



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2020 – 10:42 AM BST

PDB ID : 6WXM  
Title : X-ray crystallographic structure of a beta-hairpin peptide derived from amyloid beta 16-36  
Authors : Kreutzer, A.G.; Nowick, J.S.  
Deposited on : 2020-05-11  
Resolution : 2.30 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](mailto: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 : 2.14.3.dev2  
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) : 2.14.3.dev2

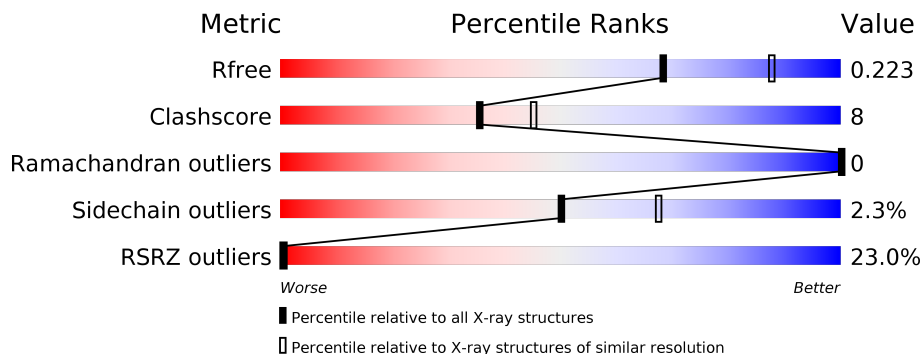
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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.



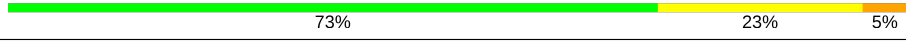


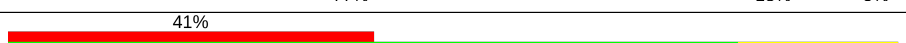
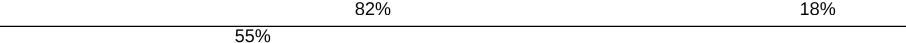
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	22	 18% 82% 14% 5%
1	B	22	 14% 86% 5% 9%
1	C	22	 73% 18% 9%
1	D	22	 23% 64% 32% 5%
1	E	22	 18% 73% 27%
1	F	22	 73% 18% 9%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	22	
1	H	22	
1	I	22	
1	J	22	
1	K	22	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	ORN	J	2	-	-	-	X
1	ORN	K	2	-	-	-	X
2	HEZ	H	102	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3926 atoms, of which 1977 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 Amyloid-beta protein.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	I	N	O	S			
1	F	22	330	105	167	1	26	28	3	0	0	0
1	H	22	330	105	167	1	26	28	3	0	0	0
1	B	22	330	105	167	1	26	28	3	0	0	0
1	I	22	330	105	167	1	26	28	3	0	0	0
1	E	22	330	105	167	1	26	28	3	0	0	0
1	A	22	330	105	167	1	26	28	3	0	0	0
1	C	22	330	105	167	1	26	28	3	0	0	0
1	D	22	330	105	167	1	26	28	3	0	0	0
1	J	22	330	105	167	1	26	28	3	0	0	0
1	G	22	330	105	167	1	26	28	3	0	0	0
1	K	22	330	105	167	1	26	28	3	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

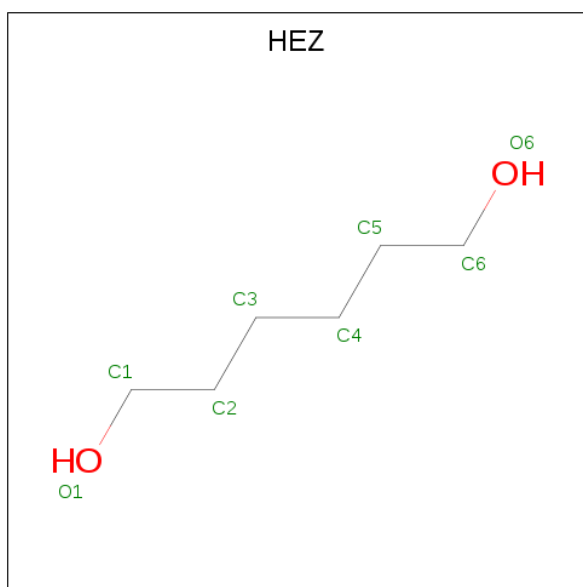
Chain	Residue	Modelled	Actual	Comment	Reference
F	1	VAL	HIS	conflict	UNP P05067
F	2	ORN	GLN	conflict	UNP P05067
F	8	CYS	ALA	conflict	UNP P05067
F	18	CYS	ILE	conflict	UNP P05067
H	1	VAL	HIS	conflict	UNP P05067
H	2	ORN	GLN	conflict	UNP P05067
H	8	CYS	ALA	conflict	UNP P05067

