WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 10:55 AM GMT

PDB ID : 1H28
Title : CDK2/CYCLIN A IN COMPLEX WITH AN 11-RESIDUE RECRUITMENT PEPTIDE FROM P107
Authors : Tews, I.; Cheng, K.Y.; Lowe, E.D.; Noble, M.E.M.; Brown, N.R.; Gul, S.; Gamblin, S.; Johnson, L.N.
Deposited on : 2002-07-31
Resolution : 2.80 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Rfree		0.312
Clashscore		36
Ramachandran outliers		4.5%
Sidechain outliers		13.0%
RSRZ outliers		6.4%

Worse *Better*

▮ Percentile relative to all X-ray structures
◻ Percentile relative to X-ray structures of similar resolution
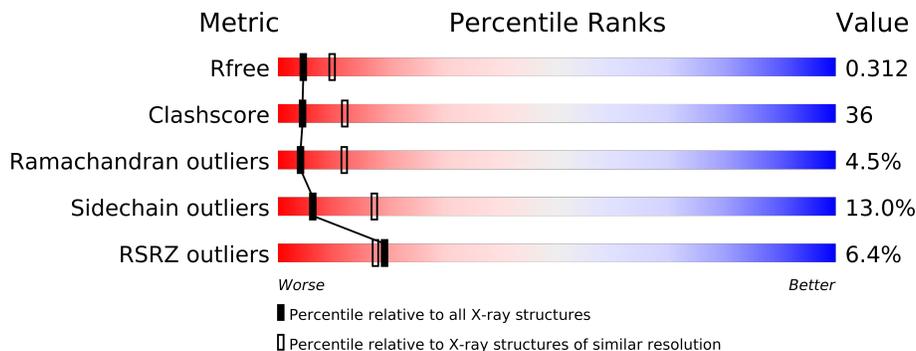
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	303	
1	C	303	
2	B	259	
2	D	259	
3	E	11	
3	F	11	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 9125 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			
1	C	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			

- Molecule 3 is a protein called RETINOBLASTOMA-LIKE PROTEIN 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	10	Total	C	N	O	0	0	0
			78	48	17	13			
3	F	8	Total	C	N	O	0	0	0
			68	43	15	10			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	11	Total	O	0	0
			11	11		
4	C	10	Total	O	0	0
			10	10		
4	D	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total 1	O 1	0	0

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: CELL DIVISION PROTEIN KINASE 2

Chain A:
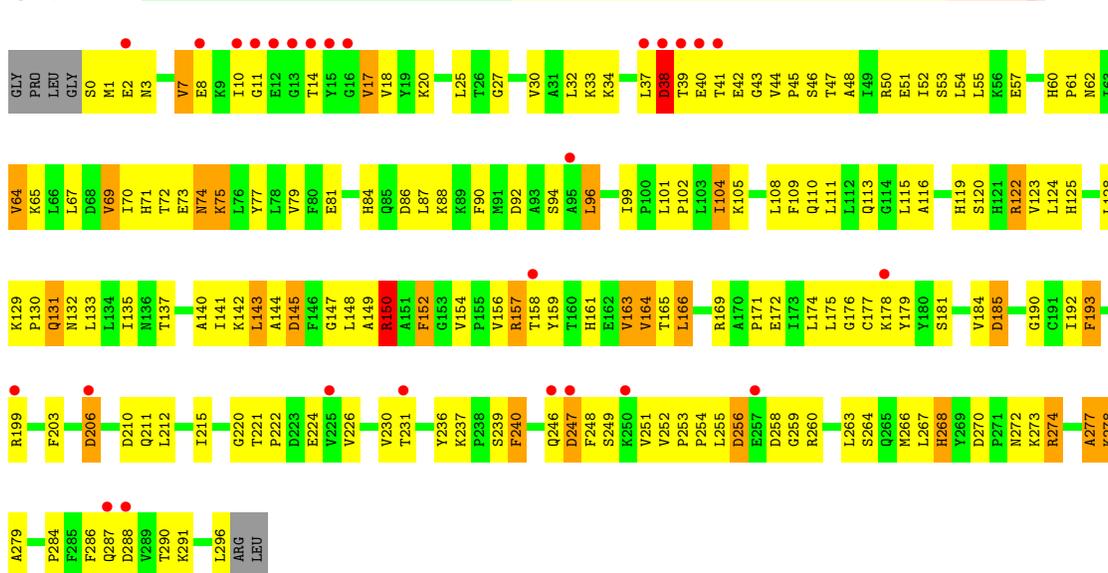

• Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain C:
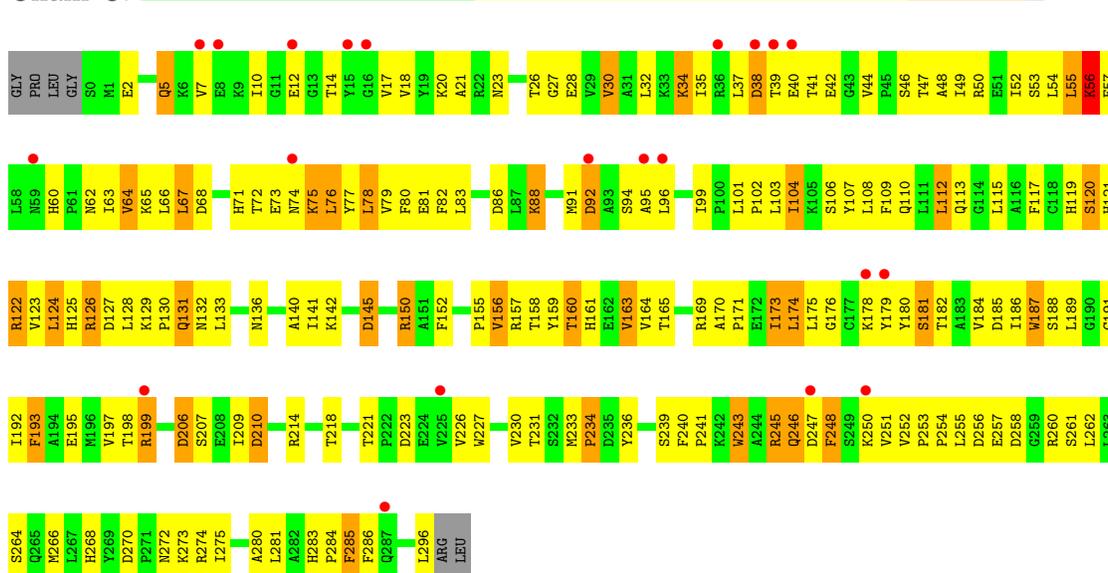
● Molecule 2: CYCLIN A2

Chain B:
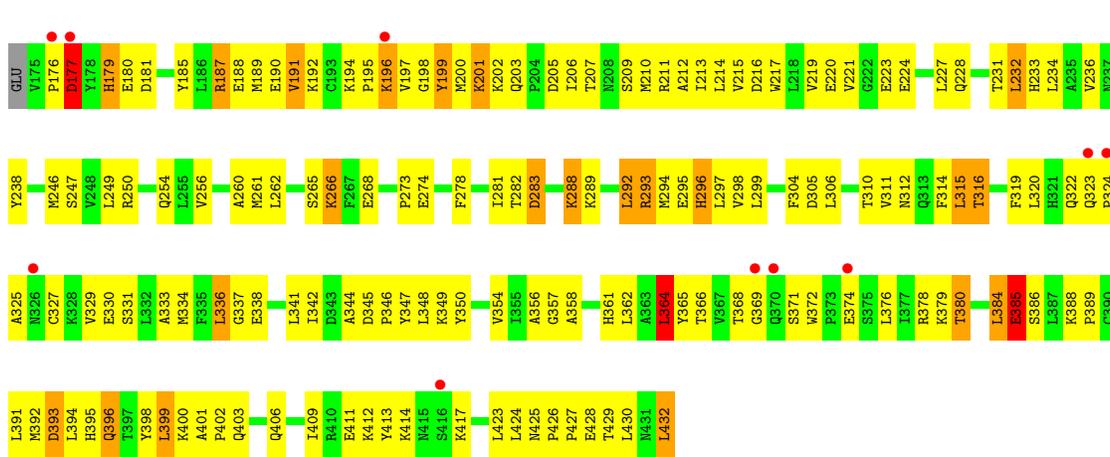
● Molecule 2: CYCLIN A2

Chain D:
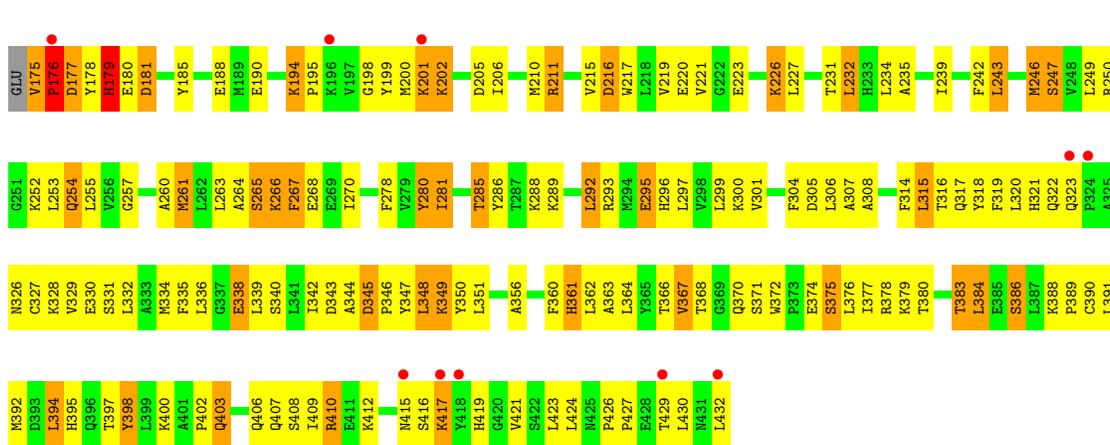
● Molecule 3: RETINOBLASTOMA-LIKE PROTEIN 1

