



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:41 PM GMT

PDB ID : 4FT4
Title : crystal structure of Zea mays ZMET2 in complex H3(1-32)K9me2 peptide and SAH
Authors : Du, J.; Patel, D.J.
Deposited on : 2012-06-27
Resolution : 2.70 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 ⓘ symbol.

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

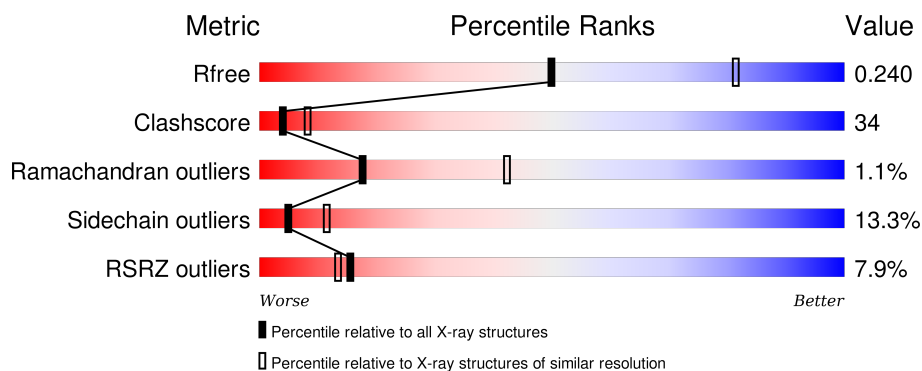
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 $\leq 5\%$. 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	784	<div> <div>11%</div> <div>38%</div> <div>41%</div> <div>9%</div> <div>12%</div> </div>
1	B	784	<div> <div>2%</div> <div>57%</div> <div>25%</div> <div>5%</div> <div>12%</div> </div>
2	P	32	<div> <div>6%</div> <div>13%</div> <div>78%</div> </div>
2	Q	32	<div> <div>13%</div> <div>6%</div> <div>84%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MLY	P	9	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11265 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 DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	693	Total	C	N	O	S	0	0	0
			5514	3521	939	1021	33			
1	A	688	Total	C	N	O	S	0	0	0
			5443	3476	931	1003	33			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	129	SER	-	EXPRESSION TAG	UNP Q9AXT8
A	129	SER	-	EXPRESSION TAG	UNP Q9AXT8

- Molecule 2 is a protein called H3(1-32)K9me2 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	0	0	0
			56	33	12	11			
2	Q	5	Total	C	N	O	0	0	0
			40	24	9	7			

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

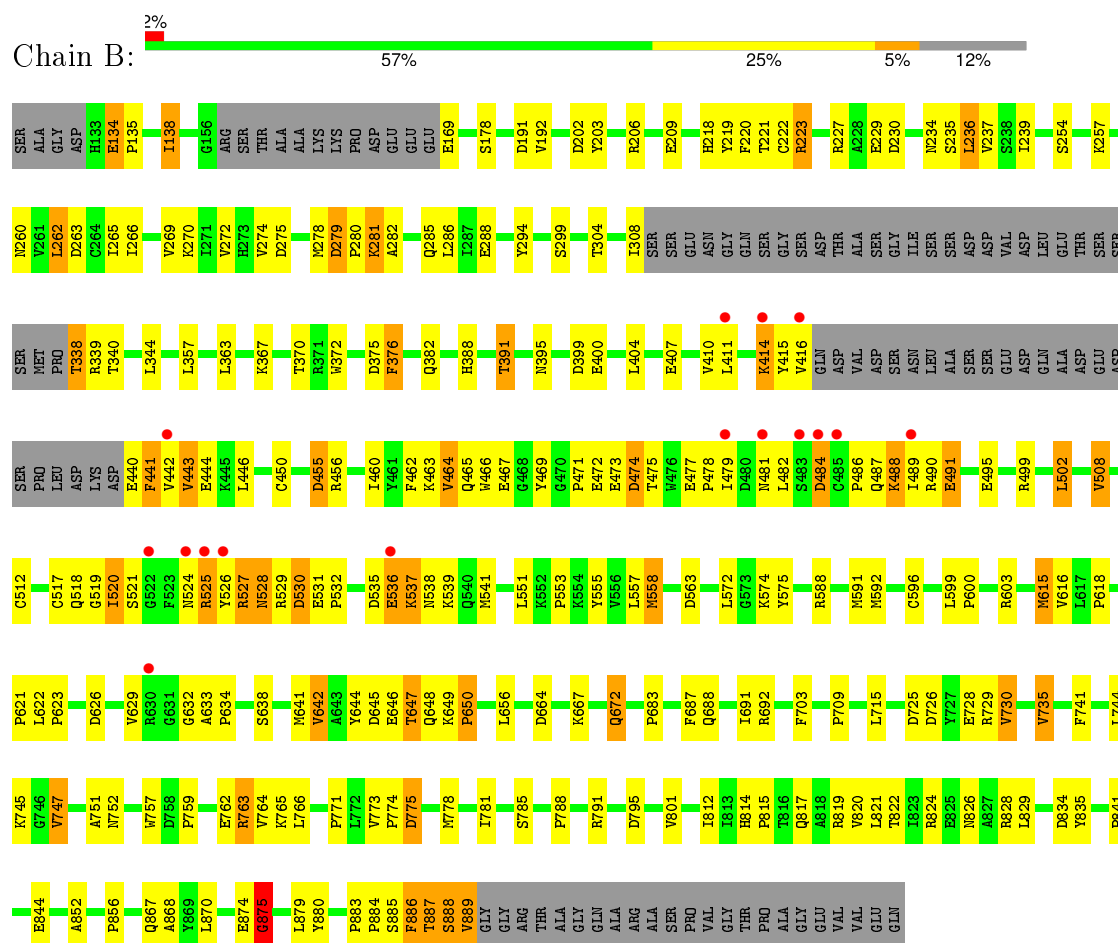
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	132	Total	O	0	0
			132	132		
4	A	27	Total	O	0	0
			27	27		
4	Q	1	Total	O	0	0
			1	1		

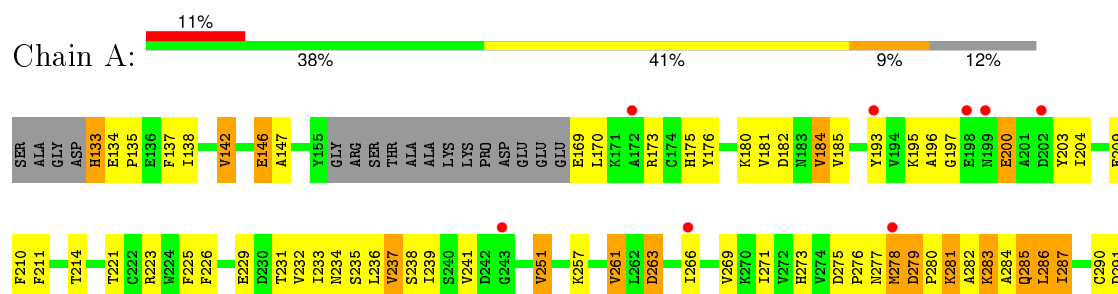
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: DNA (cytosine-5)-methyltransferase 1



• Molecule 1: DNA (cytosine-5)-methyltransferase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.64Å 111.56Å 151.48Å 90.00° 101.98° 90.00°	Depositor
Resolution (Å)	43.82 – 2.70 49.39 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.82-2.70) 97.8 (49.39-2.69)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.206 , 0.248 0.197 , 0.240	Depositor DCC
R_{free} test set	2880 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.7	EDS
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 57189 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11265	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.40	0/5577	0.56	2/7555 (0.0%)
1	B	0.47	1/5649 (0.0%)	0.50	0/7650
2	P	0.25	0/44	0.56	0/58
2	Q	0.27	0/28	0.66	0/36
All	All	0.44	1/11298 (0.0%)	0.53	2/15299 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	517	CYS	CB-SG	-5.43	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	PRO	N-CA-C	5.31	125.90	112.10
1	A	477	GLU	C-N-CD	-5.29	108.96	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	875	GLY	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	5443	0	5326	513	0
1	B	5514	0	5427	229	0
2	P	56	0	59	11	0
2	Q	40	0	45	9	0
3	A	26	0	19	5	0
3	B	26	0	19	5	0
4	A	27	0	0	2	0
4	B	132	0	0	5	0
4	Q	1	0	0	0	0
All	All	11265	0	10895	753	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 34.

