Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 01:31 pm GMT

PDB ID	:	7PZH
Title	:	Phocaeicola vulgatus sialic acid esterase at 2.06 Angstrom resolution
Authors	:	Scott, H.; Armstrong, Z.; Davies, G.J.
Deposited on	:	2021-10-12
Resolution	:	2.06 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:

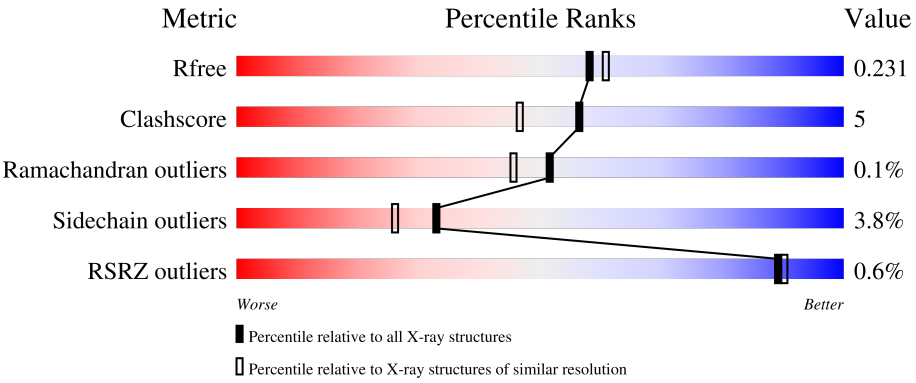
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.06 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	AAA	221	79% 11% 9%
1	BBB	221	78% 12% 10%
1	CCC	221	76% 14% 10%
1	DDD	221	% 74% 15% 10%
1	EEE	221	77% 12% 10%

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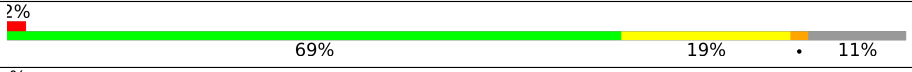
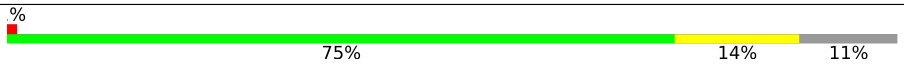
Mol	Chain	Length	Quality of chain
1	FFF	221	
1	GGG	221	
1	HHH	221	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13077 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 Lysophospholipase L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	201	Total	C	N	O	S	0	1	0
			1617	1038	271	301	7			
1	BBB	200	Total	C	N	O	S	0	0	0
			1597	1026	267	297	7			
1	CCC	200	Total	C	N	O	S	0	2	0
			1622	1042	273	300	7			
1	DDD	198	Total	C	N	O	S	0	6	0
			1628	1045	275	301	7			
1	EEE	199	Total	C	N	O	S	0	1	0
			1595	1028	267	293	7			
1	FFF	196	Total	C	N	O	S	0	2	0
			1578	1014	264	293	7			
1	HHH	196	Total	C	N	O	S	0	2	0
			1581	1017	265	292	7			
1	GGG	197	Total	C	N	O	S	0	2	0
			1592	1025	268	292	7			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	2	MET	-	initiating methionine	UNP A0A174J845
AAA	3	GLY	-	expression tag	UNP A0A174J845
AAA	4	SER	-	expression tag	UNP A0A174J845
AAA	5	SER	-	expression tag	UNP A0A174J845
AAA	6	HIS	-	expression tag	UNP A0A174J845
AAA	7	HIS	-	expression tag	UNP A0A174J845
AAA	8	HIS	-	expression tag	UNP A0A174J845
AAA	9	HIS	-	expression tag	UNP A0A174J845
AAA	10	HIS	-	expression tag	UNP A0A174J845
AAA	11	HIS	-	expression tag	UNP A0A174J845
AAA	12	GLY	-	expression tag	UNP A0A174J845
AAA	13	THR	-	expression tag	UNP A0A174J845
AAA	14	ALA	-	expression tag	UNP A0A174J845

