Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:53 PM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

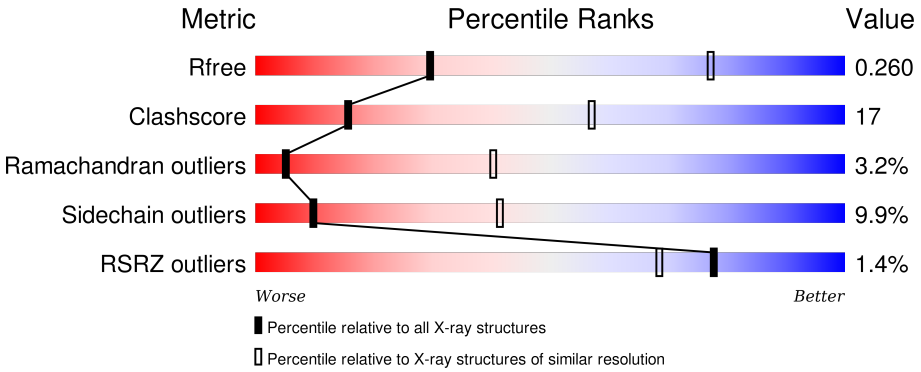
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (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. 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 <=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	2% 57% 28% • • 10%
1	B	1174	% 58% 28% • • 10%
2	C	326	% 51% 38% 7% • •
2	D	326	51% 37% 8% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22160 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

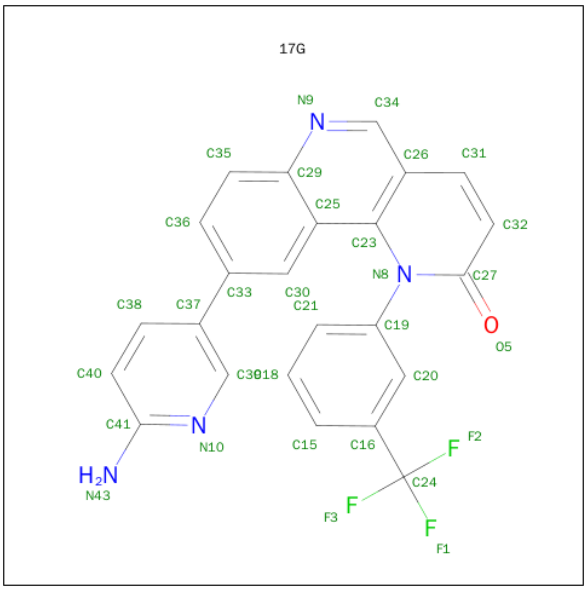
- Molecule 1 is a protein called Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1058	Total	C	N	O	S	0	0	0
			8607	5472	1520	1552	63			
1	A	1054	Total	C	N	O	S	0	0	0
			8577	5451	1517	1546	63			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	317	Total	C	N	O	S	0	0	0
			2456	1526	436	476	18			
2	C	317	Total	C	N	O	S	0	0	0
			2456	1526	436	476	18			

- Molecule 3 is 9-(6-AMINOPYRIDIN-3-YL)-1-[3-(TRIFLUOROMETHYL)PHENYL]BENZO[H][1,6]NAPHTHYRIDIN-2(1H)-ONE (three-letter code: 17G) (formula: $C_{24}H_{15}F_3N_4O$).



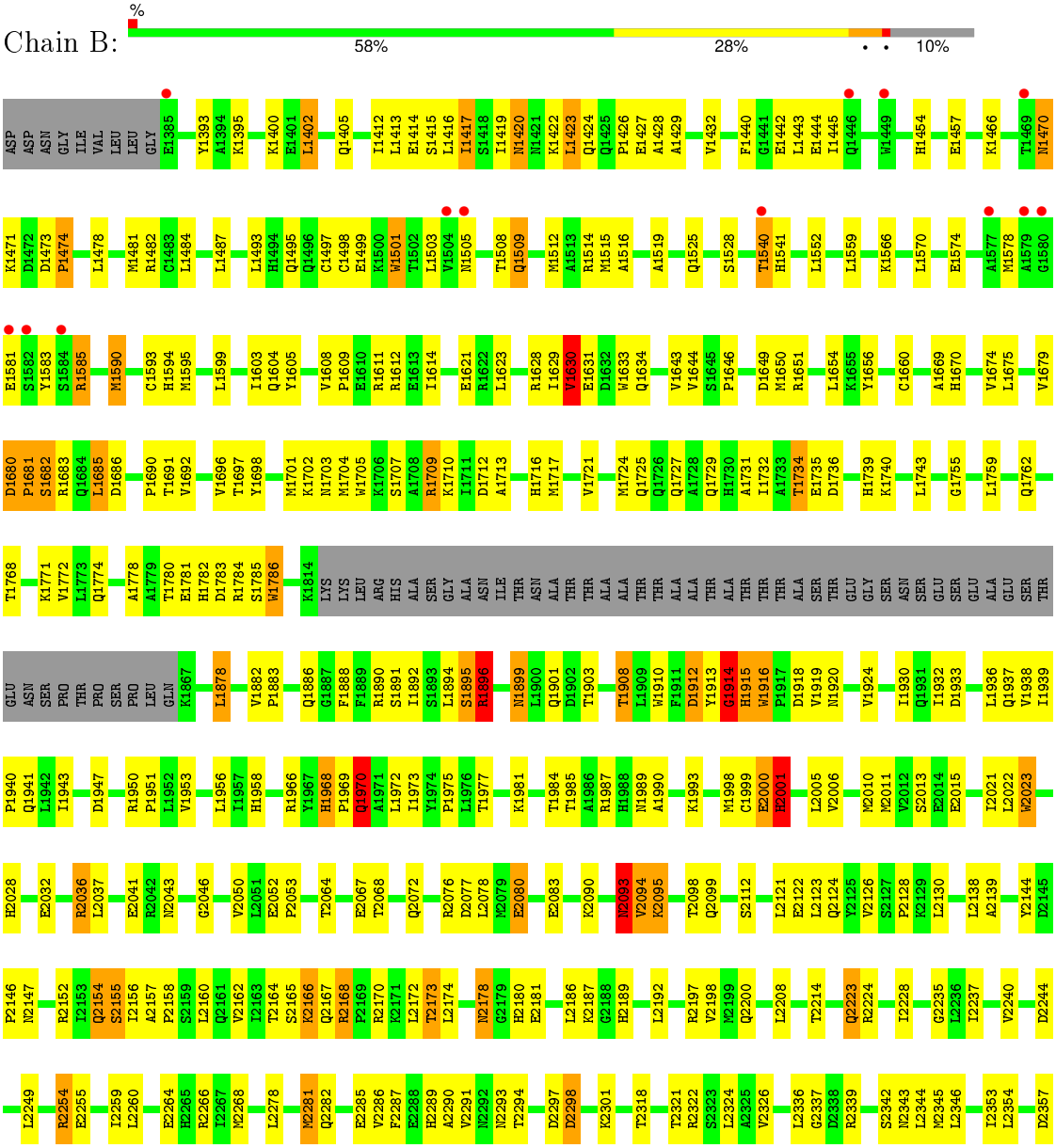
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			32	24	3	4	1		
3	A	1	Total	C	F	N	O	0	0
			32	24	3	4	1		

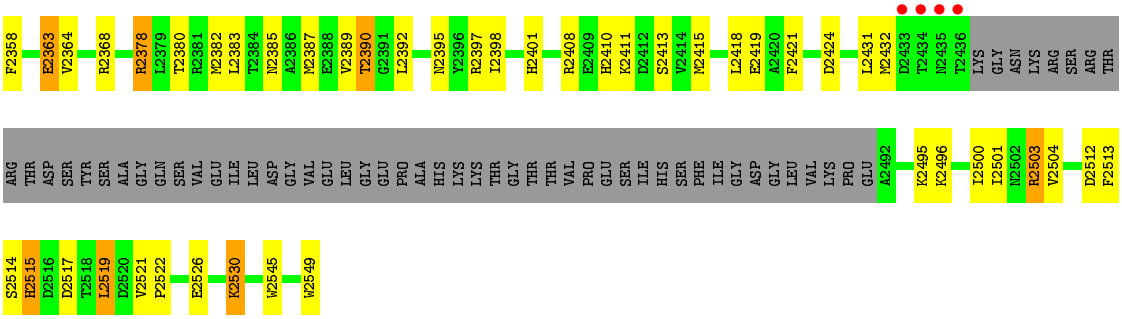
3 Residue-property plots (i)

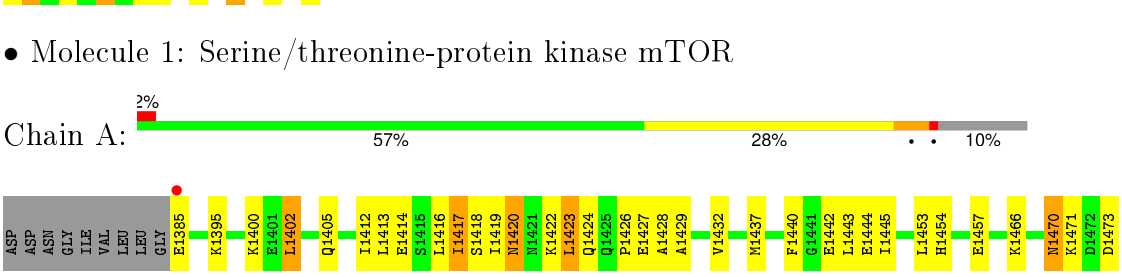
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 (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

Chain B:

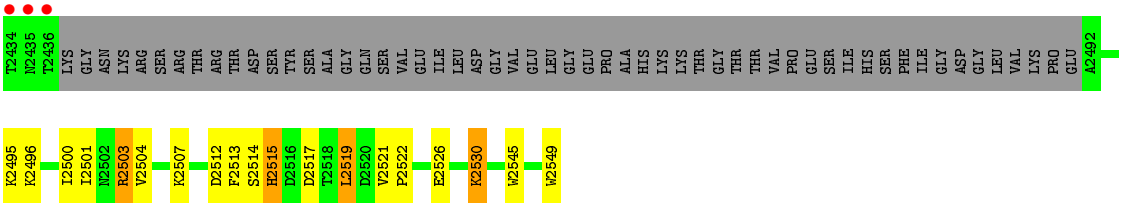






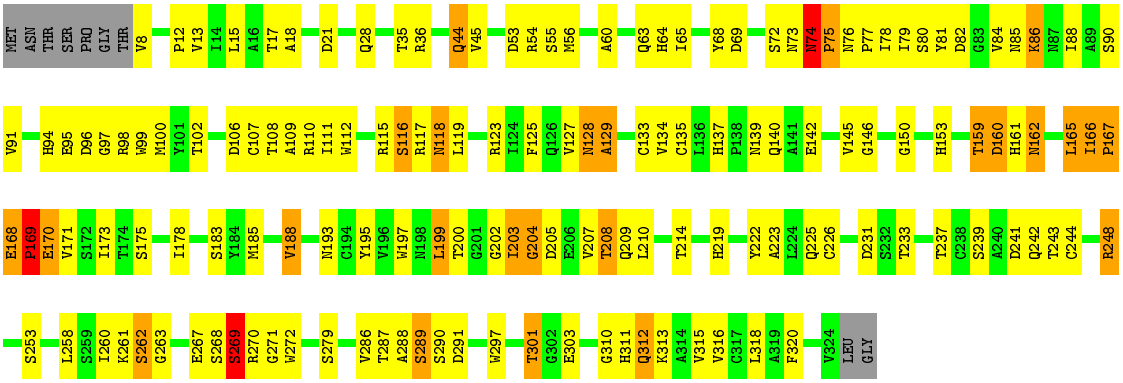
• Molecule 1: Serine/threonine-protein kinase mTOR

Chain A:



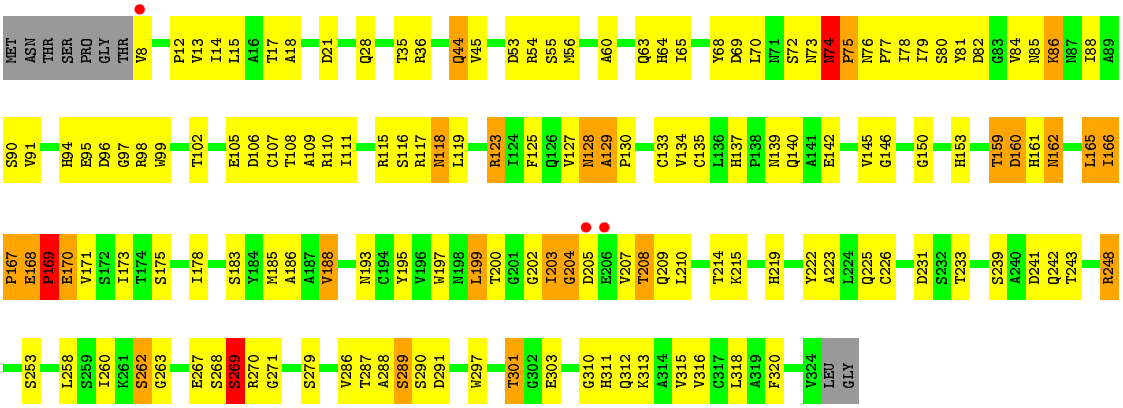
• Molecule 2: Target of rapamycin complex subunit LST8

Chain D:



• Molecule 2: Target of rapamycin complex subunit LST8

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	139.40Å 163.20Å 207.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.67 – 3.50 39.64 – 3.48	Depositor EDS
% Data completeness (in resolution range)	84.2 (39.67-3.50) 83.4 (39.64-3.48)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.224 , 0.257 0.226 , 0.260	Depositor DCC
R_{free} test set	1769 reflections (3.58%)	DCC
Wilson B-factor (Å^2)	61.7	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 36.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	1 of 57573 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	22160	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.36 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.5437e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 17G

