



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 11:01 PM GMT

PDB ID : 5EI9
Title : Human PRDM9 allele-A ZnF Domain with Associated Recombination Hotspot DNA Sequence I
Authors : Patel, A.; Horton, J.R.; Wilson, G.G.; Zhang, X.; Cheng, X.
Deposited on : 2015-10-29
Resolution : 1.92 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

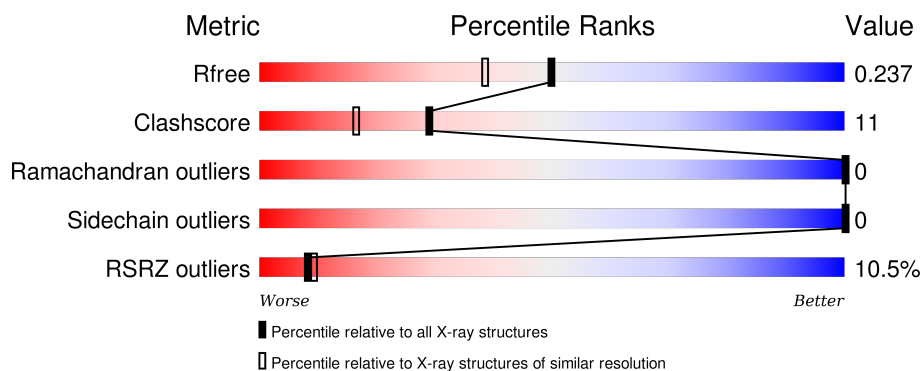
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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}	91344	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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.

Mol	Chain	Length	Quality of chain
1	A	21	
1	C	21	
2	E	144	
2	F	144	
3	B	21	

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Mol	Chain	Length	Quality of chain
3	D	21	<div> <div></div> <div>5%</div> <div>71%</div> <div>24%</div> <div>5%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3722 atoms, of which 16 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 DNA (5'-D(*AP*TP*CP*CP*AP*CP*GP*TP*GP*GP*CP*TP*AP*GP*GP*GP*AP*GP*GP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	P	0	0	0
			431	204	84	123	20			
1	C	21	Total	C	N	O	P	0	0	0
			431	204	84	123	20			

- Molecule 2 is a protein called Histone-lysine N-methyltransferase PRDM9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	F	110	Total	C	H	N	O	S	0	0	0
			912	546	8	197	153	8			
2	E	111	Total	C	H	N	O	S	0	1	0
			925	554	8	201	154	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	714	GLY	-	expression tag	UNP Q9NQV7
F	715	SER	-	expression tag	UNP Q9NQV7
E	714	GLY	-	expression tag	UNP Q9NQV7
E	715	SER	-	expression tag	UNP Q9NQV7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	21	Total	C	N	O	P	0	0	0
			423	202	77	124	20			
3	D	21	Total	C	N	O	P	0	0	0
			424	202	77	125	20			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	4	Total 4	Zn 4	0	0
4	E	4	Total 4	Zn 4	0	0

- Molecule 5 is water.

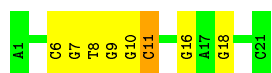
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	33	Total 33	O 33	0	0
5	F	31	Total 31	O 31	0	0
5	E	52	Total 52	O 52	0	0
5	C	18	Total 18	O 18	0	0
5	B	24	Total 24	O 24	0	0
5	D	10	Total 10	O 10	0	0

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 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.

