



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2019 – 05:53 PM EST

PDB ID : 6D02  
Title : Cross-alpha Amyloid-like Structure alphaAmL, 2nd form  
Authors : Zhang, S.-Q.; Liu, L.; Degrado, W.F.  
Deposited on : 2018-04-10  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

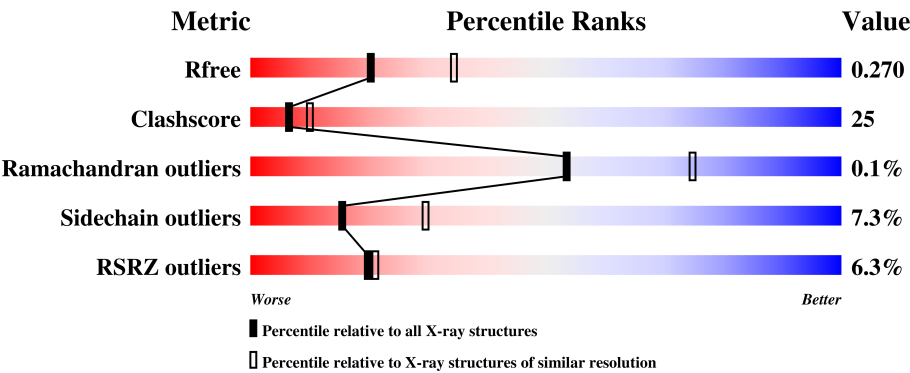
MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

# 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 2.50 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 <sub>free</sub>	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	27	<div><div>22%</div><div>37%48%11%.</div></div>
1	B	27	<div><div>11%</div><div>52%37%11%</div></div>
1	C	27	<div><div>4%</div><div>33%52%.11%</div></div>
1	D	27	<div><div>15%</div><div>26%56%7%11%</div></div>
1	E	27	<div><div>7%</div><div>37%59%. .</div></div>

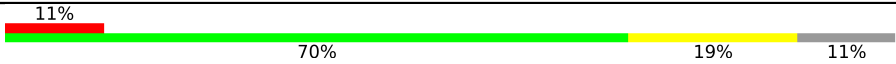

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Mol	Chain	Length	Quality of chain
1	F	27	
1	G	27	
1	H	27	
1	I	27	
1	J	27	
1	K	27	
1	L	27	
1	M	27	
1	N	27	
1	O	27	
1	P	27	
1	Q	27	
1	R	27	
1	S	27	
1	T	27	
1	U	27	
1	V	27	
1	W	27	
1	X	27	
1	Y	27	
1	Z	27	
1	a	27	
1	b	27	
1	c	27	
1	d	27	

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Mol	Chain	Length	Quality of chain
1	e	27	
1	f	27	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	E	101	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6078 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 alpha-Amyloid peptide alphaAmL.

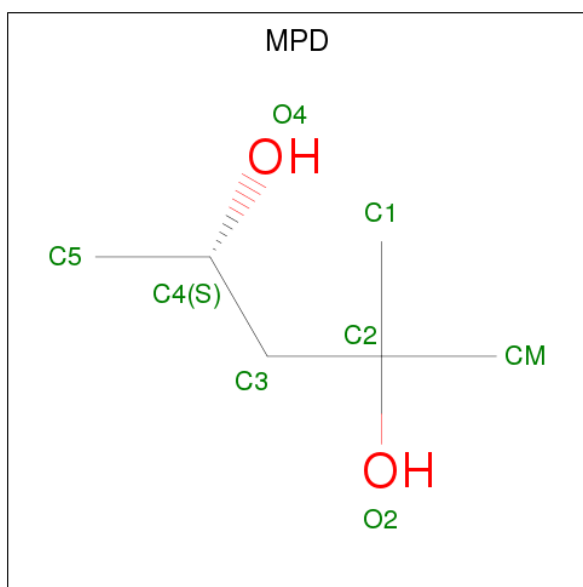
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	26	Total	C	N	O	0	0	1
			202	134	36	32			
1	B	24	Total	C	N	O	0	0	0
			158	103	28	27			
1	C	24	Total	C	N	O	0	0	0
			195	132	32	31			
1	D	24	Total	C	N	O	0	0	0
			181	123	29	29			
1	E	26	Total	C	N	O	0	0	1
			205	137	36	32			
1	F	26	Total	C	N	O	0	0	1
			184	122	34	28			
1	G	24	Total	C	N	O	0	0	0
			200	133	34	33			
1	H	24	Total	C	N	O	0	0	0
			173	117	27	29			
1	I	24	Total	C	N	O	0	0	0
			196	132	33	31			
1	J	26	Total	C	N	O	0	0	1
			175	117	30	28			
1	K	26	Total	C	N	O	0	0	1
			201	133	36	32			
1	L	24	Total	C	N	O	0	0	0
			185	125	29	31			
1	M	26	Total	C	N	O	0	0	1
			198	130	36	32			
1	N	24	Total	C	N	O	0	0	0
			174	117	28	29			
1	O	26	Total	C	N	O	0	0	1
			196	129	35	32			
1	P	24	Total	C	N	O	0	0	0
			165	113	27	25			

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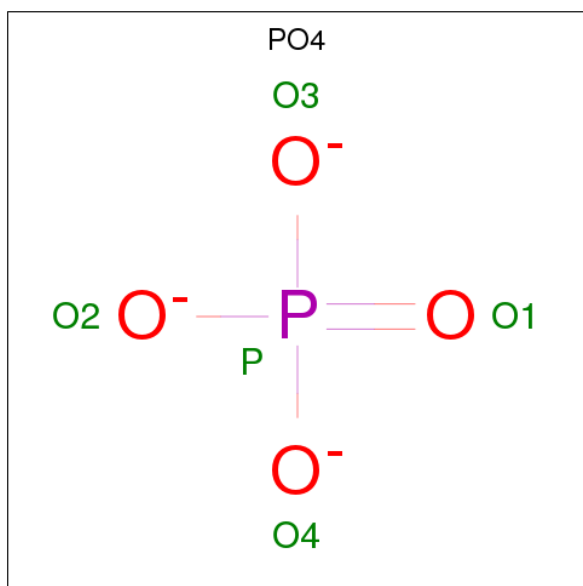
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Q	26	Total	C	N	O	0	0	1
			205	137	36	32			
1	R	26	Total	C	N	O	0	0	1
			180	118	30	32			
1	S	24	Total	C	N	O	0	0	0
			200	135	34	31			
1	T	26	Total	C	N	O	0	0	1
			176	117	31	28			
1	U	24	Total	C	N	O	0	0	0
			203	136	34	33			
1	V	24	Total	C	N	O	0	0	0
			180	124	29	27			
1	W	24	Total	C	N	O	0	0	0
			200	135	34	31			
1	X	24	Total	C	N	O	0	0	0
			175	117	29	29			
1	Y	24	Total	C	N	O	0	0	0
			194	132	31	31			
1	Z	25	Total	C	N	O	0	0	0
			160	106	26	28			
1	a	24	Total	C	N	O	0	0	0
			184	123	30	31			
1	b	23	Total	C	N	O	0	0	0
			173	117	29	27			
1	c	23	Total	C	N	O	0	0	0
			170	114	30	26			
1	d	26	Total	C	N	O	0	0	1
			189	125	32	32			
1	e	24	Total	C	N	O	0	0	0
			181	122	32	27			
1	f	23	Total	C	N	O	0	0	0
			169	115	29	25			

