



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:17 AM UTC

PDB ID : 2WMA / pdb_00002wma
Title : Structural and thermodynamic consequences of cyclization of peptide ligands for the recruitment site of cyclin A
Authors : Robertson, G.F.; Endicott, J.A.; Noble, M.E.M.; McDonnell, J.M.
Deposited on : 2009-06-30
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

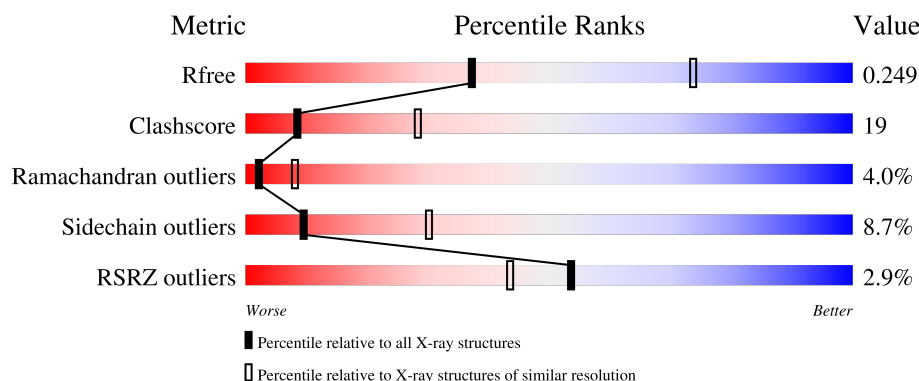
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	
1	C	303	
2	B	259	
2	D	259	
3	E	5	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8827 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 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	266	Total	C	N	O	P	S	0	0	0
			2131	1380	364	379	1	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P24941
A	-3	PRO	-	expression tag	UNP P24941
A	-2	LEU	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-4	GLY	-	expression tag	UNP P24941
C	-3	PRO	-	expression tag	UNP P24941
C	-2	LEU	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

- 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 CYCLIC RKLFN-NH2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			47	31	10	6			

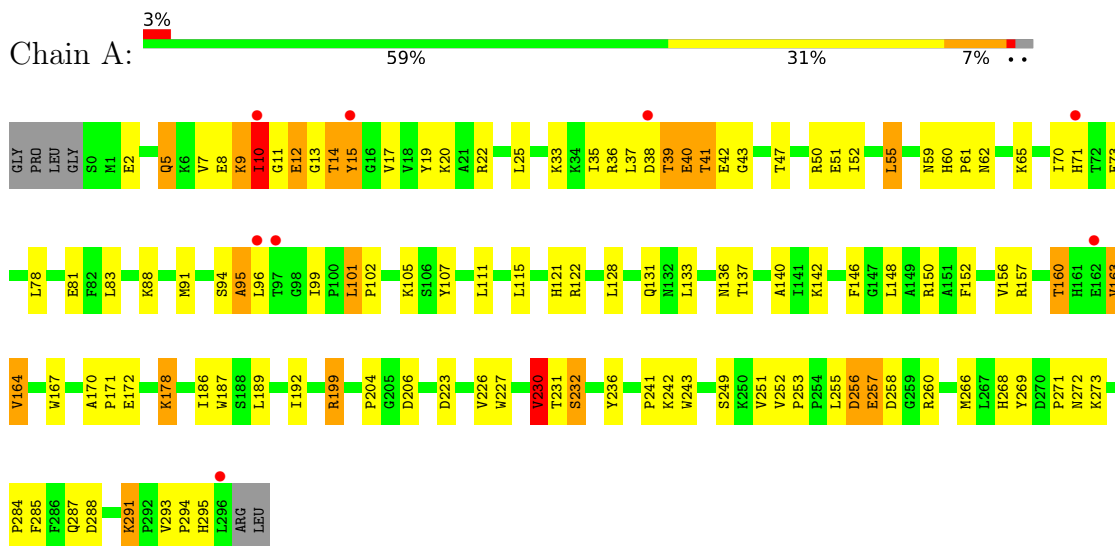
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total 32	O 32	0	0
4	B	32	Total 32	O 32	0	0
4	C	15	Total 15	O 15	0	0
4	D	16	Total 16	O 16	0	0

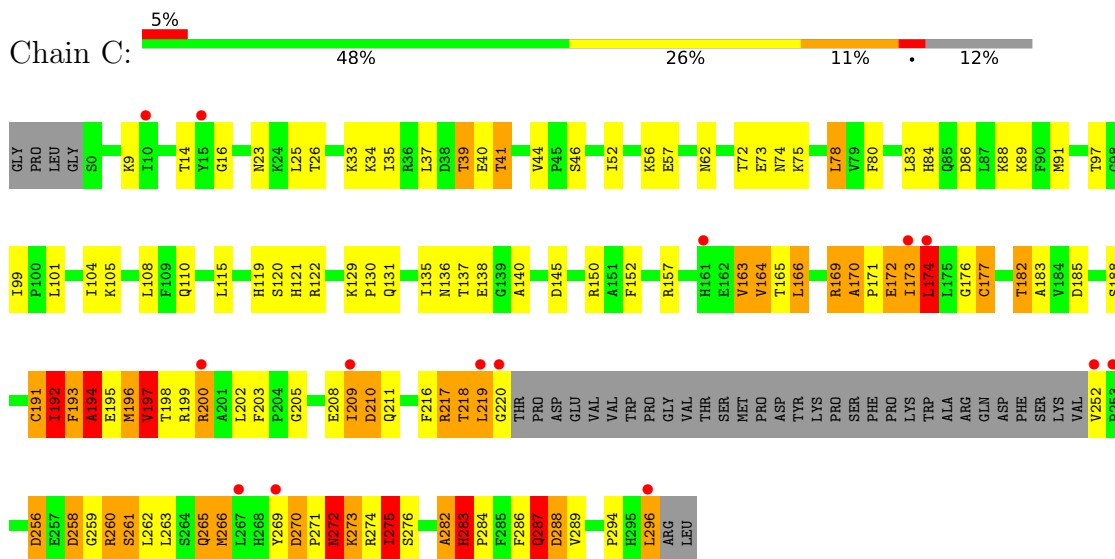
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CELL DIVISION PROTEIN KINASE 2

