Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 09:29 pm BST

PDB ID	:	2YGU
Title	:	Crystal structure of fire ant venom allergen, Sol I 2
Authors	:	Borer, A.S.; Wassmann, P.; Schirmer, T.; Markovic-Housley, Z.
Deposited on	:	2011-04-20
Resolution	:	2.60 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:

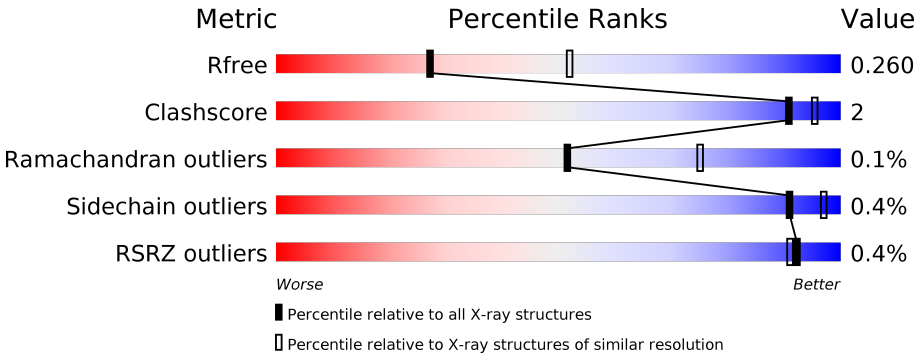
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	125	94% 6%
1	B	125	93% • 5%
1	C	125	94% • 6%
1	D	125	90% • 6%
1	E	125	% 92% • • 5%
1	F	125	% 93% • •

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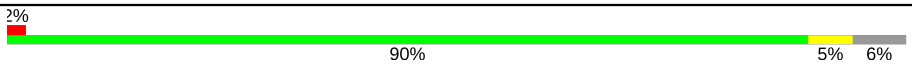
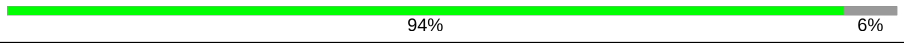
Mol	Chain	Length	Quality of chain
1	G	125	
1	H	125	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7007 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 VENOM ALLERGEN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	0	0	1
			856	523	160	163	10			
1	B	119	Total	C	N	O	S	0	0	0
			858	527	158	163	10			
1	C	118	Total	C	N	O	S	0	0	0
			870	534	160	166	10			
1	D	117	Total	C	N	O	S	0	0	0
			839	515	154	160	10			
1	E	119	Total	C	N	O	S	0	0	1
			877	536	165	166	10			
1	F	120	Total	C	N	O	S	0	0	1
			859	529	160	160	10			
1	G	118	Total	C	N	O	S	0	0	0
			875	537	162	166	10			
1	H	117	Total	C	N	O	S	0	0	0
			838	520	150	158	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	HIS	-	expression tag	UNP P35775
A	121	HIS	-	expression tag	UNP P35775
A	122	HIS	-	expression tag	UNP P35775
A	123	HIS	-	expression tag	UNP P35775
A	124	HIS	-	expression tag	UNP P35775
A	125	HIS	-	expression tag	UNP P35775
B	120	HIS	-	expression tag	UNP P35775
B	121	HIS	-	expression tag	UNP P35775
B	122	HIS	-	expression tag	UNP P35775
B	123	HIS	-	expression tag	UNP P35775
B	124	HIS	-	expression tag	UNP P35775
B	125	HIS	-	expression tag	UNP P35775
C	120	HIS	-	expression tag	UNP P35775