All (753) 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:483:SER:O	1:A:486:PRO:HD3	1.31	1.26
1:A:533:LEU:HD12	1:A:534:LYS:N	1.52	1.22
1:A:589:LEU:O	1:A:589:LEU:HD12	1.34	1.20
1:A:285:GLN:CA	1:A:285:GLN:HE21	1.56	1.18
1:A:589:LEU:HD12	1:A:589:LEU:C	1.64	1.17
1:A:481:ASN:HD22	1:A:481:ASN:C	1.47	1.16
1:A:878:PRO:C	1:A:879:LEU:HD13	1.65	1.15
1:A:285:GLN:HE21	1:A:285:GLN:HA	1.07	1.15
1:A:526:TYR:HA	1:A:529:ARG:HD2	1.21	1.14
1:A:667:LYS:H	1:A:667:LYS:HD3	1.12	1.13
1:B:260:ASN:HD21	2:Q:7:ALA:HA	0.91	1.07
1:B:416:VAL:HG22	1:B:489:ILE:HG22	1.35	1.06
1:B:471:PRO:O	1:B:472:GLU:HB2	1.55	1.05
1:A:533:LEU:HD12	1:A:534:LYS:CA	1.85	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:TYR:CD1	2:P:9:MLY:HD3	1.91	1.04
1:A:285:GLN:NE2	1:A:285:GLN:HA	1.71	1.04
1:A:781:ILE:HG22	1:A:781:ILE:O	1.57	1.04
1:A:203:TYR:HD1	2:P:9:MLY:HD3	1.13	1.03
1:B:883:PRO:HB2	1:B:884:PRO:HD2	1.39	1.02
1:A:879:LEU:HD13	1:A:879:LEU:N	1.63	1.02
1:B:886:PHE:HD1	1:B:887:THR:H	1.03	1.02
1:A:209:GLU:HB2	1:A:221:THR:HB	1.38	1.02
1:A:481:ASN:C	1:A:481:ASN:ND2	2.07	1.01
1:B:528:ASN:ND2	1:B:535:ASP:HB3	1.76	1.01
1:A:589:LEU:CD1	1:A:589:LEU:C	2.30	1.00
1:A:413:LYS:HB2	1:A:413:LYS:NZ	1.75	1.00
1:A:793:TRP:HB3	1:A:815:PRO:HB3	1.41	1.00
1:A:536:GLU:O	1:A:537:LYS:HG2	1.62	1.00
1:B:886:PHE:CD1	1:B:887:THR:N	2.29	1.00
1:A:533:LEU:C	1:A:533:LEU:CD1	2.30	0.99
1:A:878:PRO:C	1:A:879:LEU:CD1	2.30	0.99
1:B:260:ASN:ND2	2:Q:7:ALA:HA	1.77	0.98
1:A:749:VAL:CG1	1:A:756:GLU:CB	2.41	0.97
1:B:279:ASP:OD2	1:B:280:PRO:HD2	1.64	0.97
1:A:414:LYS:O	1:A:415:TYR:HB2	1.65	0.96
1:A:169:GLU:OE1	1:A:169:GLU:N	1.98	0.95
1:A:533:LEU:CD1	1:A:534:LYS:N	2.30	0.95
1:A:749:VAL:O	1:A:749:VAL:HG22	1.63	0.95
1:B:466:TRP:HH2	1:B:475:THR:HG1	0.96	0.94
1:A:481:ASN:ND2	1:A:482:LEU:HG	1.81	0.94
1:A:537:LYS:HG3	1:A:537:LYS:O	1.64	0.93
1:A:203:TYR:CE1	2:P:9:MLY:HD2	2.04	0.92
1:A:735:VAL:HG22	1:A:791:ARG:HH22	1.35	0.92
1:A:749:VAL:HG12	1:A:756:GLU:CB	1.99	0.92
1:A:371:ARG:CG	1:A:371:ARG:HH11	1.84	0.91
1:B:508:VAL:HG11	1:B:551:LEU:HD13	1.52	0.91
1:A:485:CYS:HB3	1:A:488:LYS:HB2	1.53	0.91
1:A:481:ASN:HD21	1:A:482:LEU:HG	1.35	0.91
1:A:203:TYR:CD1	2:P:9:MLY:CD	2.55	0.90
1:B:528:ASN:ND2	1:B:536:GLU:CD	2.25	0.90
1:B:442:VAL:HG13	1:B:467:GLU:HB3	1.52	0.90
1:A:879:LEU:CD1	1:A:879:LEU:N	2.30	0.90
1:A:536:GLU:OE1	1:A:537:LYS:HG2	1.72	0.90
1:A:536:GLU:HG3	1:A:536:GLU:O	1.73	0.89
1:A:533:LEU:CD1	1:A:534:LYS:HA	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLN:N	1:A:285:GLN:HE21	1.70	0.89
1:B:443:VAL:O	1:B:443:VAL:HG22	1.72	0.89
1:A:671:HIS:HB2	1:A:721:ARG:HE	1.37	0.88
1:A:203:TYR:HE1	2:P:9:MLY:HD2	1.38	0.88
1:B:519:GLY:HA2	1:B:524:ASN:CB	2.04	0.88
1:A:724:ASN:O	1:A:725:ASP:HB2	1.74	0.87
1:A:749:VAL:HG11	1:A:756:GLU:CB	2.05	0.86
1:A:635:ASN:O	1:A:636:ALA:HB3	1.76	0.85
1:A:633:ALA:HB2	1:A:641:MET:HE2	1.57	0.85
1:A:485:CYS:HA	1:A:488:LYS:HD3	1.59	0.85
1:A:770:LYS:CG	1:A:771:PRO:HD2	2.05	0.85
1:A:793:TRP:CB	1:A:815:PRO:HB3	2.06	0.85
1:A:859:ARG:HH11	1:A:859:ARG:CG	1.90	0.85
1:A:877:ASP:OD2	1:A:878:PRO:HD2	1.76	0.85
1:B:260:ASN:HD21	2:Q:7:ALA:CA	1.83	0.85
1:A:525:ARG:O	1:A:526:TYR:CG	2.30	0.84
1:A:525:ARG:O	1:A:526:TYR:CD2	2.30	0.84
1:B:528:ASN:HD22	1:B:535:ASP:HB3	1.43	0.84
1:A:748:ARG:HD2	1:A:759:PRO:HD3	1.59	0.83
1:B:745:LYS:HG2	1:B:764:VAL:HG21	1.58	0.83
1:A:533:LEU:C	1:A:533:LEU:HD13	1.98	0.83
1:A:283:LYS:HA	1:A:283:LYS:HE2	1.59	0.83
1:A:484:ASP:O	1:A:486:PRO:HD2	1.78	0.82
1:A:283:LYS:CE	1:A:283:LYS:HA	2.09	0.82
1:A:602:PHE:HE2	1:A:630:ARG:HH12	1.21	0.82
1:A:533:LEU:CD1	1:A:534:LYS:CA	2.56	0.82
1:A:196:ALA:HA	1:A:203:TYR:HE2	1.43	0.82
1:A:667:LYS:HD3	1:A:667:LYS:N	1.94	0.81
1:A:285:GLN:CA	1:A:285:GLN:NE2	2.30	0.81
1:B:191:ASP:OD1	1:B:206:ARG:HD3	1.81	0.81
1:B:883:PRO:HB2	1:B:884:PRO:CD	2.11	0.81
1:A:485:CYS:CA	1:A:488:LYS:HD3	2.12	0.80
1:A:261:VAL:HG23	1:A:263:ASP:H	1.45	0.80
1:A:536:GLU:OE1	1:A:537:LYS:CE	2.30	0.79
1:B:416:VAL:HG21	1:B:490:ARG:CA	2.13	0.79
1:B:443:VAL:CG2	1:B:443:VAL:O	2.30	0.79
1:A:735:VAL:HG22	1:A:791:ARG:NH2	1.97	0.79
1:B:279:ASP:OD2	1:B:280:PRO:CD	2.30	0.79
1:A:811:VAL:O	1:A:811:VAL:HG22	1.81	0.79
1:B:275:ASP:O	1:B:278:MET:HG2	1.83	0.79
1:A:133:HIS:HE2	1:A:180:LYS:HG2	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LYS:CA	1:A:283:LYS:CE	2.60	0.79
1:A:811:VAL:O	1:A:811:VAL:CG2	2.31	0.79
1:B:209:GLU:HB2	1:B:221:THR:HB	1.63	0.79
1:A:536:GLU:O	1:A:537:LYS:CG	2.30	0.79
1:B:886:PHE:HD1	1:B:887:THR:N	1.75	0.78
1:A:142:VAL:CG2	1:A:147:ALA:HB2	2.13	0.78
1:A:415:TYR:O	1:A:416:VAL:HG13	1.83	0.78
1:B:519:GLY:HA2	1:B:524:ASN:HB2	1.65	0.78
1:A:602:PHE:CE2	1:A:630:ARG:NH1	2.50	0.78
1:A:651:SER:O	1:A:652:LEU:HD23	1.84	0.78
1:B:715:LEU:O	1:B:824:ARG:HD2	1.82	0.78
1:B:416:VAL:CG2	1:B:490:ARG:HA	2.13	0.78
1:A:794:TRP:HH2	1:A:816:THR:HG23	1.49	0.78
1:A:536:GLU:CG	1:A:536:GLU:O	2.29	0.78
1:A:536:GLU:OE1	1:A:537:LYS:HE2	1.84	0.77
1:A:283:LYS:CA	1:A:283:LYS:HE2	2.12	0.77
1:A:781:ILE:CG2	1:A:781:ILE:O	2.30	0.77
1:B:236:LEU:HD22	1:B:575:TYR:HA	1.66	0.77
1:A:728:GLU:OE1	1:A:766:LEU:HD23	1.85	0.77
1:A:819:ARG:HG2	1:A:820:VAL:O	1.84	0.77
1:B:528:ASN:HB2	1:B:535:ASP:OD1	1.82	0.77
1:B:442:VAL:CG1	1:B:467:GLU:HB3	2.14	0.77
1:A:203:TYR:CE1	2:P:9:MLY:CD	2.66	0.77
1:A:196:ALA:HA	1:A:203:TYR:CE2	2.19	0.77
1:B:645:ASP:OD2	1:B:647:THR:HG23	1.86	0.76
1:A:725:ASP:OD1	1:A:768:SER:CB	2.34	0.76
1:B:528:ASN:HB2	1:B:535:ASP:CG	2.06	0.76
1:A:415:TYR:O	1:A:416:VAL:HG22	1.86	0.76
1:A:460:ILE:O	1:A:461:TYR:HD2	1.69	0.75
1:A:483:SER:O	1:A:486:PRO:CD	2.25	0.75
1:A:823:ILE:HD11	1:A:842:ILE:HG23	1.67	0.75
1:A:223:ARG:HB3	1:A:257:LYS:HG2	1.67	0.75
1:A:867:GLN:NE2	1:A:872:GLU:O	2.20	0.74
1:A:371:ARG:HH11	1:A:371:ARG:HG3	1.50	0.74
1:A:770:LYS:HG3	1:A:771:PRO:HD2	1.69	0.74
1:A:443:VAL:HG21	1:A:485:CYS:SG	2.27	0.74
1:A:347:TYR:O	3:A:1000:SAH:HG1	1.88	0.73
1:A:485:CYS:C	1:A:488:LYS:HD3	2.08	0.73
1:A:555:TYR:HE2	1:A:618:PRO:HD3	1.52	0.73
1:B:763:ARG:NH1	1:B:773:VAL:O	2.22	0.73
1:A:748:ARG:O	1:A:749:VAL:HG13	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:ARG:HG2	1:A:749:VAL:H	1.54	0.72
1:A:508:VAL:HG21	1:A:551:LEU:HD13	1.72	0.72
1:A:343:LEU:HD13	1:A:510:VAL:HG22	1.71	0.72
1:A:481:ASN:ND2	1:A:482:LEU:CG	2.51	0.72
1:A:659:GLY:HA3	1:A:794:TRP:HD1	1.54	0.72
1:B:763:ARG:NH2	1:B:775:ASP:OD1	2.21	0.72
1:A:691:ILE:HG12	1:A:828:ARG:HG2	1.70	0.72
1:B:223:ARG:HD2	1:B:254:SER:O	1.90	0.72
1:A:748:ARG:O	1:A:749:VAL:CG1	2.38	0.72
1:A:279:ASP:HB3	1:A:280:PRO:HD2	1.72	0.72
1:A:196:ALA:HB1	1:A:200:GLU:HB3	1.72	0.71
1:A:746:GLY:O	1:A:757:TRP:HA	1.90	0.71
1:A:501:ILE:O	1:A:502:LEU:HD23	1.90	0.71