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
H	18	CYS	ILE	conflict	UNP P05067
B	1	VAL	HIS	conflict	UNP P05067
B	2	ORN	GLN	conflict	UNP P05067
B	8	CYS	ALA	conflict	UNP P05067
B	18	CYS	ILE	conflict	UNP P05067
I	1	VAL	HIS	conflict	UNP P05067
I	2	ORN	GLN	conflict	UNP P05067
I	8	CYS	ALA	conflict	UNP P05067
I	18	CYS	ILE	conflict	UNP P05067
E	1	VAL	HIS	conflict	UNP P05067
E	2	ORN	GLN	conflict	UNP P05067
E	8	CYS	ALA	conflict	UNP P05067
E	18	CYS	ILE	conflict	UNP P05067
A	1	VAL	HIS	conflict	UNP P05067
A	2	ORN	GLN	conflict	UNP P05067
A	8	CYS	ALA	conflict	UNP P05067
A	18	CYS	ILE	conflict	UNP P05067
C	1	VAL	HIS	conflict	UNP P05067
C	2	ORN	GLN	conflict	UNP P05067
C	8	CYS	ALA	conflict	UNP P05067
C	18	CYS	ILE	conflict	UNP P05067
D	1	VAL	HIS	conflict	UNP P05067
D	2	ORN	GLN	conflict	UNP P05067
D	8	CYS	ALA	conflict	UNP P05067
D	18	CYS	ILE	conflict	UNP P05067
J	1	VAL	HIS	conflict	UNP P05067
J	2	ORN	GLN	conflict	UNP P05067
J	8	CYS	ALA	conflict	UNP P05067
J	18	CYS	ILE	conflict	UNP P05067
G	1	VAL	HIS	conflict	UNP P05067
G	2	ORN	GLN	conflict	UNP P05067
G	8	CYS	ALA	conflict	UNP P05067
G	18	CYS	ILE	conflict	UNP P05067
K	1	VAL	HIS	conflict	UNP P05067
K	2	ORN	GLN	conflict	UNP P05067
K	8	CYS	ALA	conflict	UNP P05067
K	18	CYS	ILE	conflict	UNP P05067

- Molecule 2 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	H	O	0	0
			22	6	14	2		
2	H	1	Total	C	H	O	0	0
			22	6	14	2		
2	I	1	Total	C	H	O	0	0
			22	6	14	2		
2	E	1	Total	C	H	O	0	0
			22	6	14	2		
2	A	1	Total	C	H	O	0	0
			22	6	14	2		
2	C	1	Total	C	H	O	0	0
			22	6	14	2		
2	D	1	Total	C	H	O	0	0
			22	6	14	2		
2	J	1	Total	C	H	O	0	0
			22	6	14	2		
2	J	1	Total	C	H	O	0	0
			22	6	14	2		
2	G	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	12	Total	O	0	0
			12	12		
3	H	7	Total	O	0	0
			7	7		

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
3	B	6	Total O 6 6	0	0
3	I	4	Total O 4 4	0	0
3	E	7	Total O 7 7	0	0
3	A	7	Total O 7 7	0	0
3	C	9	Total O 9 9	0	0
3	D	11	Total O 11 11	0	0
3	J	5	Total O 5 5	0	0
3	G	5	Total O 5 5	0	0
3	K	3	Total O 3 3	0	0

### 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.

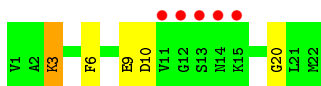
- Molecule 1: Amyloid-beta protein

Chain F: 




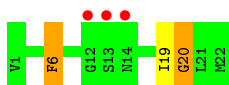
- Molecule 1: Amyloid-beta protein

Chain H: 




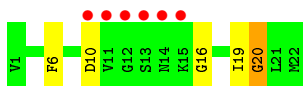
- Molecule 1: Amyloid-beta protein

Chain B: 



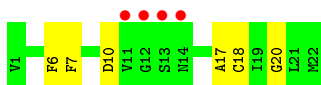
- Molecule 1: Amyloid-beta protein

Chain I: 



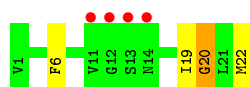
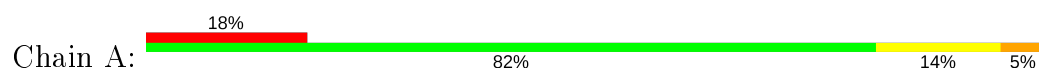
- Molecule 1: Amyloid-beta protein

Chain E: 



- Molecule 1: Amyloid-beta protein

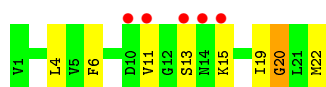




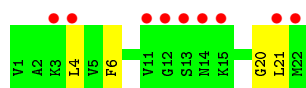
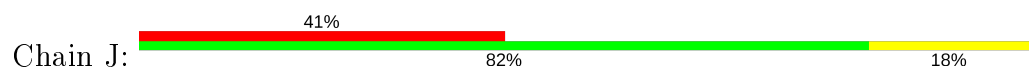
- Molecule 1: Amyloid-beta protein



