



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:52 PM UTC

PDB ID : 1T5C / pdb_00001t5c
Title : Crystal structure of the motor domain of human kinetochore protein CENP-E
Authors : Garcia-Saez, I.; Yen, T.; Wade, R.H.; Kozielski, F.; Structural Proteomics in Europe (SPINE)
Deposited on : 2004-05-04
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

<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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

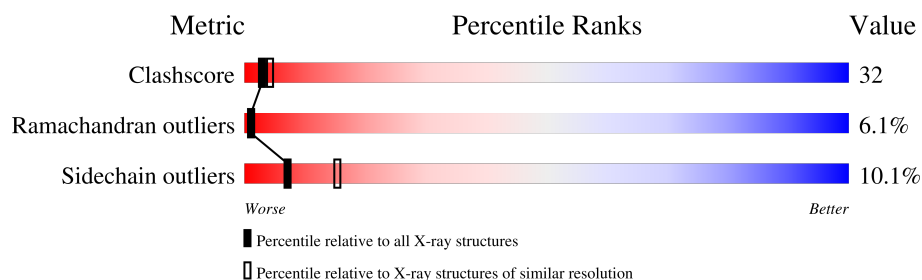
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	349	
1	B	349	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PIN	A	604	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5217 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 Centromeric protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	31	3	0
			2581	1625	452	492	12			
1	B	310	Total	C	N	O	S	102	1	0
			2474	1564	431	467	12			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	300	ALA	PRO	SEE REMARK 999	UNP Q02224
A	343	LEU	-	cloning artifact	UNP Q02224
A	344	GLU	-	cloning artifact	UNP Q02224
A	345	HIS	-	cloning artifact	UNP Q02224
A	346	HIS	-	cloning artifact	UNP Q02224
A	347	HIS	-	cloning artifact	UNP Q02224
A	348	HIS	-	cloning artifact	UNP Q02224
A	349	HIS	-	cloning artifact	UNP Q02224
A	350	HIS	-	cloning artifact	UNP Q02224
B	300	ALA	PRO	SEE REMARK 999	UNP Q02224
B	343	LEU	-	cloning artifact	UNP Q02224
B	344	GLU	-	cloning artifact	UNP Q02224
B	345	HIS	-	cloning artifact	UNP Q02224
B	346	HIS	-	cloning artifact	UNP Q02224
B	347	HIS	-	cloning artifact	UNP Q02224
B	348	HIS	-	cloning artifact	UNP Q02224
B	349	HIS	-	cloning artifact	UNP Q02224
B	350	HIS	-	cloning artifact	UNP Q02224

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

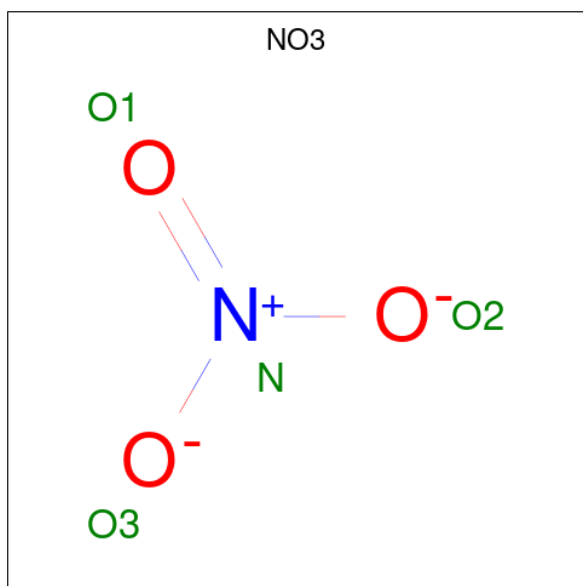
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

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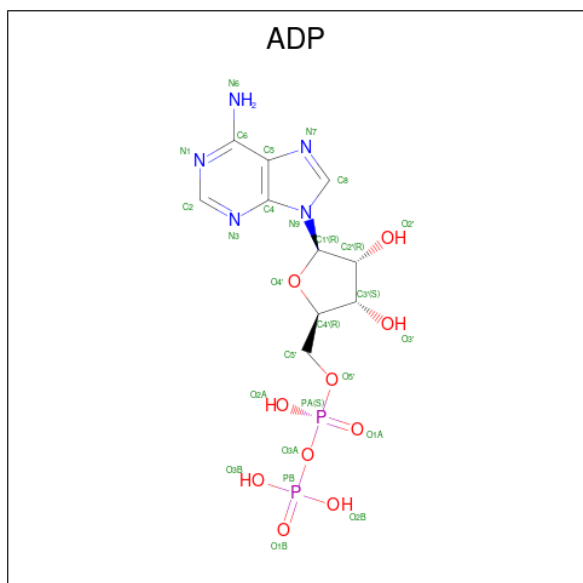
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



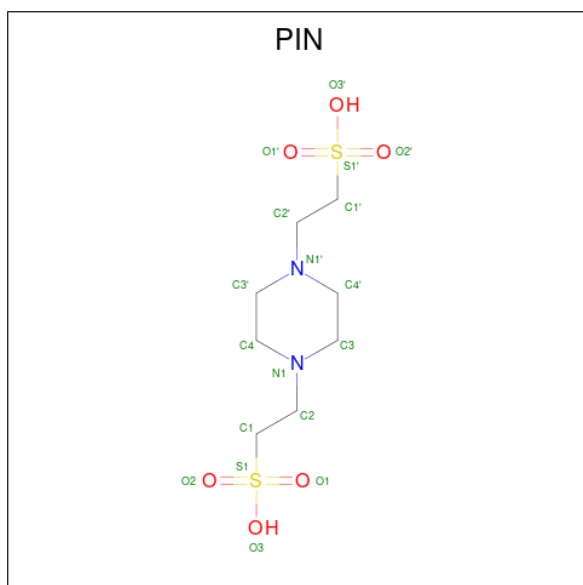
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is PIPERAZINE-N,N'-BIS(2-ETHANESULFONIC ACID) (CCD ID: PIN) (formula: C₈H₁₈N₂O₆S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			18	8	2	6	2		

- Molecule 6 is water.

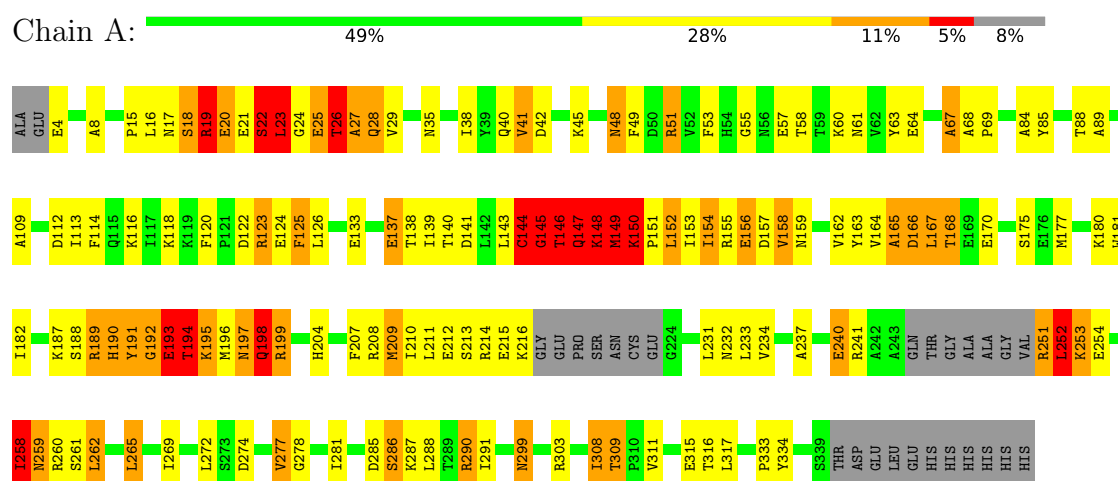
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	71	Total	O	0	0
			71	71		
6	B	13	Total	O	0	0
			13	13		

