



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:22 pm GMT

PDB ID : 1T5C
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

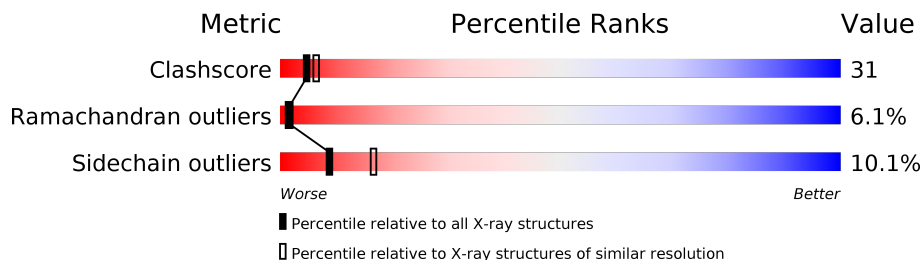
1 Overall quality at a glance

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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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 (three-letter code: MG) (formula: Mg).

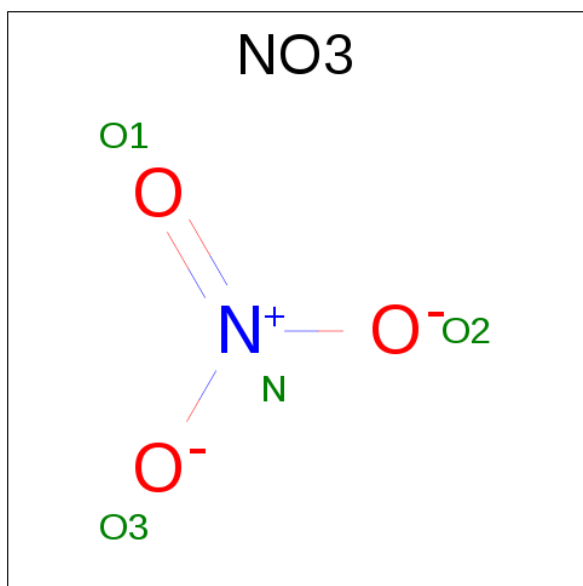
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		

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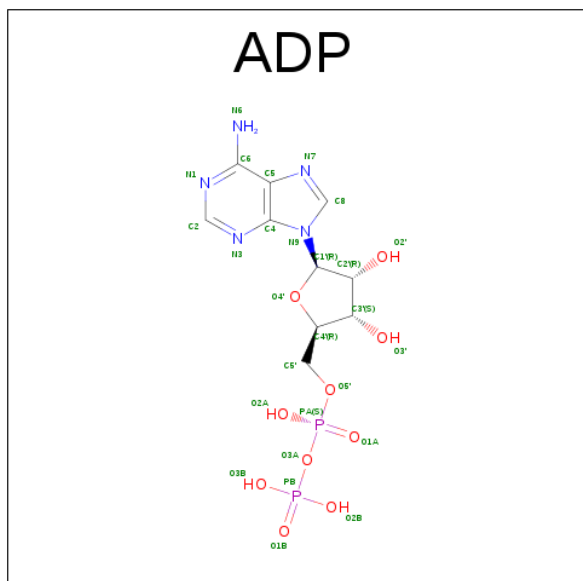
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



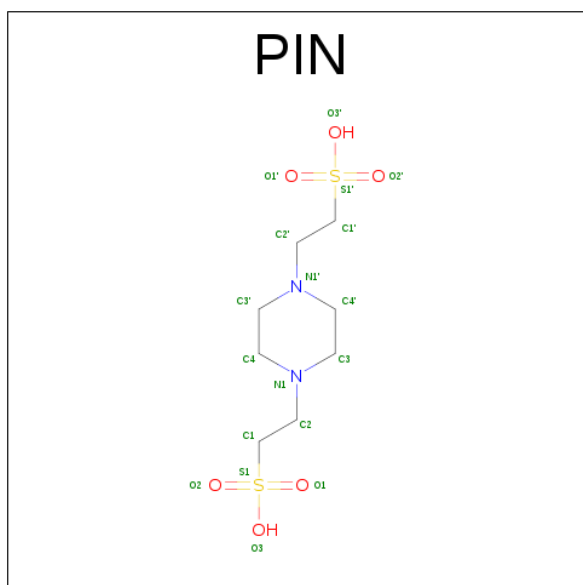
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: 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) (three-letter code: 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.

