



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2024 – 03:19 AM EDT

PDB ID : 3P2L
Title : Crystal Structure of ATP-dependent Clp protease subunit P from *Francisella tularensis*
Authors : Kim, Y.; Zhou, M.; Gu, M.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2010-10-02
Resolution : 2.29 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

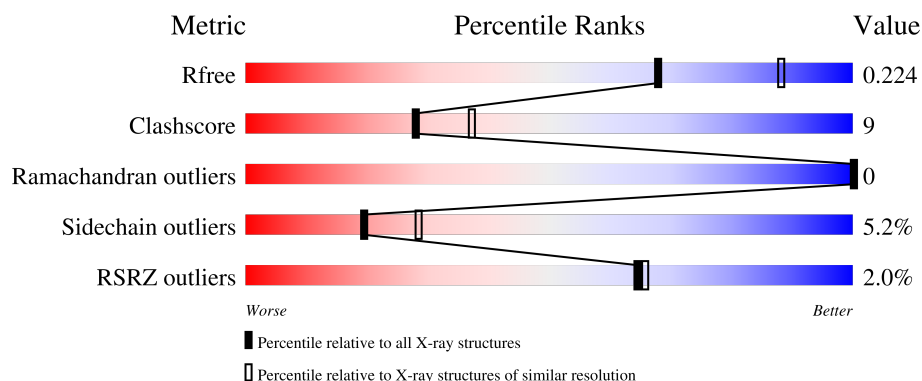
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	201	
1	B	201	
1	C	201	
1	D	201	
1	E	201	

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Mol	Chain	Length	Quality of chain
1	F	201	<div><div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>72%</div><div>16%</div><div>•</div><div>9%</div></div></div>
1	G	201	<div><div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>76%</div><div>13%</div><div>•</div><div>7%</div></div></div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10751 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	Se	0	0	0
			1468	929	253	278	1	7			
1	B	184	Total	C	N	O	S	Se	0	0	0
			1426	905	243	270	1	7			
1	C	183	Total	C	N	O	S	Se	0	0	0
			1418	899	242	269	1	7			
1	D	188	Total	C	N	O	S	Se	0	0	0
			1460	924	250	278	1	7			
1	E	182	Total	C	N	O	S	Se	0	0	0
			1410	893	241	268	1	7			
1	F	183	Total	C	N	O	S	Se	0	0	0
			1418	899	242	269	1	7			
1	G	186	Total	C	N	O	S	Se	0	1	0
			1453	920	252	273	1	7			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q5NH47
A	2	ASN	-	expression tag	UNP Q5NH47
A	3	ALA	-	expression tag	UNP Q5NH47
B	1	SER	-	expression tag	UNP Q5NH47
B	2	ASN	-	expression tag	UNP Q5NH47
B	3	ALA	-	expression tag	UNP Q5NH47
C	1	SER	-	expression tag	UNP Q5NH47
C	2	ASN	-	expression tag	UNP Q5NH47
C	3	ALA	-	expression tag	UNP Q5NH47
D	1	SER	-	expression tag	UNP Q5NH47
D	2	ASN	-	expression tag	UNP Q5NH47
D	3	ALA	-	expression tag	UNP Q5NH47
E	1	SER	-	expression tag	UNP Q5NH47
E	2	ASN	-	expression tag	UNP Q5NH47
E	3	ALA	-	expression tag	UNP Q5NH47

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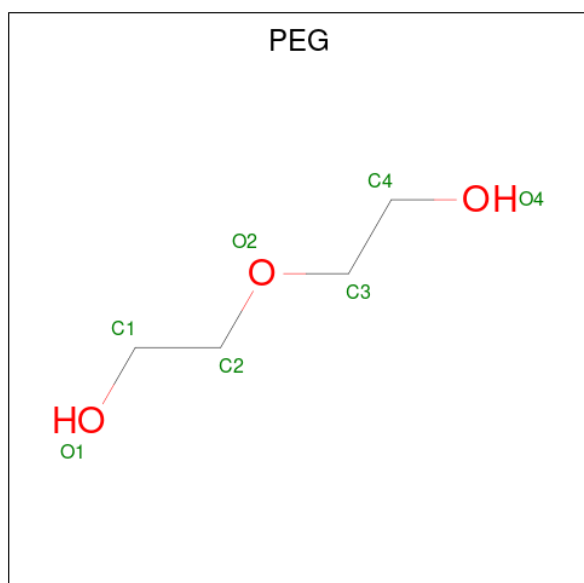
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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	SER	-	expression tag	UNP Q5NH47
F	2	ASN	-	expression tag	UNP Q5NH47
F	3	ALA	-	expression tag	UNP Q5NH47
G	1	SER	-	expression tag	UNP Q5NH47
G	2	ASN	-	expression tag	UNP Q5NH47
G	3	ALA	-	expression tag	UNP Q5NH47

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

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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



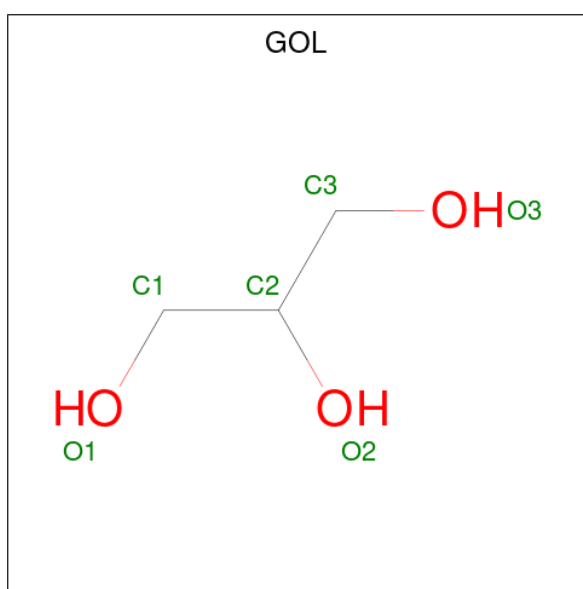
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	E	1	Total C O 7 4 3	0	0
3	E	1	Total C O 7 4 3	0	0
3	E	1	Total C O 7 4 3	0	0
3	E	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	G	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			7	4	3		
3	G	1	Total	C	O	0	0
			7	4	3		
3	G	1	Total	C	O	0	0
			7	4	3		
3	G	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



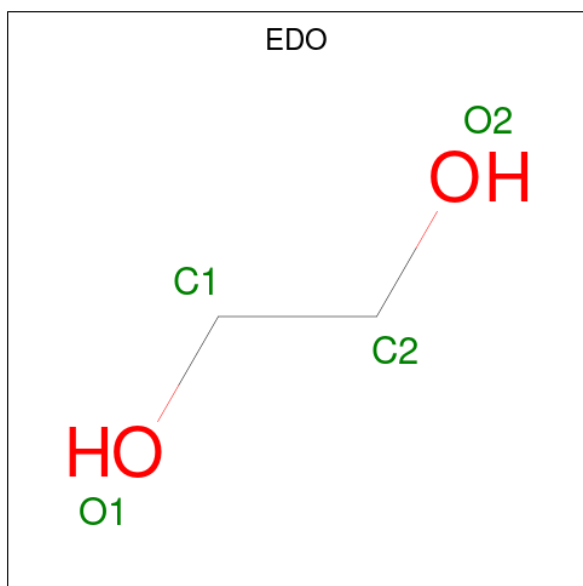
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



