



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 10:10 pm BST

PDB ID : 4DMU  
Title : Crystal structure of the von Willebrand factor A3 domain in complex with a collagen III derived triple-helical peptide  
Authors : Brondijk, T.H.C.; Huizinga, E.G.  
Deposited on : 2012-02-08  
Resolution : 2.80 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](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.

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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

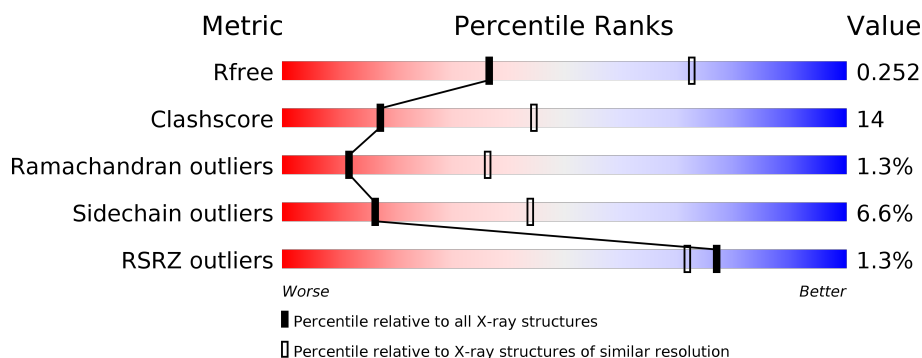
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	87	<div> <div>5%</div> <div> <div>80%</div> <div>10%</div> <div>9%</div> </div> </div>
1	C	87	<div> <div>82%</div> <div>9%</div> <div>9%</div> </div>
1	E	87	<div> <div>83%</div> <div>7%</div> <div>9%</div> </div>
1	G	87	<div> <div>2%</div> <div> <div>78%</div> <div>11%</div> <div>9%</div> </div> </div>
1	I	87	<div> <div>82%</div> <div>9%</div> <div>9%</div> </div>
1	K	87	<div> <div>70%</div> <div>22%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	192	
2	D	192	
2	F	192	
2	H	192	
2	J	192	
2	L	192	

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	HYP	A	127	-	-	-	X
1	HYP	A	227	-	-	-	X
1	HYP	A	27	-	-	-	X
1	HYP	G	127	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11651 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 Collagen III derived triple-helical peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	79	Total	C	N	O	S	0	0	0
			529	332	91	103	3			
1	C	79	Total	C	N	O	S	0	0	0
			529	332	91	103	3			
1	E	79	Total	C	N	O	S	0	0	0
			529	332	91	103	3			
1	G	79	Total	C	N	O	S	0	0	0
			529	332	91	103	3			
1	I	79	Total	C	N	O	S	0	0	0
			529	332	91	103	3			
1	K	80	Total	C	N	O	S	0	0	0
			536	337	92	104	3			

- Molecule 2 is a protein called von Willebrand factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	188	Total	C	N	O	S	0	0	0
			1406	890	241	269	6			
2	D	188	Total	C	N	O	S	0	0	0
			1406	890	241	269	6			
2	F	188	Total	C	N	O	S	0	0	0
			1406	890	241	269	6			
2	H	187	Total	C	N	O	S	0	0	0
			1400	887	240	268	5			
2	J	191	Total	C	N	O	S	0	0	0
			1426	902	244	274	6			
2	L	188	Total	C	N	O	S	0	0	0
			1406	890	241	269	6			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

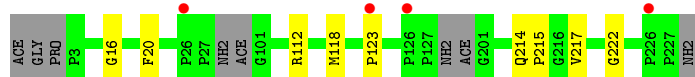
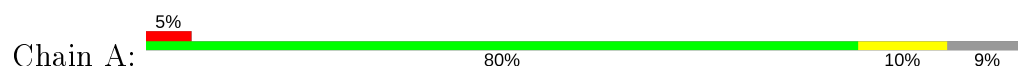


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		

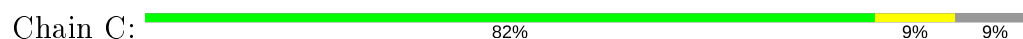
### 3 Residue-property plots [i](#)

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.

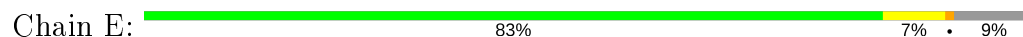
- Molecule 1: Collagen III derived triple-helical peptide



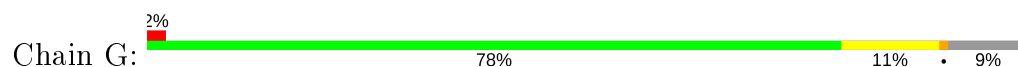
- Molecule 1: Collagen III derived triple-helical peptide



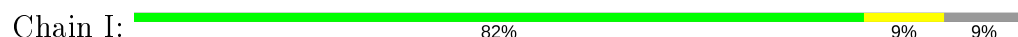
- Molecule 1: Collagen III derived triple-helical peptide



- Molecule 1: Collagen III derived triple-helical peptide

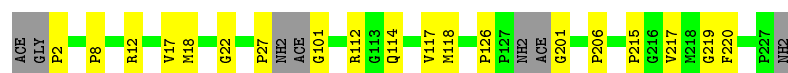


- Molecule 1: Collagen III derived triple-helical peptide



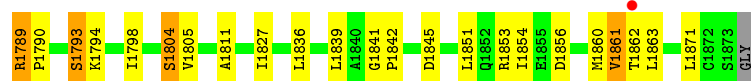
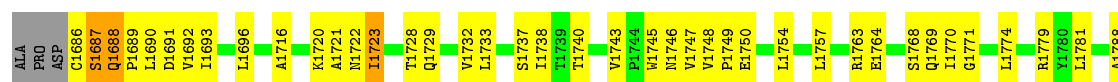
- Molecule 1: Collagen III derived triple-helical peptide