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



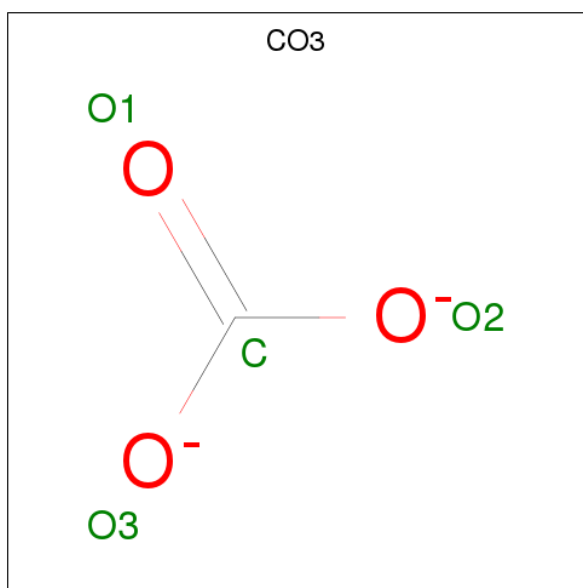
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	4	Total	O	0	0
			4	4		
5	C	5	Total	O	0	0
			5	5		
5	D	3	Total	O	0	0
			3	3		
5	E	5	Total	O	0	0
			5	5		
5	F	6	Total	O	0	0
			6	6		
5	G	4	Total	O	0	0
			4	4		
5	H	4	Total	O	0	0
			4	4		
5	J	1	Total	O	0	0
			1	1		
5	K	6	Total	O	0	0
			6	6		

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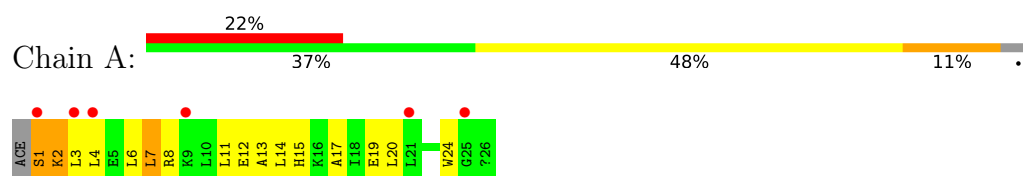
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	9	Total O 9 9	0	0
5	M	7	Total O 7 7	0	0
5	O	1	Total O 1 1	0	0
5	P	6	Total O 6 6	0	0
5	Q	4	Total O 4 4	0	0
5	R	3	Total O 3 3	0	0
5	S	4	Total O 4 4	0	0
5	T	2	Total O 2 2	0	0
5	U	3	Total O 3 3	0	0
5	V	4	Total O 4 4	0	0
5	W	3	Total O 3 3	0	0
5	X	2	Total O 2 2	0	0
5	Y	5	Total O 5 5	0	0
5	Z	6	Total O 6 6	0	0
5	a	4	Total O 4 4	0	0
5	b	4	Total O 4 4	0	0
5	c	5	Total O 5 5	0	0
5	d	1	Total O 1 1	0	0
5	e	4	Total O 4 4	0	0
5	f	3	Total O 3 3	0	0

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

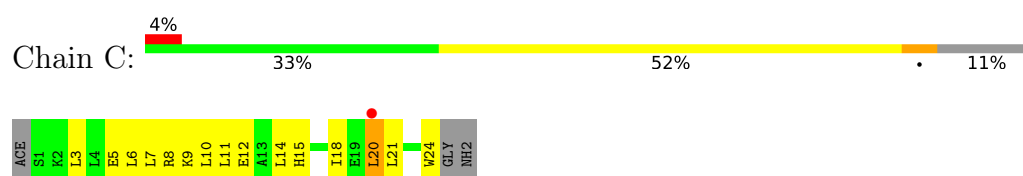
- Molecule 1: alpha-Amyloid peptide alphaAmL



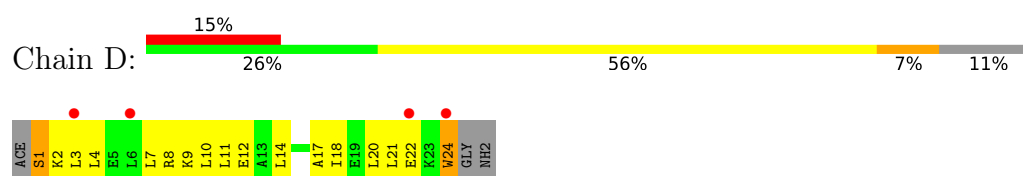
- Molecule 1: alpha-Amyloid peptide alphaAmL



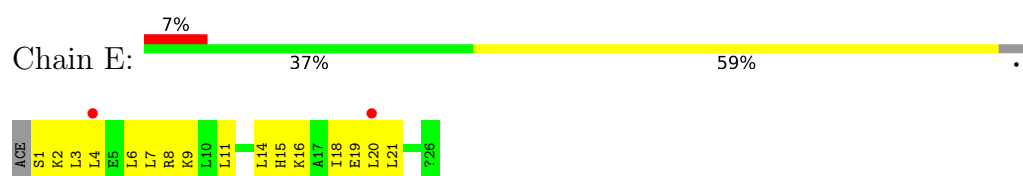
- Molecule 1: alpha-Amyloid peptide alphaAmL



- Molecule 1: alpha-Amyloid peptide alphaAmL



- Molecule 1: alpha-Amyloid peptide alphaAmL



- Molecule 1: alpha-Amyloid peptide alphaAmL





- Molecule 1: alpha-Amyloid peptide alphaAmL



- Molecule 1: alpha-Amyloid peptide alphaAmL



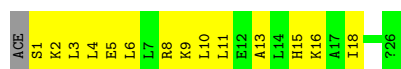
- Molecule 1: alpha-Amyloid peptide alphaAmL



- Molecule 1: alpha-Amyloid peptide alphaAmL



- Molecule 1: alpha-Amyloid peptide alphaAmL



- Molecule 1: alpha-Amyloid peptide alphaAmL



- Molecule 1: alpha-Amyloid peptide alphaAmL



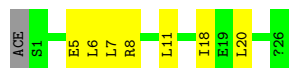
- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain N:  41% 48% 11%



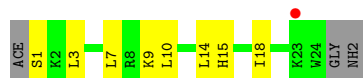
- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain O:  70% 26% 4%



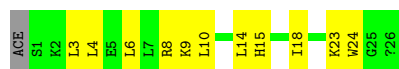
- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain P:  4% 59% 30% 7%



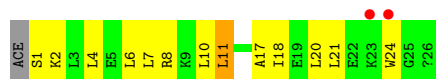
- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain Q:  56% 41% 3%



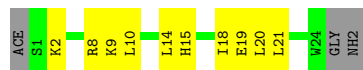
- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain R:  7% 48% 44% 1%



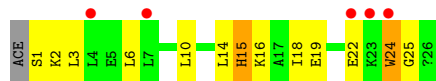
- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain S:  52% 37% 11%



- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain T:  19% 48% 41% 7% 5%



- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain U:  52% 30% 7% 11%



- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain V:  4% 33% 44% 11% 11%




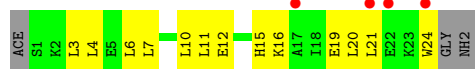
- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain W:  59% 26% 11% 11%