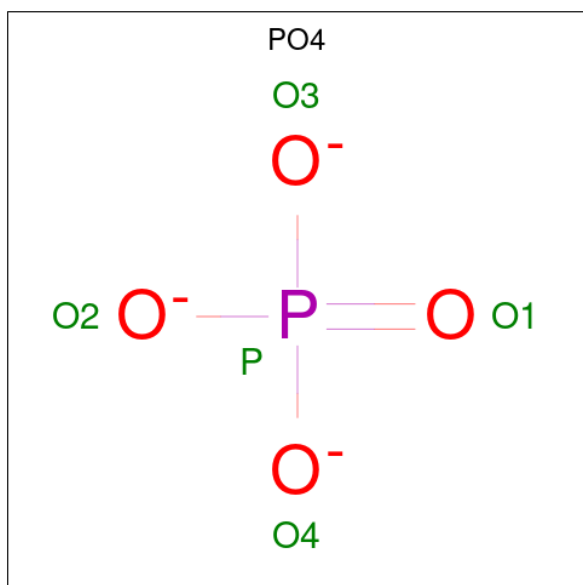
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	D	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	F	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	O	P	0	0
			5	4	1		

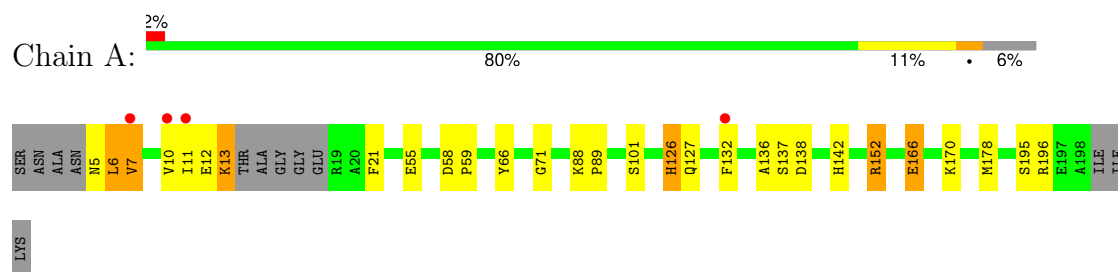
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	65	Total	O	0	0
			65	65		
7	B	62	Total	O	0	0
			62	62		
7	C	44	Total	O	0	0
			44	44		
7	D	32	Total	O	0	0
			32	32		
7	E	39	Total	O	0	0
			39	39		
7	F	42	Total	O	0	0
			42	42		
7	G	65	Total	O	0	0
			65	65		

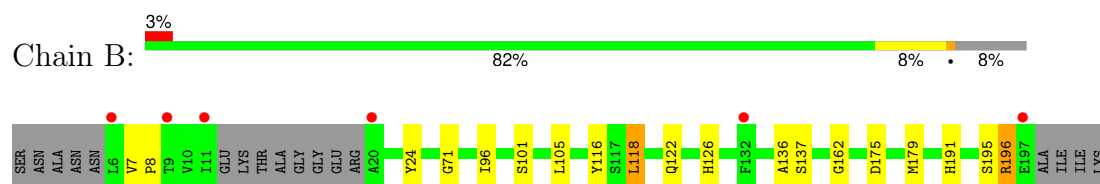
3 Residue-property plots

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.

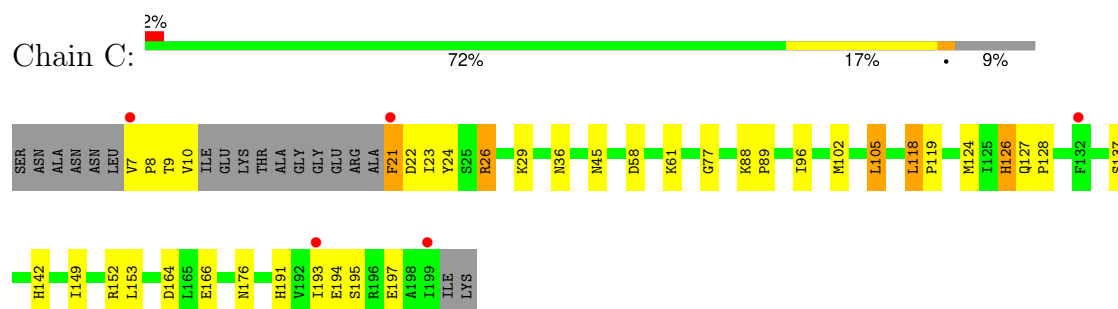
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



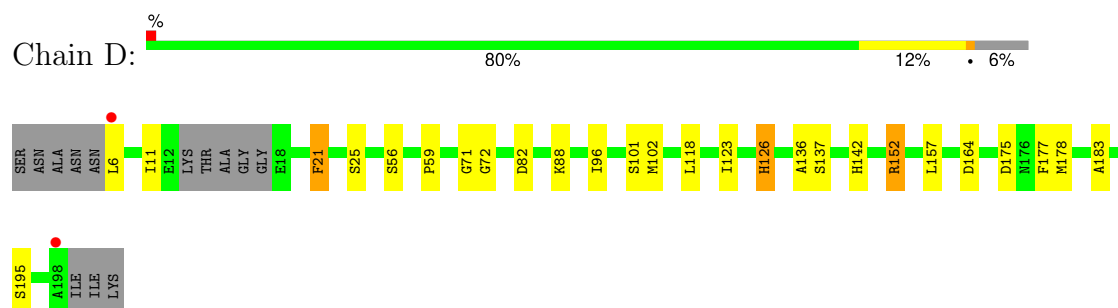
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

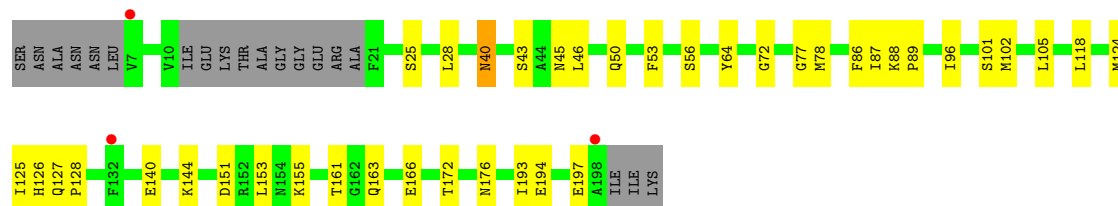


- Molecule 1: ATP-dependent Clp protease proteolytic subunit



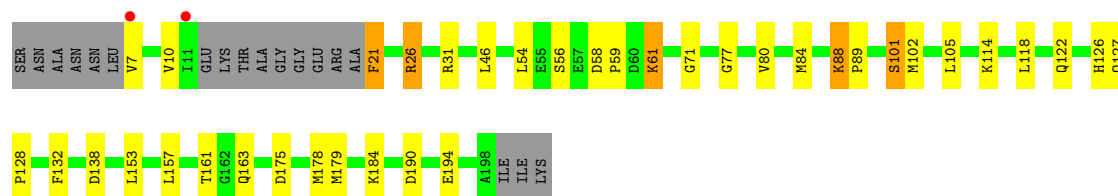
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E: 