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.35	0/8772	0.61	1/11872 (0.0%)
1	B	0.35	0/8804	0.61	1/11918 (0.0%)
2	C	0.36	0/2514	0.66	0/3426
2	D	0.40	0/2514	0.68	0/3426
All	All	0.36	0/22604	0.62	2/30642 (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	2
1	B	0	2
2	C	0	1
2	D	0	1
All	All	0	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1915	HIS	N-CA-C	5.67	126.32	111.00
1	A	1915	HIS	N-CA-C	5.65	126.26	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1914	GLY	Peptide
1	A	2000	GLU	Peptide
1	B	1914	GLY	Peptide
1	B	2000	GLU	Peptide
2	C	169	PRO	Peptide
2	D	169	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8577	0	8559	256	0
1	B	8607	0	8592	258	0
2	C	2456	0	2341	121	0
2	D	2456	0	2341	123	0
3	A	32	0	15	8	0
3	B	32	0	15	6	0
All	All	22160	0	21863	752	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (752) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:ASN:HB3	2:D:77:PRO:HD2	1.30	1.13
2:C:76:ASN:HB3	2:C:77:PRO:HD2	1.29	1.13
2:D:146:GLY:HA3	2:D:173:ILE:HD11	1.33	1.06
2:C:146:GLY:HA3	2:C:173:ILE:HD11	1.33	1.04
1:A:1418:SER:HB2	1:A:1581:GLU:HG2	1.35	1.03
1:A:1908:THR:O	1:A:1912:ASP:HB2	1.65	0.97
2:D:231:ASP:HB3	2:D:233:THR:OG1	1.64	0.96
1:B:1908:THR:O	1:B:1912:ASP:HB2	1.65	0.96
2:C:231:ASP:HB3	2:C:233:THR:OG1	1.67	0.93
1:A:1969:PRO:O	1:A:1970:GLN:HB2	1.66	0.92
1:B:1422:LYS:HE2	1:B:1581:GLU:HG3	1.50	0.92
1:A:2380:THR:HG22	1:A:2383:LEU:HG	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1969:PRO:O	1:B:1970:GLN:HB2	1.73	0.87
1:A:1892:ILE:HG21	1:A:1930:ILE:HD11	1.57	0.86
1:B:2380:THR:HG22	1:B:2383:LEU:HG	1.55	0.85
2:D:117:ARG:O	2:D:118:ASN:HB2	1.77	0.85
2:D:167:PRO:HD2	2:D:169:PRO:HG2	1.60	0.83
2:C:117:ARG:O	2:C:118:ASN:HB2	1.78	0.83
2:D:76:ASN:HB3	2:D:77:PRO:CD	2.07	0.83
2:C:76:ASN:HB3	2:C:77:PRO:CD	2.07	0.82
1:A:2344:LEU:HD13	1:A:2353:ILE:HD11	1.61	0.82
1:A:2160:LEU:HD22	1:A:2172:LEU:HA	1.63	0.81
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.13	0.80
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.15	0.80
2:C:167:PRO:HD2	2:C:169:PRO:HG2	1.63	0.79
1:A:1611:ARG:HH11	1:A:1614:ILE:HG21	1.47	0.79
1:B:1998:MET:HA	1:B:2001:HIS:HD2	1.47	0.79
1:B:1892:ILE:HG21	1:B:1930:ILE:HD11	1.66	0.78
1:B:2390:THR:O	1:B:2390:THR:HG23	1.84	0.78
1:B:2160:LEU:HD22	1:B:2172:LEU:HA	1.66	0.78
1:A:1998:MET:HA	1:A:2001:HIS:HD2	1.46	0.78
1:B:1611:ARG:HH11	1:B:1614:ILE:HG21	1.48	0.77
1:B:1428:ALA:HB2	1:B:2395:ASN:HD21	1.49	0.77
1:B:1901:GLN:HG3	1:B:2413:SER:HA	1.67	0.77
1:B:2095:LYS:O	1:B:2099:GLN:HG2	1.84	0.77
1:A:2095:LYS:O	1:A:2099:GLN:HG2	1.85	0.76
1:A:1670:HIS:HE1	1:A:1681:PRO:HB3	1.50	0.76
1:A:1958:HIS:CE1	1:A:1990:ALA:HB1	2.21	0.75
2:D:150:GLY:HA3	2:D:169:PRO:HB3	1.68	0.75
1:B:2344:LEU:HD13	1:B:2353:ILE:HD11	1.68	0.75
1:A:1427:GLU:HB2	1:A:2398:ILE:HD13	1.69	0.74
2:D:107:CYS:HB3	2:D:127:VAL:O	1.86	0.74
1:A:1422:LYS:HE2	1:A:1581:GLU:HG3	1.68	0.74
1:B:1941:GLN:HE22	1:B:2200:GLN:HE22	1.35	0.74
1:A:2421:PHE:HA	1:A:2424:ASP:HB2	1.69	0.74
1:B:2421:PHE:HA	1:B:2424:ASP:HB2	1.70	0.74
1:A:1892:ILE:CG2	1:A:1930:ILE:HD11	2.16	0.73
1:A:1901:GLN:HG3	1:A:2413:SER:HA	1.70	0.73
1:B:1427:GLU:HB2	1:B:2398:ILE:HD13	1.70	0.73
2:D:69:ASP:HB2	2:D:78:ILE:HD11	1.70	0.73
3:B:2601:17G:H8	3:B:2601:17G:C19	2.18	0.73
2:C:108:THR:OG1	2:C:110:ARG:NH1	2.21	0.73
2:C:150:GLY:HA3	2:C:169:PRO:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:123:ARG:NH2	2:D:160:ASP:OD1	2.20	0.73
1:A:2390:THR:HG23	1:A:2390:THR:O	1.89	0.73
2:C:107:CYS:HB3	2:C:127:VAL:O	1.87	0.73
2:D:95:GLU:HB2	2:D:140:GLN:NE2	2.02	0.73
2:D:108:THR:OG1	2:D:110:ARG:NH1	2.21	0.72
1:B:1958:HIS:CE1	1:B:1990:ALA:HB1	2.23	0.72
2:D:55:SER:O	2:D:56:MET:HG2	1.89	0.72
3:A:2601:17G:H8	3:A:2601:17G:C19	2.19	0.71
1:A:2093:ASN:O	1:A:2094:VAL:HB	1.91	0.71
1:B:2093:ASN:O	1:B:2094:VAL:HB	1.89	0.71
1:A:1428:ALA:HB2	1:A:2395:ASN:HD21	1.56	0.70
2:C:95:GLU:HB2	2:C:140:GLN:NE2	2.05	0.70
1:B:1422:LYS:HE2	1:B:1581:GLU:CG	2.21	0.70
2:C:69:ASP:HB2	2:C:78:ILE:HD11	1.72	0.70
1:A:2515:HIS:N	1:A:2515:HIS:ND1	2.39	0.69
1:B:2515:HIS:N	1:B:2515:HIS:ND1	2.39	0.69
1:A:2178:ASN:HD22	1:A:2180:HIS:H	1.39	0.69
2:D:289:SER:HB2	2:D:291:ASP:OD1	1.91	0.69
1:B:2178:ASN:HD22	1:B:2180:HIS:H	1.40	0.69
2:D:169:PRO:HA	2:D:171:VAL:H	1.56	0.69
2:C:279:SER:HA	2:C:320:PHE:HE2	1.59	0.68
1:A:1941:GLN:HE22	1:A:2200:GLN:HE22	1.41	0.67
1:B:2336:LEU:HG	1:B:2339:ARG:HH11	1.60	0.67
1:A:1734:THR:C	1:A:1736:ASP:H	1.95	0.67
2:C:123:ARG:NH2	2:C:160:ASP:OD1	2.26	0.67
2:C:95:GLU:H	2:C:140:GLN:HE22	1.41	0.67
1:B:1704:MET:HG2	1:B:1713:ALA:HB2	1.76	0.67
2:C:168:GLU:N	2:C:169:PRO:HD2	2.10	0.66
1:B:1783:ASP:O	1:B:1785:SER:N	2.29	0.66
2:C:188:VAL:HG13	2:C:223:ALA:HB3	1.77	0.66
2:D:168:GLU:N	2:D:169:PRO:HD2	2.11	0.66
1:A:1508:THR:O	1:A:1512:MET:HB2	1.94	0.66
1:B:1759:LEU:HG	1:B:1772:VAL:HG11	1.78	0.66
1:B:2192:LEU:HD12	1:B:2235:GLY:HA3	1.76	0.66
1:B:1508:THR:O	1:B:1512:MET:HB2	1.95	0.66
1:A:1422:LYS:HD3	1:A:1580:GLY:HA3	1.76	0.66
2:C:169:PRO:HA	2:C:171:VAL:H	1.60	0.65
1:A:1759:LEU:HG	1:A:1772:VAL:HG11	1.77	0.65
1:B:1892:ILE:CG2	1:B:1930:ILE:HD11	2.26	0.65
1:A:1704:MET:HG2	1:A:1713:ALA:HB2	1.77	0.65
2:D:95:GLU:H	2:D:140:GLN:HE22	1.43	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1418:SER:CB	1:A:1581:GLU:HG2	2.21	0.64
1:B:1428:ALA:HB2	1:B:2395:ASN:ND2	2.12	0.64
2:D:188:VAL:HG13	2:D:223:ALA:HB3	1.78	0.64
1:A:1969:PRO:O	1:A:1970:GLN:CB	2.44	0.64
1:B:2281:MET:HE1	2:D:222:TYR:CD2	2.32	0.64
2:D:134:VAL:HG22	2:D:145:VAL:HG22	1.79	0.64
1:A:1680:ASP:C	1:A:1682:SER:N	2.51	0.64
1:A:2192:LEU:HD12	1:A:2235:GLY:HA3	1.78	0.64
2:C:134:VAL:HG22	2:C:145:VAL:HG22	1.79	0.63
1:A:1783:ASP:O	1:A:1785:SER:N	2.31	0.63
2:C:55:SER:O	2:C:56:MET:HG2	1.99	0.63
1:A:1482:ARG:HA	1:A:1515:MET:HE3	1.79	0.63
1:A:1732:ILE:HD13	1:A:1740:LYS:HD2	1.80	0.63
1:B:1660:CYS:HB2	1:B:1669:ALA:HB2	1.79	0.63
2:D:279:SER:HA	2:D:320:PHE:HE2	1.63	0.63
1:A:1690:PRO:HB2	1:A:1692:VAL:HG22	1.79	0.63
1:A:2064:THR:HG22	1:A:2128:PRO:HD3	1.79	0.62
1:A:1977:THR:HG21	1:A:2013:SER:OG	1.99	0.62
1:B:1604:GLN:O	1:B:1608:VAL:HG23	1.98	0.62
1:A:1734:THR:O	1:A:1736:ASP:N	2.32	0.62
2:C:74:ASN:H	2:C:75:PRO:HD3	1.64	0.62
1:B:1654:LEU:HD21	1:B:1696:VAL:HG22	1.80	0.62
1:A:2037:LEU:HD22	1:A:2043:ASN:HD22	1.64	0.62
2:D:74:ASN:H	2:D:75:PRO:HD3	1.64	0.62
1:A:1958:HIS:HE1	1:A:1990:ALA:HB1	1.65	0.62
1:B:2363:GLU:OE2	1:B:2503:ARG:HD2	2.00	0.62
1:B:1680:ASP:C	1:B:1682:SER:N	2.53	0.61
1:A:1732:ILE:HD13	1:A:1740:LYS:HB2	1.82	0.61
1:B:1690:PRO:HB2	1:B:1692:VAL:HG22	1.82	0.61
1:A:1914:GLY:HA3	1:A:1950:ARG:HE	1.63	0.61
1:B:1914:GLY:HA3	1:B:1950:ARG:HE	1.65	0.61
1:B:1958:HIS:HE1	1:B:1990:ALA:HB1	1.66	0.61
1:A:2278:LEU:HD23	2:C:44:GLN:HG2	1.80	0.61
2:D:241:ASP:OD2	2:D:243:THR:HB	2.00	0.61
2:D:170:GLU:OE2	2:D:170:GLU:HA	2.01	0.61
1:A:2336:LEU:HG	1:A:2339:ARG:HH11	1.66	0.61
2:C:289:SER:HB2	2:C:291:ASP:OD1	2.01	0.61
1:B:1968:HIS:HB3	1:B:2144:TYR:OH	2.01	0.60
1:B:1623:LEU:HG	1:B:1633:TRP:CH2	2.36	0.60
2:C:199:LEU:HD22	2:C:210:LEU:HD22	1.84	0.60
1:B:1734:THR:C	1:B:1736:ASP:H	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:LEU:HD22	2:D:210:LEU:HD22	1.83	0.60
2:D:56:MET:HB2	2:D:68:TYR:O	2.02	0.60
1:A:1428:ALA:HB2	1:A:2395:ASN:ND2	2.17	0.60
1:B:1920:ASN:O	1:B:1924:VAL:HG23	2.00	0.60
1:A:2321:THR:HG23	1:A:2387:MET:HG2	1.83	0.60
1:B:1734:THR:O	1:B:1736:ASP:N	2.31	0.60
2:C:241:ASP:OD2	2:C:243:THR:HB	2.01	0.60
1:B:1915:HIS:HD2	1:B:1953:VAL:HG22	1.67	0.60
1:A:2380:THR:CG2	1:A:2383:LEU:HG	2.31	0.59
1:A:2278:LEU:CD2	2:C:44:GLN:HG2	2.32	0.59
1:A:2281:MET:HE1	2:C:222:TYR:CD2	2.38	0.59
2:C:137:HIS:HD2	2:C:139:ASN:H	1.49	0.59
1:A:1611:ARG:NH1	1:A:1614:ILE:HG21	2.16	0.59
1:B:1739:HIS:O	1:B:1743:LEU:HB2	2.02	0.59
1:A:1680:ASP:C	1:A:1682:SER:H	2.04	0.59
1:B:1705:TRP:CE3	1:B:1710:LYS:HB2	2.38	0.59
1:A:1968:HIS:HB3	1:A:2144:TYR:OH	2.03	0.59
1:B:1422:LYS:CE	1:B:1581:GLU:HG3	2.29	0.59
1:B:1969:PRO:O	1:B:1970:GLN:CB	2.49	0.58
1:B:2037:LEU:HD22	1:B:2043:ASN:HD22	1.68	0.58
1:B:2336:LEU:HG	1:B:2339:ARG:NH1	2.17	0.58
1:B:2298:ASP:HB2	1:B:2382:MET:CE	2.34	0.58
2:C:301:THR:HB	2:C:303:GLU:HG2	1.85	0.58
1:A:2411:LYS:O	1:A:2415:MET:HG3	2.03	0.58
1:A:1920:ASN:O	1:A:1924:VAL:HG23	2.03	0.58
1:A:1493:LEU:HD23	1:A:1519:ALA:HB2	1.85	0.58
1:B:2390:THR:O	1:B:2390:THR:CG2	2.52	0.58
1:A:1680:ASP:O	1:A:1682:SER:N	2.31	0.58
1:A:2237:ILE:HG21	3:A:2601:17G:H11	1.87	0.57
2:C:279:SER:HA	2:C:320:PHE:CE2	2.39	0.57
2:D:231:ASP:CB	2:D:233:THR:OG1	2.48	0.57
2:C:202:GLY:O	2:C:203:ILE:O	2.22	0.57
1:B:1611:ARG:NH1	1:B:1614:ILE:HG21	2.18	0.57
2:D:137:HIS:CD2	2:D:139:ASN:H	2.22	0.57
1:A:2496:LYS:HE3	1:A:2500:ILE:HD11	1.87	0.57
1:A:1481:MET:HA	1:A:1484:LEU:HD12	1.87	0.57
2:D:137:HIS:HD2	2:D:139:ASN:H	1.51	0.57
1:B:2281:MET:HA	1:B:2281:MET:CE	2.35	0.56
2:C:225:GLN:HG2	2:C:226:CYS:N	2.20	0.56
1:B:1482:ARG:HA	1:B:1515:MET:HE3	1.87	0.56
2:C:137:HIS:CD2	2:C:139:ASN:H	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:202:GLY:O	2:D:203:ILE:O	2.23	0.56
2:C:111:ILE:HD12	2:C:123:ARG:HD3	1.87	0.56
1:B:1686:ASP:O	1:A:2266:ARG:HG3	2.05	0.56
1:B:2237:ILE:HG21	3:B:2601:17G:H11	1.87	0.56
2:D:225:GLN:HG2	2:D:226:CYS:N	2.19	0.56
1:B:2297:ASP:HB3	1:B:2301:LYS:HD2	1.87	0.56
2:C:127:VAL:HG11	2:C:153:HIS:CE1	2.41	0.56
1:B:1680:ASP:O	1:B:1682:SER:N	2.32	0.56
2:D:21:ASP:HB3	2:D:313:LYS:H	1.71	0.56
1:A:1910:TRP:O	1:A:1915:HIS:NE2	2.39	0.56
2:D:159:THR:HG22	2:D:161:HIS:HD2	1.70	0.56
2:D:188:VAL:HG13	2:D:223:ALA:CB	2.35	0.56
1:A:1680:ASP:HB3	1:A:1683:ARG:H	1.71	0.56
1:B:1682:SER:O	1:B:1685:LEU:HD12	2.06	0.56
1:B:1623:LEU:HG	1:B:1633:TRP:CZ3	2.41	0.55
1:B:1481:MET:HA	1:B:1484:LEU:HD12	1.88	0.55
2:D:63:GLN:HE21	2:D:86:LYS:H	1.54	0.55
1:B:1609:PRO:HB3	1:B:1612:ARG:NH1	2.22	0.55
2:C:63:GLN:HE21	2:C:86:LYS:H	1.54	0.55
2:D:301:THR:HB	2:D:303:GLU:HG2	1.88	0.55
1:A:1674:VAL:HG11	1:A:1681:PRO:HD3	1.87	0.55
1:B:1910:TRP:O	1:B:1915:HIS:NE2	2.40	0.55
1:A:1781:GLU:OE1	1:A:1781:GLU:HA	2.07	0.55
1:B:2380:THR:HG23	1:B:2549:TRP:O	2.06	0.55
2:D:15:LEU:HD11	2:D:286:VAL:HG11	1.89	0.55
1:B:1778:ALA:O	1:B:1782:HIS:HD2	1.90	0.55
1:A:2298:ASP:HB2	1:A:2382:MET:CE	2.37	0.55
2:C:94:HIS:HB3	2:C:99:TRP:HB2	1.87	0.55
1:A:1915:HIS:HD2	1:A:1953:VAL:HG22	1.70	0.55
1:B:2282:GLN:HE21	2:D:316:VAL:HG11	1.72	0.55
1:A:1739:HIS:O	1:A:1743:LEU:HB2	2.06	0.55
2:D:117:ARG:O	2:D:118:ASN:CB	2.54	0.55
2:D:111:ILE:HD12	2:D:123:ARG:HD3	1.88	0.55
1:B:1680:ASP:C	1:B:1682:SER:H	2.07	0.55
1:B:2496:LYS:HE3	1:B:2500:ILE:HD11	1.89	0.55
1:B:1762:GLN:HB2	1:B:1768:THR:HG21	1.89	0.55
1:A:2122:GLU:O	1:A:2126:VAL:HG23	2.07	0.55
1:B:1913:TYR:HB3	1:B:1916:TRP:HE1	1.72	0.55
2:C:21:ASP:HB3	2:C:313:LYS:H	1.72	0.55
1:A:1701:MET:HE1	1:A:1716:HIS:C	2.27	0.55
2:C:258:LEU:HD22	2:C:297:TRP:CE3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:36:ARG:NH2	2:C:69:ASP:O	2.40	0.55
2:C:15:LEU:HD11	2:C:286:VAL:HG11	1.89	0.55
1:B:1680:ASP:HB3	1:B:1683:ARG:H	1.72	0.55
2:D:94:HIS:HB3	2:D:99:TRP:HB2	1.87	0.54
2:C:159:THR:HG22	2:C:161:HIS:HD2	1.71	0.54
2:C:170:GLU:OE2	2:C:170:GLU:HA	2.07	0.54
1:A:1682:SER:O	1:A:1685:LEU:HD12	2.07	0.54
2:D:279:SER:HA	2:D:320:PHE:CE2	2.41	0.54
1:A:1501:TRP:CE3	1:A:1503:LEU:HD12	2.42	0.54
2:D:36:ARG:NH2	2:D:69:ASP:O	2.40	0.54
2:C:202:GLY:HA3	2:C:208:THR:H	1.72	0.54
1:B:2411:LYS:O	1:B:2415:MET:HG3	2.08	0.54
2:C:56:MET:HB2	2:C:68:TYR:O	2.08	0.54
2:C:12:PRO:O	2:C:54:ARG:NH2	2.40	0.54
1:B:1422:LYS:C	1:B:1424:GLN:H	2.11	0.54
1:A:2336:LEU:HG	1:A:2339:ARG:NH1	2.22	0.54
2:C:288:ALA:HB2	2:C:318:LEU:HG	1.90	0.54
2:D:96:ASP:O	2:D:98:ARG:N	2.41	0.54
2:D:165:LEU:HD11	2:D:197:TRP:CH2	2.43	0.54
2:D:288:ALA:HB2	2:D:318:LEU:HG	1.90	0.54
1:A:2521:VAL:HB	1:A:2522:PRO:HD3	1.88	0.54
1:A:1583:TYR:C	1:A:1585:ARG:H	2.12	0.54
