Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 07:34 PM GMT

PDB ID	:	1G9Y
Title	:	HOMING ENDONUCLEASE I-CREI / DNA SUBSTRATE COMPLEX WITH CALCIUM
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Deposited on	:	2000-11-28
Resolution	:	2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

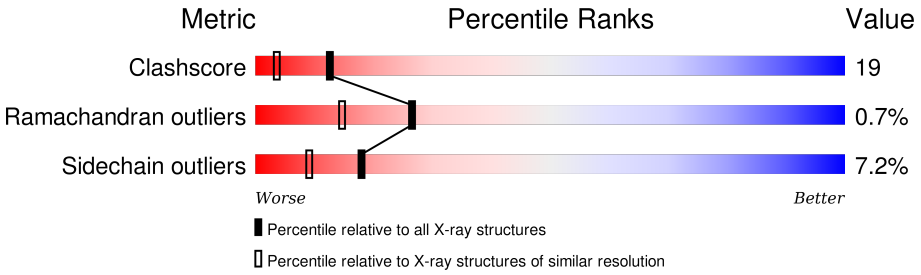
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)

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 <=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	C	24	54% 42% .
2	D	24	54% 42% .
3	A	152	73% 25% .
3	B	152	61% 34% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3890 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 DNA chain called 5'-D(*CP*GP*AP*AP*AP*CP*TP*GP*TP*CP*TP*CP *AP*CP*GP*AP*CP*GP*TP*TP*TP*TP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	24	Total	C	N	O	P	0	0	0
			485	233	85	144	23			

- Molecule 2 is a DNA chain called 5'-D(*GP*CP*AP*AP*AP*AP*CP*GP*TP*CP*GP*T P*GP*AP*GP*AP*CP*AP*GP*TP*TP*TP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	24	Total	C	N	O	P	0	0	0
			493	235	95	140	23			

- Molecule 3 is a protein called DNA ENDONUCLEASE I-CREI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	152	Total	C	N	O	S	0	0	0
			1237	796	210	230	1			
3	B	152	Total	C	N	O	S	0	0	0
			1237	796	210	230	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	THR	ALA	SEE REMARK 999	UNP P05725
A	110	GLU	TRP	SEE REMARK 999	UNP P05725
A	111	GLN	ARG	SEE REMARK 999	UNP P05725
B	242	THR	ALA	SEE REMARK 999	UNP P05725
B	310	GLU	TRP	SEE REMARK 999	UNP P05725
B	311	GLN	ARG	SEE REMARK 999	UNP P05725

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	152	Total O 152 152	0	0
5	B	130	Total O 130 130	0	0
5	C	83	Total O 83 83	0	0
5	D	70	Total O 70 70	0	0

3 Residue-property plots (i)

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

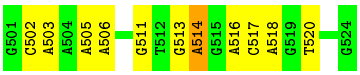
Note EDS was not executed.

• Molecule 1: 5'-D(*CP*GP*AP*AP*AP*CP*TP*GP*TP*CP*TP*CP*AP*CP*GP*AP*CP*GP*TP*TP*TP*TP*GP*C)-3'

Chain C:

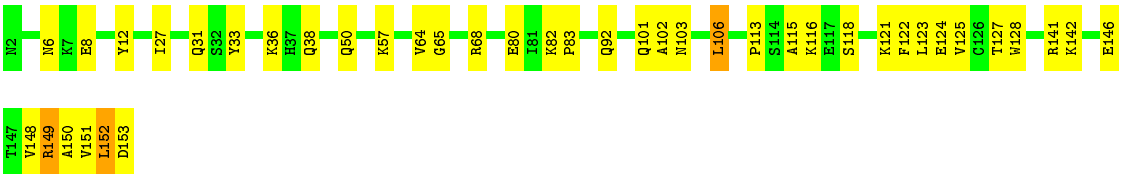
• Molecule 2: 5'-D(*GP*CP*AP*AP*AP*AP*CP*GP*TP*CP*GP*TP*GP*AP*GP*AP*CP*AP*GP*TP*TP*TP*CP*G)-3'

Chain D:



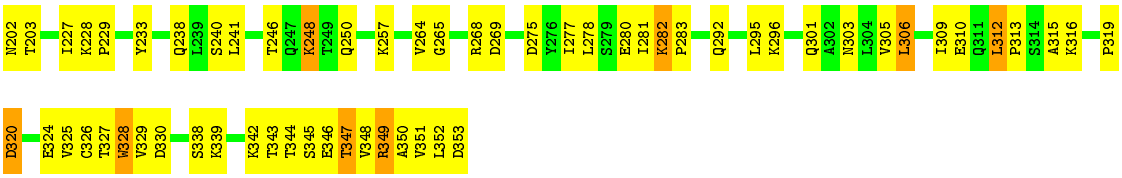
• Molecule 3: DNA ENDONUCLEASE I-CREI

Chain A:



• Molecule 3: DNA ENDONUCLEASE I-CREI

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.20Å 67.80Å 88.30Å 90.00° 91.60° 90.00°	Depositor
Resolution (Å)	26.99 – 2.05	Depositor
% Data completeness (in resolution range)	93.5 (26.99-2.05)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	5.50	Depositor
Refinement program	?	Depositor
R, R_{free}	0.207 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3890	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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: CA

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	C	0.31	0/542	0.74	0/834
2	D	0.32	0/554	0.76	0/854
3	A	0.36	0/1260	0.64	0/1700
3	B	0.36	0/1260	0.64	0/1700
All	All	0.35	0/3616	0.68	0/5088

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	C	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	418	DG	Sidechain
2	D	514	DA	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	C	485	0	273	17	0
2	D	493	0	271	15	0
3	A	1237	0	1270	39	0
3	B	1237	0	1270	65	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	152	0	0	9	0
5	B	130	0	0	9	0
5	C	83	0	0	2	0
5	D	70	0	0	2	0
All	All	3890	0	3084	127	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 (127) 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)
3:B:282:LYS:HE3	3:B:282:LYS:HA	1.50	0.94
3:B:241:LEU:HD23	3:B:305:VAL:HG13	1.50	0.93
1:C:421:DT:H2"	1:C:422:DT:H5"	1.55	0.87
3:A:118:SER:HB3	3:A:121:LYS:HB2	1.57	0.85
3:A:115:ALA:HB1	3:A:122:PHE:HA	1.64	0.80
3:B:344:THR:H	3:B:347:THR:CG2	1.95	0.79
3:A:148:VAL:O	3:A:151:VAL:HG23	1.83	0.79
3:B:353:ASP:HB2	5:B:868:HOH:O	1.84	0.77
1:C:419:DT:H71	3:B:228:LYS:HG2	1.70	0.74
3:B:281:ILE:HD11	3:B:309:ILE:HG23	1.67	0.74
3:A:92:GLN:HG3	3:A:103:ASN:HD21	1.52	0.74
3:A:92:GLN:HG3	3:A:103:ASN:ND2	2.03	0.73
3:B:344:THR:O	3:B:347:THR:HG23	1.90	0.72
1:C:421:DT:C2'	1:C:422:DT:H5"	2.21	0.71
3:A:142:LYS:HE3	5:A:897:HOH:O	1.91	0.71
1:C:419:DT:O4	3:B:228:LYS:HE3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:275:ASP:HB2	3:B:277:ILE:HD11	1.74	0.69
2:D:505:DA:H2"	2:D:506:DA:C5'	2.23	0.69
3:B:248:LYS:HE2	3:B:250:GLN:HE21	1.56	0.68
3:A:115:ALA:HA	3:A:121:LYS:HB3	1.76	0.68
2:D:505:DA:H2"	2:D:506:DA:H5'	1.76	0.68
3:A:57:LYS:HB2	3:A:57:LYS:NZ	2.09	0.67
1:C:403:DA:H1'	1:C:404:DA:H5'	1.78	0.66
3:B:350:ALA:HB3	5:B:861:HOH:O	1.96	0.64
3:A:148:VAL:C	3:A:150:ALA:H	2.02	0.63
3:B:248:LYS:CE	3:B:250:GLN:HE21	2.12	0.63
3:A:124:GLU:O	3:A:127:THR:HB	1.99	0.62
3:B:292:GLN:HG3	3:B:303:ASN:OD1	1.98	0.62
3:B:306:LEU:O	3:B:310:GLU:HG3	1.98	0.62
2:D:517:DC:H2'	2:D:518:DA:H8	1.64	0.62
3:A:12:TYR:CZ	3:B:296:LYS:HD3	2.35	0.62
