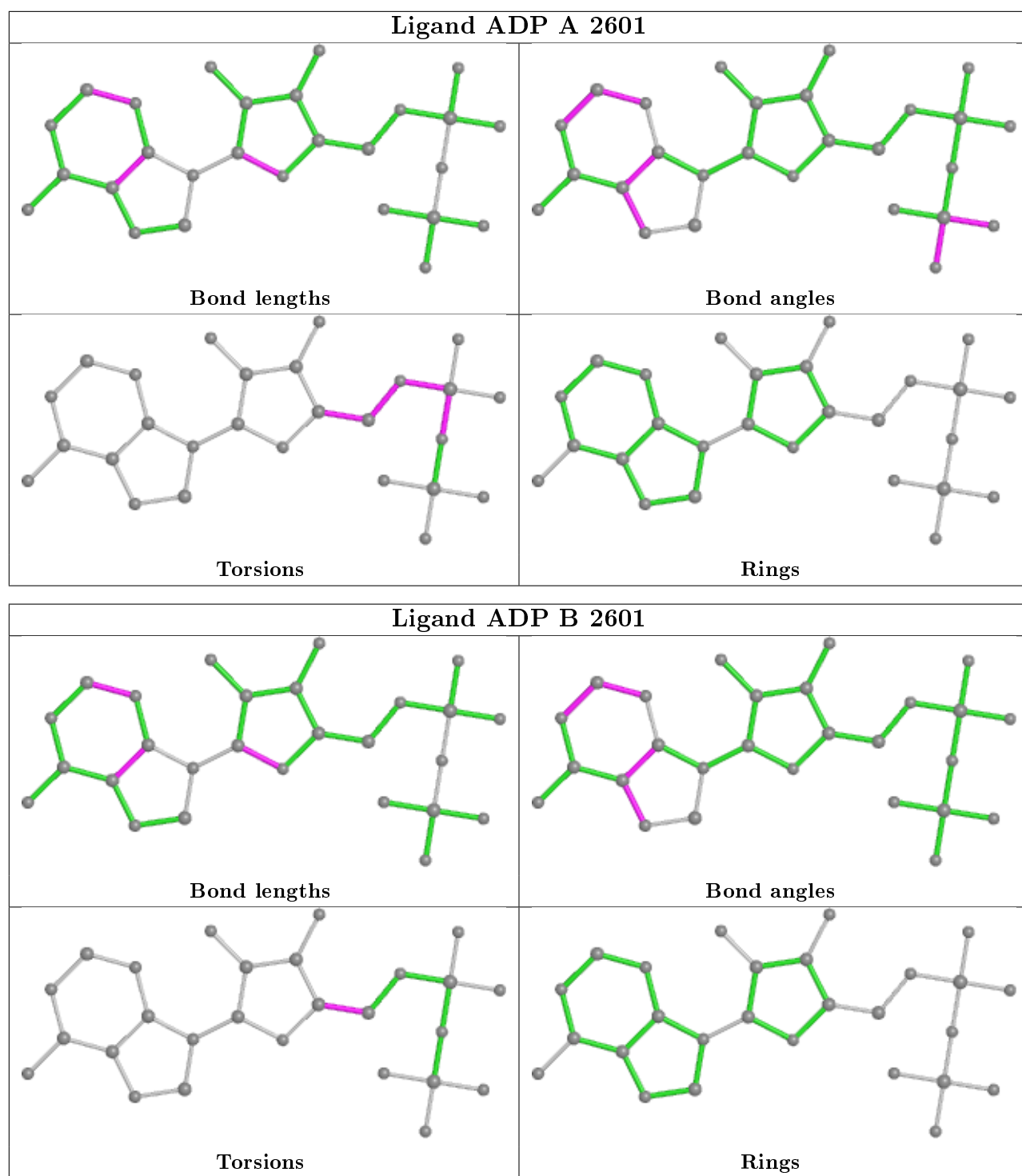
Mol	Chain	Res	Type	Atoms
3	B	2601	ADP	O4'-C4'-C5'-O5'
3	A	2601	ADP	PB-O3A-PA-O1A
3	A	2601	ADP	C5'-O5'-PA-O2A
3	B	2601	ADP	C3'-C4'-C5'-O5'
3	A	2601	ADP	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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%)	-0.18	15 (1%) 75 69	37, 70, 159, 271	0
1	B	1058/1174 (90%)	-0.27	13 (1%) 79 73	29, 59, 136, 174	0
2	C	317/326 (97%)	-0.09	0 100 100	39, 68, 116, 153	0
2	D	317/326 (97%)	-0.17	0 100 100	30, 46, 92, 130	0
All	All	2750/3000 (91%)	-0.20	28 (1%) 82 77	29, 62, 144, 271	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2436	THR	5.3
1	A	2436	THR	5.0
1	A	2435	ASN	4.7
1	A	1580	GLY	4.7
1	B	2435	ASN	4.1
1	B	1581	GLU	3.9
1	B	1580	GLY	3.7
1	B	1469	THR	2.9
1	A	1610	GLU	2.9
1	A	1578	MET	2.8
1	B	2434	THR	2.8
1	A	1599	LEU	2.7
1	B	1582	SER	2.6
1	A	1581	GLU	2.6
1	B	1578	MET	2.6
1	A	1579	ALA	2.4
1	A	2044	VAL	2.4
1	A	2097	LEU	2.3
1	B	1499	GLU	2.3
1	A	1469	THR	2.3
1	A	2434	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1385	GLU	2.2
1	B	1504	VAL	2.1
1	B	1607	LEU	2.1
1	B	2433	ASP	2.1
1	B	2432	MET	2.0
1	A	1731	ALA	2.0
1	A	1582	SER	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 carbohydrates in this entry.