Chain K:  70% 22% 8%



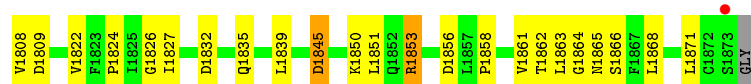
- Molecule 2: von Willebrand factor

Chain B:  65% 29%



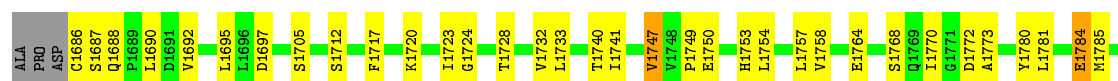
- Molecule 2: von Willebrand factor

Chain D:  69% 26%



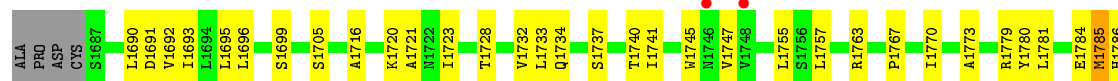
- Molecule 2: von Willebrand factor

Chain F:  67% 29%

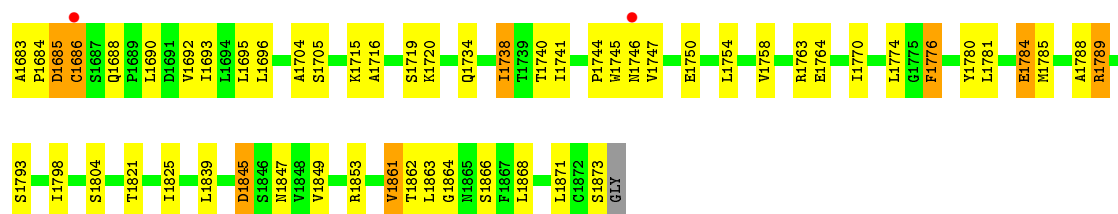


- Molecule 2: von Willebrand factor

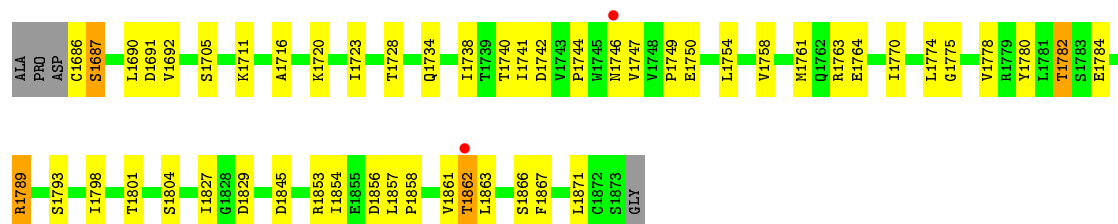
Chain H:  67% 28%



- Molecule 2: von Willebrand factor



• Molecule 2: von Willebrand factor





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	187.61Å 187.61Å 89.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.32 – 2.80 46.32 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.2 (46.32-2.80) 92.4 (46.32-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.202 , 0.253 0.199 , 0.252	Depositor DCC
$R_{free}$ test set	2099 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.9	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 9.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.518 for H, K, L 0.482 for h+k,-k,-l	Depositor
Outliers	2 of 41013 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11651	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	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 33.33 % 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 8.1368e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HYP, SO4

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	0.61	0/361	0.66	0/460
1	C	0.75	0/361	0.68	0/460
1	E	0.61	0/361	0.71	0/460
1	G	0.54	0/361	0.65	0/460
1	I	0.71	0/361	0.72	0/460
1	K	0.68	0/368	0.69	0/468
2	B	0.64	0/1431	0.73	0/1946
2	D	0.72	0/1431	0.79	1/1946 (0.1%)
2	F	0.64	0/1431	0.75	0/1946
2	H	0.57	0/1425	0.65	0/1938
2	J	0.88	0/1452	0.87	1/1976 (0.1%)
2	L	0.78	0/1431	0.80	0/1946
All	All	0.70	0/10774	0.75	2/14466 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1789	ARG	NE-CZ-NH2	5.09	122.85	120.30
2	D	1692	VAL	CB-CA-C	-5.07	101.78	111.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	529	0	487	9	0
1	C	529	0	487	12	0
1	E	529	0	487	7	0
1	G	529	0	487	12	0
1	I	529	0	487	11	0
1	K	536	0	493	17	0
2	B	1406	0	1421	56	0
2	D	1406	0	1421	46	0
2	F	1406	0	1421	43	0
2	H	1400	0	1418	46	0
2	J	1426	0	1437	46	0
2	L	1406	0	1421	50	0
3	C	5	0	0	0	0
3	F	5	0	0	1	0
3	I	5	0	0	0	0
3	K	5	0	0	1	0
All	All	11651	0	11467	319	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 14.

The worst 5 of 319 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:215:HYP:HD23	2:F:1740:THR:HG22	1.31	1.10
2:J:1770:ILE:HD12	2:J:1804:SER:HB2	1.38	1.06
1:C:215:HYP:HD23	2:D:1740:THR:HG22	1.37	1.02
1:K:215:HYP:HD23	2:L:1740:THR:HG22	1.41	0.98
2:B:1693:ILE:HG23	2:B:1733:LEU:HD13	1.49	0.91

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	56/87 (64%)	52 (93%)	4 (7%)	0	100	100
1	C	56/87 (64%)	51 (91%)	4 (7%)	1 (2%)	8	28
1	E	56/87 (64%)	53 (95%)	3 (5%)	0	100	100
1	G	56/87 (64%)	51 (91%)	4 (7%)	1 (2%)	8	28
1	I	56/87 (64%)	54 (96%)	2 (4%)	0	100	100
1	K	56/87 (64%)	53 (95%)	3 (5%)	0	100	100
2	B	186/192 (97%)	172 (92%)	9 (5%)	5 (3%)	5	17
2	D	186/192 (97%)	163 (88%)	21 (11%)	2 (1%)	14	41
2	F	186/192 (97%)	168 (90%)	14 (8%)	4 (2%)	6	22
2	H	185/192 (96%)	169 (91%)	15 (8%)	1 (0%)	29	61
2	J	189/192 (98%)	168 (89%)	19 (10%)	2 (1%)	14	41
2	L	186/192 (97%)	169 (91%)	14 (8%)	3 (2%)	9	31
All	All	1454/1674 (87%)	1323 (91%)	112 (8%)	19 (1%)	12	36

