Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 07:11 pm BST

PDB ID	:	8P6J
Title	:	Structure of the hypervariable region of Streptococcus pyogenes M3 protein in complex with a collagen peptide
Authors	:	Wojnowska, M.; Schwarz-Linek, U.
Deposited on	:	2023-05-26
Resolution	:	2.32 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

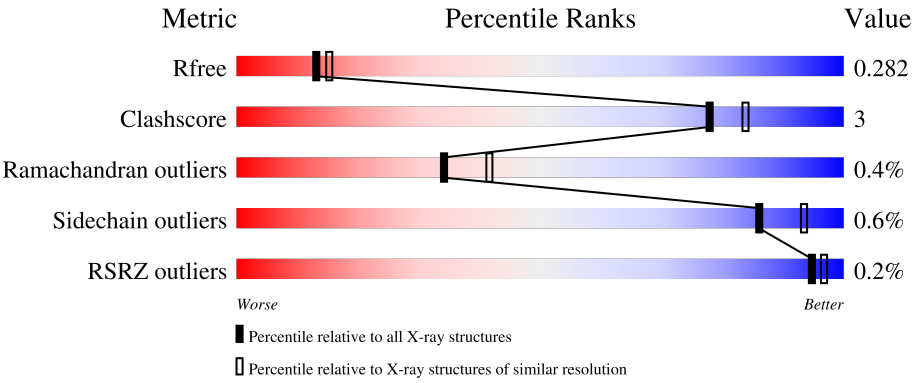
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	BBB	113	88% . 8%
1	CCC	113	88% 6% 6%
1	FFF	113	% 87% 7% 6%
1	GGG	113	81% 11% 9%
2	AAA	24	92% 8%

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Mol	Chain	Length	Quality of chain
2	DDD	24	92% 8%
2	EEE	24	96%
2	HHH	24	83% 17%
2	III	24	88% 8%
2	JJJ	24	88% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4046 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 Antiphagocytic M protein, type 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	BBB	104	Total	C	N	O	0	1	0
			801	502	139	160			
1	CCC	106	Total	C	N	O	0	0	0
			805	505	144	156			
1	FFF	106	Total	C	N	O	0	0	0
			786	492	135	159			
1	GGG	103	Total	C	N	O	0	1	0
			749	471	135	143			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	1	GLY	-	expression tag	UNP A0A0H2UWN1
BBB	2	ALA	-	expression tag	UNP A0A0H2UWN1
BBB	3	MET	-	expression tag	UNP A0A0H2UWN1
BBB	113	CYS	-	expression tag	UNP A0A0H2UWN1
CCC	1	GLY	-	expression tag	UNP A0A0H2UWN1
CCC	2	ALA	-	expression tag	UNP A0A0H2UWN1
CCC	3	MET	-	expression tag	UNP A0A0H2UWN1
CCC	113	CYS	-	expression tag	UNP A0A0H2UWN1
FFF	1	GLY	-	expression tag	UNP A0A0H2UWN1
FFF	2	ALA	-	expression tag	UNP A0A0H2UWN1
FFF	3	MET	-	expression tag	UNP A0A0H2UWN1
FFF	113	CYS	-	expression tag	UNP A0A0H2UWN1
GGG	1	GLY	-	expression tag	UNP A0A0H2UWN1
GGG	2	ALA	-	expression tag	UNP A0A0H2UWN1
GGG	3	MET	-	expression tag	UNP A0A0H2UWN1
GGG	113	CYS	-	expression tag	UNP A0A0H2UWN1

- Molecule 2 is a protein called collagen II-27 Toolkit peptide (JDM238).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	AAA	24	Total	C	N	O	0	0	0
			147	92	24	31			
2	DDD	24	Total	C	N	O	0	0	0
			148	93	24	31			
2	EEE	24	Total	C	N	O	0	0	0
			147	92	24	31			
2	HHH	24	Total	C	N	O	0	0	0
			148	93	24	31			
2	JJJ	24	Total	C	N	O	0	0	0
			147	92	24	31			
2	III	23	Total	C	N	O	0	0	0
			143	90	23	30			

- Molecule 3 is water.