Chain E:

● Molecule 3: RETINOBLASTOMA-LIKE PROTEIN 1

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	149.50Å 162.51Å 71.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.62 – 2.80 29.23 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (29.62-2.80) 95.1 (29.23-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.243 , 0.323 0.242 , 0.312	Depositor DCC
R_{free} test set	2095 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	42.2	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 27.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	1 of 41503 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9125	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.90 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.5558e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.92	2/2438 (0.1%)	1.03	10/3308 (0.3%)
1	C	0.95	1/2438 (0.0%)	1.06	12/3308 (0.4%)
2	B	1.03	0/2133	1.05	7/2897 (0.2%)
2	D	1.03	3/2133 (0.1%)	1.02	6/2897 (0.2%)
3	E	0.93	0/78	0.97	0/100
3	F	0.83	0/68	1.09	0/87
All	All	0.98	6/9288 (0.1%)	1.04	35/12597 (0.3%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	267	PHE	CD2-CE2	-7.79	1.23	1.39
2	D	261	MET	CG-SD	6.12	1.97	1.81
1	C	187	TRP	CE3-CZ3	-5.53	1.29	1.38
1	A	64	VAL	CA-CB	-5.52	1.43	1.54
2	D	281	ILE	CA-CB	-5.43	1.42	1.54
1	A	152	PHE	CD2-CE2	-5.04	1.29	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	247	ASP	CB-CG-OD2	9.71	127.04	118.30
1	C	127	ASP	CB-CG-OD2	9.23	126.61	118.30
2	B	283	ASP	CB-CG-OD2	8.61	126.05	118.30
2	B	345	ASP	CB-CG-OD2	8.50	125.95	118.30
1	A	86	ASP	CB-CG-OD2	7.71	125.24	118.30
1	A	270	ASP	CB-CG-OD2	7.68	125.21	118.30
2	B	205	ASP	CB-CG-OD2	7.55	125.09	118.30
2	B	305	ASP	CB-CG-OD2	7.53	125.07	118.30
1	C	210	ASP	CB-CG-OD2	7.32	124.88	118.30
1	C	256	ASP	CB-CG-OD2	7.18	124.76	118.30
1	C	206	ASP	CB-CG-OD2	7.12	124.71	118.30
1	C	169	ARG	NE-CZ-NH2	-6.96	116.82	120.30
2	D	177	ASP	CB-CG-OD2	6.95	124.56	118.30
1	C	86	ASP	CB-CG-OD2	6.86	124.47	118.30
2	B	393	ASP	CB-CG-OD2	6.70	124.33	118.30
1	A	206	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	247	ASP	CB-CG-OD2	6.60	124.24	118.30
1	C	92	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	210	ASP	CB-CG-OD2	6.50	124.16	118.30
2	B	181	ASP	CB-CG-OD2	6.26	123.94	118.30
1	A	185	ASP	CB-CG-OD2	6.10	123.79	118.30
1	C	76	LEU	CA-CB-CG	6.06	129.25	115.30
2	D	243	LEU	CA-CB-CG	6.05	129.22	115.30
2	D	216	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	258	ASP	CB-CG-OD2	5.87	123.58	118.30
2	D	343	ASP	CB-CG-OD2	5.54	123.28	118.30
1	C	258	ASP	CB-CG-OD2	5.52	123.27	118.30
2	B	177	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	92	ASP	CB-CG-OD2	5.48	123.23	118.30
2	D	345	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	38	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	223	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	124	LEU	CA-CB-CG	5.29	127.48	115.30
1	A	150	ARG	NE-CZ-NH1	5.21	122.91	120.30
2	D	305	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	TYR	Mainchain
1	C	160	TPO	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2429	170	0
1	C	2388	0	2430	195	0
2	B	2083	0	2107	148	2
2	D	2083	0	2107	175	2
3	E	78	0	80	8	0
3	F	68	0	72	15	0
4	A	12	0	0	3	0
4	B	11	0	0	0	0
4	C	10	0	0	6	0
4	D	3	0	0	0	0
4	F	1	0	0	1	0
All	All	9125	0	9225	654	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.