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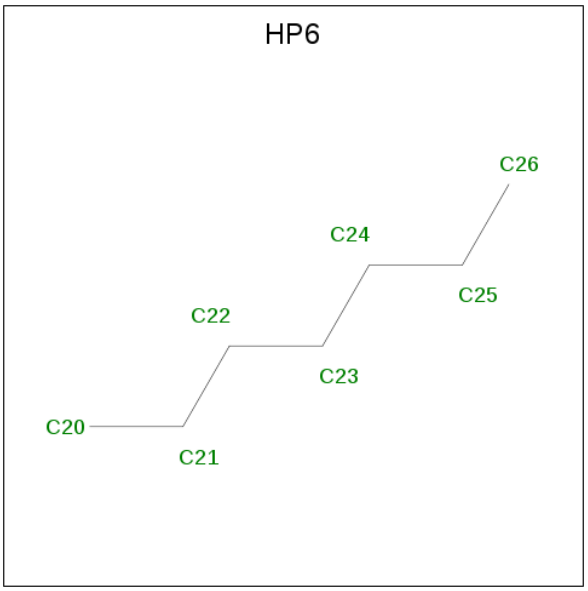
Chain	Residue	Modelled	Actual	Comment	Reference
C	121	HIS	-	expression tag	UNP P35775
C	122	HIS	-	expression tag	UNP P35775
C	123	HIS	-	expression tag	UNP P35775
C	124	HIS	-	expression tag	UNP P35775
C	125	HIS	-	expression tag	UNP P35775
D	120	HIS	-	expression tag	UNP P35775
D	121	HIS	-	expression tag	UNP P35775
D	122	HIS	-	expression tag	UNP P35775
D	123	HIS	-	expression tag	UNP P35775
D	124	HIS	-	expression tag	UNP P35775
D	125	HIS	-	expression tag	UNP P35775
E	120	HIS	-	expression tag	UNP P35775
E	121	HIS	-	expression tag	UNP P35775
E	122	HIS	-	expression tag	UNP P35775
E	123	HIS	-	expression tag	UNP P35775
E	124	HIS	-	expression tag	UNP P35775
E	125	HIS	-	expression tag	UNP P35775
F	120	HIS	-	expression tag	UNP P35775
F	121	HIS	-	expression tag	UNP P35775
F	122	HIS	-	expression tag	UNP P35775
F	123	HIS	-	expression tag	UNP P35775
F	124	HIS	-	expression tag	UNP P35775
F	125	HIS	-	expression tag	UNP P35775
G	120	HIS	-	expression tag	UNP P35775
G	121	HIS	-	expression tag	UNP P35775
G	122	HIS	-	expression tag	UNP P35775
G	123	HIS	-	expression tag	UNP P35775
G	124	HIS	-	expression tag	UNP P35775
G	125	HIS	-	expression tag	UNP P35775
H	120	HIS	-	expression tag	UNP P35775
H	121	HIS	-	expression tag	UNP P35775
H	122	HIS	-	expression tag	UNP P35775
H	123	HIS	-	expression tag	UNP P35775
H	124	HIS	-	expression tag	UNP P35775
H	125	HIS	-	expression tag	UNP P35775

- Molecule 2 is HEPTANE (three-letter code: HP6) (formula: C_7H_{16}).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 7 7	0	0
2	B	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	D	1	Total C 7 7	0	0
2	E	1	Total C 7 7	0	0
2	F	1	Total C 7 7	0	0
2	G	1	Total C 7 7	0	0
2	H	1	Total C 7 7	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	20	Total O 20 20	0	0
3	B	5	Total O 5 5	0	0
3	C	10	Total O 10 10	0	0
3	D	2	Total O 2 2	0	0

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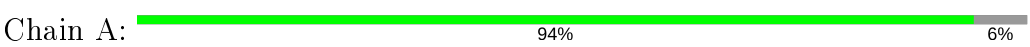
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	18	Total O 18 18	0	0
3	F	3	Total O 3 3	0	0
3	G	14	Total O 14 14	0	0
3	H	7	Total O 7 7	0	0

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 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.