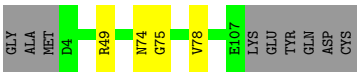
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	BBB	5	Total	O	0	0
			5	5		
3	CCC	3	Total	O	0	0
			3	3		
3	AAA	1	Total	O	0	0
			1	1		
3	DDD	1	Total	O	0	0
			1	1		
3	EEE	1	Total	O	0	0
			1	1		
3	FFF	3	Total	O	0	0
			3	3		
3	GGG	6	Total	O	0	0
			6	6		
3	HHH	2	Total	O	0	0
			2	2		
3	III	3	Total	O	0	0
			3	3		

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.

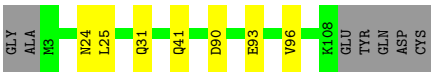
• Molecule 1: Antiphagocytic M protein, type 3

Chain BBB:



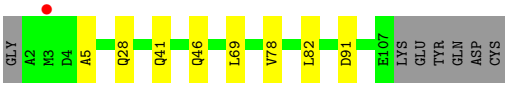
• Molecule 1: Antiphagocytic M protein, type 3

Chain CCC:



• Molecule 1: Antiphagocytic M protein, type 3

Chain FFF:



• Molecule 1: Antiphagocytic M protein, type 3

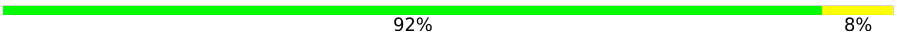
Chain GGG:

• Molecule 2: collagen II-27 Toolkit peptide (JDM238)

Chain AAA:

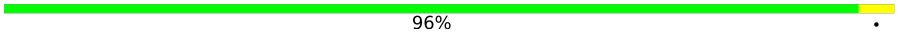
• Molecule 2: collagen II-27 Toolkit peptide (JDM238)

Chain DDD:



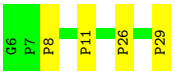
• Molecule 2: collagen II-27 Toolkit peptide (JDM238)

Chain EEE:



• Molecule 2: collagen II-27 Toolkit peptide (JDM238)

Chain HHH:

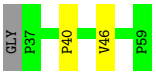


• Molecule 2: collagen II-27 Toolkit peptide (JDM238)

Chain JJJ:

• Molecule 2: collagen II-27 Toolkit peptide (JDM238)

Chain III:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	31.83Å 51.50Å 80.19Å 87.33° 84.78° 89.39°	Depositor
Resolution (Å)	79.77 – 2.32 79.77 – 2.32	Depositor EDS
% Data completeness (in resolution range)	89.6 (79.77-2.32) 77.8 (79.77-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.241 , 0.285 0.244 , 0.282	Depositor DCC
R_{free} test set	947 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	40.5	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 26.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.107 for -h,k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4046	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: HYP

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	BBB	0.68	0/810	0.74	0/1096
1	CCC	0.68	0/815	0.74	0/1102
1	FFF	0.69	0/796	0.73	0/1081
1	GGG	0.70	0/762	0.76	0/1037
2	AAA	0.69	0/90	0.68	0/115
2	DDD	0.53	0/91	0.66	0/116
2	EEE	0.59	0/90	0.69	0/115
2	HHH	0.65	0/91	0.68	0/116
2	III	0.52	0/86	0.68	0/109
2	JJJ	0.63	0/90	0.70	0/115
All	All	0.68	0/3721	0.73	0/5002

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	BBB	801	0	726	3	0
1	CCC	805	0	741	7	0
1	FFF	786	0	693	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GGG	749	0	653	9	0
2	AAA	147	0	130	0	0
2	DDD	148	0	132	1	0
2	EEE	147	0	130	0	0
2	HHH	148	0	132	1	0
2	III	143	0	128	2	0
2	JJJ	147	0	130	3	0
3	AAA	1	0	0	0	0
3	BBB	5	0	0	0	0
3	CCC	3	0	0	0	0
3	DDD	1	0	0	0	0
3	EEE	1	0	0	0	0
3	FFF	3	0	0	0	0
3	GGG	6	0	0	0	0
3	HHH	2	0	0	0	0
3	III	3	0	0	0	0
All	All	4046	0	3595	22	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 3.