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

Chain A: 



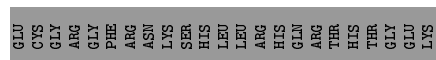
- Molecule 1: DNA (5'-D(*AP*TP*CP*CP*AP*CP*GP*TP*GP*GP*CP*TP*AP*GP*GP*GP*AP*GP*GP*CP*C)-3')

Chain C: 



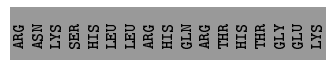
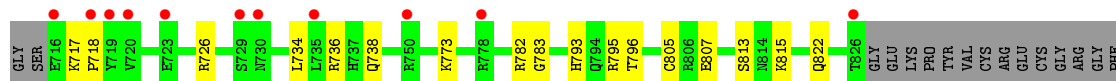
- Molecule 2: Histone-lysine N-methyltransferase PRDM9

Chain F: 

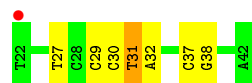


- Molecule 2: Histone-lysine N-methyltransferase PRDM9

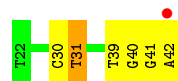
Chain E: 



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.33Å 55.74Å 76.04Å 89.85° 75.50° 86.58°	Depositor
Resolution (Å)	32.98 – 1.92 32.98 – 1.92	Depositor EDS
% Data completeness (in resolution range)	97.5 (32.98-1.92) 88.9 (32.98-1.92)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 1.92Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.214 , 0.237 0.214 , 0.237	Depositor DCC
R_{free} test set	3958 reflections (3.79%)	DCC
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.0	EDS
Estimated twinning fraction	0.016 for -h,-k,-h+l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 52370 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3722	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.58 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.4339e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	1.00	0/484	1.16	2/746 (0.3%)
1	C	0.87	0/484	1.00	3/746 (0.4%)
2	E	0.50	0/942	0.64	0/1256
2	F	0.47	0/926	0.58	0/1235
3	B	0.92	2/473 (0.4%)	0.98	2/728 (0.3%)
3	D	0.80	1/474 (0.2%)	0.93	0/729
All	All	0.72	3/3783 (0.1%)	0.86	7/5440 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	31	DT	C3'-O3'	-6.18	1.35	1.44
3	B	27	DT	C3'-O3'	-5.11	1.37	1.44
3	B	31	DT	C3'-O3'	-5.07	1.37	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	DA	O4'-C1'-N9	5.96	112.17	108.00
1	A	11	DC	C1'-O4'-C4'	-5.94	104.16	110.10
1	A	16	DG	O5'-P-OP2	-5.23	100.99	105.70
1	C	11	DC	O4'-C4'-C3'	-5.15	102.44	104.50
1	C	11	DC	C1'-O4'-C4'	-5.13	104.97	110.10
3	B	29	DC	O4'-C1'-N1	5.04	111.53	108.00
3	B	31	DT	N3-C4-O4	5.04	122.92	119.90

There are no chirality outliers.

There are no planarity outliers.

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	431	0	236	15	0
1	C	431	0	236	17	0
2	E	917	8	880	18	0
2	F	904	8	865	20	0
3	B	423	0	234	6	0
3	D	424	0	237	4	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
5	A	33	0	0	1	0
5	B	24	0	0	0	0
5	C	18	0	0	0	0
5	D	10	0	0	0	0
5	E	52	0	0	2	0
5	F	31	0	0	0	0
All	All	3706	16	2688	69	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 11.