3 Residue-property plots [i](#)

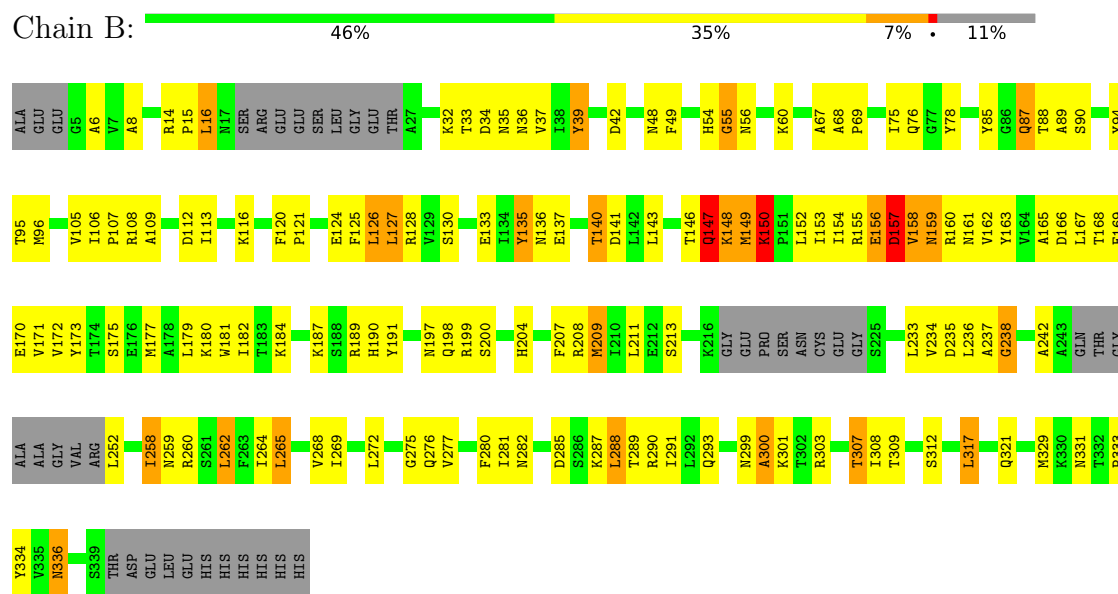
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: Centromeric protein E



• Molecule 1: Centromeric protein E



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.35Å 83.70Å 94.16Å 90.00° 103.05° 90.00°	Depositor
Resolution (Å)	12.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5217	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PIN, ADP, NO3, MG

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	0.80	7/2622 (0.3%)	1.53	68/3531 (1.9%)
1	B	0.43	0/2514	0.95	10/3388 (0.3%)
All	All	0.65	7/5136 (0.1%)	1.28	78/6919 (1.1%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	MET	SD-CE	-16.91	1.37	1.79
1	A	146	THR	N-CA	7.33	1.55	1.46
1	A	149	MET	CG-SD	-5.99	1.65	1.80
1	A	146	THR	CA-CB	5.65	1.63	1.53
1	A	149	MET	N-CA	5.44	1.53	1.46
1	A	149	MET	CA-C	5.28	1.59	1.52
1	A	19	ARG	CB-CG	5.04	1.67	1.52

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	LYS	N-CA-C	-20.56	87.78	114.31
1	A	197	ASN	N-CA-C	14.78	129.79	110.43
1	A	192	GLY	N-CA-C	-14.23	90.56	111.19
1	A	149	MET	N-CA-C	13.41	139.37	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	SER	CA-C-N	12.20	144.83	121.54
1	A	18	SER	C-N-CA	12.20	144.83	121.54
1	A	19	ARG	N-CA-CB	12.15	131.03	110.49
1	A	22	SER	CA-C-N	11.99	144.44	121.54
1	A	22	SER	C-N-CA	11.99	144.44	121.54
1	B	147	GLN	N-CA-C	11.58	135.47	110.80
1	A	146	THR	N-CA-C	11.44	135.16	110.80
1	B	301	LYS	N-CA-C	-11.35	88.17	107.80
1	A	234	VAL	N-CA-C	11.07	123.66	108.17
1	A	191	TYR	N-CA-C	-9.91	89.70	110.80
1	A	23	LEU	N-CA-CB	9.70	126.88	110.49
1	B	258	ILE	N-CA-C	9.21	122.03	108.96
1	A	252	LEU	N-CA-C	8.45	123.77	110.17
1	A	67	ALA	N-CA-C	7.99	119.77	111.14
1	A	144	CYS	N-CA-C	7.81	127.44	110.80
1	A	27	ALA	N-CA-C	-7.58	97.99	109.96
1	A	150	LYS	N-CA-C	7.56	126.52	109.81
1	A	145	GLY	CA-C-N	7.46	135.78	121.54
1	A	145	GLY	C-N-CA	7.46	135.78	121.54
1	A	147	GLN	N-CA-C	-7.46	98.52	109.11
1	A	23	LEU	CA-CB-CG	-7.42	90.31	116.30
1	A	198	GLN	N-CA-C	-7.33	95.20	110.80
1	A	158	VAL	N-CA-C	-7.11	94.56	109.34
1	A	195	LYS	CA-C-N	7.09	135.09	121.54
1	A	195	LYS	C-N-CA	7.09	135.09	121.54
1	A	146	THR	CB-CA-C	-6.76	96.97	110.42
1	A	137	GLU	CA-C-N	-6.59	113.48	122.77
1	A	137	GLU	C-N-CA	-6.59	113.48	122.77
1	A	191	TYR	CA-C-N	6.55	131.18	120.51
1	A	191	TYR	C-N-CA	6.55	131.18	120.51
1	A	23	LEU	CA-C-O	6.45	129.73	120.51
1	A	147	GLN	CA-C-N	-6.18	109.74	121.54
1	A	147	GLN	C-N-CA	-6.18	109.74	121.54
1	B	149	MET	N-CA-C	6.12	123.83	110.80
1	A	189	ARG	N-CA-C	-6.08	106.02	113.50
1	A	199	ARG	N-CA-C	-6.03	105.02	112.38
1	B	146	THR	N-CA-C	6.03	120.08	109.96
1	A	138	THR	N-CA-C	6.00	118.19	108.34
1	A	146	THR	N-CA-CB	5.96	120.56	110.49
1	A	20	GLU	N-CA-C	-5.92	97.96	108.13
1	A	149	MET	CG-SD-CE	-5.88	87.97	100.90
1	B	300	ALA	CA-C-O	-5.86	115.85	122.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ILE	N-CA-C	5.85	116.81	107.98
1	A	258	ILE	N-CA-C	5.82	117.08	109.58
1	A	23	LEU	O-C-N	5.80	130.31	122.59
1	A	190	HIS	CA-C-N	5.79	132.59	121.54
1	A	190	HIS	C-N-CA	5.79	132.59	121.54
1	A	123	ARG	N-CA-C	5.78	118.63	110.14
1	A	156	GLU	CA-C-N	5.70	132.43	121.54
1	A	156	GLU	C-N-CA	5.70	132.43	121.54
1	A	299	ASN	N-CA-C	5.63	118.51	110.68
1	A	139	ILE	CB-CA-C	-5.62	105.16	111.23
1	B	67	ALA	N-CA-C	5.61	117.19	111.14
1	A	148	LYS	N-CA-C	5.57	122.67	110.80
1	B	280	PHE	N-CA-C	-5.53	107.18	114.04
1	A	194	THR	CA-C-N	5.43	130.77	122.24
1	A	194	THR	C-N-CA	5.43	130.77	122.24
1	A	28	GLN	N-CA-C	5.42	118.40	109.72
1	A	192	GLY	CA-C-O	-5.41	116.28	121.41
1	A	309	THR	CA-C-N	5.37	126.56	119.84
1	A	309	THR	C-N-CA	5.37	126.56	119.84
1	A	125[A]	PHE	N-CA-C	5.36	117.64	108.90
1	A	125[B]	PHE	N-CA-C	5.36	117.64	108.90
1	A	22	SER	O-C-N	5.26	129.59	122.59
1	B	146	THR	CA-C-N	5.25	131.57	121.54
1	B	146	THR	C-N-CA	5.25	131.57	121.54
1	A	138	THR	CA-C-N	5.19	129.38	122.01
1	A	138	THR	C-N-CA	5.19	129.38	122.01
1	A	290	ARG	N-CA-C	-5.17	105.09	111.40
1	A	22	SER	N-CA-C	5.16	121.79	110.80
1	A	240	GLU	N-CA-C	-5.13	106.12	112.38
1	A	19	ARG	CA-CB-CG	-5.11	103.88	114.10
1	A	84	ALA	N-CA-C	-5.11	100.09	108.41
1	A	35	ASN	N-CA-C	-5.04	100.07	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	39[A]	TYR	Sidechain

