



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:54 PM GMT

PDB ID : 4JSP  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

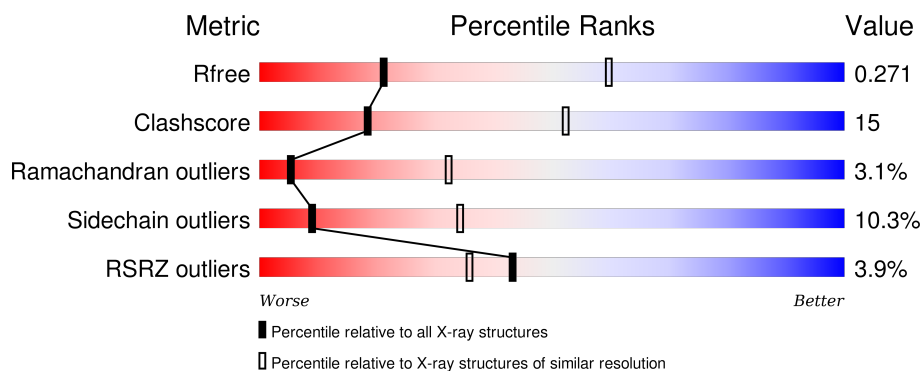
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>5%</div> <div>60% 26% • 10%</div> </div>
1	B	1174	<div> <div>3%</div> <div>60% 26% • 10%</div> </div>
2	C	326	<div> <div>2%</div> <div>53% 36% 7% • •</div> </div>
2	D	326	<div> <div>%</div> <div>51% 37% 8% • •</div> </div>

## 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.

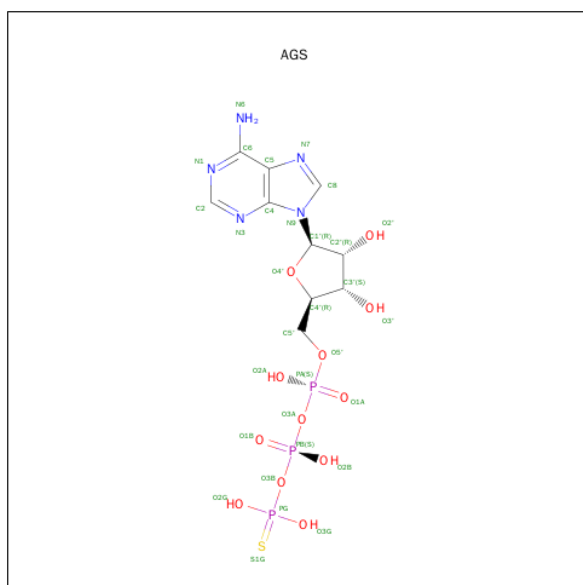
- Molecule 1 is a protein called Serine/threonine-protein kinase mTOR.

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 (three-letter code: 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		

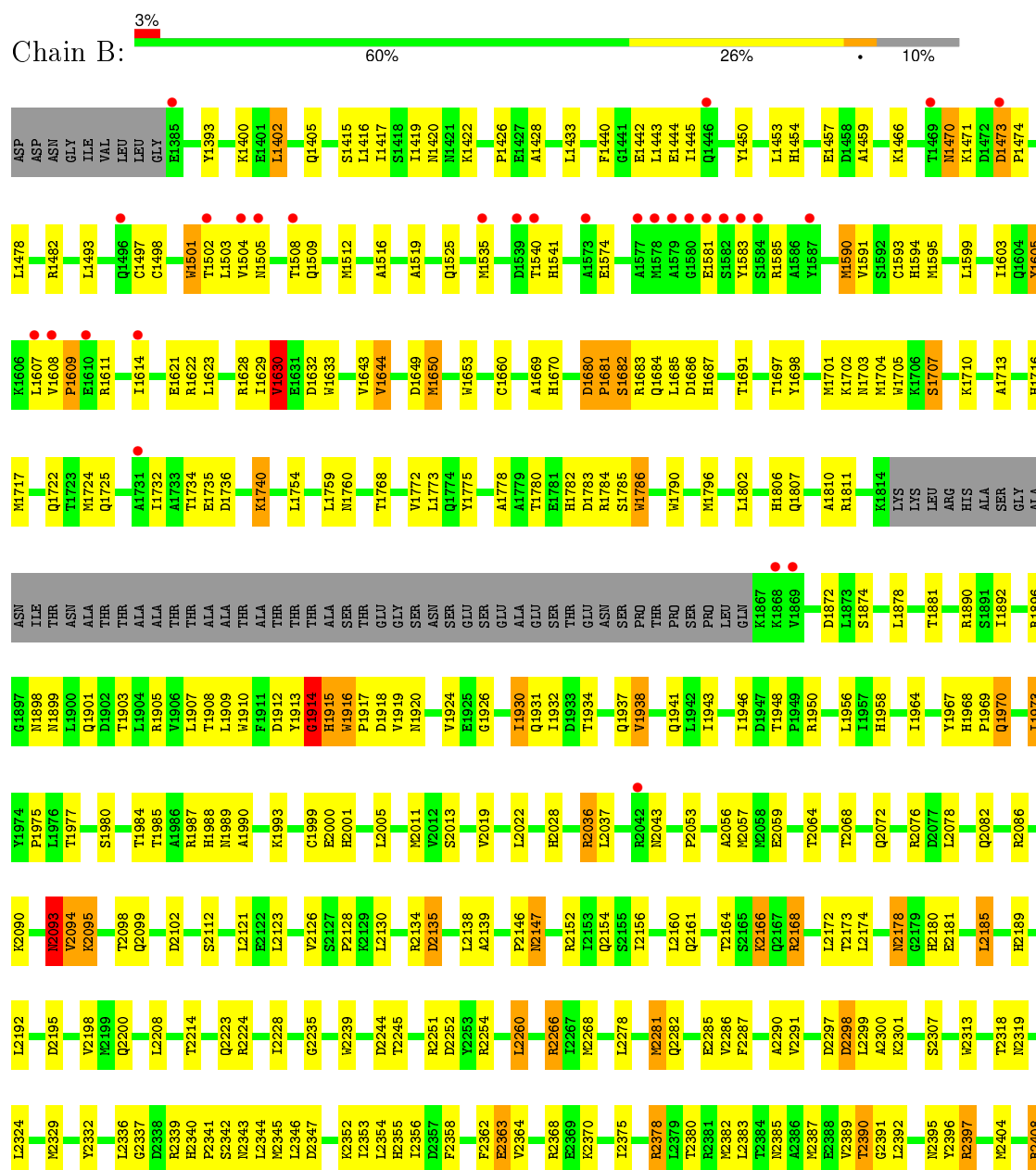
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

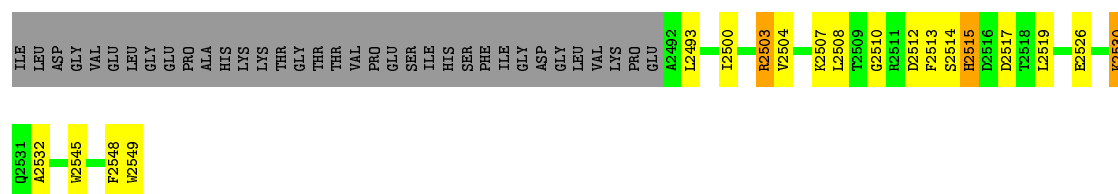
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