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1687	SER
2	F	1687	SER
2	D	1687	SER
2	F	1864	GLY
1	G	22	GLY

### 5.3.2 Protein sidechains ⓘ

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	32/33 (97%)	32 (100%)	0	100	100
1	C	32/33 (97%)	32 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	32/33 (97%)	31 (97%)	1 (3%)	40	74
1	G	32/33 (97%)	32 (100%)	0	100	100
1	I	32/33 (97%)	32 (100%)	0	100	100
1	K	33/33 (100%)	33 (100%)	0	100	100
2	B	155/157 (99%)	145 (94%)	10 (6%)	17	44
2	D	155/157 (99%)	144 (93%)	11 (7%)	14	39
2	F	155/157 (99%)	141 (91%)	14 (9%)	9	28
2	H	154/157 (98%)	141 (92%)	13 (8%)	11	31
2	J	157/157 (100%)	141 (90%)	16 (10%)	7	22
2	L	155/157 (99%)	146 (94%)	9 (6%)	20	50
All	All	1124/1140 (99%)	1050 (93%)	74 (7%)	16	44

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	1853	ARG
2	H	1785	MET
2	L	1763	ARG
2	F	1861	VAL
2	H	1705	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	1869	HIS
2	F	1753	HIS
2	J	1762	GLN
2	D	1769	GLN
2	H	1869	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