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	2581	0	2588	175	0
1	B	2474	0	2487	149	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	A	18	0	18	20	0
6	A	71	0	0	5	0
6	B	13	0	0	0	0
All	All	5217	0	5117	322	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 32.

All (322) 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:192:GLY:HA2	1:A:195:LYS:HE3	1.24	1.13
1:A:287:LYS:HG2	5:A:604:PIN:H3'2	1.18	1.09
1:B:300:ALA:O	1:B:333:PRO:HB3	1.57	1.04
1:A:141:ASP:OD2	1:A:168:THR:HG22	1.65	0.95
1:A:287:LYS:N	5:A:604:PIN:H3'1	1.81	0.94
1:A:146:THR:O	1:A:146:THR:OG1	1.78	0.94
1:A:193:GLU:O	1:A:194:THR:HG23	1.69	0.93
1:B:153:ILE:HG22	1:B:155:ARG:H	1.32	0.92
1:A:194:THR:N	1:A:197:ASN:OD1	2.04	0.91
1:B:126:LEU:HD11	1:B:171:VAL:HG13	1.52	0.91
1:A:19:ARG:NH2	1:A:27:ALA:O	2.04	0.91
1:B:130:SER:HB2	1:B:208:ARG:HG2	1.52	0.91
1:A:20:GLU:O	1:A:21:GLU:HG3	1.70	0.91
1:B:16:LEU:HD12	1:B:16:LEU:H	1.38	0.88
1:B:126:LEU:HD11	1:B:171:VAL:CG1	2.03	0.88
1:A:26:THR:HG23	1:A:27:ALA:O	1.75	0.87
1:A:23:LEU:HD23	1:A:23:LEU:C	1.98	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLU:HA	1:A:197:ASN:OD1	1.76	0.85
1:B:90:SER:CB	1:B:307:THR:HG22	2.08	0.84
1:A:170:GLU:HG2	1:A:181:TRP:CE2	2.12	0.83
1:A:277:VAL:HA	1:A:281:ILE:HD11	1.57	0.83
1:A:29:VAL:O	1:A:41:VAL:HG21	1.80	0.81
1:B:90:SER:OG	1:B:307:THR:HG22	1.82	0.80
1:A:170:GLU:HG2	1:A:181:TRP:CZ2	2.18	0.79
1:B:156:GLU:HG3	1:B:157:ASP:N	1.96	0.79
1:B:154:ILE:HG23	1:B:162:VAL:HG22	1.62	0.78
1:B:90:SER:HB2	1:B:307:THR:HG22	1.64	0.77
1:B:336:ASN:N	1:B:336:ASN:HD22	1.83	0.77
1:A:204:HIS:HE1	1:A:261[B]:SER:OG	1.68	0.77
1:B:265:LEU:O	1:B:269:ILE:HG12	1.84	0.77
1:B:154:ILE:HA	1:B:162:VAL:HG13	1.67	0.76
1:B:170:GLU:HG3	1:B:181:TRP:CZ2	2.22	0.75
1:A:258:ILE:HD12	1:A:258:ILE:H	1.52	0.75
1:A:286:SER:HA	5:A:604:PIN:H3'1	1.68	0.74
1:A:193:GLU:CA	1:A:197:ASN:OD1	2.36	0.74
1:A:60:LYS:HE2	1:A:64:GLU:OE1	1.87	0.74
1:A:143:LEU:O	1:A:168:THR:HG21	1.86	0.74
1:A:156:GLU:C	1:A:158:VAL:H	1.91	0.73
1:B:90:SER:OG	1:B:307:THR:CG2	2.37	0.73
1:B:109:ALA:O	1:B:113:ILE:HG13	1.88	0.73
1:A:22:SER:O	1:A:27:ALA:HB2	1.90	0.72
1:A:287:LYS:H	5:A:604:PIN:H3'1	1.53	0.72
1:B:182:ILE:HD11	1:B:207:PHE:CD1	2.24	0.72
1:A:153:ILE:HG22	1:A:154:ILE:H	1.55	0.72
1:A:190:HIS:CD2	1:A:193:GLU:HG3	2.24	0.72
1:A:287:LYS:H	5:A:604:PIN:C3'	2.03	0.72
1:B:299:ASN:HD21	1:B:336:ASN:HD21	1.37	0.71
1:A:286:SER:C	5:A:604:PIN:H3'1	2.15	0.71
1:B:156:GLU:O	1:B:157:ASP:HB3	1.91	0.69
1:A:260:ARG:CZ	5:A:604:PIN:H32	2.23	0.69
1:B:141:ASP:OD2	1:B:167:LEU:HD12	1.93	0.69
1:A:19:ARG:CZ	1:A:29:VAL:HG23	2.23	0.69
1:A:122:ASP:OD2	1:A:216:LYS:HE2	1.91	0.68
1:A:145:GLY:O	1:A:146:THR:HG23	1.93	0.68
1:B:135:TYR:HD2	1:B:136:ASN:N	1.91	0.68
1:B:60:LYS:HG2	1:B:108:ARG:NH2	2.09	0.68
1:B:68:ALA:HB3	1:B:69:PRO:HD3	1.76	0.68
1:A:8:ALA:HB3	1:A:303:ARG:HD3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:SER:CB	1:B:307:THR:CG2	2.72	0.68
1:A:152:LEU:HD12	1:A:152:LEU:N	2.09	0.68
1:A:204:HIS:CD2	1:A:237:ALA:H	2.12	0.67
1:A:19:ARG:HH22	1:A:28:GLN:HA	1.58	0.67
1:B:32:LYS:HE2	1:B:39[B]:TYR:CE2	2.30	0.67
1:B:133:GLU:HB3	1:B:140:THR:HG23	1.75	0.67
1:A:154:ILE:O	1:A:156:GLU:N	2.27	0.67
1:B:36:ASN:HB3	1:B:49:PHE:O	1.94	0.67
1:B:135:TYR:CE1	1:B:199:ARG:HG3	2.30	0.66
1:A:194:THR:HG22	1:A:197:ASN:HD21	1.61	0.66
1:A:286:SER:CA	5:A:604:PIN:H3'1	2.26	0.66
1:B:158:VAL:O	1:B:159:ASN:HB2	1.95	0.66
1:A:287:LYS:N	5:A:604:PIN:C3'	2.55	0.66
1:A:133:GLU:OE1	6:A:673:HOH:O	2.13	0.66
1:B:153:ILE:HG22	1:B:155:ARG:N	2.09	0.66
1:B:126:LEU:HD13	1:B:173:TYR:CE1	2.32	0.65