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F: 



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.52Å 128.82Å 98.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.45 – 2.29 40.45 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.45-2.29) 99.2 (40.45-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.186 , 0.226 0.184 , 0.224	Depositor DCC
R_{free} test set	3453 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10751	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PEG, PO4, MG, GOL

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	0.53	0/1484	0.63	0/1988
1	B	0.56	0/1442	0.66	0/1933
1	C	0.52	0/1434	0.61	0/1922
1	D	0.52	0/1476	0.61	0/1978
1	E	0.50	0/1426	0.59	0/1911
1	F	0.50	0/1434	0.61	0/1922
1	G	0.58	0/1469	0.66	0/1968
All	All	0.53	0/10165	0.63	0/13622

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	7	VAL	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1468	0	1478	39	0
1	B	1426	0	1435	17	0
1	C	1418	0	1424	35	0
1	D	1460	0	1465	22	0
1	E	1410	0	1413	33	0
1	F	1418	0	1424	25	0
1	G	1453	0	1465	41	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
3	A	21	0	30	1	0
3	B	28	0	40	4	0
3	C	21	0	30	1	0
3	D	28	0	40	3	0
3	E	28	0	40	2	0
3	F	21	0	30	1	0
3	G	35	0	50	4	0
4	A	24	0	32	3	0
4	B	12	0	16	0	0
4	C	12	0	16	1	0
4	D	12	0	16	0	0
4	E	18	0	24	1	0
4	F	6	0	8	1	0
4	G	6	0	8	0	0
5	A	8	0	12	0	0
5	C	4	0	6	0	0
5	F	4	0	6	0	0
5	G	4	0	6	0	0
6	A	5	0	0	0	0
6	B	15	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
6	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	5	0	0	0	0
6	G	10	0	0	0	0
7	A	65	0	0	2	0
7	B	62	0	0	0	0
7	C	44	0	0	0	0
7	D	32	0	0	0	0
7	E	39	0	0	1	0
7	F	42	0	0	0	0
7	G	65	0	0	0	0
All	All	10751	0	10514	183	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 9.