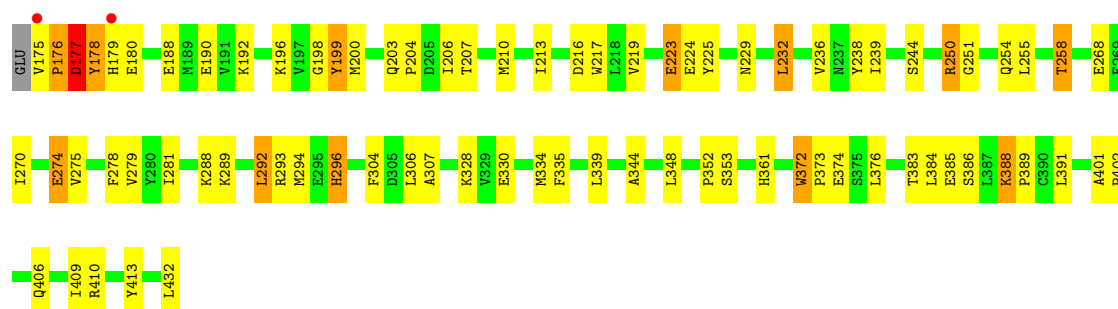


• Molecule 1: CELL DIVISION PROTEIN KINASE 2

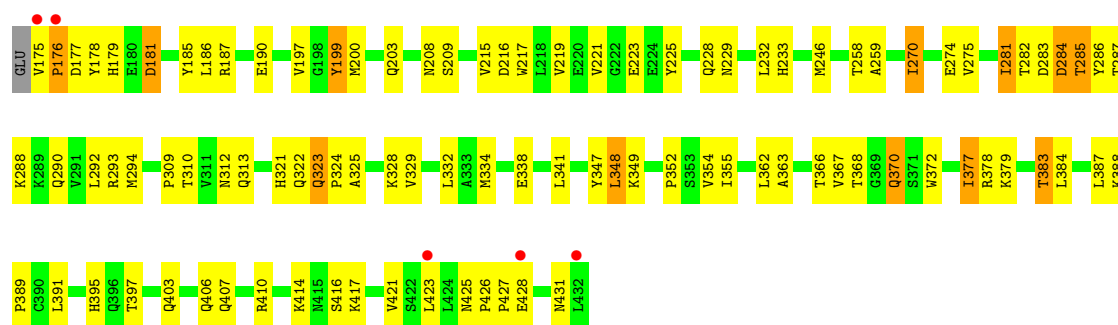


• Molecule 2: CYCLIN-A2

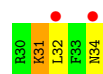




● Molecule 2: CYCLIN-A2



● Molecule 3: CYCLIC RKLFN-NH2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.79Å 131.85Å 146.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.80 98.12 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (100.00-2.80) 99.4 (98.12-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.285 (Not available) , 0.249	Depositor DCC
R_{free} test set	1764 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8827	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.68	0/2438	0.93	3/3308 (0.1%)
1	C	0.68	0/2168	1.18	23/2935 (0.8%)
2	B	0.61	0/2133	0.97	5/2897 (0.2%)
2	D	0.58	0/2133	0.94	2/2897 (0.1%)
3	E	0.42	0/47	1.16	1/60 (1.7%)
All	All	0.64	0/8919	1.01	34/12097 (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	2
2	B	0	1
All	All	0	4

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	265	GLN	N-CA-C	9.10	125.01	113.55
1	C	196	MET	N-CA-C	8.83	120.68	111.14
1	C	252	VAL	CA-C-N	8.22	128.85	120.38
1	C	252	VAL	C-N-CA	8.22	128.85	120.38
1	C	272	ASN	N-CA-C	7.88	127.59	110.80
1	C	196	MET	CA-C-N	7.75	135.64	121.70
1	C	196	MET	C-N-CA	7.75	135.64	121.70
2	B	372	TRP	CA-C-N	7.34	127.32	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	372	TRP	C-N-CA	7.34	127.32	119.76
1	C	210	ASP	N-CA-C	-7.22	100.97	110.43
1	C	191	CYS	CA-C-N	6.92	134.15	121.70
1	C	191	CYS	C-N-CA	6.92	134.15	121.70
1	A	253	PRO	N-CA-C	6.89	119.11	110.70
2	B	177	ASP	CA-C-N	6.76	133.87	121.70
2	B	177	ASP	C-N-CA	6.76	133.87	121.70
1	C	287	GLN	CA-C-N	6.48	133.37	121.70
1	C	287	GLN	C-N-CA	6.48	133.37	121.70
1	C	275	ILE	N-CA-C	6.27	117.76	110.62
1	A	230	VAL	CB-CA-C	-6.08	103.92	111.70
1	C	272	ASN	CA-C-N	6.07	132.63	121.70
1	C	272	ASN	C-N-CA	6.07	132.63	121.70
1	C	265	GLN	CA-C-N	6.06	132.61	121.70
1	C	265	GLN	C-N-CA	6.06	132.61	121.70
2	B	177	ASP	N-CA-C	5.73	123.01	110.80
1	C	196	MET	CA-C-O	-5.47	115.06	120.70
1	C	283	HIS	CA-C-N	5.46	126.66	119.84
1	C	283	HIS	C-N-CA	5.46	126.66	119.84
1	A	11	GLY	N-CA-C	5.27	118.45	111.70
1	C	191	CYS	N-CA-C	5.27	122.02	110.80
2	D	372	TRP	CA-C-N	5.26	125.20	119.78
2	D	372	TRP	C-N-CA	5.26	125.20	119.78
3	E	31	LYS	N-CA-C	-5.22	102.76	110.48
1	C	194	ALA	CA-C-N	5.21	131.08	121.70
1	C	194	ALA	C-N-CA	5.21	131.08	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	ILE	Peptide
2	B	176	PRO	Peptide
1	C	169	ARG	Peptide
1	C	260	ARG	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	2388	0	2430	96	0
1	C	2131	0	2178	128	0
2	B	2083	0	2107	66	0
2	D	2083	0	2107	63	0
3	E	47	0	49	5	0
4	A	32	0	0	3	0
4	B	32	0	0	5	0
4	C	15	0	0	0	0
4	D	16	0	0	2	0
All	All	8827	0	8871	334	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 19.