1:A:182:ILE:HD11	1:A:207:PHE:CD1	2.31	0.65
1:B:76:GLN:HA	1:B:76:GLN:HE21	1.61	0.65
1:A:258:ILE:HD12	1:A:258:ILE:N	2.10	0.65
1:B:264:ILE:O	1:B:268:VAL:HG23	1.96	0.65
1:A:19:ARG:O	1:A:19:ARG:HG3	1.96	0.65
1:B:8:ALA:HB3	1:B:303:ARG:HD3	1.77	0.65
1:A:141:ASP:CG	1:A:168:THR:HG22	2.21	0.64
1:A:193:GLU:C	1:A:194:THR:HG23	2.22	0.64
1:A:23:LEU:C	1:A:23:LEU:CD2	2.69	0.64
1:B:269:ILE:HD12	1:B:329:MET:HE1	1.80	0.64
1:A:194:THR:HG22	1:A:197:ASN:ND2	2.12	0.64
1:A:170:GLU:HG3	6:A:622:HOH:O	1.98	0.64
1:B:156:GLU:HG2	1:B:161:ASN:HB2	1.78	0.64
1:B:156:GLU:HB2	1:B:161:ASN:O	1.98	0.64
1:A:19:ARG:NH1	1:A:29:VAL:HG23	2.13	0.63
1:B:126:LEU:CD1	1:B:171:VAL:HG13	2.27	0.63
1:B:269:ILE:HD12	1:B:329:MET:CE	2.29	0.63
1:A:124:GLU:HG2	1:A:125[B]:PHE:N	2.14	0.63
1:A:251:ARG:HE	1:A:252:LEU:HG	1.62	0.63
1:A:287:LYS:CG	5:A:604:PIN:H3'2	2.11	0.63
1:B:155:ARG:HD3	1:B:155:ARG:C	2.24	0.63
1:B:130:SER:HB2	1:B:208:ARG:CG	2.29	0.62
1:A:308:ILE:HG12	1:A:316:THR:HG23	1.81	0.62
1:A:308:ILE:CG1	1:A:316:THR:HG23	2.30	0.62
1:A:147:GLN:O	1:A:148:LYS:C	2.41	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ILE:HG22	1:B:289:THR:HG21	1.80	0.61
1:A:260:ARG:HD3	1:A:285:ASP:O	2.01	0.61
1:B:35:ASN:OD1	1:B:36:ASN:N	2.32	0.61
1:A:124:GLU:HG2	1:A:125[B]:PHE:H	1.66	0.61
1:A:259:ASN:ND2	1:A:261[B]:SER:OG	2.32	0.61
1:B:282:ASN:HB2	1:B:285:ASP:OD1	2.01	0.61
1:A:25:GLU:O	1:A:26:THR:CB	2.48	0.61
1:A:197:ASN:O	1:A:198:GLN:HB2	1.99	0.61
1:B:90:SER:HB2	1:B:307:THR:CG2	2.29	0.61
1:A:123:ARG:NH1	1:A:215:GLU:HG3	2.16	0.60
1:A:286:SER:HA	5:A:604:PIN:C3'	2.31	0.60
1:A:122:ASP:OD1	1:A:215:GLU:HG2	2.02	0.60
1:A:19:ARG:NH2	1:A:28:GLN:HA	2.17	0.60
1:A:208:ARG:HG2	1:A:209:MET:N	2.17	0.60
1:A:145:GLY:O	1:A:146:THR:CG2	2.50	0.60
1:B:112:ASP:OD2	1:B:116:LYS:NZ	2.35	0.60
1:A:192:GLY:CA	1:A:195:LYS:HE3	2.16	0.59
1:A:193:GLU:C	1:A:197:ASN:OD1	2.44	0.59
1:A:25:GLU:O	1:A:26:THR:HB	2.03	0.59
1:A:156:GLU:O	1:A:158:VAL:N	2.35	0.59
1:B:150:LYS:HE3	1:B:166:ASP:C	2.27	0.59
1:B:290:ARG:O	1:B:293:GLN:HB2	2.03	0.59
1:A:182:ILE:HD11	1:A:207:PHE:CE1	2.37	0.59
1:B:16:LEU:HD12	1:B:16:LEU:N	2.16	0.58
1:B:88:THR:O	1:B:89:ALA:HB3	2.03	0.58
1:B:156:GLU:HG3	1:B:157:ASP:H	1.67	0.58
1:B:16:LEU:H	1:B:16:LEU:CD1	2.12	0.58
1:B:76:GLN:HA	1:B:76:GLN:NE2	2.18	0.58
1:A:53:PHE:HA	1:A:57:GLU:OE1	2.04	0.57
1:A:122:ASP:OD2	1:A:216:LYS:CE	2.52	0.57
1:B:170:GLU:HG3	1:B:181:TRP:CE2	2.39	0.57
1:B:165:ALA:O	1:B:166:ASP:HB2	2.03	0.57
1:B:172:VAL:HG13	1:B:177:MET:HB2	1.85	0.57
1:A:187:LYS:C	1:A:189:ARG:H	2.12	0.57
1:B:120:PHE:N	1:B:121:PRO:HD3	2.20	0.57
1:A:170:GLU:HG2	1:A:181:TRP:NE1	2.20	0.57
1:B:106:ILE:HG12	1:B:233:LEU:HD12	1.87	0.56
1:A:122:ASP:CG	1:A:216:LYS:HE2	2.30	0.56
1:B:259:ASN:HD22	1:B:262:LEU:H	1.52	0.56
1:B:309:THR:HG23	1:B:312:SER:HB3	1.88	0.56
1:A:253:LYS:CG	1:A:254:GLU:H	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ASN:HD22	1:A:333:PRO:HA	1.70	0.56
1:B:317:LEU:O	1:B:321:GLN:HG3	2.06	0.56
1:B:156:GLU:CG	1:B:161:ASN:HB2	2.36	0.56
1:B:336:ASN:N	1:B:336:ASN:ND2	2.54	0.55
1:A:260:ARG:NE	5:A:604:PIN:H32	2.21	0.55
1:B:156:GLU:O	1:B:157:ASP:CB	2.53	0.55
1:A:122:ASP:OD2	1:A:216:LYS:NZ	2.39	0.54
1:B:299:ASN:HD21	1:B:336:ASN:ND2	2.06	0.54
1:B:175:SER:O	1:B:179:LEU:HD23	2.07	0.54
1:A:28:GLN:O	1:A:311:VAL:HA	2.08	0.54
1:A:140:THR:HG22	6:A:653:HOH:O	2.07	0.54
1:A:153:ILE:HG22	1:A:154:ILE:N	2.22	0.54
1:A:287:LYS:HD3	5:A:604:PIN:H2'1	1.90	0.54
1:A:112:ASP:OD2	1:A:116:LYS:HE3	2.09	0.53
1:B:177:MET:O	1:B:180:LYS:HB2	2.09	0.53
1:A:265:LEU:O	1:A:269:ILE:HG12	2.08	0.53