126 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	HYP	G	215	1	6,8,9	0.75	0	5,10,12	1.54	1 (20%)
1	HYP	A	215	1	6,8,9	0.83	0	5,10,12	1.66	1 (20%)
1	HYP	I	24	1	6,8,9	0.66	0	5,10,12	2.11	2 (40%)
1	HYP	C	15	1	6,8,9	1.33	1 (16%)	5,10,12	1.68	2 (40%)
1	HYP	I	209	1	6,8,9	0.95	0	5,10,12	2.19	2 (40%)
1	HYP	E	9	1	6,8,9	0.66	0	5,10,12	1.16	1 (20%)
1	HYP	C	227	1	6,8,9	0.60	0	5,10,12	1.27	1 (20%)
1	HYP	A	227	1	6,8,9	0.64	0	5,10,12	2.08	2 (40%)
1	HYP	I	206	1	6,8,9	0.81	0	5,10,12	1.59	1 (20%)
1	HYP	K	215	1	6,8,9	1.12	0	5,10,12	0.74	0
1	HYP	G	121	1	6,8,9	0.68	0	5,10,12	1.87	1 (20%)
1	HYP	E	206	1	6,8,9	0.59	0	5,10,12	1.52	1 (20%)
1	HYP	C	27	1	6,8,9	0.63	0	5,10,12	1.35	1 (20%)
1	HYP	E	24	1	6,8,9	0.55	0	5,10,12	1.51	1 (20%)
1	HYP	I	224	1	6,8,9	0.53	0	5,10,12	1.98	2 (40%)
1	HYP	E	27	1	6,8,9	0.61	0	5,10,12	1.65	2 (40%)
1	HYP	I	227	1	6,8,9	0.54	0	5,10,12	1.43	1 (20%)
1	HYP	A	206	1	6,8,9	0.67	0	5,10,12	0.89	0
1	HYP	I	15	1	6,8,9	1.17	1 (16%)	5,10,12	2.16	2 (40%)
1	HYP	C	215	1	6,8,9	0.53	0	5,10,12	1.18	0
1	HYP	I	21	1	6,8,9	0.97	0	5,10,12	1.67	2 (40%)
1	HYP	G	103	1	6,8,9	0.76	0	5,10,12	1.99	2 (40%)
1	HYP	A	3	1	6,8,9	0.52	0	5,10,12	2.19	2 (40%)
1	HYP	E	15	1	6,8,9	0.94	1 (16%)	5,10,12	2.53	4 (80%)
1	HYP	G	9	1	6,8,9	0.65	0	5,10,12	1.62	1 (20%)
1	HYP	A	21	1	6,8,9	0.70	0	5,10,12	1.70	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HYP	E	127	1	6,8,9	0.68	0	5,10,12	2.25	3 (60%)
1	HYP	I	106	1	6,8,9	0.46	0	5,10,12	1.20	1 (20%)
1	HYP	I	27	1	6,8,9	0.61	0	5,10,12	1.58	2 (40%)
1	HYP	K	9	1	6,8,9	0.83	0	5,10,12	2.33	2 (40%)
1	HYP	I	9	1	6,8,9	0.56	0	5,10,12	1.29	1 (20%)
1	HYP	C	206	1	6,8,9	0.73	0	5,10,12	2.00	1 (20%)
1	HYP	E	221	1	6,8,9	0.63	0	5,10,12	1.17	0
1	HYP	E	224	1	6,8,9	0.68	0	5,10,12	1.10	0
1	HYP	I	221	1	6,8,9	0.66	0	5,10,12	0.99	0
1	HYP	A	109	1	6,8,9	0.44	0	5,10,12	1.60	1 (20%)
1	HYP	G	106	1	6,8,9	0.78	0	5,10,12	1.23	0
1	HYP	K	27	1	6,8,9	0.51	0	5,10,12	2.14	2 (40%)
1	HYP	E	21	1	6,8,9	1.06	0	5,10,12	1.47	1 (20%)
1	HYP	E	209	1	6,8,9	0.58	0	5,10,12	2.10	2 (40%)
1	HYP	C	209	1	6,8,9	1.07	0	5,10,12	2.35	3 (60%)
1	HYP	G	221	1	6,8,9	0.59	0	5,10,12	2.04	2 (40%)
1	HYP	K	224	1	6,8,9	0.72	0	5,10,12	1.46	1 (20%)
1	HYP	G	27	1	6,8,9	0.54	0	5,10,12	1.98	2 (40%)
1	HYP	A	209	1	6,8,9	0.63	0	5,10,12	1.60	2 (40%)
1	HYP	K	127	1	6,8,9	0.63	0	5,10,12	2.06	2 (40%)
1	HYP	G	3	1	6,8,9	0.60	0	5,10,12	1.98	2 (40%)
1	HYP	E	227	1	6,8,9	0.61	0	5,10,12	1.61	1 (20%)
1	HYP	G	21	1	6,8,9	0.68	0	5,10,12	1.95	1 (20%)
1	HYP	A	9	1	6,8,9	0.53	0	5,10,12	1.44	1 (20%)
1	HYP	K	227	1	6,8,9	0.66	0	5,10,12	1.20	0
1	HYP	G	224	1	6,8,9	0.54	0	5,10,12	1.71	2 (40%)
1	HYP	E	6	1	6,8,9	0.87	0	5,10,12	1.87	2 (40%)
1	HYP	K	206	1	6,8,9	0.86	0	5,10,12	1.46	1 (20%)
1	HYP	A	6	1	6,8,9	0.76	0	5,10,12	1.50	1 (20%)
1	HYP	I	121	1	6,8,9	1.00	0	5,10,12	1.17	1 (20%)
1	HYP	E	215	1	6,8,9	0.94	0	5,10,12	1.29	1 (20%)
1	HYP	G	206	1	6,8,9	0.56	0	5,10,12	1.15	0
1	HYP	G	24	1	6,8,9	0.59	0	5,10,12	1.94	1 (20%)
1	HYP	K	209	1	6,8,9	1.21	1 (16%)	5,10,12	1.73	2 (40%)
1	HYP	G	227	1	6,8,9	0.58	0	5,10,12	2.28	2 (40%)