2:D:517:DC:OP1	2:D:517:DC:H4'	1.99	0.61
1:C:418:DG:H2'	1:C:419:DT:H72	1.81	0.61
3:B:282:LYS:HE2	5:B:877:HOH:O	2.01	0.61
3:B:344:THR:HG22	3:B:347:THR:HG22	1.83	0.60
1:C:417:DC:H2'	1:C:418:DG:C8	2.37	0.60
3:B:257:LYS:HE2	5:B:873:HOH:O	2.02	0.59
2:D:517:DC:H2"	2:D:518:DA:H5'	1.84	0.58
3:A:31:GLN:NE2	3:A:36:LYS:HG3	2.18	0.58
3:B:327:THR:HG23	5:B:856:HOH:O	2.04	0.58
3:A:82:LYS:HB3	3:A:83:PRO:HD3	1.84	0.58
3:A:141:ARG:HD2	5:A:833:HOH:O	2.03	0.57
3:B:264:VAL:HG22	3:B:265:GLY:N	2.20	0.57
3:B:227:ILE:HD11	3:B:329:VAL:HG11	1.87	0.57
3:B:233:TYR:CZ	3:B:238:GLN:HB2	2.39	0.57
2:D:517:DC:H2'	2:D:518:DA:C8	2.39	0.56
2:D:502:DC:H3'	3:B:316:LYS:HE2	1.85	0.56
1:C:417:DC:H2'	1:C:418:DG:H8	1.70	0.56
3:A:57:LYS:HZ3	3:A:57:LYS:HB2	1.71	0.56
3:B:280:GLU:O	3:B:283:PRO:HD2	2.06	0.55
3:B:241:LEU:N	3:B:241:LEU:HD12	2.21	0.55
5:D:210:HOH:O	3:B:339:LYS:HG3	2.05	0.55
3:B:348:VAL:C	3:B:350:ALA:H	2.10	0.55
3:B:312:LEU:N	3:B:313:PRO:HD2	2.22	0.54
3:B:248:LYS:HE2	3:B:250:GLN:NE2	2.22	0.54
3:A:116:LYS:HE3	5:A:937:HOH:O	2.07	0.54
3:A:102:ALA:O	3:A:106:LEU:HD22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:312:LEU:HD22	3:B:316:LYS:HE3	1.88	0.54
3:A:121:LYS:HG3	5:A:938:HOH:O	2.08	0.53
3:B:343:THR:HA	3:B:347:THR:HG21	1.92	0.52
1:C:404:DA:H2"	1:C:405:DA:OP2	2.09	0.52
3:B:240:SER:C	3:B:241:LEU:HD12	2.30	0.52
3:B:344:THR:N	3:B:347:THR:CG2	2.70	0.52
1:C:421:DT:H2"	1:C:422:DT:C5'	2.32	0.51
3:A:115:ALA:HB2	3:A:125:VAL:HG21	1.91	0.51
3:B:324:GLU:O	3:B:327:THR:HB	2.10	0.51
1:C:413:DA:H1'	1:C:414:DC:O4'	2.10	0.51
3:A:150:ALA:HA	5:A:835:HOH:O	2.09	0.51
3:A:80:GLU:O	3:A:83:PRO:HD2	2.10	0.51
3:A:57:LYS:HG3	5:A:898:HOH:O	2.10	0.50
3:B:326:CYS:HA	3:B:329:VAL:HG12	1.92	0.50
3:B:320:ASP:HB2	5:B:886:HOH:O	2.11	0.50
1:C:414:DC:H5"	3:B:246:THR:HG22	1.93	0.50
3:A:149:ARG:HG2	3:A:152:LEU:HD11	1.94	0.50
3:A:80:GLU:HG3	5:A:848:HOH:O	2.11	0.50
3:A:113:PRO:HG2	5:A:866:HOH:O	2.12	0.50
3:B:344:THR:HG23	3:B:346:GLU:HB3	1.94	0.50
3:B:264:VAL:HG22	3:B:265:GLY:H	1.75	0.49
3:B:319:PRO:HD2	5:B:886:HOH:O	2.12	0.48
3:A:152:LEU:HD23	3:A:152:LEU:O	2.13	0.48
2:D:505:DA:H2"	2:D:506:DA:H5"	1.94	0.48
3:B:248:LYS:HD3	5:B:893:HOH:O	2.13	0.48
3:A:6:ASN:HD21	3:A:8:GLU:HG3	1.79	0.47
3:B:344:THR:CG2	3:B:347:THR:HG22	2.45	0.47
3:A:150:ALA:HB3	5:A:869:HOH:O	2.15	0.47
3:A:6:ASN:ND2	3:A:8:GLU:H	2.13	0.47
1:C:419:DT:O4	3:B:228:LYS:CE	2.63	0.46
2:D:520:DT:H2'	5:D:139:HOH:O	2.15	0.46
3:B:344:THR:CG2	3:B:346:GLU:HB3	2.46	0.46
2:D:505:DA:C2'	2:D:506:DA:H5"	2.46	0.46
3:A:27:ILE:HG21	3:A:148:VAL:CG2	2.46	0.46
3:B:348:VAL:O	3:B:350:ALA:N	2.47	0.46
