wwPDB X-ray Structure Validation Summary Report (i)

May 9, 2024 – 12:28 AM EDT

PDB ID	:	3EI4
Title	:	Structure of the hsDDB1-hsDDB2 complex
Authors	:	Scrima, A.; Pavletich, N.P.; Thoma, N.H.
Deposited on	:	2008-09-15
Resolution	:	3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

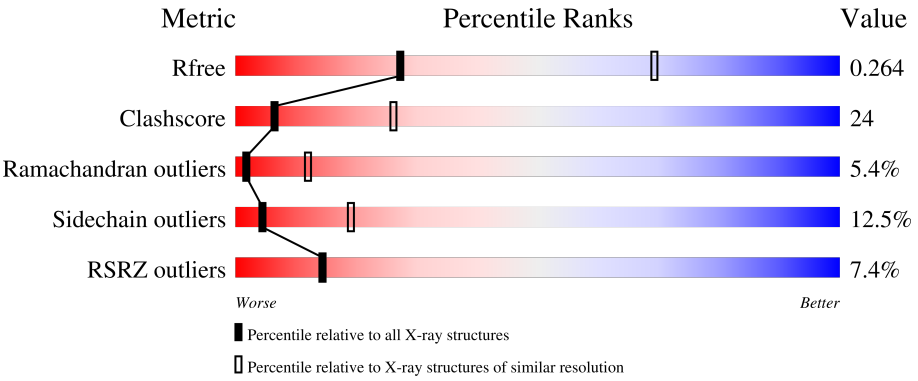
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	1158	8% 55% 36% 7%
1	C	1158	7% 56% 36% 7%
1	E	1158	9% 54% 37% 6%
2	B	436	3% 38% 37% 8% 16%
2	D	436	4% 40% 34% 9% 16%

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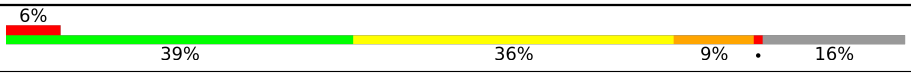
Mol	Chain	Length	Quality of chain
2	F	436	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 35241 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 damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1140	Total	C	N	O	S	0	0	0
			8861	5610	1493	1709	49			
1	C	1140	Total	C	N	O	S	0	0	0
			8861	5610	1493	1709	49			
1	E	1140	Total	C	N	O	S	0	0	0
			8861	5610	1493	1709	49			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP Q16531
A	-16	HIS	-	expression tag	UNP Q16531
A	-15	HIS	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	HIS	-	expression tag	UNP Q16531
A	-12	HIS	-	expression tag	UNP Q16531
A	-11	HIS	-	expression tag	UNP Q16531
A	-10	ARG	-	expression tag	UNP Q16531
A	-9	ARG	-	expression tag	UNP Q16531
A	-8	LEU	-	expression tag	UNP Q16531
A	-7	VAL	-	expression tag	UNP Q16531
A	-6	PRO	-	expression tag	UNP Q16531
A	-5	ARG	-	expression tag	UNP Q16531
A	-4	GLY	-	expression tag	UNP Q16531
A	-3	SER	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531
A	422	TYR	ASP	SEE REMARK 999	UNP Q16531
A	898	ASP	GLU	SEE REMARK 999	UNP Q16531
A	899	VAL	LEU	SEE REMARK 999	UNP Q16531
C	-17	MET	-	expression tag	UNP Q16531
C	-16	HIS	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	HIS	-	expression tag	UNP Q16531
C	-14	HIS	-	expression tag	UNP Q16531
C	-13	HIS	-	expression tag	UNP Q16531
C	-12	HIS	-	expression tag	UNP Q16531
C	-11	HIS	-	expression tag	UNP Q16531
C	-10	ARG	-	expression tag	UNP Q16531
C	-9	ARG	-	expression tag	UNP Q16531
C	-8	LEU	-	expression tag	UNP Q16531
C	-7	VAL	-	expression tag	UNP Q16531
C	-6	PRO	-	expression tag	UNP Q16531
C	-5	ARG	-	expression tag	UNP Q16531
C	-4	GLY	-	expression tag	UNP Q16531
C	-3	SER	-	expression tag	UNP Q16531
C	-2	GLY	-	expression tag	UNP Q16531
C	-1	GLY	-	expression tag	UNP Q16531
C	0	ARG	-	expression tag	UNP Q16531
C	422	TYR	ASP	SEE REMARK 999	UNP Q16531
C	898	ASP	GLU	SEE REMARK 999	UNP Q16531
C	899	VAL	LEU	SEE REMARK 999	UNP Q16531
E	-17	MET	-	expression tag	UNP Q16531
E	-16	HIS	-	expression tag	UNP Q16531
E	-15	HIS	-	expression tag	UNP Q16531
E	-14	HIS	-	expression tag	UNP Q16531
E	-13	HIS	-	expression tag	UNP Q16531
E	-12	HIS	-	expression tag	UNP Q16531
E	-11	HIS	-	expression tag	UNP Q16531
E	-10	ARG	-	expression tag	UNP Q16531
E	-9	ARG	-	expression tag	UNP Q16531
E	-8	LEU	-	expression tag	UNP Q16531
E	-7	VAL	-	expression tag	UNP Q16531
E	-6	PRO	-	expression tag	UNP Q16531
E	-5	ARG	-	expression tag	UNP Q16531
E	-4	GLY	-	expression tag	UNP Q16531
E	-3	SER	-	expression tag	UNP Q16531
E	-2	GLY	-	expression tag	UNP Q16531
E	-1	GLY	-	expression tag	UNP Q16531
E	0	ARG	-	expression tag	UNP Q16531
E	422	TYR	ASP	SEE REMARK 999	UNP Q16531
E	898	ASP	GLU	SEE REMARK 999	UNP Q16531
E	899	VAL	LEU	SEE REMARK 999	UNP Q16531