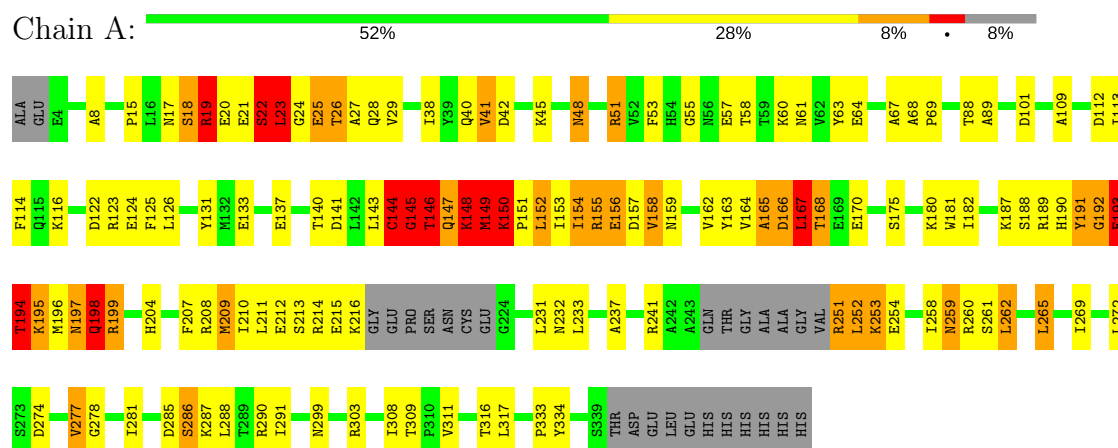
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	71	Total	O	0	0
			71	71		
6	B	13	Total	O	0	0
			13	13		

3 Residue-property plots

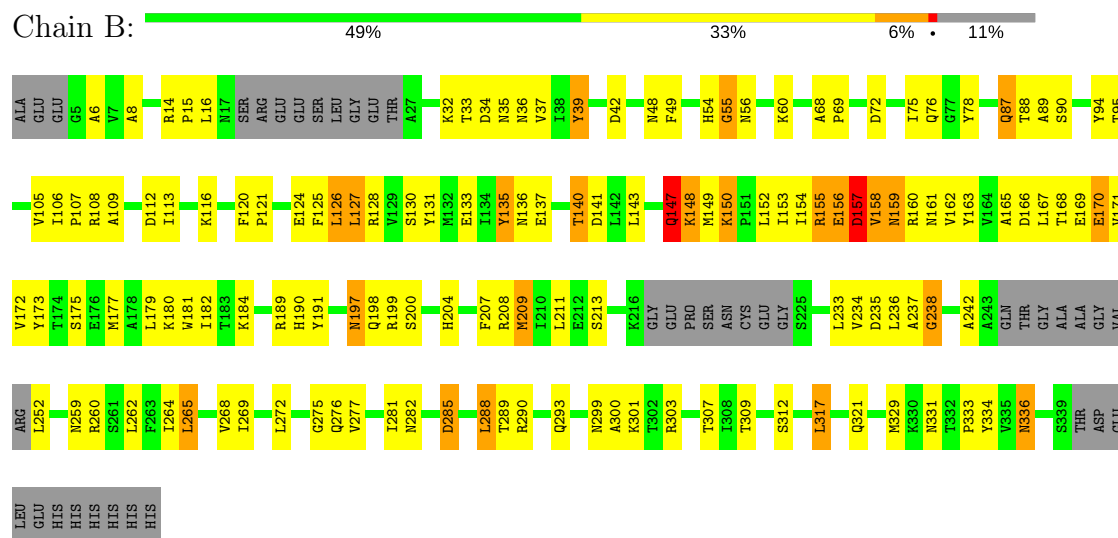
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