1:A:555:TYR:CE2	1:A:618:PRO:HD3	2.24	0.71
1:B:471:PRO:O	1:B:472:GLU:CB	2.30	0.71
1:A:794:TRP:CH2	1:A:816:THR:HG23	2.24	0.71
1:A:485:CYS:O	1:A:488:LYS:HB2	1.90	0.71
1:A:766:LEU:HB2	1:A:770:LYS:O	1.90	0.71
1:B:741:PHE:HE1	1:B:778:MET:CE	2.04	0.71
1:A:747:VAL:O	1:A:748:ARG:HB2	1.91	0.71
1:A:635:ASN:O	1:A:636:ALA:CB	2.35	0.71
1:A:770:LYS:HG2	1:A:771:PRO:HD2	1.72	0.70
1:A:793:TRP:HB2	1:A:794:TRP:CE3	2.25	0.70
1:A:560:ASN:HB3	1:A:564:ILE:HD11	1.73	0.70
1:B:883:PRO:CB	1:B:884:PRO:CD	2.68	0.70
1:B:192:VAL:HG21	1:B:265:ILE:HG23	1.73	0.70
1:B:527:ARG:N	4:B:1190:HOH:O	2.23	0.70
1:B:279:ASP:C	1:B:279:ASP:OD2	2.29	0.70
1:A:231:THR:OG1	1:A:233:ILE:HG12	1.91	0.70
1:B:645:ASP:CG	1:B:647:THR:HG23	2.11	0.70
1:A:601:GLN:NE2	1:A:830:GLN:OE1	2.24	0.69
1:A:371:ARG:HB3	1:A:372:TRP:CE3	2.28	0.69
1:A:479:ILE:O	1:A:480:ASP:C	2.30	0.69
1:A:766:LEU:CD1	1:A:772:LEU:HA	2.23	0.69
1:A:737:LYS:NZ	1:A:795:ASP:OD1	2.25	0.69
1:A:481:ASN:HD21	1:A:482:LEU:CG	2.06	0.69
1:A:416:VAL:HG12	1:A:489:ILE:HG22	1.75	0.69
1:A:488:LYS:H	1:A:488:LYS:CD	2.05	0.69
1:A:819:ARG:NH2	1:A:825:GLU:OE1	2.25	0.68
1:A:560:ASN:CB	1:A:564:ILE:HD11	2.23	0.68
1:A:749:VAL:O	1:A:749:VAL:CG2	2.37	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:LYS:HA	1:B:491:GLU:HG3	1.74	0.68
1:B:603:ARG:NH2	1:B:801:VAL:O	2.27	0.68
1:B:416:VAL:HG21	1:B:490:ARG:HA	1.73	0.68
1:A:671:HIS:CB	1:A:721:ARG:HE	2.06	0.68
1:A:279:ASP:HB3	1:A:280:PRO:CD	2.24	0.68
1:A:659:GLY:HA3	1:A:794:TRP:CD1	2.29	0.68
1:A:744:LEU:HD13	1:A:772:LEU:HD22	1.76	0.68
1:B:462:PHE:HE2	1:B:479:ILE:HD13	1.59	0.68
1:B:888:SER:O	1:B:889:VAL:C	2.30	0.68
1:A:283:LYS:HE3	1:A:286:LEU:HD12	1.74	0.68
1:B:528:ASN:HD22	1:B:536:GLU:HG3	1.59	0.68
1:A:859:ARG:HG3	1:A:859:ARG:HH11	1.58	0.68
1:A:791:ARG:NH2	1:A:815:PRO:O	2.27	0.67
1:A:413:LYS:HZ2	1:A:413:LYS:HB2	1.58	0.67
1:A:878:PRO:O	1:A:879:LEU:HD12	1.94	0.67
1:A:533:LEU:HD12	1:A:534:LYS:HA	1.61	0.67
1:A:878:PRO:CB	1:A:879:LEU:HD13	2.25	0.67
2:Q:7:ALA:O	2:Q:8:ARG:HB3	1.94	0.67
1:A:415:TYR:C	1:A:416:VAL:HG22	2.15	0.67
1:A:456:ARG:HD2	1:A:461:TYR:HD1	1.59	0.67
1:A:371:ARG:HG2	1:A:371:ARG:HH11	1.59	0.67
1:A:485:CYS:HA	1:A:488:LYS:CD	2.25	0.66
1:A:659:GLY:CA	1:A:794:TRP:CD1	2.78	0.66
1:A:195:LYS:HA	1:A:266:ILE:HD11	1.78	0.66
1:A:481:ASN:ND2	1:A:482:LEU:CB	2.58	0.66
1:B:466:TRP:HZ3	1:B:475:THR:HG23	1.61	0.66
1:B:645:ASP:OD2	1:B:647:THR:CG2	2.43	0.66
1:A:278:MET:HB3	1:A:283:LYS:HD3	1.77	0.66
1:A:882:LEU:N	1:A:882:LEU:HD12	2.10	0.66
1:A:617:LEU:HD12	1:A:618:PRO:HD2	1.77	0.65
1:A:343:LEU:HD12	1:A:344:LEU:N	2.10	0.65
1:A:384:LEU:HD23	1:A:393:VAL:HG22	1.77	0.65
1:A:737:LYS:NZ	1:A:795:ASP:OD2	2.28	0.65
1:B:664:ASP:OD1	1:B:828:ARG:NH1	2.30	0.65
1:B:591:MET:O	1:B:642:VAL:HG13	1.97	0.65
1:A:285:GLN:N	1:A:285:GLN:NE2	2.42	0.65
1:A:794:TRP:CZ3	1:A:815:PRO:HB2	2.31	0.65
1:B:279:ASP:OD2	1:B:281:LYS:N	2.30	0.65
1:B:455:ASP:OD1	1:B:455:ASP:N	2.29	0.65
1:B:645:ASP:OD1	1:B:645:ASP:N	2.29	0.65
1:A:359:LEU:C	1:A:859:ARG:HH12	2.00	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASP:OD2	1:A:277:ASN:N	2.30	0.64
1:A:560:ASN:HB3	1:A:564:ILE:CD1	2.27	0.64
1:A:295:ASP:OD1	1:A:296:MET:HG3	1.96	0.64
2:P:11:THR:OG1	2:P:11:THR:O	2.16	0.64
1:B:887:THR:OG1	1:B:888:SER:N	2.29	0.64
1:B:460:ILE:HG22	1:B:479:ILE:HB	1.80	0.64
1:A:596:CYS:HB3	1:A:623:PRO:HB3	1.80	0.64
1:A:485:CYS:HB3	1:A:488:LYS:CB	2.26	0.64
1:A:481:ASN:ND2	1:A:482:LEU:HB2	2.11	0.64
1:B:495:GLU:OE2	1:B:499:ARG:NH1	2.30	0.64
1:B:304:THR:HG21	1:B:588:ARG:HH21	1.63	0.64
1:B:528:ASN:HD22	1:B:536:GLU:CG	2.12	0.63
1:A:533:LEU:O	1:A:533:LEU:HD13	1.98	0.63
1:B:528:ASN:C	1:B:528:ASN:OD1	2.36	0.63
1:A:484:ASP:C	1:A:486:PRO:CD	2.65	0.63
1:A:414:LYS:CG	1:A:416:VAL:O	2.46	0.63
1:B:466:TRP:HB2	1:B:469:TYR:HD2	1.63	0.63
1:A:645:ASP:OD1	1:A:648:GLN:HG3	1.97	0.63
1:A:642:VAL:HG12	1:A:642:VAL:O	1.99	0.63
1:A:748:ARG:N	1:A:756:GLU:O	2.31	0.63
1:A:647:THR:O	1:A:648:GLN:NE2	2.32	0.63
1:B:481:ASN:OD1	1:A:527:ARG:NE	2.32	0.62
1:A:728:GLU:CD	1:A:766:LEU:CD2	2.68	0.62
1:A:766:LEU:HD12	1:A:772:LEU:HA	1.80	0.62
1:B:474:ASP:OD1	1:B:474:ASP:N	2.32	0.62
1:A:878:PRO:C	1:A:879:LEU:HD12	2.19	0.62
1:A:526:TYR:HA	1:A:529:ARG:CD	2.14	0.62
1:B:884:PRO:CD	1:B:885:SER:H	2.13	0.62
1:A:343:LEU:HD12	1:A:344:LEU:H	1.63	0.62
1:B:525:ARG:HG3	1:B:526:TYR:CE2	2.34	0.62
1:A:600:PRO:HG2	1:A:661:ALA:HB2	1.81	0.62
1:A:819:ARG:NH2	1:A:825:GLU:CD	2.53	0.62
1:A:684:LYS:N	1:A:688:GLN:OE1	2.27	0.62
1:B:791:ARG:HD3	1:B:815:PRO:O	2.00	0.62
1:B:416:VAL:HG23	1:B:490:ARG:HA	1.81	0.62
1:A:802:VAL:HG22	1:A:803:THR:N	2.15	0.62
1:B:399:ASP:OD2	1:B:400:GLU:N	2.33	0.62
1:B:519:GLY:CA	1:B:524:ASN:CB	2.76	0.61
1:A:867:GLN:HE21	1:A:872:GLU:C	2.02	0.61
1:A:748:ARG:C	1:A:749:VAL:HG12	2.21	0.61
1:B:415:TYR:O	1:B:416:VAL:HB	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:LEU:HD22	1:B:575:TYR:CA	2.29	0.61
1:B:683:PRO:HB3	1:B:692:ARG:HD3	1.81	0.61
1:A:482:LEU:N	1:A:482:LEU:HD23	2.13	0.61
1:B:791:ARG:NH2	1:B:814:HIS:O	2.34	0.61
1:B:528:ASN:ND2	1:B:535:ASP:CB	2.60	0.61
1:A:632:GLY:O	1:A:634:PRO:HD3	2.00	0.61
1:A:583:MET:O	1:A:584:LYS:HG2	2.01	0.61
1:B:370:THR:O	1:B:391:THR:HB	2.00	0.61
1:B:202:ASP:O	1:B:227:ARG:NH2	2.32	0.61
1:B:388:HIS:O	1:B:391:THR:HG23	2.01	0.61
2:P:8:ARG:NH2	2:P:10:SER:OG	2.34	0.61
1:A:408:TRP:O	1:A:412:CYS:SG	2.53	0.61
1:A:449:ILE:HD11	1:A:460:ILE:HG13	1.83	0.60
1:A:878:PRO:HB2	1:A:879:LEU:CD1	2.31	0.60
1:A:356:GLY:HA3	1:A:858:ALA:HB3	1.83	0.60
1:A:449:ILE:HG22	1:A:492:PHE:HZ	1.66	0.60
1:B:440:GLU:HG2	1:B:441:PHE:H	1.66	0.60
1:A:203:TYR:HD1	2:P:9:MLY:CD	1.96	0.60
1:B:134:GLU:HG3	1:B:135:PRO:HD2	1.82	0.60
1:A:340:THR:HA	1:A:367:LYS:HB3	1.83	0.60
1:A:748:ARG:CG	1:A:749:VAL:H	2.14	0.60
1:A:859:ARG:HH11	1:A:859:ARG:HG2	1.65	0.60
1:B:744:LEU:O	1:B:747:VAL:CG1	2.49	0.60
1:B:218:HIS:HB3	1:B:262:LEU:HD22	1.83	0.60
1:A:196:ALA:CA	1:A:203:TYR:HE2	2.15	0.59
1:A:636:ALA:O	1:A:639:GLN:NE2	2.29	0.59
2:Q:8:ARG:O	2:Q:8:ARG:HG2	2.02	0.59
1:B:741:PHE:HE1	1:B:778:MET:HE2	1.66	0.59
1:A:463:LYS:HA	1:A:475:THR:O	2.02	0.59
1:A:307:ASN:O	1:A:308:ILE:HB	2.01	0.59
1:A:808:HIS:C	1:A:809:ASN:OD1	2.40	0.59
1:A:748:ARG:C	1:A:749:VAL:CG1	2.70	0.59
1:A:137:PHE:C	1:A:138:ILE:HD12	2.23	0.59
1:A:594:ALA:HB3	1:A:603:ARG:HB3	1.85	0.59
1:B:672:GLN:HG3	1:B:672:GLN:O	2.02	0.59
1:A:757:TRP:NE1	1:A:763:ARG:HG2	2.18	0.59
1:B:407:GLU:O	1:B:410:VAL:HG22	2.01	0.59
1:A:484:ASP:C	1:A:486:PRO:HD2	2.22	0.59
1:A:371:ARG:NH1	1:A:371:ARG:HG3	2.16	0.59
1:A:601:GLN:HB2	1:A:798:VAL:O	2.01	0.59
1:A:737:LYS:NZ	1:A:795:ASP:CG	2.56	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:TRP:CZ3	1:B:475:THR:HG23	2.38	0.59