2:D:94:HIS:CE1	2:D:96:ASP:HB2	2.42	0.53
2:C:94:HIS:CE1	2:C:96:ASP:HB2	2.42	0.53
1:A:1977:THR:HG22	1:A:1981:LYS:HE2	1.88	0.53
1:B:1670:HIS:HE1	1:B:1681:PRO:HB3	1.73	0.53
1:B:1643:VAL:HG12	1:B:1644:VAL:HG23	1.90	0.53
2:D:202:GLY:HA3	2:D:208:THR:H	1.73	0.53
1:B:1701:MET:HE1	1:B:1716:HIS:C	2.29	0.53
2:C:17:THR:HB	2:C:311:HIS:HE1	1.73	0.53
1:B:2064:THR:HG22	1:B:2128:PRO:HD3	1.89	0.53
1:A:1913:TYR:HB3	1:A:1916:TRP:HE1	1.74	0.53
2:D:12:PRO:O	2:D:54:ARG:NH2	2.41	0.53
1:B:1936:LEU:HA	1:B:1939:ILE:HG13	1.91	0.53
1:B:1970:GLN:NE2	1:B:2139:ALA:H	2.07	0.53
1:A:1999:CYS:C	1:A:2001:HIS:H	2.12	0.53
2:C:188:VAL:HG13	2:C:223:ALA:CB	2.39	0.53
2:C:17:THR:HB	2:C:311:HIS:CE1	2.43	0.53
1:A:1705:TRP:CE3	1:A:1710:LYS:HB2	2.44	0.53
2:D:60:ALA:HB1	2:D:88:ILE:HG22	1.91	0.53
1:B:2197:ARG:NH1	1:B:2424:ASP:OD2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:ASP:CB	2:D:78:ILE:HD11	2.39	0.53
1:A:2345:MET:HE2	3:A:2601:17G:H1	1.90	0.53
1:A:2297:ASP:HB3	1:A:2301:LYS:HD2	1.90	0.53
1:A:1913:TYR:O	1:A:1915:HIS:HA	2.08	0.53
1:B:2278:LEU:HD23	2:D:44:GLN:HG2	1.90	0.53
1:B:2168:ARG:HB2	1:B:2168:ARG:CZ	2.38	0.53
1:A:1896:ARG:NH2	1:A:1933:ASP:OD2	2.42	0.53
2:D:133:CYS:SG	2:D:175:SER:HA	2.49	0.53
1:B:1478:LEU:O	1:B:1482:ARG:HG3	2.09	0.52
1:A:1595:MET:O	1:A:1599:LEU:HB2	2.09	0.52
1:A:1660:CYS:HB2	1:A:1669:ALA:HB2	1.90	0.52
1:A:1762:GLN:HB2	1:A:1768:THR:HG21	1.92	0.52
1:B:2165:SER:OG	1:B:2166:LYS:N	2.42	0.52
1:A:1725:GLN:O	1:A:1729:GLN:HG2	2.09	0.52
3:B:2601:17G:C20	3:B:2601:17G:H8	2.40	0.52
1:B:1913:TYR:O	1:B:1915:HIS:HA	2.08	0.52
2:D:82:ASP:HB2	2:D:119:LEU:HD13	1.92	0.52
2:D:135:CYS:SG	2:D:178:ILE:HG22	2.50	0.52
1:A:1778:ALA:O	1:A:1782:HIS:HD2	1.93	0.52
1:A:1416:LEU:HA	1:A:1419:ILE:HG22	1.91	0.52
2:D:166:ILE:HD12	2:D:167:PRO:O	2.10	0.52
1:A:2363:GLU:OE2	1:A:2503:ARG:HD2	2.10	0.52
2:C:115:ARG:O	2:C:116:SER:HB3	2.10	0.52
1:A:1878:LEU:HD21	1:A:1918:ASP:HB2	1.92	0.52
1:B:1583:TYR:C	1:B:1585:ARG:H	2.13	0.52
2:D:94:HIS:HE1	2:D:96:ASP:HB2	1.75	0.52
1:B:1416:LEU:HA	1:B:1419:ILE:HG22	1.91	0.52
2:D:258:LEU:HD22	2:D:297:TRP:CE3	2.45	0.52
2:D:98:ARG:HD2	2:D:115:ARG:HB2	1.92	0.51
1:A:1649:ASP:O	1:A:1651:ARG:N	2.43	0.51
1:A:2382:MET:HG3	1:A:2549:TRP:O	2.10	0.51
1:A:1611:ARG:HG2	1:A:1614:ILE:HD12	1.92	0.51
1:B:1629:ILE:HG22	1:B:1630:VAL:HG23	1.92	0.51
2:D:17:THR:HB	2:D:311:HIS:HE1	1.75	0.51
1:B:1566:LYS:O	1:B:1570:LEU:HG	2.10	0.51
2:D:115:ARG:O	2:D:116:SER:HB3	2.09	0.51
1:B:1701:MET:HE1	1:B:1717:MET:N	2.24	0.51
1:B:1781:GLU:HA	1:B:1781:GLU:OE1	2.10	0.51
1:B:1999:CYS:C	1:B:2001:HIS:H	2.14	0.51
1:A:2281:MET:HA	1:A:2281:MET:CE	2.40	0.51
2:D:200:THR:O	2:D:208:THR:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2298:ASP:HB2	1:B:2382:MET:HE2	1.91	0.51
1:A:1701:MET:HE1	1:A:1717:MET:N	2.25	0.51
1:B:2321:THR:HG23	1:B:2387:MET:HG2	1.92	0.51
2:C:165:LEU:HD11	2:C:197:TRP:CH2	2.46	0.51
1:B:2521:VAL:HB	1:B:2522:PRO:HD3	1.91	0.51
1:B:1497:CYS:SG	1:B:1516:ALA:HB2	2.51	0.51
1:A:1422:LYS:C	1:A:1424:GLN:H	2.14	0.51
1:A:2178:ASN:ND2	1:A:2180:HIS:H	2.07	0.51
1:B:1785:SER:O	1:B:1786:TRP:HB3	2.10	0.51
2:D:17:THR:HB	2:D:311:HIS:CE1	2.45	0.51
1:A:2123:LEU:HB2	1:A:2158:PRO:O	2.11	0.51
1:A:1785:SER:O	1:A:1786:TRP:HB3	2.10	0.51
2:C:142:GLU:OE2	2:C:208:THR:HB	2.10	0.51
2:C:128:ASN:O	2:C:129:ALA:HB3	2.11	0.51
1:B:2178:ASN:ND2	1:B:2180:HIS:H	2.07	0.51
1:A:2154:GLN:NE2	1:A:2155:SER:HB3	2.25	0.51
1:A:1936:LEU:HA	1:A:1939:ILE:HG13	1.93	0.51
2:C:117:ARG:O	2:C:118:ASN:CB	2.55	0.50
1:B:1501:TRP:CE3	1:B:1503:LEU:HD12	2.46	0.50
1:B:1878:LEU:HD21	1:B:1918:ASP:HB2	1.93	0.50
1:A:1631:GLU:H	1:A:1631:GLU:CD	2.15	0.50
1:B:2289:HIS:O	1:B:2293:ASN:ND2	2.44	0.50
1:B:1649:ASP:O	1:B:1651:ARG:N	2.44	0.50
1:A:2168:ARG:HB2	1:A:2168:ARG:CZ	2.42	0.50
1:B:1595:MET:O	1:B:1599:LEU:HB2	2.11	0.50
2:C:96:ASP:O	2:C:98:ARG:N	2.44	0.50
2:C:78:ILE:HG22	2:C:79:ILE:HG13	1.93	0.50
1:B:1697:THR:O	1:B:1701:MET:HG3	2.11	0.50
1:A:2289:HIS:O	1:A:2293:ASN:ND2	2.44	0.50
1:B:1732:ILE:HD13	1:B:1740:LYS:HD2	1.92	0.50
1:A:1888:PHE:O	1:A:1892:ILE:HG13	2.11	0.50
1:B:2389:VAL:O	1:B:2390:THR:HG22	2.12	0.50
1:B:2281:MET:CE	2:D:222:TYR:CD2	2.94	0.50
2:C:200:THR:O	2:C:208:THR:HA	2.12	0.50
2:C:94:HIS:HE1	2:C:96:ASP:HB2	1.76	0.50
2:D:128:ASN:O	2:D:129:ALA:HB3	2.12	0.50
2:C:135:CYS:SG	2:C:178:ILE:HG22	2.52	0.50
1:A:1495:GLN:O	1:A:1499:GLU:HB2	2.12	0.50
2:C:169:PRO:HA	2:C:171:VAL:HG22	1.93	0.50
1:A:2389:VAL:O	1:A:2390:THR:HG22	2.12	0.50
2:C:8:VAL:HG11	2:C:36:ARG:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:271:GLY:HA2	2:C:290:SER:HB2	1.92	0.50
2:D:268:SER:O	2:D:269:SER:HB3	2.10	0.50
1:B:2154:GLN:NE2	1:B:2155:SER:HB3	2.26	0.50
2:D:8:VAL:HG11	2:D:36:ARG:HG2	1.93	0.50
2:C:69:ASP:CB	2:C:78:ILE:HD11	2.42	0.50
2:D:219:HIS:HE1	2:D:243:THR:HG22	1.75	0.50
1:A:1913:TYR:O	1:A:1915:HIS:CG	2.65	0.50
1:A:1602:VAL:HG13	1:A:1643:VAL:HG23	1.93	0.50
1:A:1882:VAL:HG12	1:A:1886:GLN:HE21	1.76	0.50
2:D:94:HIS:CD2	2:D:140:GLN:HB3	2.47	0.49
1:B:1915:HIS:HE1	1:B:1919:VAL:HG11	1.78	0.49
2:D:142:GLU:OE2	2:D:208:THR:HB	2.12	0.49
1:A:1915:HIS:HE1	1:A:1919:VAL:HG11	1.77	0.49
1:B:1732:ILE:HD13	1:B:1740:LYS:HB2	1.94	0.49
1:A:1564:ILE:HG23	1:A:1596:LEU:HD22	1.94	0.49
1:B:1552:LEU:HD11	1:B:1603:ILE:HG13	1.94	0.49
2:D:127:VAL:HG11	2:D:153:HIS:CE1	2.47	0.49
2:D:185:MET:HB2	2:D:199:LEU:HD21	1.94	0.49
1:B:2254:ARG:HD2	1:B:2259:ILE:HB	1.95	0.49
2:C:133:CYS:SG	2:C:175:SER:HA	2.52	0.49
1:B:1420:ASN:HB3	1:B:1429:ALA:HB2	1.95	0.49
2:C:98:ARG:HD2	2:C:115:ARG:HB2	1.94	0.49
1:A:1734:THR:C	1:A:1736:ASP:N	2.64	0.49
1:B:2380:THR:CG2	1:B:2383:LEU:HG	2.37	0.49
1:A:1966:ARG:HA	1:A:2001:HIS:CE1	2.46	0.49
1:A:1420:ASN:HB3	1:A:1429:ALA:HB2	1.95	0.49
1:A:1732:ILE:CD1	1:A:1740:LYS:HB2	2.42	0.49
1:B:1609:PRO:HA	1:B:1612:ARG:NH1	2.28	0.49
1:A:1697:THR:O	1:A:1701:MET:HG3	2.13	0.49
2:C:64:HIS:HA	2:C:81:TYR:O	2.13	0.49
2:D:271:GLY:HA2	2:D:290:SER:HB2	1.94	0.49
1:A:2380:THR:HG23	1:A:2549:TRP:O	2.13	0.49
1:A:2390:THR:CG2	1:A:2390:THR:O	2.57	0.49
2:C:94:HIS:CD2	2:C:140:GLN:HB3	2.48	0.49
1:B:1882:VAL:HG12	1:B:1886:GLN:HE21	1.77	0.49
1:B:1977:THR:HG21	1:B:2013:SER:OG	2.13	0.49
1:A:1705:TRP:CZ3	1:A:1757:TRP:HB3	2.47	0.49
1:A:2397:ARG:NH2	1:A:2526:GLU:OE1	2.44	0.49
1:A:2530:LYS:HE2	1:A:2530:LYS:HA	1.93	0.49
1:B:1771:LYS:O	1:B:1774:GLN:HB3	2.12	0.49
2:C:74:ASN:H	2:C:75:PRO:CD	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.46	0.49
1:A:2006:VAL:O	1:A:2010:MET:HB2	2.12	0.49
2:D:72:SER:O	2:D:74:ASN:N	2.45	0.48
2:D:53:ASP:C	2:D:55:SER:H	2.16	0.48
2:D:64:HIS:HA	2:D:81:TYR:O	2.13	0.48
2:C:106:ASP:OD1	2:C:108:THR:OG1	2.24	0.48
1:A:1432:VAL:HG22	1:A:2390:THR:HG21	1.95	0.48
1:B:2278:LEU:CD2	2:D:44:GLN:HG2	2.43	0.48
1:B:2395:ASN:HA	1:B:2398:ILE:HD12	1.94	0.48
1:B:1400:LYS:HG3	1:B:1416:LEU:HD13	1.94	0.48
1:B:1896:ARG:NH2	1:B:1933:ASP:OD2	2.46	0.48
1:A:1400:LYS:HG3	1:A:1416:LEU:HD13	1.95	0.48
1:A:1629:ILE:HG22	1:A:1630:VAL:HG23	1.95	0.48
2:C:28:GLN:O	2:C:28:GLN:HG3	2.14	0.48
1:A:1943:ILE:HD13	1:A:1975:PRO:HB2	1.95	0.48
1:A:1427:GLU:HB2	1:A:2398:ILE:CD1	2.40	0.48
1:B:2281:MET:HE2	1:B:2281:MET:HA	1.95	0.48
1:A:1631:GLU:HA	1:A:1634:GLN:HE21	1.77	0.48
2:D:65:ILE:CD1	2:D:102:THR:HG21	2.43	0.48
1:A:2298:ASP:HB2	1:A:2382:MET:HE2	1.94	0.48
1:A:2187:LYS:HG3	1:A:2237:ILE:HD12	1.95	0.48
1:B:1913:TYR:O	1:B:1915:HIS:ND1	2.46	0.48
1:A:1892:ILE:HG21	1:A:1930:ILE:CD1	2.36	0.48
2:C:268:SER:O	2:C:269:SER:HB3	2.11	0.48
1:A:2249:LEU:CD1	1:A:2346:LEU:HD12	2.44	0.48
2:C:301:THR:CB	2:C:303:GLU:HG2	2.43	0.48
1:A:1654:LEU:HD21	1:A:1696:VAL:HG22	1.95	0.48
1:A:1478:LEU:O	1:A:1482:ARG:HG3	2.14	0.48
1:B:1643:VAL:HG12	1:B:1644:VAL:CG2	2.42	0.48
1:B:2006:VAL:O	1:B:2010:MET:HB2	2.13	0.48
1:B:1631:GLU:CD	1:B:1631:GLU:H	2.17	0.48
2:C:269:SER:OG	2:C:270:ARG:N	2.47	0.48
1:A:2052:GLU:HG2	1:A:2053:PRO:HD3	1.95	0.48
1:A:1429:ALA:HA	1:A:1432:VAL:HG23	1.96	0.47
2:D:106:ASP:OD1	2:D:108:THR:OG1	2.24	0.47
2:C:239:SER:HB3	2:C:241:ASP:OD2	2.14	0.47
1:A:1913:TYR:HB2	1:A:1915:HIS:CE1	2.49	0.47
1:A:2162:VAL:CG1	1:A:2168:ARG:HG2	2.44	0.47
1:A:2165:SER:OG	1:A:2166:LYS:N	2.47	0.47
1:B:1913:TYR:O	1:B:1915:HIS:CG	2.67	0.47
1:B:2530:LYS:HE2	1:B:2530:LYS:HA	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2514:SER:OG	1:B:2517:ASP:HB2	2.15	0.47
1:A:2095:LYS:HA	1:A:2098:THR:HG22	1.95	0.47
2:D:204:GLY:O	2:D:205:ASP:HB2	2.13	0.47
1:B:1413:LEU:O	1:B:1417:ILE:HG12	2.13	0.47
1:B:1703:ASN:O	1:B:1707:SER:HB2	2.14	0.47
2:C:168:GLU:N	2:C:169:PRO:CD	2.76	0.47
1:B:2249:LEU:CD1	1:B:2346:LEU:HD12	2.45	0.47
1:A:2339:ARG:HD3	1:A:2355:HIS:CE1	2.49	0.47
1:B:1977:THR:HG22	1:B:1981:LYS:HE2	1.96	0.47
1:B:2123:LEU:HB2	1:B:2158:PRO:O	2.15	0.47
1:A:1691:THR:HG23	1:A:1724:MET:HE1	1.97	0.47
2:C:204:GLY:O	2:C:205:ASP:HB2	2.13	0.47
1:A:1703:ASN:O	1:A:1707:SER:HB2	2.14	0.47
1:B:2512:ASP:N	1:B:2512:ASP:OD1	2.47	0.47
1:B:1400:LYS:HD2	1:B:1412:ILE:HG23	1.96	0.47
1:A:2146:PRO:O	1:A:2147:ASN:HB2	2.14	0.47
2:D:74:ASN:H	2:D:75:PRO:CD	2.28	0.47
2:C:53:ASP:C	2:C:55:SER:H	2.18	0.47
2:C:219:HIS:HE1	2:C:243:THR:HG22	1.78	0.47
1:A:2401:HIS:CD2	1:A:2522:PRO:HA	2.50	0.47
2:C:17:THR:CG2	2:C:311:HIS:CE1	2.97	0.47
1:A:2052:GLU:CG	1:A:2053:PRO:HD3	2.44	0.47
2:C:82:ASP:HB2	2:C:119:LEU:HD13	1.97	0.47
1:A:2046:GLY:O	1:A:2050:VAL:HG23	2.15	0.47
1:B:1493:LEU:HD23	1:B:1519:ALA:HB2	1.96	0.47
1:B:1691:THR:HG23	1:B:1724:MET:HE1	1.97	0.47
1:A:1422:LYS:HG2	1:A:1580:GLY:C	2.35	0.47
3:A:2601:17G:H8	3:A:2601:17G:C20	2.45	0.47
1:A:1505:ASN:CB	1:A:1508:THR:HB	2.45	0.47
1:B:1646:PRO:HG3	1:B:1675:LEU:HD21	1.96	0.47
1:B:1495:GLN:O	1:B:1499:GLU:HB2	2.15	0.47
1:B:1628:ARG:HB2	1:B:1633:TRP:CD1	2.50	0.47
1:B:2378:ARG:HH11	1:B:2380:THR:HG21	1.80	0.47
2:C:207:VAL:HG12	2:C:209:GLN:HG2	1.96	0.47
1:A:1913:TYR:O	1:A:1915:HIS:ND1	2.48	0.46
1:B:2397:ARG:NH2	1:B:2526:GLU:OE1	2.46	0.46
1:B:2046:GLY:O	1:B:2050:VAL:HG23	2.15	0.46
1:A:2513:PHE:HB2	1:A:2519:LEU:HD11	1.97	0.46
1:B:1947:ASP:CG	1:B:1987:ARG:HG2	2.35	0.46
1:B:1674:VAL:HG11	1:B:1681:PRO:HD3	1.97	0.46
1:B:2146:PRO:O	1:B:2147:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:VAL:HG12	2:C:102:THR:HG22	1.96	0.46
2:D:75:PRO:HB2	2:D:76:ASN:H	1.52	0.46
2:D:168:GLU:N	2:D:169:PRO:CD	2.77	0.46
2:C:203:ILE:HG22	2:C:204:GLY:N	2.30	0.46
1:A:1566:LYS:O	1:A:1570:LEU:HG	2.14	0.46
2:D:28:GLN:O	2:D:28:GLN:HG3	2.16	0.46
1:B:1611:ARG:HG2	1:B:1614:ILE:HD12	1.97	0.46
1:B:1785:SER:O	1:B:1786:TRP:CB	2.63	0.46
1:B:2419:GLU:HG2	1:B:2501:ILE:HD13	1.96	0.46
1:B:2095:LYS:HA	1:B:2098:THR:HG22	1.97	0.46
1:A:2395:ASN:HA	1:A:2398:ILE:HD12	1.97	0.46
1:A:2503:ARG:HH11	1:A:2507:LYS:CE	2.28	0.46
2:D:269:SER:OG	2:D:270:ARG:N	2.48	0.46
1:A:2392:LEU:O	1:A:2397:ARG:HB2	2.16	0.46
2:D:102:THR:O	2:D:109:ALA:HA	2.16	0.46
2:D:168:GLU:HB3	2:D:195:TYR:OH	2.16	0.46
1:B:1505:ASN:CB	1:B:1508:THR:HB	2.46	0.46
1:A:1498:CYS:HA	1:A:1501:TRP:HD1	1.80	0.46
1:A:1501:TRP:HA	1:A:1503:LEU:HG	1.97	0.46
1:B:2168:ARG:O	1:B:2170:ARG:NH1	2.49	0.46
2:C:65:ILE:CD1	2:C:102:THR:HG21	2.45	0.46
2:D:207:VAL:HG12	2:D:209:GLN:HG2	1.96	0.46
1:A:2022:LEU:HD21	1:A:2126:VAL:HG13	1.97	0.46
1:B:2162:VAL:CG1	1:B:2168:ARG:HG2	2.46	0.46
1:A:1466:LYS:O	1:A:1470:ASN:HB2	2.15	0.46
1:B:1725:GLN:O	1:B:1729:GLN:HG2	2.15	0.46
1:A:1413:LEU:O	1:A:1417:ILE:HG12	2.15	0.46
1:B:1427:GLU:HB2	1:B:2398:ILE:CD1	2.44	0.46
2:C:159:THR:C	2:C:161:HIS:H	2.19	0.46
2:D:91:VAL:HG12	2:D:102:THR:HG22	1.96	0.46
1:A:1646:PRO:HG3	1:A:1675:LEU:HD21	1.97	0.46
2:D:203:ILE:HG22	2:D:204:GLY:N	2.31	0.46
1:A:2194:GLN:HG2	1:A:2427:LEU:HD22	1.97	0.46
2:C:125:PHE:CE1	2:C:162:ASN:HB2	2.51	0.46
1:B:1429:ALA:HA	1:B:1432:VAL:HG23	1.98	0.45
2:D:288:ALA:HB1	2:D:315:VAL:HG12	1.97	0.45
1:B:1466:LYS:O	1:B:1470:ASN:HB2	2.16	0.45
2:C:72:SER:O	2:C:74:ASN:N	2.48	0.45