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: MG, PIN, ADP, NO3

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	0.62	5/2622 (0.2%)	1.10	24/3531 (0.7%)
1	B	0.35	0/2514	0.65	2/3388 (0.1%)
All	All	0.51	5/5136 (0.1%)	0.91	26/6919 (0.4%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	MET	SD-CE	-7.25	1.37	1.77
1	A	156	GLU	CB-CG	6.66	1.64	1.52
1	A	149	MET	CG-SD	-5.92	1.65	1.81
1	A	19	ARG	CB-CG	5.56	1.67	1.52
1	A	156	GLU	CG-CD	5.34	1.59	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	ARG	N-CA-CB	11.35	131.03	110.60
1	A	23	LEU	CA-CB-CG	-10.86	90.31	115.30
1	A	149	MET	N-CA-C	10.51	139.37	111.00
1	A	18	SER	C-N-CA	9.25	144.83	121.70
1	A	22	SER	C-N-CA	9.10	144.44	121.70
1	B	147	GLN	N-CA-C	9.06	135.47	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	LEU	CA-C-N	-9.03	98.14	116.20
1	A	192	GLY	N-CA-C	-9.02	90.56	113.10
1	A	146	THR	N-CA-C	8.95	135.16	111.00
1	A	195	LYS	N-CA-C	-8.60	87.78	111.00
1	B	301	LYS	N-CA-C	-8.46	88.17	111.00
1	A	23	LEU	N-CA-CB	8.24	126.88	110.40
1	A	191	TYR	N-CA-C	-7.89	89.70	111.00
1	A	149	MET	CG-SD-CE	-7.64	87.97	100.20
1	A	167	LEU	CA-CB-CG	7.42	132.36	115.30
1	A	197	ASN	N-CA-C	6.96	129.79	111.00
1	A	158	VAL	N-CA-C	-6.09	94.56	111.00
1	A	144	CYS	N-CA-C	6.09	127.44	111.00
1	A	198	GLN	N-CA-C	-5.85	95.20	111.00
1	A	150	LYS	N-CA-C	5.75	126.52	111.00
1	A	145	GLY	C-N-CA	5.63	135.78	121.70
1	A	146	THR	CB-CA-C	-5.42	96.97	111.60
1	A	146	THR	N-CA-CB	5.40	120.56	110.30
1	A	195	LYS	C-N-CA	5.36	135.09	121.70
1	A	18	SER	N-CA-CB	-5.30	102.56	110.50
1	A	155	ARG	NE-CZ-NH2	-5.05	117.78	120.30

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 [i](#)

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	168	0
1	B	2474	0	2487	140	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	306	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 31.