1:A:359:LEU:C	1:A:859:ARG:NH1	2.57	0.58
1:A:481:ASN:O	1:A:481:ASN:ND2	2.16	0.58
1:A:781:ILE:HG21	1:A:784:LYS:O	2.02	0.58
1:B:279:ASP:CG	1:B:280:PRO:HD2	2.23	0.58
1:A:456:ARG:HD2	1:A:461:TYR:CD1	2.38	0.58
1:A:664:ASP:HB2	1:A:688:GLN:CD	2.24	0.58
1:B:519:GLY:CA	1:B:524:ASN:HB3	2.34	0.58
1:B:520:ILE:HG13	1:B:563:ASP:HB3	1.84	0.58
1:A:650:PRO:HD2	1:A:651:SER:H	1.68	0.58
1:A:413:LYS:HZ3	1:A:413:LYS:HB2	1.66	0.58
1:A:387:ASN:HD21	1:A:837:ARG:H	1.51	0.58
1:B:192:VAL:CG2	1:B:265:ILE:HG23	2.34	0.58
1:B:728:GLU:HB3	1:B:766:LEU:HD22	1.85	0.58
1:A:672:GLN:HG3	1:A:718:GLN:HG2	1.84	0.58
1:B:191:ASP:OD2	1:B:206:ARG:NH1	2.37	0.57
1:A:757:TRP:CZ2	1:A:763:ARG:CZ	2.87	0.57
1:B:229:GLU:HG3	1:B:237:VAL:HG11	1.86	0.57
1:B:519:GLY:O	1:B:524:ASN:HB3	2.03	0.57
1:B:744:LEU:O	1:B:747:VAL:HG12	2.04	0.57
1:A:878:PRO:O	1:A:879:LEU:CD1	2.49	0.57
1:A:747:VAL:C	1:A:756:GLU:O	2.43	0.57
1:B:375:ASP:CG	3:B:1000:SAH:O3'	2.43	0.57
1:A:481:ASN:CG	1:A:482:LEU:HG	2.24	0.57
1:A:664:ASP:OD2	1:A:692:ARG:NH1	2.32	0.57
1:A:414:LYS:O	1:A:415:TYR:CB	2.45	0.57
1:A:671:HIS:HB2	1:A:721:ARG:NE	2.14	0.57
1:A:878:PRO:HB2	1:A:879:LEU:HD13	1.85	0.57
1:A:488:LYS:H	1:A:488:LYS:HD2	1.67	0.57
2:P:8:ARG:NH1	2:P:10:SER:OG	2.38	0.57
1:B:629:VAL:HG11	1:B:641:MET:SD	2.45	0.57
1:A:748:ARG:CD	1:A:759:PRO:HD3	2.32	0.56
1:A:877:ASP:CG	1:A:878:PRO:HD2	2.24	0.56
1:A:781:ILE:CG2	1:A:784:LYS:O	2.53	0.56
1:A:736:LYS:HA	1:A:793:TRP:CH2	2.40	0.56
1:A:633:ALA:HB2	1:A:641:MET:CE	2.31	0.56
1:A:859:ARG:HG3	1:A:859:ARG:NH1	2.20	0.56
1:A:263:ASP:N	1:A:263:ASP:OD2	2.38	0.56
1:A:763:ARG:HH22	1:A:775:ASP:CG	2.08	0.56
1:A:695:ARG:NE	1:A:835:TYR:CD1	2.74	0.56
1:A:728:GLU:CD	1:A:766:LEU:HD21	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:GLU:HA	1:B:473:GLU:OE1	2.04	0.56
1:A:415:TYR:CE1	1:A:494:GLN:HG2	2.41	0.56
2:Q:8:ARG:CG	2:Q:8:ARG:O	2.54	0.56
1:A:375:ASP:O	1:A:395:ASN:HA	2.06	0.56
1:A:664:ASP:HB3	1:A:828:ARG:HH12	1.71	0.56
1:A:564:ILE:O	1:A:570:GLY:HA2	2.06	0.56
1:A:774:PRO:HB3	1:A:776:TYR:CE2	2.40	0.56
1:A:589:LEU:HA	1:A:620:TYR:OH	2.05	0.56
1:A:209:GLU:HB2	1:A:221:THR:CB	2.26	0.56
1:B:526:TYR:C	4:B:1190:HOH:O	2.43	0.55
1:B:741:PHE:CD2	1:B:788:PRO:HB2	2.41	0.55
1:A:645:ASP:HB2	1:A:648:GLN:HG2	1.88	0.55
1:A:695:ARG:HG3	1:A:700:ASP:HB3	1.87	0.55
1:A:814:HIS:CG	1:A:815:PRO:HD2	2.41	0.55
1:A:659:GLY:HA2	1:A:794:TRP:CD1	2.40	0.55
1:B:279:ASP:OD2	1:B:280:PRO:N	2.39	0.55
1:B:828:ARG:NH2	1:B:834:ASP:OD2	2.39	0.55
1:A:802:VAL:CG2	1:A:803:THR:N	2.69	0.55
1:A:195:LYS:NZ	1:A:197:GLY:HA2	2.21	0.55
1:A:855:VAL:HG22	1:A:856:PRO:HD3	1.89	0.55
1:A:234:ASN:OD1	1:A:235:SER:N	2.39	0.55
1:A:284:ALA:C	1:A:285:GLN:HE21	2.10	0.55
1:B:884:PRO:HD2	1:B:885:SER:H	1.71	0.55
1:A:715:LEU:O	1:A:824:ARG:HD2	2.06	0.55
1:A:283:LYS:N	1:A:283:LYS:CD	2.68	0.55
1:A:650:PRO:CD	1:A:651:SER:H	2.20	0.55
1:A:828:ARG:HD2	1:A:834:ASP:OD1	2.07	0.55
1:A:872:GLU:OE1	1:A:872:GLU:N	2.39	0.55
1:A:659:GLY:CA	1:A:794:TRP:HD1	2.17	0.55
1:A:279:ASP:N	1:A:279:ASP:OD1	2.39	0.54
1:B:512:CYS:HA	1:B:557:LEU:O	2.07	0.54
1:B:416:VAL:HG21	1:B:490:ARG:N	2.22	0.54
1:A:345:ASP:OD2	1:A:354:SER:HB3	2.06	0.54
1:A:133:HIS:ND1	1:A:134:GLU:N	2.56	0.54
1:A:287:ILE:HD13	1:A:293:TYR:CE2	2.43	0.54
2:P:8:ARG:CZ	2:P:10:SER:OG	2.56	0.54
1:B:874:GLU:CD	1:B:875:GLY:N	2.61	0.54
1:A:739:ALA:HB3	1:A:791:ARG:HG2	1.90	0.54
1:A:173:ARG:HG3	1:A:214:THR:HA	1.90	0.54
1:A:416:VAL:HG12	1:A:489:ILE:CG2	2.37	0.54
1:A:537:LYS:O	1:A:537:LYS:CG	2.45	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:ARG:HB2	4:B:1190:HOH:O	2.08	0.53
1:A:749:VAL:CG1	1:A:756:GLU:N	2.71	0.53
1:A:770:LYS:HG2	1:A:771:PRO:CD	2.38	0.53
1:B:375:ASP:OD2	3:B:1000:SAH:O3'	2.25	0.53
1:A:792:LEU:C	1:A:792:LEU:HD12	2.29	0.53
1:B:508:VAL:HG22	1:B:553:PRO:HB3	1.90	0.53
1:A:728:GLU:CD	1:A:766:LEU:HD23	2.29	0.53
1:A:415:TYR:CD1	1:A:494:GLN:HG2	2.43	0.53
1:A:602:PHE:O	1:A:799:PRO:O	2.26	0.53
1:A:882:LEU:HD12	1:A:882:LEU:H	1.72	0.53
1:A:758:ASP:O	1:A:761:ILE:O	2.27	0.53
1:A:481:ASN:ND2	1:A:482:LEU:N	2.55	0.53
1:B:541:MET:SD	1:B:558:MET:CE	2.97	0.53
1:A:592:MET:SD	1:A:861:LEU:HD21	2.49	0.53
1:B:751:ALA:O	1:B:752:ASN:HB2	2.09	0.53
1:A:878:PRO:HG2	1:A:879:LEU:HD22	1.91	0.53
1:A:460:ILE:C	1:A:461:TYR:CD2	2.82	0.53
1:A:792:LEU:O	1:A:793:TRP:HB3	2.07	0.53
1:A:449:ILE:HG12	1:A:450:CYS:N	2.23	0.53
1:B:487:GLN:O	1:B:491:GLU:HG2	2.09	0.53
1:A:802:VAL:CG2	1:A:803:THR:H	2.21	0.53
1:A:469:TYR:HD1	1:A:473:GLU:HG2	1.73	0.53
1:A:446:LEU:HD23	1:A:462:PHE:HB3	1.91	0.53
1:A:832:PHE:HA	1:A:855:VAL:HG11	1.91	0.53
1:B:735:VAL:O	1:B:735:VAL:CG2	2.56	0.53
1:A:740:ASN:HA	1:A:790:GLY:HA2	1.90	0.53
1:B:416:VAL:CG2	1:B:490:ARG:CA	2.79	0.52
1:A:414:LYS:HG2	1:A:416:VAL:O	2.08	0.52
1:A:460:ILE:O	1:A:461:TYR:CD2	2.57	0.52
1:B:622:LEU:HD13	1:B:644:TYR:CE1	2.44	0.52
1:A:609:TRP:CD1	1:A:620:TYR:CE1	2.97	0.52
1:B:555:TYR:CE1	1:B:615:MET:HG2	2.44	0.52
1:A:229:GLU:OE2	1:A:229:GLU:N	2.23	0.52
1:A:588:ARG:HG3	1:A:589:LEU:N	2.23	0.52
1:A:371:ARG:HB3	1:A:372:TRP:CD2	2.44	0.52
1:B:874:GLU:CD	1:B:875:GLY:H	2.13	0.52
1:B:528:ASN:HD22	1:B:536:GLU:CD	2.09	0.52
1:A:536:GLU:OE1	1:A:537:LYS:HE3	2.07	0.52
1:A:469:TYR:CD1	1:A:473:GLU:HG2	2.44	0.52
1:A:513:GLY:HA3	1:A:544:PHE:HE1	1.75	0.52
1:A:545:MET:HA	1:A:548:VAL:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:LEU:HD13	1:A:772:LEU:CD2	2.40	0.52
1:B:596:CYS:HB3	1:B:623:PRO:HB3	1.91	0.52
1:B:239:ILE:C	1:B:239:ILE:HD12	2.29	0.52
1:A:878:PRO:CA	1:A:879:LEU:HD13	2.39	0.52
1:A:513:GLY:HA3	1:A:544:PHE:CE1	2.45	0.52
1:A:671:HIS:ND1	1:A:721:ARG:NE	2.58	0.52
1:A:344:LEU:HG	1:A:346:LEU:CD1	2.40	0.52
1:B:388:HIS:HB3	1:B:391:THR:CG2	2.39	0.52
1:A:226:PHE:O	1:A:251:VAL:HG12	2.10	0.52
1:A:349:GLY:C	1:A:351:GLY:H	2.14	0.51
1:B:415:TYR:O	1:B:416:VAL:CB	2.58	0.51
1:A:619:LYS:NZ	1:A:875:GLY:O	2.43	0.51
1:A:650:PRO:CD	1:A:651:SER:N	2.73	0.51
1:A:657:LEU:HD23	1:A:795:ASP:HA	1.93	0.51
1:B:525:ARG:HG3	1:B:526:TYR:CD2	2.46	0.51
1:A:236:LEU:HG	1:A:574:LYS:HB2	1.93	0.51
1:A:414:LYS:HG3	1:A:416:VAL:O	2.10	0.51
1:A:803:THR:HB	1:A:847:ILE:HG12	1.92	0.51
1:A:536:GLU:O	1:A:537:LYS:CB	2.58	0.50
1:A:481:ASN:HD21	1:A:482:LEU:HB2	1.76	0.50
1:B:404:LEU:HD21	1:B:502:LEU:HD21	1.93	0.50
1:A:485:CYS:HA	1:A:488:LYS:CE	2.42	0.50
1:A:241:VAL:O	1:A:241:VAL:HG13	2.12	0.50
1:A:283:LYS:N	1:A:283:LYS:HD2	2.26	0.50
1:B:541:MET:SD	1:B:558:MET:HE1	2.52	0.50
1:A:363:LEU:HB2	1:A:863:TYR:CD1	2.46	0.50
1:A:269:VAL:HG13	1:A:271:ILE:HG13	1.94	0.50
1:A:282:ALA:O	1:A:285:GLN:HB2	2.11	0.50
1:A:536:GLU:OE1	1:A:536:GLU:O	2.30	0.50
1:A:635:ASN:OD1	1:A:635:ASN:O	2.30	0.50
