



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 04:50 PM BST

PDB ID : 6ISF
Title : Structure of 9N-I DNA polymerase incorporation with dT in the active site
Authors : Linwu, S.W.; Maestre-Reyna, M.; Tsai, M.D.; Tu, Y.H.; Chang, W.H.
Deposited on : 2018-11-16
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

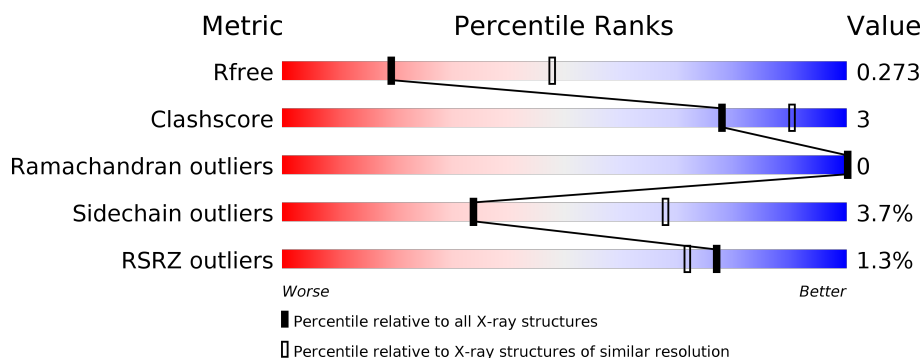
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	783	<div> <div></div> <div>86%10% ..</div> </div>
1	B	783	<div> <div></div> <div>89%7% ..</div> </div>
2	C	15	<div> <div></div> <div>87%13%</div> </div>
2	E	15	<div> <div></div> <div>100%</div> </div>
3	D	18	<div> <div>11%</div> <div>100%</div> </div>
3	F	18	<div> <div></div> <div>89%11%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13186 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 DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	757	Total	C	N	O	S	0	1	0
			5933	3832	1011	1075	15			
1	B	756	Total	C	N	O	S	0	0	0
			5877	3793	996	1073	15			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ALA	ASP	engineered mutation	UNP Q56366
A	143	ALA	GLU	engineered mutation	UNP Q56366
A	485	LEU	ALA	engineered mutation	UNP Q56366
A	776	LEU	-	expression tag	UNP Q56366
A	777	GLU	-	expression tag	UNP Q56366
A	778	HIS	-	expression tag	UNP Q56366
A	779	HIS	-	expression tag	UNP Q56366
A	780	HIS	-	expression tag	UNP Q56366
A	781	HIS	-	expression tag	UNP Q56366
A	782	HIS	-	expression tag	UNP Q56366
A	783	HIS	-	expression tag	UNP Q56366
B	141	ALA	ASP	engineered mutation	UNP Q56366
B	143	ALA	GLU	engineered mutation	UNP Q56366
B	485	LEU	ALA	engineered mutation	UNP Q56366
B	776	LEU	-	expression tag	UNP Q56366
B	777	GLU	-	expression tag	UNP Q56366
B	778	HIS	-	expression tag	UNP Q56366
B	779	HIS	-	expression tag	UNP Q56366
B	780	HIS	-	expression tag	UNP Q56366
B	781	HIS	-	expression tag	UNP Q56366
B	782	HIS	-	expression tag	UNP Q56366
B	783	HIS	-	expression tag	UNP Q56366

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	P	0	0	0
			302	145	53	90	14			
2	E	15	Total	C	N	O	P	0	0	0
			301	145	53	89	14			

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*CP*AP*GP*GP*TP*AP*AP*GP*CP*AP*GP*TP*CP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	18	Total	C	N	O	P	0	0	0
			359	170	69	103	17			
3	F	18	Total	C	N	O	P	0	0	0
			359	170	69	103	17			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	5	Total	Ca	0	0
			5	5		
4	A	2	Total	Ca	0	0
			2	2		

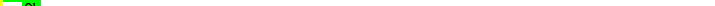

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	28	Total	O	0	0
			28	28		
5	B	19	Total	O	0	0
			19	19		
5	E	1	Total	O	0	0
			1	1		

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.