All (183) 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:B:96:ILE:HG22	1:B:118:LEU:HD22	1.47	0.97
1:G:78:MSE:HE2	1:G:102:MSE:SE	2.16	0.96
1:G:78:MSE:HE3	1:G:153:LEU:HD21	1.49	0.94
1:G:22:ASP:OD1	1:G:25:SER:HB2	1.66	0.94
1:C:96:ILE:HG22	1:C:118:LEU:HD22	1.50	0.93
1:G:78:MSE:HE3	1:G:153:LEU:CD2	2.00	0.92
1:E:78:MSE:HE3	1:E:153:LEU:HD22	1.51	0.91
1:E:78:MSE:HE2	1:E:102:MSE:SE	2.20	0.91
1:G:78:MSE:HE2	1:G:102:MSE:HE1	1.54	0.88
1:G:78:MSE:HE2	1:G:102:MSE:CE	2.06	0.86
1:A:6:LEU:HD23	1:A:6:LEU:N	1.91	0.85
1:A:6:LEU:HD22	1:D:6:LEU:HD12	1.60	0.84
1:G:96:ILE:HG22	1:G:118:LEU:HD22	1.59	0.83
1:G:78:MSE:HE1	1:G:105:LEU:HD22	1.63	0.78
1:F:132:PHE:HE2	1:F:138:ASP:HB3	1.50	0.77
1:E:78:MSE:HE3	1:E:153:LEU:CD2	2.15	0.76
1:B:196:ARG:HH22	3:B:205:PEG:H41	1.52	0.75
1:B:101:SER:HA	3:B:206:PEG:H21	1.70	0.73
1:A:6:LEU:HD12	7:A:247:HOH:O	1.91	0.70
1:A:10:VAL:HG12	1:A:13:LYS:NZ	2.07	0.69
1:E:78:MSE:CE	1:E:153:LEU:HD22	2.22	0.69
1:A:137:SER:H	1:C:127:GLN:HE22	1.41	0.69
1:C:36:ASN:HB3	4:C:208:GOL:H12	1.76	0.68
1:G:152[A]:ARG:HH21	1:G:152[A]:ARG:HB2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:VAL:HG21	1:F:26:ARG:HG2	1.75	0.68
1:A:11:ILE:HG13	1:A:12:GLU:H	1.58	0.67
1:E:40:ASN:ND2	1:E:43:SER:H	1.92	0.67
1:A:6:LEU:CD2	1:D:6:LEU:HD12	2.24	0.67
1:C:58:ASP:OD2	1:C:61:LYS:HD2	1.93	0.67
1:G:152[A]:ARG:HH21	1:G:152[A]:ARG:CB	2.09	0.66
1:A:101:SER:HA	4:A:204:GOL:H11	1.78	0.66
1:B:96:ILE:HG22	1:B:118:LEU:CD2	2.24	0.66
1:G:78:MSE:CE	1:G:102:MSE:SE	2.92	0.65
1:E:28:LEU:HD13	1:E:50:GLN:HE21	1.61	0.65
1:A:10:VAL:CG1	1:A:13:LYS:NZ	2.59	0.65
1:F:21:PHE:N	1:F:21:PHE:CD1	2.63	0.65
1:C:166:GLU:H	1:C:166:GLU:CD	2.00	0.64
1:A:136:ALA:HB3	1:C:127:GLN:HE21	1.63	0.63
1:B:136:ALA:HB3	1:G:127:GLN:HE21	1.62	0.63
1:F:59:PRO:HB3	1:F:88:LYS:HD3	1.80	0.63
1:C:96:ILE:HG22	1:C:118:LEU:CD2	2.26	0.63
1:G:78:MSE:HE1	1:G:105:LEU:CD2	2.29	0.62
1:C:21:PHE:N	1:C:21:PHE:CD2	2.66	0.62
1:B:196:ARG:HH22	3:B:205:PEG:C4	2.13	0.62
4:E:207:GOL:H31	7:E:319:HOH:O	1.99	0.62
1:E:64:TYR:CD1	3:E:203:PEG:H41	2.35	0.61
1:A:10:VAL:HG13	1:G:21:PHE:CE1	2.35	0.61
1:B:137:SER:H	1:G:127:GLN:HE22	1.47	0.61
1:C:21:PHE:N	1:C:21:PHE:HD2	1.99	0.61
1:C:9:THR:O	1:E:25:SER:HB3	2.01	0.60
1:A:152:ARG:HH21	1:A:152:ARG:HG2	1.66	0.60
1:G:78:MSE:CE	1:G:105:LEU:HD22	2.31	0.60
1:A:136:ALA:HB3	1:C:127:GLN:NE2	2.15	0.59
1:E:125:ILE:HD12	1:E:172:THR:CG2	2.32	0.59
1:F:157:LEU:HD11	3:F:204:PEG:H12	1.86	0.58
1:B:137:SER:H	1:G:127:GLN:NE2	2.03	0.57
1:D:59:PRO:HB2	1:D:88:LYS:HD3	1.86	0.57
1:G:77:GLY:HA3	1:G:102:MSE:HE2	1.86	0.57
1:C:10:VAL:CG2	1:C:26:ARG:HG3	2.35	0.56
1:A:127:GLN:HE22	1:C:137:SER:H	1.51	0.56
1:F:71:GLY:HA3	1:F:101:SER:HB3	1.88	0.56
1:A:6:LEU:N	1:A:6:LEU:CD2	2.63	0.56
1:E:124:MSE:HG2	1:E:176:ASN:O	2.06	0.56
1:C:10:VAL:HG21	1:C:26:ARG:HG3	1.88	0.55
1:F:132:PHE:CE2	1:F:138:ASP:HB3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:HIS:HB3	3:C:206:PEG:H41	1.89	0.55
1:C:77:GLY:HA3	1:C:102:MSE:HE2	1.89	0.54
1:B:179:MSE:HG3	1:C:152:ARG:NH1	2.21	0.54
1:G:152[A]:ARG:HH21	1:G:152[A]:ARG:CG	2.19	0.54
1:B:122:GLN:OE1	1:C:149:ILE:HD11	2.07	0.54
1:F:127:GLN:HB2	1:F:128:PRO:HD2	1.90	0.54
1:A:10:VAL:HG12	1:A:13:LYS:HZ2	1.71	0.53
1:A:21:PHE:CD1	1:D:11:ILE:HD12	2.43	0.53
1:C:193:ILE:HG12	1:E:86:PHE:HE1	1.74	0.53
1:A:137:SER:H	1:C:127:GLN:NE2	2.06	0.53
1:A:10:VAL:HG12	1:A:13:LYS:HZ1	1.73	0.53
1:A:10:VAL:CG1	1:A:13:LYS:HZ1	2.20	0.53
1:A:71:GLY:HA3	1:A:101:SER:HB3	1.90	0.53
1:G:78:MSE:CE	1:G:153:LEU:CD2	2.84	0.52
1:E:127:GLN:HB2	1:E:128:PRO:HD2	1.91	0.52
1:D:136:ALA:HB3	1:E:127:GLN:NE2	2.25	0.52
1:D:136:ALA:HB3	1:E:127:GLN:HE21	1.74	0.52
1:E:72:GLY:HA2	3:E:205:PEG:H22	1.91	0.51
1:G:78:MSE:CE	1:G:102:MSE:HE1	2.33	0.51
1:G:21:PHE:N	1:G:21:PHE:CD2	2.77	0.51
1:C:124:MSE:HA	1:C:176:ASN:O	2.10	0.51
1:D:71:GLY:HA3	1:D:101:SER:HB3	1.93	0.51
1:D:21:PHE:HB2	1:D:25:SER:HB2	1.93	0.50
1:B:71:GLY:HA3	1:B:101:SER:HB3	1.92	0.50
1:A:132:PHE:HE2	1:A:138:ASP:HB3	1.76	0.50
1:F:80:VAL:O	1:F:84:MSE:HG3	2.11	0.50
1:D:123:ILE:HD12	1:D:183:ALA:CB	2.41	0.50
1:D:142:HIS:HE1	1:F:175:ASP:OD2	1.95	0.50
1:E:78:MSE:HE2	1:E:102:MSE:CE	2.43	0.49
1:G:59:PRO:HB3	1:G:88:LYS:HD2	1.95	0.49
1:A:132:PHE:CE2	1:A:138:ASP:HB3	2.47	0.49
1:E:77:GLY:HA3	1:E:102:MSE:HE2	1.94	0.49
1:F:77:GLY:HA3	1:F:102:MSE:HE2	1.95	0.49
1:E:88:LYS:N	1:E:89:PRO:CD	2.76	0.48
1:B:162:GLY:O	3:B:211:PEG:H41	2.13	0.48