1:A:279:ASP:CB	1:A:280:PRO:CD	2.88	0.50
1:A:415:TYR:O	1:A:416:VAL:CG1	2.57	0.50
1:A:349:GLY:O	1:A:350:CYS:SG	2.70	0.50
1:A:852:ALA:HA	3:A:1000:SAH:C	2.40	0.50
1:A:732:GLN:OE1	1:A:772:LEU:HD21	2.12	0.50
1:B:134:GLU:HG3	1:B:135:PRO:CD	2.41	0.49
1:B:781:ILE:O	1:B:781:ILE:HG22	2.11	0.49
1:B:888:SER:O	1:B:889:VAL:O	2.30	0.49
1:A:276:PRO:O	1:A:278:MET:O	2.30	0.49
1:B:529:ARG:O	1:B:532:PRO:HD3	2.12	0.49
1:A:667:LYS:H	1:A:667:LYS:CD	1.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:PHE:CE1	1:B:778:MET:CE	2.91	0.49
1:A:384:LEU:HD23	1:A:393:VAL:CG2	2.41	0.49
1:A:182:ASP:O	1:A:184:VAL:HG12	2.11	0.49
1:A:624:THR:O	1:A:624:THR:HG22	2.12	0.49
1:A:812:ILE:O	1:A:812:ILE:CG1	2.61	0.49
1:A:449:ILE:HD11	1:A:460:ILE:CG1	2.41	0.49
1:A:622:LEU:HD13	1:A:644:TYR:CE1	2.47	0.49
1:A:133:HIS:ND1	1:A:133:HIS:C	2.65	0.49
1:B:375:ASP:OD1	3:B:1000:SAH:O3'	2.30	0.49
1:A:645:ASP:OD1	1:A:648:GLN:CG	2.60	0.49
1:A:793:TRP:O	1:A:796:GLU:HG2	2.11	0.49
1:B:236:LEU:HD13	1:B:574:LYS:HB2	1.95	0.49
1:A:281:LYS:HD2	1:A:282:ALA:N	2.27	0.49
1:A:449:ILE:HG22	1:A:492:PHE:CZ	2.46	0.49
1:B:555:TYR:HE2	1:B:618:PRO:HD3	1.78	0.49
1:A:586:GLN:NE2	1:A:615:MET:O	2.44	0.49
1:A:645:ASP:O	1:A:646:GLU:HB2	2.12	0.49
1:B:446:LEU:CD2	1:B:464:VAL:HG12	2.43	0.49
1:B:688:GLN:HA	1:B:691:ILE:HD11	1.94	0.49
1:B:191:ASP:CG	1:B:206:ARG:HH11	2.16	0.48
1:A:867:GLN:NE2	1:A:873:SER:HA	2.27	0.48
1:A:481:ASN:HD21	1:A:482:LEU:CB	2.24	0.48
1:B:339:ARG:HD3	1:B:870:LEU:CD2	2.43	0.48
1:B:338:THR:HG21	1:B:367:LYS:HE3	1.94	0.48
1:A:275:ASP:O	1:A:278:MET:HB2	2.13	0.48
1:B:525:ARG:CG	1:B:526:TYR:CE2	2.96	0.48
1:B:440:GLU:HG2	1:B:441:PHE:N	2.28	0.48
1:B:622:LEU:HD21	1:B:879:LEU:HD13	1.94	0.48
1:A:488:LYS:N	1:A:488:LYS:CD	2.74	0.48
1:A:385:LYS:HB2	1:A:393:VAL:HG21	1.96	0.48
1:A:376:PHE:C	1:A:376:PHE:CD2	2.86	0.48
1:B:528:ASN:ND2	1:B:536:GLU:CG	2.74	0.48
1:A:349:GLY:HA3	4:A:1114:HOH:O	2.13	0.48
1:A:146:GLU:C	1:A:146:GLU:OE1	2.52	0.48
1:A:415:TYR:O	1:A:416:VAL:CG2	2.59	0.48
1:A:819:ARG:HH22	1:A:825:GLU:CD	2.15	0.48
1:B:828:ARG:HD2	1:B:834:ASP:OD1	2.13	0.48
1:A:641:MET:HG3	1:A:643:ALA:H	1.78	0.48
1:A:463:LYS:HB2	1:A:476:TRP:CZ3	2.49	0.48
1:A:137:PHE:O	1:A:138:ILE:HD12	2.14	0.48
1:A:235:SER:C	1:A:237:VAL:H	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:ASP:C	1:B:532:PRO:HD3	2.34	0.48
1:A:477:GLU:HA	1:A:478:PRO:HD3	1.26	0.48
1:A:566:LYS:HD2	1:A:566:LYS:HA	1.61	0.48
1:A:619:LYS:HD3	1:A:877:ASP:O	2.14	0.48
1:A:413:LYS:CG	1:A:414:LYS:N	2.77	0.48
1:A:307:ASN:O	1:A:308:ILE:CB	2.61	0.48
1:A:235:SER:OG	1:A:236:LEU:N	2.45	0.48
1:A:729:ARG:O	1:A:732:GLN:N	2.43	0.47
1:A:663:SER:OG	1:A:688:GLN:NE2	2.39	0.47
1:A:235:SER:O	1:A:237:VAL:N	2.47	0.47
1:A:460:ILE:C	1:A:461:TYR:HD2	2.16	0.47
1:A:488:LYS:N	1:A:488:LYS:HD2	2.28	0.47
1:B:519:GLY:C	1:B:524:ASN:HB3	2.35	0.47
1:B:484:ASP:C	1:B:486:PRO:HD3	2.34	0.47
1:B:521:SER:HB3	1:B:563:ASP:OD2	2.13	0.47
1:A:512:CYS:HA	1:A:557:LEU:O	2.13	0.47
3:B:1000:SAH:H4'	3:B:1000:SAH:HG2	1.68	0.47
1:A:142:VAL:HG22	1:A:147:ALA:HB2	1.94	0.47
1:A:650:PRO:HD2	1:A:651:SER:N	2.30	0.47
1:A:181:VAL:O	1:A:184:VAL:HG13	2.14	0.47
1:B:220:PHE:HE1	1:B:222:CYS:HG	1.60	0.47
1:A:484:ASP:C	1:A:486:PRO:HD3	2.34	0.47
1:A:353:MET:O	1:A:357:LEU:HG	2.15	0.47
1:B:272:VAL:HG21	1:B:286:LEU:HG	1.97	0.47
1:A:667:LYS:HA	1:A:817:GLN:HE22	1.79	0.47
1:B:841:PRO:HG2	1:B:844:GLU:CG	2.44	0.47
1:B:884:PRO:CG	1:B:885:SER:N	2.78	0.47
1:B:886:PHE:C	1:B:887:THR:HG23	2.35	0.47
1:B:535:ASP:HB3	1:B:536:GLU:HG3	1.97	0.47
1:B:762:GLU:O	1:B:763:ARG:C	2.50	0.46
1:B:826:ASN:ND2	4:B:1187:HOH:O	2.46	0.46
1:B:382:GLN:NE2	4:B:1201:HOH:O	2.27	0.46
3:A:1000:SAH:O3'	4:A:1114:HOH:O	2.20	0.46
1:B:294:TYR:HE1	1:B:308:ILE:HD13	1.80	0.46
1:B:525:ARG:O	1:B:525:ARG:HD2	2.15	0.46
1:B:725:ASP:O	1:B:729:ARG:HG3	2.15	0.46
1:A:485:CYS:O	1:A:488:LYS:CB	2.61	0.46
1:B:781:ILE:HB	1:B:785:SER:HB2	1.97	0.46
1:B:531:GLU:N	1:B:532:PRO:HD3	2.30	0.46
1:A:176:TYR:O	1:A:210:PHE:HB2	2.16	0.46
1:A:619:LYS:HE3	1:A:875:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:TYR:HA	1:B:260:ASN:O	2.16	0.46
1:A:291:ASP:O	1:A:292:LEU:HD23	2.16	0.46
1:A:703:PHE:O	1:A:704:GLY:C	2.53	0.46
1:A:479:ILE:HG13	1:A:480:ASP:N	2.22	0.46
1:A:645:ASP:O	1:A:646:GLU:CB	2.64	0.46
1:A:135:PRO:HG3	1:A:263:ASP:OD2	2.15	0.46
1:B:528:ASN:HD21	1:B:536:GLU:CD	2.17	0.46
1:B:304:THR:HG21	1:B:588:ARG:NH2	2.31	0.46
1:B:632:GLY:O	1:B:634:PRO:HD3	2.16	0.46
1:A:485:CYS:O	1:A:488:LYS:N	2.48	0.46
1:A:622:LEU:HD13	1:A:644:TYR:HE1	1.81	0.46
1:A:133:HIS:CE1	1:A:134:GLU:O	2.69	0.45
1:B:227:ARG:HB2	1:B:230:ASP:OD2	2.16	0.45
1:B:592:MET:HB3	1:B:592:MET:HE2	1.75	0.45
1:A:444:GLU:HG3	1:A:445:LYS:N	2.29	0.45
1:B:416:VAL:HG22	1:B:489:ILE:CG2	2.26	0.45
1:B:411:LEU:O	1:B:415:TYR:N	2.50	0.45
1:A:569:ASP:O	1:A:574:LYS:HE3	2.16	0.45
1:A:813:ILE:HA	1:A:820:VAL:HA	1.99	0.45
1:A:822:THR:OG1	1:A:825:GLU:HG3	2.15	0.45
1:A:387:ASN:HD21	1:A:837:ARG:N	2.13	0.45
1:A:349:GLY:H	3:A:1000:SAH:HG2	1.81	0.45
1:A:808:HIS:N	1:A:808:HIS:CD2	2.84	0.45
1:A:589:LEU:CD1	1:A:640:CYS:HB3	2.46	0.45
1:A:545:MET:HA	1:A:548:VAL:CG1	2.46	0.45
1:A:485:CYS:N	1:A:486:PRO:CD	2.80	0.45
1:A:657:LEU:HB3	1:A:794:TRP:O	2.17	0.45
1:A:356:GLY:HA3	1:A:858:ALA:CB	2.45	0.45
1:A:283:LYS:O	1:A:287:ILE:HG13	2.17	0.45
1:A:626:ASP:N	1:A:652:LEU:HB3	2.32	0.45
1:A:788:PRO:O	1:A:790:GLY:N	2.50	0.45
1:B:667:LYS:HG2	1:B:817:GLN:CD	2.37	0.45
1:B:599:LEU:HD11	1:B:856:PRO:HD2	1.99	0.45
1:A:732:GLN:OE1	1:A:772:LEU:HD11	2.17	0.45
1:B:357:LEU:HD11	1:B:557:LEU:HD23	1.99	0.45
1:A:363:LEU:HD23	1:A:363:LEU:N	2.32	0.45
2:Q:6:THR:OG1	2:Q:6:THR:O	2.32	0.45
1:A:749:VAL:O	1:A:754:ILE:O	2.35	0.45
1:B:338:THR:CG2	1:B:367:LYS:HE3	2.47	0.45
1:A:449:ILE:CG1	1:A:450:CYS:N	2.80	0.45
1:A:279:ASP:CB	1:A:280:PRO:HD2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:ARG:NH1	1:A:773:VAL:O	2.49	0.45
1:A:463:LYS:HB2	1:A:476:TRP:CE3	2.52	0.45
1:B:812:ILE:HG23	1:B:820:VAL:HG22	1.99	0.45
1:B:735:VAL:HG23	1:B:735:VAL:O	2.16	0.44
1:A:657:LEU:HG	1:A:795:ASP:C	2.38	0.44
1:B:648:GLN:O	1:B:650:PRO:HD3	2.16	0.44
1:B:414:LYS:O	1:B:414:LYS:HG3	2.15	0.44
1:A:531:GLU:OE2	1:A:534:LYS:NZ	2.38	0.44
1:A:283:LYS:HE3	1:A:283:LYS:HA	1.93	0.44
1:B:488:LYS:HA	1:B:491:GLU:CG	2.43	0.44
1:A:781:ILE:HB	1:A:785:SER:HB2	2.00	0.44
1:B:481:ASN:O	1:B:481:ASN:OD1	2.36	0.44
1:A:479:ILE:C	1:A:481:ASN:N	2.65	0.44
1:A:687:PHE:CE1	1:A:691:ILE:HD13	2.52	0.44
1:B:741:PHE:CE1	1:B:778:MET:HE2	2.49	0.44
1:B:642:VAL:O	1:B:642:VAL:HG22	2.17	0.44
1:B:538:ASN:ND2	1:B:572:LEU:HD11	2.33	0.44
1:A:621:PRO:HD3	1:A:864:CYS:SG	2.58	0.44