1	HYP	E	106	1	6,8,9	0.85	0	5,10,12	1.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HYP	I	215	1	6,8,9	0.95	0	5,10,12	1.13	0
1	HYP	K	103	1	6,8,9	0.80	0	5,10,12	1.97	2 (40%)
1	HYP	G	109	1	6,8,9	0.62	0	5,10,12	0.88	0
1	HYP	I	124	1	6,8,9	0.62	0	5,10,12	1.58	1 (20%)
1	HYP	K	115	1	6,8,9	0.79	0	5,10,12	2.11	1 (20%)
1	HYP	G	6	1	6,8,9	0.62	0	5,10,12	2.01	2 (40%)
1	HYP	I	115	1	6,8,9	1.27	0	5,10,12	1.97	1 (20%)
1	HYP	E	203	1	6,8,9	0.69	0	5,10,12	1.19	0
1	HYP	A	103	1	6,8,9	0.56	0	5,10,12	2.48	3 (60%)
1	HYP	G	209	1	6,8,9	0.80	0	5,10,12	1.47	0
1	HYP	C	6	1	6,8,9	0.94	0	5,10,12	1.81	2 (40%)
1	HYP	A	224	1	6,8,9	0.66	0	5,10,12	1.47	0
1	HYP	G	15	1	6,8,9	0.90	0	5,10,12	2.09	1 (20%)
1	HYP	A	127	1	6,8,9	0.55	0	5,10,12	2.22	2 (40%)
1	HYP	C	9	1	6,8,9	0.48	0	5,10,12	1.08	0
1	HYP	C	124	1	6,8,9	0.58	0	5,10,12	2.33	2 (40%)
1	HYP	E	115	1	6,8,9	0.87	0	5,10,12	1.65	1 (20%)
1	HYP	A	115	1	6,8,9	0.88	0	5,10,12	1.92	2 (40%)
1	HYP	E	121	1	6,8,9	1.03	0	5,10,12	1.66	1 (20%)
1	HYP	C	121	1	6,8,9	0.43	0	5,10,12	1.48	1 (20%)
1	HYP	I	103	1	6,8,9	0.72	0	5,10,12	2.19	2 (40%)
1	HYP	I	127	1	6,8,9	0.69	0	5,10,12	2.34	3 (60%)
1	HYP	A	15	1	6,8,9	1.00	0	5,10,12	1.86	2 (40%)
1	HYP	K	124	1	6,8,9	0.55	0	5,10,12	2.18	2 (40%)
1	HYP	A	106	1	6,8,9	0.70	0	5,10,12	1.72	1 (20%)
1	HYP	G	124	1	6,8,9	0.58	0	5,10,12	2.38	2 (40%)
1	HYP	E	124	1	6,8,9	0.73	0	5,10,12	1.99	2 (40%)
1	HYP	A	27	1	6,8,9	0.56	0	5,10,12	1.81	2 (40%)
1	HYP	I	3	1	6,8,9	0.62	0	5,10,12	2.00	2 (40%)
1	HYP	E	3	1	6,8,9	0.67	0	5,10,12	1.97	2 (40%)
1	HYP	I	6	1	6,8,9	0.95	0	5,10,12	1.39	0
1	HYP	K	109	1	6,8,9	0.59	0	5,10,12	1.01	0
1	HYP	A	24	1	6,8,9	0.62	0	5,10,12	1.92	2 (40%)
1	HYP	G	203	1	6,8,9	0.58	0	5,10,12	1.32	1 (20%)
1	HYP	C	203	1	6,8,9	0.74	0	5,10,12	1.45	0
1	HYP	A	121	1	6,8,9	0.72	0	5,10,12	0.88	0
1	HYP	K	3	1	6,8,9	0.63	0	5,10,12	1.81	2 (40%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HYP	E	109	1	6,8,9	0.73	0	5,10,12	1.51	1 (20%)
1	HYP	C	106	1	6,8,9	0.78	0	5,10,12	1.46	1 (20%)
1	HYP	A	124	1	6,8,9	0.58	0	5,10,12	2.00	2 (40%)
1	HYP	C	221	1	6,8,9	0.54	0	5,10,12	1.57	1 (20%)
1	HYP	K	221	1	6,8,9	0.63	0	5,10,12	1.32	0
1	HYP	C	224	1	6,8,9	0.62	0	5,10,12	1.54	0
1	HYP	C	127	1	6,8,9	0.66	0	5,10,12	2.39	3 (60%)
1	HYP	G	127	1	6,8,9	0.83	0	5,10,12	2.32	3 (60%)
1	HYP	K	6	1	6,8,9	0.87	0	5,10,12	1.28	0
1	HYP	K	121	1	6,8,9	0.91	0	5,10,12	1.70	1 (20%)
1	HYP	C	115	1	6,8,9	0.96	0	5,10,12	1.66	1 (20%)
1	HYP	A	221	1	6,8,9	0.56	0	5,10,12	1.64	1 (20%)
1	HYP	C	24	1	6,8,9	0.60	0	5,10,12	1.66	1 (20%)
1	HYP	C	21	1	6,8,9	0.66	0	5,10,12	1.75	3 (60%)
1	HYP	I	203	1	6,8,9	0.79	0	5,10,12	1.81	1 (20%)
1	HYP	C	109	1	6,8,9	0.68	0	5,10,12	1.32	1 (20%)
1	HYP	K	203	1	6,8,9	0.83	0	5,10,12	1.69	1 (20%)
1	HYP	G	115	1	6,8,9	0.60	0	5,10,12	1.70	1 (20%)
1	HYP	K	15	1	6,8,9	0.82	0	5,10,12	1.59	1 (20%)
1	HYP	K	24	1	6,8,9	0.60	0	5,10,12	2.06	1 (20%)
1	HYP	K	21	1	6,8,9	1.02	0	5,10,12	0.91	0
1	HYP	I	109	1	6,8,9	0.77	0	5,10,12	1.32	1 (20%)
1	HYP	C	3	1	6,8,9	0.81	0	5,10,12	2.38	3 (60%)
1	HYP	K	106	1	6,8,9	0.66	0	5,10,12	1.35	0
1	HYP	E	103	1	6,8,9	0.71	0	5,10,12	1.53	1 (20%)
1	HYP	C	103	1	6,8,9	0.83	0	5,10,12	1.52	1 (20%)
1	HYP	A	203	1	6,8,9	0.64	0	5,10,12	1.55	1 (20%)