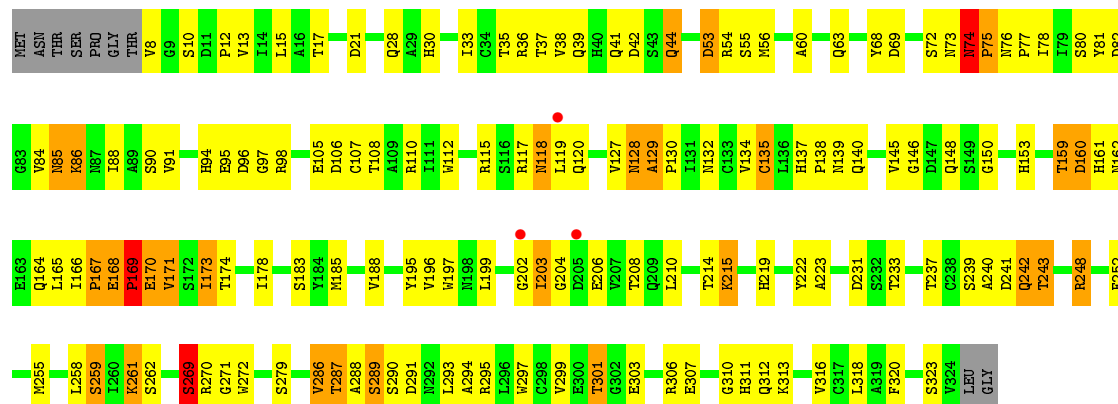
- Molecule 1: Serine/threonine-protein kinase mTOR



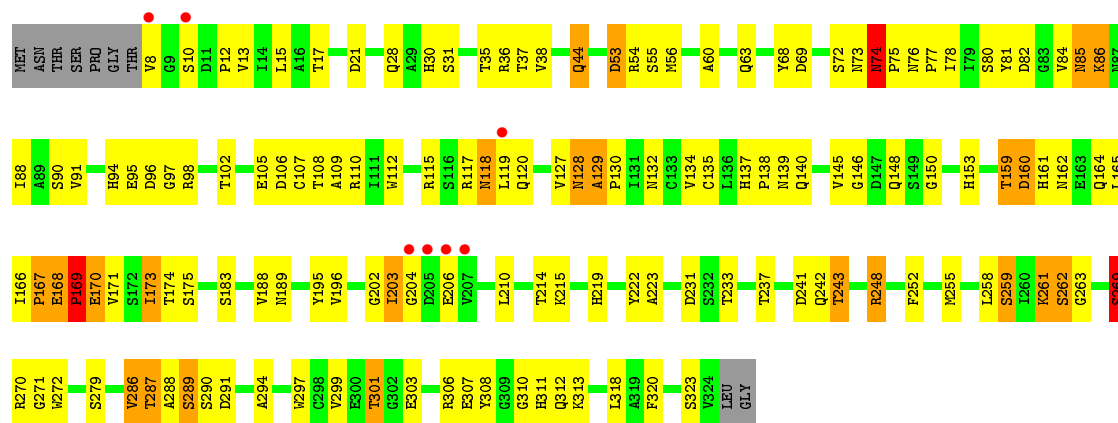




- Molecule 2: Target of rapamycin complex subunit LST8



- Molecule 2: Target of rapamycin complex subunit LST8



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.40 Å   163.20 Å   207.80 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	100.00 – 3.30 74.20 – 3.19	Depositor EDS
% Data completeness (in resolution range)	89.9 (100.00-3.30) 87.4 (74.20-3.19)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 3.19 Å)	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	1770 reflections (2.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.6	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 33.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	4 of 77327 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	22194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.35	0/8805	0.60	2/11920 (0.0%)
1	B	0.36	0/8805	0.60	1/11920 (0.0%)
2	C	0.38	0/2514	0.66	0/3426
2	D	0.43	0/2514	0.68	0/3426
All	All	0.37	0/22638	0.62	3/30692 (0.0%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1915	HIS	N-CA-C	5.96	127.09	111.00
1	B	1915	HIS	N-CA-C	5.88	126.89	111.00
1	A	1610	GLU	N-CA-C	5.77	126.58	111.00

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	237	6
1	B	8608	0	8593	233	0
2	C	2456	0	2341	110	0
2	D	2456	0	2341	119	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	22194	0	21892	683	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 15.