1:A:2093:ASN:HD22	1:A:2095:LYS:H	1.63	0.45
1:A:1943:ILE:HA	1:A:1946:ILE:HG13	1.99	0.45
1:A:1440:PHE:HB3	1:A:1442:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1970:GLN:NE2	1:A:2139:ALA:H	2.14	0.45
1:B:1966:ARG:HA	1:B:2001:HIS:CE1	2.50	0.45
2:D:301:THR:CB	2:D:303:GLU:HG2	2.45	0.45
1:A:1643:VAL:HG12	1:A:1644:VAL:HG23	1.98	0.45
1:B:1470:ASN:HB3	1:B:1471:LYS:H	1.57	0.45
2:D:169:PRO:HA	2:D:171:VAL:HG22	1.98	0.45
2:D:95:GLU:HB2	2:D:140:GLN:HE22	1.76	0.45
2:D:17:THR:CG2	2:D:311:HIS:CE1	2.99	0.45
1:B:2052:GLU:HG2	1:B:2053:PRO:HD3	1.97	0.45
2:C:185:MET:HB2	2:C:199:LEU:HD21	1.99	0.45
1:A:1882:VAL:N	1:A:1883:PRO:HD2	2.32	0.45
1:B:1414:GLU:O	1:B:1417:ILE:HG13	2.17	0.45
2:D:242:GLN:NE2	2:D:261:LYS:HA	2.30	0.45
2:D:262:SER:OG	2:D:267:GLU:HG2	2.17	0.45
1:B:2015:GLU:HB3	1:B:2130:LEU:CD1	2.46	0.45
1:A:1947:ASP:CG	1:A:1987:ARG:HG2	2.36	0.45
1:A:2378:ARG:HH11	1:A:2380:THR:HG21	1.82	0.45
1:A:2346:LEU:HD23	1:A:2353:ILE:HG13	1.98	0.45
3:A:2601:17G:H9	3:A:2601:17G:H11	1.70	0.45
1:A:2287:PHE:O	1:A:2291:VAL:HG23	2.17	0.45
1:B:1727:GLN:O	1:B:1731:ALA:HB3	2.17	0.45
2:D:125:PHE:CE1	2:D:162:ASN:HB2	2.52	0.45
1:B:1432:VAL:HG22	1:B:2390:THR:HG21	1.99	0.45
1:B:2093:ASN:HD22	1:B:2095:LYS:H	1.63	0.45
1:B:1634:GLN:HG2	1:B:1656:TYR:OH	2.17	0.45
1:A:1895:SER:HB2	1:A:1899:ASN:HB3	1.98	0.45
1:A:1623:LEU:HD13	1:A:1640:ARG:NH1	2.32	0.45
1:B:1989:ASN:HB3	1:B:1993:LYS:NZ	2.32	0.45
1:B:1440:PHE:HB3	1:B:1442:GLU:HB2	1.98	0.45
1:A:2514:SER:OG	1:A:2517:ASP:HB2	2.17	0.45
2:C:75:PRO:HB2	2:C:76:ASN:H	1.52	0.45
2:D:248:ARG:HG3	2:D:253:SER:OG	2.17	0.45
1:B:1631:GLU:HA	1:B:1634:GLN:HE21	1.82	0.45
1:A:2223:GLN:HB3	1:A:2354:LEU:HD13	1.99	0.45
1:B:1590:MET:O	1:B:1594:HIS:HB2	2.17	0.45
1:B:2392:LEU:O	1:B:2397:ARG:HB2	2.17	0.44
1:B:2036:ARG:HD3	1:B:2036:ARG:HA	1.73	0.44
1:A:2324:LEU:HA	1:A:2353:ILE:HG21	1.99	0.44
1:B:1629:ILE:O	1:B:1630:VAL:C	2.54	0.44
1:A:2418:LEU:O	1:A:2422:VAL:HG23	2.17	0.44
3:B:2601:17G:H11	3:B:2601:17G:H9	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1913:TYR:HB2	1:B:1915:HIS:CE1	2.52	0.44
1:B:2052:GLU:CG	1:B:2053:PRO:HD3	2.46	0.44
1:B:2208:LEU:HD22	1:B:2410:HIS:CG	2.52	0.44
1:B:2513:PHE:HB2	1:B:2519:LEU:HD11	1.99	0.44
1:A:2209:LEU:O	1:A:2215:SER:HB2	2.17	0.44
2:C:248:ARG:HG3	2:C:253:SER:OG	2.18	0.44
1:A:1974:TYR:O	1:A:1978:VAL:HG23	2.18	0.44
1:B:1501:TRP:HH2	1:B:1509:GLN:OE1	2.01	0.44
1:B:2122:GLU:O	1:B:2126:VAL:HG23	2.17	0.44
1:B:2023:TRP:CD2	1:B:2067:GLU:HG2	2.53	0.44
1:B:2240:VAL:HG21	1:B:2354:LEU:HD21	1.99	0.44
1:B:1759:LEU:HD21	1:B:1772:VAL:HG21	1.99	0.44
2:D:188:VAL:HA	2:D:193:ASN:O	2.17	0.44
2:D:242:GLN:HB2	2:D:260:ILE:HG13	1.99	0.44
1:A:1530:GLU:HA	1:A:1550:LEU:HD11	1.99	0.44
1:B:2268:MET:HG2	1:B:2286:VAL:HG12	1.98	0.44
1:A:2322:ARG:O	1:A:2326:VAL:HG23	2.18	0.44
1:A:2344:LEU:CD1	1:A:2353:ILE:HD11	2.41	0.44
1:A:2345:MET:CE	3:A:2601:17G:H1	2.47	0.44
2:C:15:LEU:HD13	2:C:320:PHE:HD1	1.83	0.44
2:C:188:VAL:HA	2:C:193:ASN:O	2.17	0.44
1:A:1759:LEU:HD21	1:A:1772:VAL:HG21	1.98	0.44
2:D:159:THR:C	2:D:161:HIS:H	2.21	0.44
1:B:2278:LEU:HB3	1:B:2282:GLN:HB2	1.99	0.44
1:A:1717:MET:O	1:A:1721:VAL:HG23	2.16	0.44
1:A:1416:LEU:HA	1:A:1419:ILE:CG2	2.48	0.44
2:C:102:THR:O	2:C:109:ALA:HA	2.18	0.44
2:C:231:ASP:CB	2:C:233:THR:OG1	2.53	0.44
2:C:195:TYR:CE2	2:C:215:LYS:HG3	2.53	0.44
3:A:2601:17G:C19	3:A:2601:17G:C30	2.90	0.44
1:A:1785:SER:O	1:A:1786:TRP:CB	2.65	0.44
1:A:1710:LYS:NZ	1:A:1760:ASN:HD21	2.16	0.44
1:A:2023:TRP:CD2	1:A:2067:GLU:HG2	2.53	0.44
1:A:2170:ARG:HB2	1:A:2186:LEU:HB3	2.00	0.44
1:B:1895:SER:HB2	1:B:1899:ASN:HB3	2.00	0.44
1:B:2418:LEU:HD13	1:B:2504:VAL:HG11	1.99	0.44
1:B:1755:GLY:HA2	1:B:1772:VAL:HG12	2.00	0.43
2:D:239:SER:HB3	2:D:241:ASP:OD2	2.18	0.43
1:B:2167:GLN:O	1:B:2168:ARG:C	2.55	0.43
1:B:1498:CYS:HA	1:B:1501:TRP:HD1	1.82	0.43
2:C:270:ARG:HD2	2:C:270:ARG:HA	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1698:TYR:O	1:B:1702:LYS:HG2	2.17	0.43
1:B:2322:ARG:O	1:B:2326:VAL:HG23	2.18	0.43
1:B:1892:ILE:HD11	1:B:1903:THR:HA	2.00	0.43
1:A:1755:GLY:HA2	1:A:1772:VAL:HG12	2.00	0.43
2:D:237:THR:O	2:D:244:CYS:HA	2.18	0.43
1:A:2512:ASP:N	1:A:2512:ASP:OD1	2.50	0.43
1:A:1595:MET:HG2	1:A:1639:VAL:HG21	2.00	0.43
2:C:128:ASN:O	2:C:129:ALA:CB	2.66	0.43
1:A:2028:HIS:HE1	1:A:2112:SER:OG	2.00	0.43
1:B:1393:TYR:CZ	1:B:1422:LYS:HD2	2.53	0.43
1:B:2378:ARG:NH1	1:B:2380:THR:HG21	2.33	0.43
1:B:2170:ARG:HB2	1:B:2186:LEU:HB3	2.00	0.43
2:D:267:GLU:O	2:D:267:GLU:HG3	2.18	0.43
1:A:1594:HIS:HE1	1:A:1622:ARG:HD2	1.82	0.43
2:C:166:ILE:HD12	2:C:167:PRO:O	2.18	0.43
1:A:1999:CYS:C	1:A:2001:HIS:N	2.70	0.43
1:B:2093:ASN:ND2	1:B:2095:LYS:H	2.16	0.43
1:A:1564:ILE:HD13	1:A:1600:GLU:HG3	2.00	0.43
1:B:2022:LEU:HD21	1:B:2126:VAL:HG13	2.00	0.43
1:B:1416:LEU:HA	1:B:1419:ILE:CG2	2.49	0.43
1:B:2324:LEU:HA	1:B:2353:ILE:HG21	2.00	0.43
1:B:1623:LEU:O	1:B:1633:TRP:HH2	2.01	0.43
1:A:2281:MET:HA	1:A:2281:MET:HE2	2.00	0.43
1:A:1400:LYS:HD2	1:A:1412:ILE:HG23	2.00	0.43
1:B:1402:LEU:O	1:B:1405:GLN:HB2	2.19	0.43
1:A:1771:LYS:O	1:A:1774:GLN:HB3	2.18	0.43
1:B:2345:MET:HE2	3:B:2601:17G:H1	2.01	0.43
1:B:1950:ARG:HA	1:B:1951:PRO:HD3	1.90	0.43
1:A:1414:GLU:O	1:A:1417:ILE:HG13	2.19	0.43
2:D:262:SER:HB2	2:D:263:GLY:H	1.60	0.43
1:B:1423:LEU:HD12	1:B:1423:LEU:HA	1.92	0.43
1:B:1734:THR:C	1:B:1736:ASP:N	2.71	0.43
1:A:1972:LEU:O	1:A:1975:PRO:HG2	2.19	0.43
1:A:1470:ASN:HB3	1:A:1471:LYS:H	1.59	0.43
1:A:2254:ARG:HD2	1:A:2259:ILE:HB	2.01	0.43
1:B:1892:ILE:HG21	1:B:1930:ILE:CD1	2.42	0.43
2:D:15:LEU:HD13	2:D:320:PHE:HD1	1.84	0.43
1:B:1501:TRP:HA	1:B:1503:LEU:HG	2.00	0.43
1:A:2167:GLN:O	1:A:2168:ARG:C	2.57	0.43
1:B:1514:ARG:HH21	1:B:1540:THR:HG21	1.84	0.43
1:A:1473:ASP:HA	1:A:1474:PRO:HD2	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2282:GLN:HE21	2:C:316:VAL:HG11	1.84	0.42
1:A:1900:LEU:HD23	1:A:2204:LEU:HD22	2.01	0.42
1:A:2036:ARG:HD3	1:A:2036:ARG:HA	1.74	0.42
1:A:2378:ARG:NH1	1:A:2380:THR:HG21	2.34	0.42
2:D:166:ILE:O	2:D:166:ILE:HG13	2.19	0.42
2:D:78:ILE:HG22	2:D:79:ILE:HG13	2.01	0.42
2:C:127:VAL:HG11	2:C:153:HIS:HE1	1.81	0.42
1:A:2240:VAL:O	3:A:2601:17G:H7	2.19	0.42
1:A:1590:MET:O	1:A:1594:HIS:HB2	2.20	0.42
1:B:1890:ARG:O	1:B:1894:LEU:HG	2.19	0.42
1:A:1721:VAL:HG11	1:A:1751:PHE:CZ	2.54	0.42
1:B:1574:GLU:HG2	1:B:1585:ARG:NH2	2.34	0.42
2:D:270:ARG:HA	2:D:270:ARG:HD2	1.87	0.42
1:A:2080:GLU:O	1:A:2083:GLU:HB3	2.19	0.42
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.53	0.42
1:A:2281:MET:CE	2:C:222:TYR:CD2	3.02	0.42
1:A:2093:ASN:ND2	1:A:2095:LYS:H	2.17	0.42
1:A:1602:VAL:HG13	1:A:1643:VAL:CG2	2.48	0.42
1:A:1629:ILE:O	1:A:1630:VAL:C	2.57	0.42
1:B:2198:VAL:HG11	1:B:2358:PHE:CD2	2.54	0.42
1:A:2319:ASN:HB3	1:A:2352:LYS:HG2	2.00	0.42
2:C:262:SER:HB2	2:C:263:GLY:H	1.57	0.42
1:A:2340:HIS:HB2	1:A:2341:PRO:CD	2.49	0.42
1:B:1970:GLN:C	1:B:1972:LEU:N	2.73	0.42
2:C:95:GLU:HB2	2:C:140:GLN:HE22	1.80	0.42
1:A:1882:VAL:HG12	1:A:1886:GLN:NE2	2.35	0.42
2:C:242:GLN:HB2	2:C:260:ILE:HG13	2.01	0.42
1:B:2156:ILE:HG12	1:B:2174:LEU:HD22	2.01	0.42
1:B:1972:LEU:O	1:B:1975:PRO:HG2	2.19	0.42
2:C:168:GLU:HB3	2:C:195:TYR:OH	2.20	0.42
2:D:95:GLU:HB2	2:D:140:GLN:HE21	1.80	0.42
1:B:1604:GLN:O	1:B:1608:VAL:CG2	2.65	0.42
2:C:288:ALA:HB1	2:C:315:VAL:HG12	2.01	0.42
1:A:1933:ASP:O	1:A:1934:THR:C	2.58	0.42
1:A:1437:MET:SD	1:A:1453:LEU:HD11	2.59	0.42
1:B:1717:MET:O	1:B:1721:VAL:HG23	2.18	0.42
2:D:128:ASN:O	2:D:129:ALA:CB	2.67	0.42
1:A:1643:VAL:HG12	1:A:1644:VAL:CG2	2.48	0.42
1:B:1882:VAL:HG12	1:B:1886:GLN:NE2	2.35	0.42
2:C:60:ALA:HB1	2:C:88:ILE:HG22	2.02	0.42
1:A:1423:LEU:HD12	1:A:1423:LEU:HA	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2281:MET:HE2	1:B:2281:MET:CA	2.50	0.41
2:C:262:SER:OG	2:C:267:GLU:HG2	2.20	0.41
1:A:1791:HIS:O	1:A:1795:VAL:HG23	2.20	0.41
1:B:2285:GLU:HG3	2:D:272:TRP:CE2	2.55	0.41
2:D:18:ALA:HB1	2:D:45:VAL:HG21	2.02	0.41
1:B:2346:LEU:HD23	1:B:2353:ILE:HG13	2.01	0.41
1:B:2187:LYS:HG3	1:B:2237:ILE:HD12	2.02	0.41
1:B:2240:VAL:O	3:B:2601:17G:H7	2.20	0.41
1:B:1680:ASP:OD2	1:B:1683:ARG:HB2	2.20	0.41
2:C:44:GLN:H	2:C:44:GLN:HG3	1.56	0.41
1:B:1939:ILE:N	1:B:1940:PRO:HD2	2.36	0.41
1:B:1497:CYS:SG	1:B:1516:ALA:CB	3.09	0.41
1:A:2199:MET:SD	1:A:2224:ARG:HB2	2.60	0.41
2:D:231:ASP:HB3	2:D:233:THR:HG1	1.75	0.41
2:C:166:ILE:HG13	2:C:166:ILE:O	2.20	0.41
2:D:69:ASP:HB2	2:D:78:ILE:CD1	2.47	0.41
1:B:2339:ARG:HH21	1:B:2343:ASN:HB3	1.85	0.41
1:A:1680:ASP:OD2	1:A:1683:ARG:HB2	2.20	0.41
1:B:1712:ASP:OD1	1:A:2266:ARG:NH2	2.53	0.41
1:B:1882:VAL:N	1:B:1883:PRO:HD2	2.36	0.41
1:B:1882:VAL:CG1	1:B:1886:GLN:HE21	2.33	0.41
1:A:1807:GLN:O	1:A:1810:ALA:HB3	2.20	0.41
1:B:1473:ASP:HA	1:B:1474:PRO:HD2	1.72	0.41
1:A:1402:LEU:O	1:A:1405:GLN:HB2	2.21	0.41
2:C:186:ALA:HA	2:C:195:TYR:O	2.20	0.41
2:D:44:GLN:HG3	2:D:44:GLN:H	1.53	0.41
2:C:105:GLU:HA	2:C:130:PRO:HB3	2.01	0.41
1:A:2139:ALA:HA	1:A:2151:ILE:O	2.21	0.41
1:B:2382:MET:HG3	1:B:2549:TRP:O	2.21	0.41
2:D:167:PRO:HB2	2:D:168:GLU:H	1.64	0.41
1:B:1621:GLU:C	1:B:1623:LEU:H	2.24	0.41
1:A:1628:ARG:HB2	1:A:1633:TRP:CD1	2.55	0.41
2:C:8:VAL:HG21	2:C:36:ARG:HD3	2.03	0.41
2:D:286:VAL:HB	2:D:318:LEU:HD13	2.03	0.41
1:A:2503:ARG:HH11	1:A:2507:LYS:HE3	1.86	0.41
1:B:2401:HIS:CD2	1:B:2522:PRO:HA	2.56	0.41
1:B:2028:HIS:HE1	1:B:2112:SER:OG	2.03	0.41
2:D:312:GLN:H	2:D:312:GLN:HG2	1.64	0.41
1:A:1634:GLN:HG2	1:A:1656:TYR:OH	2.21	0.41
1:A:1890:ARG:O	1:A:1894:LEU:HG	2.20	0.41
2:D:100:MET:HB3	2:D:112:TRP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1999:CYS:C	1:B:2001:HIS:N	2.73	0.41
2:D:65:ILE:HD13	2:D:102:THR:HG21	2.02	0.41
2:C:267:GLU:O	2:C:267:GLU:HG3	2.20	0.41
1:B:2080:GLU:O	1:B:2083:GLU:HB3	2.21	0.41
2:C:76:ASN:CB	2:C:77:PRO:HD2	2.21	0.41
1:B:1943:ILE:CD1	1:B:1975:PRO:HB2	2.51	0.41
2:C:178:ILE:HD11	2:C:199:LEU:HD11	2.02	0.41
1:B:1916:TRP:N	1:B:1916:TRP:CD1	2.80	0.41
1:A:1915:HIS:CE1	1:A:1919:VAL:HG11	2.55	0.41
1:A:1583:TYR:C	1:A:1585:ARG:N	2.75	0.41
1:B:2121:LEU:HA	1:B:2121:LEU:HD23	1.86	0.41
1:B:2287:PHE:O	1:B:2291:VAL:HG23	2.21	0.41
1:B:2297:ASP:HB2	1:B:2298:ASP:H	1.67	0.41
1:B:2197:ARG:HB3	1:B:2421:PHE:CD2	2.56	0.41
1:A:1493:LEU:CD2	1:A:1519:ALA:HB2	2.51	0.41
1:A:1717:MET:HG3	1:A:1754:LEU:HG	2.02	0.41
2:C:14:ILE:HD13	2:C:70:LEU:HD13	2.03	0.41
1:B:1609:PRO:HB3	1:B:1612:ARG:HH11	1.86	0.40
1:A:2419:GLU:HG2	1:A:2501:ILE:HD13	2.02	0.40
1:A:1916:TRP:N	1:A:1916:TRP:CD1	2.80	0.40
1:B:1605:TYR:CG	1:B:1643:VAL:HG11	2.56	0.40
1:A:1621:GLU:C	1:A:1623:LEU:H	2.24	0.40
1:A:2418:LEU:HD13	1:A:2504:VAL:HG11	2.02	0.40
1:A:1892:ILE:HD11	1:A:1903:THR:HA	2.03	0.40
1:B:1915:HIS:CE1	1:B:1919:VAL:HG11	2.56	0.40
1:A:2299:LEU:O	1:A:2303:LEU:HG	2.22	0.40
2:C:95:GLU:HB2	2:C:140:GLN:HE21	1.81	0.40
1:A:2064:THR:HG21	1:A:2126:VAL:O	2.22	0.40
1:B:2530:LYS:HA	1:B:2530:LYS:CE	2.50	0.40
2:D:262:SER:CB	2:D:267:GLU:HG2	2.51	0.40
1:B:2032:GLU:O	1:B:2036:ARG:HG2	2.21	0.40
1:A:2173:THR:HB	1:A:2183:VAL:HG13	2.04	0.40
1:B:1888:PHE:O	1:B:1892:ILE:HG13	2.20	0.40
1:A:2415:MET:O	1:A:2419:GLU:HB2	2.21	0.40
1:A:1880:TYR:O	1:A:1883:PRO:HG2	2.22	0.40
2:C:65:ILE:HD13	2:C:102:THR:HG21	2.02	0.40
1:B:2268:MET:HG3	1:B:2290:ALA:HB2	2.04	0.40
1:A:1980:SER:O	1:A:1988:HIS:HB2	2.22	0.40
1:B:2223:GLN:HB3	1:B:2354:LEU:HD13	2.04	0.40
1:B:1608:VAL:HA	1:B:1609:PRO:HD3	1.81	0.40
1:B:2157:ALA:HB3	1:B:2173:THR:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2264:GLU:HG3	1:B:2294:THR:HG21	2.03	0.40
2:C:18:ALA:HB1	2:C:45:VAL:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1046/1174 (89%)	922 (88%)	96 (9%)	28 (3%)	6	44
1	B	1052/1174 (90%)	925 (88%)	97 (9%)	30 (3%)	6	42
2	C	315/326 (97%)	275 (87%)	26 (8%)	14 (4%)	3	30
2	D	315/326 (97%)	272 (86%)	29 (9%)	14 (4%)	3	30
All	All	2728/3000 (91%)	2394 (88%)	248 (9%)	86 (3%)	5	40