All (69) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:DG:H2''	1:C:15:DG:H5'	1.43	1.01
1:C:14:DG:H5''	1:C:14:DG:H8	1.33	0.92
1:C:14:DG:H5''	1:C:14:DG:C8	2.11	0.86
2:E:783:GLY:O	5:E:1101:HOH:O	2.01	0.79
1:A:11:DC:OP1	2:E:782:ARG:NH2	2.17	0.78
1:A:6:DC:H2'	1:A:7:DG:C8	2.21	0.74
1:C:14:DG:H2''	1:C:15:DG:C5'	2.21	0.69
2:E:734:LEU:O	2:E:738:GLN:HG2	1.94	0.67
1:A:18:DG:N7	2:E:736:ARG:NH1	2.41	0.67
2:F:749:CYS:HB3	2:F:752:CYS:HB2	1.78	0.66
1:A:18:DG:O6	2:E:736:ARG:NH2	2.21	0.66
2:E:717:LYS:CB	2:E:718:PRO:HD2	2.28	0.63
2:F:765:HIS:O	2:F:766:GLN:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:815:LYS:HE2	3:B:31:DT:OP2	2.02	0.59
2:F:821:HIS:ND1	1:C:8:DT:OP1	2.35	0.59
1:A:10:DG:H3'	2:E:796:THR:HG21	1.86	0.58
2:F:756:PHE:HE2	1:C:14:DG:H5'	1.68	0.58
3:D:41:DG:H2'	3:D:42:DA:O4'	2.04	0.57
1:A:9:DG:H4'	1:A:10:DG:OP1	2.05	0.57
1:A:6:DC:H2''	1:A:7:DG:O5'	2.06	0.56
2:E:822:GLN:NE2	5:E:1103:HOH:O	2.38	0.55
2:F:752:CYS:SG	2:F:765:HIS:NE2	2.80	0.55
1:C:3:DC:H2''	1:C:4:DC:H5'	1.89	0.54
3:D:30:DC:H2''	3:D:31:DT:H5'	1.89	0.54
1:A:6:DC:H2'	1:A:7:DG:H8	1.73	0.53
3:D:39:DT:H2''	3:D:40:DG:C8	2.43	0.53
5:A:107:HOH:O	2:E:773:LYS:HE2	2.08	0.53
1:A:11:DC:OP2	2:E:796:THR:HG21	2.10	0.52
3:B:30:DC:H2''	3:B:31:DT:H5'	1.90	0.52
1:C:14:DG:H2'	1:C:15:DG:C8	2.45	0.52
1:C:14:DG:C2'	1:C:15:DG:H5'	2.30	0.51
2:F:752:CYS:CB	2:F:754:ARG:H	2.24	0.50
2:E:717:LYS:CB	2:E:718:PRO:CD	2.90	0.50
1:A:6:DC:H2''	1:A:7:DG:C5'	2.42	0.49
2:F:744:GLU:OE2	2:F:746:PRO:HG3	2.12	0.49
1:A:6:DC:H4'	1:A:7:DG:OP1	2.13	0.49
2:F:765:HIS:CD2	2:F:766:GLN:N	2.81	0.48
2:F:765:HIS:CD2	2:F:766:GLN:H	2.31	0.48
2:F:752:CYS:HB3	2:F:754:ARG:HG3	1.95	0.48
2:F:743:GLY:HA2	2:F:757:ARG:HH21	1.78	0.48
1:C:14:DG:H2'	1:C:15:DG:H8	1.77	0.48
1:A:9:DG:H2''	1:A:10:DG:O5'	2.14	0.47
3:B:30:DC:C2'	3:B:31:DT:H5'	2.45	0.47
2:F:765:HIS:ND1	1:C:14:DG:OP1	2.48	0.47
2:F:767:ARG:HA	2:F:770:THR:OG1	2.15	0.47
3:B:37:DC:H2''	3:B:38:DG:C8	2.50	0.46
1:C:1:DA:H4'	1:C:2:DT:O5'	2.16	0.46
1:C:11:DC:H2''	1:C:12:DT:C5'	2.46	0.45
2:F:801:LYS:HA	2:F:813:SER:HA	1.97	0.45
2:E:726[B]:ARG:NH1	2:E:726[B]:ARG:HG3	2.32	0.45
1:A:7:DG:C2'	1:A:8:DT:H71	2.46	0.45
2:F:752:CYS:HB3	2:F:754:ARG:H	1.82	0.45
3:D:40:DG:H2'	3:D:41:DG:C8	2.52	0.44
2:F:796:THR:HG21	1:C:10:DG:H3'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:795:ARG:HD2	2:E:813:SER:O	2.17	0.43
3:B:31:DT:H2''	3:B:32:DA:C8	2.53	0.43
2:E:726[B]:ARG:HG3	2:E:726[B]:ARG:HH11	1.83	0.43
1:A:7:DG:H2'	1:A:8:DT:H71	2.00	0.43
1:C:14:DG:C2'	1:C:15:DG:C5'	2.93	0.42
2:F:759:LYS:O	2:F:762:LEU:HB3	2.19	0.42
2:F:765:HIS:O	2:F:766:GLN:CB	2.65	0.42
2:E:805:CYS:SG	2:E:807:GLU:HB3	2.58	0.42
2:F:718:PRO:HG2	2:F:719:TYR:CD2	2.54	0.42
2:F:764:ARG:O	2:F:767:ARG:HB2	2.21	0.41
1:A:10:DG:H3'	2:E:796:THR:CG2	2.50	0.41
2:E:793:HIS:O	2:E:796:THR:HG23	2.21	0.41
3:B:37:DC:H2''	3:B:38:DG:H8	1.85	0.40
1:C:2:DT:H2''	1:C:3:DC:O5'	2.20	0.40
1:C:11:DC:H2''	1:C:12:DT:H5'	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	110/144 (76%)	108 (98%)	2 (2%)	0	100	100
2	F	108/144 (75%)	105 (97%)	3 (3%)	0	100	100
All	All	218/288 (76%)	213 (98%)	5 (2%)	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	
2	E	98/128 (77%)	98 (100%)	0	100	100
2	F	97/128 (76%)	97 (100%)	0	100	100
All	All	195/256 (76%)	195 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 8 ligands modelled in this entry, 8 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 [i](#)