All (306) 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:H	1:B:16:LEU:HD12	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: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:A:23:LEU:HD23	1:A:23:LEU:C	1.98	0.81
1:B:156:GLU:HG3	1:B:157:ASP:N	1.96	0.80
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: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:HD22	1:B:336:ASN:N	1.83	0.77
1:A:204:HIS:HE1	1:A:261[B]:SER:OG	1.68	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:109:ALA:O	1:B:113:ILE:HG13	1.88	0.73
1:B:90:SER:OG	1:B:307:THR:CG2	2.37	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: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:156:GLU:C	1:A:158:VAL:H	1.91	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
1:B:90:SER:CB	1:B:307:THR:CG2	2.72	0.68
1:A:152:LEU:N	1:A:152:LEU:HD12	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:133:GLU:HB3	1:B:140:THR:HG23	1.75	0.67
1:B:32:LYS:HE2	1:B:39[B]:TYR:CE2	2.30	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:A:286:SER:C	5:A:604:PIN:H3'1	2.15	0.66
1:B:269:ILE:HD12	1:B:329:MET:HE1	1.77	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE21	1:B:76:GLN:HA	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: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: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: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:197:ASN:O	1:A:198:GLN:HB2	1.99	0.61
1:A:25:GLU:O	1:A:26:THR:CB	2.48	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:23:LEU:CD2	1:A:23:LEU:C	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASP:CG	1:A:168:THR:HG22	2.21	0.60
1:A:193:GLU:C	1:A:194:THR:HG23	2.22	0.60
1:A:192:GLY:CA	1:A:195:LYS:HE3	2.16	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: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:155:ARG:HD3	1:B:155:ARG:C	2.24	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:NE2	1:B:76:GLN:HA	2.18	0.58
1:A:122:ASP:OD2	1:A:216:LYS:CE	2.52	0.57
1:A:53:PHE:HA	1:A:57:GLU:OE1	2.04	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:147:GLN:O	1:A:148:LYS:C	2.41	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: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
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:ND2	1:B:336:ASN:N	2.54	0.55
1:A:260:ARG:NE	5:A:604:PIN:H32	2.21	0.55
1:A:193:GLU:C	1:A:197:ASN:OD1	2.44	0.55
1:B:156:GLU:O	1:B:157:ASP:CB	2.53	0.55
1:B:150:LYS:HE3	1:B:166:ASP:C	2.27	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:197:ASN:HB3	1:A:198:GLN:OE1	2.09	0.53
1:A:208:ARG:HD3	1:A:210:ILE:HG13	1.91	0.53
1:A:187:LYS:C	1:A:189:ARG:H	2.12	0.52
1:B:135:TYR:CD1	1:B:199:ARG:HG3	2.44	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:122:ASP:CG	1:A:216:LYS:HE2	2.30	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:CD1	1:A:258:ILE:H	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:334:TYR:O	1:B:336:ASN:ND2	2.44	0.50
1:B:37:VAL:HG22	1:B:48:ASN:HB3	1.94	0.50
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: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:150:LYS:HE3	1:B:166:ASP:HB2	1.93	0.49
1:A:253:LYS:CG	1:A:254:GLU:N	2.75	0.49
1:A:123:ARG:HB3	1:A:214:ARG:O	2.12	0.49
1:B:272:LEU:HD21	1:B:281:ILE:HD13	1.94	0.49
1:A:154:ILE:HG23	1:A:154:ILE:O	2.11	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:NZ	1:A:253:LYS:HB2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LYS:HA	6:A:669:HOH:O	2.12	0.48
1:B:135:TYR:C	1:B:135:TYR:CD2	2.87	0.48
1:A:123:ARG:HH11	1:A:123:ARG:HG2	1.79	0.48