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1525	GLN
1	B	1630	VAL
1	B	1650	MET
1	B	1709	ARG
1	B	1896	ARG
1	B	1970	GLN
1	B	2094	VAL
1	B	2298	ASP
2	D	73	ASN
2	D	74	ASN
2	D	97	GLY
2	D	118	ASN
2	D	203	ILE

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Mol	Chain	Res	Type
2	D	269	SER
1	A	1525	GLN
1	A	1630	VAL
1	A	1650	MET
1	A	1709	ARG
1	A	1896	ARG
1	A	1970	GLN
1	A	2094	VAL
1	A	2298	ASP
2	C	73	ASN
2	C	74	ASN
2	C	97	GLY
2	C	118	ASN
2	C	203	ILE
2	C	269	SER
1	B	1445	ILE
1	B	1470	ASN
1	B	1735	GLU
1	B	1914	GLY
1	B	1937	GLN
1	B	2093	ASN
1	B	2364	VAL
2	D	35	THR
2	D	75	PRO
2	D	167	PRO
2	D	169	PRO
2	D	204	GLY
1	A	1445	ILE
1	A	1734	THR
1	A	1735	GLU
1	A	1914	GLY
1	A	1937	GLN
1	A	2093	ASN
1	A	2364	VAL
2	C	35	THR
2	C	75	PRO
2	C	167	PRO
2	C	169	PRO
2	C	204	GLY
1	B	1444	GLU
1	B	1681	PRO
1	B	1682	SER