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	HYP	G	215	1	-	0/0/11/13	0/1/1/1
1	HYP	A	215	1	-	0/0/11/13	0/1/1/1
1	HYP	I	24	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	C	15	1	-	0/0/11/13	0/1/1/1
1	HYP	I	209	1	-	0/0/11/13	0/1/1/1
1	HYP	E	9	1	-	0/0/11/13	0/1/1/1
1	HYP	C	227	1	-	0/0/11/13	0/1/1/1
1	HYP	A	227	1	-	0/0/11/13	0/1/1/1
1	HYP	I	206	1	-	0/0/11/13	0/1/1/1
1	HYP	K	215	1	-	0/0/11/13	0/1/1/1
1	HYP	G	121	1	-	0/0/11/13	0/1/1/1
1	HYP	E	206	1	-	0/0/11/13	0/1/1/1
1	HYP	C	27	1	-	0/0/11/13	0/1/1/1
1	HYP	E	24	1	-	0/0/11/13	0/1/1/1
1	HYP	I	224	1	-	0/0/11/13	0/1/1/1
1	HYP	E	27	1	-	0/0/11/13	0/1/1/1
1	HYP	I	227	1	-	0/0/11/13	0/1/1/1
1	HYP	A	206	1	-	0/0/11/13	0/1/1/1
1	HYP	I	15	1	-	0/0/11/13	0/1/1/1
1	HYP	C	215	1	-	0/0/11/13	0/1/1/1
1	HYP	I	21	1	-	0/0/11/13	0/1/1/1
1	HYP	G	103	1	-	0/0/11/13	0/1/1/1
1	HYP	A	3	1	-	0/0/11/13	0/1/1/1
1	HYP	E	15	1	-	0/0/11/13	0/1/1/1
1	HYP	G	9	1	-	0/0/11/13	0/1/1/1
1	HYP	A	21	1	-	0/0/11/13	0/1/1/1
1	HYP	E	127	1	-	0/0/11/13	0/1/1/1
1	HYP	I	106	1	-	0/0/11/13	0/1/1/1
1	HYP	I	27	1	-	0/0/11/13	0/1/1/1
1	HYP	K	9	1	-	0/0/11/13	0/1/1/1
1	HYP	I	9	1	-	0/0/11/13	0/1/1/1
1	HYP	C	206	1	-	0/0/11/13	0/1/1/1
1	HYP	E	221	1	-	0/0/11/13	0/1/1/1
1	HYP	E	224	1	-	0/0/11/13	0/1/1/1
1	HYP	I	221	1	-	0/0/11/13	0/1/1/1
1	HYP	A	109	1	-	0/0/11/13	0/1/1/1
1	HYP	G	106	1	-	0/0/11/13	0/1/1/1
1	HYP	K	27	1	-	0/0/11/13	0/1/1/1
1	HYP	E	21	1	-	0/0/11/13	0/1/1/1
1	HYP	E	209	1	-	0/0/11/13	0/1/1/1
1	HYP	C	209	1	-	0/0/11/13	0/1/1/1
1	HYP	G	221	1	-	0/0/11/13	0/1/1/1
1	HYP	K	224	1	-	0/0/11/13	0/1/1/1
1	HYP	G	27	1	-	0/0/11/13	0/1/1/1
1	HYP	A	209	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	K	127	1	-	0/0/11/13	0/1/1/1
1	HYP	G	3	1	-	0/0/11/13	0/1/1/1
1	HYP	E	227	1	-	0/0/11/13	0/1/1/1
1	HYP	G	21	1	-	0/0/11/13	0/1/1/1
1	HYP	A	9	1	-	0/0/11/13	0/1/1/1
1	HYP	K	227	1	-	0/0/11/13	0/1/1/1
1	HYP	G	224	1	-	0/0/11/13	0/1/1/1
1	HYP	E	6	1	-	0/0/11/13	0/1/1/1
1	HYP	K	206	1	-	0/0/11/13	0/1/1/1
1	HYP	A	6	1	-	0/0/11/13	0/1/1/1
1	HYP	I	121	1	-	0/0/11/13	0/1/1/1
1	HYP	E	215	1	-	0/0/11/13	0/1/1/1
1	HYP	G	206	1	-	0/0/11/13	0/1/1/1
1	HYP	G	24	1	-	0/0/11/13	0/1/1/1
1	HYP	K	209	1	-	0/0/11/13	0/1/1/1
1	HYP	G	227	1	-	0/0/11/13	0/1/1/1
1	HYP	E	106	1	-	0/0/11/13	0/1/1/1
1	HYP	I	215	1	-	0/0/11/13	0/1/1/1
1	HYP	K	103	1	-	0/0/11/13	0/1/1/1
1	HYP	G	109	1	-	0/0/11/13	0/1/1/1
1	HYP	I	124	1	-	0/0/11/13	0/1/1/1
1	HYP	K	115	1	-	0/0/11/13	0/1/1/1
1	HYP	G	6	1	-	0/0/11/13	0/1/1/1
1	HYP	I	115	1	-	0/0/11/13	0/1/1/1
1	HYP	E	203	1	-	0/0/11/13	0/1/1/1
1	HYP	A	103	1	-	0/0/11/13	0/1/1/1
1	HYP	G	209	1	-	0/0/11/13	0/1/1/1
1	HYP	C	6	1	-	0/0/11/13	0/1/1/1
1	HYP	A	224	1	-	0/0/11/13	0/1/1/1
1	HYP	G	15	1	-	0/0/11/13	0/1/1/1
1	HYP	A	127	1	-	0/0/11/13	0/1/1/1
1	HYP	C	9	1	-	0/0/11/13	0/1/1/1
1	HYP	C	124	1	-	0/0/11/13	0/1/1/1
1	HYP	E	115	1	-	0/0/11/13	0/1/1/1
1	HYP	A	115	1	-	0/0/11/13	0/1/1/1
1	HYP	E	121	1	-	0/0/11/13	0/1/1/1
1	HYP	C	121	1	-	0/0/11/13	0/1/1/1
1	HYP	I	103	1	-	0/0/11/13	0/1/1/1
1	HYP	I	127	1	-	0/0/11/13	0/1/1/1
1	HYP	A	15	1	-	0/0/11/13	0/1/1/1
1	HYP	K	124	1	-	0/0/11/13	0/1/1/1
1	HYP	A	106	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	G	124	1	-	0/0/11/13	0/1/1/1
1	HYP	E	124	1	-	0/0/11/13	0/1/1/1
1	HYP	A	27	1	-	0/0/11/13	0/1/1/1
1	HYP	I	3	1	-	0/0/11/13	0/1/1/1
1	HYP	E	3	1	-	0/0/11/13	0/1/1/1
1	HYP	I	6	1	-	0/0/11/13	0/1/1/1
1	HYP	K	109	1	-	0/0/11/13	0/1/1/1
1	HYP	A	24	1	-	0/0/11/13	0/1/1/1
1	HYP	G	203	1	-	0/0/11/13	0/1/1/1
1	HYP	C	203	1	-	0/0/11/13	0/1/1/1
1	HYP	A	121	1	-	0/0/11/13	0/1/1/1
1	HYP	K	3	1	-	0/0/11/13	0/1/1/1
1	HYP	E	109	1	-	0/0/11/13	0/1/1/1
1	HYP	C	106	1	-	0/0/11/13	0/1/1/1
1	HYP	A	124	1	-	0/0/11/13	0/1/1/1
1	HYP	C	221	1	-	0/0/11/13	0/1/1/1
1	HYP	K	221	1	-	0/0/11/13	0/1/1/1
1	HYP	C	224	1	-	0/0/11/13	0/1/1/1
1	HYP	C	127	1	-	0/0/11/13	0/1/1/1
1	HYP	G	127	1	-	0/0/11/13	0/1/1/1
1	HYP	K	6	1	-	0/0/11/13	0/1/1/1
1	HYP	K	121	1	-	0/0/11/13	0/1/1/1
1	HYP	C	115	1	-	0/0/11/13	0/1/1/1
1	HYP	A	221	1	-	0/0/11/13	0/1/1/1
1	HYP	C	24	1	-	0/0/11/13	0/1/1/1
1	HYP	C	21	1	-	0/0/11/13	0/1/1/1
1	HYP	I	203	1	-	0/0/11/13	0/1/1/1
1	HYP	C	109	1	-	0/0/11/13	0/1/1/1
1	HYP	K	203	1	-	0/0/11/13	0/1/1/1
1	HYP	G	115	1	-	0/0/11/13	0/1/1/1
1	HYP	K	15	1	-	0/0/11/13	0/1/1/1
1	HYP	K	24	1	-	0/0/11/13	0/1/1/1
1	HYP	K	21	1	-	0/0/11/13	0/1/1/1
1	HYP	I	109	1	-	0/0/11/13	0/1/1/1
1	HYP	C	3	1	-	0/0/11/13	0/1/1/1
1	HYP	K	106	1	-	0/0/11/13	0/1/1/1
1	HYP	E	103	1	-	0/0/11/13	0/1/1/1
1	HYP	C	103	1	-	0/0/11/13	0/1/1/1
1	HYP	A	203	1	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	15	HYP	CB-CA	-2.50	1.48	1.54
1	K	209	HYP	CB-CA	-2.40	1.49	1.54
1	I	15	HYP	CB-CA	-2.17	1.49	1.54
1	E	15	HYP	CB-CA	-2.02	1.50	1.54