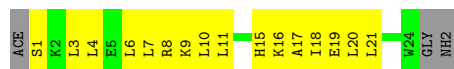
- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain X:  15% 41% 48% 11%



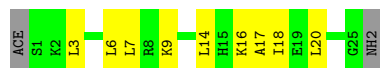
- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain Y:  30% 59% 11%




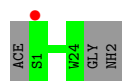
- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain Z:  59% 33% 7% 11%



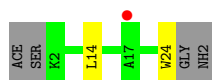
- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain a:  4% 89% 11%

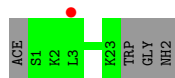
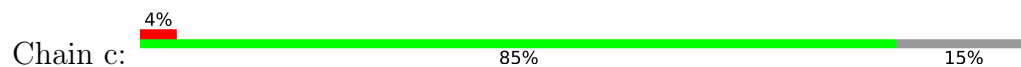


- Molecule 1: alpha-Amyloid peptide alphaAmL

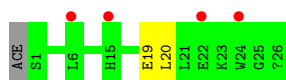
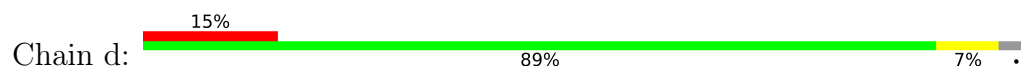
Chain b:  4% 78% 7% 15%



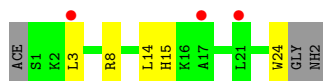
- Molecule 1: alpha-Amyloid peptide alphaAmL



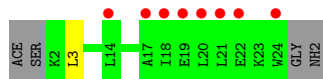
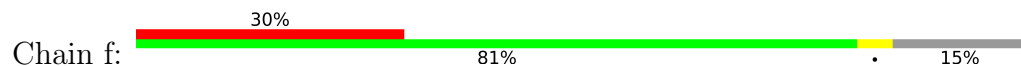
- Molecule 1: alpha-Amyloid peptide alphaAmL



- Molecule 1: alpha-Amyloid peptide alphaAmL



- Molecule 1: alpha-Amyloid peptide alphaAmL



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.55Å 107.78Å 99.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.50 76.13 – 2.48	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.50) 97.9 (76.13-2.48)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.232 , 0.277 0.235 , 0.270	Depositor DCC
$R_{free}$ test set	2015 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.4	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 78.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.447 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6078	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9293e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, MPD, PO4, NH2

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	0.45	0/203	0.67	0/270
1	B	0.29	0/160	0.45	0/219
1	C	0.39	0/196	0.55	0/261
1	D	0.49	0/183	0.61	0/248
1	E	0.47	0/206	0.66	0/274
1	F	0.42	0/185	0.53	0/250
1	G	0.44	0/202	0.56	0/269
1	H	0.30	0/175	0.54	0/240
1	I	0.72	0/198	0.68	0/265
1	J	0.34	0/176	0.57	0/240
1	K	0.60	0/202	0.57	0/269
1	L	0.66	0/186	0.71	0/249
1	M	0.64	0/199	0.76	0/265
1	N	0.41	0/176	0.57	0/240
1	O	0.43	0/195	0.68	0/258
1	P	0.34	0/166	0.58	0/226
1	Q	0.44	0/206	0.59	0/274
1	R	0.60	0/181	0.59	0/246
1	S	0.42	0/202	0.57	0/269
1	T	0.35	0/177	0.50	0/240
1	U	0.48	0/205	0.64	0/273
1	V	0.41	0/181	0.59	0/243
1	W	0.46	0/202	0.62	0/269
1	X	0.46	0/177	0.52	0/240
1	Y	0.43	0/196	0.54	0/262
1	Z	0.51	0/159	0.62	0/216
1	a	0.36	0/186	0.50	0/250
1	b	0.49	0/175	0.66	0/239
1	c	0.41	0/170	0.54	0/228
1	d	0.41	0/190	0.66	0/255
1	e	0.33	0/183	0.59	0/247
1	f	0.30	0/171	0.44	0/231



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.46	0/5969	0.60	0/8025

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	202	0	225	24	0
1	B	158	0	132	13	0
1	C	195	0	226	25	0
1	D	181	0	192	29	0
1	E	205	0	234	34	0
1	F	184	0	188	20	0
1	G	200	0	224	11	0
1	H	173	0	170	4	0
1	I	196	0	220	12	0
1	J	175	0	171	9	0
1	K	201	0	223	15	0
1	L	185	0	204	13	0
1	M	198	0	214	21	0
1	N	174	0	172	11	0
1	O	196	0	226	6	0
1	P	165	0	170	11	0
1	Q	205	0	234	14	0
1	R	180	0	170	18	0
1	S	200	0	231	10	0
1	T	176	0	173	16	0
1	U	203	0	233	9	0
1	V	180	0	205	11	0
1	W	200	0	231	13	0
1	X	175	0	174	20	0
1	Y	194	0	220	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	160	0	158	12	0
1	a	184	0	191	0	0
1	b	173	0	173	0	0
1	c	170	0	191	0	0
1	d	189	0	194	0	0
1	e	181	0	192	0	0
1	f	169	0	173	0	0
2	A	8	0	14	4	0
3	E	5	0	0	3	0
3	I	5	0	0	1	0
3	M	5	0	0	1	0
4	Q	4	0	0	0	0
5	A	6	0	0	0	0
5	B	4	0	0	1	0
5	C	5	0	0	2	0
5	D	3	0	0	0	0
5	E	5	0	0	0	0
5	F	6	0	0	0	0
5	G	4	0	0	1	0
5	H	4	0	0	1	0
5	J	1	0	0	1	0
5	K	6	0	0	0	0
5	L	9	0	0	1	0
5	M	7	0	0	3	0
5	O	1	0	0	0	0
5	P	6	0	0	0	0
5	Q	4	0	0	0	0
5	R	3	0	0	0	0
5	S	4	0	0	3	0
5	T	2	0	0	1	0
5	U	3	0	0	2	0
5	V	4	0	0	0	0
5	W	3	0	0	0	0
5	X	2	0	0	0	0
5	Y	5	0	0	1	0
5	Z	6	0	0	1	0
5	a	4	0	0	0	0
5	b	4	0	0	0	0
5	c	5	0	0	0	0
5	d	1	0	0	0	0
5	e	4	0	0	0	0
5	f	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6078	0	6348	305	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 25.