All (22) 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:GGG:14:ARG:O	1:GGG:18:LEU:HD23	1.81	0.81
1:BBB:75:GLY:O	1:BBB:78:VAL:HG12	1.93	0.69
1:CCC:24:ASN:ND2	2:JJJ:73:PRO:HB3	2.08	0.68
1:CCC:24:ASN:CG	2:JJJ:73:PRO:HB3	2.19	0.62
1:FFF:78:VAL:HG12	1:GGG:78:VAL:HG12	1.81	0.62
1:CCC:31:GLN:NE2	2:JJJ:76:VAL:HG22	2.25	0.51
1:BBB:49:ARG:NH2	2:DDD:47:HYP:O	2.43	0.51
1:CCC:90:ASP:HA	1:CCC:93:GLU:HG2	1.93	0.49
1:GGG:82:LEU:O	1:GGG:85:VAL:HG12	2.12	0.48
1:GGG:46:GLN:O	1:GGG:49:ARG:HG2	2.15	0.47
1:CCC:93:GLU:HA	1:CCC:96:VAL:HG22	1.97	0.46
1:FFF:69:LEU:HD21	2:III:40:PRO:HG3	1.98	0.46
1:GGG:41:GLN:NE2	1:GGG:41:GLN:HA	2.32	0.45
1:GGG:82:LEU:HA	1:GGG:85:VAL:HG12	1.99	0.45
1:FFF:82:LEU:HD22	1:GGG:78:VAL:HG13	1.99	0.44
1:FFF:28:GLN:CD	2:HHH:8:HYP:HG	2.39	0.43
1:CCC:41:GLN:NE2	1:CCC:41:GLN:HA	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GGG:102:LYS:C	1:GGG:104:ASP:H	2.24	0.41
1:FFF:41:GLN:NE2	1:FFF:41:GLN:HA	2.36	0.41
1:GGG:14:ARG:O	1:GGG:18:LEU:CD2	2.62	0.41
1:BBB:74:ASN:HB3	1:CCC:25:LEU:HD22	2.02	0.40
1:FFF:46:GLN:HG3	2:III:46:VAL:HG22	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	BBB	103/113 (91%)	102 (99%)	1 (1%)	0	100	100
1	CCC	104/113 (92%)	103 (99%)	1 (1%)	0	100	100
1	FFF	104/113 (92%)	101 (97%)	2 (2%)	1 (1%)	15	17
1	GGG	102/113 (90%)	97 (95%)	4 (4%)	1 (1%)	15	17
2	AAA	16/24 (67%)	16 (100%)	0	0	100	100
2	DDD	16/24 (67%)	16 (100%)	0	0	100	100
2	EEE	16/24 (67%)	16 (100%)	0	0	100	100
2	HHH	16/24 (67%)	16 (100%)	0	0	100	100
2	III	15/24 (62%)	15 (100%)	0	0	100	100
2	JJJ	16/24 (67%)	16 (100%)	0	0	100	100
All	All	508/596 (85%)	498 (98%)	8 (2%)	2 (0%)	34	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	FFF	5	ALA
1	GGG	103	ILE

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	BBB	75/100 (75%)	75 (100%)	0	100	100
1	CCC	75/100 (75%)	75 (100%)	0	100	100
1	FFF	71/100 (71%)	70 (99%)	1 (1%)	67	80
1	GGG	63/100 (63%)	62 (98%)	1 (2%)	62	77
2	AAA	7/8 (88%)	7 (100%)	0	100	100
2	DDD	7/8 (88%)	7 (100%)	0	100	100
2	EEE	7/8 (88%)	7 (100%)	0	100	100
2	HHH	7/8 (88%)	7 (100%)	0	100	100
2	III	7/8 (88%)	7 (100%)	0	100	100
2	JJJ	7/8 (88%)	7 (100%)	0	100	100
All	All	326/448 (73%)	324 (99%)	2 (1%)	86	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	FFF	91	ASP
1	GGG	27	ASP