- Molecule 1: Amyloid-beta protein



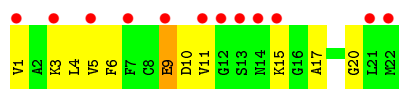
- Molecule 1: Amyloid-beta protein



- Molecule 1: Amyloid-beta protein



- Molecule 1: Amyloid-beta protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.19Å 122.13Å 58.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.28 – 2.30 36.28 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (36.28-2.30) 94.6 (36.28-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.82 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.171 , 0.218 0.176 , 0.223	Depositor DCC
$R_{free}$ test set	1441 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtrriage
Anisotropy	0.401	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3926	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ORN, SAR, PHI, HEZ

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	0.48	0/135	0.53	0/174
1	B	0.58	0/135	0.73	0/174
1	C	0.47	0/135	0.74	0/174
1	D	0.50	0/135	0.85	0/174
1	E	0.59	0/135	0.73	0/174
1	F	0.54	0/135	0.81	0/174
1	G	0.57	0/135	0.60	0/174
1	H	0.46	0/135	0.59	0/174
1	I	0.81	0/135	0.98	0/174
1	J	0.52	0/135	0.68	0/174
1	K	1.05	1/135 (0.7%)	0.71	0/174
All	All	0.62	1/1485 (0.1%)	0.73	0/1914

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	9	GLU	CD-OE2	-9.73	1.15	1.25

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	163	167	166	1	0
1	B	163	167	165	3	0
1	C	163	167	165	7	0
1	D	163	167	166	4	0
1	E	163	167	165	3	0
1	F	163	167	165	6	0
1	G	163	167	165	3	0
1	H	163	167	166	3	0
1	I	163	167	165	3	0
1	J	163	167	165	2	0
1	K	163	167	165	3	2
2	A	8	14	14	0	0
2	C	8	14	14	1	0
2	D	8	14	14	0	0
2	E	8	14	14	0	0
2	G	8	14	14	0	0
2	H	16	28	28	0	0
2	I	8	14	14	1	0
2	J	16	28	28	0	0
3	A	7	0	0	0	0
3	B	6	0	0	0	0
3	C	9	0	0	0	0
3	D	11	0	0	0	0
3	E	7	0	0	0	0
3	F	12	0	0	0	0
3	G	5	0	0	0	0
3	H	7	0	0	0	0
3	I	4	0	0	0	0
3	J	5	0	0	0	0
3	K	3	0	0	0	0
All	All	1949	1977	1958	31	2

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 8.

All (31) 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:E:17:ALA:HB1	1:K:17:ALA:HB1	1.70	0.74
1:C:1:VAL:O	1:C:2:ORN:HB2	1.97	0.65
1:F:15:LYS:NZ	1:H:9:GLU:OE2	2.40	0.54
1:F:22:MET:SD	1:C:6:PHI:I	3.36	0.54

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3:LYS:H	1:H:3:LYS:HD3	1.73	0.52
1:F:6:PHI:I	1:C:22:MET:SD	3.38	0.51
1:I:10:ASP:HA	1:I:16:GLY:HA2	1.92	0.50
1:E:10:ASP:OD1	1:E:10:ASP:N	2.45	0.48
1:K:1:VAL:N	1:K:3:LYS:O	2.46	0.48
1:D:4:LEU:HD13	1:D:22:MET:HE2	1.95	0.47
1:F:20:SAR:HN3	1:C:20:SAR:HN3	1.96	0.47
1:I:16:GLY:HA3	2:I:101:HEZ:H51	1.97	0.46
1:G:11:VAL:HG22	1:G:15:LYS:O	2.15	0.45
1:I:19:ILE:HA	1:I:20:SAR:HN1	1.62	0.45
1:E:7:PHE:O	1:E:18:CYS:HB3	2.17	0.45
1:K:10:ASP:OD1	1:K:11:VAL:N	2.51	0.44
1:J:4:LEU:HA	1:J:21:LEU:O	2.18	0.44
1:B:6:PHI:I	1:C:19:ILE:HD11	2.88	0.43
1:J:4:LEU:H	1:J:4:LEU:HD23	1.82	0.43
1:B:6:PHI:I	1:C:19:ILE:HG12	2.89	0.42
1:H:10:ASP:OD1	1:H:10:ASP:N	2.51	0.42
1:D:4:LEU:HB2	1:D:22:MET:CE	2.50	0.42
1:G:19:ILE:HA	1:G:20:SAR:HN1	1.88	0.42
2:C:101:HEZ:H62	1:G:21:LEU:HD21	2.01	0.42
1:B:19:ILE:HA	1:B:20:SAR:HN1	1.88	0.42
1:F:13:SER:OG	1:F:13:SER:O	2.33	0.42
1:D:11:VAL:HG23	1:D:15:LYS:O	2.21	0.41
1:D:19:ILE:HA	1:D:20:SAR:HN1	1.86	0.41
1:A:19:ILE:HA	1:A:20:SAR:HN1	1.81	0.41
1:F:19:ILE:HA	1:F:20:SAR:HN1	1.80	0.41
1:C:1:VAL:C	1:C:2:ORN:HB2	2.42	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5:VAL:CG2	1:K:9:GLU:OE2[4_566]	2.08	0.12
1:K:4:LEU:O	1:K:9:GLU:OE1[4_566]	2.16	0.04