All (334) 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:C:260:ARG:N	1:C:261:SER:HB2	1.54	1.23
1:C:260:ARG:H	1:C:261:SER:CB	1.56	1.19
1:C:170:ALA:HB1	1:C:171:PRO:HA	1.25	1.17
1:C:287:GLN:CB	1:C:288:ASP:HB2	1.74	1.17
2:B:254:GLN:HG3	3:E:32:LEU:HD12	1.23	1.11
1:C:194:ALA:HB1	1:C:195:GLU:HB3	1.33	1.09
1:C:193:PHE:H	1:C:194:ALA:HB2	1.19	1.07
1:C:176:GLY:HA3	1:C:177:CYS:HB2	1.36	1.06
1:A:12:GLU:HB3	1:A:13:GLY:HA2	1.34	1.06
1:C:287:GLN:HB2	1:C:288:ASP:CB	1.83	1.06
1:C:194:ALA:HB3	1:C:196:MET:N	1.69	1.05
1:C:193:PHE:N	1:C:194:ALA:HB2	1.73	1.01
1:A:60:HIS:HD2	1:A:62:ASN:H	1.09	0.99
1:C:284:PRO:O	1:C:287:GLN:HG2	1.66	0.96
1:C:272:ASN:H	1:C:274:ARG:H	1.14	0.94
1:C:287:GLN:HB2	1:C:288:ASP:HB2	0.97	0.94
1:C:260:ARG:H	1:C:261:SER:HB2	0.78	0.92
1:C:194:ALA:HB3	1:C:195:GLU:C	1.95	0.92
1:C:217:ARG:HG3	1:C:217:ARG:HH11	1.38	0.88
1:A:14:THR:HG22	1:A:15:TYR:H	1.36	0.88
1:A:150:ARG:NH2	2:B:268:GLU:O	2.05	0.88
1:C:176:GLY:CA	1:C:177:CYS:HB2	2.03	0.87
1:C:170:ALA:HB1	1:C:171:PRO:CA	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:GLY:HA3	1:C:177:CYS:CB	2.04	0.86
1:C:272:ASN:N	1:C:274:ARG:H	1.74	0.85
1:A:9:LYS:HD3	1:A:9:LYS:H	1.42	0.84
1:C:194:ALA:CB	1:C:195:GLU:HB3	2.07	0.84
1:C:169:ARG:HH11	1:C:174:LEU:HD22	1.43	0.83
1:A:12:GLU:CB	1:A:13:GLY:HA2	2.07	0.81
2:D:284:ASP:HA	2:D:286:TYR:H	1.46	0.79
1:A:88:LYS:HD2	1:A:131:GLN:HE21	1.48	0.79
1:A:291:LYS:HB3	4:A:2032:HOH:O	1.81	0.78
1:A:60:HIS:CD2	1:A:62:ASN:H	2.00	0.77
2:B:254:GLN:HG3	3:E:32:LEU:CD1	2.13	0.76
1:C:210:ASP:O	1:C:211:GLN:HB3	1.86	0.75
1:A:61:PRO:O	1:A:142:LYS:HE2	1.87	0.75
1:C:193:PHE:N	1:C:194:ALA:CB	2.50	0.74
1:C:193:PHE:O	1:C:193:PHE:CD1	2.41	0.74
1:A:160:TPO:HG22	2:B:270:ILE:HG23	1.70	0.73
1:C:129:LYS:HD3	1:C:165:THR:OG1	1.89	0.73
2:D:216:ASP:HB2	2:D:406:GLN:HG3	1.71	0.73
1:C:217:ARG:HH11	1:C:217:ARG:CG	2.01	0.72
1:C:194:ALA:HB3	1:C:195:GLU:CA	2.19	0.72
1:A:12:GLU:HB3	1:A:13:GLY:CA	2.15	0.72
1:A:133:LEU:HD11	1:A:192:ILE:HD13	1.71	0.72
1:C:287:GLN:CA	1:C:288:ASP:HB2	2.20	0.71
2:B:391:LEU:HD23	2:B:432:LEU:HD21	1.71	0.71
1:C:217:ARG:O	1:C:218:THR:OG1	2.06	0.70
1:C:262:LEU:O	1:C:265:GLN:HB2	1.90	0.70
2:D:284:ASP:HA	2:D:286:TYR:N	2.06	0.70
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.73	0.70
1:A:121:HIS:O	1:A:122:ARG:HG3	1.92	0.69
1:C:282:ALA:HA	1:C:283:HIS:O	1.91	0.69
2:B:216:ASP:HB2	2:B:406:GLN:HG2	1.76	0.67
2:B:177:ASP:HB3	2:B:178:TYR:CD2	2.30	0.67
1:A:83:LEU:HD21	1:A:142:LYS:HD2	1.77	0.67
2:D:384:LEU:HA	2:D:387:LEU:HB2	1.76	0.67
1:C:131:GLN:N	1:C:131:GLN:OE1	2.28	0.67
1:C:194:ALA:H	1:C:197:VAL:HG11	1.61	0.66
1:A:249:SER:HA	1:A:260:ARG:HD3	1.78	0.65
1:A:178:LYS:H	1:A:178:LYS:HD3	1.61	0.65
1:A:150:ARG:NH1	1:A:160:TPO:O2P	2.30	0.65
1:C:99:ILE:HD12	1:C:196:MET:O	1.97	0.64
2:D:395:HIS:HE1	2:D:427:PRO:O	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:GLU:OE2	2:B:353:SER:N	2.24	0.64
2:D:270:ILE:HD13	2:D:270:ILE:H	1.62	0.64
2:B:190:GLU:HG2	2:B:352:PRO:HD2	1.79	0.64
1:C:194:ALA:CB	1:C:195:GLU:CA	2.75	0.64
1:A:39:THR:OG1	2:B:292:LEU:HD23	1.98	0.63
2:D:332:LEU:HD23	2:D:363:ALA:HA	1.81	0.63
1:A:227:TRP:O	1:A:230:VAL:HG22	1.98	0.63
1:C:191:CYS:N	1:C:192:ILE:O	2.32	0.63
2:D:270:ILE:HG12	4:D:2009:HOH:O	1.99	0.63
1:C:272:ASN:H	1:C:274:ARG:N	1.90	0.63
1:C:115:LEU:HD11	1:C:185:ASP:HB3	1.81	0.62
1:C:219:LEU:HD11	1:C:269:TYR:HB2	1.80	0.62
2:B:344:ALA:O	2:B:348:LEU:HB2	1.99	0.62
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.81	0.61
2:D:384:LEU:HD12	2:D:384:LEU:H	1.65	0.61
1:C:194:ALA:CB	1:C:195:GLU:CB	2.77	0.61
2:B:207:THR:OG1	2:B:210:MET:HG3	2.01	0.61
1:A:178:LYS:H	1:A:178:LYS:CD	2.13	0.61
1:C:169:ARG:HH11	1:C:174:LEU:CD2	2.11	0.61
1:C:120:SER:HB2	1:C:121:HIS:HD2	1.66	0.60
1:A:242:LYS:HE3	4:A:2024:HOH:O	2.02	0.59