All (654) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:277:ALA:O	1:A:279:ALA:N	1.76	1.18
2:B:207:THR:OG1	2:B:210:MET:HG3	1.49	1.12
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.35	1.05
2:D:415:ASN:OD1	2:D:417:LYS:N	1.89	1.05
2:B:336:LEU:HD13	2:B:362:LEU:HD23	1.42	1.02
1:C:245:ARG:HG3	1:C:245:ARG:HH11	1.19	1.02
2:D:321:HIS:ND1	2:D:375:SER:OG	1.87	1.00
2:D:366:THR:HG23	2:D:427:PRO:HD3	1.44	0.99
1:C:88:LYS:HE3	1:C:131:GLN:NE2	1.77	0.98
1:C:227:TRP:O	1:C:230:VAL:HG23	1.66	0.95
2:D:175:VAL:O	2:D:177:ASP:N	2.00	0.93
1:A:0:SER:HA	4:A:2001:HOH:O	1.69	0.93
1:C:156:VAL:HG12	1:C:159:TYR:HE2	1.33	0.91
2:B:329:VAL:HG11	2:B:364:LEU:HD12	1.52	0.91
1:C:88:LYS:HB2	1:C:130:PRO:HB2	1.53	0.90
1:C:72:THR:HB	1:C:75:LYS:O	1.71	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:361:HIS:HD2	2:B:372:TRP:H	1.11	0.89
1:A:50:ARG:HH22	1:A:150:ARG:NH2	1.71	0.88
2:D:211:ARG:HH11	2:D:211:ARG:HG2	1.40	0.87
1:C:99:ILE:HG23	1:C:103:LEU:HD23	1.57	0.86
1:A:135:ILE:HG22	1:A:141:ILE:HG13	1.56	0.86
1:A:72:THR:O	1:A:74:ASN:N	2.07	0.86
1:A:88:LYS:HB2	1:A:130:PRO:HB2	1.56	0.85
1:A:116:ALA:HB2	1:A:277:ALA:HB1	1.59	0.85
1:A:7:VAL:HG11	1:A:20:LYS:HD3	1.59	0.85
1:C:248:PHE:HB3	1:C:260:ARG:HD2	1.60	0.84
1:A:129:LYS:NZ	1:A:165:THR:OG1	2.11	0.83
1:A:81:GLU:OE1	1:A:142:LYS:NZ	2.10	0.82
1:A:39:THR:HG21	2:B:289:LYS:HG2	1.59	0.82
2:B:266:LYS:NZ	2:B:295:GLU:OE1	2.11	0.82
1:A:50:ARG:NH2	1:A:150:ARG:NH2	2.26	0.81
3:F:659:ARG:NH2	3:F:663:GLU:HA	1.94	0.81
1:A:255:LEU:HD23	1:A:260:ARG:N	1.96	0.80
1:C:60:HIS:CD2	1:C:62:ASN:H	1.99	0.80
2:B:391:LEU:HD23	2:B:432:LEU:HD11	1.65	0.79
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.62	0.79
1:C:71:HIS:HE1	2:D:304:PHE:HE2	1.29	0.79
1:C:253:PRO:HB2	1:C:254:PRO:CD	2.11	0.79
1:A:266:MET:O	1:A:274:ARG:HD3	1.82	0.79
1:A:252:VAL:HG12	1:A:255:LEU:HB2	1.64	0.79
2:D:281:ILE:O	3:F:657:LYS:HA	1.83	0.79
1:C:268:HIS:NE2	1:C:273:LYS:HD2	1.99	0.78
2:D:329:VAL:HG22	2:D:367:VAL:HG21	1.64	0.78
1:C:119:HIS:HE1	1:C:185:ASP:OD2	1.65	0.78
1:C:245:ARG:HG3	1:C:245:ARG:NH1	1.98	0.78
1:C:117:PHE:O	1:C:120:SER:HB2	1.84	0.77
2:D:332:LEU:HD23	2:D:363:ALA:HA	1.65	0.77
2:B:336:LEU:CD1	2:B:362:LEU:HD23	2.14	0.76
1:C:83:LEU:HD11	1:C:142:LYS:HD2	1.66	0.76
1:C:49:ILE:O	1:C:53:SER:OG	2.03	0.76
1:C:21:ALA:HB3	1:C:30:VAL:HG22	1.67	0.76
1:C:245:ARG:HH11	1:C:245:ARG:CG	1.96	0.76
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.16	0.75
2:B:319:PHE:O	2:B:322:GLN:HB2	1.85	0.75
1:A:64:VAL:HG23	1:A:143:LEU:O	1.86	0.75
1:A:154:VAL:O	2:B:316:THR:HG23	1.88	0.74
2:B:342:ILE:HD11	2:B:409:ILE:HD12	1.69	0.74
1:C:251:VAL:HG12	1:C:252:VAL:HG13	1.69	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:400:LYS:HA	2:D:403:GLN:HE21	1.51	0.73
1:A:96:LEU:HD12	1:A:96:LEU:H	1.54	0.73
1:C:60:HIS:HD2	1:C:62:ASN:H	1.36	0.73
2:D:285:THR:HG21	3:F:659:ARG:HG3	1.71	0.72
1:A:1:MET:O	4:A:2002:HOH:O	2.07	0.72
2:D:265:SER:O	2:D:267:PHE:N	2.22	0.72
2:D:347:TYR:OH	2:D:394:LEU:HA	1.89	0.72
1:C:296:LEU:O	4:C:2010:HOH:O	2.08	0.72
1:C:39:THR:HA	2:D:292:LEU:HD23	1.70	0.72
1:C:88:LYS:HE3	1:C:131:GLN:HE22	1.53	0.72
1:A:40:GLU:O	2:B:288:LYS:NZ	2.18	0.72
1:A:224:GLU:OE2	1:A:231:THR:OG1	2.07	0.71
1:A:247:ASP:OD2	1:A:249:SER:OG	2.06	0.71
1:C:50:ARG:NH2	1:C:160:TPO:O2P	2.22	0.71
1:A:178:LYS:HE2	1:A:179:TYR:CE1	2.25	0.71
1:A:172:GLU:OE1	1:A:172:GLU:N	2.22	0.71
1:C:156:VAL:HG12	1:C:159:TYR:CE2	2.23	0.71
2:D:400:LYS:HA	2:D:403:GLN:NE2	2.06	0.70
2:D:175:VAL:C	2:D:177:ASP:H	1.93	0.70
2:D:278:PHE:O	2:D:281:ILE:HG22	1.91	0.70
1:A:72:THR:HG23	1:A:72:THR:O	1.90	0.69
1:C:39:THR:O	2:D:292:LEU:CD2	2.40	0.69
1:C:157:ARG:NH1	2:D:268:GLU:OE2	2.22	0.69
2:B:398:TYR:CE2	2:B:426:PRO:HB3	2.27	0.69
1:A:154:VAL:O	2:B:316:THR:CG2	2.41	0.69
2:B:412:LYS:HD3	2:B:413:TYR:CE1	2.27	0.69
2:B:223:GLU:OE2	2:B:412:LYS:HE3	1.92	0.69
1:A:2:GLU:OE1	1:C:73:GLU:HG2	1.91	0.69
2:B:411:GLU:O	2:B:414:LYS:HB2	1.93	0.69
2:D:306:LEU:O	2:D:308:ALA:N	2.19	0.69
3:F:661:PHE:O	3:F:663:GLU:N	2.21	0.68
1:A:108:LEU:HD23	1:A:286:PHE:HZ	1.56	0.68
2:B:196:LYS:O	2:B:199:TYR:HB3	1.92	0.68
1:A:33:LYS:NZ	1:A:51:GLU:OE2	2.26	0.68
1:A:25:LEU:HD12	2:D:297:LEU:HD22	1.76	0.68
1:A:10:ILE:HG12	1:A:18:VAL:O	1.94	0.68
1:A:239:SER:O	1:A:240:PHE:O	2.12	0.68
3:F:662:GLY:O	3:F:663:GLU:HB2	1.94	0.67
1:C:54:LEU:O	1:C:57:GLU:HB3	1.95	0.67
1:C:37:LEU:O	1:C:38:ASP:CB	2.42	0.67
1:C:181:SER:OG	1:C:182:THR:N	2.27	0.67
1:C:81:GLU:HG3	1:C:81:GLU:O	1.95	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:221:VAL:HG13	2:D:281:ILE:CD1	2.25	0.67
1:C:160:TPO:N	1:C:160:TPO:O3P	2.28	0.67
1:C:37:LEU:O	1:C:38:ASP:HB2	1.94	0.67
1:C:181:SER:O	1:C:184:VAL:HG22	1.95	0.67
2:B:254:GLN:NE2	3:E:660:LEU:HG	2.09	0.66
2:B:361:HIS:CD2	2:B:372:TRP:H	2.03	0.66
3:F:658:ARG:HG2	3:F:660:LEU:HD23	1.77	0.66
2:D:363:ALA:O	2:D:367:VAL:HG22	1.96	0.66
1:A:157:ARG:NH2	2:B:268:GLU:OE1	2.24	0.66
1:C:115:LEU:HD11	1:C:119:HIS:CE1	2.30	0.66
1:A:239:SER:O	1:A:240:PHE:C	2.31	0.66
2:D:383:THR:N	2:D:386:SER:OG	2.28	0.66
2:B:203:GLN:NE2	2:B:246:MET:O	2.28	0.66
2:D:384:LEU:HG	2:D:432:LEU:HD22	1.78	0.66
1:A:105:LYS:NZ	1:A:288:ASP:OD1	2.27	0.65
2:B:200:MET:SD	2:B:206:ILE:HG13	2.36	0.65
1:C:101:LEU:HB3	1:C:102:PRO:HD3	1.78	0.65
1:C:112:LEU:CD2	1:C:189:LEU:HD13	2.26	0.65
1:C:39:THR:CB	2:D:289:LYS:HD3	2.27	0.65
1:C:74:ASN:O	1:C:75:LYS:HB3	1.95	0.65
1:C:52:ILE:O	1:C:56:LYS:HG2	1.97	0.65
2:B:344:ALA:O	2:B:348:LEU:HB2	1.96	0.65
1:C:245:ARG:NH1	1:C:245:ARG:CG	2.59	0.64
2:D:211:ARG:NH1	2:D:211:ARG:HG2	2.09	0.64
2:D:364:LEU:HG	2:D:370:GLN:HB2	1.79	0.64
1:C:68:ASP:O	1:C:79:VAL:HG23	1.98	0.64
2:B:361:HIS:O	2:B:362:LEU:C	2.35	0.64
2:B:388:LYS:HB3	2:B:389:PRO:CD	2.27	0.64
2:B:361:HIS:NE2	2:B:371:SER:OG	2.31	0.64
2:D:332:LEU:O	2:D:335:PHE:HB3	1.98	0.64
2:D:400:LYS:O	2:D:403:GLN:HG2	1.97	0.64
2:B:299:LEU:HD23	2:B:306:LEU:HD21	1.80	0.64
1:A:50:ARG:HH22	1:A:150:ARG:HH21	1.43	0.64
1:A:10:ILE:HD11	1:A:18:VAL:HG12	1.79	0.64
2:D:366:THR:CG2	2:D:427:PRO:HD3	2.23	0.64
1:C:99:ILE:HG22	1:C:104:ILE:HG13	1.80	0.64
2:B:223:GLU:CD	2:B:412:LYS:HE3	2.18	0.64
1:A:37:LEU:O	1:A:38:ASP:HB2	1.98	0.64
1:C:112:LEU:HD23	1:C:189:LEU:HD13	1.80	0.63
1:C:10:ILE:HD13	1:C:82:PHE:HE1	1.63	0.63
2:D:299:LEU:HD22	2:D:304:PHE:CE1	2.34	0.63
2:B:342:ILE:CD1	2:B:409:ILE:HD12	2.28	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:65:LYS:HB3	1:A:81:GLU:OE2	1.97	0.63
1:A:2:GLU:HG2	1:A:2:GLU:O	1.98	0.63
2:D:221:VAL:HG13	2:D:281:ILE:HD12	1.79	0.63
2:D:361:HIS:CD2	2:D:362:LEU:N	2.66	0.63
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.14	0.63
2:D:416:SER:O	2:D:419:HIS:N	2.31	0.63
1:A:39:THR:CG2	2:B:289:LYS:HG2	2.29	0.63
2:B:412:LYS:HD3	2:B:413:TYR:HE1	1.62	0.62
1:A:247:ASP:OD2	1:A:249:SER:N	2.32	0.62
1:C:210:ASP:O	1:C:214:ARG:HG3	1.99	0.62
1:C:42:GLU:O	2:D:266:LYS:NZ	2.24	0.62
1:C:231:THR:HG22	1:C:236:TYR:CE2	2.35	0.62
1:C:155:PRO:HD2	2:D:316:THR:HG22	1.80	0.62
1:A:251:VAL:HG12	1:A:252:VAL:HG23	1.81	0.62
1:C:248:PHE:CB	1:C:260:ARG:HD2	2.27	0.62
1:A:108:LEU:HD23	1:A:286:PHE:CZ	2.34	0.62
2:D:384:LEU:HG	2:D:432:LEU:CD2	2.29	0.62
2:D:402:PRO:HA	2:D:407:GLN:HE22	1.64	0.62