1:B:260:ARG:HD3	1:B:285:ASP:O	2.08	0.53
1:A:48:ASN:ND2	1:B:42:ASP:CG	2.67	0.53
1:A:162:VAL:HG12	1:A:163:TYR:N	2.24	0.53
1:A:253:LYS:HG3	1:A:254:GLU:H	1.74	0.53
1:A:208:ARG:HD3	1:A:210:ILE:HG13	1.91	0.53
1:B:96:MET:HE2	1:B:234:VAL:O	2.09	0.53
1:A:215:GLU:O	1:A:216:LYS:C	2.52	0.52
1:A:177:MET:HE3	1:A:177:MET:HA	1.91	0.52
1:B:135:TYR:CD1	1:B:199:ARG:HG3	2.44	0.52
1:B:135:TYR:C	1:B:135:TYR:CD2	2.87	0.52
1:A:133:GLU:HB3	1:A:140:THR:HG23	1.92	0.52
1:B:182:ILE:HD11	1:B:207:PHE:CE1	2.44	0.52
1:A:19:ARG:O	1:A:19:ARG:CG	2.57	0.52
1:A:204:HIS:HD2	1:A:237:ALA:H	1.58	0.51
1:B:260:ARG:O	1:B:264:ILE:HG12	2.11	0.51
1:B:152:LEU:HD23	1:B:290:ARG:HD3	1.93	0.51
1:B:37:VAL:CG1	1:B:39[A]:TYR:CE1	2.94	0.51
1:A:192:GLY:HA2	1:A:195:LYS:CE	2.17	0.51
1:A:258:ILE:H	1:A:258:ILE:CD1	2.20	0.51
1:A:260:ARG:HD2	5:A:604:PIN:H41	1.91	0.51
1:B:126:LEU:HD21	1:B:171:VAL:HG11	1.93	0.51
1:B:237:ALA:O	1:B:262:LEU:HD21	2.11	0.51
1:A:152:LEU:N	1:A:152:LEU:CD1	2.73	0.50
1:B:37:VAL:HG22	1:B:48:ASN:HB3	1.94	0.50
1:B:334:TYR:O	1:B:336:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLU:H	1:A:199:ARG:HD2	1.76	0.50
1:A:58:THR:H	1:A:61:ASN:HD22	1.58	0.50
1:A:41:VAL:HG12	1:A:42:ASP:CG	2.36	0.50
1:A:252:LEU:HD23	1:A:253:LYS:N	2.26	0.50
1:A:158:VAL:O	1:A:159:ASN:HB2	2.12	0.50
1:A:211:LEU:HD12	1:A:211:LEU:N	2.27	0.50
1:A:287:LYS:HG2	5:A:604:PIN:C3'	2.13	0.50
1:B:15:PRO:HB3	1:B:55:GLY:O	2.11	0.50
1:B:35:ASN:OD1	1:B:35:ASN:C	2.55	0.49
1:B:150:LYS:HE3	1:B:166:ASP:HB2	1.93	0.49
1:A:18:SER:HB3	1:A:21:GLU:CD	2.37	0.49
1:A:253:LYS:CG	1:A:254:GLU:N	2.75	0.49
1:B:157:ASP:CG	1:B:158:VAL:N	2.70	0.49
1:A:123:ARG:HB3	1:A:214:ARG:O	2.12	0.49
1:A:193:GLU:C	1:A:194:THR:CG2	2.85	0.49
1:B:272:LEU:HD21	1:B:281:ILE:HD13	1.94	0.49
1:A:309:THR:O	1:A:309:THR:HG23	2.12	0.49
1:A:148:LYS:HE2	1:A:195:LYS:NZ	2.27	0.49
1:A:15:PRO:HG3	1:A:55:GLY:O	2.13	0.49
1:A:253:LYS:HB2	1:A:253:LYS:NZ	2.28	0.48
1:A:154:ILE:O	1:A:154:ILE:HG23	2.11	0.48
1:A:148:LYS:HA	6:A:669:HOH:O	2.12	0.48
1:A:63:TYR:CD1	1:A:67:ALA:HB3	2.49	0.48
1:A:123:ARG:HG2	1:A:123:ARG:HH11	1.79	0.48
1:B:60:LYS:HE2	1:B:108:ARG:HH22	1.77	0.48
1:B:128:ARG:HA	1:B:170:GLU:O	2.12	0.48
1:B:268:VAL:HG13	1:B:281:ILE:CG2	2.43	0.48
1:A:277:VAL:HA	1:A:281:ILE:CD1	2.37	0.48
1:B:54:HIS:O	1:B:56:ASN:N	2.42	0.48
1:B:252:LEU:HD12	1:B:252:LEU:N	2.28	0.48
1:A:150:LYS:H	1:A:150:LYS:HD2	1.79	0.48
1:B:6:ALA:HB1	1:B:331:ASN:HB2	1.96	0.48
1:B:34:ASP:O	1:B:35:ASN:OD1	2.31	0.48
1:A:299:ASN:HD21	1:A:334:TYR:H	1.62	0.47
1:A:189:ARG:HD2	6:A:673:HOH:O	2.14	0.47
1:B:237:ALA:O	1:B:238:GLY:C	2.57	0.47
1:B:75:ILE:HG22	1:B:75:ILE:O	2.14	0.47
1:A:26:THR:CG2	1:A:27:ALA:O	2.57	0.47
1:B:95:THR:O	1:B:105:VAL:HG23	2.14	0.47
1:A:88:THR:OG1	1:A:240:GLU:OE2	2.29	0.47
1:A:109:ALA:O	1:A:113:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:TYR:CD1	1:B:94:TYR:C	2.92	0.46
1:B:112:ASP:OD1	1:B:116:LYS:CE	2.63	0.46
1:A:122:ASP:CG	1:A:216:LYS:CE	2.89	0.46
1:B:154:ILE:HG22	1:B:154:ILE:O	2.16	0.46
1:B:155:ARG:C	1:B:155:ARG:CD	2.89	0.46
1:B:156:GLU:CG	1:B:157:ASP:H	2.26	0.46
1:A:252:LEU:HD23	1:A:253:LYS:H	1.80	0.46
1:B:199:ARG:O	1:B:200:SER:C	2.58	0.46
1:B:143:LEU:CB	1:B:168:THR:HG21	2.46	0.45
1:B:211:LEU:N	1:B:211:LEU:HD12	2.32	0.45
1:A:150:LYS:HA	1:A:151:PRO:HD3	1.68	0.45
1:B:90:SER:OG	1:B:307:THR:HG21	2.13	0.45
1:B:135:TYR:HD2	1:B:135:TYR:C	2.23	0.45
1:A:38:ILE:HG23	1:A:38:ILE:O	2.16	0.45
1:B:234:VAL:HG12	1:B:235:ASP:N	2.31	0.45
1:B:8:ALA:HB3	1:B:303:ARG:CD	2.44	0.45
1:B:125:PHE:O	1:B:126:LEU:HB2	2.16	0.45