All (683) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:167:PRO:HD2	2:C:169:PRO:HG2	1.55	0.86
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: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:H8	3:B:3000:AGS:O2A	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
2:C:95:GLU:HB2	2:C:140:GLN:NE2	2.01	0.75
1:B:1704:MET:HG2	1:B:1713:ALA:HB2	1.67	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:C:69:ASP:HB2	2:C:78:ILE:HD11	1.71	0.72
2:D:95:GLU:HB2	2:D:140:GLN:NE2	2.04	0.72
3:A:3000:AGS:H8	3:A:3000:AGS:O2A	1.90	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
2:C:168:GLU:N	2:C:169:PRO:HD2	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:168:GLU:N	2:D:169:PRO:HD2	2.05	0.72
1:B:1941:GLN:HE22	1:B:2200:GLN:HE22	1.36	0.72
1:B:1901:GLN:HG3	1:B:2413:SER:HA	1.72	0.72
2:D:63:GLN:HE21	2:D:86:LYS:H	1.38	0.71
1:B:1778:ALA:O	1:B:1782:HIS:HD2	1.72	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:1701:MET:HE1	1:B:1717:MET:N	2.06	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: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
2:C:63:GLN:HE21	2:C:86:LYS:H	1.41	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:A:2281:MET:HE1	2:C:222:TYR:CD2	2.28	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:2022:LEU:HD21	1:A:2126:VAL:HG13	1.77	0.67
1:A:1913:TYR:HB2	1:A:1915:HIS:CE1	2.29	0.67
1:A:1778:ALA:O	1:A:1782:HIS:HD2	1.78	0.67
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.28	0.66
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1701:MET:HE1	1:A:1717:MET:N	2.10	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:B:2281:MET:HE1	2:D:222:TYR:CD2	2.30	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
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: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
2:C:107:CYS:HB3	2:C:127:VAL:O	1.95	0.65
2:C:17:THR:HB	2:C:311:HIS:HE1	1.62	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:2387:MET:HE1	1:A:2396:TYR:HB2	1.78	0.64
1:A:1926:GLY:O	1:A:1930:ILE:HG22	1.96	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: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:H	2.01	0.64
1:B:2390:THR:HG23	1:B:2390:THR:O	1.97	0.64
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
1:A:2382:MET:HG3	1:A:2549:TRP:O	1.97	0.63
2:D:279:SER:HA	2:D:320:PHE:CE2	2.34	0.63
1:B:1680:ASP:C	1:B:1682:SER:H	2.02	0.63
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
1:A:1680:ASP:C	1:A:1682:SER:N	2.53	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
2:C:36:ARG:NH2	2:C:69:ASP:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:2339:ARG:HH21	1:B:2343:ASN:HB3	1.64	0.62
1:B:1759:LEU:HG	1:B:1772:VAL:HG11	1.80	0.62
2:C:94:HIS:CD2	2:C:140:GLN:HB3	2.34	0.62
1:A:1703:ASN:O	1:A:1707:SER:HB2	1.99	0.62
2:C:279:SER:HA	2:C:320:PHE:CE2	2.35	0.62
1:B:1703:ASN:O	1:B:1707:SER:HB2	1.99	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
2:D:169:PRO:HA	2:D:171:VAL:H	1.64	0.62
1:B:2251:ARG:NH1	1:B:2252:ASP:OD1	2.32	0.62
2:C:118:ASN:HD22	2:C:120:GLN:HB2	1.64	0.62
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.32	0.62
1:B:1705:TRP:HZ2	1:B:1760:ASN:HD22	1.48	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
1:B:1680:ASP:C	1:B:1682:SER:N	2.53	0.61
2:D:94:HIS:CD2	2:D:140:GLN:HB3	2.35	0.61
1:B:1691:THR:HG22	1:B:1691:THR:O	2.00	0.61
1:B:2387:MET:HE1	1:B:2396:TYR:HB2	1.82	0.61
1:A:1913:TYR:O	1:A:1915:HIS:HA	2.00	0.61
1:B:1422:LYS:HE2	1:B:1581:GLU:CG	2.30	0.61
1:B:2380:THR:HG23	1:B:2549:TRP:O	2.01	0.60
1:B:2093:ASN:O	1:B:2094:VAL:HB	2.01	0.60
1:A:1583:TYR:C	1:A:1585:ARG:H	2.05	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
1:A:1734:THR:C	1:A:1736:ASP:H	2.04	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
1:A:2380:THR:HG23	1:A:2549:TRP:O	2.02	0.59
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
2:C:169:PRO:HA	2:C:171:VAL:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2390:THR:O	1:A:2390:THR:HG23	2.01	0.59
1:A:2339:ARG:HH21	1:A:2343:ASN:HB3	1.68	0.59
1:B:1583:TYR:C	1:B:1585:ARG:H	2.06	0.59
2:D:94:HIS:CE1	2:D:96:ASP:HB2	2.38	0.59
2:C:248:ARG:O	2:C:252:PHE:N	2.34	0.58
1:A:1691:THR:O	1:A:1691:THR:HG22	2.03	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
2:C:54:ARG:HD2	2:C:323:SER:HB2	1.85	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:D:137:HIS:CD2	2:D:138:PRO:HD2	2.38	0.58
1:B:1892:ILE:HD11	1:B:1903:THR:HA	1.85	0.58
2:C:21:ASP:HB3	2:C:313:LYS:H	1.68	0.58
1:A:2319:ASN:HB3	1:A:2352:LYS:HG2	1.85	0.58
1:A:2298:ASP:HB2	1:A:2382:MET:CE	2.33	0.58
1:B:2281:MET:HE1	2:D:222:TYR:CG	2.38	0.58
1:B:2514:SER:OG	1:B:2517:ASP:HB2	2.04	0.58
2:D:168:GLU:HB3	2:D:195:TYR:OH	2.04	0.58
2:D:105:GLU:HA	2:D:130:PRO:HB3	1.85	0.58
2:D:128:ASN:O	2:D:129:ALA:HB3	2.03	0.58
1:B:1497:CYS:SG	1:B:1516:ALA:HB2	2.44	0.58
1:B:2298:ASP:HB2	1:B:2382:MET:HE2	1.85	0.58
1:A:1907:LEU:HD11	1:A:1938:VAL:CG1	2.34	0.58
1:B:2287:PHE:O	1:B:2291:VAL:HG23	2.04	0.58
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
2:D:21:ASP:HB3	2:D:313:LYS:H	1.69	0.57
1:A:2515:HIS:N	1:A:2515:HIS:ND1	2.53	0.57
2:D:94:HIS:HD2	2:D:140:GLN:HB3	1.70	0.57
1:B:1680:ASP:O	1:B:1682:SER:N	2.30	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:N	1:B:2515:HIS:ND1	2.53	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
1:A:2387:MET:HE1	1:A:2396:TYR:CB	2.35	0.56
2:C:132:ASN:HD21	2:C:148:GLN:HG2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:137:HIS:CD2	2:C:139:ASN:H	2.22	0.56
2:D:137:HIS:CD2	2:D: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
2:C:128:ASN:O	2:C:129:ALA:HB3	2.05	0.55
1:A:2037:LEU:HD22	1:A:2043:ASN:HD22	1.71	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: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
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
2:D:106:ASP:OD1	2:D:108:THR:OG1	2.18	0.55
1:B:2056:ALA:HA	1:B:2059:GLU:HB2	1.88	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:A:2503:ARG:HH11	1:A:2507:LYS:CE	2.02	0.55
1:A:2408:ARG:HG2	1:A:2508:LEU:O	2.06	0.55
1:B:2146:PRO:O	1:B:2147:ASN:HB2	2.07	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
2:C:269:SER:OG	2:C:270:ARG:N	2.41	0.54
2:C:117:ARG:O	2:C:118:ASN:CB	2.55	0.54
2:D:117:ARG:O	2:D:118:ASN:CB	2.55	0.54
1:B:2095:LYS:O	1:B:2099:GLN:HG2	2.07	0.54
2:D:82:ASP:HB2	2:D:119:LEU:HD13	1.90	0.54
1:B:2282:GLN:HE21	2:D:316:VAL:HG11	1.72	0.54
1:B:1428:ALA:HB2	1:B:2395:ASN:HD21	1.72	0.54
1:A:2178:ASN:HD22	1:A:2180:HIS:H	1.56	0.54
1:A:1508:THR:O	1:A:1512:MET:HB2	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:96:ASP:O	2:C:98:ARG:N	2.37	0.53
2:D:96:ASP:O	2:D:98:ARG:N	2.38	0.53
1:B:1402:LEU:O	1:B:1405:GLN:HB2	2.08	0.53
1:A:1422:LYS:HE2	1:A:1581:GLU:HG3	1.90	0.53
1:B:1623:LEU:HG	1:B:1633:TRP:CZ3	2.43	0.53
2:C:195:TYR:CE2	2:C:215:LYS:HG3	2.43	0.53
1:A:1754:LEU:HD13	1:A:1775:TYR:CE2	2.43	0.53
1:B:2387:MET:HE1	1:B:2396:TYR:CB	2.38	0.53
1:A:1590:MET:O	1:A:1594:HIS:HB2	2.09	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
1:A:1393:TYR:CZ	1:A:1422:LYS:HD2	2.44	0.53
1:A:2281:MET:HE1	2:C:222:TYR:CG	2.44	0.52
1:B:2530:LYS:HA	1:B:2530:LYS:CE	2.39	0.52
1:B:1508:THR:O	1:B:1512:MET:HB2	2.09	0.52
2:D:127:VAL:HG11	2:D:153:HIS:CE1	2.44	0.52
1:A:1698:TYR:O	1:A:1702:LYS:HG2	2.09	0.52
1:B:2178:ASN:HD22	1:B:2180:HIS:H	1.57	0.52
1:B:1807:GLN:O	1:B:1810:ALA:HB3	2.08	0.52
2:D:269:SER:OG	2:D:270:ARG:N	2.43	0.52
1:A:2056:ALA:HA	1:A:2059:GLU:HB2	1.90	0.52
1:B:1913:TYR:CB	1:B:1915:HIS:CE1	2.92	0.52
1:B:1590:MET:O	1:B:1594:HIS:HB2	2.10	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
2:C:168:GLU:HB3	2:C:195:TYR:OH	2.10	0.52
1:A:1913:TYR:CB	1:A:1915:HIS:CE1	2.92	0.52
2:C:259:SER:HB2	2:C:261:LYS:HE3	1.92	0.52
2:C:38:VAL:HG11	2:C:68:TYR:CD2	2.44	0.52