3:F:659:ARG:HH21	3:F:663:GLU:HA	1.63	0.62
1:C:88:LYS:HA	1:C:91:MET:HE2	1.82	0.61
1:A:67:LEU:HD12	1:A:79:VAL:HG12	1.82	0.61
1:C:35:ILE:HD12	1:C:78:LEU:HD21	1.80	0.61
2:D:177:ASP:HB3	2:D:178:TYR:CD2	2.35	0.61
1:C:39:THR:OG1	2:D:289:LYS:HD3	1.99	0.61
1:C:5:GLN:HE21	1:C:5:GLN:HA	1.65	0.61
2:B:236:VAL:HG21	2:B:341:LEU:HD22	1.82	0.61
1:C:268:HIS:CE1	1:C:273:LYS:HD2	2.35	0.61
1:C:126:ARG:NH2	1:C:160:TPO:O1P	2.30	0.61
2:B:234:LEU:HD23	2:B:310:THR:HG21	1.81	0.61
1:A:253:PRO:HB2	1:A:254:PRO:HD3	1.83	0.61
1:C:283:HIS:ND1	1:C:284:PRO:HD2	2.14	0.61
1:A:190:GLY:HA2	1:A:266:MET:CE	2.31	0.60
1:C:161:HIS:O	1:C:163:VAL:N	2.33	0.60
2:D:285:THR:HG22	3:F:659:ARG:HD2	1.83	0.60
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.84	0.60
2:D:216:ASP:HB2	2:D:406:GLN:HG2	1.83	0.60
1:A:51:GLU:O	1:A:55:LEU:HB2	2.02	0.60
2:D:254:GLN:HG3	2:D:254:GLN:O	2.01	0.60
1:A:277:ALA:O	1:A:278:LYS:C	2.37	0.60
1:A:96:LEU:N	1:A:96:LEU:HD12	2.17	0.60
2:B:203:GLN:NE2	2:B:247:SER:HA	2.16	0.60
1:A:116:ALA:HB2	1:A:277:ALA:CB	2.31	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.84	0.60
2:D:289:LYS:HD2	2:D:293:ARG:HH21	1.67	0.60
2:D:368:THR:CB	2:D:370:GLN:HE21	2.14	0.60
2:D:176:PRO:HA	2:D:179:HIS:CG	2.37	0.59
2:D:360:PHE:HD2	2:D:372:TRP:CZ3	2.20	0.59
1:C:230:VAL:HG12	1:C:236:TYR:CD1	2.38	0.59
1:A:190:GLY:HA2	1:A:266:MET:HE3	1.83	0.59
1:A:157:ARG:HH11	1:A:157:ARG:HG3	1.68	0.59
2:D:247:SER:O	2:D:247:SER:OG	2.16	0.58
1:C:136:ASN:HD21	1:C:140:ALA:HB3	1.66	0.58
2:D:402:PRO:HB3	2:D:410:ARG:CZ	2.33	0.58
1:A:90:PHE:CE2	1:A:99:ILE:HD12	2.39	0.58
2:D:265:SER:O	2:D:266:LYS:C	2.41	0.58
1:C:55:LEU:C	1:C:57:GLU:H	2.07	0.58
1:C:39:THR:CA	2:D:292:LEU:HD23	2.34	0.58
2:D:253:LEU:HD12	2:D:253:LEU:O	2.03	0.58
1:A:239:SER:C	1:A:240:PHE:O	2.39	0.58
2:B:428:GLU:O	2:B:428:GLU:HG2	2.04	0.58
3:F:658:ARG:NE	4:F:2001:HOH:O	2.20	0.57
2:D:178:TYR:O	2:D:180:GLU:N	2.38	0.57
1:A:61:PRO:O	1:A:142:LYS:HD3	2.05	0.57
2:B:203:GLN:HE22	2:B:247:SER:HA	1.67	0.57
1:C:110:GLN:HE22	1:C:140:ALA:HA	1.69	0.57
1:A:54:LEU:HD13	1:A:123:VAL:HG13	1.86	0.57
1:A:1:MET:CE	1:A:70:ILE:HD13	2.35	0.57
1:A:177:CYS:SG	1:A:178:LYS:N	2.77	0.57
1:C:218:THR:HA	1:C:246:GLN:HG3	1.86	0.57
2:D:263:LEU:HD23	2:D:295:GLU:OE2	2.04	0.57
1:C:128:LEU:HB2	4:C:2004:HOH:O	2.04	0.57
2:D:388:LYS:N	2:D:389:PRO:CD	2.67	0.57
2:D:338:GLU:OE2	2:D:412:LYS:NZ	2.33	0.57
2:B:216:ASP:OD1	2:B:406:GLN:HB3	2.04	0.57
1:C:230:VAL:HG12	1:C:236:TYR:CE1	2.40	0.57
2:B:283:ASP:O	2:B:283:ASP:OD1	2.23	0.57
1:C:65:LYS:NZ	1:C:67:LEU:HD23	2.20	0.57
1:C:129:LYS:HE2	1:C:132:ASN:ND2	2.20	0.56
2:B:338:GLU:OE2	2:B:412:LYS:NZ	2.33	0.56
2:B:401:ALA:N	2:B:402:PRO:CD	2.69	0.56
1:C:109:PHE:CE2	1:C:113:GLN:NE2	2.73	0.56
3:F:659:ARG:CZ	3:F:663:GLU:HA	2.34	0.56
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.41	0.56
2:D:371:SER:O	2:D:372:TRP:C	2.44	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:84:HIS:CD2	1:A:296:LEU:HD13	2.41	0.56
1:C:21:ALA:HB3	1:C:30:VAL:CG2	2.34	0.56
2:B:391:LEU:HD23	2:B:432:LEU:CD1	2.32	0.56
1:C:108:LEU:CD2	1:C:193:PHE:CD2	2.88	0.56
2:B:365:TYR:O	2:B:369:GLY:HA2	2.04	0.56
2:D:234:LEU:O	2:D:235:ALA:C	2.40	0.56
1:A:256:ASP:O	1:A:260:ARG:HG3	2.05	0.56
1:C:7:VAL:HB	1:C:20:LYS:HB3	1.88	0.56
2:B:396:GLN:O	2:B:399:LEU:N	2.39	0.56
1:C:145:ASP:OD1	1:C:145:ASP:C	2.44	0.56
2:B:215:VAL:HG22	2:B:236:VAL:HG22	1.88	0.56
1:C:113:GLN:HA	1:C:281:LEU:HD11	1.88	0.56
2:D:254:GLN:HG2	2:D:286:TYR:HE2	1.71	0.55
1:C:268:HIS:CE1	1:C:273:LYS:HB3	2.42	0.55
2:D:220:GLU:HG3	2:D:408:SER:HB3	1.87	0.55
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.88	0.55
2:D:265:SER:O	2:D:268:GLU:N	2.40	0.55
2:B:187:ARG:NH1	2:B:187:ARG:HG3	2.20	0.55
1:A:124:LEU:HG	1:A:152:PHE:HD2	1.72	0.55
1:A:122:ARG:HA	1:A:152:PHE:CZ	2.41	0.55
2:D:416:SER:O	2:D:417:LYS:C	2.45	0.55
1:C:39:THR:O	2:D:292:LEU:HD23	2.06	0.55
2:B:200:MET:SD	2:B:206:ILE:CD1	2.95	0.55
2:D:321:HIS:HD1	2:D:375:SER:HG	0.57	0.55
1:A:42:GLU:O	2:B:266:LYS:NZ	2.38	0.55
1:C:178:LYS:HG2	1:C:179:TYR:CE1	2.42	0.55
2:D:336:LEU:HD13	2:D:362:LEU:HD23	1.88	0.55
2:D:319:PHE:CZ	2:D:330:GLU:HA	2.42	0.55
1:C:272:ASN:HB3	4:C:2009:HOH:O	2.07	0.55
2:D:314:PHE:O	2:D:315:LEU:C	2.44	0.55
2:D:227:LEU:N	2:D:227:LEU:HD23	2.22	0.55
1:C:35:ILE:O	1:C:35:ILE:HG22	2.06	0.54
1:C:101:LEU:HB3	1:C:102:PRO:CD	2.37	0.54
1:A:2:GLU:OE1	1:C:73:GLU:CG	2.55	0.54
1:A:1:MET:CE	1:A:70:ILE:CD1	2.86	0.54
2:D:317:GLN:NE2	2:D:379:LYS:NZ	2.56	0.54
2:D:175:VAL:N	2:D:176:PRO:CD	2.70	0.54
1:A:255:LEU:HD23	1:A:259:GLY:C	2.26	0.54
1:C:34:LYS:HB2	1:C:77:TYR:CE1	2.42	0.54
2:D:329:VAL:HG22	2:D:367:VAL:CG2	2.37	0.54
1:C:109:PHE:O	1:C:113:GLN:HB2	2.07	0.54
2:B:221:VAL:HG11	2:B:281:ILE:HD13	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:383:THR:N	2:D:386:SER:HG	2.04	0.54
1:C:193:PHE:CD1	1:C:193:PHE:C	2.82	0.54
1:A:226:VAL:O	1:A:226:VAL:HG22	2.07	0.54
1:A:110:GLN:HE22	1:A:140:ALA:HA	1.72	0.54
2:B:361:HIS:CD2	2:B:371:SER:OG	2.61	0.54
1:A:32:LEU:CD2	1:A:79:VAL:HG22	2.39	0.54
2:B:210:MET:HE1	2:B:250:ARG:HG2	1.90	0.53
1:C:50:ARG:O	1:C:54:LEU:HD12	2.08	0.53
1:A:172:GLU:O	1:A:177:CYS:HB2	2.08	0.53
1:A:171:PRO:HD2	1:A:172:GLU:OE1	2.07	0.53
2:D:392:MET:O	2:D:395:HIS:HB3	2.08	0.53
1:A:27:GLY:HA3	2:D:249:LEU:HD12	1.90	0.53
2:D:374:GLU:HA	2:D:377:ILE:HD12	1.90	0.53
1:A:122:ARG:HD2	1:A:122:ARG:O	2.08	0.53
2:D:175:VAL:C	2:D:177:ASP:N	2.56	0.53
2:B:185:TYR:O	2:B:188:GLU:HB3	2.09	0.53
2:B:294:MET:O	2:B:295:GLU:C	2.47	0.53
2:D:368:THR:HB	2:D:370:GLN:HE21	1.73	0.53
2:D:376:LEU:O	2:D:380:THR:OG1	2.16	0.53
2:B:221:VAL:CG1	2:B:281:ILE:HD13	2.39	0.53
2:D:415:ASN:OD1	2:D:416:SER:N	2.42	0.53
2:D:326:ASN:HB3	2:D:329:VAL:HG23	1.91	0.53
1:C:55:LEU:C	1:C:57:GLU:N	2.60	0.53
2:D:210:MET:CE	2:D:250:ARG:HB2	2.39	0.53
1:C:193:PHE:C	1:C:193:PHE:HD1	2.12	0.52
2:B:211:ARG:O	2:B:214:LEU:HB3	2.08	0.52
2:B:234:LEU:HD23	2:B:310:THR:CG2	2.40	0.52
2:B:203:GLN:HB3	2:B:206:ILE:HG12	1.91	0.52
1:A:211:GLN:O	1:A:215:ILE:HG13	2.09	0.52
1:C:63:ILE:O	1:C:64:VAL:C	2.47	0.52
1:A:181:SER:O	1:A:184:VAL:HG22	2.10	0.52
1:C:170:ALA:HB1	1:C:171:PRO:CD	2.39	0.52
3:E:659:ARG:HE	3:E:663:GLU:HA	1.73	0.52
1:C:156:VAL:CG1	1:C:159:TYR:HE2	2.14	0.52
2:D:221:VAL:HG22	2:D:281:ILE:CD1	2.39	0.52
1:C:39:THR:HB	2:D:289:LYS:HD3	1.91	0.52
1:A:42:GLU:HA	1:A:42:GLU:OE1	2.09	0.52
1:C:160:TPO:HG23	1:C:161:HIS:N	2.25	0.52
1:C:37:LEU:HD22	1:C:44:VAL:HA	1.91	0.52
1:A:236:TYR:C	1:A:236:TYR:CD2	2.82	0.52
2:B:330:GLU:O	2:B:333:ALA:HB3	2.10	0.52
2:D:216:ASP:CB	2:D:406:GLN:HG2	2.40	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:155:PRO:CD	2:D:316:THR:HG22	2.39	0.52
1:C:40:GLU:O	2:D:288:LYS:NZ	2.43	0.52
1:A:60:HIS:HD2	1:A:62:ASN:H	1.55	0.51
2:D:285:THR:CG2	3:F:659:ARG:HD2	2.40	0.51
1:A:101:LEU:HB3	1:A:102:PRO:HD3	1.92	0.51
2:B:196:LYS:HB2	2:B:196:LYS:NZ	2.25	0.51
1:C:178:LYS:HG2	1:C:179:TYR:CD1	2.45	0.51
1:C:266:MET:O	1:C:274:ARG:HD3	2.10	0.51
1:C:57:GLU:HG3	2:D:185:TYR:OH	2.11	0.51
2:B:262:LEU:O	2:B:265:SER:HB2	2.11	0.51
2:B:211:ARG:HD3	2:B:344:ALA:HB2	1.91	0.51
1:A:38:ASP:HB3	4:A:2004:HOH:O	2.10	0.51
2:B:189:MET:O	2:B:190:GLU:C	2.49	0.51
1:A:17:VAL:HG12	1:A:18:VAL:H	1.75	0.51