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

42 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	$\#\|Z\| > 2$
2	HYP	AAA	8	2	6,8,9	0.62	0	5,10,12	0.75	0
2	HYP	AAA	26	2	6,8,9	0.47	0	5,10,12	0.82	0
2	HYP	DDD	53	2	6,8,9	0.54	0	5,10,12	0.80	0
2	HYP	JJJ	83	2	6,8,9	0.55	0	5,10,12	0.86	0
2	HYP	III	59	2	6,8,9	0.56	0	5,10,12	1.40	0
2	HYP	DDD	59	2	6,8,9	0.60	0	5,10,12	1.10	1 (20%)
2	HYP	JJJ	77	2	6,8,9	0.57	0	5,10,12	1.03	0
2	HYP	EEE	86	2	6,8,9	0.44	0	5,10,12	0.91	0
2	HYP	JJJ	71	2	6,8,9	0.50	0	5,10,12	1.02	0
2	HYP	JJJ	89	2	6,8,9	0.55	0	5,10,12	1.18	1 (20%)
2	HYP	III	56	2	6,8,9	0.49	0	5,10,12	0.82	0
2	HYP	HHH	26	2	6,8,9	0.56	0	5,10,12	1.11	1 (20%)
2	HYP	DDD	38	2	6,8,9	0.45	0	5,10,12	0.78	0
2	HYP	DDD	44	2	6,8,9	0.55	0	5,10,12	0.69	0
2	HYP	AAA	11	2	6,8,9	0.45	0	5,10,12	1.02	1 (20%)
2	HYP	EEE	71	2	6,8,9	0.44	0	5,10,12	0.87	0
2	HYP	DDD	56	2	6,8,9	0.53	0	5,10,12	0.84	0
2	HYP	III	38	2	6,8,9	0.54	0	5,10,12	0.72	0
2	HYP	III	53	2	6,8,9	0.38	0	5,10,12	0.83	0
2	HYP	III	44	2	6,8,9	0.57	0	5,10,12	0.81	0
2	HYP	EEE	74	2	6,8,9	0.61	0	5,10,12	0.82	0
2	HYP	HHH	11	2	6,8,9	0.58	0	5,10,12	0.97	1 (20%)
2	HYP	HHH	29	2	6,8,9	0.46	0	5,10,12	1.17	1 (20%)
2	HYP	HHH	23	2	6,8,9	0.53	0	5,10,12	0.78	0
2	HYP	HHH	14	2	6,8,9	0.61	0	5,10,12	0.66	0
2	HYP	AAA	17	2	6,8,9	0.87	0	5,10,12	1.04	0
2	HYP	AAA	29	2	6,8,9	0.59	0	5,10,12	1.25	1 (20%)
2	HYP	AAA	14	2	6,8,9	0.59	0	5,10,12	0.71	0
2	HYP	DDD	41	2	6,8,9	0.56	0	5,10,12	1.08	0
2	HYP	JJJ	86	2	6,8,9	0.49	0	5,10,12	0.88	0
2	HYP	HHH	8	2	6,8,9	0.50	0	5,10,12	0.74	0
2	HYP	III	47	2	6,8,9	0.51	0	5,10,12	0.90	0
2	HYP	DDD	47	2	6,8,9	0.70	0	5,10,12	1.05	0
2	HYP	III	41	2	6,8,9	0.45	0	5,10,12	0.93	0
2	HYP	HHH	17	2	6,8,9	0.68	0	5,10,12	0.91	0
2	HYP	JJJ	68	2	6,8,9	0.58	0	5,10,12	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HYP	JJJ	74	2	6,8,9	0.52	0	5,10,12	0.73	0
2	HYP	EEE	68	2	6,8,9	0.59	0	5,10,12	0.71	0
2	HYP	AAA	23	2	6,8,9	0.46	0	5,10,12	0.84	0
2	HYP	EEE	77	2	6,8,9	0.49	0	5,10,12	1.05	0
2	HYP	EEE	89	2	6,8,9	0.51	0	5,10,12	1.13	1 (20%)