- Molecule 2 is a protein called DNA damage-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	368	Total	C	N	O	S	0	0	0
			2886	1841	513	515	17			
2	D	368	Total	C	N	O	S	0	0	0
			2886	1841	513	515	17			
2	F	368	Total	C	N	O	S	0	0	0
			2886	1841	513	515	17			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	MET	-	expression tag	UNP Q92466
B	-7	HIS	-	expression tag	UNP Q92466
B	-6	HIS	-	expression tag	UNP Q92466
B	-5	HIS	-	expression tag	UNP Q92466
B	-4	HIS	-	expression tag	UNP Q92466
B	-3	HIS	-	expression tag	UNP Q92466
B	-2	HIS	-	expression tag	UNP Q92466
B	-1	ARG	-	expression tag	UNP Q92466
B	0	ARG	-	expression tag	UNP Q92466
B	1	LEU	-	expression tag	UNP Q92466
B	2	VAL	-	expression tag	UNP Q92466
B	3	PRO	-	expression tag	UNP Q92466
B	4	ARG	-	expression tag	UNP Q92466
B	5	GLY	-	expression tag	UNP Q92466
B	6	SER	-	expression tag	UNP Q92466
B	7	GLY	-	expression tag	UNP Q92466
B	8	GLY	-	expression tag	UNP Q92466
B	9	ARG	-	expression tag	UNP Q92466
D	-8	MET	-	expression tag	UNP Q92466
D	-7	HIS	-	expression tag	UNP Q92466
D	-6	HIS	-	expression tag	UNP Q92466
D	-5	HIS	-	expression tag	UNP Q92466
D	-4	HIS	-	expression tag	UNP Q92466
D	-3	HIS	-	expression tag	UNP Q92466
D	-2	HIS	-	expression tag	UNP Q92466
D	-1	ARG	-	expression tag	UNP Q92466
D	0	ARG	-	expression tag	UNP Q92466
D	1	LEU	-	expression tag	UNP Q92466
D	2	VAL	-	expression tag	UNP Q92466
D	3	PRO	-	expression tag	UNP Q92466
D	4	ARG	-	expression tag	UNP Q92466
D	5	GLY	-	expression tag	UNP Q92466
D	6	SER	-	expression tag	UNP Q92466