1:A:25:LEU:O	2:D:252:LYS:HG3	2.10	0.51
2:B:217:TRP:CE3	3:E:660:LEU:HD11	2.46	0.51
2:B:388:LYS:N	2:B:389:PRO:HD2	2.26	0.51
1:C:160:TPO:HA	2:D:270:ILE:HG23	1.92	0.51
1:A:52:ILE:O	1:A:53:SER:C	2.49	0.51
1:C:231:THR:HG22	1:C:236:TYR:CZ	2.46	0.51
3:E:657:LYS:O	3:E:658:ARG:HB2	2.12	0.50
2:B:249:LEU:HD12	1:C:27:GLY:HA3	1.92	0.50
1:C:101:LEU:N	1:C:102:PRO:HD2	2.26	0.50
2:D:221:VAL:HG22	2:D:281:ILE:HD11	1.93	0.50
1:C:128:LEU:CB	4:C:2004:HOH:O	2.59	0.50
2:D:350:TYR:CE1	2:D:390:CYS:HB2	2.47	0.50
1:A:132:ASN:OD1	1:A:145:ASP:HB3	2.12	0.50
1:C:123:VAL:HG12	1:C:124:LEU:N	2.25	0.50
1:A:266:MET:O	1:A:274:ARG:CD	2.58	0.50
2:D:306:LEU:C	2:D:308:ALA:H	2.12	0.50
2:D:205:ASP:O	2:D:206:ILE:CG2	2.59	0.50
2:B:342:ILE:HD11	2:B:409:ILE:CD1	2.39	0.50
2:B:398:TYR:CD2	2:B:426:PRO:HB3	2.46	0.50
2:B:187:ARG:HH11	2:B:187:ARG:CG	2.24	0.50
1:C:101:LEU:O	1:C:104:ILE:HB	2.12	0.50
2:B:278:PHE:O	2:B:282:THR:HG23	2.12	0.50
1:C:253:PRO:CB	1:C:254:PRO:CD	2.83	0.50
2:D:175:VAL:N	2:D:176:PRO:HD2	2.26	0.50
1:A:268:HIS:HB2	1:A:274:ARG:HA	1.92	0.50
2:D:339:LEU:HD23	2:D:409:ILE:HG21	1.92	0.50
2:B:322:GLN:CD	2:B:325:ALA:HA	2.33	0.50
1:C:108:LEU:HD11	1:C:112:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:40:GLU:H	2:B:292:LEU:HD23	1.75	0.50
1:A:115:LEU:HD21	1:A:185:ASP:HB3	1.93	0.50
1:C:284:PRO:C	1:C:286:PHE:N	2.62	0.49
2:D:395:HIS:O	2:D:398:TYR:HB3	2.12	0.49
1:C:197:VAL:HG21	1:C:255:LEU:HD13	1.94	0.49
1:A:174:LEU:HD13	1:A:212:LEU:HD23	1.93	0.49
2:D:361:HIS:HD2	2:D:391:LEU:HD11	1.76	0.49
1:A:124:LEU:HG	1:A:152:PHE:CD2	2.46	0.49
1:C:233:MET:O	1:C:234:PRO:C	2.50	0.49
2:D:200:MET:SD	2:D:206:ILE:HG13	2.52	0.49
2:D:327:CYS:SG	2:D:328:LYS:N	2.86	0.49
3:F:659:ARG:HH21	3:F:663:GLU:CA	2.25	0.49
1:C:60:HIS:HD2	1:C:62:ASN:N	2.08	0.49
2:B:409:ILE:O	2:B:412:LYS:HB3	2.13	0.49
1:A:37:LEU:O	1:A:38:ASP:CB	2.61	0.49
2:B:203:GLN:OE1	2:B:247:SER:HA	2.13	0.49
2:B:314:PHE:O	2:B:315:LEU:C	2.49	0.49
1:A:1:MET:C	1:A:3:ASN:H	2.16	0.49
1:C:241:PRO:HB2	1:C:243:TRP:CZ3	2.48	0.49
2:B:227:LEU:HD21	2:B:273:PRO:CG	2.43	0.49
1:C:39:THR:O	2:D:292:LEU:HD22	2.11	0.48
2:D:326:ASN:OD1	2:D:329:VAL:HG23	2.12	0.48
1:C:180:TYR:C	1:C:180:TYR:CD1	2.86	0.48
2:D:296:HIS:CD2	2:D:300:LYS:HE2	2.48	0.48
1:A:7:VAL:HG12	1:A:8:GLU:N	2.28	0.48
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.95	0.48
1:A:124:LEU:O	1:A:149:ALA:HA	2.13	0.48
2:B:336:LEU:O	2:B:337:GLY:C	2.51	0.48
1:C:260:ARG:O	1:C:264:SER:HB3	2.13	0.48
1:A:47:THR:O	1:A:51:GLU:N	2.40	0.48
2:B:278:PHE:HD1	2:B:281:ILE:HD11	1.78	0.48
1:C:57:GLU:CG	2:D:185:TYR:OH	2.61	0.48
2:D:255:LEU:HB2	2:D:286:TYR:CZ	2.47	0.48
1:C:209:ILE:CG2	1:C:210:ASP:N	2.76	0.48
2:D:392:MET:CE	2:D:430:LEU:HD12	2.44	0.48
1:A:284:PRO:O	1:A:287:GLN:HG2	2.14	0.48
2:D:246:MET:HG2	2:D:301:VAL:HG11	1.96	0.48
1:C:95:ALA:O	1:C:199:ARG:NH1	2.44	0.48
1:C:83:LEU:HA	1:C:83:LEU:HD23	1.49	0.48
2:B:346:PRO:O	2:B:348:LEU:N	2.47	0.48
1:C:284:PRO:O	1:C:286:PHE:N	2.47	0.48
1:C:123:VAL:CG1	1:C:124:LEU:N	2.76	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:378:ARG:CB	2:D:378:ARG:HH11	2.27	0.48
1:C:65:LYS:HZ3	1:C:67:LEU:HD23	1.77	0.48
2:D:260:ALA:O	2:D:261:MET:C	2.52	0.48
1:C:99:ILE:CG2	1:C:104:ILE:HG13	2.43	0.47
1:A:131:GLN:N	1:A:131:GLN:OE1	2.47	0.47
2:B:400:LYS:HG2	2:B:403:GLN:HE21	1.79	0.47
2:B:384:LEU:O	2:B:385:GLU:C	2.53	0.47
1:A:190:GLY:O	1:A:193:PHE:HB3	2.13	0.47
1:C:10:ILE:HD11	1:C:20:LYS:HA	1.96	0.47
2:B:198:GLY:O	2:B:201:LYS:HG3	2.14	0.47
1:A:266:MET:O	1:A:274:ARG:HG3	2.14	0.47
1:A:237:LYS:HG2	1:A:240:PHE:CZ	2.49	0.47
2:B:299:LEU:HD21	2:B:306:LEU:HD11	1.96	0.47
1:A:2:GLU:CG	1:A:2:GLU:O	2.63	0.47
1:A:17:VAL:C	1:A:18:VAL:HG23	2.35	0.47
2:B:329:VAL:HG11	2:B:364:LEU:CD1	2.35	0.47
1:A:171:PRO:HA	1:A:174:LEU:HB2	1.97	0.47
2:B:398:TYR:CZ	2:B:426:PRO:HB3	2.49	0.47
2:D:366:THR:HG23	2:D:427:PRO:CD	2.31	0.47
1:C:88:LYS:HB2	1:C:130:PRO:CB	2.36	0.47
1:C:103:LEU:O	1:C:104:ILE:C	2.53	0.47
2:B:428:GLU:O	2:B:429:THR:HG23	2.15	0.47
2:D:205:ASP:O	2:D:206:ILE:HG23	2.14	0.47
2:B:293:ARG:CG	1:C:2:GLU:OE2	2.63	0.47
2:D:254:GLN:HG2	2:D:286:TYR:CE2	2.49	0.47
1:A:11:GLY:O	1:A:18:VAL:HB	2.14	0.47
2:B:201:LYS:HB2	2:B:201:LYS:HE2	1.64	0.47
1:A:267:LEU:HA	1:A:267:LEU:HD23	1.71	0.47
2:D:252:LYS:O	2:D:255:LEU:N	2.47	0.47
2:D:226:LYS:HE3	2:D:226:LYS:HB3	1.52	0.47
1:C:156:VAL:HG22	4:C:2006:HOH:O	2.15	0.47
1:C:46:SER:O	1:C:50:ARG:HG3	2.14	0.47
1:A:33:LYS:NZ	1:A:51:GLU:CD	2.68	0.47
2:D:178:TYR:O	2:D:181:ASP:N	2.46	0.46
1:C:74:ASN:O	1:C:75:LYS:CB	2.63	0.46
2:B:398:TYR:O	2:B:398:TYR:CD1	2.68	0.46
1:A:259:GLY:O	1:A:260:ARG:C	2.52	0.46
2:D:360:PHE:CD2	2:D:372:TRP:CZ3	3.03	0.46
1:A:64:VAL:HG12	1:A:65:LYS:N	2.29	0.46
1:A:226:VAL:CG2	1:A:226:VAL:O	2.63	0.46
2:B:190:GLU:O	2:B:191:VAL:C	2.53	0.46
2:D:210:MET:HE3	2:D:250:ARG:HB2	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:241:PRO:HB2	1:C:243:TRP:CE3	2.50	0.46
1:C:106:SER:O	1:C:107:TYR:C	2.52	0.46
1:A:10:ILE:HG13	1:A:11:GLY:N	2.30	0.46
1:C:17:VAL:HG12	1:C:18:VAL:N	2.30	0.46
2:B:398:TYR:O	2:B:398:TYR:HD1	1.99	0.46
2:D:199:TYR:C	2:D:199:TYR:CD1	2.88	0.46
2:B:256:VAL:HG22	2:B:294:MET:CE	2.46	0.46
1:C:64:VAL:CG1	1:C:65:LYS:N	2.78	0.46
1:C:129:LYS:HE3	1:C:131:GLN:HG2	1.98	0.46
1:A:268:HIS:CD2	1:A:273:LYS:HB3	2.50	0.46
2:D:360:PHE:HD2	2:D:372:TRP:CE3	2.32	0.46
2:D:397:THR:O	2:D:398:TYR:C	2.55	0.46
2:D:231:THR:HG23	2:D:264:ALA:C	2.36	0.46
2:D:190:GLU:HG3	2:D:351:LEU:HD22	1.97	0.45
2:B:350:TYR:OH	2:B:389:PRO:O	2.32	0.45
1:C:125:HIS:O	1:C:126:ARG:HB2	2.16	0.45
1:C:108:LEU:CD1	1:C:112:LEU:HD21	2.46	0.45
1:C:170:ALA:HB1	1:C:171:PRO:HD2	1.97	0.45
1:A:165:THR:O	1:A:166:LEU:C	2.54	0.45
1:A:166:LEU:HD13	1:A:169:ARG:NH1	2.31	0.45
1:A:125:HIS:NE2	1:A:144:ALA:O	2.35	0.45
1:C:30:VAL:HB	1:C:80:PHE:O	2.17	0.45
1:C:284:PRO:O	1:C:285:PHE:C	2.55	0.45
2:D:239:ILE:HD11	2:D:257:GLY:HA2	1.99	0.45
1:A:203:PHE:O	1:A:211:GLN:NE2	2.46	0.45
1:C:39:THR:C	2:D:292:LEU:HD23	2.37	0.45
1:C:261:SER:O	1:C:262:LEU:C	2.54	0.45
2:D:288:LYS:HB3	2:D:288:LYS:HE2	1.56	0.45
2:B:296:HIS:O	2:B:297:LEU:C	2.55	0.45
2:D:360:PHE:CD2	2:D:372:TRP:HZ3	2.35	0.45
1:A:64:VAL:HG21	1:A:144:ALA:HB2	1.98	0.45
1:C:284:PRO:C	1:C:286:PHE:H	2.20	0.45
1:A:90:PHE:HE2	1:A:99:ILE:HD12	1.79	0.45
1:A:87:LEU:HG	1:A:87:LEU:O	2.17	0.45
2:B:219:VAL:HG21	2:B:409:ILE:CG1	2.47	0.45
2:D:423:LEU:O	2:D:424:LEU:C	2.49	0.45
2:B:394:LEU:HD12	2:B:394:LEU:HA	1.59	0.45
1:A:129:LYS:HA	1:A:192:ILE:HD11	1.99	0.45
2:D:252:LYS:O	2:D:253:LEU:C	2.54	0.45
2:D:253:LEU:HD12	2:D:253:LEU:C	2.35	0.45
2:B:423:LEU:O	2:B:424:LEU:C	2.54	0.45
1:A:252:VAL:CG1	1:A:255:LEU:HB2	2.42	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:200:MET:SD	2:B:206:ILE:CG1	3.05	0.44
1:A:45:PRO:O	1:A:48:ALA:HB3	2.16	0.44
1:A:248:PHE:CE2	1:A:264:SER:HB3	2.52	0.44
1:A:172:GLU:O	1:A:177:CYS:CB	2.65	0.44
1:A:142:LYS:O	1:A:143:LEU:C	2.55	0.44
1:C:55:LEU:O	1:C:57:GLU:N	2.50	0.44
2:B:312:ASN:OD1	2:B:334:MET:CE	2.65	0.44
2:B:358:ALA:HA	2:B:391:LEU:HD13	1.99	0.44
2:D:217:TRP:O	2:D:221:VAL:HG23	2.18	0.44
2:D:281:ILE:O	2:D:281:ILE:HG12	2.17	0.44
1:C:10:ILE:HD11	1:C:20:LYS:CA	2.47	0.44
2:D:318:TYR:HA	2:D:376:LEU:HD21	1.99	0.44