The worst 5 of 161 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	124	HYP	CG-CB-CA	3.84	108.81	103.96
1	C	206	HYP	CB-CG-CD	-3.81	98.59	103.27
1	K	115	HYP	CB-CG-CD	3.79	107.91	103.27
1	K	24	HYP	CB-CG-CD	3.77	107.89	103.27
1	C	124	HYP	CG-CB-CA	3.77	108.72	103.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	215	HYP	1	0
1	A	215	HYP	2	0
1	E	9	HYP	1	0
1	K	215	HYP	1	0
1	C	215	HYP	1	0
1	K	27	HYP	1	0
1	G	21	HYP	2	0
1	K	206	HYP	1	0
1	E	215	HYP	2	0
1	I	215	HYP	1	0
1	C	9	HYP	1	0
1	I	3	HYP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
3	SO4	I	301	-	4,4,4	0.36	0	6,6,6	0.54	0
3	SO4	F	1901	-	4,4,4	0.34	0	6,6,6	0.55	0
3	SO4	K	301	-	4,4,4	0.27	0	6,6,6	0.45	0
3	SO4	C	301	-	4,4,4	0.32	0	6,6,6	0.67	0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1901	SO4	1	0
3	K	301	SO4	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	58/87 (66%)	0.29	4 (6%) 16 10	42, 61, 124, 149	0
1	C	58/87 (66%)	-0.33	0 100 100	23, 43, 89, 98	0
1	E	58/87 (66%)	-0.42	0 100 100	31, 41, 74, 87	0
1	G	58/87 (66%)	0.02	2 (3%) 45 35	53, 67, 119, 134	0
1	I	58/87 (66%)	-0.34	0 100 100	19, 36, 78, 85	0
1	K	59/87 (67%)	-0.40	0 100 100	25, 42, 85, 94	0
2	B	188/192 (97%)	-0.19	1 (0%) 91 88	36, 55, 84, 103	0
2	D	188/192 (97%)	-0.25	2 (1%) 80 75	27, 45, 64, 79	0
2	F	188/192 (97%)	-0.10	2 (1%) 80 75	35, 55, 78, 89	0
2	H	187/192 (97%)	0.19	4 (2%) 63 54	54, 67, 98, 116	0
2	J	191/192 (99%)	-0.24	2 (1%) 82 77	20, 34, 56, 73	0
2	L	188/192 (97%)	-0.22	2 (1%) 80 75	21, 42, 76, 99	0
All	All	1479/1674 (88%)	-0.15	19 (1%) 77 72	19, 51, 86, 149	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	PRO	6.5
1	A	26	PRO	5.8
1	A	126	PRO	5.0
2	L	1862	THR	3.6
1	A	123	PRO	3.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	HYP	G	127	8/9	0.41	0.51	126,133,134,135	0
1	HYP	A	127	8/9	0.67	0.66	148,156,161,161	0
1	HYP	A	227	8/9	0.70	0.72	157,165,167,170	0
1	HYP	K	3	8/9	0.72	0.21	74,79,85,86	0
1	HYP	G	24	8/9	0.74	0.23	97,100,102,103	0
1	HYP	A	27	8/9	0.75	0.48	132,137,143,145	0
1	HYP	C	3	8/9	0.75	0.24	78,83,91,95	0
1	HYP	A	3	8/9	0.77	0.20	81,87,93,97	0
1	HYP	K	227	8/9	0.77	0.26	103,107,113,114	0
1	HYP	G	224	8/9	0.77	0.30	119,122,129,130	0
1	HYP	E	227	8/9	0.78	0.29	85,87,93,94	0
1	HYP	I	227	8/9	0.79	0.28	94,100,104,104	0
1	HYP	G	227	8/9	0.81	0.76	143,146,153,157	0
1	HYP	G	27	8/9	0.81	0.24	126,130,132,133	0
1	HYP	G	3	8/9	0.81	0.33	71,73,78,80	0
1	HYP	C	227	8/9	0.83	0.37	108,114,116,118	0
1	HYP	K	127	8/9	0.84	0.17	90,95,97,102	0
1	HYP	A	124	8/9	0.85	0.26	111,117,119,119	0
1	HYP	E	127	8/9	0.86	0.20	91,95,97,97	0
1	HYP	A	24	8/9	0.86	0.32	101,105,110,110	0
1	HYP	G	124	8/9	0.87	0.21	105,107,113,116	0
1	HYP	C	221	8/9	0.88	0.21	61,62,70,72	0
1	HYP	I	3	8/9	0.88	0.17	66,70,75,77	0
1	HYP	C	27	8/9	0.88	0.16	98,102,107,109	0
1	HYP	E	27	8/9	0.89	0.21	78,81,89,90	0
1	HYP	A	224	8/9	0.89	0.28	116,121,124,125	0
1	HYP	G	221	8/9	0.89	0.16	96,100,104,104	0
1	HYP	A	21	8/9	0.89	0.21	75,78,81,81	0
1	HYP	C	127	8/9	0.90	0.23	99,106,108,113	0
1	HYP	G	121	8/9	0.90	0.19	88,90,97,100	0
1	HYP	E	3	8/9	0.90	0.23	55,58,62,64	0
1	HYP	C	224	8/9	0.91	0.25	80,84,90,93	0
1	HYP	K	27	8/9	0.92	0.15	88,90,99,102	0
1	HYP	G	9	8/9	0.92	0.19	55,58,62,63	0
1	HYP	K	24	8/9	0.92	0.12	59,63,64,64	0
1	HYP	I	103	8/9	0.92	0.19	55,59,67,69	0
1	HYP	K	124	8/9	0.93	0.22	64,67,71,73	0
1	HYP	K	103	8/9	0.93	0.17	69,75,84,86	0
1	HYP	G	103	8/9	0.93	0.13	65,66,71,72	0
1	HYP	G	21	8/9	0.93	0.17	78,81,82,83	0
1	HYP	C	124	8/9	0.93	0.20	66,70,72,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	HYP	A	221	8/9	0.93	0.29	86,91,92,93	0
1	HYP	C	24	8/9	0.93	0.20	67,70,73,74	0
1	HYP	G	115	8/9	0.93	0.17	62,64,68,69	0
1	HYP	I	24	8/9	0.93	0.14	55,59,61,62	0
1	HYP	I	127	8/9	0.93	0.34	85,89,94,98	0