1:A:724:ASN:O	1:A:725:ASP:CB	2.54	0.44
3:A:1000:SAH:HG2	3:A:1000:SAH:H4'	1.51	0.44
1:A:883:PRO:HG2	1:A:884:PRO:HD3	1.99	0.44
1:A:368:LEU:HA	1:A:368:LEU:HD23	1.81	0.44
1:A:748:ARG:CG	1:A:749:VAL:N	2.80	0.44
1:A:499:ARG:HA	1:A:499:ARG:HD2	1.68	0.44
1:A:522:GLY:O	1:A:525:ARG:HB2	2.18	0.44
1:A:819:ARG:CG	1:A:820:VAL:O	2.60	0.43
1:B:528:ASN:CB	1:B:535:ASP:OD1	2.59	0.43
1:A:133:HIS:HE2	1:A:180:LYS:HE3	1.84	0.43
1:B:599:LEU:HA	1:B:600:PRO:HD3	1.83	0.43
1:B:884:PRO:CD	1:B:885:SER:N	2.77	0.43
1:A:371:ARG:NH1	1:A:371:ARG:CG	2.54	0.43
1:A:884:PRO:O	1:A:885:SER:C	2.57	0.43
1:A:229:GLU:CD	1:A:229:GLU:H	2.12	0.43
1:A:487:GLN:O	1:A:490:ARG:HB3	2.18	0.43
1:B:462:PHE:CE2	1:B:479:ILE:HD13	2.48	0.43
1:A:239:ILE:HD12	1:A:239:ILE:C	2.38	0.43
1:A:589:LEU:HD11	1:A:640:CYS:HB3	2.00	0.43
1:A:196:ALA:CB	1:A:200:GLU:HB3	2.47	0.43
1:A:388:HIS:ND1	1:A:702:SER:OG	2.32	0.43
1:A:482:LEU:C	1:A:484:ASP:N	2.70	0.43
1:A:236:LEU:HD13	1:A:236:LEU:HA	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:TRP:CD2	1:A:618:PRO:HG2	2.54	0.43
1:A:753:ASN:O	1:A:784:LYS:HB3	2.19	0.43
1:A:882:LEU:HA	1:A:883:PRO:HD3	1.88	0.43
1:A:787:LYS:N	1:A:788:PRO:CD	2.82	0.43
1:A:876:SER:OG	1:A:876:SER:O	2.30	0.43
1:A:878:PRO:HB2	1:A:879:LEU:HD11	2.01	0.43
1:B:202:ASP:OD2	1:B:266:ILE:HD13	2.18	0.43
1:B:220:PHE:HE1	1:B:222:CYS:SG	2.40	0.43
1:B:416:VAL:HG21	1:B:490:ARG:HG3	2.00	0.42
1:B:886:PHE:O	1:B:887:THR:C	2.57	0.42
1:A:346:LEU:HD21	1:A:547:ILE:HG21	2.01	0.42
1:A:671:HIS:CD2	1:A:673:PRO:HD3	2.54	0.42
1:A:649:LYS:HA	1:A:650:PRO:HD3	1.82	0.42
1:A:564:ILE:HG23	1:A:572:LEU:HB2	2.01	0.42
1:A:689:ARG:HB2	1:A:689:ARG:CZ	2.48	0.42
1:B:703:PHE:CE1	1:B:709:PRO:HD3	2.54	0.42
1:B:376:PHE:CD2	1:B:376:PHE:C	2.90	0.42
1:A:804:ARG:HB3	1:A:806:GLU:OE1	2.20	0.42
1:A:589:LEU:CD1	1:A:590:GLY:N	2.81	0.42
1:A:359:LEU:O	1:A:859:ARG:NH1	2.37	0.42
1:A:630:ARG:C	1:A:632:GLY:H	2.23	0.42
1:B:687:PHE:O	1:B:691:ILE:HG13	2.18	0.42
1:B:819:ARG:NH1	1:B:822:THR:HG23	2.35	0.42
1:A:398:ALA:O	1:A:401:PHE:HB3	2.18	0.42
2:Q:7:ALA:O	2:Q:8:ARG:CB	2.65	0.42
1:A:794:TRP:HH2	1:A:816:THR:CG2	2.24	0.42
1:A:882:LEU:N	1:A:882:LEU:CD1	2.79	0.42
1:A:367:LYS:NZ	1:A:369:GLU:OE2	2.52	0.42
1:A:664:ASP:HB3	1:A:828:ARG:NH1	2.34	0.42
1:A:195:LYS:HZ3	1:A:197:GLY:HA2	1.84	0.42
1:B:463:LYS:HE2	1:B:474:ASP:HB2	2.01	0.42
1:B:416:VAL:HG21	1:B:490:ARG:CB	2.50	0.42
1:B:527:ARG:HB2	1:B:527:ARG:HE	1.40	0.42
1:B:482:LEU:C	1:B:484:ASP:N	2.73	0.42
1:A:447:VAL:HG12	1:A:447:VAL:O	2.18	0.42
1:A:399:ASP:OD1	1:A:400:GLU:N	2.53	0.42
1:A:728:GLU:OE1	1:A:766:LEU:CD2	2.57	0.42
1:A:356:GLY:O	1:A:859:ARG:HA	2.19	0.42
1:A:348:SER:O	1:A:350:CYS:N	2.53	0.42
1:B:481:ASN:C	1:B:482:LEU:HD23	2.40	0.42
1:A:735:VAL:HA	1:A:791:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:GLU:OE1	1:A:537:LYS:CG	2.58	0.42
1:A:592:MET:HE2	1:A:592:MET:HB3	1.88	0.42
1:B:222:CYS:O	1:B:257:LYS:HA	2.19	0.42
1:A:479:ILE:HG22	1:A:479:ILE:H	1.55	0.42
1:B:633:ALA:HA	1:B:634:PRO:HD2	1.79	0.42
1:A:273:HIS:HB2	1:A:294:TYR:CE2	2.55	0.42
1:A:369:GLU:HG3	1:A:371:ARG:HD3	2.01	0.41
1:B:278:MET:HE2	1:B:282:ALA:HB3	2.02	0.41
1:A:612:LEU:C	1:A:614:SER:N	2.73	0.41
1:A:622:LEU:HG	1:A:879:LEU:HB3	2.03	0.41
1:A:792:LEU:HD23	1:A:811:VAL:HG23	2.00	0.41
1:A:387:ASN:ND2	1:A:837:ARG:H	2.17	0.41
1:A:353:MET:HG3	1:A:853:VAL:HG11	2.01	0.41
1:A:560:ASN:CG	1:A:564:ILE:HD11	2.40	0.41
1:A:415:TYR:O	1:A:416:VAL:CB	2.69	0.41
1:A:758:ASP:HA	1:A:759:PRO:HD3	1.93	0.41
1:A:630:ARG:C	1:A:632:GLY:N	2.73	0.41
1:A:594:ALA:CB	1:A:603:ARG:HB3	2.50	0.41
1:A:855:VAL:N	1:A:856:PRO:CD	2.84	0.41
1:A:447:VAL:O	1:A:447:VAL:CG1	2.67	0.41
1:B:537:LYS:HG2	1:B:539:LYS:HB2	2.01	0.41
1:A:696:LYS:HE2	1:A:706:GLY:HA2	2.03	0.41
1:A:344:LEU:HD13	1:A:372:TRP:HB2	2.03	0.41
1:A:740:ASN:OD1	1:A:742:ARG:N	2.38	0.41
1:B:757:TRP:O	1:B:759:PRO:HD3	2.21	0.41
1:A:204:ILE:HG22	1:A:225:PHE:CD2	2.56	0.41
1:A:612:LEU:C	1:A:614:SER:H	2.24	0.41
1:A:877:ASP:CG	1:A:878:PRO:CD	2.88	0.41
1:A:802:VAL:HG22	1:A:803:THR:H	1.82	0.41
1:B:672:GLN:CG	1:B:672:GLN:O	2.68	0.41
1:A:812:ILE:O	1:A:812:ILE:HG13	2.21	0.41
1:B:344:LEU:CD1	1:B:372:TRP:HB2	2.51	0.41
1:B:477:GLU:HA	1:B:478:PRO:HD3	1.95	0.41
1:A:482:LEU:H	1:A:482:LEU:HD23	1.81	0.41
1:B:203:TYR:CE2	2:Q:7:ALA:HB3	2.56	0.41
1:A:196:ALA:CB	1:A:203:TYR:CE2	3.03	0.41
1:B:528:ASN:ND2	1:B:536:GLU:OE2	2.54	0.41
1:A:658:LEU:CD2	1:A:792:LEU:HD13	2.50	0.41
1:A:536:GLU:CD	1:A:536:GLU:O	2.58	0.41
1:B:209:GLU:HB2	1:B:221:THR:CB	2.43	0.41
1:A:825:GLU:O	1:A:829:LEU:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:GLN:NE2	1:A:872:GLU:C	2.66	0.41
1:A:233:ILE:HG13	1:A:233:ILE:O	2.20	0.41
1:A:696:LYS:NZ	1:A:706:GLY:H	2.19	0.41
1:A:677:MET:O	1:A:714:LEU:HB3	2.21	0.41
1:B:616:VAL:O	1:B:868:ALA:HB1	2.20	0.41
1:A:833:PRO:HG2	1:A:836:TYR:HB2	2.02	0.41
1:B:835:TYR:C	1:B:835:TYR:CD1	2.95	0.41
1:B:621:PRO:HA	1:B:880:TYR:O	2.20	0.41
1:B:884:PRO:CG	1:B:885:SER:H	2.33	0.41
1:B:763:ARG:NH1	1:B:771:PRO:HB2	2.35	0.41
1:B:726:ASP:O	1:B:730:VAL:HG13	2.20	0.41
1:A:751:ALA:O	1:A:752:ASN:CB	2.69	0.41
1:A:564:ILE:CG2	1:A:573:GLY:N	2.84	0.40
1:B:491:GLU:H	1:B:491:GLU:HG2	1.54	0.40
1:B:202:ASP:OD2	1:B:266:ILE:CD1	2.69	0.40
1:A:175:HIS:CD2	1:A:211:PHE:HB3	2.56	0.40
1:A:603:ARG:CZ	1:A:830:GLN:HE22	2.34	0.40
1:B:814:HIS:CG	1:B:815:PRO:HD2	2.56	0.40
1:B:886:PHE:CG	1:B:887:THR:N	2.69	0.40
1:A:749:VAL:HG13	1:A:754:ILE:O	2.22	0.40
1:A:500:LYS:C	1:A:502:LEU:N	2.74	0.40
1:A:513:GLY:C	1:A:515:PRO:HD3	2.42	0.40
1:A:363:LEU:CD2	1:A:363:LEU:N	2.84	0.40
1:A:364:SER:OG	1:A:863:TYR:O	2.39	0.40
1:A:778:MET:O	1:A:783:GLY:HA2	2.22	0.40
1:B:886:PHE:C	1:B:887:THR:CG2	2.90	0.40
1:A:271:ILE:HA	1:A:292:LEU:O	2.20	0.40
1:A:193:TYR:CE1	1:A:204:ILE:HG13	2.56	0.40
1:A:722:LEU:CD1	1:A:730:VAL:HG21	2.52	0.40
1:B:138:ILE:HG12	1:B:178:SER:HB3	2.03	0.40
1:B:285:GLN:O	1:B:288:GLU:HB3	2.22	0.40
1:B:626:ASP:OD1	1:B:626:ASP:C	2.60	0.40
1:A:482:LEU:O	1:A:483:SER:C	2.58	0.40
1:A:482:LEU:O	1:A:485:CYS:N	2.54	0.40
1:A:671:HIS:CG	1:A:721:ARG:HE	2.40	0.40
1:A:133:HIS:NE2	1:A:180:LYS:HE3	2.37	0.40
1:A:649:LYS:HD2	1:A:650:PRO:HD2	2.02	0.40
1:B:773:VAL:HA	1:B:774:PRO:HD2	1.93	0.40
1:B:852:ALA:HA	3:B:1000:SAH:C	2.52	0.40
1:B:751:ALA:O	1:B:752:ASN:CB	2.70	0.40
1:A:451:TYR:HA	1:A:459:GLY:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:SER:HB3	1:A:683:PRO:HD2	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	680/784 (87%)	631 (93%)	38 (6%)	11 (2%)	12	30
1	B	685/784 (87%)	660 (96%)	22 (3%)	3 (0%)	39	69
2	P	4/32 (12%)	4 (100%)	0	0	100	100
2	Q	2/32 (6%)	1 (50%)	0	1 (50%)	0	0
All	All	1371/1632 (84%)	1296 (94%)	60 (4%)	15 (1%)	17	42