6.4 Ligands [i](#)

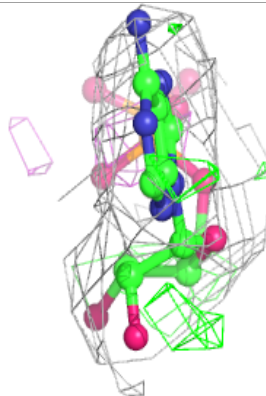
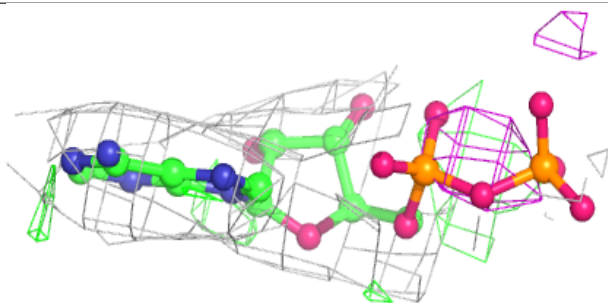
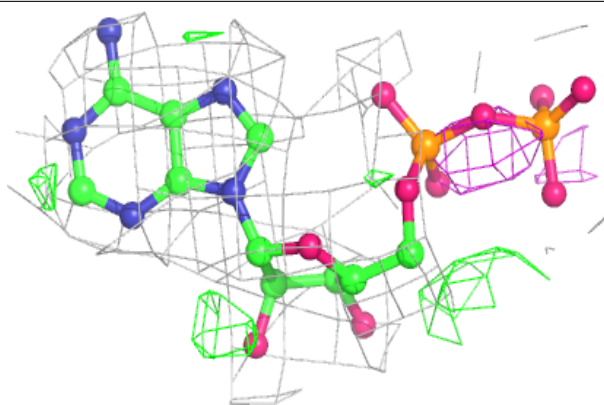
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MGF	A	2604	4/4	0.84	0.31	75,76,78,79	0
5	MGF	B	2604	4/4	0.89	0.20	57,59,59,60	0
3	ADP	A	2601	27/27	0.90	0.18	64,69,81,82	0
3	ADP	B	2601	27/27	0.93	0.15	50,54,62,62	0
4	MG	A	2603	1/1	0.93	0.15	72,72,72,72	0
4	MG	B	2602	1/1	0.93	0.10	57,57,57,57	0
4	MG	B	2603	1/1	0.94	0.15	57,57,57,57	0
4	MG	A	2602	1/1	0.95	0.07	74,74,74,74	0

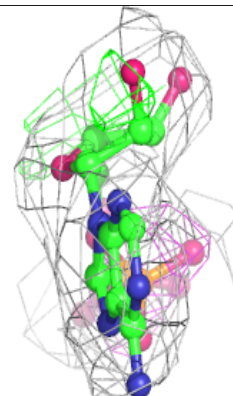
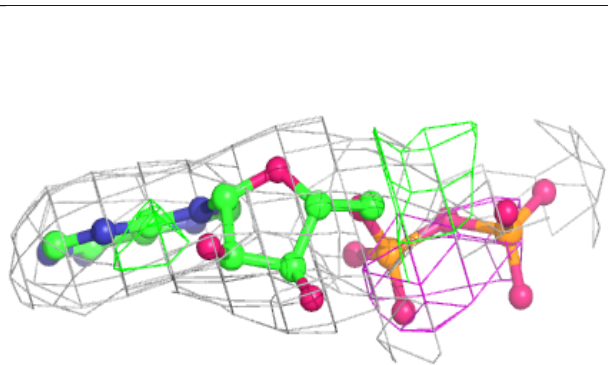
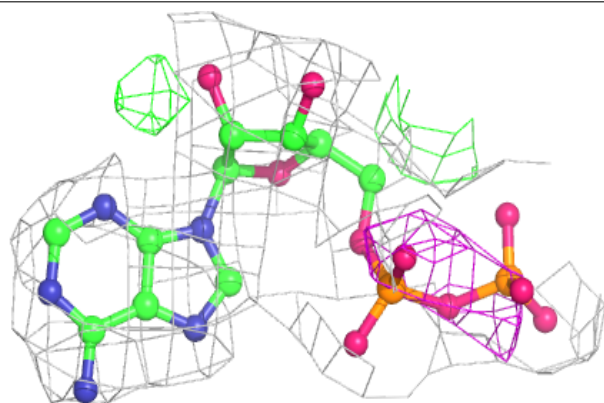
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP 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 ADP 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.