- Chain A:
-
- 86%
- 10%
- •
- M1 E251 N569 L574 F582 V589 T590 E599 L608 R612 R613 T618 R620 E621 T622 L627 I630 L650 R671 R674 R678 V682 G696 Q736 V737 L738 P739 E742 L745 K746 F748 V757 GLN LYS THR GLN LYS VAL Cys
- T9 E35 I48 V51 R58 V65 K66 K73 R89 P90 V93 P94 K124 G125 L126 M129 L145 E150 E151 T154 I157 L158 D164 T172 I176 E189 V198 K201 D202 K220 K221 R222 C223 E224 Q242
- R265 R266 L275 K285 E293 R307 K317 F327 P328 L333 V344 S347 S348 T349 N365 R375 R381 Y388 N399 R406 T415 H416 Y431 K443 D465 L466 L467 W516 Y520 D540 T541 D542 K557 L564

- Chain B:
-
- 89% 7%
- 0% 100%
- •

- Chain C:  87% 13%
- 

- Molecule 2: DNA (5'-D(P*GP*CP*GP*GP*AP*CP*TP*GP*CP*TP*TP*AP*CP*CP*T)-3')

Chain E:  100%


There are no outlier residues recorded for this chain.

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

Chain D:  11% 100%



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

Chain F:  89% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.09Å 107.36Å 255.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.38 – 2.80 86.64 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.38-2.80) 99.5 (86.64-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.232 , 0.272 0.235 , 0.273	Depositor DCC
R_{free} test set	3128 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13186	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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 [i](#)

5.1 Standard geometry [i](#)

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	A	0.75	1/6076 (0.0%)	0.79	0/8231
1	B	0.75	0/6013	0.80	0/8160
2	C	0.30	0/337	0.73	0/518
2	E	0.32	0/336	0.79	0/517
3	D	0.35	0/403	0.72	0/620
3	F	0.35	0/403	0.74	0/620
All	All	0.72	1/13568 (0.0%)	0.79	0/18666

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	GLU	CD-OE1	6.41	1.32	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5933	0	5682	42	0
1	B	5877	0	5611	29	0
2	C	302	0	171	2	0
2	E	301	0	168	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	359	0	197	0	0
3	F	359	0	197	2	0
4	A	2	0	0	0	0
4	B	5	0	0	0	0
5	A	28	0	0	0	0
5	B	19	0	0	0	0
5	E	1	0	0	0	0
All	All	13186	0	12026	72	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 3.