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	883	PRO
1	B	650	PRO
1	B	875	GLY
1	A	704	GLY
1	A	748	ARG
1	A	789	PHE
1	A	349	GLY
1	A	478	PRO
1	A	725	ASP
1	A	350	CYS
1	A	485	CYS
1	B	886	PHE
1	A	490	ARG
2	Q	8	ARG

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Mol	Chain	Res	Type
1	A	650	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	580/668 (87%)	492 (85%)	88 (15%)	3	9
1	B	596/668 (89%)	530 (89%)	66 (11%)	8	17
2	P	5/21 (24%)	3 (60%)	2 (40%)	0	0
2	Q	3/21 (14%)	1 (33%)	2 (67%)	0	0
All	All	1184/1378 (86%)	1026 (87%)	158 (13%)	5	11

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	134	GLU
1	B	138	ILE
1	B	169	GLU
1	B	223	ARG
1	B	234	ASN
1	B	235	SER
1	B	236	LEU
1	B	262	LEU
1	B	263	ASP
1	B	269	VAL
1	B	270	LYS
1	B	274	VAL
1	B	279	ASP
1	B	281	LYS
1	B	299	SER
1	B	338	THR
1	B	340	THR
1	B	363	LEU
1	B	376	PHE
1	B	391	THR

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Mol	Chain	Res	Type
1	B	395	ASN
1	B	414	LYS
1	B	441	PHE
1	B	443	VAL
1	B	444	GLU
1	B	450	CYS
1	B	455	ASP
1	B	456	ARG
1	B	464	VAL
1	B	465	GLN
1	B	474	ASP
1	B	484	ASP
1	B	488	LYS
1	B	491	GLU
1	B	502	LEU
1	B	508	VAL
1	B	518	GLN
1	B	520	ILE
1	B	525	ARG
1	B	527	ARG
1	B	528	ASN
1	B	530	ASP
1	B	536	GLU
1	B	537	LYS
1	B	558	MET
1	B	615	MET
1	B	638	SER
1	B	642	VAL
1	B	646	GLU
1	B	647	THR
1	B	649	LYS
1	B	656	LEU
1	B	672	GLN
1	B	730	VAL
1	B	735	VAL
1	B	747	VAL
1	B	763	ARG
1	B	765	LYS
1	B	775	ASP
1	B	795	ASP
1	B	821	LEU
1	B	829	LEU