## 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	17/22 (77%)	17 (100%)	0	0	100	100
1	B	17/22 (77%)	17 (100%)	0	0	100	100
1	C	17/22 (77%)	17 (100%)	0	0	100	100
1	D	17/22 (77%)	15 (88%)	2 (12%)	0	100	100
1	E	17/22 (77%)	15 (88%)	2 (12%)	0	100	100
1	F	17/22 (77%)	17 (100%)	0	0	100	100
1	G	17/22 (77%)	17 (100%)	0	0	100	100
1	H	17/22 (77%)	14 (82%)	3 (18%)	0	100	100
1	I	17/22 (77%)	15 (88%)	2 (12%)	0	100	100
1	J	17/22 (77%)	16 (94%)	1 (6%)	0	100	100
1	K	17/22 (77%)	16 (94%)	1 (6%)	0	100	100
All	All	187/242 (77%)	176 (94%)	11 (6%)	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	16/16 (100%)	15 (94%)	1 (6%)	18	24
1	B	16/16 (100%)	16 (100%)	0	100	100
1	C	16/16 (100%)	16 (100%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	16/16 (100%)	15 (94%)	1 (6%)	18	24
1	E	16/16 (100%)	16 (100%)	0	100	100
1	F	16/16 (100%)	16 (100%)	0	100	100
1	G	16/16 (100%)	16 (100%)	0	100	100
1	H	16/16 (100%)	15 (94%)	1 (6%)	18	24
1	I	16/16 (100%)	16 (100%)	0	100	100
1	J	16/16 (100%)	16 (100%)	0	100	100
1	K	16/16 (100%)	15 (94%)	1 (6%)	18	24
All	All	176/176 (100%)	172 (98%)	4 (2%)	50	67

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	3	LYS
1	A	22	MET
1	D	13	SER
1	K	15	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	14	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](#)

33 non-standard protein/DNA/RNA residues 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
1	SAR	H	20	1	4,4,5	2.29	1 (25%)	1,3,5	2.54	1 (100%)
1	PHI	A	6	1	11,12,13	1.74	3 (27%)	12,15,17	1.50	1 (8%)
1	ORN	F	2	1	6,7,8	0.78	0	2,7,9	0.43	0
1	ORN	D	2	1	6,7,8	0.75	0	2,7,9	0.27	0
1	ORN	I	2	1	6,7,8	0.79	0	2,7,9	0.20	0
1	SAR	A	20	1	4,4,5	2.11	1 (25%)	1,3,5	2.37	1 (100%)
1	SAR	I	20	1	4,4,5	2.18	1 (25%)	1,3,5	1.69	0
1	ORN	C	2	1	6,7,8	0.96	0	2,7,9	0.31	0
1	ORN	B	2	1	6,7,8	0.84	0	2,7,9	0.30	0
1	ORN	A	2	1	6,7,8	1.16	0	2,7,9	0.19	0
1	PHI	J	6	1	11,12,13	1.64	3 (27%)	12,15,17	1.26	1 (8%)
1	PHI	I	6	1	11,12,13	1.68	3 (27%)	12,15,17	1.94	2 (16%)
1	PHI	K	6	1	11,12,13	1.67	3 (27%)	12,15,17	1.08	1 (8%)
1	ORN	K	2	1	6,7,8	0.78	0	2,7,9	0.31	0
1	ORN	J	2	1	6,7,8	0.68	0	2,7,9	0.22	0
1	SAR	E	20	1	4,4,5	2.30	1 (25%)	1,3,5	1.93	0
1	SAR	B	20	1	4,4,5	2.03	1 (25%)	1,3,5	1.64	0
1	SAR	K	20	1	4,4,5	2.35	1 (25%)	1,3,5	0.85	0
1	PHI	B	6	1	11,12,13	1.66	3 (27%)	12,15,17	1.23	1 (8%)
1	SAR	G	20	1	4,4,5	2.30	1 (25%)	1,3,5	0.70	0
1	ORN	E	2	1	6,7,8	1.13	0	2,7,9	0.30	0
1	PHI	E	6	1	11,12,13	1.66	3 (27%)	12,15,17	1.62	1 (8%)
1	PHI	G	6	1	11,12,13	1.62	3 (27%)	12,15,17	1.05	1 (8%)
1	SAR	C	20	1	4,4,5	1.98	1 (25%)	1,3,5	2.41	1 (100%)
1	ORN	H	2	1	6,7,8	0.60	0	2,7,9	0.26	0
1	SAR	D	20	1	4,4,5	2.06	1 (25%)	1,3,5	2.72	1 (100%)
1	SAR	F	20	1	4,4,5	2.02	1 (25%)	1,3,5	2.48	1 (100%)
1	ORN	G	2	1	6,7,8	0.94	0	2,7,9	0.19	0
1	PHI	F	6	1	11,12,13	1.61	3 (27%)	12,15,17	1.57	2 (16%)
1	PHI	D	6	1	11,12,13	1.64	3 (27%)	12,15,17	1.40	1 (8%)
1	PHI	H	6	1	11,12,13	1.70	3 (27%)	12,15,17	1.34	1 (8%)
1	PHI	C	6	1	11,12,13	1.56	3 (27%)	12,15,17	1.47	1 (8%)
1	SAR	J	20	1	4,4,5	2.27	1 (25%)	1,3,5	2.23	1 (100%)