1:A:2130:LEU:HD22	1:A:2156:ILE:HD13	1.91	0.52
2:D:72:SER:O	2:D:74:ASN:N	2.42	0.52
1:B:1698:TYR:O	1:B:1702:LYS:HG2	2.10	0.52
1:A:1701:MET:HE1	1:A:1716:HIS:C	2.30	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:A:1915:HIS:HE1	1:A:1919:VAL:HG11	1.75	0.51
1:B:1943:ILE:O	1:B:1987:ARG:NH2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1611:ARG:HG2	1:B:1614:ILE:HD12	1.93	0.51
1:A:1422:LYS:HG2	1:A:1580:GLY:C	2.31	0.51
1:B:1701:MET:HE1	1:B:1716:HIS:C	2.30	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:2337:GLY:O	1:B:2339:ARG:NH1	2.44	0.51
2:C:72:SER:O	2:C:74:ASN:N	2.43	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:D:76:ASN:CB	2:D:77:PRO:HD2	2.30	0.51
1:B:1938:VAL:O	1:B:1938:VAL:CG1	2.59	0.51
1:B:1643:VAL:HG12	1:B:1644:VAL:HG22	1.92	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:2530:LYS:CE	1:A:2530:LYS:HA	2.41	0.50
1:A:1698:TYR:CE2	1:A:1702:LYS:HD3	2.47	0.50
2:C:127:VAL:HG11	2:C:153:HIS:CE1	2.47	0.50
1:B:1660:CYS:HB2	1:B:1669:ALA:HB2	1.92	0.50
2:C:255:MET:HE1	2:C:299:VAL:HG12	1.93	0.50
1:B:2428:ASN:HB3	1:B:2493:LEU:HD13	1.94	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:C:271:GLY:HA2	2:C:290:SER:HB2	1.93	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
2:C:168:GLU:N	2:C:169:PRO:CD	2.73	0.50
1:B:1393:TYR:CZ	1:B:1422:LYS:HD2	2.47	0.50
2:D:248:ARG:O	2:D:252:PHE:N	2.43	0.49
2:C:196:VAL:HG11	2:C:252:PHE:CZ	2.47	0.49
2:D:255:MET:HE1	2:D:299:VAL:HG12	1.94	0.49
1:A:1908:THR:O	1:A:1912:ASP:HB2	2.12	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: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:B:1686:ASP:O	1:A:2266:ARG:HG3	2.12	0.49
1:A:2298:ASP:HB2	1:A:2382:MET:HE1	1.94	0.49
1:B:2421:PHE:CD1	1:B:2430:ARG:NH2	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:53:ASP:HB2	2:C:55:SER:OG	2.12	0.49
1:B:1930:ILE:HD11	1:B:1934:THR:HG21	1.95	0.49
1:B:1621:GLU:C	1:B:1623:LEU:H	2.15	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
2:C:94:HIS:CE1	2:C:96:ASP:HB2	2.48	0.49
1:A:1913:TYR:O	1:A:1915:HIS:CG	2.65	0.49
2:C:219:HIS:NE2	2:C:237:THR:CG2	2.76	0.49
1:B:2130:LEU:HD22	1:B:2156:ILE:HD13	1.94	0.49
1:A:1621:GLU:C	1:A:1623:LEU:H	2.15	0.49
2:C:134:VAL:HG22	2:C:145:VAL:HG22	1.94	0.49
1:A:1466:LYS:O	1:A:1470:ASN:HB2	2.12	0.49
2:D:168:GLU:N	2:D:169:PRO:CD	2.74	0.49
1:B:2319:ASN:HB3	1:B:2352:LYS:HG2	1.94	0.49
1:A:1878:LEU:HD21	1:A:1918:ASP:CB	2.42	0.49
1:B:1930:ILE:HG12	1:B:1931:GLN:N	2.28	0.49
2:D:231:ASP:CB	2:D:233:THR:OG1	2.50	0.48
1:A:2298:ASP:HB2	1:A:2382:MET:HE2	1.94	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
2:C:95:GLU:HB2	2:C:140:GLN:HE21	1.73	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
1:B:1938:VAL:O	1:B:1938:VAL:HG13	2.13	0.48
2:C:98:ARG:HD2	2:C:115:ARG:HB2	1.96	0.48
2:D:306:ARG:HG2	2:D:307:GLU:H	1.78	0.48
2:D:41:GLN:O	2:D:42:ASP:HB2	2.13	0.48
1:A:1530:GLU:HA	1:A:1550:LEU:HD11	1.95	0.48
1:B:1393:TYR:O	1:B:1419:ILE:HD11	2.13	0.48
1:B:1734:THR:C	1:B:1736:ASP:H	2.13	0.48
1:B:1943:ILE:O	1:B:1946:ILE:HG13	2.14	0.48
1:B:2512:ASP:N	1:B:2512:ASP:OD1	2.36	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
2:D:202:GLY:O	2:D:203:ILE:O	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1970:GLN:NE2	1:A:2139:ALA:H	2.12	0.48
1:B:2281:MET:HA	1:B:2281:MET:CE	2.44	0.48
1:B:1649:ASP:HB2	1:B:1653:TRP:CD1	2.49	0.48
1:A:2421:PHE:CD1	1:A:2430:ARG:NH2	2.73	0.47
2:D:98:ARG:HD2	2:D:115:ARG:HB2	1.96	0.47
1:B:2208:LEU:HD22	1:B:2410:HIS:CG	2.49	0.47
1:A:2019:VAL:HG22	1:A:2126:VAL:HG12	1.96	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: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
1:B:1754:LEU:HD13	1:B:1775:TYR:CE2	2.49	0.47
2:D:134:VAL:HG22	2:D:145:VAL:HG22	1.95	0.47
1:B:1908:THR:O	1:B:1912:ASP:HB2	2.14	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
2:D:167:PRO:HD2	2:D:169:PRO:CG	2.33	0.47
1:A:2297:ASP:O	1:A:2300:ALA:N	2.48	0.47
1:B:1705:TRP:HZ2	1:B:1760:ASN:ND2	2.10	0.47
1:A:1943:ILE:O	1:A:1946:ILE:HG13	2.15	0.47
1:A:2408:ARG:NH2	1:A:2510:GLY:HA3	2.30	0.47
1:B:1684:GLN:HB3	1:B:1687:HIS:CD2	2.50	0.47
1:A:1428:ALA:HB2	1:A:2395:ASN:ND2	2.30	0.47
2:D:69:ASP:CB	2:D:78:ILE:HD11	2.38	0.47
1:A:2130:LEU:HD22	1:A:2156:ILE:CD1	2.45	0.47
1:B:2166:LYS:O	1:B:2166:LYS:HE2	2.15	0.47
1:A:1498:CYS:HA	1:A:1501:TRP:HD1	1.80	0.47
1:B:1498:CYS:HA	1:B:1501:TRP:HD1	1.79	0.47
1:A:1660:CYS:HB2	1:A:1669:ALA:HB2	1.97	0.47
1:B:2036:ARG:HD3	1:B:2036:ARG:HA	1.70	0.47
1:A:1791:HIS:O	1:A:1795:VAL:HG23	2.15	0.47
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:A:2281:MET:CE	2:C:222:TYR:CD2	2.98	0.46
1:A:1670:HIS:HE1	1:A:1681:PRO:CB	2.27	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:165:LEU:HD23	2:D:210:LEU:HD12	1.97	0.46
1:B:1970:GLN:NE2	1:B:2139:ALA:H	2.12	0.46
1:A:1938:VAL:O	1:A:1938:VAL:CG1	2.63	0.46
2:C:159:THR:HB	2:C:161:HIS:HB2	1.96	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:B:1705:TRP:CE3	1:B:1710:LYS:HB2	2.51	0.46
1:A:1440:PHE:HB3	1:A:1442:GLU:HB2	1.97	0.46
1:B:1943:ILE:HD13	1:B:1975:PRO:HB2	1.98	0.46
1:B:1607:LEU:O	1:B:1609:PRO:HD3	2.15	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:1881:THR:HG23	1:B:1909:LEU:HD22	1.98	0.46
1:B:2513:PHE:HB2	1:B:2519:LEU:HD11	1.98	0.46
1:B:2245:THR:HA	1:B:2345:MET:HB3	1.96	0.46
2:C:28:GLN:O	2:C:28:GLN:HG3	2.16	0.46
1:A:1490:TRP:CE3	1:A:1519:ALA:HA	2.50	0.46
2:D:86:LYS:HE2	2:D:105:GLU:HB3	1.97	0.46
1:A:2339:ARG:HD3	1:A:2355:HIS:CE1	2.51	0.46
1:B:2208:LEU:HD22	1:B:2410:HIS:CD2	2.51	0.46
1:B:1501:TRP:HA	1:B:1503:LEU:HG	1.98	0.46
1:A:2345:MET:HG3	1:A:2354:LEU:HD23	1.98	0.46
1:A:1505:ASN:HB2	1:A:1508:THR:HB	1.97	0.46
2:C:287:THR:O	2:C:294:ALA:HA	2.16	0.46
1:A:2028:HIS:HE1	1:A:2112:SER:OG	1.99	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:1958:HIS:CE1	1:B:1990:ALA:HB1	2.51	0.46
1:A:1595:MET:HG2	1:A:1639:VAL:HG21	1.97	0.45
1:A:1973:ILE:HG13	1:A:1973:ILE:H	1.57	0.45
1:B:1915:HIS:HE1	1:B:1919:VAL:HG11	1.81	0.45
2:C:86:LYS:HE2	2:C:105:GLU:HB3	1.97	0.45
2:D:159:THR:C	2:D:161:HIS:H	2.20	0.45
1:A:1473:ASP:HA	1:A:1474:PRO:HD2	1.83	0.45
1:B:2028:HIS:HE1	1:B:2112:SER:OG	1.99	0.45
1:B:2329:MET:SD	1:B:2404:MET:HE2	2.55	0.45
1:A:1943:ILE:HD13	1:A:1975:PRO:HB2	1.98	0.45
1:A:1594:HIS:HE1	1:A:1622:ARG:HD2	1.81	0.45
2:C:159:THR:C	2:C:161:HIS:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2375:ILE:HA	1:B:2375:ILE:HD13	1.74	0.45
2:C:82:ASP:HB2	2:C:119:LEU:HD13	1.99	0.45
2:D:288:ALA:HB2	2:D:318:LEU:HG	1.98	0.45
1:B:1784:ARG:O	1:B:1790:TRP:NE1	2.39	0.45
1:B:1722:GLN:HA	1:B:1725:GLN:NE2	2.30	0.45
1:B:1478:LEU:O	1:B:1482:ARG:HG3	2.16	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
1:B:1473:ASP:HA	1:B:1474:PRO:HD2	1.83	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:1400:LYS:HG3	1:B:1416:LEU:HD13	1.99	0.45
2:D:169:PRO:CA	2:D:171:VAL:H	2.30	0.45
2:D:86:LYS:HB2	2:D:105:GLU:HB2	1.97	0.45
1:B:1710:LYS:NZ	1:B:1760:ASN:HD21	2.14	0.45
1:A:1977:THR:HG21	1:A:2013:SER:OG	2.17	0.45
1:B:1907:LEU:HD11	1:B:1938:VAL:HG13	1.99	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:A:1915:HIS:CE1	1:A:1919:VAL:HG11	2.52	0.45
1:A:1432:VAL:HG22	1:A:2390:THR:HG21	1.98	0.45
1:B:1705:TRP:CZ2	1:B:1760:ASN:ND2	2.81	0.45
1:A:1938:VAL:O	1:A:1938:VAL:HG13	2.16	0.45
1:B:1973:ILE:HG13	1:B:1973:ILE:H	1.60	0.45
2:D:195:TYR:CE2	2:D:215:LYS:HG3	2.52	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
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
2:D:242:GLN:NE2	2:D:261:LYS:HB3	2.33	0.44
1:B:1643:VAL:HG12	1:B:1644:VAL:CG2	2.47	0.44
1:B:1913:TYR:O	1:B:1915:HIS:ND1	2.50	0.44
1:A:2260:LEU:HD12	1:A:2261:LEU:N	2.33	0.44
1:A:2260:LEU:HD21	1:A:2266:ARG:NH1	2.32	0.44
1:A:1629:ILE:HG22	1:A:1630:VAL:HG23	2.00	0.44
2:D:271:GLY:HA2	2:D:290:SER:HB2	1.99	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