1:A:63:TYR:CD1	1:A:67:ALA:HB3	2.49	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:A:48:ASN:ND2	1:B:42:ASP:CG	2.67	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:252:LEU:HD12	1:B:252:LEU:N	2.28	0.48
1:B:54:HIS:O	1:B:56:ASN:N	2.42	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:215:GLU:O	1:A:216:LYS:C	2.52	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:75:ILE:O	1:B:75:ILE:HG22	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:109:ALA:O	1:A:113:ILE:HG13	2.15	0.47
1:B:112:ASP:OD1	1:B:116:LYS:CE	2.63	0.46
1:B:154:ILE:O	1:B:154:ILE:HG22	2.16	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: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:A:38:ILE:HG23	1:A:38:ILE:O	2.16	0.45
1:A:41:VAL:HG12	1:A:42:ASP:CG	2.36	0.45
1:B:234:VAL:HG12	1:B:235:ASP:N	2.31	0.45
1:B:125:PHE:O	1:B:126:LEU:HB2	2.16	0.45
1:B:8:ALA:HB3	1:B:303:ARG:CD	2.44	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:153:ILE:CG2	1:B:155:ARG:H	2.17	0.45
1:B:135:TYR:HE1	1:B:199:ARG:HG3	1.81	0.45
1:A:18:SER:HB3	1:A:21:GLU:CD	2.37	0.45
1:A:19:ARG:HA	1:A:19:ARG:HD2	1.56	0.45
1:A:308:ILE:HG13	1:A:316:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ASP:CG	1:B:158:VAL:N	2.70	0.45
1:B:35:ASN:OD1	1:B:35:ASN:C	2.55	0.45
1:A:193:GLU:C	1:A:194:THR:CG2	2.85	0.45
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:269:ILE:HG23	1:B:329:MET:HE2	2.00	0.43
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:113:ILE:HG21	1:A:209:MET:HE1	2.00	0.43
1:A:232:ASN:O	1:A:233:LEU:HD23	2.18	0.43
1:A:40:GLN:OE1	1:A:45:LYS:HB2	2.18	0.43
1:A:260:ARG:HB3	5:A:604:PIN:H22	1.99	0.43
1:B:124:GLU:O	1:B:213:SER:HA	2.18	0.43
5:A:604:PIN:H42	5:A:604:PIN:H11	1.74	0.43
1:A:192:GLY:O	1:A:193:GLU:HB2	2.18	0.43
1:A:21:GLU:O	1:A:26:THR:HA	2.18	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:A:48:ASN:ND2	1:B:42:ASP:OD1	2.52	0.43
1:B:237:ALA:O	1:B:238:GLY:C	2.57	0.43
1:B:33:THR:OG1	1:B:54:HIS:HD2	2.03	0.42
1:A:208:ARG:HB2	1:A:232:ASN:ND2	2.35	0.42
1:B:106:ILE:HG12	1:B:233:LEU:CD1	2.49	0.42
1:B:78:TYR:HE1	1:B:334:TYR:HA	1.85	0.42
1:A:192:GLY:HA3	1:A:199:ARG:NH1	2.34	0.42
1:A:156:GLU:C	1:A:158:VAL:N	2.67	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:OE1	1:A:198:GLN:N	2.53	0.42
1:B:150:LYS:HE3	1:B:166:ASP:CB	2.49	0.42
1:B:94:TYR:C	1:B:94:TYR:CD1	2.92	0.42
1:A:272:LEU:HD21	1:A:281:ILE:HD13	2.02	0.41
1:B:172:VAL:CG1	1:B:177:MET:HB2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:CD2	1:A:291:ILE:HG13	2.50	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:122:ASP:CG	1:A:216:LYS:CE	2.89	0.41
1:A:262:LEU:HA	1:A:262:LEU:HD12	1.83	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:199:ARG:O	1:B:200:SER:C	2.58	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:274:ASP:OD2	1:B:39[A]:TYR:OH	2.39	0.41
1:A:260:ARG:HB3	5:A:604:PIN:H12	2.02	0.41
1:B:197:ASN:HD22	1:B:198:GLN:N	2.18	0.41
1:B:135:TYR:C	1:B:135:TYR:HD2	2.23	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: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:A:286:SER:HA	5:A:604:PIN:C4	2.52	0.40
1:B:204:HIS:ND1	1:B:288:LEU:HG	2.37	0.40
1:A:123:ARG:NH1	1:A:123:ARG:HG2	2.36	0.40
1:A:23:LEU:HD23	1:A:24:GLY:N	2.35	0.40
1:B:155:ARG:CD	1:B:155:ARG:C	2.89	0.40
1:B:156:GLU:CD	1:B:161:ASN:HB2	2.41	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:168:THR:HG22	1:B:169:GLU:N	2.36	0.40
1:B:127:LEU:HD13	1:B:209:MET:CE	2.51	0.40
1:B:262:LEU:HA	1:B:262:LEU:HD12	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%)	2	2
All	All	622/698 (89%)	512 (82%)	72 (12%)	38 (6%)	2	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