2:B:177:ASP:HB2	4:B:2001:HOH:O	2.03	0.59
1:C:261:SER:O	1:C:265:GLN:HG3	2.01	0.59
1:A:71:HIS:CE1	2:B:304:PHE:HE2	2.20	0.59
1:C:108:LEU:HD22	1:C:193:PHE:CD1	2.38	0.59
2:D:368:THR:HG23	2:D:370:GLN:H	1.67	0.59
2:B:384:LEU:HD12	4:B:2026:HOH:O	2.03	0.58
1:A:95:ALA:HA	1:A:199:ARG:HH11	1.69	0.58
1:A:14:THR:O	1:A:15:TYR:HB2	2.03	0.58
2:B:254:GLN:CG	3:E:32:LEU:HD12	2.16	0.58
1:C:16:GLY:HA3	1:C:34:LYS:O	2.03	0.58
1:A:157:ARG:HH22	2:B:268:GLU:HG3	1.69	0.57
1:C:188:SER:O	1:C:191:CYS:HB2	2.04	0.57
1:A:231:THR:HA	1:A:236:TYR:CD1	2.39	0.57
2:D:190:GLU:OE2	2:D:352:PRO:HD2	2.04	0.57
1:C:39:THR:C	1:C:41:THR:H	2.13	0.57
1:A:172:GLU:HG2	1:A:271:PRO:HG3	1.86	0.57
1:A:15:TYR:HD1	1:A:35:ILE:HG12	1.68	0.57
1:C:40:GLU:O	2:D:288:LYS:HD3	2.04	0.57
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.86	0.57
1:C:170:ALA:CB	1:C:171:PRO:HA	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:VAL:HG12	1:A:252:VAL:HG23	1.86	0.57
2:B:289:LYS:O	2:B:293:ARG:HG3	2.05	0.56
1:A:170:ALA:HB1	1:A:172:GLU:OE2	2.06	0.56
2:D:323:GLN:HA	2:D:324:PRO:C	2.31	0.56
2:D:368:THR:HG23	2:D:370:GLN:HB2	1.87	0.56
2:D:287:THR:OG1	2:D:290:GLN:HG3	2.06	0.56
2:D:407:GLN:OE1	2:D:410:ARG:HD3	2.06	0.56
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.71	0.55
2:D:366:THR:HG23	2:D:427:PRO:HD3	1.87	0.55
1:A:59:ASN:OD1	1:A:65:LYS:HE2	2.07	0.55
2:D:221:VAL:HG22	2:D:281:ILE:HG21	1.88	0.55
1:C:270:ASP:OD1	1:C:273:LYS:HG2	2.07	0.55
1:A:2:GLU:HG2	1:C:73:GLU:OE1	2.07	0.54
1:C:194:ALA:HB3	1:C:196:MET:H	1.65	0.54
2:D:181:ASP:OD1	2:D:181:ASP:N	2.41	0.54
1:A:121:HIS:C	1:A:122:ARG:HG3	2.31	0.54
1:A:156:VAL:HG22	2:B:175:VAL:HG21	1.90	0.54
1:C:199:ARG:HG2	1:C:200:ARG:N	2.22	0.54
1:A:13:GLY:HA3	1:A:14:THR:C	2.32	0.54
2:D:282:THR:O	2:D:285:THR:OG1	2.26	0.54
2:D:309:PRO:HA	2:D:313:GLN:NE2	2.22	0.54
1:C:262:LEU:HB2	1:C:283:HIS:CE1	2.43	0.54
1:C:193:PHE:CD1	1:C:193:PHE:C	2.84	0.53
2:D:176:PRO:HA	2:D:179:HIS:CE1	2.42	0.53
2:D:197:VAL:HG23	2:D:349:LYS:HB3	1.89	0.53
2:D:347:TYR:C	2:D:349:LYS:H	2.16	0.53
2:B:294:MET:HE2	1:C:25:LEU:HB3	1.89	0.53
1:C:183:ALA:CB	1:C:271:PRO:HB3	2.38	0.53
1:C:260:ARG:N	1:C:261:SER:CB	2.37	0.53
1:A:60:HIS:HD2	1:A:62:ASN:N	1.91	0.53
1:C:119:HIS:CG	1:C:182:THR:OG1	2.62	0.53
2:D:197:VAL:CG2	2:D:349:LYS:HB3	2.38	0.53
1:C:173:ILE:HG22	1:C:174:LEU:HB2	1.90	0.53
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.44	0.52
2:B:275:VAL:HG11	2:B:292:LEU:HD13	1.90	0.52
2:B:373:PRO:HD2	2:B:376:LEU:HD12	1.91	0.52
1:C:192:ILE:HA	1:C:194:ALA:HB2	1.91	0.52
2:D:176:PRO:O	2:D:178:TYR:N	2.40	0.52
2:D:259:ALA:CB	2:D:294:MET:HG3	2.40	0.52
1:C:219:LEU:HD13	1:C:220:GLY:H	1.72	0.52
1:A:62:ASN:HA	1:A:142:LYS:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:TYR:CZ	2:B:306:LEU:HD22	2.45	0.52
1:A:230:VAL:C	1:A:232:SER:H	2.16	0.52
1:C:256:ASP:OD1	1:C:256:ASP:N	2.41	0.52
1:A:71:HIS:NE2	2:B:296:HIS:ND1	2.57	0.52
2:D:233:HIS:CD2	2:D:341:LEU:HD21	2.44	0.52
1:C:121:HIS:O	1:C:122:ARG:HG3	2.09	0.52
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.90	0.52
2:D:282:THR:C	2:D:284:ASP:H	2.18	0.51
1:C:170:ALA:CB	1:C:171:PRO:CA	2.79	0.51
2:B:199:TYR:HB2	2:B:244:SER:HA	1.92	0.51
2:D:186:LEU:HD22	2:D:309:PRO:HB3	1.91	0.51
1:A:107:TYR:O	1:A:111:LEU:HG	2.10	0.51
1:C:157:ARG:HD2	2:D:228:GLN:OE1	2.11	0.51
1:C:193:PHE:N	1:C:194:ALA:CA	2.74	0.51
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.79	0.51
2:B:179:HIS:CD2	2:B:180:GLU:H	2.29	0.51
1:C:172:GLU:O	1:C:177:CYS:CB	2.59	0.51
1:C:192:ILE:N	1:C:194:ALA:HB1	2.26	0.51
1:A:293:VAL:HG12	1:A:294:PRO:O	2.11	0.50
2:B:188:GLU:CB	4:B:2005:HOH:O	2.59	0.50
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.93	0.50
2:B:236:VAL:HA	2:B:239:ILE:HD12	1.93	0.50
1:C:173:ILE:CG2	1:C:174:LEU:HB2	2.42	0.50
1:A:40:GLU:C	1:A:42:GLU:H	2.18	0.50