2:C:169:PRO:CA	2:C:171:VAL:H	2.31	0.44
2:C:21:ASP:HB3	2:C:313:LYS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2430:ARG:H	1:A:2430:ARG:HG3	1.71	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:B:2345:MET:HG3	1:B:2354:LEU:HD23	1.99	0.44
1:A:2245:THR:HA	1:A:2345:MET:HB3	1.99	0.44
1:B:2297:ASP:O	1:B:2300:ALA:N	2.51	0.44
1:B:2198:VAL:HG11	1:B:2358:PHE:CD2	2.53	0.44
1:B:1759:LEU:HD11	1:B:1796:MET:HE3	2.00	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:1910:TRP:HD1	1:B:1910:TRP:O	2.01	0.43
1:B:2130:LEU:HD22	1:B:2156:ILE:CD1	2.49	0.43
1:A:1681:PRO:HG2	1:A:1683:ARG:HE	1.84	0.43
1:B:1802:LEU:HD22	1:B:1806:HIS:NE2	2.33	0.43
1:B:2019:VAL:HG22	1:B:2126:VAL:HG12	1.99	0.43
1:A:2095:LYS:HA	1:A:2098:THR:HG22	1.99	0.43
2:D:82:ASP:H	2:D:119:LEU:HD22	1.84	0.43
2:D:81:TYR:CD2	2:D:112:TRP:CE3	3.07	0.43
1:A:2036:ARG:HA	1:A:2036:ARG:HD3	1.71	0.43
1:B:1670:HIS:HE1	1:B:1681:PRO:HB3	1.82	0.43
1:A:2324:LEU:HA	1:A:2353:ILE:HG21	2.01	0.43
1:A:2146:PRO:O	1:A:2147:ASN:CB	2.66	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
2:C:168:GLU:HB3	2:C:195:TYR:HH	1.84	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:1999:CYS:C	1:A:2001:HIS:H	2.22	0.43
1:B:2307:SER:CB	1:B:2313:TRP:HB2	2.49	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:2285:GLU:HB2	2:C:272:TRP:CZ3	2.54	0.43
2:D:270:ARG:HA	2:D:270:ARG:HD2	1.76	0.43
2:C:203:ILE:HA	2:C:206:GLU:HG2	2.01	0.43
1:B:2168:ARG:CZ	1:B:2168:ARG:HB2	2.48	0.43
1:A:1705:TRP:CE3	1:A:1710:LYS:HB2	2.54	0.43
1:A:1705:TRP:HZ2	1:A:1760:ASN:ND2	2.10	0.43
1:A:1916:TRP:HA	1:A:1917:PRO:HD2	1.73	0.43
1:B:2297:ASP:O	1:B:2298:ASP:C	2.57	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:1605:TYR:CG	1:B:1643:VAL:HG11	2.54	0.42
2:D:68:TYR:CE2	2:D:77:PRO:HD3	2.54	0.42
1:B:1773:LEU:HG	1:B:1796:MET:HG3	2.01	0.42
1:A:2270:ARG:O	2:C:313:LYS:NZ	2.43	0.42
1:B:2093:ASN:HB3	1:B:2094:VAL:H	1.62	0.42
1:B:1505:ASN:HB2	1:B:1508:THR:HB	2.00	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
2:D:95:GLU:HB2	2:D:140:GLN:HE22	1.83	0.42
1:A:2168:ARG:HB2	1:A:2168:ARG:CZ	2.49	0.42
1:B:1914:GLY:HA3	1:B:1950:ARG:HE	1.84	0.42
1:A:2297:ASP:O	1:A:2298:ASP:C	2.57	0.42
1:A:1691:THR:HG23	1:A:1724:MET:HE1	2.02	0.42
1:A:2340:HIS:HB2	1:A:2341:PRO:CD	2.49	0.42
1:A:1722:GLN:HA	1:A:1725:GLN:NE2	2.34	0.42
2:C:262:SER:HB2	2:C:263:GLY:H	1.56	0.42
1:B:1905:ARG:HD3	1:B:1905:ARG:HA	1.75	0.42
1:A:2281:MET:CE	2:C:222:TYR:CE2	3.03	0.42
1:B:2340:HIS:HB2	1:B:2341:PRO:CD	2.49	0.42
1:B:1440:PHE:HB3	1:B:1442:GLU:HB2	2.00	0.42
2:D:287:THR:O	2:D:294:ALA:HA	2.19	0.42
2:D:44:GLN:HG3	2:D:44:GLN:H	1.42	0.42
2:C:17:THR:HB	2:C:311:HIS:CE1	2.47	0.42
1:B:2095:LYS:HA	1:B:2098:THR:HG22	2.00	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
2:C:82:ASP:H	2:C:119:LEU:HD22	1.85	0.42
1:B:1433:LEU:HD23	1:B:1453:LEU:CD2	2.50	0.42
1:A:2187:LYS:HD2	1:A:2237:ILE:CD1	2.50	0.42
2:D:17:THR:HB	2:D:311:HIS:CE1	2.47	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:A:1495:GLN:O	1:A:1499:GLU:HB2	2.20	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:1393:TYR:CE2	1:A:1422:LYS:HD2	2.55	0.42
2:D:15:LEU:HD11	2:D:286:VAL:HG11	2.02	0.42
1:B:1943:ILE:HG12	1:B:1946:ILE:HD11	2.02	0.42
1:A:1726:GLN:HA	1:A:1729:GLN:HG2	2.01	0.42
1:B:1591:VAL:HG21	1:B:1632:ASP:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2134:ARG:O	1:A:2135:ASP:C	2.58	0.42
1:B:1938:VAL:HG22	1:B:1941:GLN:HE21	1.85	0.42
1:B:1778:ALA:O	1:B:1782:HIS:CD2	2.62	0.42
1:B:2336:LEU:HG	1:B:2339:ARG:HH11	1.85	0.42
2:C:294:ALA:HB3	2:C:308:TYR:HB2	2.02	0.42
2:D:135:CYS:SG	2:D:178:ILE:HG22	2.60	0.42
1:A:1762:GLN:HB2	1:A:1768:THR:HG21	2.01	0.42
1:A:1618:ILE:H	1:A:1618:ILE:HG13	1.73	0.42
1:A:1502:THR:HG22	1:A:1504:VAL:HG23	2.01	0.42
2:C:86:LYS:HB2	2:C:105:GLU:HB2	2.00	0.41
1:A:1552:LEU:HD22	1:A:1602:VAL:HG12	2.02	0.41
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:2160:LEU:HD22	1:A:2172:LEU:HA	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:A:1734:THR:C	1:A:1736:ASP:N	2.71	0.41
1:A:1943:ILE:HG12	1:A:1946:ILE:HD11	2.02	0.41
2:C:159:THR:C	2:C:161:HIS:N	2.72	0.41
1:A:2380:THR:HG22	1:A:2383:LEU:CG	2.49	0.41
1:A:1583:TYR:C	1:A:1585:ARG:N	2.72	0.41
2:C:255:MET:CE	2:C:299:VAL:HG12	2.50	0.41
1:B:2260:LEU:HD21	1:B:2266:ARG:NH1	2.35	0.41
1:A:2344:LEU:CD1	1:A:2353:ILE:HD11	2.44	0.41
1:B:1629:ILE:O	1:B:1630:VAL:C	2.59	0.41
2:C:28:GLN:OE1	2:C:30:HIS:CE1	2.73	0.41
1:A:1905:ARG:HA	1:A:1905:ARG:HD3	1.77	0.41
2:C:168:GLU:OE1	2:C:189:ASN:ND2	2.52	0.41
1:B:2380:THR:CG2	1:B:2383:LEU:HG	2.48	0.41
2:C:28:GLN:NE2	2:C:31:SER:OG	2.54	0.41
2:D:159:THR:C	2:D:161:HIS:N	2.72	0.41
1:B:1910:TRP:C	1:B:1910:TRP:CD1	2.94	0.41
1:A:1881:THR:HG23	1:A:1909:LEU:HD22	2.02	0.41
1:B:2268:MET:HG3	1:B:2290:ALA:HB2	2.01	0.41
1:A:1914:GLY:HA3	1:A:1950:ARG:HE	1.85	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:A:1910:TRP:O	1:A:1910:TRP:HD1	2.04	0.41
2:C:102:THR:O	2:C:109:ALA:HA	2.20	0.41
2:D:75:PRO:HB2	2:D:76:ASN:H	1.63	0.41
1:B:2297:ASP:O	1:B:2299:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2339:ARG:HD3	1:B:2355:HIS:CE1	2.55	0.41
1:B:1583:TYR:C	1:B:1585:ARG:N	2.73	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:B:2307:SER:OG	1:B:2313:TRP:HB2	2.21	0.41
1:B:1948:THR:HG22	1:B:1950:ARG:H	1.86	0.41
2:D:28:GLN:HE21	2:D:33:ILE:HD12	1.85	0.41
1:B:1977:THR:HG21	1:B:2013:SER:OG	2.21	0.41
1:A:2268:MET:HG3	1:A:2290:ALA:HB2	2.02	0.41
1:B:1999:CYS:C	1:B:2001:HIS:H	2.24	0.41
2:C:85:ASN:H	2:C:85:ASN:ND2	2.19	0.41
2:D:188:VAL:HG13	2:D:223:ALA:CB	2.48	0.41
1:A:1892:ILE:HG21	1:A:1930:ILE:HD11	2.03	0.41
1:A:2339:ARG:NH2	1:A:2356:ILE:O	2.53	0.41
2:D:68:TYR:HE2	2:D:77:PRO:HD3	1.86	0.41
1:A:1874:SER:O	1:A:1878:LEU:HB2	2.21	0.41
1:B:1874:SER:O	1:B:1878:LEU:HB2	2.21	0.41
1:A:1807:GLN:O	1:A:1811:ARG:HG2	2.21	0.41
2:D:255:MET:CE	2:D:299:VAL:HG12	2.50	0.41
2:D:39:GLN:HB3	2:D:41:GLN:NE2	2.36	0.41
2:D:165:LEU:HD11	2:D:197:TRP:CH2	2.56	0.41
1:A:1488:GLY:HA3	1:A:1634:GLN:OE1	2.21	0.41
1:B:2160:LEU:HD22	1:B:2172:LEU:HA	2.02	0.41
2:C:81:TYR:CD2	2:C:112:TRP:CE3	3.09	0.41
1:A:2500:ILE:O	1:A:2504:VAL:HG23	2.20	0.41
1:B:2332:TYR:CZ	1:B:2507:LYS:HD3	2.56	0.41
2:C:270:ARG:HD2	2:C:270:ARG:HA	1.77	0.41
1:B:2268:MET:HG2	1:B:2286:VAL:HG12	2.03	0.41
1:A:2363:GLU:OE1	1:A:2363:GLU:HA	2.21	0.40
1:B:1691:THR:HG23	1:B:1724:MET:HE1	2.02	0.40
1:B:1681:PRO:HG2	1:B:1683:ARG:HE	1.86	0.40
1:B:1502:THR:HG22	1:B:1504:VAL:HG23	2.03	0.40
1:A:2053:PRO:O	1:A:2057:MET:HB2	2.21	0.40
1:B:2363:GLU:OE1	1:B:2363:GLU:HA	2.21	0.40
2:C:98:ARG:O	2:C:98:ARG:HG3	2.20	0.40
2:D:239:SER:OG	2:D:240:ALA:N	2.54	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:1497:CYS:SG	1:B:1516:ALA:CB	3.09	0.40
1:B:1470:ASN:HB3	1:B:1471:LYS:H	1.59	0.40
2:D:28:GLN:O	2:D:28:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1910:TRP:CD1	1:A:1910:TRP:C	2.95	0.40
1:A:1895:SER:HB2	1:A:1899:ASN:HB3	2.02	0.40
1:A:2329:MET:SD	1:A:2404:MET:HE2	2.61	0.40
1:A:1423:LEU:HA	1:A:1423:LEU:HD12	1.96	0.40
1:B:2134:ARG:O	1:B:2135:ASP:C	2.60	0.40
2:D:185:MET:HB2	2:D:199:LEU:HD21	2.03	0.40
1:B:2298:ASP:HB2	1:B:2382:MET:HE1	2.00	0.40
1:A:1710:LYS:NZ	1:A:1760:ASN:HD21	2.19	0.40
2:C:86:LYS:CB	2:C:105:GLU:HB2	2.51	0.40
1:B:1574:GLU:HG2	1:B:1585:ARG:HH22	1.86	0.40
1:A:1691:THR:CG2	1:A:1691:THR:O	2.70	0.40
1:A:2166:LYS:O	1:A:2166:LYS:HE2	2.21	0.40
1:B:2121:LEU:HA	1:B:2121:LEU:HD23	1.88	0.40
1:A:2408:ARG:CG	1:A:2508:LEU:O	2.67	0.40
1:B:1732:ILE:HD13	1:B:1740:LYS:HB2	2.02	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%)	6 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1052/1174 (90%)	940 (89%)	84 (8%)	28 (3%)	6	35
2	C	315/326 (97%)	270 (86%)	31 (10%)	14 (4%)	3	22
2	D	315/326 (97%)	273 (87%)	27 (9%)	15 (5%)	3	20
All	All	2734/3000 (91%)	2421 (89%)	227 (8%)	86 (3%)	5	32