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Mol	Chain	Res	Type
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%)	5	10
1	B	273/303 (90%)	253 (93%)	20 (7%)	16	31
All	All	558/606 (92%)	502 (90%)	56 (10%)	9	17

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

Mol	Chain	Res	Type
1	A	17	ASN
1	A	23	LEU
1	A	25	GLU
1	A	48	ASN
1	A	51	ARG
1	A	101	ASP
1	A	131	TYR
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

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Mol	Chain	Res	Type
1	A	191	TYR
1	A	193	GLU
1	A	194	THR
1	A	198	GLN
1	A	199	ARG
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	259	ASN
1	A	262	LEU
1	A	265	LEU
1	A	286	SER
1	A	288	LEU
1	A	290	ARG
1	A	317	LEU
1	B	72	ASP
1	B	127	LEU
1	B	131	TYR
1	B	135	TYR
1	B	137	GLU
1	B	140	THR
1	B	147	GLN
1	B	148	LYS
1	B	155	ARG
1	B	157	ASP
1	B	170	GLU
1	B	184	LYS
1	B	190	HIS
1	B	197	ASN
1	B	209	MET
1	B	265	LEU
1	B	285	ASP
1	B	288	LEU
1	B	317	LEU
1	B	336	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	61	ASN
1	A	87	GLN
1	A	161	ASN
1	A	190	HIS
1	A	204	HIS
1	A	232	ASN
1	A	259	ASN
1	A	293	GLN
1	A	299	ASN
1	A	336	ASN
1	B	54	HIS
1	B	61	ASN
1	B	76	GLN
1	B	87	GLN
1	B	147	GLN
1	B	197	ASN
1	B	198	GLN
1	B	257	ASN
1	B	259	ASN
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 carbohydrates 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
4	ADP	A	600	2	25,29,29	1.79	7 (28%)	24,45,45	2.66	3 (12%)
3	NO3	A	603	-	1,3,3	0.31	0	0,3,3	0.00	-
5	PIN	A	604	-	18,18,18	2.33	6 (33%)	22,26,26	3.02	7 (31%)
4	ADP	B	700	2	25,29,29	1.91	8 (32%)	24,45,45	2.70	3 (12%)

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
4	ADP	A	600	2	-	0/12/32/32	0/3/3/3
3	NO3	A	603	-	-	0/0/0/0	0/0/0/0
5	PIN	A	604	-	-	0/12/22/22	0/1/1/1
4	ADP	B	700	2	-	0/12/32/32	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	604	PIN	C1-S1	-4.89	1.70	1.77
5	A	604	PIN	C1'-S1'	-2.72	1.73	1.77
5	A	604	PIN	O1-S1	-2.59	1.37	1.45
4	A	600	ADP	C5-N7	-2.35	1.31	1.39
4	B	700	ADP	C5-N7	-2.34	1.31	1.39
4	B	700	ADP	PB-O3A	-2.28	1.56	1.60
4	A	600	ADP	PB-O3A	-2.26	1.56	1.60
5	A	604	PIN	O1'-S1'	-2.19	1.38	1.45
4	B	700	ADP	C5-C4	2.27	1.45	1.40
4	B	700	ADP	C5'-C4'	2.56	1.59	1.51
4	A	600	ADP	C5'-C4'	2.60	1.59	1.51
4	A	600	ADP	C2-N1	2.84	1.39	1.33
4	B	700	ADP	C2-N1	2.92	1.39	1.33
4	B	700	ADP	C4-N3	2.94	1.39	1.35
4	A	600	ADP	O4'-C1'	3.20	1.45	1.41
4	A	600	ADP	C4-N3	3.28	1.40	1.35
4	A	600	ADP	C2-N3	3.57	1.38	1.32
5	A	604	PIN	O3'-S1'	3.88	1.60	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	700	ADP	O4'-C1'	4.19	1.47	1.41
4	B	700	ADP	C2-N3	4.37	1.39	1.32
5	A	604	PIN	O3-S1	5.23	1.65	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	700	ADP	N3-C2-N1	-12.20	118.23	128.86
4	A	600	ADP	N3-C2-N1	-11.92	118.47	128.86
5	A	604	PIN	O3'-S1'-C1'	-3.26	102.05	106.06
5	A	604	PIN	O3-S1-O2	-2.29	106.11	111.37
4	B	700	ADP	C4-C5-N7	-2.29	107.20	109.41
4	A	600	ADP	C4-C5-N7	-2.06	107.42	109.41
4	A	600	ADP	C4'-O4'-C1'	2.02	111.91	109.77
4	B	700	ADP	C4'-O4'-C1'	2.17	112.08	109.77
5	A	604	PIN	C4-C3'-N1'	2.70	116.09	110.63
5	A	604	PIN	C2'-N1'-C4'	3.38	119.92	111.26
5	A	604	PIN	O1-S1-C1	4.92	111.02	106.79
5	A	604	PIN	O2-S1-C1	5.25	111.30	106.79
5	A	604	PIN	O1'-S1'-C1'	9.77	115.19	106.79

There are no chirality outliers.

There are no torsion outliers.

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.