2	HYP	EEE	83	2	6,8,9	0.54	0	5,10,12	0.78	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	HYP	AAA	8	2	-	0/0/11/13	0/1/1/1
2	HYP	AAA	26	2	-	0/0/11/13	0/1/1/1
2	HYP	DDD	53	2	-	0/0/11/13	0/1/1/1
2	HYP	JJJ	83	2	-	0/0/11/13	0/1/1/1
2	HYP	III	59	2	-	0/0/11/13	0/1/1/1
2	HYP	DDD	59	2	-	0/0/11/13	0/1/1/1
2	HYP	JJJ	77	2	-	0/0/11/13	0/1/1/1
2	HYP	EEE	86	2	-	0/0/11/13	0/1/1/1
2	HYP	JJJ	71	2	-	0/0/11/13	0/1/1/1
2	HYP	JJJ	89	2	-	0/0/11/13	0/1/1/1
2	HYP	III	56	2	-	0/0/11/13	0/1/1/1
2	HYP	HHH	26	2	-	0/0/11/13	0/1/1/1
2	HYP	DDD	38	2	-	0/0/11/13	0/1/1/1
2	HYP	DDD	44	2	-	0/0/11/13	0/1/1/1
2	HYP	AAA	11	2	-	0/0/11/13	0/1/1/1
2	HYP	EEE	71	2	-	0/0/11/13	0/1/1/1
2	HYP	DDD	56	2	-	0/0/11/13	0/1/1/1
2	HYP	III	38	2	-	0/0/11/13	0/1/1/1
2	HYP	III	53	2	-	0/0/11/13	0/1/1/1
2	HYP	III	44	2	-	0/0/11/13	0/1/1/1
2	HYP	EEE	74	2	-	0/0/11/13	0/1/1/1
2	HYP	HHH	11	2	-	0/0/11/13	0/1/1/1
2	HYP	HHH	29	2	-	0/0/11/13	0/1/1/1
2	HYP	HHH	23	2	-	0/0/11/13	0/1/1/1
2	HYP	HHH	14	2	-	0/0/11/13	0/1/1/1
2	HYP	AAA	17	2	-	0/0/11/13	0/1/1/1
2	HYP	AAA	29	2	-	0/0/11/13	0/1/1/1
2	HYP	AAA	14	2	-	0/0/11/13	0/1/1/1
2	HYP	DDD	41	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	JJJ	86	2	-	0/0/11/13	0/1/1/1
2	HYP	HHH	8	2	-	0/0/11/13	0/1/1/1
2	HYP	III	47	2	-	0/0/11/13	0/1/1/1
2	HYP	DDD	47	2	-	0/0/11/13	0/1/1/1
2	HYP	III	41	2	-	0/0/11/13	0/1/1/1
2	HYP	HHH	17	2	-	0/0/11/13	0/1/1/1
2	HYP	JJJ	68	2	-	0/0/11/13	0/1/1/1
2	HYP	JJJ	74	2	-	0/0/11/13	0/1/1/1
2	HYP	EEE	68	2	-	0/0/11/13	0/1/1/1
2	HYP	AAA	23	2	-	0/0/11/13	0/1/1/1
2	HYP	EEE	77	2	-	0/0/11/13	0/1/1/1
2	HYP	EEE	89	2	-	0/0/11/13	0/1/1/1
2	HYP	EEE	83	2	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	JJJ	89	HYP	O-C-CA	-2.53	118.15	124.78
2	HHH	29	HYP	O-C-CA	-2.53	118.15	124.78
2	EEE	89	HYP	O-C-CA	-2.53	118.16	124.78
2	AAA	29	HYP	O-C-CA	-2.51	118.19	124.78
2	DDD	59	HYP	O-C-CA	-2.35	118.61	124.78
2	HHH	26	HYP	O-C-CA	-2.35	118.62	124.78
2	AAA	11	HYP	O-C-CA	-2.21	118.97	124.78
2	HHH	11	HYP	O-C-CA	-2.02	119.48	124.78