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Mol	Chain	Res	Type
1	B	867	GLN
1	B	887	THR
1	B	888	SER
1	B	889	VAL
1	A	133	HIS
1	A	142	VAL
1	A	146	GLU
1	A	170	LEU
1	A	184	VAL
1	A	185	VAL
1	A	200	GLU
1	A	232	VAL
1	A	237	VAL
1	A	238	SER
1	A	251	VAL
1	A	261	VAL
1	A	263	ASP
1	A	278	MET
1	A	279	ASP
1	A	281	LYS
1	A	283	LYS
1	A	285	GLN
1	A	286	LEU
1	A	287	ILE
1	A	290	CYS
1	A	338	THR
1	A	363	LEU
1	A	368	LEU
1	A	371	ARG
1	A	376	PHE
1	A	407	GLU
1	A	410	VAL
1	A	411	LEU
1	A	413	LYS
1	A	416	VAL
1	A	442	VAL
1	A	444	GLU
1	A	455	ASP
1	A	457	GLU
1	A	460	ILE
1	A	464	VAL
1	A	475	THR

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Mol	Chain	Res	Type
1	A	479	ILE
1	A	481	ASN
1	A	484	ASP
1	A	499	ARG
1	A	510	VAL
1	A	521	SER
1	A	533	LEU
1	A	535	ASP
1	A	536	GLU
1	A	537	LYS
1	A	558	MET
1	A	589	LEU
1	A	614	SER
1	A	627	VAL
1	A	644	TYR
1	A	647	THR
1	A	653	LYS
1	A	657	LEU
1	A	665	LEU
1	A	667	LYS
1	A	675	ASP
1	A	693	LEU
1	A	694	SER
1	A	699	LEU
1	A	716	ASP
1	A	747	VAL
1	A	754	ILE
1	A	763	ARG
1	A	765	LYS
1	A	766	LEU
1	A	767	SER
1	A	772	LEU
1	A	779	SER
1	A	781	ILE
1	A	782	LYS
1	A	793	TRP
1	A	808	HIS
1	A	809	ASN
1	A	819	ARG
1	A	821	LEU
1	A	824	ARG
1	A	834	ASP

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Mol	Chain	Res	Type
1	A	859	ARG
1	A	867	GLN
1	A	872	GLU
1	A	873	SER
1	A	874	GLU
1	A	876	SER
1	A	879	LEU
1	A	882	LEU
2	P	6	THR
2	P	11	THR
2	Q	6	THR
2	Q	8	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	234	ASN
1	B	260	ASN
1	B	528	ASN
1	B	752	ASN
1	B	810	GLN
1	A	285	GLN
1	A	481	ASN
1	A	487	GLN
1	A	867	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
2	MLY	P	9	2	9,10,11	0.82	1 (11%)	9,11,13	1.00	0
2	MLY	Q	9	2	9,10,11	0.99	1 (11%)	9,11,13	1.68	2 (22%)

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
2	MLY	P	9	2	-	0/7/9/11	0/0/0/0
2	MLY	Q	9	2	-	0/7/9/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	9	MLY	CB-CA	-2.68	1.51	1.53
2	P	9	MLY	CB-CA	-2.05	1.51	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	9	MLY	CD-CE-NZ	-3.97	103.70	113.92
2	Q	9	MLY	O-C-CA	-2.24	119.66	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	9	MLY	7	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	SAH	A	1000	-	20,28,28	1.16	2 (10%)	19,40,40	2.14	4 (21%)
3	SAH	B	1000	-	20,28,28	1.71	5 (25%)	19,40,40	5.20	12 (63%)

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	SAH	A	1000	-	-	0/7/31/31	0/3/3/3
3	SAH	B	1000	-	-	0/7/31/31	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1000	SAH	C5-C4	-3.10	1.33	1.40
3	A	1000	SAH	C5'-SD	-2.33	1.76	1.81
3	B	1000	SAH	C2'-C3'	-2.17	1.47	1.53
3	B	1000	SAH	O4'-C4'	2.52	1.50	1.45
3	B	1000	SAH	C2-N1	3.03	1.39	1.33
3	A	1000	SAH	C5-C4	3.08	1.47	1.40
3	B	1000	SAH	C2-N3	4.47	1.40	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1000	SAH	N3-C2-N1	-13.82	118.31	128.89
3	B	1000	SAH	O4'-C4'-C5'	-11.67	77.06	108.85
3	B	1000	SAH	O4'-C4'-C3'	-7.34	90.36	105.15
3	A	1000	SAH	N3-C2-N1	-6.76	123.72	128.89
3	B	1000	SAH	C5'-SD-CG	-4.08	90.16	102.41
3	B	1000	SAH	C4'-O4'-C1'	-3.77	105.58	109.72
3	B	1000	SAH	C1'-N9-C4	-3.54	121.61	126.94
3	B	1000	SAH	C2'-C1'-N9	-3.54	108.89	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1000	SAH	C4-C5-N7	-3.10	106.63	109.48
3	A	1000	SAH	C2'-C1'-N9	-2.99	109.72	114.29
3	B	1000	SAH	C4'-C5'-SD	-2.60	105.50	113.53
3	B	1000	SAH	C4-C5-N7	-2.14	107.51	109.48
3	B	1000	SAH	C2'-C3'-C4'	-2.13	98.23	102.61
3	A	1000	SAH	CB-CG-SD	-2.12	109.49	113.57
3	B	1000	SAH	CB-CG-SD	2.64	118.67	113.57
3	B	1000	SAH	C5'-C4'-C3'	7.09	133.37	114.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	SAH	5	0
3	B	1000	SAH	5	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	688/784 (87%)	0.61	90 (13%) 5 4	56, 88, 149, 228	0
1	B	693/784 (88%)	0.04	16 (2%) 64 64	24, 45, 106, 159	0
2	P	6/32 (18%)	0.64	0 100 100	105, 130, 135, 135	0
2	Q	4/32 (12%)	4.52	4 (100%) 0 0	119, 128, 143, 164	0
All	All	1391/1632 (85%)	0.34	110 (7%) 15 13	24, 71, 137, 228	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	628	VAL	10.5
1	A	629	VAL	9.6
1	A	479	ILE	8.5
1	A	416	VAL	7.8
1	A	748	ARG	7.7
2	Q	6	THR	7.7
1	A	750	GLY	7.0
1	A	526	TYR	6.0
1	A	744	LEU	5.9
1	A	482	LEU	5.5
1	A	745	LYS	5.0
1	A	626	ASP	4.9
1	B	526	TYR	4.8
1	A	415	TYR	4.6
1	A	199	ASN	4.6
1	A	739	ALA	4.6
1	A	198	GLU	4.4
1	A	485	CYS	4.3
2	Q	7	ALA	4.1
1	A	764	VAL	4.1
1	A	481	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	749	VAL	4.0
1	B	416	VAL	4.0
1	B	479	ILE	3.7
1	B	481	ASN	3.6
1	B	525	ARG	3.6
1	A	757	TRP	3.6
2	Q	8	ARG	3.5
1	A	741	PHE	3.4
1	A	874	GLU	3.4
1	A	761	ILE	3.3
1	A	497	HIS	3.2
1	A	774	PRO	3.2
1	A	528	ASN	3.2
1	A	411	LEU	3.2
1	A	793	TRP	3.1
1	A	243	GLY	3.1
1	B	485	CYS	3.0
1	A	733	ILE	2.9
1	B	630	ARG	2.9
1	A	490	ARG	2.9
1	A	643	ALA	2.9
1	B	484	ASP	2.9
1	A	742	ARG	2.8
1	A	651	SER	2.8
1	A	870	LEU	2.8
2	Q	10	SER	2.8
1	A	734	PRO	2.7
1	A	454	SER	2.7
1	A	483	SER	2.7
1	A	818	ALA	2.7
1	A	414	LYS	2.7
1	A	193	TYR	2.6
1	A	778	MET	2.6
1	A	746	GLY	2.6
1	A	478	PRO	2.6
1	B	536	GLU	2.6
1	A	480	ASP	2.6
1	A	732	GLN	2.6
1	A	654	LYS	2.6
1	A	484	ASP	2.6
1	A	738	GLY	2.5
1	B	411	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	446	LEU	2.5
1	A	631	GLY	2.5
1	A	648	GLN	2.5
1	A	488	LYS	2.4
1	A	533	LEU	2.4
1	A	755	VAL	2.4
1	B	522	GLY	2.4
1	A	642	VAL	2.4
1	A	492	PHE	2.4
1	A	760	GLU	2.4
1	A	202	ASP	2.3
1	A	789	PHE	2.3
1	A	529	ARG	2.3
1	B	483	SER	2.3
1	A	630	ARG	2.3
1	A	772	LEU	2.3
1	A	494	GLN	2.3
1	B	524	ASN	2.3
1	A	650	PRO	2.3
1	A	743	ASP	2.3
1	A	751	ALA	2.3
1	A	266	ILE	2.3
1	A	278	MET	2.2
1	B	414	LYS	2.2
1	B	442	VAL	2.2
1	A	759	PRO	2.2
1	A	378	SER	2.2
1	A	644	TYR	2.2
1	A	534	LYS	2.1
1	A	740	ASN	2.1
1	B	489	ILE	2.1
1	A	462	PHE	2.1
1	A	727	TYR	2.1
1	A	747	VAL	2.1
1	A	766	LEU	2.1
1	A	338	THR	2.1
1	A	489	ILE	2.1
1	A	366	LEU	2.1
1	A	652	LEU	2.1
1	A	441	PHE	2.1
1	A	762	GLU	2.1
1	A	349	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	172	ALA	2.1
1	A	413	LYS	2.0
1	A	729	ARG	2.0
1	A	722	LEU	2.0
1	A	469	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MLY	Q	9	11/12	0.85	0.26	-	76,96,108,114	0
2	MLY	P	9	11/12	0.88	0.29	-	81,87,108,112	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SAH	A	1000	26/26	0.90	0.24	0.98	36,63,83,93	0
3	SAH	B	1000	26/26	0.96	0.24	0.87	11,36,55,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.