1:C:86:ASP:HB2	1:C:89:LYS:H	1.76	0.50
1:A:95:ALA:HA	1:A:199:ARG:HD2	1.93	0.50
2:B:229:ASN:HD22	2:B:334:MET:HE2	1.76	0.50
1:C:199:ARG:HG2	1:C:200:ARG:H	1.77	0.50
1:A:50:ARG:NH1	1:A:160:TPO:O3P	2.39	0.50
1:C:272:ASN:N	1:C:274:ARG:N	2.52	0.49
1:C:196:MET:N	1:C:197:VAL:HG12	2.27	0.49
2:D:323:GLN:HA	2:D:325:ALA:N	2.27	0.49
2:B:217:TRP:HH2	2:B:258:THR:HG23	1.76	0.49
1:A:258:ASP:HB3	1:A:285:PHE:HA	1.95	0.49
1:C:194:ALA:CB	1:C:196:MET:N	2.59	0.49
1:A:5:GLN:HE22	1:A:22:ARG:NH2	2.10	0.49
1:A:39:THR:HG23	1:A:41:THR:H	1.78	0.49
1:C:193:PHE:O	1:C:193:PHE:HD1	1.94	0.48
1:A:71:HIS:HE1	2:B:304:PHE:CE2	2.32	0.48
1:C:217:ARG:HG3	1:C:217:ARG:NH1	2.18	0.48
1:C:23:ASN:HB3	1:C:26:THR:OG1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:383:THR:OG1	2:B:385:GLU:HB3	2.14	0.48
1:A:71:HIS:CE1	2:B:304:PHE:CE2	3.01	0.48
2:B:278:PHE:HA	2:B:281:ILE:HG12	1.95	0.48
1:A:36:ARG:NH1	1:A:36:ARG:HB3	2.29	0.47
2:D:414:LYS:HG2	2:D:423:LEU:HG	1.96	0.47
1:A:256:ASP:O	1:A:257:GLU:CB	2.61	0.47
1:C:84:HIS:HB3	1:C:135:ILE:O	2.14	0.47
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.49	0.47
1:A:9:LYS:C	1:A:10:ILE:HG13	2.40	0.47
1:A:15:TYR:CD1	1:A:35:ILE:HG12	2.48	0.47
2:B:335:PHE:HB2	2:B:413:TYR:CD2	2.50	0.47
2:B:361:HIS:HD2	2:B:391:LEU:HD21	1.80	0.47
1:C:52:ILE:O	1:C:56:LYS:HB2	2.15	0.47
2:B:279:VAL:HG21	2:B:288:LYS:HG3	1.97	0.47
1:C:72:THR:HB	1:C:75:LYS:H	1.80	0.47
1:C:91:MET:CE	1:C:195:GLU:HG2	2.45	0.47
1:A:9:LYS:H	1:A:9:LYS:CD	2.21	0.46
1:A:288:ASP:HB3	4:A:2029:HOH:O	2.15	0.46
1:C:171:PRO:C	1:C:173:ILE:H	2.23	0.46
1:A:284:PRO:O	1:A:287:GLN:HG2	2.15	0.46
1:C:33:LYS:HD3	1:C:80:PHE:HE1	1.79	0.46
1:C:209:ILE:HG13	1:C:210:ASP:N	2.29	0.46
1:C:35:ILE:HD12	1:C:78:LEU:HD21	1.96	0.46
1:A:71:HIS:CD2	2:B:296:HIS:CE1	3.03	0.46
1:A:137:THR:O	1:A:293:VAL:HG13	2.16	0.46
1:C:121:HIS:C	1:C:122:ARG:HG3	2.40	0.46
1:C:203:PHE:HB2	1:C:211:GLN:HE22	1.79	0.46
1:C:265:GLN:HB3	1:C:275:ILE:HB	1.96	0.46
2:D:425:ASN:OD1	2:D:426:PRO:HD2	2.16	0.46
2:B:198:GLY:O	2:B:200:MET:N	2.48	0.46
1:C:208:GLU:O	1:C:209:ILE:HG12	2.16	0.46
1:C:263:LEU:C	1:C:265:GLN:H	2.23	0.46
2:D:312:ASN:ND2	2:D:334:MET:SD	2.89	0.46
1:A:7:VAL:HG12	1:A:8:GLU:HG2	1.98	0.46
1:C:163:VAL:HG13	1:C:164:VAL:HG23	1.98	0.46
1:A:14:THR:HG22	1:A:15:TYR:N	2.17	0.46
1:A:51:GLU:O	1:A:55:LEU:HB2	2.16	0.45
1:C:197:VAL:HG13	1:C:198:THR:HG23	1.97	0.45
1:A:122:ARG:NH2	2:B:307:ALA:HB1	2.32	0.45
3:E:31:LYS:HD3	3:E:34:ASN:O	2.15	0.45
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:THR:HG22	1:C:137:THR:O	2.15	0.45
1:A:223:ASP:H	1:A:226:VAL:HG12	1.81	0.45
2:B:372:TRP:CZ2	2:B:376:LEU:HB3	2.52	0.45
2:D:215:VAL:O	2:D:219:VAL:HG23	2.16	0.45
1:C:173:ILE:HB	1:C:174:LEU:HB2	1.98	0.45
1:C:270:ASP:HA	1:C:271:PRO:HD3	1.82	0.45
1:C:286:PHE:O	1:C:287:GLN:C	2.59	0.45
2:B:177:ASP:N	2:B:179:HIS:H	2.15	0.45
1:C:202:LEU:HD13	1:C:203:PHE:CZ	2.52	0.45
2:B:401:ALA:HB3	2:B:402:PRO:HD3	1.99	0.45
1:C:91:MET:HE3	1:C:196:MET:HG2	1.99	0.44
2:D:282:THR:O	2:D:284:ASP:N	2.51	0.44
1:A:55:LEU:HD22	1:A:146:PHE:HB2	1.99	0.44
1:A:189:LEU:HB3	1:A:266:MET:HE1	1.99	0.44
2:B:219:VAL:HG21	2:B:409:ILE:HG13	1.98	0.44
2:B:391:LEU:HD23	2:B:432:LEU:CD2	2.45	0.44
2:D:384:LEU:HD12	2:D:384:LEU:N	2.31	0.44
1:A:9:LYS:HD3	1:A:9:LYS:N	2.21	0.44
2:D:310:THR:OG1	2:D:313:GLN:HG3	2.17	0.44
1:A:40:GLU:OE1	1:A:43:GLY:O	2.34	0.44
1:A:105:LYS:HG2	1:A:285:PHE:CZ	2.52	0.44
1:C:271:PRO:O	1:C:272:ASN:CG	2.61	0.44
2:D:225:TYR:CE1	2:D:281:ILE:HD11	2.52	0.44
1:C:294:PRO:HG2	1:C:296:LEU:HD21	2.00	0.44
1:C:170:ALA:HA	1:C:171:PRO:O	2.18	0.44
2:D:200:MET:HG2	2:D:208:ASN:N	2.33	0.44
2:D:229:ASN:ND2	4:D:2003:HOH:O	2.51	0.44
2:D:199:TYR:CE2	2:D:348:LEU:HD21	2.52	0.44
2:B:401:ALA:HB1	2:B:410:ARG:HD2	2.00	0.44
1:C:282:ALA:HA	1:C:283:HIS:C	2.43	0.44