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%)	848 (91%)	83 (9%)	12	43
1	B	931/1024 (91%)	845 (91%)	86 (9%)	11	40
2	C	269/276 (98%)	230 (86%)	39 (14%)	4	18
2	D	269/276 (98%)	229 (85%)	40 (15%)	4	17
All	All	2400/2600 (92%)	2152 (90%)	248 (10%)	9	34

All (248) 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	1443	LEU
1	B	1457	GLU
1	B	1501	TRP
1	B	1509	GLN
1	B	1535	MET
1	B	1540	THR
1	B	1541	HIS

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Mol	Chain	Res	Type
1	B	1590	MET
1	B	1593	CYS
1	B	1603	ILE
1	B	1605	TYR
1	B	1608	VAL
1	B	1630	VAL
1	B	1644	VAL
1	B	1650	MET
1	B	1685	LEU
1	B	1740	LYS
1	B	1768	THR
1	B	1780	THR
1	B	1872	ASP
1	B	1890	ARG
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	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	2036	ARG
1	B	2068	THR
1	B	2072	GLN
1	B	2076	ARG
1	B	2078	LEU
1	B	2090	LYS
1	B	2093	ASN
1	B	2095	LYS
1	B	2102	ASP
1	B	2123	LEU
1	B	2138	LEU
1	B	2152	ARG
1	B	2154	GLN
1	B	2161	GLN