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	15	GLU	-	expression tag	UNP A0A174J845
AAA	16	ASN	-	expression tag	UNP A0A174J845
AAA	17	LEU	-	expression tag	UNP A0A174J845
AAA	18	TYR	-	expression tag	UNP A0A174J845
AAA	19	PHE	-	expression tag	UNP A0A174J845
AAA	20	GLN	-	expression tag	UNP A0A174J845
AAA	21	GLY	-	expression tag	UNP A0A174J845
BBB	2	MET	-	initiating methionine	UNP A0A174J845
BBB	3	GLY	-	expression tag	UNP A0A174J845
BBB	4	SER	-	expression tag	UNP A0A174J845
BBB	5	SER	-	expression tag	UNP A0A174J845
BBB	6	HIS	-	expression tag	UNP A0A174J845
BBB	7	HIS	-	expression tag	UNP A0A174J845
BBB	8	HIS	-	expression tag	UNP A0A174J845
BBB	9	HIS	-	expression tag	UNP A0A174J845
BBB	10	HIS	-	expression tag	UNP A0A174J845
BBB	11	HIS	-	expression tag	UNP A0A174J845
BBB	12	GLY	-	expression tag	UNP A0A174J845
BBB	13	THR	-	expression tag	UNP A0A174J845
BBB	14	ALA	-	expression tag	UNP A0A174J845
BBB	15	GLU	-	expression tag	UNP A0A174J845
BBB	16	ASN	-	expression tag	UNP A0A174J845
BBB	17	LEU	-	expression tag	UNP A0A174J845
BBB	18	TYR	-	expression tag	UNP A0A174J845
BBB	19	PHE	-	expression tag	UNP A0A174J845
BBB	20	GLN	-	expression tag	UNP A0A174J845
BBB	21	GLY	-	expression tag	UNP A0A174J845
CCC	2	MET	-	initiating methionine	UNP A0A174J845
CCC	3	GLY	-	expression tag	UNP A0A174J845
CCC	4	SER	-	expression tag	UNP A0A174J845
CCC	5	SER	-	expression tag	UNP A0A174J845
CCC	6	HIS	-	expression tag	UNP A0A174J845
CCC	7	HIS	-	expression tag	UNP A0A174J845
CCC	8	HIS	-	expression tag	UNP A0A174J845
CCC	9	HIS	-	expression tag	UNP A0A174J845
CCC	10	HIS	-	expression tag	UNP A0A174J845
CCC	11	HIS	-	expression tag	UNP A0A174J845
CCC	12	GLY	-	expression tag	UNP A0A174J845
CCC	13	THR	-	expression tag	UNP A0A174J845
CCC	14	ALA	-	expression tag	UNP A0A174J845
CCC	15	GLU	-	expression tag	UNP A0A174J845
CCC	16	ASN	-	expression tag	UNP A0A174J845

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	17	LEU	-	expression tag	UNP A0A174J845
CCC	18	TYR	-	expression tag	UNP A0A174J845
CCC	19	PHE	-	expression tag	UNP A0A174J845
CCC	20	GLN	-	expression tag	UNP A0A174J845
CCC	21	GLY	-	expression tag	UNP A0A174J845
DDD	2	MET	-	initiating methionine	UNP A0A174J845
DDD	3	GLY	-	expression tag	UNP A0A174J845
DDD	4	SER	-	expression tag	UNP A0A174J845
DDD	5	SER	-	expression tag	UNP A0A174J845
DDD	6	HIS	-	expression tag	UNP A0A174J845
DDD	7	HIS	-	expression tag	UNP A0A174J845
DDD	8	HIS	-	expression tag	UNP A0A174J845
DDD	9	HIS	-	expression tag	UNP A0A174J845
DDD	10	HIS	-	expression tag	UNP A0A174J845
DDD	11	HIS	-	expression tag	UNP A0A174J845
DDD	12	GLY	-	expression tag	UNP A0A174J845
DDD	13	THR	-	expression tag	UNP A0A174J845
DDD	14	ALA	-	expression tag	UNP A0A174J845
DDD	15	GLU	-	expression tag	UNP A0A174J845
DDD	16	ASN	-	expression tag	UNP A0A174J845
DDD	17	LEU	-	expression tag	UNP A0A174J845
DDD	18	TYR	-	expression tag	UNP A0A174J845
DDD	19	PHE	-	expression tag	UNP A0A174J845
DDD	20	GLN	-	expression tag	UNP A0A174J845
DDD	21	GLY	-	expression tag	UNP A0A174J845
EEE	2	MET	-	initiating methionine	UNP A0A174J845
EEE	3	GLY	-	expression tag	UNP A0A174J845
EEE	4	SER	-	expression tag	UNP A0A174J845
EEE	5	SER	-	expression tag	UNP A0A174J845
EEE	6	HIS	-	expression tag	UNP A0A174J845
EEE	7	HIS	-	expression tag	UNP A0A174J845
EEE	8	HIS	-	expression tag	UNP A0A174J845
EEE	9	HIS	-	expression tag	UNP A0A174J845
EEE	10	HIS	-	expression tag	UNP A0A174J845
EEE	11	HIS	-	expression tag	UNP A0A174J845
EEE	12	GLY	-	expression tag	UNP A0A174J845
EEE	13	THR	-	expression tag	UNP A0A174J845
EEE	14	ALA	-	expression tag	UNP A0A174J845
EEE	15	GLU	-	expression tag	UNP A0A174J845
EEE	16	ASN	-	expression tag	UNP A0A174J845
EEE	17	LEU	-	expression tag	UNP A0A174J845
EEE	18	TYR	-	expression tag	UNP A0A174J845