1:A:37:LEU:O	1:A:38:ASP:CG	2.61	0.43
1:A:52:ILE:HD11	1:A:78:LEU:HD21	2.00	0.43
1:A:256:ASP:O	1:A:257:GLU:HB2	2.18	0.43
1:C:37:LEU:HD22	1:C:44:VAL:HG22	1.99	0.43
1:C:194:ALA:H	1:C:197:VAL:CG1	2.28	0.43
1:C:192:ILE:HA	1:C:194:ALA:CB	2.47	0.43
1:A:227:TRP:CE3	1:A:269:TYR:HB3	2.54	0.43
1:A:5:GLN:HE21	1:A:5:GLN:HB3	1.46	0.43
1:C:62:ASN:ND2	1:C:110:GLN:HB3	2.34	0.43
1:A:230:VAL:C	1:A:232:SER:N	2.74	0.43
1:C:169:ARG:HD2	1:C:174:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:THR:O	1:A:15:TYR:CB	2.67	0.43
1:C:172:GLU:O	1:C:177:CYS:HB3	2.18	0.43
1:A:136:ASN:ND2	1:A:140:ALA:HB3	2.34	0.42
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.34	0.42
2:D:377:ILE:HD13	2:D:383:THR:HG22	2.01	0.42
1:A:115:LEU:HD23	1:A:186:ILE:HD13	2.00	0.42
2:B:188:GLU:HB2	4:B:2005:HOH:O	2.19	0.42
2:B:196:LYS:HE3	2:B:199:TYR:HA	2.01	0.42
2:D:217:TRP:CH2	2:D:282:THR:HG22	2.54	0.42
2:B:330:GLU:O	2:B:334:MET:HG2	2.19	0.42
1:C:258:ASP:HA	1:C:259:GLY:HA2	1.73	0.42
1:A:7:VAL:HB	1:A:20:LYS:HG2	2.01	0.42
2:D:175:VAL:HA	2:D:176:PRO:HD3	1.72	0.42
2:B:223:GLU:O	2:B:224:GLU:C	2.62	0.42
1:C:78:LEU:HD23	1:C:78:LEU:N	2.34	0.42
1:C:88:LYS:HB2	1:C:130:PRO:HB2	2.02	0.42
1:C:101:LEU:HA	1:C:104:ILE:HD12	2.01	0.42
1:C:193:PHE:C	1:C:196:MET:HB2	2.44	0.42
2:B:216:ASP:HB2	2:B:406:GLN:CG	2.47	0.42
2:D:203:GLN:NE2	2:D:246:MET:O	2.48	0.42
1:A:25:LEU:HD21	2:D:293:ARG:HB2	2.01	0.42
1:C:157:ARG:CZ	2:D:228:GLN:HG3	2.50	0.41
2:D:199:TYR:CD2	2:D:348:LEU:HD21	2.55	0.41
2:D:329:VAL:HG23	2:D:367:VAL:HB	2.02	0.41
1:C:216:PHE:HD1	1:C:219:LEU:HB3	1.85	0.41
2:B:250:ARG:HG3	2:B:251:GLY:N	2.35	0.41
1:C:171:PRO:O	1:C:173:ILE:N	2.54	0.41
1:C:172:GLU:O	1:C:177:CYS:HB2	2.20	0.41
1:A:33:LYS:HB3	1:A:78:LEU:HB2	2.02	0.41
1:A:241:PRO:HB2	1:A:243:TRP:CH2	2.55	0.41
2:B:213:ILE:HG22	3:E:32:LEU:HD22	2.02	0.41
2:B:274:GLU:H	2:B:274:GLU:HG2	1.66	0.41
1:C:259:GLY:HA3	1:C:262:LEU:HB3	2.02	0.41
2:D:321:HIS:CE1	2:D:379:LYS:HD2	2.56	0.41
2:D:328:LYS:O	2:D:421:VAL:HG11	2.21	0.41
1:A:101:LEU:N	1:A:102:PRO:CD	2.83	0.41
2:B:391:LEU:CD2	2:B:432:LEU:HD21	2.44	0.41
1:C:39:THR:O	1:C:41:THR:N	2.51	0.41
1:C:205:GLY:HA3	1:C:211:GLN:HB2	2.02	0.41
1:C:57:GLU:CG	2:D:185:TYR:OH	2.68	0.41
2:D:347:TYR:C	2:D:349:LYS:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:TYR:CD1	2:B:199:TYR:C	2.98	0.41
2:B:339:LEU:HD23	2:B:339:LEU:HA	1.94	0.41
1:C:173:ILE:CB	1:C:174:LEU:HB2	2.51	0.41
1:A:25:LEU:HD11	2:D:293:ARG:HB3	2.03	0.41
1:A:95:ALA:HA	1:A:199:ARG:NH1	2.36	0.41
1:A:252:VAL:HG11	1:A:255:LEU:HD22	2.01	0.41
1:C:266:MET:N	1:C:275:ILE:HG22	2.35	0.41
2:D:187:ARG:HD2	2:D:187:ARG:HA	1.78	0.41
2:D:347:TYR:OH	2:D:397:THR:OG1	2.30	0.41
2:D:354:VAL:O	2:D:355:ILE:C	2.64	0.41
1:A:163:VAL:CG1	1:A:164:VAL:HG23	2.51	0.41
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.86	0.40
2:B:188:GLU:HB3	4:B:2005:HOH:O	2.20	0.40
1:A:65:LYS:H	1:A:81:GLU:HG2	1.86	0.40
1:A:171:PRO:HD3	1:A:187:TRP:CE2	2.56	0.40
2:B:203:GLN:HA	2:B:204:PRO:HD2	1.95	0.40
2:B:255:LEU:HG	2:B:294:MET:HG2	2.02	0.40
2:D:258:THR:OG1	2:D:282:THR:HG21	2.22	0.40
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.57	0.40
2:B:203:GLN:HB3	2:B:206:ILE:HG12	2.04	0.40
1:C:203:PHE:HB2	1:C:211:GLN:NE2	2.37	0.40
1:A:268:HIS:NE2	1:A:273:LYS:HD2	2.37	0.40
2:D:270:ILE:H	2:D:270:ILE:CD1	2.29	0.40
2:D:275:VAL:HG21	2:D:292:LEU:HD21	2.03	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	294/303 (97%)	266 (90%)	21 (7%)	7 (2%)	4 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	261/303 (86%)	204 (78%)	34 (13%)	23 (9%)	0	1
2	B	256/259 (99%)	240 (94%)	12 (5%)	4 (2%)	7	27
2	D	256/259 (99%)	233 (91%)	14 (6%)	9 (4%)	3	10
3	E	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
All	All	1070/1129 (95%)	945 (88%)	82 (8%)	43 (4%)	2	8