All (305) 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:Z:16:LYS:O	1:Z:20:LEU:HD12	1.48	1.09
1:C:20:LEU:O	1:C:24:TRP:HB2	1.56	1.06
1:R:7:LEU:O	1:R:11:LEU:HD12	1.60	1.00
1:D:14:LEU:O	1:D:18:ILE:HD12	4.88	0.92
1:E:20:LEU:HD13	1:F:3:LEU:HD11	1.56	0.87
1:W:21:LEU:HD22	1:X:7:LEU:HD11	1.59	0.85
1:R:7:LEU:C	1:R:11:LEU:HD12	1.99	0.82
1:W:3:LEU:HD21	1:X:21:LEU:HA	1.62	0.81
1:S:15:HIS:HA	1:S:18:ILE:HD12	1.63	0.79
1:K:15:HIS:HB2	1:M:8:ARG:NH2	1.99	0.78
1:D:20:LEU:HD11	1:F:6:LEU:HD12	26.02	0.77
1:Q:9:LYS:HD3	1:S:9:LYS:HD3	1.67	0.77
1:B:18:ILE:HG21	1:D:21:LEU:HD22	31.95	0.76
1:V:7:LEU:O	1:V:11:LEU:HD12	1.86	0.75
1:W:14:LEU:HD12	1:X:10:LEU:HB2	1.68	0.75
1:W:4:LEU:HD23	1:X:21:LEU:HD11	1.68	0.75
1:E:15:HIS:HA	1:E:18:ILE:HD12	1.86	0.74
1:E:1:SER:OG	1:E:2:LYS:N	2.20	0.74
1:T:14:LEU:O	1:T:18:ILE:HG12	1.87	0.74
1:A:4:LEU:HA	1:A:7:LEU:HD12	6.09	0.72
1:X:4:LEU:HA	1:X:7:LEU:HD12	1.71	0.72
1:U:2:LYS:NZ	5:U:101:HOH:O	2.23	0.72
1:L:9:LYS:NZ	5:L:101:HOH:O	2.20	0.71
1:P:7:LEU:HA	1:P:10:LEU:HD12	1.70	0.71
1:E:3:LEU:HD23	1:E:3:LEU:H	5.26	0.70
1:K:15:HIS:HA	1:K:18:ILE:HD12	1.74	0.70
1:B:15:HIS:HA	1:B:18:ILE:HD12	6.80	0.69
1:W:17:ALA:O	1:W:21:LEU:HD23	1.92	0.69
1:M:4:LEU:HA	1:M:7:LEU:HD12	1.72	0.69
1:B:18:ILE:HG22	1:D:22:GLU:HG3	33.46	0.68
1:F:18:ILE:HA	1:F:21:LEU:HD12	1.75	0.68
1:M:8:ARG:NH1	5:M:201:HOH:O	2.25	0.68
1:E:11:LEU:HA	1:E:14:LEU:HD12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:15:HIS:HA	1:P:18:ILE:HD12	1.77	0.67
1:F:8:ARG:HA	1:F:11:LEU:HD12	2.34	0.66
1:G:3:LEU:H	1:G:3:LEU:HD12	1.61	0.66
1:D:21:LEU:HA	1:D:24:TRP:HD1	4.80	0.66
1:W:21:LEU:HB3	1:X:3:LEU:HD22	1.78	0.65
1:J:21:LEU:O	1:J:26:NH2:N	2.29	0.65
1:M:26:NH2:N	5:M:202:HOH:O	2.29	0.65
1:X:21:LEU:HD22	1:Z:18:ILE:HG12	1.79	0.64
1:E:3:LEU:HD12	1:E:6:LEU:HB3	1.80	0.64
1:A:15:HIS:NE2	1:A:19:GLU:OE2	2.30	0.64
1:A:14:LEU:HD23	5:C:101:HOH:O	17.63	0.64
1:P:14:LEU:HD13	1:P:18:ILE:HD11	1.80	0.63
1:I:21:LEU:HA	1:J:3:LEU:HD21	1.80	0.63
1:Q:23:LYS:HG2	1:Q:24:TRP:CD1	2.34	0.63
1:A:12:GLU:OE2	1:Y:9:LYS:NZ	78.60	0.63
1:Y:18:ILE:HA	1:Y:21:LEU:HD12	1.80	0.63
1:C:14:LEU:HG	1:D:10:LEU:HD22	5.46	0.62
1:E:16:LYS:O	1:E:20:LEU:HG	1.99	0.62
1:E:21:LEU:HB2	1:F:3:LEU:CD2	2.28	0.62
1:C:8:ARG:NH1	5:C:101:HOH:O	10.82	0.62
1:C:20:LEU:O	1:C:24:TRP:CB	2.42	0.62
1:R:1:SER:HG	1:T:24:TRP:HZ3	1.47	0.62
1:Z:16:LYS:C	1:Z:20:LEU:HD12	2.18	0.62
1:A:14:LEU:HD11	1:B:7:LEU:HA	1.81	0.61
1:E:9:LYS:HG2	1:G:9:LYS:HD2	1.82	0.61
1:T:18:ILE:HG21	1:V:21:LEU:HD22	1.82	0.61
1:F:3:LEU:HD12	1:F:3:LEU:H	4.38	0.61
1:N:19:GLU:HA	1:N:22:GLU:HG2	1.82	0.61
1:M:14:LEU:O	1:M:18:ILE:HG13	2.00	0.61
1:V:13:ALA:HA	1:V:16:LYS:HD2	1.82	0.60
1:M:12:GLU:O	1:M:16:LYS:HG2	2.02	0.60
1:E:15:HIS:O	1:E:19:GLU:HG3	2.02	0.60
1:A:11:LEU:O	1:A:14:LEU:N	2.95	0.59
1:R:18:ILE:HA	1:R:21:LEU:HD12	1.83	0.59
1:C:15:HIS:HA	1:C:18:ILE:HD12	2.22	0.59
1:E:20:LEU:CD1	1:F:3:LEU:HD11	2.28	0.59
1:S:14:LEU:HD12	1:T:10:LEU:HB3	1.85	0.59
1:A:2:LYS:HB3	1:C:20:LEU:HD11	1.85	0.58
1:O:11:LEU:HB3	1:Q:8:ARG:HG2	1.85	0.58
1:I:6:LEU:HD21	1:L:6:LEU:HD11	1.85	0.58
1:P:3:LEU:H	1:P:3:LEU:HD12	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:20:LEU:HB3	1:N:3:LEU:HD11	1.84	0.58
1:Q:3:LEU:O	1:Q:6:LEU:HG	2.04	0.58
1:Q:14:LEU:HD13	1:R:10:LEU:HB2	1.85	0.58
1:T:18:ILE:O	1:T:22:GLU:HG3	2.03	0.58
1:W:18:ILE:HA	1:W:21:LEU:HD21	1.86	0.58
1:M:14:LEU:HD13	1:N:10:LEU:HB3	1.85	0.57
1:A:15:HIS:O	1:A:19:GLU:HG3	2.04	0.57
1:C:8:ARG:O	1:C:12:GLU:HG3	2.14	0.57
1:A:13:ALA:HB2	1:C:9:LYS:HB2	1.87	0.56
1:A:14:LEU:HD11	1:B:7:LEU:HD22	1.86	0.56
1:D:20:LEU:HD11	1:F:6:LEU:CD1	26.67	0.56
1:S:10:LEU:HD21	1:T:14:LEU:HA	1.87	0.56
1:X:20:LEU:O	1:X:24:TRP:HB2	2.05	0.56
1:Z:14:LEU:HD13	1:Z:18:ILE:HD13	1.87	0.56
1:Y:16:LYS:HA	1:Y:19:GLU:HG2	1.87	0.56
1:C:5:GLU:O	1:C:9:LYS:HG2	2.04	0.56
1:S:21:LEU:HD13	1:T:3:LEU:HD12	1.88	0.56
1:I:6:LEU:HD13	1:K:13:ALA:O	2.06	0.56
1:Y:17:ALA:HB3	1:Z:7:LEU:HD12	1.88	0.56
1:K:11:LEU:O	1:M:8:ARG:NH2	2.39	0.55
1:B:15:HIS:O	1:B:19:GLU:HG2	4.22	0.55
1:N:23:LYS:NZ	1:P:1:SER:OG	2.39	0.55
1:R:6:LEU:HD23	1:T:16:LYS:HB3	1.88	0.55
1:Z:17:ALA:HA	1:Z:20:LEU:HD13	1.89	0.55
1:R:8:ARG:HA	1:R:11:LEU:CD1	2.36	0.55
1:C:11:LEU:HD21	1:E:4:LEU:HB3	1.88	0.55
1:Y:15:HIS:ND1	5:Y:101:HOH:O	2.31	0.55
2:A:101:MPD:H31	1:E:15:HIS:HE1	1.72	0.54
1:D:2:LYS:HD3	1:F:23:LYS:HE2	41.17	0.54
1:E:4:LEU:O	1:E:8:ARG:HB3	2.07	0.54
1:F:16:LYS:HD3	1:H:6:LEU:HA	1.89	0.54
1:E:21:LEU:HB2	1:F:3:LEU:HD21	1.90	0.54
1:L:2:LYS:H	1:L:2:LYS:HD3	1.72	0.54
1:Z:9:LYS:NZ	5:Z:102:HOH:O	2.29	0.54
1:C:10:LEU:HD21	1:D:14:LEU:HA	1.88	0.54
1:M:15:HIS:HA	1:M:18:ILE:HD12	1.89	0.54
1:N:13:ALA:HA	1:P:9:LYS:HE3	1.89	0.54
1:X:15:HIS:NE2	1:X:19:GLU:OE2	2.41	0.54
1:Y:18:ILE:HG13	1:Z:7:LEU:HD11	1.88	0.54
1:Y:17:ALA:HA	1:Y:20:LEU:HD12	1.89	0.54
1:P:14:LEU:CD1	1:P:18:ILE:HD11	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:HD12	1:Y:16:LYS:HB3	63.74	0.54
1:Q:23:LYS:HG2	1:Q:24:TRP:HD1	1.71	0.53
1:A:8:ARG:NH2	2:A:101:MPD:O2	2.41	0.53
1:E:7:LEU:O	1:E:11:LEU:HG	2.32	0.53
1:P:14:LEU:O	1:P:18:ILE:HG13	2.07	0.53
1:X:6:LEU:CD2	1:X:10:LEU:HD11	2.38	0.53
1:Y:4:LEU:O	1:Y:7:LEU:HB3	2.07	0.53
1:I:8:ARG:O	1:I:12:GLU:HG3	2.08	0.53
1:D:1:SER:N	1:D:4:LEU:HD12	2.23	0.53
1:E:14:LEU:HG	1:F:10:LEU:HB3	1.91	0.53