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Mol	Chain	Res	Type
1	B	1784	ARG
1	B	2000	GLU
1	B	2357	ASP
1	B	2368	ARG
2	D	129	ALA
1	A	1444	GLU
1	A	1454	HIS
1	A	1470	ASN
1	A	1681	PRO
1	A	1682	SER
1	A	1784	ARG
1	A	2000	GLU
1	A	2357	ASP
2	C	129	ALA
1	B	1426	PRO
1	B	1734	THR
1	B	2001	HIS
2	D	208	THR
1	A	1426	PRO
1	A	2001	HIS
1	B	1454	HIS
1	B	1786	TRP
1	A	1786	TRP
2	C	208	THR
2	C	310	GLY
1	B	1415	SER
2	D	310	GLY
1	A	2072	GLN
1	B	1474	PRO
1	A	1474	PRO
1	B	1680	ASP

5.3.2 Protein sidechains (i)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	927/1024 (90%)	838 (90%)	89 (10%)	10 43
1	B	930/1024 (91%)	839 (90%)	91 (10%)	10 42
2	C	269/276 (98%)	240 (89%)	29 (11%)	8 37
2	D	269/276 (98%)	240 (89%)	29 (11%)	8 37
All	All	2395/2600 (92%)	2157 (90%)	238 (10%)	10 41

All (238) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1395	LYS
1	B	1402	LEU
1	B	1417	ILE
1	B	1420	ASN
1	B	1423	LEU
1	B	1443	LEU
1	B	1457	GLU
1	B	1487	LEU
1	B	1501	TRP
1	B	1509	GLN
1	B	1528	SER
1	B	1540	THR
1	B	1541	HIS
1	B	1559	LEU
1	B	1578	MET
1	B	1585	ARG
1	B	1590	MET
1	B	1593	CYS
1	B	1630	VAL
1	B	1679	VAL
1	B	1685	LEU
1	B	1709	ARG
1	B	1780	THR
1	B	1878	LEU
1	B	1891	SER
1	B	1895	SER
1	B	1896	ARG
1	B	1899	ASN
1	B	1908	THR
1	B	1912	ASP