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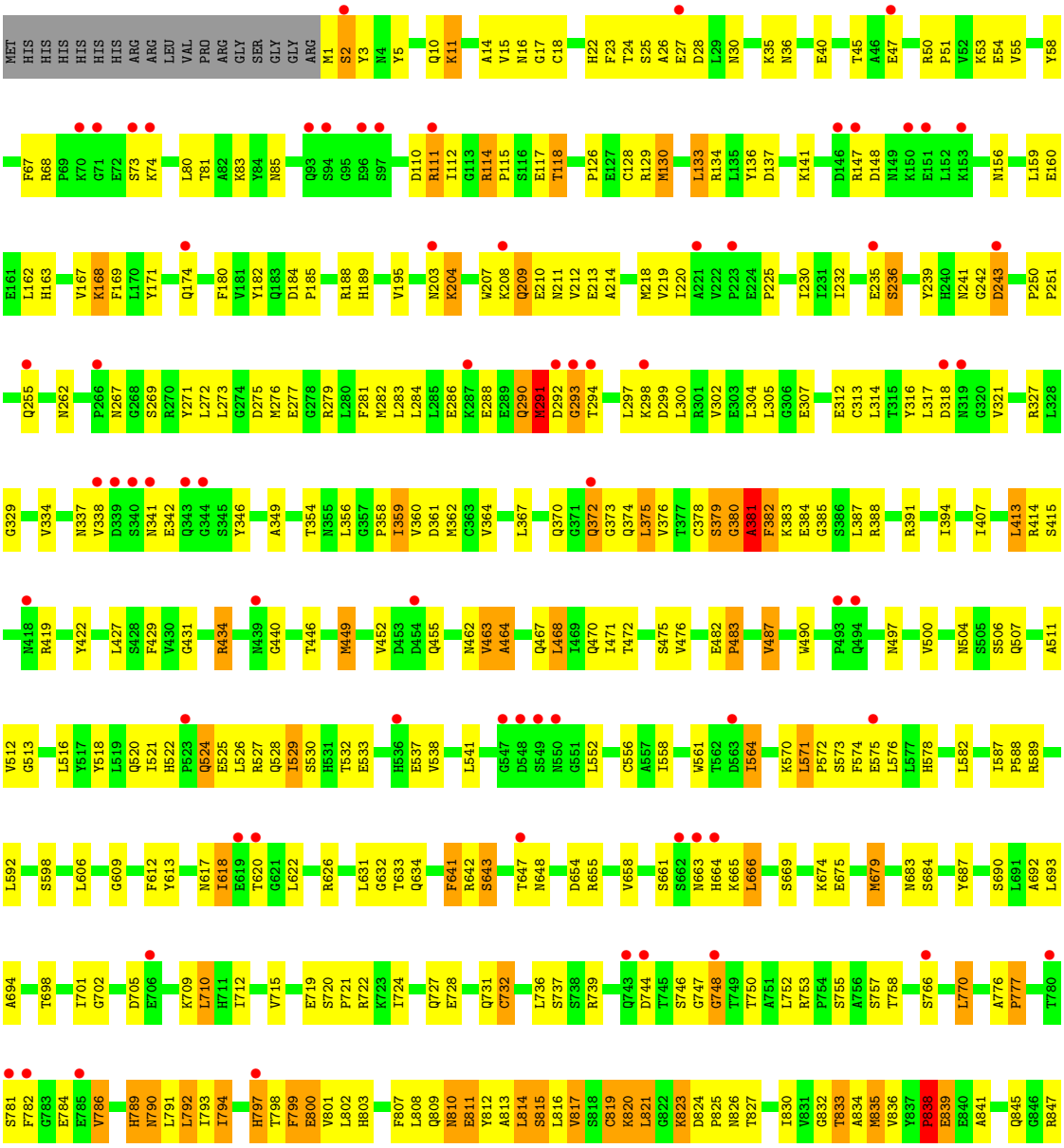
Chain	Residue	Modelled	Actual	Comment	Reference
D	7	GLY	-	expression tag	UNP Q92466
D	8	GLY	-	expression tag	UNP Q92466
D	9	ARG	-	expression tag	UNP Q92466
F	-8	MET	-	expression tag	UNP Q92466
F	-7	HIS	-	expression tag	UNP Q92466
F	-6	HIS	-	expression tag	UNP Q92466
F	-5	HIS	-	expression tag	UNP Q92466
F	-4	HIS	-	expression tag	UNP Q92466
F	-3	HIS	-	expression tag	UNP Q92466
F	-2	HIS	-	expression tag	UNP Q92466
F	-1	ARG	-	expression tag	UNP Q92466
F	0	ARG	-	expression tag	UNP Q92466
F	1	LEU	-	expression tag	UNP Q92466
F	2	VAL	-	expression tag	UNP Q92466
F	3	PRO	-	expression tag	UNP Q92466
F	4	ARG	-	expression tag	UNP Q92466
F	5	GLY	-	expression tag	UNP Q92466
F	6	SER	-	expression tag	UNP Q92466
F	7	GLY	-	expression tag	UNP Q92466
F	8	GLY	-	expression tag	UNP Q92466
F	9	ARG	-	expression tag	UNP Q92466

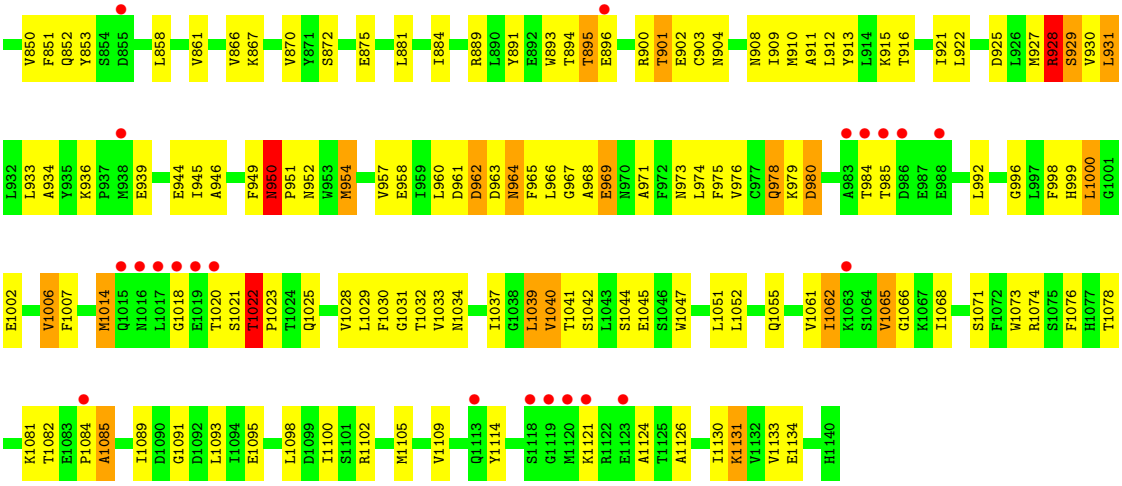
3 Residue-property plots (i)

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 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 damage-binding protein 1