1	HYP	E	203	8/9	0.94	0.15	44,47,52,54	0
1	HYP	G	209	8/9	0.94	0.15	51,53,56,60	0
1	HYP	E	24	8/9	0.94	0.15	66,68,73,74	0
1	HYP	G	203	8/9	0.94	0.16	62,65,70,71	0
1	HYP	C	203	8/9	0.94	0.21	52,55,61,63	0
1	HYP	A	106	8/9	0.94	0.18	55,56,59,61	0
1	HYP	A	9	8/9	0.94	0.22	45,47,50,53	0
1	HYP	G	206	8/9	0.94	0.14	55,57,60,62	0
1	HYP	A	109	8/9	0.95	0.16	45,48,51,54	0
1	HYP	G	215	8/9	0.95	0.21	61,63,65,65	0
1	HYP	G	15	8/9	0.95	0.20	57,58,62,63	0
1	HYP	I	121	8/9	0.95	0.20	40,41,46,48	0
1	HYP	A	121	8/9	0.95	0.17	80,82,86,86	0
1	HYP	C	21	8/9	0.95	0.17	42,44,46,49	0
1	HYP	I	203	8/9	0.95	0.13	52,57,66,67	0
1	HYP	K	203	8/9	0.95	0.21	60,63,67,70	0
1	HYP	I	221	8/9	0.95	0.18	53,55,62,63	0
1	HYP	A	115	8/9	0.95	0.23	45,46,48,51	0
1	HYP	E	121	8/9	0.95	0.18	46,47,50,51	0
1	HYP	A	203	8/9	0.95	0.13	61,63,67,67	0
1	HYP	K	6	8/9	0.96	0.16	49,51,55,56	0
1	HYP	K	224	8/9	0.96	0.15	77,80,87,88	0
1	HYP	C	121	8/9	0.96	0.15	45,47,50,50	0
1	HYP	I	206	8/9	0.96	0.14	33,37,42,47	0
1	HYP	I	27	8/9	0.96	0.18	84,88,92,95	0
1	HYP	E	224	8/9	0.96	0.13	63,66,67,68	0
1	HYP	K	121	8/9	0.96	0.20	48,49,55,56	0
1	HYP	G	6	8/9	0.96	0.12	60,63,67,68	0
1	HYP	I	224	8/9	0.96	0.14	70,73,82,86	0
1	HYP	A	103	8/9	0.96	0.13	70,72,75,76	0
1	HYP	E	15	8/9	0.96	0.18	31,32,33,34	0
1	HYP	C	109	8/9	0.96	0.13	36,39,47,47	0
1	HYP	C	6	8/9	0.96	0.12	53,58,66,69	0
1	HYP	G	106	8/9	0.96	0.14	57,59,62,63	0
1	HYP	K	15	8/9	0.96	0.14	28,30,35,36	0
1	HYP	A	206	8/9	0.96	0.15	49,50,52,53	0
1	HYP	E	21	8/9	0.96	0.16	49,52,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	HYP	E	103	8/9	0.96	0.16	44,45,47,48	0
1	HYP	A	6	8/9	0.96	0.12	58,61,67,67	0
1	HYP	I	9	8/9	0.97	0.15	31,34,40,40	0
1	HYP	C	206	8/9	0.97	0.19	35,36,39,41	0
1	HYP	K	221	8/9	0.97	0.15	54,57,62,62	0
1	HYP	A	15	8/9	0.97	0.17	44,46,46,47	0
1	HYP	E	221	8/9	0.97	0.18	51,53,56,57	0
1	HYP	E	6	8/9	0.97	0.15	43,45,49,50	0
1	HYP	K	206	8/9	0.97	0.16	45,48,55,55	0
1	HYP	E	124	8/9	0.97	0.18	65,67,69,72	0
1	HYP	C	15	8/9	0.97	0.16	21,22,23,25	0
1	HYP	A	209	8/9	0.97	0.16	43,44,46,47	0
1	HYP	I	209	8/9	0.97	0.14	22,25,28,33	0
1	HYP	K	21	8/9	0.97	0.17	41,44,45,45	0
1	HYP	K	109	8/9	0.97	0.16	31,35,39,42	0
1	HYP	C	9	8/9	0.97	0.15	34,41,46,49	0
1	HYP	A	215	8/9	0.97	0.17	51,53,56,58	0
1	HYP	C	215	8/9	0.97	0.16	32,35,38,38	0
1	HYP	I	6	8/9	0.97	0.14	44,47,50,52	0
1	HYP	I	109	8/9	0.97	0.15	26,28,31,32	0
1	HYP	K	9	8/9	0.97	0.15	36,38,40,41	0
1	HYP	K	106	8/9	0.97	0.17	46,51,58,59	0
1	HYP	I	124	8/9	0.97	0.16	56,61,62,62	0
1	HYP	C	103	8/9	0.97	0.14	59,63,66,66	0
1	HYP	C	106	8/9	0.97	0.16	46,49,51,54	0
1	HYP	I	115	8/9	0.98	0.14	22,24,31,34	0
1	HYP	I	106	8/9	0.98	0.13	36,38,43,44	0
1	HYP	K	215	8/9	0.98	0.17	28,29,32,34	0
1	HYP	K	209	8/9	0.98	0.15	32,36,42,45	0
1	HYP	E	209	8/9	0.98	0.14	30,31,33,34	0
1	HYP	E	109	8/9	0.98	0.12	35,37,39,41	0
1	HYP	E	106	8/9	0.98	0.12	36,37,38,39	0
1	HYP	I	215	8/9	0.98	0.15	22,25,27,28	0
1	HYP	E	9	8/9	0.98	0.15	35,38,42,43	0
1	HYP	G	109	8/9	0.98	0.13	54,55,58,59	0
1	HYP	E	206	8/9	0.98	0.14	34,36,38,39	0
1	HYP	E	115	8/9	0.98	0.17	32,33,36,38	0
1	HYP	K	115	8/9	0.98	0.14	27,29,31,33	0
1	HYP	I	21	8/9	0.98	0.16	34,36,37,39	0
1	HYP	I	15	8/9	0.98	0.15	19,21,25,29	0
1	HYP	C	115	8/9	0.98	0.14	27,30,37,39	0
1	HYP	E	215	8/9	0.99	0.14	37,38,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	HYP	C	209	8/9	0.99	0.15	25,27,29,29	0

### 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. 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( $\text{\AA}^2$ )	Q<0.9
3	SO4	F	1901	5/5	0.91	0.18	70,73,74,74	0
3	SO4	I	301	5/5	0.96	0.13	44,50,50,52	0
3	SO4	K	301	5/5	0.96	0.12	53,56,59,59	0
3	SO4	C	301	5/5	0.97	0.12	43,49,49,49	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.