1:F:88:LYS:HB2	1:F:89:PRO:HD3	1.95	0.48
1:C:8:PRO:O	1:C:22:ASP:HA	2.14	0.47
1:C:164:ASP:HB3	1:C:166:GLU:OE1	2.14	0.47
1:E:40:ASN:C	1:E:40:ASN:HD22	2.17	0.47
1:E:101:SER:OG	1:E:102:MSE:N	2.48	0.47
1:E:78:MSE:HE2	1:E:102:MSE:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:ILE:HG22	1:E:118:LEU:HD22	1.97	0.47
1:A:66:TYR:OH	3:A:203:PEG:H41	2.15	0.47
1:B:175:ASP:OD2	1:C:142:HIS:HE1	1.98	0.47
1:E:151:ASP:OD1	1:E:155:LYS:HE3	2.15	0.47
1:A:101:SER:CA	4:A:204:GOL:H11	2.43	0.46
1:A:55:GLU:HG3	1:A:89:PRO:HD3	1.97	0.46
1:F:26:ARG:HA	1:F:26:ARG:HD2	1.64	0.46
1:F:105:LEU:HD13	1:F:153:LEU:HD22	1.97	0.46
1:B:136:ALA:HB3	1:G:127:GLN:NE2	2.28	0.46
1:E:124:MSE:HA	1:E:176:ASN:O	2.16	0.46
1:C:127:GLN:HB2	1:C:128:PRO:HD2	1.98	0.46
1:E:125:ILE:HD12	1:E:172:THR:HG22	1.98	0.46
1:E:78:MSE:HE1	1:E:105:LEU:HD13	1.98	0.46
1:A:142:HIS:HE1	1:D:175:ASP:OD2	1.99	0.46
1:A:178:MSE:HE2	4:A:206:GOL:H32	1.98	0.45
1:G:164:ASP:HB3	1:G:166:GLU:OE1	2.16	0.45
1:F:46:LEU:HD23	1:F:46:LEU:HA	1.61	0.45
1:D:82:ASP:HB3	1:F:118:LEU:HD13	1.99	0.45
1:F:161:THR:OG1	1:F:163:GLN:HB2	2.15	0.45
1:B:24:TYR:OH	1:C:45:ASN:ND2	2.45	0.45
1:D:126:HIS:C	1:D:126:HIS:CD2	2.88	0.45
1:E:161:THR:OG1	1:E:163:GLN:HB2	2.17	0.45
1:G:11:ILE:HA	1:G:19:ARG:O	2.17	0.45
1:G:20:ALA:C	1:G:21:PHE:CD2	2.90	0.45
1:G:101:SER:C	3:G:204:PEG:H21	2.36	0.45
1:C:105:LEU:HD13	1:C:153:LEU:HD22	1.99	0.45
1:D:137:SER:H	1:E:127:GLN:HE22	1.65	0.45
1:A:11:ILE:HG13	1:A:12:GLU:N	2.30	0.44
1:G:101:SER:O	3:G:204:PEG:H31	2.16	0.44
1:A:10:VAL:O	1:A:21:PHE:HB3	2.17	0.44
1:E:87:ILE:HG13	1:E:89:PRO:HD2	2.00	0.44
1:D:177:PHE:O	3:D:206:PEG:H11	2.17	0.44
1:D:72:GLY:HA2	3:D:204:PEG:H31	2.00	0.44
1:E:78:MSE:HE1	1:E:105:LEU:HD22	1.99	0.44
1:F:31:ARG:NE	1:F:61:LYS:HB3	2.33	0.44
1:G:128:PRO:HB2	1:G:146:ILE:HD11	2.00	0.43
1:A:127:GLN:NE2	1:C:137:SER:H	2.15	0.43
1:F:132:PHE:HE2	1:F:138:ASP:CB	2.24	0.43
1:D:178:MSE:HG2	3:D:206:PEG:H22	2.01	0.43
1:G:166:GLU:H	1:G:166:GLU:CD	2.21	0.43
1:F:122:GLN:HG2	1:F:179:MSE:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:MSE:HE2	4:F:205:GOL:H32	2.00	0.43
1:A:196:ARG:HD2	1:G:55:GLU:OE2	2.19	0.42
1:G:21:PHE:HB3	1:G:25:SER:HB3	2.01	0.42
1:G:29:LYS:HE3	1:G:29:LYS:HB2	1.77	0.42
1:C:88:LYS:HB2	1:C:89:PRO:HD3	2.01	0.42
1:C:126:HIS:CD2	1:C:126:HIS:C	2.92	0.42
1:G:152[A]:ARG:CG	1:G:152[A]:ARG:NH2	2.80	0.42
1:G:157:LEU:HD11	3:G:204:PEG:H41	2.00	0.42
1:D:157:LEU:HD23	1:D:157:LEU:HA	1.90	0.42
1:B:116:TYR:CD1	1:B:191:HIS:HB2	2.54	0.42
1:A:166:GLU:O	1:A:170:LYS:HG3	2.20	0.42
1:C:24:TYR:OH	1:E:45:ASN:ND2	2.42	0.42
1:G:126:HIS:CD2	1:G:126:HIS:C	2.93	0.42
1:B:7:VAL:HA	1:B:8:PRO:HD3	1.88	0.41
1:D:101:SER:OG	1:D:102:MSE:N	2.49	0.41
1:A:6:LEU:CD1	7:A:247:HOH:O	2.59	0.41
1:C:118:LEU:HD12	1:C:118:LEU:HA	1.81	0.41
1:A:126:HIS:CD2	1:A:126:HIS:C	2.93	0.41
1:C:119:PRO:HG3	1:C:194:GLU:HG2	2.02	0.41
1:F:88:LYS:N	1:F:89:PRO:CD	2.83	0.41
1:C:23:ILE:HD12	1:C:23:ILE:HA	1.89	0.41
1:F:58:ASP:HA	1:F:59:PRO:HD3	1.87	0.41
1:G:196:ARG:HH22	3:G:203:PEG:H11	1.86	0.41
1:G:128:PRO:HG3	1:G:153:LEU:HD12	2.03	0.41
1:A:88:LYS:N	1:A:89:PRO:CD	2.84	0.41
1:A:196:ARG:NH1	1:G:55:GLU:OE1	2.48	0.41
1:D:126:HIS:HB3	1:D:175:ASP:HA	2.03	0.41
1:E:140:GLU:O	1:E:144:LYS:HG3	2.21	0.41
1:G:101:SER:OG	1:G:102:MSE:N	2.53	0.41
1:F:54:LEU:HD23	1:F:54:LEU:HA	1.88	0.41
1:D:152:ARG:HE	1:D:152:ARG:HB2	1.76	0.40
1:F:184:LYS:HE3	1:F:190:ASP:O	2.21	0.40
1:A:137:SER:N	1:C:127:GLN:HE22	2.13	0.40
1:E:53:PHE:O	1:E:56:SER:HB3	2.22	0.40
1:A:58:ASP:HA	1:A:59:PRO:HD2	1.87	0.40
1:D:96:ILE:HG22	1:D:118:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	185/201 (92%)	181 (98%)	4 (2%)	0	100	100
1	B	180/201 (90%)	176 (98%)	4 (2%)	0	100	100
1	C	179/201 (89%)	174 (97%)	5 (3%)	0	100	100
1	D	184/201 (92%)	179 (97%)	5 (3%)	0	100	100
1	E	178/201 (89%)	174 (98%)	4 (2%)	0	100	100
1	F	179/201 (89%)	174 (97%)	5 (3%)	0	100	100
1	G	183/201 (91%)	178 (97%)	5 (3%)	0	100	100
All	All	1268/1407 (90%)	1236 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	159/160 (99%)	151 (95%)	8 (5%)	20	30
1	B	155/160 (97%)	150 (97%)	5 (3%)	34	50
1	C	154/160 (96%)	145 (94%)	9 (6%)	17	24
1	D	158/160 (99%)	152 (96%)	6 (4%)	28	42
1	E	153/160 (96%)	146 (95%)	7 (5%)	23	33
1	F	154/160 (96%)	144 (94%)	10 (6%)	14	20
1	G	157/160 (98%)	144 (92%)	13 (8%)	9	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1090/1120 (97%)	1032 (95%)	58 (5%)	19	28