5:C:839:HOH:O	2:D:513:DG:N2	2.49	0.45
3:A:148:VAL:C	3:A:150:ALA:N	2.69	0.45
3:A:92:GLN:CG	3:A:103:ASN:HD21	2.25	0.45
2:D:511:DG:H4'	3:B:339:LYS:HD2	1.99	0.45
1:C:418:DG:H5"	3:B:342:LYS:HB2	1.98	0.44
3:B:275:ASP:HB2	3:B:277:ILE:CD1	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:292:GLN:HA	3:B:295:LEU:HD12	1.98	0.44
3:B:282:LYS:HB3	3:B:283:PRO:HD3	1.99	0.44
3:B:281:ILE:HG13	3:B:309:ILE:HG12	1.99	0.44
5:C:857:HOH:O	3:B:229:PRO:HG2	2.17	0.44
1:C:416:DA:H2"	1:C:417:DC:O5'	2.17	0.44
2:D:503:DA:N7	3:B:233:TYR:OH	2.45	0.44
3:B:344:THR:H	3:B:347:THR:HG21	1.76	0.44
3:A:33:TYR:CZ	3:A:38:GLN:HB2	2.53	0.44
3:A:64:VAL:HG22	3:A:65:GLY:N	2.32	0.43
3:B:346:GLU:OE1	3:B:349:ARG:NH1	2.51	0.43
3:B:349:ARG:C	3:B:351:VAL:H	2.22	0.43
2:D:516:DA:H2"	2:D:517:DC:O5'	2.19	0.43
3:B:338:SER:HB3	5:B:817:HOH:O	2.19	0.43
3:B:326:CYS:O	3:B:345:SER:HB3	2.19	0.43
3:A:36:LYS:HD2	3:A:36:LYS:N	2.33	0.43
3:B:282:LYS:CE	3:B:282:LYS:HA	2.32	0.42
2:D:513:DG:H1'	2:D:514:DA:O4'	2.19	0.42
3:B:326:CYS:C	3:B:329:VAL:HG12	2.40	0.42
3:B:248:LYS:HE2	3:B:250:GLN:HG2	2.00	0.42
3:A:152:LEU:O	3:A:153:ASP:CB	2.68	0.42
3:A:148:VAL:O	3:A:150:ALA:N	2.52	0.41
3:B:315:ALA:HB2	3:B:325:VAL:HG21	2.01	0.41
1:C:417:DC:H4'	1:C:417:DC:OP1	2.20	0.41
3:A:33:TYR:CE2	3:A:38:GLN:HB2	2.56	0.41
1:C:403:DA:H2"	1:C:404:DA:O5'	2.21	0.41
3:B:328:TRP:N	3:B:328:TRP:CE3	2.88	0.41
3:B:350:ALA:C	3:B:352:LEU:H	2.23	0.40
3:B:330:ASP:OD1	3:B:344:THR:OG1	2.35	0.40
3:A:146:GLU:O	3:A:149:ARG:HB3	2.22	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
3	A	150/152 (99%)	140 (93%)	9 (6%)	1 (1%)	26 15
3	B	150/152 (99%)	139 (93%)	10 (7%)	1 (1%)	26 15
All	All	300/304 (99%)	279 (93%)	19 (6%)	2 (1%)	26 15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	349	ARG
3	A	149	ARG

5.3.2 Protein sidechains (i)

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
3	A	139/139 (100%)	132 (95%)	7 (5%)	30 20
3	B	139/139 (100%)	126 (91%)	13 (9%)	11 4
All	All	278/278 (100%)	258 (93%)	20 (7%)	18 9

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	50	GLN
3	A	68	ARG
3	A	101	GLN
3	A	106	LEU
3	A	123	LEU
3	A	128	TRP
3	A	152	LEU
3	B	202	ASN
3	B	203	THR
3	B	248	LYS
3	B	268	ARG
3	B	269	ASP
3	B	278	LEU
3	B	282	LYS

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Mol	Chain	Res	Type
3	B	301	GLN
3	B	306	LEU
3	B	312	LEU
3	B	320	ASP
3	B	328	TRP
3	B	347	THR

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

Mol	Chain	Res	Type
3	A	6	ASN
3	A	31	GLN
3	A	50	GLN
3	A	99	GLN
3	A	103	ASN
3	B	202	ASN
3	B	206	ASN
3	B	226	GLN
3	B	250	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.