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Mol	Chain	Res	Type
1	B	2164	THR
1	B	2166	LYS
1	B	2168	ARG
1	B	2173	THR
1	B	2178	ASN
1	B	2181	GLU
1	B	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	2260	LEU
1	B	2266	ARG
1	B	2281	MET
1	B	2301	LYS
1	B	2318	THR
1	B	2342	SER
1	B	2347	ASP
1	B	2363	GLU
1	B	2378	ARG
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	2530	LYS
1	B	2548	PHE
2	D	10	SER
2	D	13	VAL
2	D	37	THR
2	D	44	GLN
2	D	53	ASP
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	135	CYS
2	D	159	THR
2	D	160	ASP
2	D	162	ASN
2	D	164	GLN
2	D	166	ILE
2	D	168	GLU
2	D	169	PRO
2	D	170	GLU
2	D	171	VAL
2	D	173	ILE
2	D	174	THR
2	D	183	SER
2	D	214	THR
2	D	215	LYS
2	D	242	GLN
2	D	243	THR
2	D	248	ARG
2	D	259	SER
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	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
1	A	1590	MET
1	A	1593	CYS

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Mol	Chain	Res	Type
1	A	1603	ILE
1	A	1605	TYR
1	A	1608	VAL
1	A	1630	VAL
1	A	1644	VAL
1	A	1650	MET
1	A	1680	ASP
1	A	1685	LEU
1	A	1740	LYS
1	A	1768	THR
1	A	1780	THR
1	A	1872	ASP
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	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	2036	ARG
1	A	2068	THR
1	A	2072	GLN
1	A	2076	ARG
1	A	2078	LEU
1	A	2090	LYS
1	A	2093	ASN
1	A	2095	LYS
1	A	2102	ASP
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	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	2301	LYS
1	A	2342	SER
1	A	2347	ASP
1	A	2363	GLU
1	A	2378	ARG
1	A	2385	ASN
1	A	2390	THR
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	2530	LYS
1	A	2548	PHE
2	C	10	SER
2	C	13	VAL
2	C	37	THR
2	C	44	GLN
2	C	53	ASP
2	C	74	ASN
2	C	80	SER
2	C	84	VAL
2	C	85	ASN
2	C	86	LYS
2	C	90	SER

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Mol	Chain	Res	Type
2	C	91	VAL
2	C	128	ASN
2	C	135	CYS
2	C	159	THR
2	C	160	ASP
2	C	162	ASN
2	C	164	GLN
2	C	166	ILE
2	C	168	GLU
2	C	169	PRO
2	C	170	GLU
2	C	173	ILE
2	C	174	THR
2	C	175	SER
2	C	183	SER
2	C	214	THR
2	C	242	GLN
2	C	243	THR
2	C	248	ARG
2	C	259	SER
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1594	HIS
1	B	1670	HIS
1	B	1687	HIS
1	B	1695	GLN
1	B	1730	HIS
1	B	1760	ASN
1	B	1782	HIS
1	B	1898	ASN
1	B	1941	GLN
1	B	1970	GLN