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	6	LEU
1	A	7	VAL
1	A	13	LYS
1	A	126	HIS
1	A	152	ARG
1	A	166	GLU
1	A	195	SER
1	B	105	LEU
1	B	118	LEU
1	B	126	HIS
1	B	195	SER
1	B	196	ARG
1	C	7	VAL
1	C	21	PHE
1	C	26	ARG
1	C	29	LYS
1	C	105	LEU
1	C	118	LEU
1	C	126	HIS
1	C	195	SER
1	C	197	GLU
1	D	21	PHE
1	D	56	SER
1	D	126	HIS
1	D	152	ARG
1	D	164	ASP
1	D	195	SER
1	E	40	ASN
1	E	46	LEU
1	E	126	HIS
1	E	166	GLU
1	E	193	ILE
1	E	194	GLU
1	E	197	GLU
1	F	7	VAL
1	F	21	PHE

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Mol	Chain	Res	Type
1	F	26	ARG
1	F	56	SER
1	F	61	LYS
1	F	88	LYS
1	F	101	SER
1	F	114	LYS
1	F	126	HIS
1	F	194	GLU
1	G	6	LEU
1	G	7	VAL
1	G	9	THR
1	G	19	ARG
1	G	21	PHE
1	G	25	SER
1	G	73	MSE
1	G	105	LEU
1	G	126	HIS
1	G	137	SER
1	G	152[A]	ARG
1	G	152[B]	ARG
1	G	194	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	127	GLN
1	A	142	HIS
1	A	154	ASN
1	B	50	GLN
1	B	154	ASN
1	C	45	ASN
1	C	50	GLN
1	C	127	GLN
1	C	142	HIS
1	C	154	ASN
1	D	45	ASN
1	D	50	GLN
1	D	142	HIS
1	D	154	ASN
1	D	163	GLN
1	E	40	ASN

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Mol	Chain	Res	Type
1	E	45	ASN
1	E	50	GLN
1	E	127	GLN
1	E	142	HIS
1	E	154	ASN
1	E	191	HIS
1	F	154	ASN
1	G	127	GLN
1	G	142	HIS
1	G	154	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 63 ligands modelled in this entry, 7 are monoatomic - leaving 56 for Mogul analysis.