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Mol	Chain	Res	Type
1	B	1916	TRP
1	B	1932	ILE
1	B	1938	VAL
1	B	1956	LEU
1	B	1968	HIS
1	B	1970	GLN
1	B	1973	ILE
1	B	1984	THR
1	B	1985	THR
1	B	2001	HIS
1	B	2005	LEU
1	B	2011	MET
1	B	2021	ILE
1	B	2023	TRP
1	B	2036	ARG
1	B	2041	GLU
1	B	2068	THR
1	B	2072	GLN
1	B	2076	ARG
1	B	2077	ASP
1	B	2078	LEU
1	B	2080	GLU
1	B	2090	LYS
1	B	2093	ASN
1	B	2095	LYS
1	B	2124	GLN
1	B	2138	LEU
1	B	2152	ARG
1	B	2154	GLN
1	B	2155	SER
1	B	2164	THR
1	B	2166	LYS
1	B	2168	ARG
1	B	2173	THR
1	B	2178	ASN
1	B	2181	GLU
1	B	2189	HIS
1	B	2214	THR
1	B	2223	GLN
1	B	2224	ARG
1	B	2228	ILE
1	B	2244	ASP

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Mol	Chain	Res	Type
1	B	2254	ARG
1	B	2255	GLU
1	B	2260	LEU
1	B	2266	ARG
1	B	2281	MET
1	B	2318	THR
1	B	2342	SER
1	B	2363	GLU
1	B	2378	ARG
1	B	2385	ASN
1	B	2390	THR
1	B	2408	ARG
1	B	2431	LEU
1	B	2432	MET
1	B	2495	LYS
1	B	2503	ARG
1	B	2515	HIS
1	B	2519	LEU
1	B	2530	LYS
2	D	13	VAL
2	D	44	GLN
2	D	74	ASN
2	D	80	SER
2	D	84	VAL
2	D	85	ASN
2	D	86	LYS
2	D	90	SER
2	D	116	SER
2	D	128	ASN
2	D	159	THR
2	D	160	ASP
2	D	162	ASN
2	D	165	LEU
2	D	166	ILE
2	D	168	GLU
2	D	169	PRO
2	D	170	GLU
2	D	183	SER
2	D	188	VAL
2	D	199	LEU
2	D	214	THR
2	D	248	ARG

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Mol	Chain	Res	Type
2	D	262	SER
2	D	269	SER
2	D	287	THR
2	D	289	SER
2	D	301	THR
2	D	312	GLN
1	A	1385	GLU
1	A	1395	LYS
1	A	1402	LEU
1	A	1417	ILE
1	A	1420	ASN
1	A	1423	LEU
1	A	1443	LEU
1	A	1457	GLU
1	A	1487	LEU
1	A	1501	TRP
1	A	1509	GLN
1	A	1528	SER
1	A	1540	THR
1	A	1541	HIS
1	A	1559	LEU
1	A	1578	MET
1	A	1585	ARG
1	A	1590	MET
1	A	1593	CYS
1	A	1630	VAL
1	A	1679	VAL
1	A	1685	LEU
1	A	1709	ARG
1	A	1780	THR
1	A	1878	LEU
1	A	1891	SER
1	A	1895	SER
1	A	1896	ARG
1	A	1899	ASN
1	A	1908	THR
1	A	1912	ASP
1	A	1916	TRP
1	A	1932	ILE
1	A	1956	LEU
1	A	1968	HIS
1	A	1970	GLN

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Mol	Chain	Res	Type
1	A	1973	ILE
1	A	1984	THR
1	A	1985	THR
1	A	2001	HIS
1	A	2005	LEU
1	A	2011	MET
1	A	2023	TRP
1	A	2036	ARG
1	A	2041	GLU
1	A	2068	THR
1	A	2072	GLN
1	A	2076	ARG
1	A	2077	ASP
1	A	2078	LEU
1	A	2080	GLU
1	A	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	2155	SER
1	A	2164	THR
1	A	2166	LYS
1	A	2168	ARG
1	A	2173	THR
1	A	2178	ASN
1	A	2181	GLU
1	A	2189	HIS
1	A	2223	GLN
1	A	2224	ARG
1	A	2228	ILE
1	A	2244	ASP
1	A	2254	ARG
1	A	2260	LEU
1	A	2266	ARG
1	A	2281	MET
1	A	2318	THR
1	A	2342	SER
1	A	2363	GLU
1	A	2378	ARG

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Mol	Chain	Res	Type
1	A	2385	ASN
1	A	2390	THR
1	A	2408	ARG
1	A	2415	MET
1	A	2431	LEU
1	A	2432	MET
1	A	2495	LYS
1	A	2503	ARG
1	A	2515	HIS
1	A	2519	LEU
1	A	2530	LYS
2	C	13	VAL
2	C	44	GLN
2	C	74	ASN
2	C	80	SER
2	C	84	VAL
2	C	85	ASN
2	C	86	LYS
2	C	90	SER
2	C	123	ARG
2	C	128	ASN
2	C	159	THR
2	C	160	ASP
2	C	162	ASN
2	C	165	LEU
2	C	166	ILE
2	C	168	GLU
2	C	169	PRO
2	C	170	GLU
2	C	183	SER
2	C	188	VAL
2	C	199	LEU
2	C	214	THR
2	C	248	ARG
2	C	262	SER
2	C	269	SER
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 (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1439	HIS
1	B	1496	GLN
1	B	1505	ASN
1	B	1594	HIS
1	B	1670	HIS
1	B	1687	HIS
1	B	1760	ASN
1	B	1782	HIS
1	B	1797	ASN
1	B	1886	GLN
1	B	1898	ASN
1	B	1941	GLN
1	B	1958	HIS
1	B	1970	GLN
1	B	2001	HIS
1	B	2028	HIS
1	B	2082	GLN
1	B	2093	ASN
1	B	2154	GLN
1	B	2167	GLN
1	B	2178	ASN
1	B	2189	HIS
1	B	2233	ASN
1	B	2247	HIS
1	B	2262	ASN
1	B	2319	ASN
1	B	2355	HIS
1	B	2395	ASN
1	B	2401	HIS
1	B	2502	ASN
2	D	30	HIS
2	D	63	GLN
2	D	85	ASN
2	D	94	HIS
2	D	122	GLN
2	D	137	HIS
2	D	140	GLN
2	D	153	HIS
2	D	161	HIS
2	D	242	GLN
2	D	311	HIS
2	D	312	GLN
1	A	1439	HIS

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Mol	Chain	Res	Type
1	A	1496	GLN
1	A	1505	ASN
1	A	1594	HIS
1	A	1670	HIS
1	A	1687	HIS
1	A	1716	HIS
1	A	1760	ASN
1	A	1782	HIS
1	A	1886	GLN
1	A	1898	ASN
1	A	1941	GLN
1	A	1958	HIS
1	A	1970	GLN
1	A	2001	HIS
1	A	2028	HIS
1	A	2082	GLN
1	A	2093	ASN
1	A	2154	GLN
1	A	2167	GLN
1	A	2178	ASN
1	A	2189	HIS
1	A	2223	GLN
1	A	2233	ASN
1	A	2247	HIS
1	A	2262	ASN
1	A	2319	ASN
1	A	2395	ASN
1	A	2401	HIS
1	A	2502	ASN
2	C	30	HIS
2	C	63	GLN
2	C	85	ASN
2	C	94	HIS
2	C	122	GLN
2	C	137	HIS
2	C	140	GLN
2	C	153	HIS
2	C	161	HIS
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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	17G	A	2601	-	34,36,36	1.26	4 (11%)	49,54,54	1.46	9 (18%)
3	17G	B	2601	-	34,36,36	1.18	4 (11%)	49,54,54	1.66	12 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	17G	A	2601	-	-	0/14/14/14	0/5/5/5
3	17G	B	2601	-	-	0/14/14/14	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2601	17G	C19-N8	-3.87	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2601	17G	C37-C33	-3.69	1.39	1.49
3	B	2601	17G	C37-C33	-3.43	1.40	1.49
3	B	2601	17G	C19-N8	-3.12	1.42	1.46
3	A	2601	17G	C27-N8	2.11	1.41	1.37
3	B	2601	17G	C27-N8	2.15	1.41	1.37
3	B	2601	17G	C34-N9	2.62	1.34	1.30
3	A	2601	17G	C34-N9	2.65	1.34	1.30

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2601	17G	C20-C19-N8	-3.37	115.78	119.27
3	B	2601	17G	C21-C19-C20	-3.17	118.63	121.50
3	A	2601	17G	C20-C19-N8	-3.06	116.10	119.27
3	A	2601	17G	C27-N8-C19	-2.99	115.89	119.39
3	B	2601	17G	C26-C34-N9	-2.96	120.27	124.83
3	B	2601	17G	C31-C26-C34	-2.94	116.64	122.64
3	B	2601	17G	C27-N8-C19	-2.87	116.04	119.39
3	A	2601	17G	C31-C26-C34	-2.70	117.13	122.64
3	A	2601	17G	C26-C34-N9	-2.60	120.82	124.83
3	B	2601	17G	C37-C39-N10	-2.37	120.51	124.34
3	B	2601	17G	C27-N8-C23	-2.04	118.94	120.92
3	A	2601	17G	C34-N9-C29	2.01	120.93	117.92
3	B	2601	17G	C34-C26-C23	2.01	120.78	117.33
3	A	2601	17G	C34-C26-C23	2.05	120.84	117.33
3	B	2601	17G	C34-N9-C29	2.22	121.25	117.92
3	A	2601	17G	C31-C26-C23	2.52	122.03	117.94
3	A	2601	17G	C32-C27-N8	2.78	121.47	118.84
3	B	2601	17G	C31-C26-C23	2.87	122.58	117.94
3	B	2601	17G	C32-C27-N8	3.14	121.81	118.84
3	A	2601	17G	C21-C19-N8	3.38	124.08	119.22
3	B	2601	17G	C21-C19-N8	4.41	125.54	119.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2601	17G	8	0
3	B	2601	17G	6	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1054/1174 (89%)	-0.17	19 (1%) 71 62	37, 70, 153, 188	0
1	B	1058/1174 (90%)	-0.27	17 (1%) 74 65	32, 61, 135, 180	0
2	C	317/326 (97%)	-0.20	3 (0%) 85 78	38, 70, 118, 156	0
2	D	317/326 (97%)	-0.35	0 100 100	29, 49, 97, 141	0
All	All	2746/3000 (91%)	-0.23	39 (1%) 78 68	29, 63, 144, 188	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1580	GLY	6.7
1	B	1446	GLN	5.3
1	B	1581	GLU	4.5
1	A	2436	THR	4.3
1	B	1582	SER	4.3
1	A	1582	SER	4.0
1	A	1581	GLU	4.0
1	B	2434	THR	3.4
2	C	8	VAL	3.4
1	A	2435	ASN	3.3
1	A	2434	THR	3.2
1	B	1469	THR	3.1
1	B	2436	THR	3.0
1	B	2433	ASP	2.9
2	C	205	ASP	2.9
1	B	1385	GLU	2.8
1	A	2038	TYR	2.8
1	B	1504	VAL	2.8
1	A	1385	GLU	2.8
1	B	1584	SER	2.8
1	B	2435	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1584	SER	2.6
1	B	1449	TRP	2.6
1	A	1579	ALA	2.5
1	A	2043	ASN	2.5
1	A	1586	ALA	2.4
1	B	1579	ALA	2.4
1	A	1554	GLN	2.4
1	B	1577	ALA	2.3
1	B	1580	GLY	2.3
1	A	2433	ASP	2.3
1	B	1505	ASN	2.3
1	A	1558	SER	2.3
1	A	2044	VAL	2.3
1	A	2097	LEU	2.2
1	A	1587	TYR	2.2
2	C	206	GLU	2.2
1	B	1540	THR	2.1
1	A	1583	TYR	2.1

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^{th} 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^2)	Q<0.9
3	17G	B	2601	32/32	0.96	0.21	0.30	36,37,38,38	0
3	17G	A	2601	32/32	0.96	0.20	-0.12	38,40,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.