1:I:6:LEU:HD12	1:K:13:ALA:HB1	1.90	0.53
1:A:2:LYS:HA	1:Y:16:LYS:NZ	59.87	0.53
1:Z:3:LEU:O	1:Z:6:LEU:HB3	2.09	0.53
1:Q:14:LEU:HD13	1:R:10:LEU:CB	2.39	0.53
1:R:8:ARG:HA	1:R:11:LEU:HD12	1.89	0.53
1:B:18:ILE:HD13	1:D:21:LEU:HD21	29.28	0.52
1:S:15:HIS:O	1:S:19:GLU:HG3	2.08	0.52
1:D:21:LEU:HA	1:D:24:TRP:CD1	5.55	0.52
1:I:14:LEU:HA	1:J:10:LEU:HD13	1.92	0.52
1:Y:8:ARG:O	1:Y:11:LEU:N	2.43	0.52
1:R:8:ARG:CA	1:R:11:LEU:HD12	2.40	0.52
1:C:21:LEU:HB2	1:D:3:LEU:HD22	1.92	0.51
1:L:14:LEU:HD21	1:M:4:LEU:HD22	1.90	0.51
1:I:12:GLU:OE1	1:K:9:LYS:NZ	2.37	0.51
1:K:4:LEU:HB3	1:K:8:ARG:HE	1.75	0.51
1:E:20:LEU:HG	1:F:3:LEU:HD23	6.25	0.51
1:K:4:LEU:O	1:K:8:ARG:HG3	2.11	0.51
1:M:4:LEU:O	1:M:8:ARG:HG2	2.10	0.51
1:R:7:LEU:O	1:R:11:LEU:CD1	2.48	0.51
1:L:15:HIS:O	1:L:18:ILE:HG12	2.10	0.51
1:M:7:LEU:HD11	1:N:21:LEU:HD22	1.93	0.51
1:E:8:ARG:HA	1:E:11:LEU:HD12	2.84	0.51
1:E:15:HIS:NE2	1:E:19:GLU:OE1	2.44	0.51
1:D:8:ARG:HA	1:D:11:LEU:HD12	1.92	0.50
1:K:3:LEU:HD12	1:K:6:LEU:HB3	1.92	0.50
1:W:18:ILE:HA	1:W:21:LEU:CD2	2.41	0.50
1:Y:19:GLU:HG3	1:Y:20:LEU:N	2.26	0.50
1:D:14:LEU:O	1:D:18:ILE:HG12	2.12	0.50
1:T:22:GLU:HG2	1:V:22:GLU:HB3	1.93	0.49
1:Z:16:LYS:O	1:Z:20:LEU:CD1	2.40	0.49
1:M:17:ALA:HB1	1:N:7:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:8:ARG:NH2	5:S:101:HOH:O	2.45	0.49
1:Y:7:LEU:O	1:Y:10:LEU:HB3	2.12	0.49
1:E:21:LEU:HD13	1:F:3:LEU:HB2	5.10	0.49
1:A:8:ARG:O	1:A:12:GLU:HG3	2.12	0.49
1:G:21:LEU:HA	1:G:24:TRP:CD1	2.47	0.49
1:X:12:GLU:O	1:X:16:LYS:HE3	2.13	0.49
1:E:11:LEU:HD23	1:F:14:LEU:HD11	4.09	0.49
1:K:1:SER:O	1:K:4:LEU:HB2	2.13	0.48
1:T:3:LEU:HD22	1:T:6:LEU:HD23	1.95	0.48
1:O:11:LEU:HD13	1:Q:8:ARG:HG2	1.95	0.48
1:V:6:LEU:HA	1:X:16:LYS:HD2	1.94	0.48
1:I:14:LEU:HD21	1:J:14:LEU:HD22	1.95	0.48
1:J:20:LEU:HD22	1:L:3:LEU:HA	1.95	0.48
1:Q:4:LEU:O	1:Q:8:ARG:HG3	2.14	0.48
1:U:3:LEU:N	5:U:102:HOH:O	2.34	0.48
1:Y:1:SER:O	1:Y:1:SER:OG	2.30	0.48
1:E:15:HIS:ND1	1:E:15:HIS:O	4.41	0.48
1:W:21:LEU:HD22	1:X:3:LEU:HD22	1.94	0.48
1:B:4:LEU:O	1:B:7:LEU:N	2.37	0.48
1:A:1:SER:C	1:A:3:LEU:HD23	2.35	0.48
1:U:9:LYS:HD3	1:W:9:LYS:HG2	1.95	0.47
1:D:9:LYS:HD3	1:D:9:LYS:HA	2.15	0.47
2:A:101:MPD:O2	1:C:9:LYS:NZ	2.46	0.47
1:L:7:LEU:HD23	1:L:11:LEU:HD23	1.97	0.47
1:D:2:LYS:HB2	1:D:2:LYS:HE3	1.41	0.47
5:S:101:HOH:O	1:U:14:LEU:HD23	2.14	0.47
1:I:21:LEU:CA	1:J:3:LEU:HD21	2.44	0.46
1:E:8:ARG:NH2	3:E:101:PO4:O3	2.44	0.46
1:E:16:LYS:HZ3	1:E:19:GLU:CB	6.63	0.46
1:E:18:ILE:O	1:E:21:LEU:N	3.20	0.46
1:Y:3:LEU:HD12	1:Y:6:LEU:HB3	1.97	0.46
1:G:1:SER:O	1:G:5:GLU:HG2	2.15	0.46
1:S:20:LEU:HD23	1:S:20:LEU:HA	1.78	0.46
1:R:24:TRP:HH2	1:T:1:SER:H3	1.59	0.46
1:G:24:TRP:O	5:G:101:HOH:O	2.21	0.46
1:C:5:GLU:O	1:C:8:ARG:HG2	4.06	0.46
1:X:16:LYS:HA	1:X:19:GLU:OE1	2.16	0.46
1:D:1:SER:OG	1:D:2:LYS:N	2.48	0.46
1:K:5:GLU:HA	1:K:8:ARG:HD2	1.98	0.46
1:O:5:GLU:CD	1:O:8:ARG:HH21	2.19	0.46
1:T:3:LEU:HD13	1:T:3:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:15:HIS:O	1:Q:18:ILE:HB	2.16	0.45
1:X:6:LEU:O	1:X:6:LEU:HD23	2.16	0.45
1:G:17:ALA:HA	1:G:20:LEU:HD12	1.98	0.45
1:Z:16:LYS:C	1:Z:20:LEU:CD1	2.84	0.45
1:D:9:LYS:NZ	1:D:12:GLU:OE2	2.25	0.45
1:I:14:LEU:O	1:I:18:ILE:HG13	2.16	0.45
1:N:16:LYS:HA	1:N:19:GLU:HG2	1.99	0.45
1:A:14:LEU:HD12	1:A:14:LEU:HA	1.56	0.45
1:A:14:LEU:HD12	1:A:17:ALA:HB3	1.98	0.45
1:E:11:LEU:HD23	1:E:14:LEU:HD13	1.99	0.45
1:N:7:LEU:O	1:N:11:LEU:HD12	2.16	0.45
1:V:2:LYS:HG2	1:V:3:LEU:N	2.32	0.45
1:J:20:LEU:HD13	1:L:2:LYS:HG2	1.99	0.45
1:R:17:ALA:O	1:R:21:LEU:HD12	2.16	0.45
1:F:3:LEU:O	1:F:6:LEU:HB3	2.18	0.44
1:I:8:ARG:NH1	3:I:101:PO4:O4	2.46	0.44
1:R:8:ARG:N	1:R:11:LEU:HD12	2.32	0.44
1:K:8:ARG:HH12	1:M:18:ILE:HD12	1.81	0.44
1:P:1:SER:HB3	1:P:3:LEU:HD12	1.99	0.44
1:A:3:LEU:H	1:A:3:LEU:HD23	1.83	0.44
1:S:15:HIS:NE2	1:S:19:GLU:OE2	2.51	0.44
1:V:23:LYS:HG3	1:V:24:TRP:CD1	2.53	0.44
1:A:20:LEU:O	1:A:24:TRP:HD1	4.85	0.44
1:B:19:GLU:HG3	5:B:102:HOH:O	6.41	0.44
1:F:14:LEU:O	1:F:18:ILE:HG23	5.44	0.44
1:O:18:ILE:HD13	1:O:18:ILE:HA	1.77	0.44
1:U:6:LEU:HD13	1:W:13:ALA:O	2.17	0.44
1:A:7:LEU:O	1:A:8:ARG:C	2.56	0.44
1:M:5:GLU:HA	1:M:8:ARG:HE	1.82	0.44
5:S:101:HOH:O	1:U:14:LEU:CD2	2.66	0.44
1:Q:3:LEU:HA	1:Q:6:LEU:CD2	2.48	0.44
1:V:2:LYS:HG2	1:V:3:LEU:H	1.82	0.43
1:C:7:LEU:HD11	1:D:18:ILE:HD13	1.99	0.43
1:E:16:LYS:NZ	1:E:19:GLU:CB	6.92	0.43
1:J:24:TRP:NE1	5:J:101:HOH:O	2.32	0.43
1:L:3:LEU:O	1:L:6:LEU:HB3	2.17	0.43
1:T:24:TRP:O	5:T:101:HOH:O	2.21	0.43
1:V:12:GLU:O	1:V:16:LYS:HG3	2.18	0.43
1:A:4:LEU:HA	1:A:4:LEU:HD23	1.68	0.43
1:D:14:LEU:HD21	1:E:4:LEU:HD22	2.01	0.43
1:E:4:LEU:HB2	3:E:101:PO4:P	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:LYS:HG3	1:D:2:LYS:H	1.97	0.43
1:C:14:LEU:HD21	1:D:11:LEU:HD23	2.00	0.43
1:Q:10:LEU:CD1	1:R:10:LEU:HD12	2.49	0.43
1:W:21:LEU:HB3	1:X:3:LEU:CD2	2.47	0.43
1:B:14:LEU:HA	1:B:14:LEU:HD23	3.56	0.42
1:I:14:LEU:HB3	1:J:10:LEU:HB3	2.01	0.42
1:M:10:LEU:HD21	1:N:14:LEU:HA	2.00	0.42
1:N:23:LYS:HG2	1:N:24:TRP:HE3	1.83	0.42
1:T:1:SER:OG	1:T:2:LYS:N	2.52	0.42
1:E:21:LEU:HA	1:E:21:LEU:HD12	2.79	0.42
1:A:2:LYS:HE2	1:A:2:LYS:HB2	1.59	0.42
1:C:7:LEU:HD11	1:D:18:ILE:HG13	4.46	0.42
1:G:11:LEU:HA	1:G:11:LEU:HD23	1.88	0.42
1:M:1:SER:N	5:M:203:HOH:O	2.38	0.42
1:D:7:LEU:O	1:D:11:LEU:HG	2.20	0.42