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	$\# Z > 2$
5	EDO	A	210	-	3,3,3	0.49	0	2,2,2	0.37	0
4	GOL	A	204	-	5,5,5	0.46	0	5,5,5	0.51	0
6	PO4	C	209	2	4,4,4	0.67	0	6,6,6	0.93	0
4	GOL	D	205	-	5,5,5	0.46	0	5,5,5	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	F	206	-	3,3,3	0.49	0	2,2,2	0.32	0
4	GOL	A	211	-	5,5,5	0.48	0	5,5,5	0.19	0
6	PO4	A	212	2	4,4,4	0.75	0	6,6,6	0.60	0
3	PEG	E	205	-	6,6,6	0.46	0	5,5,5	0.71	0
6	PO4	F	208	2	4,4,4	0.70	0	6,6,6	0.62	0
4	GOL	G	210	-	5,5,5	0.41	0	5,5,5	0.51	0
4	GOL	E	207	-	5,5,5	0.45	0	5,5,5	0.63	0
4	GOL	E	208	-	5,5,5	0.53	0	5,5,5	0.52	0
3	PEG	G	209	-	6,6,6	0.47	0	5,5,5	0.40	0
3	PEG	D	208	-	6,6,6	0.46	0	5,5,5	0.58	0
6	PO4	G	211	2	4,4,4	0.94	0	6,6,6	0.39	0
4	GOL	D	207	-	5,5,5	0.41	0	5,5,5	0.23	0
4	GOL	B	208	-	5,5,5	0.42	0	5,5,5	0.25	0
3	PEG	B	205	-	6,6,6	0.51	0	5,5,5	0.49	0
3	PEG	D	204	-	6,6,6	0.50	0	5,5,5	0.32	0
3	PEG	F	203	-	6,6,6	0.55	0	5,5,5	0.34	0
3	PEG	A	203	-	6,6,6	0.63	0	5,5,5	0.65	0
3	PEG	B	206	-	6,6,6	0.76	0	5,5,5	0.61	0
3	PEG	G	204	-	6,6,6	0.51	0	5,5,5	0.50	0
3	PEG	C	204	-	6,6,6	0.45	0	5,5,5	0.34	0
3	PEG	F	204	-	6,6,6	0.47	0	5,5,5	0.30	0
6	PO4	G	207	-	4,4,4	0.85	0	6,6,6	0.35	0
3	PEG	C	206	-	6,6,6	0.48	0	5,5,5	0.28	0
6	PO4	B	204	2	4,4,4	0.89	0	6,6,6	0.41	0
4	GOL	C	205	-	5,5,5	0.63	0	5,5,5	0.63	0
4	GOL	A	206	-	5,5,5	0.30	0	5,5,5	0.56	0
5	EDO	G	208	-	3,3,3	0.53	0	2,2,2	0.13	0
3	PEG	D	206	-	6,6,6	0.58	0	5,5,5	0.43	0
4	GOL	B	209	-	5,5,5	0.51	0	5,5,5	0.51	0
3	PEG	G	205	-	6,6,6	0.57	0	5,5,5	0.23	0
3	PEG	B	211	-	6,6,6	0.62	0	5,5,5	0.48	0
3	PEG	G	206	-	6,6,6	0.71	0	5,5,5	0.37	0
4	GOL	C	208	-	5,5,5	0.65	0	5,5,5	0.84	0
3	PEG	E	206	-	6,6,6	0.57	0	5,5,5	0.18	0
4	GOL	E	209	-	5,5,5	0.49	0	5,5,5	0.21	0
5	EDO	A	208	-	3,3,3	0.69	0	2,2,2	0.11	0
5	EDO	C	207	-	3,3,3	0.48	0	2,2,2	0.25	0
6	PO4	D	209	2	4,4,4	0.93	0	6,6,6	0.50	0
4	GOL	F	205	-	5,5,5	0.42	0	5,5,5	0.59	0
3	PEG	E	203	-	6,6,6	0.56	0	5,5,5	0.16	0
6	PO4	B	203	-	4,4,4	0.89	0	6,6,6	0.48	0
3	PEG	C	203	-	6,6,6	0.59	0	5,5,5	0.57	0
6	PO4	B	210	-	4,4,4	0.88	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	D	203	-	6,6,6	0.53	0	5,5,5	0.27	0
4	GOL	A	209	-	5,5,5	0.36	0	5,5,5	0.14	0
3	PEG	A	205	-	6,6,6	0.48	0	5,5,5	0.25	0
3	PEG	G	203	-	6,6,6	0.70	0	5,5,5	0.49	0
6	PO4	E	210	2	4,4,4	0.74	0	6,6,6	0.75	0
3	PEG	F	207	-	6,6,6	0.60	0	5,5,5	0.33	0
3	PEG	E	204	-	6,6,6	0.44	0	5,5,5	0.50	0
3	PEG	B	207	-	6,6,6	0.47	0	5,5,5	0.21	0
3	PEG	A	207	-	6,6,6	0.63	0	5,5,5	0.29	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
5	EDO	A	210	-	-	1/1/1/1	-
4	GOL	A	204	-	-	4/4/4/4	-
4	GOL	D	205	-	-	2/4/4/4	-
5	EDO	F	206	-	-	1/1/1/1	-
4	GOL	A	211	-	-	0/4/4/4	-
3	PEG	E	205	-	-	1/4/4/4	-
4	GOL	G	210	-	-	0/4/4/4	-
4	GOL	E	207	-	-	1/4/4/4	-
4	GOL	E	208	-	-	0/4/4/4	-
3	PEG	G	209	-	-	4/4/4/4	-
3	PEG	D	208	-	-	3/4/4/4	-
4	GOL	D	207	-	-	0/4/4/4	-
4	GOL	B	208	-	-	0/4/4/4	-
3	PEG	B	205	-	-	3/4/4/4	-
3	PEG	D	204	-	-	2/4/4/4	-
3	PEG	F	203	-	-	1/4/4/4	-
3	PEG	A	203	-	-	4/4/4/4	-
3	PEG	B	206	-	-	2/4/4/4	-
3	PEG	G	204	-	-	1/4/4/4	-
3	PEG	C	204	-	-	1/4/4/4	-
3	PEG	F	204	-	-	2/4/4/4	-
3	PEG	C	206	-	-	1/4/4/4	-
4	GOL	C	205	-	-	2/4/4/4	-
4	GOL	A	206	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	G	208	-	-	1/1/1/1	-
3	PEG	D	206	-	-	1/4/4/4	-
4	GOL	B	209	-	-	4/4/4/4	-
3	PEG	G	205	-	-	2/4/4/4	-
3	PEG	B	211	-	-	1/4/4/4	-
3	PEG	G	206	-	-	2/4/4/4	-
4	GOL	C	208	-	-	4/4/4/4	-
3	PEG	E	206	-	-	1/4/4/4	-
4	GOL	E	209	-	-	4/4/4/4	-
5	EDO	A	208	-	-	1/1/1/1	-
5	EDO	C	207	-	-	1/1/1/1	-
4	GOL	F	205	-	-	4/4/4/4	-
3	PEG	E	203	-	-	3/4/4/4	-
3	PEG	C	203	-	-	3/4/4/4	-
3	PEG	D	203	-	-	3/4/4/4	-
4	GOL	A	209	-	-	4/4/4/4	-
3	PEG	A	205	-	-	0/4/4/4	-
3	PEG	G	203	-	-	2/4/4/4	-
3	PEG	F	207	-	-	2/4/4/4	-
3	PEG	E	204	-	-	2/4/4/4	-
3	PEG	B	207	-	-	2/4/4/4	-
3	PEG	A	207	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	204	GOL	O1-C1-C2-C3
4	A	204	GOL	C1-C2-C3-O3
4	A	209	GOL	O1-C1-C2-C3
4	A	209	GOL	C1-C2-C3-O3
4	B	209	GOL	O1-C1-C2-C3
4	C	208	GOL	O1-C1-C2-O2
4	C	208	GOL	O1-C1-C2-C3
4	C	208	GOL	C1-C2-C3-O3
4	C	208	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	D	205	GOL	O1-C1-C2-C3
4	E	209	GOL	O1-C1-C2-C3
4	F	205	GOL	O1-C1-C2-C3
4	F	205	GOL	C1-C2-C3-O3
4	A	204	GOL	O1-C1-C2-O2
4	D	205	GOL	O1-C1-C2-O2
3	E	203	PEG	O2-C3-C4-O4
3	G	204	PEG	O1-C1-C2-O2
3	B	205	PEG	O1-C1-C2-O2
3	B	205	PEG	O2-C3-C4-O4
3	B	207	PEG	O2-C3-C4-O4
3	C	203	PEG	O1-C1-C2-O2
3	D	204	PEG	O2-C3-C4-O4
3	D	206	PEG	O1-C1-C2-O2
3	F	204	PEG	O2-C3-C4-O4
3	G	203	PEG	O1-C1-C2-O2
4	B	209	GOL	C1-C2-C3-O3
4	C	205	GOL	C1-C2-C3-O3
3	C	203	PEG	O2-C3-C4-O4
3	D	203	PEG	O1-C1-C2-O2
3	F	207	PEG	O1-C1-C2-O2
4	A	204	GOL	O2-C2-C3-O3
4	B	209	GOL	O1-C1-C2-O2
4	E	209	GOL	O1-C1-C2-O2
4	F	205	GOL	O1-C1-C2-O2
3	A	203	PEG	O1-C1-C2-O2
3	D	203	PEG	O2-C3-C4-O4
3	G	209	PEG	O1-C1-C2-O2
3	B	211	PEG	O1-C1-C2-O2
3	D	208	PEG	O1-C1-C2-O2
3	G	209	PEG	O2-C3-C4-O4
4	A	209	GOL	O1-C1-C2-O2
4	A	209	GOL	O2-C2-C3-O3
4	F	205	GOL	O2-C2-C3-O3
3	C	204	PEG	O1-C1-C2-O2
3	F	203	PEG	O1-C1-C2-O2
4	A	206	GOL	O1-C1-C2-O2
4	B	209	GOL	O2-C2-C3-O3
4	C	205	GOL	O2-C2-C3-O3
3	A	203	PEG	O2-C3-C4-O4
3	G	203	PEG	C4-C3-O2-C2
3	G	205	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
3	D	203	PEG	C1-C2-O2-C3
4	E	209	GOL	C1-C2-C3-O3
3	E	203	PEG	C4-C3-O2-C2
3	B	206	PEG	O2-C3-C4-O4
3	B	206	PEG	C4-C3-O2-C2
5	F	206	EDO	O1-C1-C2-O2
3	A	203	PEG	C1-C2-O2-C3
3	B	205	PEG	C1-C2-O2-C3
3	D	208	PEG	C1-C2-O2-C3
3	G	209	PEG	C4-C3-O2-C2
3	E	205	PEG	C1-C2-O2-C3
3	C	206	PEG	O1-C1-C2-O2
3	E	206	PEG	O1-C1-C2-O2
3	D	208	PEG	C4-C3-O2-C2
3	G	206	PEG	O1-C1-C2-O2
3	A	203	PEG	C4-C3-O2-C2
5	A	208	EDO	O1-C1-C2-O2
3	G	209	PEG	C1-C2-O2-C3
3	D	204	PEG	C1-C2-O2-C3
4	E	207	GOL	O2-C2-C3-O3
4	E	209	GOL	O2-C2-C3-O3
5	G	208	EDO	O1-C1-C2-O2
3	E	203	PEG	O1-C1-C2-O2
3	E	204	PEG	O1-C1-C2-O2
5	A	210	EDO	O1-C1-C2-O2
3	E	204	PEG	C4-C3-O2-C2
3	F	204	PEG	C1-C2-O2-C3
3	C	203	PEG	C1-C2-O2-C3
3	F	207	PEG	C1-C2-O2-C3
3	G	206	PEG	O2-C3-C4-O4
3	B	207	PEG	O1-C1-C2-O2
3	G	205	PEG	O2-C3-C4-O4
5	C	207	EDO	O1-C1-C2-O2

There are no ring outliers.