1:A:126:LEU:HB3	1:A:212:GLU:HB2	1.98	0.45
1:A:137:GLU:HB2	5:A:604:PIN:C3	2.46	0.45
1:B:135:TYR:HE1	1:B:199:ARG:HG3	1.81	0.45
1:B:153:ILE:CG2	1:B:155:ARG:H	2.17	0.45
1:B:156:GLU:CD	1:B:161:ASN:HB2	2.41	0.45
1:A:19:ARG:HD2	1:A:19:ARG:HA	1.56	0.45
1:A:308:ILE:HG13	1:A:316:THR:HG23	1.99	0.45
1:B:291:ILE:C	1:B:293:GLN:H	2.24	0.45
1:A:19:ARG:HH22	1:A:27:ALA:C	2.25	0.44
1:A:20:GLU:O	1:A:21:GLU:CG	2.54	0.44
1:B:37:VAL:HG12	1:B:39[A]:TYR:CE1	2.53	0.44
1:B:76:GLN:HE21	1:B:76:GLN:CA	2.25	0.44
1:B:14:ARG:HD2	1:B:15:PRO:O	2.17	0.44
1:B:155:ARG:HD3	1:B:156:GLU:N	2.33	0.44
1:A:19:ARG:HH22	1:A:28:GLN:CA	2.28	0.44
1:B:152:LEU:HD12	1:B:163:TYR:O	2.18	0.44
1:B:112:ASP:CG	1:B:116:LYS:NZ	2.76	0.44
1:B:87:GLN:HG2	1:B:88:THR:N	2.33	0.43
1:A:147:GLN:O	1:A:148:LYS:O	2.35	0.43
1:A:40:GLN:OE1	1:A:45:LYS:HB2	2.18	0.43
1:A:232:ASN:O	1:A:233:LEU:HD23	2.18	0.43
1:A:260:ARG:HB3	5:A:604:PIN:H22	1.99	0.43
1:A:315:GLU:H	1:A:315:GLU:CD	2.26	0.43
1:B:124:GLU:O	1:B:213:SER:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:604:PIN:H42	5:A:604:PIN:H11	1.74	0.43
1:A:21:GLU:O	1:A:26:THR:HA	2.18	0.43
1:A:49:PHE:C	1:A:51:ARG:H	2.26	0.43
1:A:192:GLY:O	1:A:193:GLU:HB2	2.18	0.43
1:A:48:ASN:ND2	1:B:42:ASP:OD1	2.52	0.43
1:A:85:TYR:CD1	1:A:85:TYR:C	2.97	0.43
1:A:124:GLU:O	1:A:213:SER:HA	2.19	0.43
1:A:251:ARG:HD3	1:A:252:LEU:N	2.33	0.43
1:B:152:LEU:CD2	1:B:290:ARG:HD3	2.49	0.43
1:B:269:ILE:HG23	1:B:329:MET:HE2	2.00	0.43
1:A:118:LYS:C	1:A:120:PHE:H	2.27	0.43
1:B:33:THR:OG1	1:B:54:HIS:HD2	2.03	0.42
1:B:269:ILE:HD12	1:B:329:MET:HE2	2.01	0.42
1:A:208:ARG:HB2	1:A:232:ASN:ND2	2.35	0.42
1:B:78:TYR:HE1	1:B:334:TYR:HA	1.85	0.42
1:B:106:ILE:HG12	1:B:233:LEU:CD1	2.49	0.42
1:A:192:GLY:HA3	1:A:199:ARG:NH1	2.34	0.42
1:B:150:LYS:CE	1:B:166:ASP:C	2.93	0.42
1:A:88:THR:O	1:A:89:ALA:HB3	2.19	0.42
1:B:88:THR:O	1:B:89:ALA:CB	2.66	0.42
1:A:164:VAL:HB	1:A:167:LEU:HD22	2.02	0.42
1:B:150:LYS:HE3	1:B:165:ALA:O	2.19	0.42
1:A:198:GLN:N	1:A:198:GLN:OE1	2.53	0.42
1:B:150:LYS:HE3	1:B:166:ASP:CB	2.49	0.42
1:A:272:LEU:HD21	1:A:281:ILE:HD13	2.02	0.41
1:B:85:TYR:CD1	1:B:85:TYR:C	2.97	0.41
1:B:172:VAL:CG1	1:B:177:MET:HB2	2.49	0.41
1:A:152:LEU:CD2	1:A:291:ILE:HG13	2.50	0.41
1:A:187:LYS:C	1:A:189:ARG:N	2.78	0.41
1:A:68:ALA:HB3	1:A:69:PRO:HD3	2.01	0.41
1:B:143:LEU:HB2	1:B:168:THR:HG21	2.03	0.41
1:A:164:VAL:O	1:A:166:ASP:N	2.53	0.41
1:A:262:LEU:HA	1:A:262:LEU:HD12	1.83	0.41
1:A:16:LEU:C	1:A:18:SER:H	2.29	0.41
1:B:106:ILE:HB	1:B:107:PRO:CD	2.50	0.41
1:A:123:ARG:HH11	1:A:215:GLU:HG3	1.86	0.41
1:B:125:PHE:CE1	1:B:213:SER:HB3	2.55	0.41
1:B:143:LEU:HD22	1:B:181:TRP:HE3	1.86	0.41
1:A:260:ARG:HB3	5:A:604:PIN:H12	2.02	0.41
1:A:274:ASP:OD2	1:B:39[A]:TYR:OH	2.39	0.41
1:B:197:ASN:HD22	1:B:198:GLN:N	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ASN:HD22	1:B:197:ASN:C	2.28	0.41
1:A:153:ILE:HB	1:A:163:TYR:CZ	2.56	0.41
1:B:133:GLU:OE1	1:B:189:ARG:HD2	2.21	0.41
1:A:113:ILE:HG21	1:A:209:MET:HE1	2.03	0.40
1:A:114:PHE:CD2	1:A:175:SER:HB3	2.56	0.40
1:A:151:PRO:HD2	1:A:165:ALA:HB3	2.03	0.40
1:B:287:LYS:O	1:B:288:LEU:C	2.63	0.40
1:A:286:SER:HA	5:A:604:PIN:C4	2.52	0.40
1:B:187:LYS:C	1:B:189:ARG:H	2.28	0.40
1:B:204:HIS:ND1	1:B:288:LEU:HG	2.37	0.40
1:A:23:LEU:HD23	1:A:24:GLY:N	2.35	0.40
1:A:123:ARG:NH1	1:A:123:ARG:HG2	2.36	0.40
1:B:275:GLY:O	1:B:277:VAL:HG13	2.21	0.40
1:A:150:LYS:H	1:A:150:LYS:CD	2.32	0.40
1:B:127:LEU:HD13	1:B:209:MET:CE	2.51	0.40
1:B:168:THR:HG22	1:B:169:GLU:N	2.36	0.40
1:B:262:LEU:HD12	1:B:262:LEU:HA	1.84	0.40
1:A:144:CYS:HB3	1:A:145:GLY:H	1.21	0.40