2:D:211:ARG:HH12	2:D:215:VAL:HG21	1.82	0.44
1:A:1:MET:C	1:A:3:ASN:N	2.71	0.44
2:B:199:TYR:CD1	2:B:199:TYR:C	2.91	0.44
2:D:361:HIS:CD2	2:D:391:LEU:HD11	2.51	0.44
1:A:111:LEU:HD21	1:A:133:LEU:HD22	2.00	0.44
2:B:212:ALA:O	2:B:213:ILE:C	2.54	0.44
2:D:201:LYS:HE3	2:D:202:LYS:NZ	2.32	0.44
1:A:50:ARG:NH2	1:A:150:ARG:CZ	2.80	0.44
1:C:119:HIS:CE1	1:C:185:ASP:OD2	2.57	0.44
2:D:292:LEU:HA	2:D:292:LEU:HD12	1.75	0.44
1:C:209:ILE:HG23	1:C:210:ASP:N	2.33	0.44
2:D:317:GLN:NE2	2:D:379:LYS:HZ1	2.16	0.44
1:A:109:PHE:O	1:A:113:GLN:HG3	2.18	0.44
2:D:342:ILE:HD11	2:D:409:ILE:HD12	2.00	0.44
2:B:385:GLU:O	2:B:386:SER:C	2.56	0.44
2:B:293:ARG:HG2	1:C:2:GLU:OE2	2.18	0.44
2:D:345:ASP:HA	2:D:346:PRO:HA	1.74	0.44
1:A:1:MET:HE3	1:A:70:ILE:CD1	2.48	0.44
1:A:71:HIS:CE1	2:B:304:PHE:CE1	3.05	0.44
1:A:268:HIS:CB	1:A:274:ARG:HA	2.48	0.44
2:B:187:ARG:HH11	2:B:187:ARG:HG3	1.82	0.44
1:C:227:TRP:HB3	1:C:230:VAL:CG2	2.48	0.44
1:C:115:LEU:CD1	1:C:119:HIS:CE1	3.00	0.44
1:C:48:ALA:O	1:C:49:ILE:C	2.53	0.44
2:B:214:LEU:HD12	2:B:214:LEU:O	2.17	0.44
1:C:233:MET:HE2	1:C:233:MET:HB2	1.69	0.44
1:C:12:GLU:HA	1:C:17:VAL:HA	2.00	0.44
1:C:17:VAL:HG12	1:C:18:VAL:H	1.81	0.44
1:A:71:HIS:HE1	2:B:304:PHE:CD1	2.36	0.44
2:D:278:PHE:O	2:D:281:ILE:CG2	2.62	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:350:TYR:CD1	2:D:390:CYS:HB2	2.53	0.43
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.82	0.43
2:B:190:GLU:O	2:B:192:LYS:N	2.51	0.43
1:C:18:VAL:HA	1:C:32:LEU:O	2.18	0.43
1:C:71:HIS:CE1	2:D:304:PHE:HE2	2.21	0.43
1:C:112:LEU:HD13	1:C:280:ALA:HB3	2.00	0.43
2:D:242:PHE:O	2:D:246:MET:HB2	2.18	0.43
1:C:239:SER:O	1:C:240:PHE:C	2.57	0.43
1:C:261:SER:HB3	1:C:283:HIS:CE1	2.53	0.43
2:D:315:LEU:HD13	2:D:356:ALA:HB1	2.00	0.43
2:D:194:LYS:HA	2:D:195:PRO:HD3	1.87	0.43
2:B:354:VAL:O	2:B:357:GLY:N	2.52	0.43
2:B:288:LYS:O	2:B:289:LYS:C	2.56	0.43
2:B:203:GLN:CD	2:B:247:SER:HA	2.38	0.43
1:A:115:LEU:HD11	1:A:185:ASP:HB3	2.00	0.43
2:B:315:LEU:HD13	2:B:356:ALA:HB1	2.01	0.43
1:C:221:THR:OG1	1:C:241:PRO:O	2.24	0.43
1:A:72:THR:CG2	1:A:72:THR:O	2.60	0.43
2:B:203:GLN:HE22	2:B:246:MET:C	2.21	0.43
2:B:247:SER:OG	1:C:28:GLU:OE2	2.37	0.43
2:B:281:ILE:O	3:E:657:LYS:HA	2.18	0.43
1:A:203:PHE:HB2	1:A:211:GLN:HE22	1.84	0.43
3:E:661:PHE:O	3:E:663:GLU:N	2.52	0.43
2:B:401:ALA:N	2:B:402:PRO:HD3	2.33	0.43
2:B:374:GLU:O	2:B:374:GLU:HG3	2.19	0.43
1:A:46:SER:HB3	2:B:266:LYS:HG2	2.01	0.43
1:C:160:TPO:HA	2:D:270:ILE:CG2	2.49	0.43
2:B:249:LEU:HD12	1:C:27:GLY:CA	2.48	0.43
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.54	0.43
1:A:277:ALA:O	1:A:279:ALA:CA	2.60	0.43
1:A:33:LYS:NZ	1:A:51:GLU:OE1	2.52	0.43
1:C:63:ILE:O	1:C:64:VAL:O	2.37	0.43
1:A:17:VAL:C	1:A:18:VAL:CG2	2.87	0.43
2:D:384:LEU:HA	2:D:384:LEU:HD12	1.69	0.43
2:B:395:HIS:O	2:B:396:GLN:C	2.58	0.42
2:D:232:LEU:O	2:D:232:LEU:HD22	2.19	0.42
2:B:366:THR:OG1	2:B:427:PRO:HD3	2.19	0.42
1:A:40:GLU:H	2:B:292:LEU:CD2	2.32	0.42
1:A:220:GLY:O	1:A:221:THR:C	2.55	0.42
3:F:661:PHE:C	3:F:663:GLU:H	2.16	0.42
1:A:1:MET:HE3	1:A:70:ILE:HD12	2.01	0.42
1:A:105:LYS:O	1:A:286:PHE:HE1	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:415:ASN:OD1	2:D:417:LYS:CB	2.67	0.42
1:A:57:GLU:OE2	2:B:189:MET:CE	2.67	0.42
1:C:121:HIS:O	1:C:122:ARG:HD2	2.18	0.42
1:C:227:TRP:CD2	1:C:230:VAL:HG22	2.55	0.42
2:D:350:TYR:CZ	2:D:390:CYS:HA	2.55	0.42
1:C:176:GLY:O	1:C:234:PRO:HG2	2.19	0.42
2:D:372:TRP:CH2	2:D:376:LEU:HD13	2.54	0.42
2:B:294:MET:O	2:B:298:VAL:HG23	2.20	0.42
1:A:247:ASP:OD2	1:A:249:SER:CB	2.67	0.42
1:A:174:LEU:C	1:A:176:GLY:H	2.23	0.42
2:D:372:TRP:CZ3	2:D:376:LEU:HD13	2.55	0.42
1:A:221:THR:HA	1:A:222:PRO:HD3	1.95	0.42
1:A:278:LYS:HE2	2:B:177:ASP:O	2.20	0.42
1:C:71:HIS:HE1	2:D:304:PHE:CE2	2.21	0.42
2:B:323:GLN:HA	2:B:324:PRO:HA	1.80	0.42
1:A:158:THR:HG23	1:A:178:LYS:O	2.20	0.42
2:B:233:HIS:CD2	2:B:311:VAL:HB	2.55	0.42
1:C:131:GLN:CD	1:C:131:GLN:H	2.22	0.42
1:A:252:VAL:HG21	1:A:263:LEU:CD2	2.50	0.42
2:B:322:GLN:O	2:B:324:PRO:HA	2.20	0.42
2:D:362:LEU:HA	2:D:362:LEU:HD12	1.81	0.42
2:D:317:GLN:NE2	2:D:379:LYS:HZ3	2.18	0.41
2:D:255:LEU:HB2	2:D:286:TYR:CE1	2.55	0.41
1:C:173:ILE:O	1:C:175:LEU:N	2.53	0.41
2:B:346:PRO:HG3	2:B:393:ASP:OD2	2.20	0.41
2:D:223:GLU:CD	2:D:412:LYS:HD2	2.40	0.41
2:D:344:ALA:O	2:D:348:LEU:HB2	2.20	0.41
1:A:42:GLU:OE2	2:B:274:GLU:HG2	2.20	0.41
1:A:174:LEU:CD1	1:A:212:LEU:HD23	2.49	0.41
2:B:214:LEU:HD12	2:B:214:LEU:C	2.40	0.41
1:A:110:GLN:O	1:A:113:GLN:HB2	2.20	0.41
2:D:323:GLN:HA	2:D:323:GLN:OE1	2.20	0.41
1:C:91:MET:HB2	1:C:91:MET:HE2	1.87	0.41
2:D:254:GLN:CG	2:D:254:GLN:O	2.68	0.41
1:C:110:GLN:HB2	1:C:141:ILE:CG2	2.50	0.41
2:D:317:GLN:O	2:D:320:LEU:HB2	2.20	0.41
2:D:331:SER:HB2	2:D:421:VAL:HG11	2.01	0.41
2:B:376:LEU:O	2:B:380:THR:HG23	2.21	0.41
1:C:186:ILE:O	1:C:187:TRP:C	2.57	0.41
2:D:280:TYR:CE1	3:F:657:LYS:HD3	2.55	0.41
2:D:198:GLY:C	2:D:200:MET:N	2.74	0.41
2:D:190:GLU:O	2:D:194:LYS:HB3	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:23:ASN:CG	1:C:26:THR:OG1	2.58	0.41
1:C:270:ASP:C	1:C:270:ASP:OD1	2.59	0.41
1:C:88:LYS:HD3	1:C:92:ASP:OD2	2.20	0.41
1:C:157:ARG:O	1:C:158:THR:C	2.59	0.41
1:C:173:ILE:HG22	1:C:174:LEU:N	2.35	0.41
1:C:136:ASN:OD1	1:C:140:ALA:N	2.41	0.41
1:A:99:ILE:HG22	1:A:104:ILE:HG13	2.02	0.41
2:D:346:PRO:O	2:D:349:LYS:HG2	2.21	0.41
2:D:348:LEU:HA	2:D:348:LEU:HD12	1.78	0.41
2:B:388:LYS:O	2:B:392:MET:N	2.45	0.41
1:C:173:ILE:O	1:C:174:LEU:C	2.59	0.41
3:E:659:ARG:HH21	3:E:663:GLU:N	2.19	0.41
2:B:398:TYR:C	2:B:398:TYR:CD1	2.92	0.41
1:C:262:LEU:HD23	1:C:285:PHE:CD2	2.56	0.41
2:B:283:ASP:C	2:B:283:ASP:OD1	2.59	0.41
1:A:110:GLN:O	1:A:111:LEU:C	2.58	0.41
1:A:57:GLU:OE2	2:B:189:MET:HE2	2.20	0.41
2:B:423:LEU:C	2:B:424:LEU:O	2.57	0.41
1:A:69:VAL:HG22	1:A:71:HIS:CE1	2.56	0.41
3:E:655:SER:OG	3:E:655:SER:O	2.31	0.41
1:A:75:LYS:HZ2	1:A:75:LYS:HB2	1.85	0.41
1:A:75:LYS:NZ	1:A:77:TYR:OH	2.48	0.41
2:D:326:ASN:HB3	2:D:329:VAL:CG2	2.51	0.41
1:C:189:LEU:O	1:C:193:PHE:N	2.40	0.41
2:D:398:TYR:CD2	2:D:426:PRO:HB3	2.56	0.41
2:B:260:ALA:O	2:B:261:MET:C	2.55	0.41
2:B:194:LYS:HA	2:B:195:PRO:HD3	1.81	0.41
4:C:2006:HOH:O	2:D:175:VAL:HG21	2.22	0.40
1:A:190:GLY:HA2	1:A:266:MET:HE1	2.02	0.40
1:C:173:ILE:HD11	1:C:184:VAL:HG11	2.04	0.40
1:A:157:ARG:HD3	2:B:228:GLN:OE1	2.21	0.40
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.76	0.40
1:C:188:SER:O	1:C:192:ILE:HG13	2.22	0.40
1:A:115:LEU:HD13	1:A:128:LEU:HD11	2.03	0.40
1:C:188:SER:O	1:C:189:LEU:C	2.60	0.40
1:A:1:MET:CE	1:A:70:ILE:HD12	2.52	0.40
1:C:150:ARG:HH21	1:C:160:TPO:P	2.44	0.40
1:A:174:LEU:HB3	1:A:212:LEU:HD21	2.02	0.40
2:B:238:TYR:OH	2:B:306:LEU:HB3	2.21	0.40
2:D:342:ILE:HD13	2:D:342:ILE:HG21	1.91	0.40
1:A:71:HIS:CE1	2:B:304:PHE:HE1	2.39	0.40
3:F:662:GLY:O	3:F:663:GLU:CB	2.66	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:265:SER:C	2:D:267:PHE:N	2.74	0.40
1:C:191:CYS:O	1:C:195:GLU:HB2	2.22	0.40
2:B:176:PRO:HA	2:B:179:HIS:ND1	2.36	0.40
2:D:338:GLU:C	2:D:340:SER:N	2.72	0.40
2:B:216:ASP:CB	2:B:406:GLN:HG2	2.51	0.40
2:B:315:LEU:HD12	2:B:315:LEU:HA	1.94	0.40
1:A:41:THR:C	1:A:43:GLY:H	2.25	0.40
2:B:180:GLU:OE1	2:B:180:GLU:HA	2.21	0.40