17 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	204	GOL	2	0
3	E	205	PEG	1	0
4	E	207	GOL	1	0
3	B	205	PEG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	204	PEG	1	0
3	A	203	PEG	1	0
3	B	206	PEG	1	0
3	G	204	PEG	3	0
3	F	204	PEG	1	0
3	C	206	PEG	1	0
4	A	206	GOL	1	0
3	D	206	PEG	2	0
3	B	211	PEG	1	0
4	C	208	GOL	1	0
4	F	205	GOL	1	0
3	E	203	PEG	1	0
3	G	203	PEG	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 ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	182/201 (90%)	-0.34	4 (2%) 62 63	38, 50, 86, 115	2 (1%)
1	B	177/201 (88%)	-0.37	6 (3%) 48 50	37, 49, 87, 123	0
1	C	176/201 (87%)	-0.20	5 (2%) 55 56	42, 57, 90, 146	0
1	D	181/201 (90%)	-0.28	2 (1%) 77 78	44, 57, 91, 125	0
1	E	175/201 (87%)	-0.23	3 (1%) 69 69	49, 60, 82, 120	0
1	F	176/201 (87%)	-0.20	2 (1%) 77 78	48, 60, 90, 133	0
1	G	179/201 (89%)	-0.47	3 (1%) 69 69	28, 47, 79, 133	2 (1%)
All	All	1246/1407 (88%)	-0.30	25 (2%) 64 66	28, 56, 87, 146	4 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	VAL	7.2
1	B	6	LEU	4.8
1	B	20	ALA	4.5
1	C	7	VAL	4.4
1	B	11	ILE	4.1
1	E	7	VAL	3.5
1	C	199	ILE	3.2
1	D	6	LEU	3.1
1	G	6	LEU	3.1
1	F	11	ILE	2.9
1	C	132	PHE	2.8
1	F	7	VAL	2.7
1	A	10	VAL	2.7
1	A	132	PHE	2.7
1	E	198	ALA	2.5
1	G	132	PHE	2.5
1	C	193	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	198	ALA	2.4
1	G	152[A]	ARG	2.3
1	C	21	PHE	2.3
1	E	132	PHE	2.3
1	A	11	ILE	2.2
1	B	9	THR	2.1
1	B	132	PHE	2.0
1	B	197	GLU	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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
6	PO4	C	209	5/5	0.38	0.13	173,177,177,178	0
6	PO4	D	209	5/5	0.39	0.14	151,153,153,154	0
6	PO4	E	210	5/5	0.45	0.14	198,199,201,201	0
6	PO4	G	211	5/5	0.45	0.15	156,157,160,161	0
6	PO4	A	212	5/5	0.55	0.15	165,168,168,169	0
6	PO4	F	208	5/5	0.62	0.11	176,176,177,177	0
6	PO4	B	204	5/5	0.63	0.16	144,147,147,148	0
6	PO4	B	203	5/5	0.63	0.10	130,132,134,135	0
6	PO4	G	207	5/5	0.67	0.11	110,120,120,124	0
3	PEG	C	206	7/7	0.69	0.14	84,97,107,108	0
5	EDO	A	208	4/4	0.71	0.18	65,72,77,78	0
4	GOL	D	207	6/6	0.74	0.14	93,100,102,102	0
4	GOL	F	205	6/6	0.75	0.15	80,92,97,102	0
4	GOL	G	210	6/6	0.75	0.17	77,88,90,92	0
4	GOL	B	208	6/6	0.77	0.18	90,98,102,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	206	6/6	0.77	0.16	76,79,86,89	0
4	GOL	C	208	6/6	0.79	0.14	66,88,92,93	0
4	GOL	E	208	6/6	0.79	0.17	80,91,97,97	0
4	GOL	E	207	6/6	0.83	0.11	84,90,92,93	0
3	PEG	G	206	7/7	0.83	0.14	62,74,82,82	0
5	EDO	C	207	4/4	0.83	0.23	83,83,86,88	0
4	GOL	A	204	6/6	0.83	0.16	50,71,75,84	0
4	GOL	A	211	6/6	0.84	0.13	84,87,88,88	0
4	GOL	E	209	6/6	0.84	0.12	84,86,97,100	0
4	GOL	D	205	6/6	0.84	0.16	71,77,82,87	0
4	GOL	B	209	6/6	0.84	0.16	78,88,90,92	0
4	GOL	C	205	6/6	0.84	0.14	70,76,77,81	0
5	EDO	A	210	4/4	0.85	0.18	65,71,72,73	0
3	PEG	D	206	7/7	0.85	0.14	76,79,83,85	0
5	EDO	G	208	4/4	0.85	0.19	72,74,77,79	0
3	PEG	E	206	7/7	0.85	0.17	95,99,104,105	0
3	PEG	A	207	7/7	0.86	0.15	84,85,88,90	0
3	PEG	F	207	7/7	0.86	0.15	79,82,86,86	0
3	PEG	B	211	7/7	0.86	0.14	65,69,83,85	0
3	PEG	C	203	7/7	0.87	0.14	87,88,90,90	0
6	PO4	B	210	5/5	0.87	0.11	138,141,142,142	0
3	PEG	F	203	7/7	0.87	0.14	80,81,86,87	0
3	PEG	D	208	7/7	0.87	0.14	85,88,92,92	0
3	PEG	A	203	7/7	0.88	0.14	68,70,81,83	0
3	PEG	E	203	7/7	0.88	0.14	81,83,85,85	0
5	EDO	F	206	4/4	0.89	0.16	72,73,74,80	0
3	PEG	D	203	7/7	0.89	0.12	75,77,83,84	0
3	PEG	E	205	7/7	0.89	0.15	84,86,89,91	0
3	PEG	G	209	7/7	0.89	0.11	64,67,73,77	0
3	PEG	B	207	7/7	0.89	0.12	63,67,73,75	0
3	PEG	B	206	7/7	0.89	0.17	60,72,82,83	0
3	PEG	C	204	7/7	0.90	0.12	64,69,78,83	0
3	PEG	G	203	7/7	0.90	0.12	65,67,67,71	0
3	PEG	G	204	7/7	0.90	0.15	59,65,83,88	0
3	PEG	G	205	7/7	0.90	0.11	71,74,82,83	0
3	PEG	D	204	7/7	0.90	0.12	64,68,82,84	0
3	PEG	F	204	7/7	0.91	0.12	74,75,79,82	0
4	GOL	A	209	6/6	0.92	0.09	74,79,81,85	0
3	PEG	B	205	7/7	0.92	0.13	76,77,79,81	0
3	PEG	A	205	7/7	0.93	0.11	71,72,79,83	0
3	PEG	E	204	7/7	0.93	0.13	66,76,79,81	0
2	MG	D	202	1/1	0.97	0.05	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	G	202	1/1	0.98	0.04	38,38,38,38	0
2	MG	C	202	1/1	0.98	0.05	46,46,46,46	0
2	MG	A	202	1/1	0.98	0.04	44,44,44,44	0
2	MG	B	202	1/1	0.99	0.06	34,34,34,34	0
2	MG	E	202	1/1	0.99	0.04	50,50,50,50	0
2	MG	F	202	1/1	0.99	0.07	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.