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Chain	Residue	Modelled	Actual	Comment	Reference
EEE	19	PHE	-	expression tag	UNP A0A174J845
EEE	20	GLN	-	expression tag	UNP A0A174J845
EEE	21	GLY	-	expression tag	UNP A0A174J845
FFF	2	MET	-	initiating methionine	UNP A0A174J845
FFF	3	GLY	-	expression tag	UNP A0A174J845
FFF	4	SER	-	expression tag	UNP A0A174J845
FFF	5	SER	-	expression tag	UNP A0A174J845
FFF	6	HIS	-	expression tag	UNP A0A174J845
FFF	7	HIS	-	expression tag	UNP A0A174J845
FFF	8	HIS	-	expression tag	UNP A0A174J845
FFF	9	HIS	-	expression tag	UNP A0A174J845
FFF	10	HIS	-	expression tag	UNP A0A174J845
FFF	11	HIS	-	expression tag	UNP A0A174J845
FFF	12	GLY	-	expression tag	UNP A0A174J845
FFF	13	THR	-	expression tag	UNP A0A174J845
FFF	14	ALA	-	expression tag	UNP A0A174J845
FFF	15	GLU	-	expression tag	UNP A0A174J845
FFF	16	ASN	-	expression tag	UNP A0A174J845
FFF	17	LEU	-	expression tag	UNP A0A174J845
FFF	18	TYR	-	expression tag	UNP A0A174J845
FFF	19	PHE	-	expression tag	UNP A0A174J845
FFF	20	GLN	-	expression tag	UNP A0A174J845
FFF	21	GLY	-	expression tag	UNP A0A174J845
HHH	2	MET	-	initiating methionine	UNP A0A174J845
HHH	3	GLY	-	expression tag	UNP A0A174J845
HHH	4	SER	-	expression tag	UNP A0A174J845
HHH	5	SER	-	expression tag	UNP A0A174J845
HHH	6	HIS	-	expression tag	UNP A0A174J845
HHH	7	HIS	-	expression tag	UNP A0A174J845
HHH	8	HIS	-	expression tag	UNP A0A174J845
HHH	9	HIS	-	expression tag	UNP A0A174J845
HHH	10	HIS	-	expression tag	UNP A0A174J845
HHH	11	HIS	-	expression tag	UNP A0A174J845
HHH	12	GLY	-	expression tag	UNP A0A174J845
HHH	13	THR	-	expression tag	UNP A0A174J845
HHH	14	ALA	-	expression tag	UNP A0A174J845
HHH	15	GLU	-	expression tag	UNP A0A174J845
HHH	16	ASN	-	expression tag	UNP A0A174J845
HHH	17	LEU	-	expression tag	UNP A0A174J845
HHH	18	TYR	-	expression tag	UNP A0A174J845
HHH	19	PHE	-	expression tag	UNP A0A174J845
HHH	20	GLN	-	expression tag	UNP A0A174J845

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Chain	Residue	Modelled	Actual	Comment	Reference
HHH	21	GLY	-	expression tag	UNP A0A174J845
GGG	2	MET	-	initiating methionine	UNP A0A174J845
GGG	3	GLY	-	expression tag	UNP A0A174J845
GGG	4	SER	-	expression tag	UNP A0A174J845
GGG	5	SER	-	expression tag	UNP A0A174J845
GGG	6	HIS	-	expression tag	UNP A0A174J845
GGG	7	HIS	-	expression tag	UNP A0A174J845
GGG	8	HIS	-	expression tag	UNP A0A174J845
GGG	9	HIS	-	expression tag	UNP A0A174J845
GGG	10	HIS	-	expression tag	UNP A0A174J845
GGG	11	HIS	-	expression tag	UNP A0A174J845
GGG	12	GLY	-	expression tag	UNP A0A174J845
GGG	13	THR	-	expression tag	UNP A0A174J845
GGG	14	ALA	-	expression tag	UNP A0A174J845
GGG	15	GLU	-	expression tag	UNP A0A174J845
GGG	16	ASN	-	expression tag	UNP A0A174J845
GGG	17	LEU	-	expression tag	UNP A0A174J845
GGG	18	TYR	-	expression tag	UNP A0A174J845
GGG	19	PHE	-	expression tag	UNP A0A174J845
GGG	20	GLN	-	expression tag	UNP A0A174J845
GGG	21	GLY	-	expression tag	UNP A0A174J845

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total Mg 1 1	0	0
2	BBB	1	Total Mg 1 1	0	0
2	CCC	1	Total Mg 1 1	0	0
2	DDD	1	Total Mg 1 1	0	0
2	EEE	1	Total Mg 1 1	0	0
2	FFF	1	Total Mg 1 1	0	0
2	HHH	1	Total Mg 1 1	0	0
2	GGG	1	Total Mg 1 1	0	0

- Molecule 3 is water.

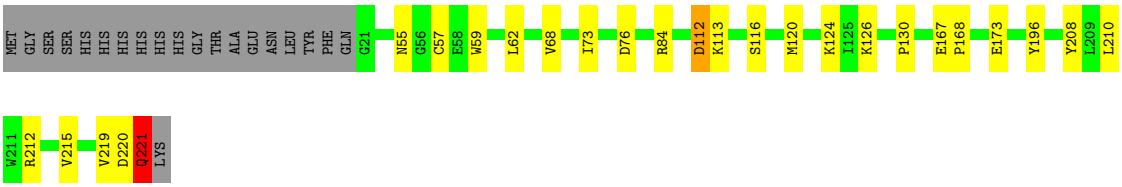
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	44	Total O 44 44	0	0
3	BBB	44	Total O 44 44	0	0
3	CCC	38	Total O 38 38	0	0
3	DDD	26	Total O 26 26	0	0
3	EEE	34	Total O 34 34	0	0
3	FFF	23	Total O 23 23	0	0
3	HHH	23	Total O 23 23	0	0
3	GGG	27	Total O 27 27	0	0

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.