All (72) 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:B:146:TYR:CB	1:B:292:ALA:HB1	1.84	1.06
1:A:220:LYS:O	1:A:224:GLU:HG3	1.72	0.89
1:A:266[A]:ARG:NH1	1:A:347:SER:O	2.07	0.87
1:B:146:TYR:CB	1:B:292:ALA:CB	2.57	0.81
1:A:265:ARG:NH2	1:A:696:GLY:O	2.12	0.81
1:A:388:TYR:O	1:A:540:ASP:O	2.07	0.71
1:B:643:VAL:HG21	1:B:741:VAL:HG21	1.75	0.69
1:B:713:ARG:NH1	1:B:728:ASP:OD2	2.32	0.62
1:A:151:GLU:O	1:A:154:THR:CG2	2.49	0.61
1:A:93:VAL:HB	1:A:94:PRO:HD3	1.84	0.58
1:B:544:LEU:O	1:B:544:LEU:HD12	2.05	0.57
1:B:457:LEU:O	1:B:461:GLN:HG3	2.05	0.56
1:A:35:GLU:OE1	1:A:66:LYS:HE2	2.05	0.55
1:A:541:THR:O	1:A:542:ASP:OD1	2.24	0.55
1:B:639:ALA:HA	1:B:642:ILE:HD12	1.90	0.54
1:B:45:ASP:OD2	1:B:70:LYS:NZ	2.24	0.54
1:A:630:ILE:HD13	1:A:748:PHE:CE2	2.43	0.54
1:A:157:ILE:HG13	1:A:222:ARG:HG3	1.90	0.53
1:A:145:LEU:HB2	1:A:158:LEU:HD21	1.90	0.52
1:B:58:ARG:NH2	1:B:92:ASP:OD1	2.41	0.52
1:A:415:THR:O	1:A:443:LYS:NZ	2.42	0.51
1:B:407:SER:OG	1:B:487:LYS:NZ	2.43	0.50
1:A:220:LYS:O	1:A:224:GLU:CG	2.53	0.49
1:A:742:GLU:O	1:A:746:LYS:N	2.44	0.49
1:A:151:GLU:O	1:A:154:THR:HG22	2.11	0.49
1:B:643:VAL:CG2	1:B:741:VAL:HG21	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ILE:O	1:A:51:VAL:HG22	2.14	0.48
1:B:591:LYS:HD3	3:F:6:DT:H5''	1.95	0.47
1:A:416:HIS:HE2	1:A:520:TYR:HH	1.63	0.47
1:A:674:LYS:NZ	2:C:-4:DC:OP1	2.47	0.47
1:B:650:LEU:HD13	1:B:655:VAL:HG21	1.97	0.47
1:A:1:MET:HG3	1:A:129:MET:HA	1.98	0.47
1:B:193:ARG:O	1:B:197:VAL:HG23	2.15	0.46
1:B:544:LEU:C	1:B:544:LEU:HD12	2.36	0.46
1:B:157:ILE:HG22	1:B:190:MET:HE1	1.97	0.46
3:F:18:DG:OP2	3:F:18:DG:H4'	2.14	0.46
1:A:172:THR:HG21	1:A:176:ILE:HD12	1.97	0.46
1:A:242:GLN:NE2	1:A:251:GLU:OE2	2.48	0.46
1:B:207:ILE:HD13	1:B:323:GLY:HA3	1.98	0.46
1:B:156:PRO:HA	1:B:222:ARG:HE	1.81	0.46
1:B:157:ILE:N	1:B:187:GLU:OE2	2.47	0.46
1:B:650:LEU:HD23	1:B:733:ILE:HG13	1.98	0.46
1:A:399:ASN:HA	1:A:582:PHE:CZ	2.50	0.46
1:B:101:ARG:NH1	1:B:108:ASP:OD1	2.49	0.46
1:A:73:LYS:HE2	1:A:365:ASN:OD1	2.17	0.45
1:A:738:LEU:HB2	1:A:739:PRO:HD3	2.00	0.44
1:A:333:LEU:HG	1:A:344:VAL:HG11	1.99	0.43
1:A:678:PRO:O	1:A:682:VAL:HG23	2.18	0.43
1:A:612:ARG:NH2	2:C:-1:DA:O4'	2.52	0.43
1:A:164:ASP:OD2	1:A:201:LYS:NZ	2.52	0.43
1:A:333:LEU:HG	1:A:344:VAL:CG1	2.48	0.43
1:A:124:LYS:HB3	1:A:126:LEU:HG	2.01	0.43
1:A:612:ARG:O	1:A:620:LYS:HD3	2.18	0.43
1:A:568:ASN:N	1:A:569:PRO:CD	2.82	0.42
1:B:159:MET:HG3	1:B:172:THR:HB	2.02	0.42
1:A:327:PHE:N	1:A:328:PRO:CD	2.82	0.42
1:B:70:LYS:HE2	1:B:81:GLU:HG2	2.02	0.42
1:A:150:GLU:HG2	1:A:154:THR:HG23	2.02	0.42
1:B:612:ARG:O	1:B:620:LYS:HD3	2.20	0.42
1:B:625:ARG:NH2	1:B:642:ILE:HG23	2.35	0.42
1:A:198:VAL:O	1:A:202:ASP:N	2.52	0.41
1:A:589:VAL:HG12	1:A:590:THR:HG23	2.02	0.41
1:A:58:ARG:O	1:A:58:ARG:CG	2.68	0.41
1:B:400:ILE:CD1	1:B:586:GLY:HA3	2.50	0.41
1:A:89:HIS:CG	1:A:90:PRO:HD2	2.56	0.41
1:B:70:LYS:HE2	1:B:81:GLU:CG	2.51	0.41
1:A:557:LYS:NZ	1:A:599:GLU:OE1	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LEU:HD23	1:A:275:LEU:HA	1.96	0.40
1:B:528:LEU:HD12	1:B:528:LEU:HA	1.96	0.40
1:A:589:VAL:HG21	1:A:608:LEU:HD21	2.04	0.40
1:A:399:ASN:HA	1:A:582:PHE:CE1	2.57	0.40
1:B:638:GLU:HA	1:B:641:ARG:NH1	2.35	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	756/783 (97%)	717 (95%)	39 (5%)	0	100	100
1	B	754/783 (96%)	714 (95%)	40 (5%)	0	100	100
All	All	1510/1566 (96%)	1431 (95%)	79 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	563/675 (83%)	541 (96%)	22 (4%)	32	66
1	B	562/675 (83%)	541 (96%)	21 (4%)	34	68
All	All	1125/1350 (83%)	1082 (96%)	43 (4%)	34	67