1:A:11:LEU:HD21	1:C:7:LEU:HD23	20.36	0.42
1:C:3:LEU:O	1:C:6:LEU:HB3	2.19	0.42
1:D:8:ARG:O	1:D:12:GLU:HG2	5.93	0.42
1:G:7:LEU:HD23	1:G:7:LEU:HA	1.77	0.42
1:H:3:LEU:O	1:H:3:LEU:HD23	2.20	0.42
1:L:2:LYS:N	1:L:2:LYS:HD3	2.35	0.42
1:W:3:LEU:HG	1:X:21:LEU:HD12	2.01	0.42
1:C:7:LEU:HD12	1:C:7:LEU:HA	1.86	0.42
1:U:1:SER:O	1:U:5:GLU:OE2	2.38	0.42
1:U:1:SER:O	1:U:5:GLU:HB2	2.20	0.42
1:C:21:LEU:HA	1:D:3:LEU:HD23	4.19	0.42
1:Q:4:LEU:HG	1:Q:4:LEU:H	1.44	0.42
1:C:14:LEU:HA	1:C:14:LEU:HD12	1.76	0.41
1:X:6:LEU:HD21	1:X:10:LEU:HD11	2.02	0.41
1:C:7:LEU:HD22	1:D:21:LEU:HD12	2.01	0.41
1:G:14:LEU:HA	1:G:14:LEU:HD23	1.81	0.41
1:G:14:LEU:HG	1:H:10:LEU:HB3	2.02	0.41
1:A:2:LYS:HA	1:Y:16:LYS:HZ3	59.31	0.41
1:H:21:LEU:HD23	5:H:101:HOH:O	2.20	0.41
1:E:16:LYS:CE	1:E:16:LYS:HA	4.47	0.41
1:E:4:LEU:HB2	3:E:101:PO4:O1	2.20	0.41
1:F:24:TRP:CE3	1:F:24:TRP:HA	2.56	0.41
2:A:101:MPD:H4	2:A:101:MPD:HM1	1.69	0.41
1:B:24:TRP:HA	1:B:24:TRP:CE3	4.39	0.41
1:D:17:ALA:O	1:D:20:LEU:HB2	2.21	0.41
1:M:12:GLU:OE1	3:M:101:PO4:O3	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:GLU:HA	1:C:8:ARG:NE	3.98	0.41
1:F:7:LEU:O	1:F:11:LEU:HG	3.14	0.41
1:G:21:LEU:HA	1:G:24:TRP:HD1	1.86	0.41
1:P:14:LEU:HD13	1:P:18:ILE:CD1	2.50	0.41
1:P:18:ILE:HG21	1:R:21:LEU:HB3	2.02	0.41
1:B:16:LYS:HA	1:B:16:LYS:HD3	1.95	0.41
1:O:6:LEU:HD23	1:O:7:LEU:N	2.36	0.41
1:S:14:LEU:O	1:S:18:ILE:HG13	2.21	0.41
1:V:14:LEU:O	1:V:18:ILE:HG13	2.21	0.41
1:E:7:LEU:HD21	1:F:21:LEU:HD11	2.03	0.41
1:L:14:LEU:O	1:L:18:ILE:HG23	2.21	0.41
1:O:6:LEU:C	1:O:6:LEU:HD23	2.41	0.41
1:K:15:HIS:CD2	1:M:8:ARG:NH1	2.89	0.40
1:L:19:GLU:O	1:L:22:GLU:HG3	2.20	0.40
1:T:19:GLU:HA	1:T:22:GLU:CD	2.41	0.40
1:B:2:LYS:C	1:Z:20:LEU:HD21	91.85	0.40
1:R:1:SER:OG	1:R:2:LYS:N	2.53	0.40
1:U:12:GLU:O	1:U:15:HIS:N	2.54	0.40
1:X:6:LEU:HD23	1:X:6:LEU:C	2.42	0.40
1:K:10:LEU:HA	1:K:10:LEU:HD12	1.83	0.40
1:C:14:LEU:HD23	1:C:14:LEU:HA	4.41	0.40
1:K:2:LYS:HE3	1:K:2:LYS:HB2	1.79	0.40
1:L:14:LEU:HD21	1:M:4:LEU:CD2	2.52	0.40
1:Q:3:LEU:HD21	1:R:20:LEU:HD12	2.03	0.40
1:T:15:HIS:HD1	1:T:15:HIS:C	2.25	0.40
1:V:9:LYS:HB2	1:X:16:LYS:NZ	2.36	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	24/27 (89%)	21 (88%)	3 (12%)	0	100	100
1	B	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
1	C	22/27 (82%)	19 (86%)	3 (14%)	0	100	100
1	D	22/27 (82%)	18 (82%)	4 (18%)	0	100	100
1	E	24/27 (89%)	22 (92%)	2 (8%)	0	100	100
1	F	24/27 (89%)	21 (88%)	3 (12%)	0	100	100
1	G	22/27 (82%)	22 (100%)	0	0	100	100
1	H	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
1	I	22/27 (82%)	22 (100%)	0	0	100	100
1	J	24/27 (89%)	20 (83%)	4 (17%)	0	100	100
1	K	24/27 (89%)	22 (92%)	2 (8%)	0	100	100
1	L	22/27 (82%)	22 (100%)	0	0	100	100
1	M	24/27 (89%)	22 (92%)	2 (8%)	0	100	100
1	N	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
1	O	24/27 (89%)	19 (79%)	5 (21%)	0	100	100
1	P	22/27 (82%)	22 (100%)	0	0	100	100
1	Q	24/27 (89%)	20 (83%)	4 (17%)	0	100	100
1	R	24/27 (89%)	23 (96%)	1 (4%)	0	100	100
1	S	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
1	T	24/27 (89%)	23 (96%)	0	1 (4%)	3	3
1	U	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
1	V	22/27 (82%)	22 (100%)	0	0	100	100
1	W	22/27 (82%)	18 (82%)	4 (18%)	0	100	100
1	X	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
1	Y	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
1	Z	23/27 (85%)	23 (100%)	0	0	100	100
1	a	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
1	b	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
1	c	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
1	d	24/27 (89%)	20 (83%)	4 (17%)	0	100	100
1	e	22/27 (82%)	19 (86%)	3 (14%)	0	100	100
1	f	21/27 (78%)	19 (90%)	2 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	724/864 (84%)	662 (91%)	61 (8%)	1 (0%)	53 75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	25	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	20/22 (91%)	17 (85%)	3 (15%)	3 6
1	B	10/22 (46%)	9 (90%)	1 (10%)	8 16
1	C	20/22 (91%)	19 (95%)	1 (5%)	27 49
1	D	17/22 (77%)	15 (88%)	2 (12%)	6 11
1	E	21/22 (96%)	21 (100%)	0	100 100
1	F	15/22 (68%)	15 (100%)	0	100 100
1	G	21/22 (96%)	19 (90%)	2 (10%)	9 18
1	H	15/22 (68%)	15 (100%)	0	100 100
1	I	20/22 (91%)	19 (95%)	1 (5%)	27 49
1	J	14/22 (64%)	14 (100%)	0	100 100
1	K	20/22 (91%)	19 (95%)	1 (5%)	27 49
1	L	18/22 (82%)	15 (83%)	3 (17%)	2 4
1	M	19/22 (86%)	18 (95%)	1 (5%)	25 46
1	N	15/22 (68%)	14 (93%)	1 (7%)	18 34
1	O	20/22 (91%)	19 (95%)	1 (5%)	27 49
1	P	13/22 (59%)	13 (100%)	0	100 100
1	Q	21/22 (96%)	21 (100%)	0	100 100
1	R	15/22 (68%)	13 (87%)	2 (13%)	4 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	21/22 (96%)	20 (95%)	1 (5%)	28	51
1	T	14/22 (64%)	12 (86%)	2 (14%)	3	6
1	U	22/22 (100%)	19 (86%)	3 (14%)	4	7
1	V	17/22 (77%)	14 (82%)	3 (18%)	2	3
1	W	21/22 (96%)	20 (95%)	1 (5%)	28	51
1	X	15/22 (68%)	14 (93%)	1 (7%)	18	34
1	Y	20/22 (91%)	20 (100%)	0	100	100
1	Z	12/22 (54%)	12 (100%)	0	100	100
1	a	17/22 (77%)	17 (100%)	0	100	100
1	b	15/22 (68%)	13 (87%)	2 (13%)	4	8
1	c	16/22 (73%)	16 (100%)	0	100	100
1	d	17/22 (77%)	15 (88%)	2 (12%)	6	11
1	e	16/22 (73%)	11 (69%)	5 (31%)	0	0
1	f	14/22 (64%)	13 (93%)	1 (7%)	16	31
All	All	551/704 (78%)	511 (93%)	40 (7%)	15	29