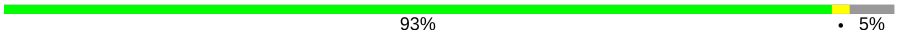
- Molecule 1: VENOM ALLERGEN 2

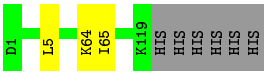
Chain A:



- Molecule 1: VENOM ALLERGEN 2

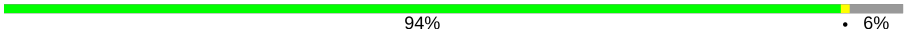
Chain B:





- Molecule 1: VENOM ALLERGEN 2

Chain C:

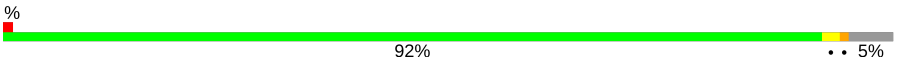


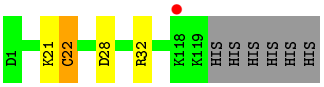
- Molecule 1: VENOM ALLERGEN 2

Chain D:

- Molecule 1: VENOM ALLERGEN 2

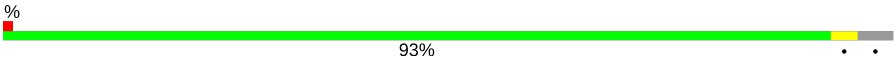
Chain E:

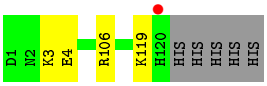




- Molecule 1: VENOM ALLERGEN 2

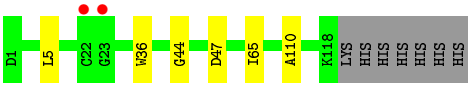
Chain F:





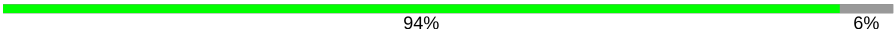
• Molecule 1: VENOM ALLERGEN 2

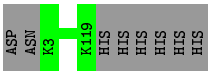
Chain G:



• Molecule 1: VENOM ALLERGEN 2

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	110.21Å 139.16Å 62.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 69.58 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.6 (15.00-2.60) 94.3 (69.58-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.237 , 0.270 0.235 , 0.260	Depositor DCC
R_{free} test set	1441 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 29.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7007	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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 45.89 % 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 1.2378e-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

Bond lengths and bond angles in the following residue types are not validated in this section: HP6

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	0.49	0/866	0.60	0/1175
1	B	0.46	0/866	0.56	0/1175
1	C	0.45	0/880	0.56	0/1194
1	D	0.44	0/849	0.54	0/1155
1	E	0.50	0/885	0.59	0/1199
1	F	0.46	0/867	0.58	0/1177
1	G	0.49	0/885	0.59	0/1200
1	H	0.45	0/848	0.55	0/1152
All	All	0.47	0/6946	0.57	0/9427

There are no bond length outliers.

There are no bond angle outliers.

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	856	0	836	0	0
1	B	858	0	828	4	0
1	C	870	0	853	0	0
1	D	839	0	800	3	0
1	E	877	0	863	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	859	0	829	4	0
1	G	875	0	862	5	0
1	H	838	0	805	0	0
2	A	7	0	16	0	0
2	B	7	0	16	0	0
2	C	7	0	16	0	0
2	D	7	0	16	2	0
2	E	7	0	16	2	0
2	F	7	0	16	0	0
2	G	7	0	16	3	0
2	H	7	0	16	1	0
3	A	20	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
3	D	2	0	0	0	0
3	E	18	0	0	1	0
3	F	3	0	0	0	0
3	G	14	0	0	0	0
3	H	7	0	0	0	0
All	All	7007	0	6804	23	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 2.