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
1	SAR	H	20	1	-	1/1/2/3	-
1	PHI	A	6	1	-	2/5/6/8	0/1/1/1
1	ORN	F	2	1	-	1/5/6/8	-
1	ORN	D	2	1	-	0/5/6/8	-
1	ORN	I	2	1	-	0/5/6/8	-
1	SAR	A	20	1	-	1/1/2/3	-
1	SAR	I	20	1	-	1/1/2/3	-
1	ORN	C	2	1	-	1/5/6/8	-
1	ORN	B	2	1	-	1/5/6/8	-
1	ORN	A	2	1	-	0/5/6/8	-
1	PHI	J	6	1	-	2/5/6/8	0/1/1/1
1	PHI	I	6	1	-	2/5/6/8	0/1/1/1
1	PHI	K	6	1	-	1/5/6/8	0/1/1/1
1	ORN	K	2	1	-	1/5/6/8	-
1	ORN	J	2	1	-	2/5/6/8	-
1	SAR	E	20	1	-	1/1/2/3	-
1	SAR	B	20	1	-	1/1/2/3	-
1	SAR	K	20	1	-	1/1/2/3	-
1	PHI	B	6	1	-	2/5/6/8	0/1/1/1
1	SAR	G	20	1	-	1/1/2/3	-
1	ORN	E	2	1	-	0/5/6/8	-
1	PHI	E	6	1	-	3/5/6/8	0/1/1/1
1	PHI	G	6	1	-	2/5/6/8	0/1/1/1
1	SAR	C	20	1	-	1/1/2/3	-
1	ORN	H	2	1	-	2/5/6/8	-
1	SAR	D	20	1	-	1/1/2/3	-
1	SAR	F	20	1	-	1/1/2/3	-
1	ORN	G	2	1	-	0/5/6/8	-
1	PHI	F	6	1	-	2/5/6/8	0/1/1/1
1	PHI	D	6	1	-	2/5/6/8	0/1/1/1
1	PHI	H	6	1	-	1/5/6/8	0/1/1/1
1	PHI	C	6	1	-	2/5/6/8	0/1/1/1
1	SAR	J	20	1	-	1/1/2/3	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	20	SAR	CA-C	-4.57	1.33	1.49
1	E	20	SAR	CA-C	-4.51	1.33	1.49
1	H	20	SAR	CA-C	-4.50	1.33	1.49
1	G	20	SAR	CA-C	-4.45	1.34	1.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	20	SAR	CA-C	-4.43	1.34	1.49
1	I	20	SAR	CA-C	-4.31	1.34	1.49
1	A	20	SAR	CA-C	-4.18	1.35	1.49
1	D	20	SAR	CA-C	-4.12	1.35	1.49
1	B	20	SAR	CA-C	-4.04	1.35	1.49
1	F	20	SAR	CA-C	-4.03	1.35	1.49
1	C	20	SAR	CA-C	-3.88	1.36	1.49
1	H	6	PHI	CD1-CG	3.32	1.46	1.38
1	A	6	PHI	CD1-CG	3.30	1.45	1.38
1	E	6	PHI	CD1-CG	3.30	1.45	1.38
1	A	6	PHI	CE2-CZ	3.24	1.45	1.38
1	D	6	PHI	CD1-CG	3.23	1.45	1.38
1	K	6	PHI	CD1-CG	3.21	1.45	1.38
1	I	6	PHI	CD1-CG	3.17	1.45	1.38
1	J	6	PHI	CD1-CG	3.13	1.45	1.38
1	G	6	PHI	CD1-CG	3.11	1.45	1.38
1	B	6	PHI	CD1-CG	3.10	1.45	1.38
1	E	6	PHI	CE2-CZ	2.98	1.45	1.38
1	H	6	PHI	CE2-CZ	2.92	1.45	1.38
1	I	6	PHI	CE2-CZ	2.90	1.45	1.38
1	F	6	PHI	CE2-CZ	2.84	1.45	1.38
1	B	6	PHI	CE2-CZ	2.83	1.45	1.38
1	G	6	PHI	CE2-CZ	2.83	1.45	1.38
1	C	6	PHI	CD1-CG	2.78	1.44	1.38
1	F	6	PHI	CD1-CG	2.77	1.44	1.38
1	J	6	PHI	CE2-CZ	2.68	1.44	1.38
1	C	6	PHI	CE2-CZ	2.67	1.44	1.38
1	K	6	PHI	CE2-CZ	2.67	1.44	1.38
1	D	6	PHI	CE2-CZ	2.66	1.44	1.38
1	J	6	PHI	O-C	2.47	1.29	1.19
1	F	6	PHI	O-C	2.44	1.29	1.19
1	C	6	PHI	O-C	2.41	1.29	1.19
1	E	6	PHI	O-C	2.41	1.29	1.19
1	G	6	PHI	O-C	2.38	1.29	1.19
1	B	6	PHI	O-C	2.38	1.29	1.19
1	I	6	PHI	O-C	2.36	1.29	1.19
1	A	6	PHI	O-C	2.36	1.29	1.19
1	K	6	PHI	O-C	2.31	1.29	1.19
1	H	6	PHI	O-C	2.29	1.29	1.19
1	D	6	PHI	O-C	2.15	1.28	1.19