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	2	LYS
1	A	7	LEU
1	B	3	LEU
1	C	20	LEU
1	D	1	SER
1	D	24	TRP
1	G	7	LEU
1	G	14	LEU
1	I	2	LYS
1	K	16	LYS
1	L	1	SER
1	L	2	LYS
1	L	19	GLU
1	M	8	ARG
1	N	15	HIS
1	O	20	LEU
1	R	4	LEU

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Mol	Chain	Res	Type
1	R	11	LEU
1	S	2	LYS
1	T	15	HIS
1	T	24	TRP
1	U	5	GLU
1	U	14	LEU
1	U	16	LYS
1	V	2	LYS
1	V	7	LEU
1	V	11	LEU
1	W	21	LEU
1	X	11	LEU
1	b	14	LEU
1	b	24	TRP
1	d	19	GLU
1	d	20	LEU
1	e	3	LEU
1	e	8	ARG
1	e	14	LEU
1	e	15	HIS
1	e	24	TRP
1	f	3	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	15	HIS
1	K	15	HIS
1	Q	15	HIS
1	W	15	HIS

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	MPD	A	101	-	7,7,7	0.29	0	9,10,10	0.66	0
3	PO4	E	101	-	4,4,4	0.81	0	6,6,6	0.46	0
3	PO4	I	101	-	4,4,4	0.87	0	6,6,6	0.55	0
3	PO4	M	101	-	4,4,4	0.77	0	6,6,6	0.39	0
4	CO3	Q	101	-	0,3,3	0.00	-	0,3,3	0.00	-