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	TYR
2	B	176	PRO
1	C	170	ALA
1	C	177	CYS
1	C	192	ILE
1	C	256	ASP
2	D	176	PRO
2	D	177	ASP
2	D	284	ASP
2	D	322	GLN
1	A	95	ALA
1	A	257	GLU
2	B	177	ASP
1	C	164	VAL
1	C	173	ILE
1	C	193	PHE
1	C	194	ALA
1	C	218	THR
1	C	287	GLN
1	C	288	ASP
2	D	283	ASP
2	D	285	THR
1	A	12	GLU
1	A	41	THR
1	A	164	VAL
2	B	178	TYR
1	C	197	VAL
1	C	266	MET
1	C	272	ASN
1	C	273	LYS
1	C	282	ALA
1	C	283	HIS

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Mol	Chain	Res	Type
2	D	199	TYR
2	D	348	LEU
1	C	200	ARG
1	C	261	SER
2	D	323	GLN
1	A	10	ILE
1	C	145	ASP
1	C	166	LEU
1	C	174	LEU
1	C	258	ASP
2	B	388	LYS

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%)	235 (90%)	26 (10%)	7	24
1	C	231/265 (87%)	204 (88%)	27 (12%)	5	18
2	B	232/233 (100%)	220 (95%)	12 (5%)	21	53
2	D	232/233 (100%)	213 (92%)	19 (8%)	10	33
3	E	5/5 (100%)	5 (100%)	0	100	100
All	All	961/1001 (96%)	877 (91%)	84 (9%)	9	30