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	6	PHI	CG-CB-CA	-4.97	104.04	114.10
1	I	6	PHI	CG-CB-CA	-4.62	104.74	114.10
1	D	6	PHI	CG-CB-CA	-4.35	105.30	114.10
1	A	6	PHI	CG-CB-CA	-4.26	105.47	114.10
1	C	6	PHI	CG-CB-CA	-4.00	105.99	114.10
1	H	6	PHI	CG-CB-CA	-3.66	106.68	114.10
1	F	6	PHI	CG-CB-CA	-3.66	106.69	114.10
1	I	6	PHI	CB-CA-C	-3.03	105.78	111.47
1	B	6	PHI	CG-CB-CA	-2.99	108.04	114.10
1	D	20	SAR	O-C-CA	-2.72	117.55	125.42
1	G	6	PHI	CG-CB-CA	-2.71	108.61	114.10
1	J	6	PHI	CG-CB-CA	-2.67	108.69	114.10
1	K	6	PHI	CG-CB-CA	-2.55	108.93	114.10
1	H	20	SAR	O-C-CA	-2.54	118.08	125.42
1	F	20	SAR	O-C-CA	-2.48	118.26	125.42
1	C	20	SAR	O-C-CA	-2.41	118.45	125.42
1	A	20	SAR	O-C-CA	-2.37	118.58	125.42
1	J	20	SAR	O-C-CA	-2.23	118.98	125.42
1	F	6	PHI	CB-CG-CD1	-2.20	116.53	120.91

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	H	20	SAR	C-CA-N-CN
1	A	6	PHI	C-CA-CB-CG
1	A	20	SAR	C-CA-N-CN
1	I	20	SAR	C-CA-N-CN
1	E	20	SAR	C-CA-N-CN
1	B	20	SAR	C-CA-N-CN
1	K	20	SAR	C-CA-N-CN
1	B	6	PHI	C-CA-CB-CG
1	G	20	SAR	C-CA-N-CN
1	E	6	PHI	C-CA-CB-CG
1	E	6	PHI	O-C-CA-CB
1	C	20	SAR	C-CA-N-CN
1	D	20	SAR	C-CA-N-CN
1	F	20	SAR	C-CA-N-CN
1	D	6	PHI	C-CA-CB-CG
1	J	20	SAR	C-CA-N-CN
1	J	6	PHI	N-CA-CB-CG
1	I	6	PHI	N-CA-CB-CG
1	G	6	PHI	N-CA-CB-CG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	F	6	PHI	N-CA-CB-CG
1	D	6	PHI	N-CA-CB-CG
1	C	6	PHI	N-CA-CB-CG
1	J	2	ORN	C-CA-CB-CG
1	J	2	ORN	CA-CB-CG-CD
1	H	2	ORN	CA-CB-CG-CD
1	A	6	PHI	N-CA-CB-CG
1	B	6	PHI	N-CA-CB-CG
1	E	6	PHI	N-CA-CB-CG
1	C	2	ORN	CA-CB-CG-CD
1	J	6	PHI	C-CA-CB-CG
1	I	6	PHI	C-CA-CB-CG
1	K	6	PHI	C-CA-CB-CG
1	G	6	PHI	C-CA-CB-CG
1	F	6	PHI	C-CA-CB-CG
1	H	6	PHI	C-CA-CB-CG
1	C	6	PHI	C-CA-CB-CG
1	K	2	ORN	C-CA-CB-CG
1	F	2	ORN	CA-CB-CG-CD
1	B	2	ORN	CA-CB-CG-CD
1	H	2	ORN	NE-CD-CG-CB

There are no ring outliers.