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:379:LYS:O	2:D:378:ARG:NH2[2_665]	1.84	0.36
2:B:378:ARG:NH1	2:D:320:LEU:O[2_665]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/303 (97%)	232 (79%)	47 (16%)	15 (5%)	3	9
1	C	294/303 (97%)	242 (82%)	37 (13%)	15 (5%)	3	9
2	B	256/259 (99%)	204 (80%)	42 (16%)	10 (4%)	5	15
2	D	256/259 (99%)	201 (78%)	48 (19%)	7 (3%)	8	25
3	E	8/11 (73%)	4 (50%)	2 (25%)	2 (25%)	0	0
3	F	6/11 (54%)	4 (67%)	1 (17%)	1 (17%)	0	0
All	All	1114/1146 (97%)	887 (80%)	177 (16%)	50 (4%)	4	12

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	73	GLU

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Mol	Chain	Res	Type
1	A	137	THR
1	A	277	ALA
1	A	278	LYS
2	B	197	VAL
1	C	14	THR
1	C	145	ASP
1	C	174	LEU
2	D	176	PRO
2	D	266	LYS
1	A	145	ASP
1	A	164	VAL
1	A	175	LEU
2	B	320	LEU
2	B	347	TYR
1	C	38	ASP
1	C	75	LYS
1	C	164	VAL
1	C	173	ILE
2	D	179	HIS
2	D	307	ALA
2	D	417	LYS
3	E	658	ARG
3	F	662	GLY
1	A	38	ASP
1	A	143	LEU
2	B	191	VAL
2	B	364	LEU
1	C	41	THR
1	C	56	LYS
1	C	285	PHE
3	E	655	SER
1	A	193	PHE
1	A	256	ASP
2	B	385	GLU
2	B	396	GLN
1	C	64	VAL
1	C	120	SER
2	B	179	HIS
2	B	336	LEU
1	C	104	ILE
1	C	234	PRO
2	D	265	SER