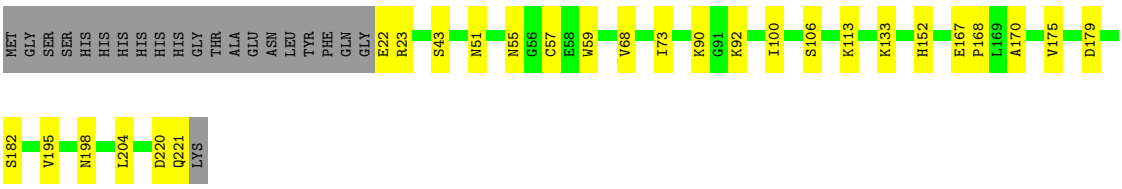
• Molecule 1: Lysophospholipase L1

Chain AAA:



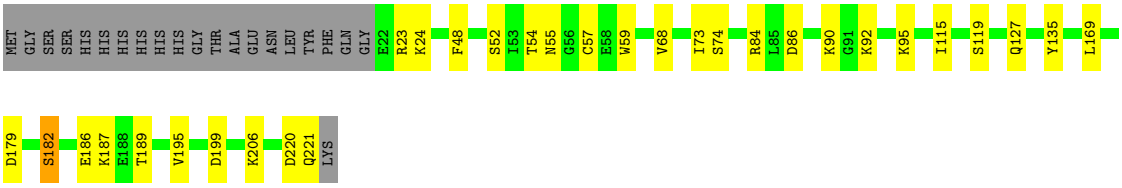
• Molecule 1: Lysophospholipase L1

Chain BBB:



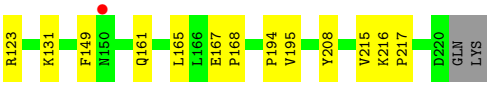
• Molecule 1: Lysophospholipase L1

Chain CCC:



• Molecule 1: Lysophospholipase L1

Chain DDD:

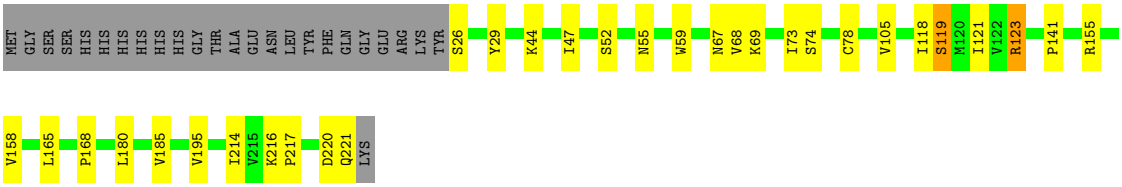


• Molecule 1: Lysophospholipase L1

Chain EEE:

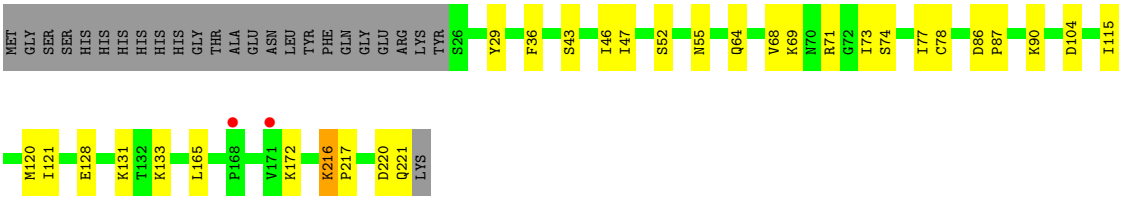
• Molecule 1: Lysophospholipase L1

Chain FFF:



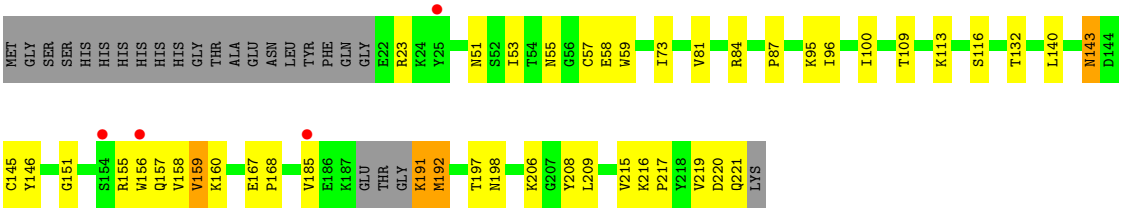
• Molecule 1: Lysophospholipase L1

Chain HHH:



• Molecule 1: Lysophospholipase L1

Chain GGG:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	93.23Å 93.23Å 353.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.74 – 2.06 80.74 – 2.06	Depositor EDS
% Data completeness (in resolution range)	100.0 (80.74-2.06) 100.0 (80.74-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.185 , 0.226 0.192 , 0.231	Depositor DCC
R_{free} test set	5355 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 31.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.146 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.847 for h, k, l 0.153 for -k, -h, -l	Depositor
Outliers	0 of 106770 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13077	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: MG

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	AAA	0.80	0/1649	0.92	2/2226 (0.1%)
1	BBB	0.81	0/1629	0.87	0/2202
1	CCC	0.78	0/1654	0.89	0/2232
1	DDD	0.78	0/1661	0.87	0/2245
1	EEE	0.79	0/1628	0.87	0/2200
1	FFF	0.77	0/1609	0.89	0/2174
1	GGG	0.78	1/1623 (0.1%)	0.88	0/2191
1	HHH	0.73	0/1612	0.86	0/2177
All	All	0.78	1/13065 (0.0%)	0.88	2/17647 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	GGG	58	GLU	CD-OE2	-7.45	1.17	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	221	GLN	CA-C-O	-5.82	107.87	120.10
1	AAA	84	ARG	NE-CZ-NH2	-5.11	117.74	120.30

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	AAA	1617	0	1633	13	0
1	BBB	1597	0	1604	16	0
1	CCC	1622	0	1644	15	0
1	DDD	1628	0	1643	24	0
1	EEE	1595	0	1618	12	0
1	FFF	1578	0	1594	16	0
1	GGG	1592	0	1605	22	0
1	HHH	1581	0	1602	16	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
2	CCC	1	0	0	0	0
2	DDD	1	0	0	0	0
2	EEE	1	0	0	0	0
2	FFF	1	0	0	0	0
2	GGG	1	0	0	0	0
2	HHH	1	0	0	0	0
3	AAA	44	0	0	2	0
3	BBB	44	0	0	0	0
3	CCC	38	0	0	0	0
3	DDD	26	0	0	0	0
3	EEE	34	0	0	0	0
3	FFF	23	0	0	0	0
3	GGG	27	0	0	0	0
3	HHH	23	0	0	0	0
All	All	13077	0	12943	129	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 5.