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	MPD	A	101	-	-	0/5/5/5	0/0/0/0
3	PO4	E	101	-	-	0/0/0/0	0/0/0/0
3	PO4	I	101	-	-	0/0/0/0	0/0/0/0
3	PO4	M	101	-	-	0/0/0/0	0/0/0/0
4	CO3	Q	101	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	101	MPD	4	0
3	E	101	PO4	3	0
3	I	101	PO4	1	0
3	M	101	PO4	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	25/27 (92%)	0.82	6 (24%) 0 0	49, 59, 106, 311	0
1	B	24/27 (88%)	0.65	3 (12%) 4 3	59, 74, 86, 96	0
1	C	24/27 (88%)	0.00	1 (4%) 36 39	36, 46, 65, 90	0
1	D	24/27 (88%)	0.58	4 (16%) 1 1	52, 62, 77, 86	0
1	E	25/27 (92%)	0.23	2 (8%) 12 12	32, 43, 76, 96	0
1	F	25/27 (92%)	0.22	2 (8%) 12 12	47, 59, 87, 101	0
1	G	24/27 (88%)	-0.12	0 100 100	26, 37, 55, 58	0
1	H	24/27 (88%)	-0.28	0 100 100	47, 59, 77, 92	0
1	I	24/27 (88%)	0.03	0 100 100	31, 38, 64, 81	0
1	J	25/27 (92%)	-0.14	0 100 100	47, 58, 76, 103	0
1	K	25/27 (92%)	0.04	0 100 100	17, 34, 58, 66	0
1	L	24/27 (88%)	-0.00	0 100 100	42, 57, 86, 108	0
1	M	25/27 (92%)	-0.27	0 100 100	27, 32, 61, 71	0
1	N	24/27 (88%)	-0.21	0 100 100	45, 58, 71, 81	0
1	O	25/27 (92%)	-0.23	0 100 100	24, 34, 57, 74	0
1	P	24/27 (88%)	0.01	1 (4%) 36 39	49, 59, 69, 70	0
1	Q	25/27 (92%)	-0.07	0 100 100	28, 36, 55, 69	0
1	R	25/27 (92%)	0.50	2 (8%) 12 12	39, 57, 76, 88	0
1	S	24/27 (88%)	-0.09	0 100 100	32, 41, 57, 64	0
1	T	25/27 (92%)	0.59	5 (20%) 1 1	47, 61, 82, 104	0
1	U	24/27 (88%)	-0.06	0 100 100	30, 41, 57, 75	0
1	V	24/27 (88%)	0.19	1 (4%) 36 39	48, 58, 81, 99	0
1	W	24/27 (88%)	-0.14	0 100 100	30, 39, 52, 63	0
1	X	24/27 (88%)	0.22	4 (16%) 1 1	50, 62, 90, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	Y	24/27 (88%)	-0.06	0 100 100	33, 44, 65, 72	0
1	Z	25/27 (92%)	-0.42	0 100 100	48, 63, 75, 76	0
1	a	24/27 (88%)	0.07	1 (4%) 36 39	36, 50, 63, 83	0
1	b	23/27 (85%)	0.13	1 (4%) 35 38	55, 70, 85, 123	0
1	c	23/27 (85%)	-0.14	1 (4%) 35 38	34, 48, 58, 63	0
1	d	25/27 (92%)	0.51	4 (16%) 1 1	51, 68, 99, 114	0
1	e	24/27 (88%)	0.62	3 (12%) 4 3	45, 55, 67, 72	0
1	f	23/27 (85%)	2.01	8 (34%) 0 0	67, 75, 101, 108	0
All	All	777/864 (89%)	0.16	49 (6%) 20 21	17, 55, 86, 311	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	24	TRP	10.5
1	f	24	TRP	9.9
1	f	21	LEU	7.8
1	a	1	SER	6.0
1	f	20	LEU	4.5
1	A	9	LYS	4.4
1	A	1	SER	4.3
1	D	24	TRP	4.2
1	e	21	LEU	4.1
1	d	15	HIS	4.0
1	f	18	ILE	3.9
1	F	24	TRP	3.9
1	f	14	LEU	3.9
1	e	17	ALA	3.6
1	A	3	LEU	3.5
1	B	24	TRP	3.4
1	X	21	LEU	3.4
1	e	3	LEU	3.4
1	d	24	TRP	3.3
1	D	6	LEU	3.2
1	E	20	LEU	3.2
1	X	22	GLU	3.1
1	T	23	LYS	3.1
1	T	22	GLU	3.0
1	F	22	GLU	3.0
1	f	22	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	19	GLU	2.9
1	B	16	LYS	2.9
1	D	3	LEU	2.8
1	C	20	LEU	2.8
1	f	17	ALA	2.8
1	D	22	GLU	2.7
1	X	24	TRP	2.7
1	b	17	ALA	2.7
1	A	4	LEU	2.7
1	R	23	LYS	2.6
1	E	4	LEU	2.6
1	d	22	GLU	2.6
1	d	6	LEU	2.6
1	X	17	ALA	2.5
1	T	7	LEU	2.5
1	V	20	LEU	2.5
1	f	19	GLU	2.4
1	T	4	LEU	2.4
1	c	3	LEU	2.4
1	A	25	GLY	2.3
1	T	24	TRP	2.2
1	A	21	LEU	2.1
1	P	23	LYS	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	M	101	5/5	0.90	0.12	52,54,55,56	0
4	CO3	Q	101	4/4	0.95	0.12	20,26,28,30	0
2	MPD	A	101	8/8	0.95	0.09	5,26,36,39	0
3	PO4	I	101	5/5	0.96	0.24	27,34,39,40	0
3	PO4	E	101	5/5	0.96	0.15	38,45,47,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.