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Mol	Chain	Res	Type
2	B	327	CYS
2	D	201	LYS
1	A	104	ILE
1	A	147	GLY
1	A	240	PHE
1	C	275	ILE

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	261/265 (98%)	232 (89%)	29 (11%)	9	25
1	C	261/265 (98%)	226 (87%)	35 (13%)	6	16
2	B	232/233 (100%)	202 (87%)	30 (13%)	6	18
2	D	232/233 (100%)	197 (85%)	35 (15%)	4	12
3	E	7/7 (100%)	7 (100%)	0	100	100
3	F	6/7 (86%)	5 (83%)	1 (17%)	3	9
All	All	999/1010 (99%)	869 (87%)	130 (13%)	6	17

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	17	VAL
1	A	30	VAL
1	A	34	LYS
1	A	44	VAL
1	A	69	VAL
1	A	74	ASN
1	A	75	LYS
1	A	94	SER
1	A	96	LEU
1	A	120	SER
1	A	122	ARG
1	A	131	GLN

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Mol	Chain	Res	Type
1	A	148	LEU
1	A	150	ARG
1	A	156	VAL
1	A	157	ARG
1	A	161	HIS
1	A	163	VAL
1	A	166	LEU
1	A	199	ARG
1	A	206	ASP
1	A	230	VAL
1	A	246	GLN
1	A	268	HIS
1	A	272	ASN
1	A	274	ARG
1	A	290	THR
1	A	291	LYS
2	B	177	ASP
2	B	187	ARG
2	B	196	LYS
2	B	199	TYR
2	B	201	LYS
2	B	202	LYS
2	B	209	SER
2	B	220	GLU
2	B	224	GLU
2	B	231	THR
2	B	232	LEU
2	B	266	LYS
2	B	288	LYS
2	B	292	LEU
2	B	293	ARG
2	B	296	HIS
2	B	315	LEU
2	B	316	THR
2	B	331	SER
2	B	349	LYS
2	B	364	LEU
2	B	368	THR
2	B	380	THR
2	B	384	LEU
2	B	385	GLU
2	B	399	LEU

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Mol	Chain	Res	Type
2	B	417	LYS
2	B	425	ASN
2	B	430	LEU
2	B	432	LEU
1	C	5	GLN
1	C	30	VAL
1	C	34	LYS
1	C	47	THR
1	C	55	LEU
1	C	56	LYS
1	C	66	LEU
1	C	67	LEU
1	C	76	LEU
1	C	78	LEU
1	C	88	LYS
1	C	94	SER
1	C	96	LEU
1	C	112	LEU
1	C	122	ARG
1	C	126	ARG
1	C	131	GLN
1	C	133	LEU
1	C	150	ARG
1	C	156	VAL
1	C	163	VAL
1	C	165	THR
1	C	181	SER
1	C	193	PHE
1	C	198	THR
1	C	199	ARG
1	C	206	ASP
1	C	207	SER
1	C	226	VAL
1	C	243	TRP
1	C	245	ARG
1	C	246	GLN
1	C	248	PHE
1	C	250	LYS
1	C	257	GLU
2	D	175	VAL
2	D	176	PRO
2	D	179	HIS

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Mol	Chain	Res	Type
2	D	181	ASP
2	D	188	GLU
2	D	194	LYS
2	D	202	LYS
2	D	211	ARG
2	D	226	LYS
2	D	232	LEU
2	D	243	LEU
2	D	246	MET
2	D	247	SER
2	D	254	GLN
2	D	280	TYR
2	D	285	THR
2	D	292	LEU
2	D	295	GLU
2	D	315	LEU
2	D	322	GLN
2	D	334	MET
2	D	338	GLU
2	D	348	LEU
2	D	349	LYS
2	D	361	HIS
2	D	367	VAL
2	D	375	SER
2	D	383	THR
2	D	384	LEU
2	D	386	SER
2	D	394	LEU
2	D	398	TYR
2	D	403	GLN
2	D	410	ARG
2	D	429	THR
3	F	663	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	74	ASN
1	A	85	GLN
1	A	119	HIS
1	A	268	HIS

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Mol	Chain	Res	Type
2	B	317	GLN
2	B	370	GLN
2	B	395	HIS
2	B	403	GLN
1	C	5	GLN
1	C	60	HIS
1	C	71	HIS
1	C	85	GLN
1	C	113	GLN
1	C	119	HIS
1	C	131	GLN
2	D	179	HIS
2	D	254	GLN
2	D	296	HIS
2	D	317	GLN
2	D	361	HIS
2	D	370	GLN
2	D	396	GLN
2	D	403	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	#$|Z| > 2$
1	TPO	A	160	1	10,10,11	5.78	5 (50%)	12,14,16	2.62	7 (58%)
1	TPO	C	160	1	10,10,11	6.34	2 (20%)	12,14,16	3.44	5 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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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
1	TPO	A	160	1	-	0/9/11/13	0/0/0/0
1	TPO	C	160	1	-	0/9/11/13	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	O-C	19.64	1.24	1.11
1	A	160	TPO	O-C	17.28	1.23	1.11
1	A	160	TPO	P-O1P	3.29	1.62	1.51
1	A	160	TPO	OG1-CB	-2.88	1.39	1.45
1	A	160	TPO	P-O3P	2.62	1.64	1.54
1	A	160	TPO	CA-C	2.61	1.53	1.48
1	C	160	TPO	P-O1P	2.01	1.58	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	160	TPO	OG1-CB-CA	7.17	119.57	107.55
1	C	160	TPO	C-CA-N	-6.51	101.35	111.94
1	C	160	TPO	OG1-P-O1P	5.13	121.11	106.79
1	A	160	TPO	OG1-CB-CA	4.54	115.16	107.55
1	A	160	TPO	O2P-P-OG1	3.97	118.53	107.09
1	A	160	TPO	OG1-CB-CG2	-3.95	103.53	110.13
1	A	160	TPO	O3P-P-OG1	-2.68	99.36	107.09
1	C	160	TPO	O3P-P-OG1	-2.54	99.79	107.09
1	C	160	TPO	O3P-P-O2P	2.42	117.05	107.61
1	A	160	TPO	C-CA-N	-2.26	108.26	111.94
1	A	160	TPO	P-OG1-CB	-2.09	110.96	120.17
1	A	160	TPO	CG2-CB-CA	2.04	117.38	113.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	297/303 (98%)	0.23	27 (9%)	9	8	13, 32, 60, 75	0
1	C	297/303 (98%)	0.19	21 (7%)	16	14	12, 32, 58, 71	0
2	B	258/259 (99%)	-0.01	10 (3%)	37	37	9, 25, 48, 59	0
2	D	258/259 (99%)	0.06	10 (3%)	37	37	11, 28, 47, 64	0
3	E	10/11 (90%)	1.03	4 (40%)	1	0	33, 41, 46, 46	0
3	F	8/11 (72%)	0.49	0	100	100	42, 45, 54, 57	0
All	All	1128/1146 (98%)	0.14	72 (6%)	19	17	9, 29, 54, 75	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	323	GLN	7.6
1	A	39	THR	5.3
1	A	40	GLU	5.3
1	C	39	THR	4.9
2	D	432	LEU	4.3
1	C	287	GLN	4.2
1	C	40	GLU	4.2
1	A	95	ALA	4.1
1	C	92	ASP	4.1
1	A	41	THR	4.1
1	C	199	ARG	4.1
1	A	12	GLU	4.0
1	C	74	ASN	4.0
1	A	247	ASP	3.9
1	C	36	ARG	3.7
2	B	324	PRO	3.7
3	E	654	GLY	3.6
2	B	416	SER	3.6
1	C	178	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	177	ASP	3.3
1	A	231	THR	3.3
1	A	225	VAL	3.2
1	A	16	GLY	3.2
1	A	287	GLN	3.2
1	C	59	ASN	3.1
1	C	16	GLY	3.1
1	A	13	GLY	3.1
1	C	15	TYR	3.1
1	C	95	ALA	3.1
1	A	250	LYS	3.0
1	A	206	ASP	3.0
1	A	37	LEU	3.0
1	C	225	VAL	3.0
1	A	246	GLN	3.0
2	D	429	THR	3.0
1	A	257	GLU	2.9
1	A	178	LYS	2.9
2	B	196	LYS	2.9
1	C	247	ASP	2.8
2	D	176	PRO	2.8
2	D	324	PRO	2.7
1	C	12	GLU	2.6
1	C	96	LEU	2.6
2	B	369	GLY	2.6
1	A	199	ARG	2.6
2	B	370	GLN	2.6
2	D	323	GLN	2.6
3	E	663	GLU	2.6
1	A	15	TYR	2.5
2	B	374	GLU	2.5
3	E	662	GLY	2.4
1	C	38	ASP	2.4
1	C	250	LYS	2.4
2	B	176	PRO	2.4
1	A	38	ASP	2.4
2	D	196	LYS	2.4
1	C	8	GLU	2.3
1	A	10	ILE	2.3
1	A	288	ASP	2.3
1	A	8	GLU	2.3
1	A	2	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	417	LYS	2.2
2	D	418	TYR	2.2
1	A	11	GLY	2.2
1	C	179	TYR	2.2
3	E	655	SER	2.1
2	D	201	LYS	2.1
2	D	415	ASN	2.1
1	C	7	VAL	2.0
2	B	326	ASN	2.0
1	A	14	THR	2.0
1	A	158	THR	2.0

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

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	TPO	C	160	11/12	0.11	-1.44	14,19,24,25	0
1	TPO	A	160	11/12	0.11	-1.65	4,14,21,27	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.