All (129) 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:220:ASP:C	1:GGG:221:GLN:N	2.01	1.13
1:AAA:220:ASP:C	1:AAA:221:GLN:N	2.11	1.04
1:GGG:220:ASP:O	1:GGG:221:GLN:N	2.00	0.93
1:CCC:220:ASP:O	1:CCC:221:GLN:N	2.01	0.93
1:BBB:220:ASP:C	1:BBB:221:GLN:N	2.25	0.90
1:DDD:86[B]:ASP:OD1	1:DDD:90[B]:LYS:NZ	2.06	0.88
1:FFF:220:ASP:C	1:FFF:221:GLN:N	2.31	0.84
1:CCC:24:LYS:HE3	1:DDD:149:PHE:CE1	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:130:PRO:HD2	3:AAA:443:HOH:O	1.87	0.75
1:AAA:126:LYS:NZ	1:AAA:173:GLU:O	2.22	0.72
1:HHH:220:ASP:O	1:HHH:221:GLN:N	2.26	0.68
1:AAA:124:LYS:NZ	3:AAA:401:HOH:O	2.26	0.68
1:DDD:86[B]:ASP:OD1	1:DDD:90[B]:LYS:CE	2.42	0.67
1:EEE:144:ASP:O	1:EEE:147:GLY:N	2.29	0.65
1:HHH:86:ASP:HB2	1:HHH:87:PRO:HD3	1.78	0.64
1:BBB:167:GLU:HB3	1:BBB:168:PRO:HD3	1.84	0.59
1:BBB:23:ARG:N	1:BBB:23:ARG:HD2	2.17	0.59
1:GGG:167:GLU:HB3	1:GGG:168:PRO:HD3	1.83	0.59
1:BBB:23:ARG:HD2	1:BBB:23:ARG:H	1.68	0.59
1:AAA:62:LEU:HD21	1:AAA:212:ARG:HB2	1.86	0.58
1:FFF:123:ARG:HD3	1:HHH:128:GLU:OE2	2.04	0.58
1:GGG:96:ILE:HD12	1:GGG:132:THR:HG21	1.86	0.57
1:GGG:53:ILE:O	1:GGG:208:TYR:OH	2.18	0.57
1:CCC:186:GLU:HB2	1:CCC:189:THR:OG1	2.06	0.56
1:DDD:131:LYS:HA	1:DDD:131:LYS:HE2	1.87	0.56
1:FFF:119:SER:O	1:FFF:123:ARG:HG3	2.05	0.56
1:BBB:220:ASP:O	1:BBB:221:GLN:O	2.24	0.56
1:GGG:206:LYS:HA	1:GGG:209:LEU:HD12	1.87	0.55
1:CCC:24:LYS:HE3	1:DDD:149:PHE:CZ	2.42	0.54
1:CCC:95[B]:LYS:NZ	1:CCC:135:TYR:OH	2.39	0.54
1:DDD:167:GLU:HB3	1:DDD:168:PRO:HD3	1.90	0.53
1:FFF:105:VAL:HG22	1:FFF:158:VAL:HG11	1.91	0.52
1:FFF:216:LYS:NZ	1:FFF:220:ASP:OD2	2.42	0.51
1:EEE:193:ASN:OD1	1:EEE:195:VAL:HG12	2.11	0.51
1:DDD:29:TYR:HA	1:DDD:73:ILE:HG21	1.92	0.51
1:FFF:29:TYR:HA	1:FFF:73:ILE:HG21	1.94	0.50
1:AAA:167:GLU:HB3	1:AAA:168:PRO:HD3	1.92	0.50
1:CCC:73:ILE:HD12	1:CCC:84:ARG:NE	2.26	0.50
1:HHH:78:CYS:O	1:HHH:121:ILE:HD11	2.11	0.50
1:EEE:180:LEU:HD23	1:EEE:214:ILE:HG21	1.94	0.50
1:GGG:145:CYS:SG	1:GGG:146:TYR:N	2.86	0.49
1:BBB:179:ASP:OD2	1:BBB:182:SER:OG	2.17	0.48
1:HHH:64[A]:GLN:HA	1:HHH:64[A]:GLN:OE1	2.12	0.48
1:GGG:216:LYS:N	1:GGG:217:PRO:CD	2.76	0.48
1:GGG:192:MET:O	1:GGG:192:MET:HG3	2.12	0.48
1:DDD:86[B]:ASP:CG	1:DDD:90[B]:LYS:NZ	2.65	0.48
1:FFF:59:TRP:HB3	1:FFF:68:VAL:HG12	1.95	0.48
1:HHH:115:ILE:HG13	1:HHH:165:LEU:HD12	1.94	0.48
1:EEE:179:ASP:OD2	1:EEE:182:SER:OG	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HHH:77:ILE:HB	1:HHH:104:ASP:OD1	2.14	0.48
1:HHH:47:ILE:HD13	1:HHH:69:LYS:HB2	1.96	0.47
1:HHH:216:LYS:N	1:HHH:217:PRO:CD	2.77	0.47
1:DDD:118:ILE:O	1:DDD:122:VAL:HG23	2.13	0.47
1:DDD:86[B]:ASP:HB3	1:DDD:87:PRO:HD3	1.96	0.47
1:GGG:53:ILE:HG21	1:GGG:140:LEU:HD12	1.96	0.47
1:DDD:43:SER:HA	1:DDD:92:LYS:O	2.14	0.47
1:FFF:118:ILE:HA	1:FFF:121:ILE:HD12	1.97	0.47
1:CCC:90:LYS:O	1:CCC:92:LYS:HG2	2.14	0.47
1:FFF:165:LEU:C	1:FFF:168:PRO:HD2	2.35	0.47
1:HHH:86:ASP:HB2	1:HHH:87:PRO:CD	2.43	0.47
1:CCC:48:PHE:HB3	1:CCC:54:THR:HG23	1.97	0.47
1:BBB:51:ASN:HA	1:BBB:73:ILE:O	2.15	0.47
1:GGG:81:VAL:HG21	1:GGG:100:ILE:HD13	1.97	0.47
1:BBB:57:CYS:HB3	1:BBB:59:TRP:CE2	2.50	0.46
1:GGG:84:ARG:O	1:GGG:87:PRO:HD2	2.15	0.46
1:BBB:59:TRP:HB3	1:BBB:68:VAL:HG12	1.98	0.46
1:DDD:216:LYS:N	1:DDD:217:PRO:CD	2.79	0.46
1:FFF:44:LYS:HE2	1:FFF:67:ASN:OD1	2.15	0.46
1:CCC:199:ASP:OD2	1:DDD:31:GLN:NE2	2.49	0.46