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Mol	Chain	Res	Type
1	B	2003	ASN
1	B	2028	HIS
1	B	2082	GLN
1	B	2093	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	2502	ASN
2	D	22	HIS
2	D	30	HIS
2	D	40	HIS
2	D	41	GLN
2	D	63	GLN
2	D	85	ASN
2	D	94	HIS
2	D	118	ASN
2	D	128	ASN
2	D	132	ASN
2	D	137	HIS
2	D	140	GLN
2	D	153	HIS
2	D	161	HIS
2	D	198	ASN
2	D	242	GLN
2	D	311	HIS
2	D	312	GLN
1	A	1594	HIS
1	A	1670	HIS
1	A	1687	HIS
1	A	1695	GLN
1	A	1719	HIS
1	A	1760	ASN
1	A	1782	HIS
1	A	1898	ASN
1	A	1941	GLN
1	A	1970	GLN
1	A	2001	HIS

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Mol	Chain	Res	Type
1	A	2003	ASN
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
2	C	22	HIS
2	C	30	HIS
2	C	40	HIS
2	C	41	GLN
2	C	63	GLN
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	161	HIS
2	C	198	ASN
2	C	242	GLN
2	C	311	HIS
2	C	312	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	A	3000	4	24,33,33	2.30	3 (12%)	28,52,52	2.21	5 (17%)
3	AGS	B	3000	4	24,33,33	2.33	4 (16%)	28,52,52	1.95	5 (17%)

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	A	3000	4	-	0/15/38/38	0/3/3/3
3	AGS	B	3000	4	-	0/15/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3000	AGS	O4'-C1'	2.23	1.44	1.41
3	B	3000	AGS	PG-O2G	2.25	1.63	1.55
3	A	3000	AGS	PG-O2G	2.27	1.63	1.55
3	A	3000	AGS	C5-C4	2.96	1.47	1.40
3	B	3000	AGS	C5-C4	3.02	1.47	1.40
3	B	3000	AGS	PG-S1G	9.93	2.09	1.90
3	A	3000	AGS	PG-S1G	9.97	2.09	1.90

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3000	AGS	N3-C2-N1	-7.78	122.94	128.89
3	B	3000	AGS	N3-C2-N1	-7.09	123.46	128.89
3	A	3000	AGS	PA-O3A-PB	-4.95	118.84	132.73
3	A	3000	AGS	PB-O3B-PG	-3.56	120.73	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3000	AGS	PA-O3A-PB	-3.23	123.66	132.73
3	A	3000	AGS	C4-C5-N7	-3.18	106.55	109.48
3	B	3000	AGS	C2'-C1'-N9	-3.00	109.70	114.29
3	B	3000	AGS	PB-O3B-PG	-2.76	123.40	132.67
3	B	3000	AGS	C4-C5-N7	-2.31	107.36	109.48
3	A	3000	AGS	C2'-C1'-N9	-2.01	111.23	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1058/1174 (90%)	0.21	62 (5%) 26 20	30, 64, 156, 230	0
1	B	1058/1174 (90%)	0.11	35 (3%) 50 43	25, 54, 134, 177	0
2	C	317/326 (97%)	0.08	7 (2%) 65 59	36, 63, 113, 157	0
2	D	317/326 (97%)	-0.01	3 (0%) 85 82	27, 43, 94, 127	0
All	All	2750/3000 (91%)	0.13	107 (3%) 43 36	25, 57, 143, 230	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1580	GLY	6.8
1	A	1599	LEU	6.5
1	B	2433	ASP	5.9
1	A	1385	GLU	5.8
1	B	2434	THR	5.6
1	B	1581	GLU	5.1
1	B	1582	SER	4.9
1	A	1581	GLU	4.9
1	A	1469	THR	4.8
1	A	1603	ILE	4.7
1	A	1579	ALA	4.5
1	A	1596	LEU	4.4
1	A	1558	SER	4.3
1	A	1610	GLU	4.3
1	B	1607	LEU	4.3
1	A	2436	THR	4.2
1	A	2435	ASN	4.1
2	C	205	ASP	3.8
1	A	1619	TRP	3.8
2	C	119	LEU	3.8
1	B	1504	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	2433	ASP	3.8
1	B	1577	ALA	3.8
1	B	2436	THR	3.7
1	B	1385	GLU	3.7
1	A	1606	LYS	3.6
1	A	1642	LEU	3.5
1	A	2434	THR	3.5
1	A	2044	VAL	3.4
1	A	1468	ASP	3.4
1	A	1582	SER	3.4
1	B	1573	ALA	3.4
1	B	1578	MET	3.3
1	B	1496	GLN	3.3
1	B	1731	ALA	3.3
1	B	1508	THR	3.2
1	B	1608	VAL	3.2
1	B	1587	TYR	3.1
1	B	2435	ASN	3.1
1	B	2432	MET	3.1
1	A	2090	LYS	3.1
1	A	1608	VAL	3.0
1	B	1868	LYS	3.0
1	A	1578	MET	3.0
2	C	207	VAL	2.9
1	A	2431	LEU	2.9
1	B	1583	TYR	2.9
1	A	2038	TYR	2.9
1	A	1604	GLN	2.8
1	A	2428	ASN	2.8
1	A	1595	MET	2.8
2	C	10	SER	2.8
1	A	1868	LYS	2.8
1	B	1540	THR	2.7
2	D	202	GLY	2.7
1	A	1504	VAL	2.7
1	A	1586	ALA	2.7
1	B	1469	THR	2.6
1	B	1580	GLY	2.6
1	B	1579	ALA	2.5
1	A	2049	GLU	2.5
1	A	1730	HIS	2.5
1	B	1614	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1386	ARG	2.5
1	A	1570	LEU	2.5
1	B	1446	GLN	2.5
1	B	2042	ARG	2.4
1	A	1600	GLU	2.4
1	A	1614	ILE	2.4
1	A	2089	MET	2.4
2	C	8	VAL	2.4
1	A	1620	TRP	2.4
1	B	1584	SER	2.4
1	B	1869	VAL	2.4
1	A	1584	SER	2.4
1	A	1587	TYR	2.4
1	A	2037	LEU	2.4
1	A	2045	LYS	2.3
1	A	1418	SER	2.3
1	A	1549	VAL	2.3
1	A	1607	LEU	2.3
1	A	1731	ALA	2.3
1	A	1559	LEU	2.3
1	A	1528	SER	2.3
2	C	204	GLY	2.3
1	A	1583	TYR	2.2
2	D	205	ASP	2.2
1	A	1653	TRP	2.2
1	B	1473	ASP	2.2
2	C	206	GLU	2.1
1	A	1509	GLN	2.1
1	B	1505	ASN	2.1
1	A	2432	MET	2.1
1	A	1615	ILE	2.1
1	A	1496	GLN	2.1
1	B	1610	GLU	2.1
1	B	1535	MET	2.1
1	A	1444	GLU	2.1
1	A	1527	ASP	2.1
1	A	1563	CYS	2.0
1	B	1502	THR	2.0
1	A	2097	LEU	2.0
1	A	1564	ILE	2.0
1	B	1539	ASP	2.0
1	A	1546	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1573	ALA	2.0
2	D	119	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	AGS	B	3000	31/31	0.92	0.21	-0.25	50,56,79,84	0
3	AGS	A	3000	31/31	0.92	0.19	-1.01	51,60,81,85	0
4	MG	A	3002	1/1	0.82	0.21	-	72,72,72,72	0
4	MG	B	3001	1/1	0.87	0.25	-	63,63,63,63	0
4	MG	B	3002	1/1	0.88	0.10	-	69,69,69,69	0
4	MG	A	3001	1/1	0.91	0.16	-	66,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.