There are no symmetry-related clashes.

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	319/349 (91%)	268 (84%)	30 (9%)	21 (7%)	1	1
1	B	303/349 (87%)	244 (80%)	42 (14%)	17 (6%)	1	1
All	All	622/698 (89%)	512 (82%)	72 (12%)	38 (6%)	1	1

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	23	LEU
1	A	26	THR
1	A	41	VAL
1	A	146	THR
1	A	149	MET
1	A	155	ARG
1	A	157	ASP
1	A	196	MET
1	B	126	LEU
1	B	147	GLN
1	B	148	LYS
1	B	149	MET
1	B	156	GLU
1	B	157	ASP
1	A	148	LYS
1	A	165	ALA
1	A	166	ASP
1	A	194	THR
1	A	277	VAL
1	A	278	GLY
1	B	160	ARG
1	B	242	ALA
1	B	276	GLN
1	A	22	SER
1	A	51	ARG
1	A	145	GLY
1	A	188	SER
1	B	87	GLN
1	B	158	VAL
1	B	191	TYR
1	A	193	GLU
1	B	159	ASN
1	B	236	LEU
1	A	150	LYS
1	B	238	GLY
1	B	55	GLY
1	B	150	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	285/303 (94%)	249 (87%)	36 (13%)	4	9
1	B	273/303 (90%)	253 (93%)	20 (7%)	13	27
All	All	558/606 (92%)	502 (90%)	56 (10%)	7	15

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	17	ASN
1	A	23	LEU
1	A	25	GLU
1	A	26	THR
1	A	48	ASN
1	A	144	CYS
1	A	146	THR
1	A	147	GLN
1	A	148	LYS
1	A	149	MET
1	A	150	LYS
1	A	152	LEU
1	A	154	ILE
1	A	167	LEU
1	A	168	THR
1	A	180	LYS
1	A	191	TYR
1	A	193	GLU
1	A	194	THR
1	A	198	GLN
1	A	209	MET
1	A	231	LEU
1	A	241	ARG
1	A	251	ARG
1	A	252	LEU
1	A	253	LYS
1	A	258	ILE
1	A	259	ASN
1	A	262	LEU
1	A	265	LEU

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Mol	Chain	Res	Type
1	A	286	SER
1	A	288	LEU
1	A	290	ARG
1	A	308	ILE
1	A	317	LEU
1	B	16	LEU
1	B	127	LEU
1	B	135	TYR
1	B	137	GLU
1	B	140	THR
1	B	147	GLN
1	B	148	LYS
1	B	150	LYS
1	B	157	ASP
1	B	184	LYS
1	B	190	HIS
1	B	209	MET
1	B	258	ILE
1	B	262	LEU
1	B	265	LEU
1	B	288	LEU
1	B	307	THR
1	B	308	ILE
1	B	317	LEU
1	B	336	ASN

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

Mol	Chain	Res	Type
1	A	36	ASN
1	A	48	ASN
1	A	61	ASN
1	A	161	ASN
1	A	190	HIS
1	A	204	HIS
1	A	259	ASN
1	A	293	GLN
1	A	299	ASN
1	A	321	GLN
1	A	336	ASN
1	B	36	ASN
1	B	54	HIS

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Mol	Chain	Res	Type
1	B	61	ASN
1	B	76	GLN
1	B	87	GLN
1	B	147	GLN
1	B	161	ASN
1	B	197	ASN
1	B	198	GLN
1	B	257	ASN
1	B	259	ASN
1	B	321	GLN
1	B	336	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NO3	A	603	-	1,3,3	0.34	0	0,3,3	-	-
5	PIN	A	604	-	18,18,18	2.35	7 (38%)	24,26,26	2.05	8 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	A	600	2	28,29,29	1.85	8 (28%)	43,45,45	1.98	9 (20%)
4	ADP	B	700	2	28,29,29	1.93	10 (35%)	43,45,45	1.96	7 (16%)

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
5	PIN	A	604	-	-	2/12/22/22	0/1/1/1
4	ADP	A	600	2	-	6/16/32/32	0/3/3/3
4	ADP	B	700	2	-	7/16/32/32	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	604	PIN	C1-S1	-5.30	1.70	1.77
5	A	604	PIN	O3-S1	4.75	1.65	1.47
4	A	600	ADP	C5-N7	-4.18	1.31	1.39
4	B	700	ADP	C5-N7	-4.17	1.31	1.39
4	B	700	ADP	C5-C4	3.66	1.45	1.39
5	A	604	PIN	O3'-S1'	3.55	1.60	1.47
4	A	600	ADP	C4-N3	3.19	1.40	1.34
4	B	700	ADP	C2-N3	3.10	1.39	1.33
4	B	700	ADP	C2-N1	3.07	1.39	1.33
4	A	600	ADP	C5-C4	3.04	1.44	1.39
4	A	600	ADP	C2-N1	2.99	1.39	1.33
5	A	604	PIN	C1'-S1'	-2.99	1.73	1.77
4	B	700	ADP	C4-N3	2.92	1.39	1.34
4	B	700	ADP	C4-N9	-2.84	1.31	1.37
4	A	600	ADP	C4-N9	-2.81	1.31	1.37
4	A	600	ADP	C5'-C4'	2.74	1.59	1.51
4	B	700	ADP	C5'-C4'	2.70	1.59	1.51
5	A	604	PIN	O1-S1	-2.69	1.37	1.45
4	B	700	ADP	C6-N1	2.56	1.42	1.35
4	A	600	ADP	C2-N3	2.36	1.38	1.33
5	A	604	PIN	O1'-S1'	-2.28	1.38	1.45
4	B	700	ADP	O4'-C1'	2.18	1.47	1.42
4	A	600	ADP	C6-N1	2.18	1.41	1.35
4	B	700	ADP	C1'-N9	2.06	1.52	1.46
5	A	604	PIN	C4'-C3	2.05	1.58	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	700	ADP	N3-C2-N1	-6.84	118.23	128.58
4	A	600	ADP	N3-C2-N1	-6.68	118.47	128.58
5	A	604	PIN	O1'-S1'-C1'	5.60	115.19	106.73
4	B	700	ADP	C5-C4-N3	-4.69	120.25	126.72
4	A	600	ADP	C5-C4-N3	-4.69	120.26	126.72
4	B	700	ADP	C2-N3-C4	4.39	122.55	111.83
4	A	600	ADP	C2-N3-C4	4.29	122.31	111.83
4	A	600	ADP	N3-C4-N9	3.70	133.46	127.17
4	B	700	ADP	N3-C4-N9	3.63	133.34	127.17
4	B	700	ADP	C5-N7-C8	3.31	108.66	103.45
5	A	604	PIN	C2'-N1'-C4'	3.26	119.92	111.24
4	A	600	ADP	C5-N7-C8	3.23	108.53	103.45
5	A	604	PIN	C1'-C2'-N1'	3.18	124.38	112.36
5	A	604	PIN	O2-S1-C1	3.03	111.30	106.73
4	B	700	ADP	C4-C5-N7	-2.96	107.20	110.58
5	A	604	PIN	O1-S1-C1	2.84	111.02	106.73
4	A	600	ADP	C4-C5-N7	-2.77	107.42	110.58
4	A	600	ADP	N9-C8-N7	-2.75	110.03	113.94
5	A	604	PIN	C4-C3'-N1'	2.70	116.09	110.65
4	B	700	ADP	N9-C8-N7	-2.63	110.20	113.94
4	A	600	ADP	PA-O5'-C5'	2.41	135.14	121.35
4	A	600	ADP	O2'-C2'-C1'	2.15	117.51	110.10
5	A	604	PIN	O3-S1-O2	-2.11	106.11	111.40
5	A	604	PIN	O3'-S1'-C1'	-2.02	102.05	106.00