1:FFF:180:LEU:HD23	1:FFF:214:ILE:HG21	1.97	0.46
1:CCC:52:SER:HB3	1:CCC:74:SER:HA	1.99	0.45
1:EEE:46:ILE:O	1:EEE:68:VAL:HA	2.16	0.45
1:AAA:112:ASP:OD2	1:AAA:112:ASP:N	2.48	0.45
1:DDD:73:ILE:HD12	1:DDD:84:ARG:NE	2.32	0.45
1:FFF:216:LYS:HB3	1:FFF:217:PRO:HD3	1.99	0.45
1:GGG:113:LYS:O	1:GGG:116:SER:HB3	2.16	0.45
1:FFF:52:SER:HB3	1:FFF:74:SER:HA	1.98	0.45
1:CCC:179:ASP:OD2	1:CCC:182:SER:HB2	2.17	0.45
1:CCC:195:VAL:HG22	1:CCC:206:LYS:HE3	1.97	0.45
1:FFF:105:VAL:O	1:FFF:155:ARG:CD	2.65	0.44
1:EEE:57:CYS:HB3	1:EEE:59:TRP:CE2	2.53	0.44
1:EEE:92:LYS:HD3	1:EEE:129:SER:HB2	1.99	0.44
1:GGG:57:CYS:HB3	1:GGG:59:TRP:CE2	2.52	0.44
1:FFF:141:PRO:HG3	1:FFF:185:VAL:HB	2.00	0.44
1:EEE:33:ALA:O	1:EEE:37:GLU:HG2	2.17	0.44
1:HHH:36:PHE:CD1	1:HHH:71:ARG:HD3	2.53	0.44
1:BBB:43:SER:HA	1:BBB:92:LYS:O	2.18	0.44
1:HHH:90[B]:LYS:HA	1:HHH:90[B]:LYS:HD2	1.82	0.44
1:BBB:198:ASN:HB3	1:BBB:204:LEU:HD21	2.00	0.44
1:FFF:47:ILE:HD13	1:FFF:69:LYS:HB2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:73:ILE:O	1:AAA:76:ASP:HB2	2.18	0.43
1:AAA:120:MET:CE	1:DDD:194:PRO:HG2	2.48	0.43
1:GGG:156:TRP:CD2	1:GGG:191:LYS:HE2	2.54	0.43
1:EEE:186:GLU:HG3	1:EEE:193:ASN:HA	2.00	0.43
1:GGG:197:THR:OG1	1:GGG:198:ASN:N	2.50	0.43
1:BBB:220:ASP:O	1:BBB:221:GLN:N	2.51	0.43
1:CCC:57:CYS:HB3	1:CCC:59:TRP:CE2	2.53	0.43
1:EEE:167:GLU:N	1:EEE:168:PRO:HD2	2.34	0.43
1:GGG:158:VAL:O	1:GGG:159:VAL:C	2.57	0.43
1:GGG:143:ASN:ND2	1:GGG:191:LYS:HB3	2.34	0.42
1:BBB:100:ILE:HD12	1:BBB:100:ILE:HA	1.96	0.42
1:BBB:106:SER:HB3	1:BBB:152:HIS:CD2	2.54	0.42
1:GGG:51:ASN:HA	1:GGG:73:ILE:O	2.20	0.42
1:AAA:196:TYR:CZ	1:AAA:210:LEU:HD22	2.54	0.42
1:DDD:92:LYS:HA	1:DDD:92:LYS:HD3	1.89	0.42
1:GGG:95[B]:LYS:NZ	1:GGG:219:VAL:O	2.48	0.42
1:CCC:115:ILE:HG23	1:CCC:169:LEU:HD22	2.01	0.42
1:HHH:46:ILE:O	1:HHH:68:VAL:HA	2.20	0.42
1:DDD:33:ALA:O	1:DDD:37:GLU:HG3	2.19	0.42
1:DDD:115:ILE:HG13	1:DDD:165:LEU:HB2	2.02	0.41
1:DDD:161:GLN:O	1:DDD:165:LEU:HG	2.20	0.41
1:GGG:151:GLY:O	1:GGG:155:ARG:NH1	2.53	0.41
1:AAA:215:VAL:HG13	1:AAA:219:VAL:HG23	2.02	0.41
1:BBB:23:ARG:H	1:BBB:23:ARG:CD	2.30	0.41
1:EEE:95[A]:LYS:HA	1:EEE:133:LYS:O	2.21	0.41
1:HHH:29:TYR:HA	1:HHH:73:ILE:HG21	2.02	0.41
1:DDD:73:ILE:O	1:DDD:76:ASP:HB2	2.21	0.41
1:DDD:57:CYS:HB2	1:DDD:208:TYR:CE1	2.56	0.41
1:HHH:86:ASP:CB	1:HHH:87:PRO:HD3	2.49	0.41
1:BBB:170:ALA:HB1	1:BBB:175:VAL:O	2.20	0.41
1:EEE:30:GLU:O	1:EEE:34:THR:HG23	2.20	0.41
1:AAA:59:TRP:HB3	1:AAA:68:VAL:HG12	2.02	0.41
1:GGG:109:THR:CG2	1:GGG:113:LYS:HB3	2.51	0.41
1:AAA:57:CYS:HB2	1:AAA:208:TYR:CE1	2.56	0.40
1:DDD:119:SER:HB2	1:DDD:123:ARG:HH11	1.87	0.40
1:DDD:131:LYS:HA	1:DDD:131:LYS:CE	2.46	0.40
1:CCC:59:TRP:HB3	1:CCC:68:VAL:HG12	2.02	0.40
1:DDD:86[B]:ASP:CG	1:DDD:90[B]:LYS:HZ1	2.18	0.40
1:HHH:52:SER:HB3	1:HHH:74:SER:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	199/221 (90%)	195 (98%)	4 (2%)	0	100	100
1	BBB	197/221 (89%)	191 (97%)	6 (3%)	0	100	100
1	CCC	199/221 (90%)	193 (97%)	6 (3%)	0	100	100
1	DDD	202/221 (91%)	193 (96%)	9 (4%)	0	100	100
1	EEE	198/221 (90%)	192 (97%)	6 (3%)	0	100	100
1	FFF	195/221 (88%)	180 (92%)	14 (7%)	1 (0%)	29	19
1	GGG	194/221 (88%)	180 (93%)	13 (7%)	1 (0%)	29	19
1	HHH	195/221 (88%)	180 (92%)	15 (8%)	0	100	100
All	All	1579/1768 (89%)	1504 (95%)	73 (5%)	2 (0%)	51	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	FFF	78	CYS
1	GGG	159	VAL