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
2	HHH	8	HYP	1	0
2	DDD	47	HYP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	BBB	104/113 (92%)	-0.41	0 100 100	31, 44, 60, 77	0
1	CCC	106/113 (93%)	-0.31	0 100 100	32, 47, 64, 76	0
1	FFF	106/113 (93%)	-0.24	1 (0%) 84 88	30, 45, 81, 97	0
1	GGG	103/113 (91%)	-0.38	0 100 100	28, 46, 74, 84	0
2	AAA	17/24 (70%)	-0.58	0 100 100	36, 42, 51, 53	0
2	DDD	17/24 (70%)	-0.37	0 100 100	36, 41, 61, 72	0
2	EEE	17/24 (70%)	-0.38	0 100 100	36, 41, 57, 58	0
2	HHH	17/24 (70%)	-0.47	0 100 100	38, 41, 51, 59	0
2	III	16/24 (66%)	-0.59	0 100 100	35, 41, 48, 64	0
2	JJJ	17/24 (70%)	-0.37	0 100 100	37, 45, 56, 61	0
All	All	520/596 (87%)	-0.36	1 (0%) 95 97	28, 45, 72, 97	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	FFF	3	MET	2.3

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^{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	HYP	DDD	38	8/9	0.90	0.13	49,60,64,65	0
2	HYP	AAA	8	8/9	0.91	0.10	46,49,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HYP	EEE	86	8/9	0.91	0.12	45,53,55,60	0
2	HYP	JJJ	77	8/9	0.92	0.15	39,43,48,48	0
2	HYP	HHH	11	8/9	0.92	0.14	46,47,50,54	0
2	HYP	DDD	59	8/9	0.92	0.15	58,61,62,63	0
2	HYP	HHH	8	8/9	0.93	0.09	52,54,54,54	0
2	HYP	III	38	8/9	0.93	0.15	46,59,62,67	0
2	HYP	JJJ	89	8/9	0.93	0.13	62,64,67,71	0
2	HYP	DDD	56	8/9	0.94	0.12	61,69,73,83	0
2	HYP	AAA	23	8/9	0.94	0.12	39,41,45,47	0
2	HYP	DDD	41	8/9	0.95	0.14	33,35,36,37	0
2	HYP	AAA	14	8/9	0.95	0.11	41,47,48,49	0
2	HYP	DDD	44	8/9	0.95	0.14	37,41,47,47	0
2	HYP	III	44	8/9	0.95	0.09	36,37,39,41	0
2	HYP	JJJ	86	8/9	0.95	0.11	47,54,57,58	0
2	HYP	AAA	17	8/9	0.95	0.11	32,33,37,37	0
2	HYP	EEE	77	8/9	0.95	0.14	36,38,40,40	0
2	HYP	III	59	8/9	0.95	0.10	55,56,58,58	0
2	HYP	DDD	53	8/9	0.96	0.11	44,45,46,47	0
2	HYP	HHH	23	8/9	0.96	0.10	37,39,41,41	0
2	HYP	AAA	26	8/9	0.96	0.15	41,46,48,50	0
2	HYP	JJJ	71	8/9	0.96	0.10	44,45,47,50	0
2	HYP	EEE	68	8/9	0.96	0.10	40,53,56,56	0
2	HYP	DDD	47	8/9	0.96	0.09	34,38,39,40	0
2	HYP	III	56	8/9	0.96	0.14	45,54,57,60	0
2	HYP	AAA	11	8/9	0.96	0.11	38,40,41,42	0
2	HYP	EEE	89	8/9	0.96	0.14	59,62,66,67	0
2	HYP	HHH	29	8/9	0.96	0.11	47,52,54,55	0
2	HYP	HHH	14	8/9	0.96	0.14	42,42,43,44	0
2	HYP	JJJ	74	8/9	0.96	0.11	40,41,46,54	0
2	HYP	AAA	29	8/9	0.97	0.09	40,42,43,45	0
2	HYP	EEE	83	8/9	0.97	0.12	47,48,49,51	0
2	HYP	EEE	71	8/9	0.97	0.08	39,42,43,44	0
2	HYP	HHH	26	8/9	0.97	0.13	40,44,54,56	0
2	HYP	JJJ	83	8/9	0.97	0.09	43,44,47,47	0
2	HYP	JJJ	68	8/9	0.97	0.08	43,47,48,48	0
2	HYP	III	47	8/9	0.98	0.06	37,38,41,46	0
2	HYP	EEE	74	8/9	0.98	0.08	35,37,39,44	0
2	HYP	III	53	8/9	0.98	0.07	38,40,41,41	0
2	HYP	HHH	17	8/9	0.98	0.07	35,36,39,40	0
2	HYP	III	41	8/9	0.98	0.10	36,39,39,40	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.