11 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	20	SAR	1	0
1	I	20	SAR	1	0
1	C	2	ORN	2	0
1	B	20	SAR	1	0
1	B	6	PHI	2	0
1	G	20	SAR	1	0
1	C	20	SAR	1	0
1	D	20	SAR	1	0
1	F	20	SAR	2	0
1	F	6	PHI	1	0
1	C	6	PHI	1	0

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

10 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	HEZ	J	102	-	7,7,7	0.33	0	6,6,6	0.74	0
2	HEZ	A	101	-	7,7,7	0.31	0	6,6,6	0.79	0
2	HEZ	D	101	-	7,7,7	0.41	0	6,6,6	0.53	0
2	HEZ	H	102	-	7,7,7	0.34	0	6,6,6	0.46	0
2	HEZ	E	101	-	7,7,7	0.33	0	6,6,6	0.68	0
2	HEZ	H	101	-	7,7,7	0.37	0	6,6,6	0.56	0
2	HEZ	G	101	-	7,7,7	0.39	0	6,6,6	0.59	0
2	HEZ	J	101	-	7,7,7	0.39	0	6,6,6	0.57	0
2	HEZ	I	101	-	7,7,7	0.33	0	6,6,6	0.66	0
2	HEZ	C	101	-	7,7,7	0.34	0	6,6,6	0.71	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	HEZ	J	102	-	-	4/5/5/5	-
2	HEZ	A	101	-	-	2/5/5/5	-
2	HEZ	D	101	-	-	2/5/5/5	-
2	HEZ	H	102	-	-	1/5/5/5	-
2	HEZ	E	101	-	-	0/5/5/5	-
2	HEZ	H	101	-	-	1/5/5/5	-
2	HEZ	G	101	-	-	1/5/5/5	-
2	HEZ	J	101	-	-	3/5/5/5	-
2	HEZ	I	101	-	-	3/5/5/5	-
2	HEZ	C	101	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	102	HEZ	C2-C3-C4-C5
2	J	101	HEZ	C2-C3-C4-C5
2	J	101	HEZ	C3-C4-C5-C6
2	D	101	HEZ	C1-C2-C3-C4
2	C	101	HEZ	C3-C4-C5-C6
2	J	102	HEZ	C4-C5-C6-O6
2	H	102	HEZ	O1-C1-C2-C3
2	J	102	HEZ	O1-C1-C2-C3
2	J	101	HEZ	C4-C5-C6-O6
2	A	101	HEZ	C1-C2-C3-C4
2	D	101	HEZ	C2-C3-C4-C5
2	H	101	HEZ	C2-C3-C4-C5
2	J	102	HEZ	C1-C2-C3-C4
2	G	101	HEZ	C2-C3-C4-C5
2	I	101	HEZ	C4-C5-C6-O6
2	I	101	HEZ	O1-C1-C2-C3
2	A	101	HEZ	O1-C1-C2-C3
2	I	101	HEZ	C3-C4-C5-C6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	101	HEZ	1	0
2	C	101	HEZ	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	19/22 (86%)	0.52	4 (21%) 1 1	28, 53, 102, 106	0
1	B	19/22 (86%)	1.01	3 (15%) 2 2	30, 44, 124, 138	0
1	C	19/22 (86%)	-0.12	0 100 100	29, 34, 59, 69	0
1	D	19/22 (86%)	1.92	5 (26%) 0 0	32, 57, 167, 227	0
1	E	19/22 (86%)	1.89	4 (21%) 1 1	37, 51, 159, 162	0
1	F	19/22 (86%)	0.28	0 100 100	29, 37, 78, 78	0
1	G	19/22 (86%)	-0.10	0 100 100	30, 38, 78, 94	0
1	H	19/22 (86%)	1.91	5 (26%) 0 0	37, 55, 159, 163	0
1	I	19/22 (86%)	1.84	6 (31%) 0 0	34, 49, 148, 149	0
1	J	19/22 (86%)	2.65	9 (47%) 0 0	29, 73, 153, 170	0
1	K	19/22 (86%)	3.14	12 (63%) 0 0	58, 97, 168, 182	0
All	All	209/242 (86%)	1.36	48 (22%) 0 1	28, 55, 152, 227	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	13	SER	14.6
1	D	13	SER	13.6
1	H	12	GLY	11.1
1	E	13	SER	10.4
1	K	13	SER	10.4
1	D	14	ASN	9.5
1	I	13	SER	8.6
1	K	14	ASN	7.8
1	J	14	ASN	7.2
1	I	12	GLY	7.0
1	B	14	ASN	6.9
1	H	11	VAL	6.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	J	12	GLY	6.8
1	E	12	GLY	6.6
1	H	13	SER	6.6
1	B	13	SER	6.5
1	K	11	VAL	5.9
1	K	1	VAL	5.9
1	D	15	LYS	5.6
1	D	11	VAL	5.5
1	I	11	VAL	5.5
1	I	14	ASN	5.2
1	J	11	VAL	4.9
1	H	14	ASN	4.9
1	E	11	VAL	4.5
1	E	14	ASN	4.4
1	J	15	LYS	3.9
1	K	3	LYS	3.9
1	K	7	PHE	3.7
1	K	22	MET	3.4
1	I	10	ASP	3.3
1	K	21	LEU	3.3
1	I	15	LYS	3.1
1	A	12	GLY	3.1
1	D	10	ASP	3.0
1	J	3	LYS	2.9
1	A	14	ASN	2.9
1	H	15	LYS	2.7
1	K	5	VAL	2.7
1	K	15	LYS	2.7
1	A	11	VAL	2.6
1	K	12	GLY	2.6
1	J	4	LEU	2.5
1	J	22	MET	2.3
1	B	12	GLY	2.2
1	A	13	SER	2.1
1	J	21	LEU	2.1
1	K	9	GLU	2.1