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	AAA	180/196 (92%)	175 (97%)	5 (3%)	43	37
1	BBB	177/196 (90%)	171 (97%)	6 (3%)	37	30
1	CCC	181/196 (92%)	174 (96%)	7 (4%)	32	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	DDD	181/196 (92%)	174 (96%)	7 (4%)	32 25
1	EEE	177/196 (90%)	170 (96%)	7 (4%)	31 24
1	FFF	176/196 (90%)	171 (97%)	5 (3%)	43 37
1	GGG	176/196 (90%)	167 (95%)	9 (5%)	24 15
1	HHH	176/196 (90%)	169 (96%)	7 (4%)	31 24
All	All	1424/1568 (91%)	1371 (96%)	53 (4%)	33 27

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	55	ASN
1	AAA	112	ASP
1	AAA	113	LYS
1	AAA	116	SER
1	AAA	221	GLN
1	BBB	22	GLU
1	BBB	55	ASN
1	BBB	90	LYS
1	BBB	113	LYS
1	BBB	133	LYS
1	BBB	195	VAL
1	CCC	23	ARG
1	CCC	55	ASN
1	CCC	86	ASP
1	CCC	119	SER
1	CCC	127	GLN
1	CCC	182	SER
1	CCC	187	LYS
1	DDD	23	ARG
1	DDD	42	THR
1	DDD	55	ASN
1	DDD	116	SER
1	DDD	119	SER
1	DDD	195	VAL
1	DDD	215	VAL
1	EEE	55	ASN
1	EEE	113	LYS
1	EEE	123	ARG
1	EEE	131	LYS
1	EEE	133	LYS

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Mol	Chain	Res	Type
1	EEE	172	LYS
1	EEE	195	VAL
1	FFF	26	SER
1	FFF	55	ASN
1	FFF	119	SER
1	FFF	123	ARG
1	FFF	195	VAL
1	HHH	43	SER
1	HHH	55	ASN
1	HHH	120	MET
1	HHH	131	LYS
1	HHH	133	LYS
1	HHH	172	LYS
1	HHH	216	LYS
1	GGG	23	ARG
1	GGG	55	ASN
1	GGG	143	ASN
1	GGG	157	GLN
1	GGG	160	LYS
1	GGG	185	VAL
1	GGG	191	LYS
1	GGG	192	MET
1	GGG	215	VAL

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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	CCC	1
1	HHH	1
1	FFF	1
1	BBB	1
1	AAA	1
1	GGG	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CCC	220:ASP	C	221:GLN	N	2.92
1	HHH	220:ASP	C	221:GLN	N	2.76
1	FFF	220:ASP	C	221:GLN	N	2.31
1	BBB	220:ASP	C	221:GLN	N	2.25
1	AAA	220:ASP	C	221:GLN	N	2.11
1	GGG	220:ASP	C	221:GLN	N	2.01

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	AAA	201/221 (90%)	-0.48	0	100	100	21, 32, 49, 65	0
1	BBB	200/221 (90%)	-0.45	0	100	100	22, 33, 51, 69	0
1	CCC	200/221 (90%)	-0.41	0	100	100	25, 36, 53, 76	0
1	DDD	198/221 (89%)	-0.27	2 (1%)	82	83	26, 43, 60, 71	0
1	EEE	199/221 (90%)	-0.37	1 (0%)	91	91	24, 38, 56, 70	0
1	FFF	196/221 (88%)	-0.24	0	100	100	27, 43, 58, 69	0
1	GGG	197/221 (89%)	-0.08	4 (2%)	65	67	26, 45, 84, 106	0
1	HHH	196/221 (88%)	-0.12	2 (1%)	82	83	30, 46, 60, 75	0
All	All	1587/1768 (89%)	-0.31	9 (0%)	89	90	21, 39, 60, 106	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	25	TYR	3.5
1	GGG	156	TRP	2.7
1	EEE	25	TYR	2.7
1	GGG	154	SER	2.7
1	GGG	25	TYR	2.6
1	DDD	150[A]	ASN	2.5
1	GGG	185	VAL	2.1
1	HHH	168	PRO	2.1
1	HHH	171	VAL	2.0

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

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

6.3 Carbohydrates (i)

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^{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	MG	BBB	301	1/1	0.89	0.08	35,35,35,35	0
2	MG	DDD	301	1/1	0.90	0.07	43,43,43,43	0
2	MG	EEE	301	1/1	0.90	0.14	32,32,32,32	0
2	MG	CCC	301	1/1	0.95	0.06	32,32,32,32	0
2	MG	AAA	301	1/1	0.96	0.10	36,36,36,36	0
2	MG	FFF	301	1/1	0.97	0.05	38,38,38,38	0
2	MG	GGG	301	1/1	0.97	0.06	62,62,62,62	0
2	MG	HHH	301	1/1	0.98	0.04	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.