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	ADP	PA-O3A-PB-O2B
4	A	600	ADP	C5'-O5'-PA-O1A
4	A	600	ADP	C5'-O5'-PA-O2A
4	A	600	ADP	C5'-O5'-PA-O3A
4	B	700	ADP	PA-O3A-PB-O2B
4	B	700	ADP	C5'-O5'-PA-O1A
4	B	700	ADP	C5'-O5'-PA-O2A
4	B	700	ADP	C5'-O5'-PA-O3A
5	A	604	PIN	S1-C1-C2-N1
5	A	604	PIN	C1-C2-N1-C4
4	A	600	ADP	C3'-C4'-C5'-O5'
4	A	600	ADP	O4'-C4'-C5'-O5'

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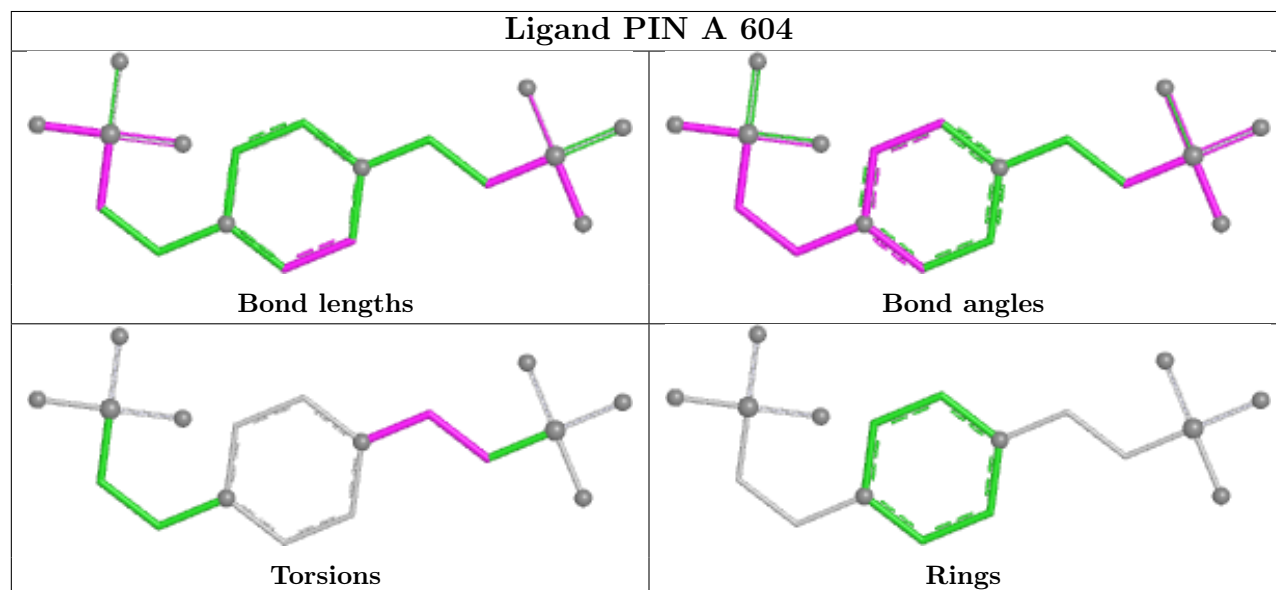
Mol	Chain	Res	Type	Atoms
4	B	700	ADP	C3'-C4'-C5'-O5'
4	B	700	ADP	O4'-C4'-C5'-O5'
4	B	700	ADP	PA-O3A-PB-O3B

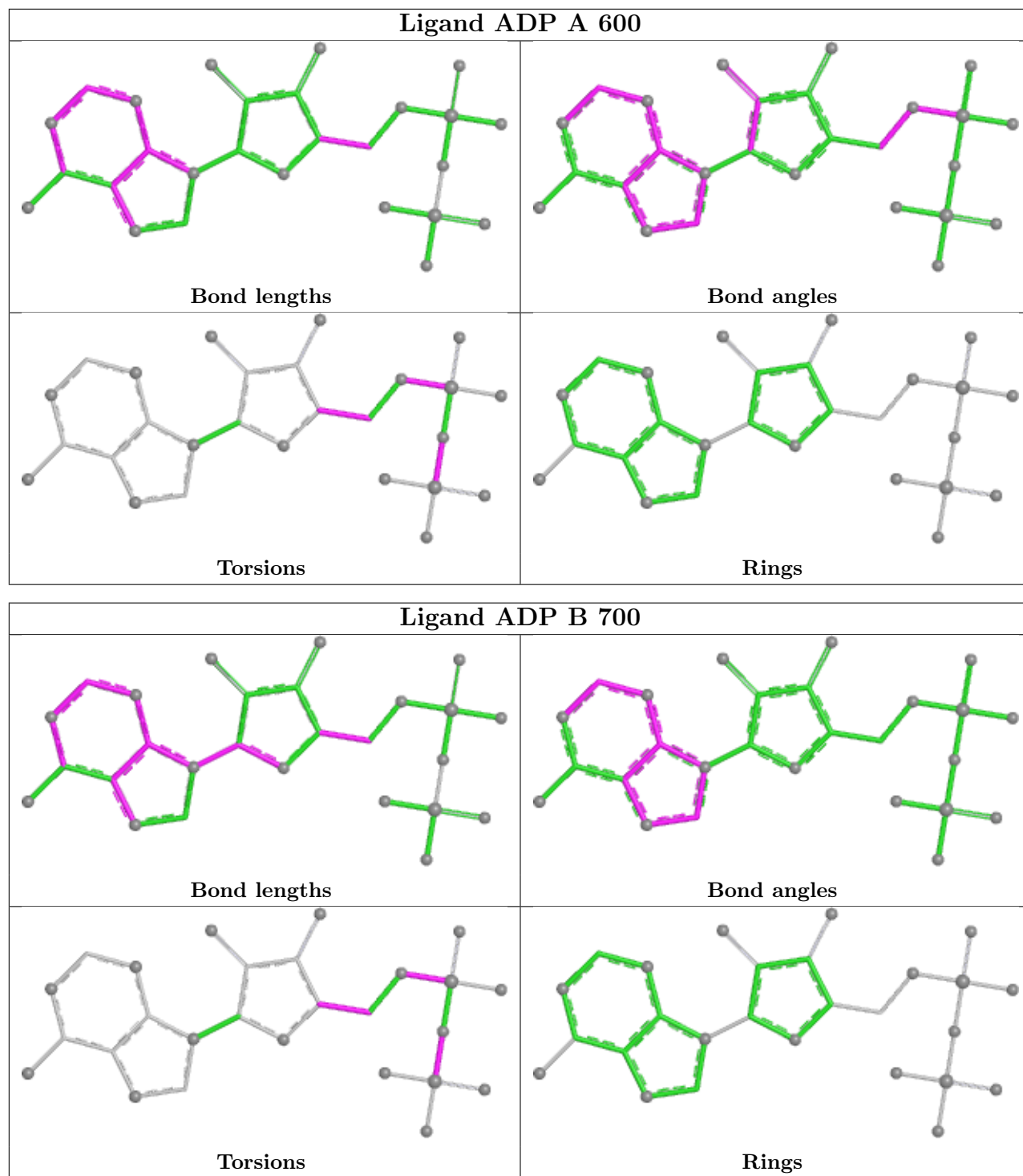
There are no ring outliers.

1 monomer is involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	PIN	20	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.