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	65	VAL
1	A	124	LYS
1	A	154	THR
1	A	266[A]	ARG
1	A	266[B]	ARG
1	A	285	LYS
1	A	307	ARG
1	A	317	LYS
1	A	349	THR
1	A	375	ARG
1	A	406	ARG
1	A	457	LEU
1	A	516	TRP
1	A	541	THR
1	A	542	ASP
1	A	564	LEU
1	A	574	LEU
1	A	613	ARG
1	A	627	LEU
1	A	671	ARG
1	A	745	LEU
1	B	44	ASP
1	B	81	GLU
1	B	140	PHE
1	B	159	MET
1	B	180	TYR
1	B	201	LYS
1	B	222	ARG
1	B	241	ILE
1	B	329	MET
1	B	363	LYS
1	B	453	LEU
1	B	478	LEU
1	B	484	ARG
1	B	487	LYS
1	B	516	TRP
1	B	542	ASP
1	B	548	ILE
1	B	627	LEU
1	B	648	GLU
1	B	743	ARG

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Mol	Chain	Res	Type
1	B	751	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	91	GLN
1	B	491	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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 [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	757/783 (96%)	0.23	9 (1%) 79 73	34, 62, 96, 119	3 (0%)
1	B	756/783 (96%)	0.27	10 (1%) 77 72	36, 62, 104, 141	1 (0%)
2	C	15/15 (100%)	-0.04	0 100 100	33, 47, 60, 66	0
2	E	15/15 (100%)	0.18	0 100 100	34, 40, 58, 61	0
3	D	18/18 (100%)	0.46	2 (11%) 5 3	34, 46, 80, 110	2 (11%)
3	F	18/18 (100%)	0.11	0 100 100	34, 48, 67, 89	0
All	All	1579/1632 (96%)	0.25	21 (1%) 77 72	33, 62, 101, 141	6 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	292	ALA	3.4
1	B	299	TRP	2.9
1	A	51	VAL	2.8
3	D	1	DA	2.7
1	A	736	GLN	2.7
3	D	18	DG	2.7
1	B	541	THR	2.5
1	A	650	LEU	2.5
1	B	153	GLY	2.4
1	B	587	PHE	2.4
1	B	586	GLY	2.3
1	B	149	GLY	2.3
1	A	293	GLU	2.3
1	B	750	TYR	2.3
1	A	618	ILE	2.2
1	A	381	ARG	2.1
1	A	622	THR	2.1
1	A	455	ASP	2.1
1	B	152	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	431	TYR	2.1
1	B	246	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [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(\AA^2)	Q<0.9
4	CA	B	801	1/1	0.72	0.15	85,85,85,85	0
4	CA	B	802	1/1	0.77	0.14	104,104,104,104	0
4	CA	A	802	1/1	0.85	0.19	101,101,101,101	0
4	CA	B	804	1/1	0.86	0.08	90,90,90,90	0
4	CA	B	805	1/1	0.92	0.17	75,75,75,75	0
4	CA	A	801	1/1	0.92	0.09	80,80,80,80	0
4	CA	B	803	1/1	0.97	0.09	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.