All (23) 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:E:1120:HP6:H202	2:E:1120:HP6:H241	1.50	0.93
1:E:21:LYS:CA	1:E:22:CYS:N	2.39	0.86
1:F:3:LYS:CA	1:F:4:GLU:N	2.43	0.81
1:B:64:LYS:CA	1:B:65:ILE:N	2.45	0.80
1:G:110:ALA:HB2	2:G:1119:HP6:C26	2.19	0.73
1:B:64:LYS:CA	1:B:64:LYS:O	2.39	0.70
1:F:3:LYS:O	1:F:3:LYS:CA	2.40	0.70
1:B:64:LYS:O	1:B:65:ILE:N	2.25	0.69
1:E:21:LYS:O	1:E:22:CYS:N	2.25	0.69
1:D:116:ALA:O	1:D:117:ARG:CB	2.41	0.69
1:E:21:LYS:CA	1:E:21:LYS:O	2.42	0.68
1:F:3:LYS:O	1:F:4:GLU:N	2.27	0.67
1:G:110:ALA:HB2	2:G:1119:HP6:H263	1.79	0.65
2:E:1120:HP6:C20	2:E:1120:HP6:H241	2.28	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:SER:OG	2:D:1118:HP6:H263	2.08	0.54
1:G:36:TRP:CE2	2:G:1119:HP6:H262	2.46	0.51
1:D:58:SER:OG	2:D:1118:HP6:C26	2.61	0.49
1:E:32:ARG:HA	3:E:2004:HOH:O	2.14	0.47
1:B:5:LEU:HD21	1:B:65:ILE:HA	1.98	0.45
1:G:44:GLY:HA2	1:G:47:ASP:OD1	2.18	0.43
2:H:1120:HP6:H231	2:H:1120:HP6:H263	1.60	0.41
1:E:28:ASP:OD2	1:F:106:ARG:NH1	2.53	0.41
1:G:5:LEU:HD21	1:G:65:ILE:HA	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
1	A	115/125 (92%)	113 (98%)	2 (2%)	0	100 100
1	B	115/125 (92%)	112 (97%)	3 (3%)	0	100 100
1	C	116/125 (93%)	115 (99%)	1 (1%)	0	100 100
1	D	115/125 (92%)	114 (99%)	1 (1%)	0	100 100
1	E	115/125 (92%)	113 (98%)	2 (2%)	0	100 100
1	F	116/125 (93%)	114 (98%)	1 (1%)	1 (1%)	17 35
1	G	116/125 (93%)	115 (99%)	1 (1%)	0	100 100
1	H	115/125 (92%)	114 (99%)	1 (1%)	0	100 100
All	All	923/1000 (92%)	910 (99%)	12 (1%)	1 (0%)	51 75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	119	LYS

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	89/108 (82%)	89 (100%)	0	100 100
1	B	87/108 (81%)	87 (100%)	0	100 100
1	C	91/108 (84%)	90 (99%)	1 (1%)	73 88
1	D	83/108 (77%)	82 (99%)	1 (1%)	71 87
1	E	92/108 (85%)	91 (99%)	1 (1%)	73 88
1	F	85/108 (79%)	85 (100%)	0	100 100
1	G	91/108 (84%)	91 (100%)	0	100 100
1	H	82/108 (76%)	82 (100%)	0	100 100
All	All	700/864 (81%)	697 (100%)	3 (0%)	91 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	22	CYS
1	D	22	CYS
1	E	22	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	B	95	GLN
1	C	95	GLN
1	D	95	GLN
1	E	95	GLN
1	F	95	GLN
1	G	95	GLN
1	H	95	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

8 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	HP6	E	1120	-	6,6,6	0.54	0	5,5,5	0.34	0
2	HP6	B	1120	-	6,6,6	0.40	0	5,5,5	0.47	0
2	HP6	H	1120	-	6,6,6	0.45	0	5,5,5	0.42	0
2	HP6	D	1118	-	6,6,6	0.52	0	5,5,5	0.66	0
2	HP6	G	1119	-	6,6,6	0.33	0	5,5,5	0.54	0
2	HP6	C	1119	-	6,6,6	0.33	0	5,5,5	0.69	0
2	HP6	F	1121	-	6,6,6	0.43	0	5,5,5	0.42	0
2	HP6	A	1118	-	6,6,6	0.53	0	5,5,5	0.45	0