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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	ORN	K	2	8/9	0.36	0.81	142,182,195,195	0
1	ORN	J	2	8/9	0.60	0.61	127,152,170,170	0
1	SAR	K	20	5/6	0.87	0.23	62,74,79,79	0
1	ORN	A	2	8/9	0.89	0.14	47,61,79,79	0
1	ORN	E	2	8/9	0.90	0.13	58,70,80,80	0
1	ORN	F	2	8/9	0.92	0.13	35,44,53,53	0
1	ORN	I	2	8/9	0.93	0.10	52,63,76,76	0
1	ORN	C	2	8/9	0.93	0.14	48,60,71,71	0
1	ORN	B	2	8/9	0.93	0.16	47,61,74,74	0
1	ORN	D	2	8/9	0.93	0.13	51,65,80,80	0
1	ORN	H	2	8/9	0.93	0.29	70,86,95,95	0
1	ORN	G	2	8/9	0.93	0.13	39,51,65,65	0
1	SAR	D	20	5/6	0.94	0.10	40,44,51,51	0
1	SAR	A	20	5/6	0.95	0.16	36,44,46,46	0
1	SAR	J	20	5/6	0.95	0.11	40,51,78,78	0
1	SAR	F	20	5/6	0.97	0.16	26,31,38,38	0
1	SAR	H	20	5/6	0.97	0.14	50,57,62,62	0
1	SAR	E	20	5/6	0.97	0.15	38,42,47,47	0
1	SAR	G	20	5/6	0.98	0.14	24,30,36,36	0
1	SAR	B	20	5/6	0.98	0.16	21,28,34,34	0
1	SAR	C	20	5/6	0.98	0.16	23,28,33,33	0
1	SAR	I	20	5/6	0.98	0.10	33,39,47,47	0
1	PHI	I	6	12/13	0.99	0.14	26,30,37,37	0
1	PHI	G	6	12/13	0.99	0.15	33,40,48,53	0
1	PHI	B	6	12/13	0.99	0.16	23,29,39,40	0
1	PHI	C	6	12/13	0.99	0.16	19,23,32,34	0
1	PHI	K	6	12/13	0.99	0.13	42,57,70,79	0
1	PHI	E	6	12/13	1.00	0.18	32,39,44,47	0
1	PHI	F	6	12/13	1.00	0.18	28,34,39,41	0
1	PHI	D	6	12/13	1.00	0.14	26,31,42,45	0
1	PHI	H	6	12/13	1.00	0.12	31,35,40,42	0
1	PHI	A	6	12/13	1.00	0.16	26,29,35,36	0
1	PHI	J	6	12/13	1.00	0.13	27,32,40,45	0

### 6.3 Carbohydrates

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	HEZ	H	102	8/8	0.59	0.45	165,198,198,198	0
2	HEZ	H	101	8/8	0.70	0.23	65,78,82,82	0
2	HEZ	J	102	8/8	0.81	0.16	65,78,80,80	0
2	HEZ	G	101	8/8	0.81	0.19	55,68,78,78	0
2	HEZ	J	101	8/8	0.81	0.27	65,80,91,94	0
2	HEZ	C	101	8/8	0.83	0.18	63,76,78,79	0
2	HEZ	I	101	8/8	0.86	0.33	60,72,85,87	0
2	HEZ	D	101	8/8	0.86	0.19	60,73,84,84	0
2	HEZ	A	101	8/8	0.90	0.17	53,64,73,79	0
2	HEZ	E	101	8/8	0.91	0.17	58,71,79,81	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.