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	9	LYS
1	A	10	ILE
1	A	14	THR
1	A	17	VAL
1	A	19	TYR
1	A	39	THR
1	A	40	GLU

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Mol	Chain	Res	Type
1	A	47	THR
1	A	55	LEU
1	A	73	GLU
1	A	94	SER
1	A	96	LEU
1	A	101	LEU
1	A	128	LEU
1	A	148	LEU
1	A	163	VAL
1	A	178	LYS
1	A	199	ARG
1	A	206	ASP
1	A	230	VAL
1	A	232	SER
1	A	256	ASP
1	A	272	ASN
1	A	291	LYS
1	A	295	HIS
2	B	192	LYS
2	B	199	TYR
2	B	223	GLU
2	B	232	LEU
2	B	250	ARG
2	B	258	THR
2	B	274	GLU
2	B	292	LEU
2	B	296	HIS
2	B	328	LYS
2	B	374	GLU
2	B	386	SER
1	C	9	LYS
1	C	14	THR
1	C	39	THR
1	C	41	THR
1	C	46	SER
1	C	74	ASN
1	C	78	LEU
1	C	83	LEU
1	C	97	THR
1	C	105	LYS
1	C	138	GLU
1	C	150	ARG

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Mol	Chain	Res	Type
1	C	163	VAL
1	C	166	LEU
1	C	172	GLU
1	C	174	LEU
1	C	182	THR
1	C	192	ILE
1	C	197	VAL
1	C	209	ILE
1	C	217	ARG
1	C	219	LEU
1	C	270	ASP
1	C	275	ILE
1	C	276	SER
1	C	289	VAL
1	C	296	LEU
2	D	181	ASP
2	D	209	SER
2	D	223	GLU
2	D	232	LEU
2	D	270	ILE
2	D	274	GLU
2	D	281	ILE
2	D	338	GLU
2	D	362	LEU
2	D	370	GLN
2	D	377	ILE
2	D	378	ARG
2	D	383	THR
2	D	391	LEU
2	D	403	GLN
2	D	416	SER
2	D	417	LYS
2	D	428	GLU
2	D	431	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	60	HIS
1	A	85	GLN
2	B	179	HIS

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Mol	Chain	Res	Type
2	B	183	HIS
2	B	290	GLN
1	C	23	ASN
1	C	62	ASN
1	C	74	ASN
1	C	121	HIS
1	C	268	HIS
2	D	179	HIS
2	D	254	GLN
2	D	312	ASN
2	D	313	GLN
2	D	370	GLN
2	D	395	HIS
2	D	419	HIS
2	D	431	ASN

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	$\# Z > 2$
1	TPO	A	160	1	8,10,11	0.99	0	10,14,16	1.53	2 (20%)
1	TPO	C	160	1	8,10,11	0.89	0	10,14,16	1.20	0

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
1	TPO	A	160	1	-	5/9/11/13	-
1	TPO	C	160	1	-	0/9/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	P-OG1-CB	2.31	129.59	123.33
1	A	160	TPO	O3P-P-O2P	2.28	116.33	107.80

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	160	TPO	N-CA-CB-CG2
1	A	160	TPO	N-CA-CB-OG1
1	A	160	TPO	C-CA-CB-CG2
1	A	160	TPO	O-C-CA-CB
1	A	160	TPO	CG2-CB-OG1-P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	160	TPO	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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	296/303 (97%)	-0.24	8 (2%) 56 46	22, 35, 67, 79	0
1	C	265/303 (87%)	0.31	14 (5%) 32 24	32, 53, 78, 83	0
2	B	258/259 (99%)	-0.32	2 (0%) 82 75	25, 39, 55, 65	0
2	D	258/259 (99%)	0.15	5 (1%) 66 57	30, 53, 82, 93	0
3	E	5/5 (100%)	1.62	2 (40%) 1 0	62, 63, 68, 71	0
All	All	1082/1129 (95%)	-0.02	31 (2%) 53 43	22, 44, 78, 93	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	432	LEU	5.4
1	C	252	VAL	4.5
2	B	175	VAL	3.7
2	D	175	VAL	3.7
1	C	269	TYR	3.4
1	C	15	TYR	3.4
1	C	174	LEU	3.3
1	C	220	GLY	3.3
1	A	96	LEU	3.2
1	C	253	PRO	3.2
1	C	173	ILE	3.1
3	E	34	ASN	2.7
1	C	200	ARG	2.7
1	A	162	GLU	2.5
1	C	219	LEU	2.5
1	C	209	ILE	2.4
1	C	161	HIS	2.4
1	C	10	ILE	2.3
2	B	179	HIS	2.3
1	A	10	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	71	HIS	2.2
1	A	38	ASP	2.2
2	D	176	PRO	2.2
1	C	267	LEU	2.2
1	C	296	LEU	2.2
2	D	423	LEU	2.1
1	A	296	LEU	2.0
3	E	32	LEU	2.0
1	A	97	THR	2.0
1	A	15	TYR	2.0
2	D	428	GLU	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	C	160	11/12	0.95	0.09	50,53,55,55	0
1	TPO	A	160	11/12	0.96	0.07	39,41,42,42	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.