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
2	HP6	E	1120	-	-	1/4/4/4	-
2	HP6	B	1120	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HP6	H	1120	-	-	4/4/4/4	-
2	HP6	D	1118	-	-	3/4/4/4	-
2	HP6	G	1119	-	-	1/4/4/4	-
2	HP6	C	1119	-	-	3/4/4/4	-
2	HP6	F	1121	-	-	3/4/4/4	-
2	HP6	A	1118	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1120	HP6	C21-C22-C23-C24
2	F	1121	HP6	C21-C22-C23-C24
2	H	1120	HP6	C23-C24-C25-C26
2	B	1120	HP6	C23-C24-C25-C26
2	B	1120	HP6	C21-C22-C23-C24
2	H	1120	HP6	C22-C23-C24-C25
2	F	1121	HP6	C22-C23-C24-C25
2	H	1120	HP6	C21-C22-C23-C24
2	B	1120	HP6	C20-C21-C22-C23
2	H	1120	HP6	C20-C21-C22-C23
2	C	1119	HP6	C23-C24-C25-C26
2	A	1118	HP6	C21-C22-C23-C24
2	G	1119	HP6	C20-C21-C22-C23
2	D	1118	HP6	C21-C22-C23-C24
2	A	1118	HP6	C20-C21-C22-C23
2	A	1118	HP6	C22-C23-C24-C25
2	C	1119	HP6	C21-C22-C23-C24
2	D	1118	HP6	C20-C21-C22-C23
2	C	1119	HP6	C20-C21-C22-C23
2	D	1118	HP6	C22-C23-C24-C25
2	F	1121	HP6	C23-C24-C25-C26

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1120	HP6	2	0
2	H	1120	HP6	1	0
2	D	1118	HP6	2	0
2	G	1119	HP6	3	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

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	117/125 (93%)	-0.50	0 100 100	12, 25, 57, 76	0
1	B	119/125 (95%)	-0.28	0 100 100	18, 37, 70, 98	0
1	C	118/125 (94%)	-0.34	0 100 100	19, 37, 75, 95	0
1	D	117/125 (93%)	-0.11	0 100 100	26, 52, 76, 104	0
1	E	119/125 (95%)	-0.40	1 (0%) 86 84	17, 28, 69, 85	0
1	F	120/125 (96%)	-0.30	1 (0%) 86 84	18, 38, 67, 93	0
1	G	118/125 (94%)	-0.47	2 (1%) 70 66	12, 29, 64, 98	0
1	H	117/125 (93%)	-0.33	0 100 100	14, 32, 62, 88	0
All	All	945/1000 (94%)	-0.34	4 (0%) 92 91	12, 35, 71, 104	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	118	LYS	3.2
1	F	120	HIS	2.9
1	G	22	CYS	2.4
1	G	23	GLY	2.4

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 carbohydrates in this entry.

6.4 Ligands

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, 95^{th} 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(Å^2)	Q<0.9
2	HP6	D	1118	7/7	0.74	0.32	32,35,43,52	0
2	HP6	E	1120	7/7	0.86	0.20	17,30,36,43	0
2	HP6	G	1119	7/7	0.86	0.26	19,22,41,47	0
2	HP6	B	1120	7/7	0.88	0.24	38,42,51,51	0
2	HP6	C	1119	7/7	0.90	0.27	24,25,38,51	0
2	HP6	F	1121	7/7	0.90	0.18	15,27,41,45	0
2	HP6	A	1118	7/7	0.92	0.18	14,31,39,41	0
2	HP6	H	1120	7/7	0.93	0.16	16,18,23,29	0

6.5 Other polymers

There are no such residues in this entry.