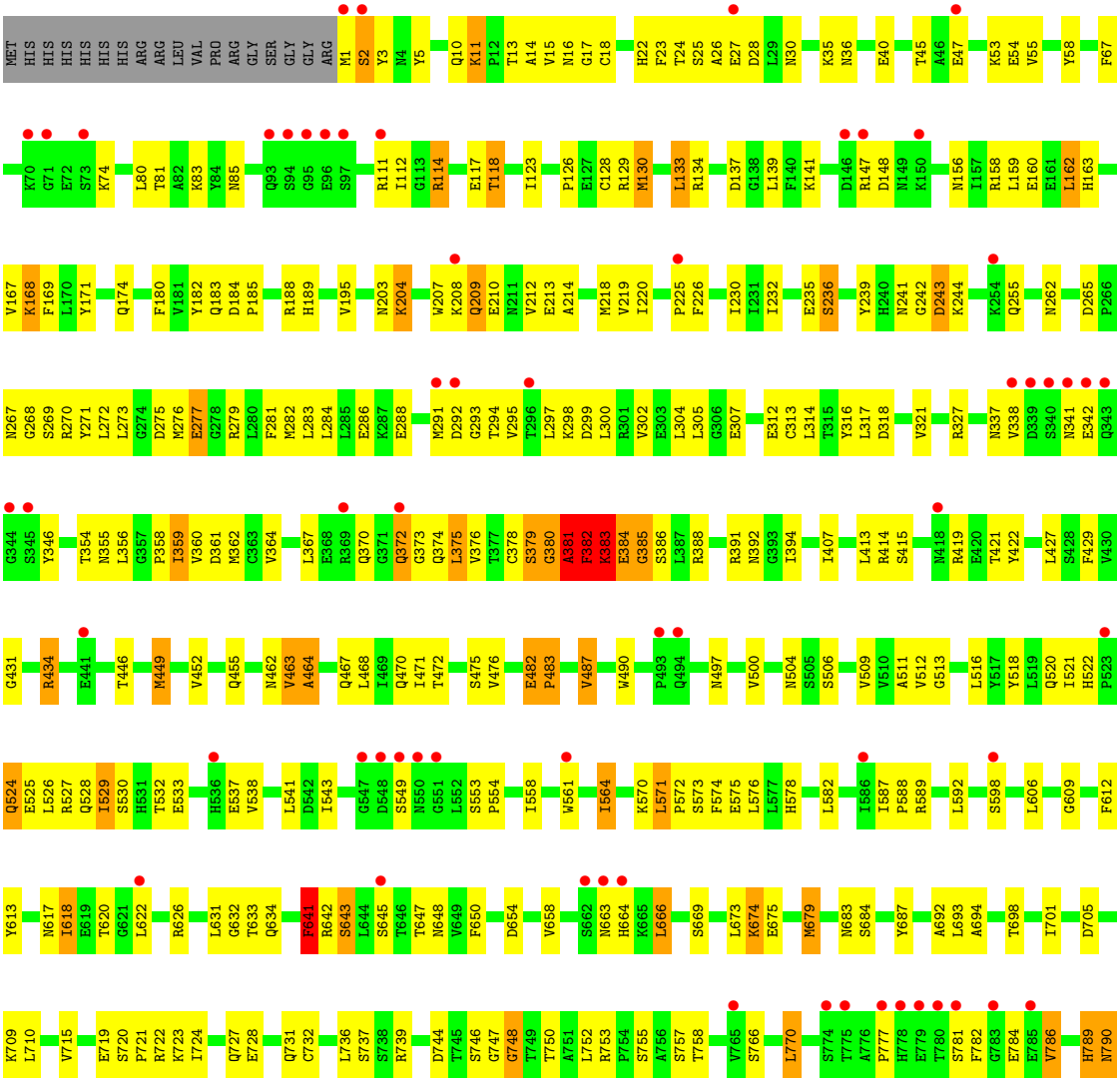
Chain A:

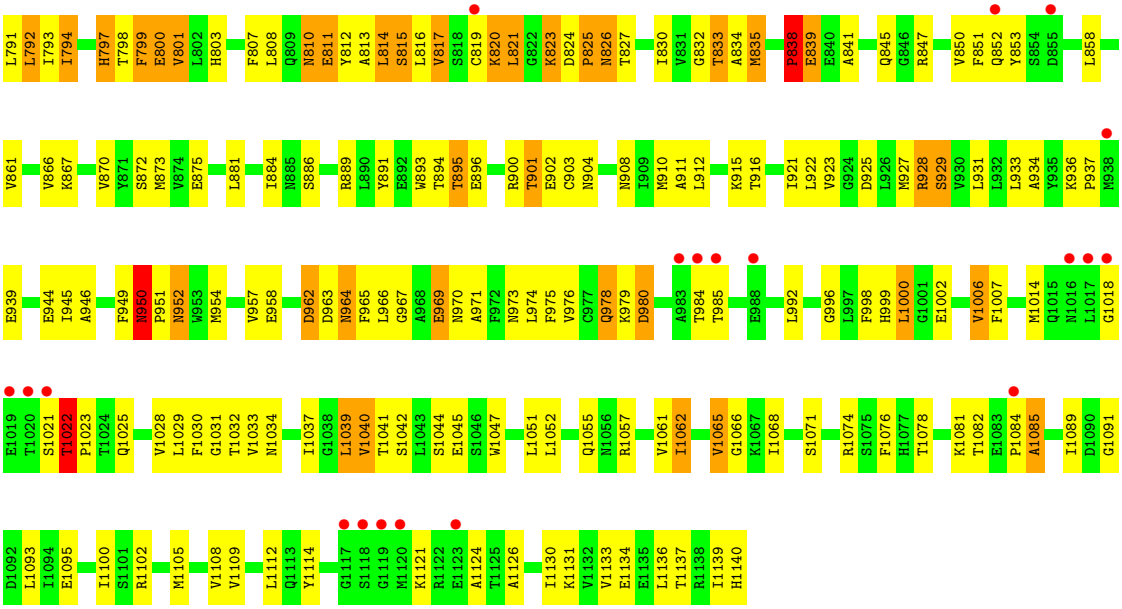




• Molecule 1: DNA damage-binding protein 1

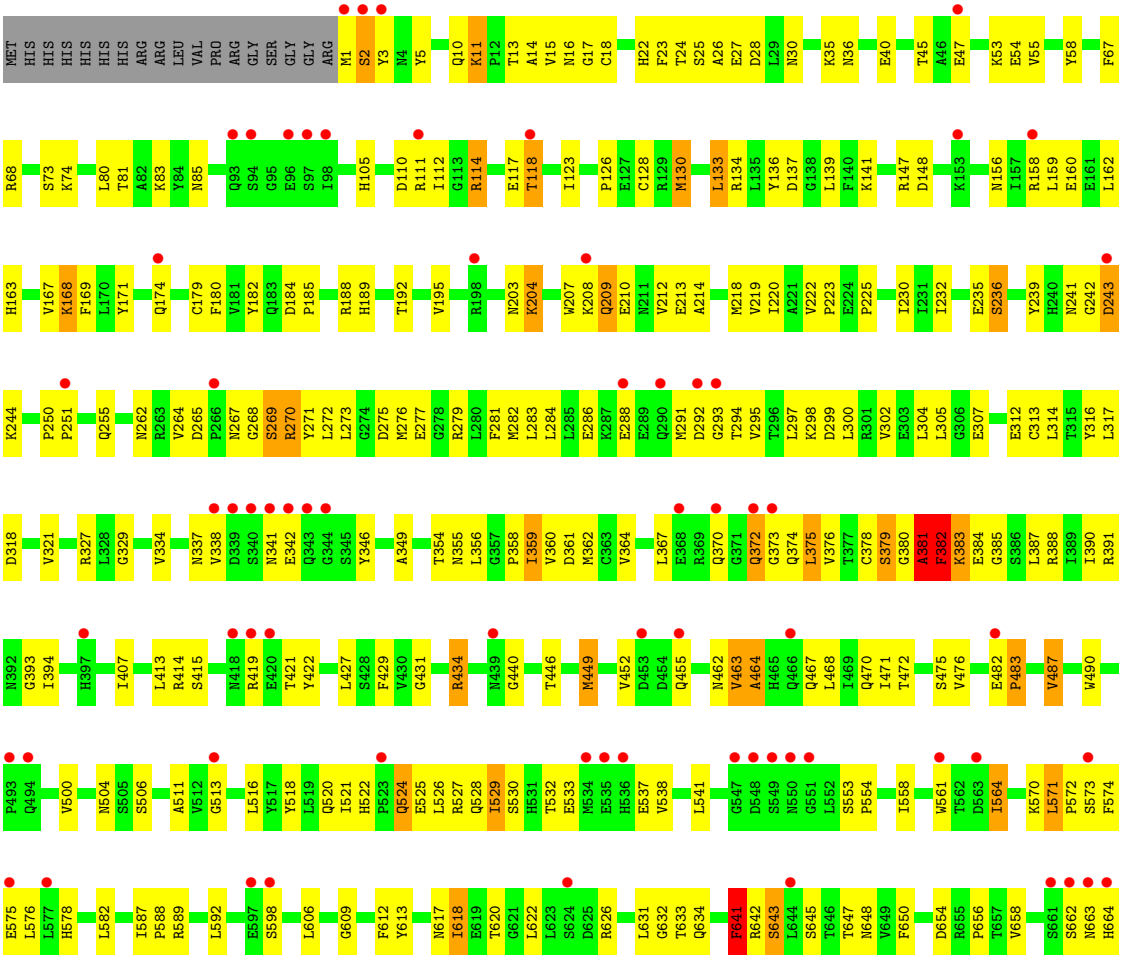
Chain C:

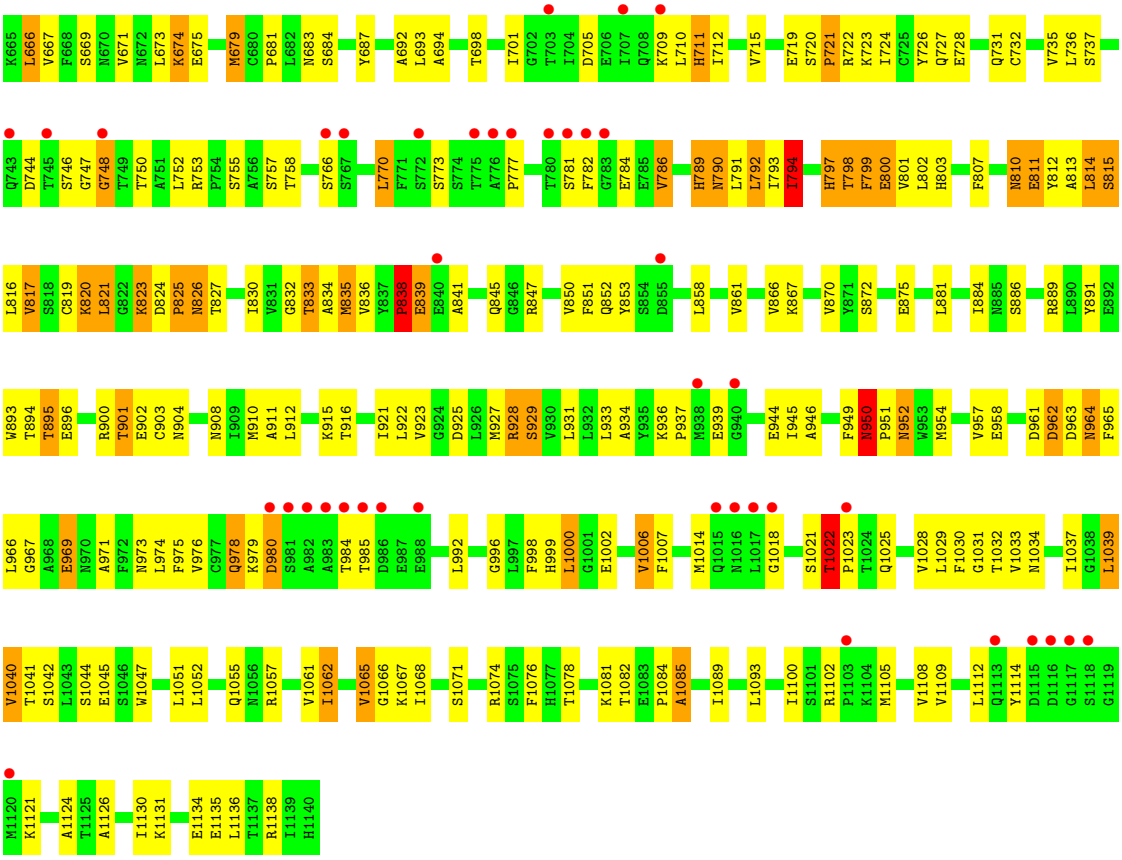




• Molecule 1: DNA damage-binding protein 1

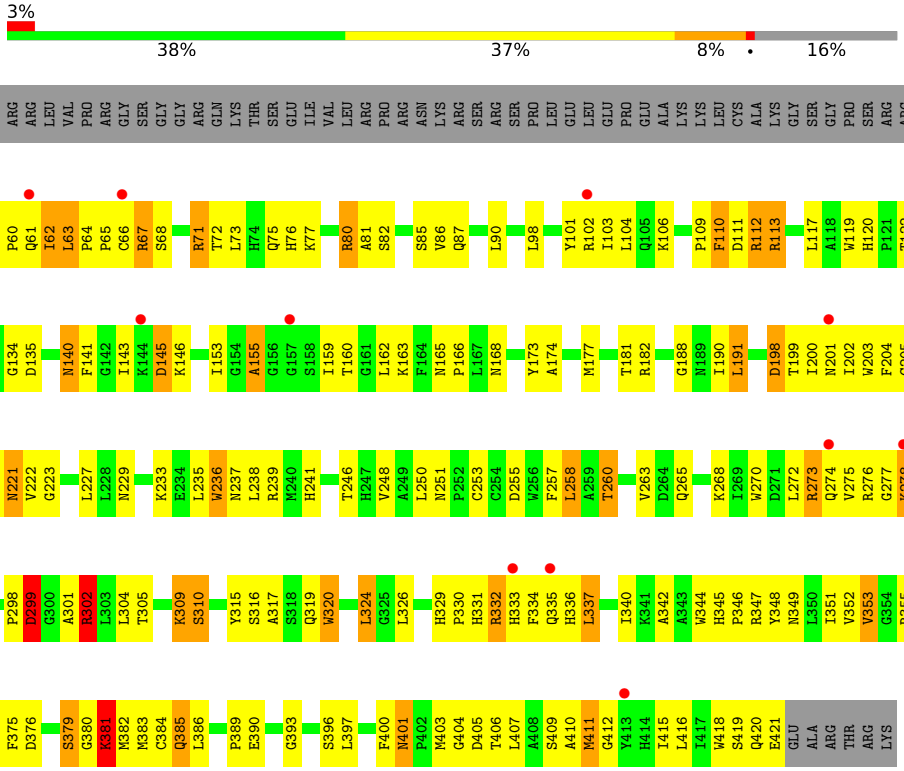
Chain E:





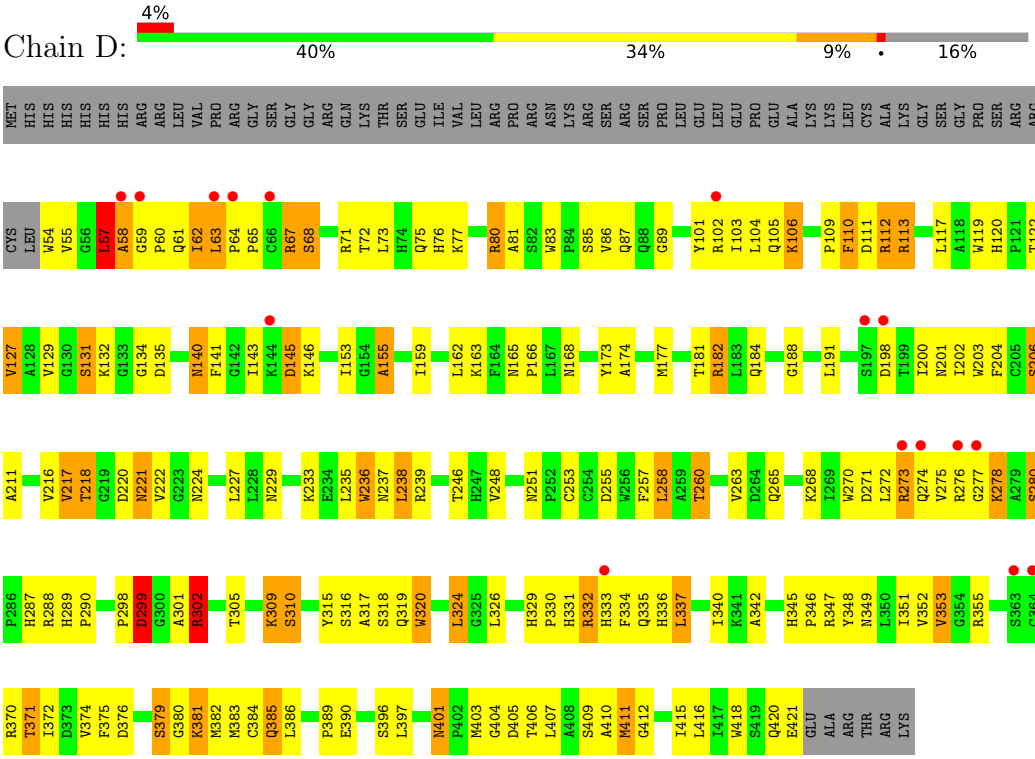
• Molecule 2: DNA damage-binding protein 2

Chain B:



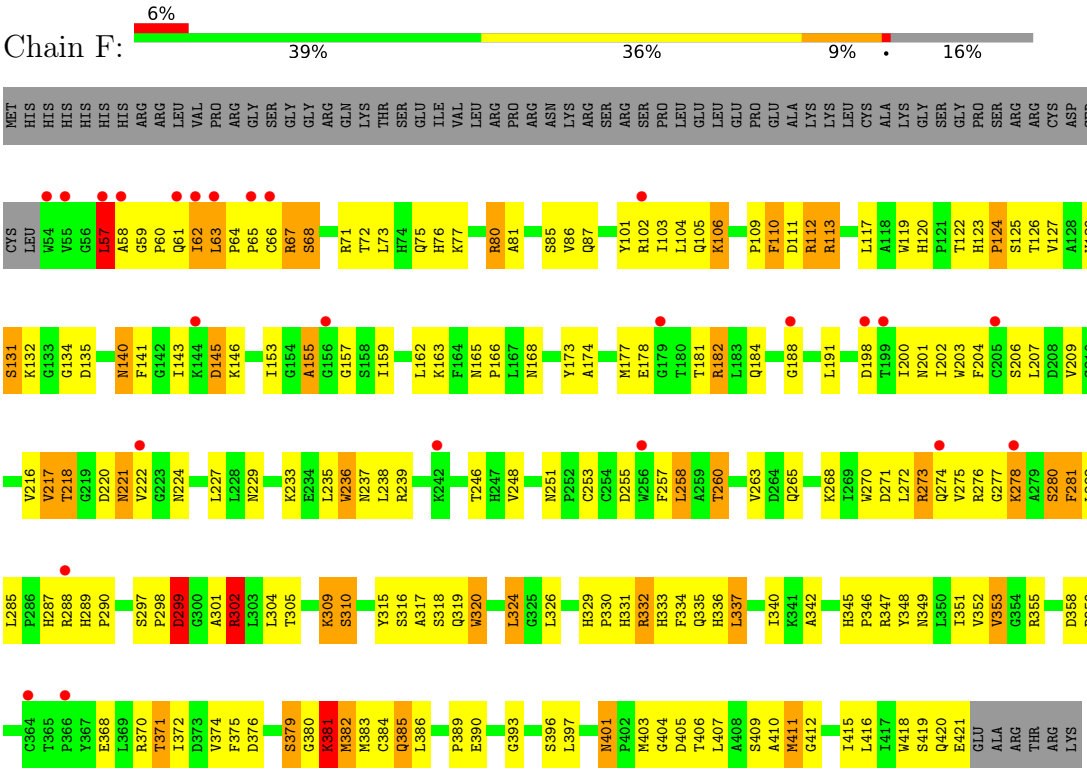
• Molecule 2: DNA damage-binding protein 2

Chain D:



• Molecule 2: DNA damage-binding protein 2

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	268.50Å 268.50Å 471.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 3.30 19.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	80.2 (25.00-3.30) 86.8 (19.98-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.4.0062	Depositor
R, R_{free}	0.254 , 0.288 0.266 , 0.264	Depositor DCC
R_{free} test set	1368 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 83.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	35241	wwPDB-VP
Average B, all atoms (Å^2)	63.0	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 33.92 % 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 7.4042e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.59	2/9026 (0.0%)	0.72	2/12239 (0.0%)
1	C	0.50	1/9026 (0.0%)	0.68	2/12239 (0.0%)
1	E	0.51	2/9026 (0.0%)	0.69	5/12239 (0.0%)
2	B	0.65	0/2970	0.78	4/4042 (0.1%)
2	D	0.57	0/2970	0.74	2/4042 (0.0%)
2	F	0.55	0/2970	0.73	2/4042 (0.0%)
All	All	0.55	5/35988 (0.0%)	0.71	17/48843 (0.0%)

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	A	0	6
1	C	0	7
1	E	0	5
2	B	0	2
2	D	0	1
2	F	0	2
All	All	0	23

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	381	ALA	CA-CB	-5.83	1.40	1.52
1	A	819	CYS	CB-SG	-5.80	1.72	1.81
1	C	384	GLU	C-O	-5.73	1.12	1.23
1	E	711	HIS	N-CA	-5.17	1.36	1.46
1	A	732	CYS	CB-SG	-5.08	1.73	1.81

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	794	ILE	CG1-CB-CG2	-5.98	98.24	111.40
1	E	802	LEU	CA-CB-CG	5.92	128.91	115.30
2	D	57	LEU	CA-CB-CG	5.89	128.84	115.30
2	B	57	LEU	CA-CB-CG	5.88	128.81	115.30
2	F	57	LEU	CA-CB-CG	5.76	128.54	115.30

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	MET	Peptide
1	A	293	GLY	Peptide
1	A	379	SER	Peptide
1	A	380	GLY	Peptide
1	A	381	ALA	Peptide

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	8861	0	8781	397	0
1	C	8861	0	8781	386	0
1	E	8861	0	8781	400	0
2	B	2886	0	2836	195	0
2	D	2886	0	2836	181	0
2	F	2886	0	2836	188	0
All	All	35241	0	34851	1677	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 24.

The worst 5 of 1677 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)
2:B:208:ASP:O	2:B:209:VAL:CG1	1.66	1.43
1:A:791:LEU:HD22	1:A:814:LEU:O	1.25	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:791:LEU:HD22	1:E:814:LEU:O	1.25	1.26
1:C:791:LEU:HD22	1:C:814:LEU:O	1.27	1.23
2:D:287:HIS:CE1	2:D:305:THR:HG21	1.75	1.22

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	1138/1158 (98%)	953 (84%)	130 (11%)	55 (5%)	2 14
1	C	1138/1158 (98%)	944 (83%)	135 (12%)	59 (5%)	2 13
1	E	1138/1158 (98%)	949 (83%)	131 (12%)	58 (5%)	2 13
2	B	366/436 (84%)	303 (83%)	39 (11%)	24 (7%)	1 8
2	D	366/436 (84%)	303 (83%)	40 (11%)	23 (6%)	1 9
2	F	366/436 (84%)	308 (84%)	35 (10%)	23 (6%)	1 9
All	All	4512/4782 (94%)	3760 (83%)	510 (11%)	242 (5%)	2 12

5 of 242 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	26	ALA
1	A	204	LYS
1	A	243	ASP
1	A	381	ALA

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	984/1014 (97%)	868 (88%)	116 (12%)	5 21
1	C	984/1014 (97%)	876 (89%)	108 (11%)	6 24
1	E	984/1014 (97%)	875 (89%)	109 (11%)	6 23
2	B	315/378 (83%)	264 (84%)	51 (16%)	2 10
2	D	315/378 (83%)	265 (84%)	50 (16%)	2 11
2	F	315/378 (83%)	262 (83%)	53 (17%)	2 9
All	All	3897/4176 (93%)	3410 (88%)	487 (12%)	4 19

5 of 487 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	786	VAL
2	F	117	LEU
2	D	127	VAL
2	F	71	ARG
2	F	326	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	467	GLN
2	F	237	ASN
1	E	522	HIS
1	E	950	ASN
2	F	385	GLN

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)

There are no ligands in this entry.

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, 95^{th} 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	1140/1158 (98%)	0.45	91 (7%)	12	11	23, 63, 97, 120	0
1	C	1140/1158 (98%)	0.45	81 (7%)	16	16	23, 63, 95, 120	0
1	E	1140/1158 (98%)	0.54	108 (9%)	8	8	22, 64, 96, 120	0
2	B	368/436 (84%)	0.14	13 (3%)	44	42	24, 55, 86, 141	0
2	D	368/436 (84%)	0.15	17 (4%)	32	30	24, 55, 88, 136	0
2	F	368/436 (84%)	0.31	26 (7%)	16	16	25, 56, 85, 139	0
All	All	4524/4782 (94%)	0.41	336 (7%)	14	14	22, 62, 94, 141	0

The worst 5 of 336 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	548	ASP	9.5
1	C	780	THR	8.9
1	C	1117	GLY	8.8
1	E	984	THR	8.3
1	A	1120	MET	8.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.