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	21/21 (100%)	0.77	0 100 100	34, 51, 83, 87	0
1	C	21/21 (100%)	0.93	1 (4%) 34 38	42, 54, 99, 100	0
2	E	111/144 (77%)	0.79	11 (9%) 9 11	31, 43, 71, 78	0
2	F	110/144 (76%)	0.92	18 (16%) 2 3	35, 50, 74, 82	0
3	B	21/21 (100%)	0.61	1 (4%) 34 38	38, 55, 85, 88	0
3	D	21/21 (100%)	0.63	1 (4%) 34 38	46, 65, 97, 101	0
All	All	305/372 (81%)	0.82	32 (10%) 8 9	31, 49, 83, 101	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	826	THR	8.3
2	F	753	GLY	5.5
2	F	826	THR	5.2
2	F	750	ARG	5.0
2	E	719	TYR	4.7
2	E	729	SER	4.5
2	E	750	ARG	4.4
2	E	716	GLU	4.3
2	F	718	PRO	4.2
1	C	1	DA	4.1
2	E	718	PRO	4.1
2	F	770	THR	3.7
2	E	720	VAL	3.4
2	F	717	LYS	3.4
2	F	771	GLY	3.4
2	E	778	ARG	3.2
2	F	752	CYS	3.2
2	F	823	ARG	3.0
2	F	754	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	723	GLU	2.9
2	F	719	TYR	2.8
2	E	730	ASN	2.8
2	F	768	THR	2.7
2	E	735	LEU	2.5
2	F	729	SER	2.5
3	D	42	DA	2.4
2	F	778	ARG	2.3
2	F	813	SER	2.3
2	F	751	GLU	2.2
3	B	22	DT	2.2
2	F	742	THR	2.1
2	F	825	HIS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	ZN	E	1003	1/1	0.96	0.11	0.08	37,37,37,37	0
4	ZN	E	1004	1/1	0.96	0.11	-0.50	42,42,42,42	0
4	ZN	F	1001	1/1	0.99	0.08	-0.53	38,38,38,38	0
4	ZN	E	1002	1/1	0.98	0.06	-1.08	41,41,41,41	0
4	ZN	F	1004	1/1	0.95	0.07	-1.33	54,54,54,54	0
4	ZN	E	1001	1/1	0.99	0.06	-1.46	49,49,49,49	0
4	ZN	F	1003	1/1	0.97	0.07	-1.63	41,41,41,41	0
4	ZN	F	1002	1/1	0.86	0.05	-2.54	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.