



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 26, 2023 – 08:13 PM EDT

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

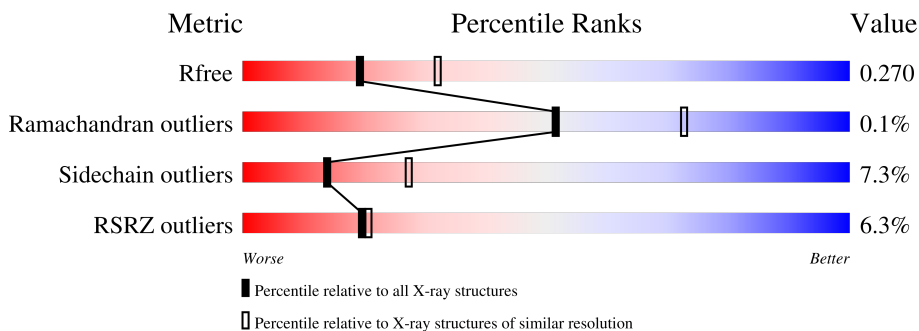
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	27	
1	B	27	
1	C	27	
1	D	27	
1	E	27	
1	F	27	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	27	81% 7% 11%
1	H	27	89% 11%
1	I	27	85% 11%
1	J	27	96% 11%
1	K	27	93% 11%
1	L	27	78% 11% 11%
1	M	27	93% 11%
1	N	27	85% 11%
1	O	27	93% 11%
1	P	27	4% 89% 11%
1	Q	27	96% 11%
1	R	27	7% 89% 7% 11%
1	S	27	85% 11%
1	T	27	19% 85% 11% 11%
1	U	27	78% 11% 11%
1	V	27	4% 78% 11% 11%
1	W	27	85% 11%
1	X	27	15% 85% 11%
1	Y	27	89% 11%
1	Z	27	93% 7%
1	a	27	4% 89% 11%
1	b	27	4% 78% 7% 15%
1	c	27	4% 85% 15%
1	d	27	15% 89% 7% 11%
1	e	27	11% 70% 19% 11%

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	f	27	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '30%', a green segment in the middle labeled '81%', and a grey segment on the right labeled '15%'. A small yellow dot is visible on the green segment.</p>

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

*Continued on next page...*

Continued from previous page...

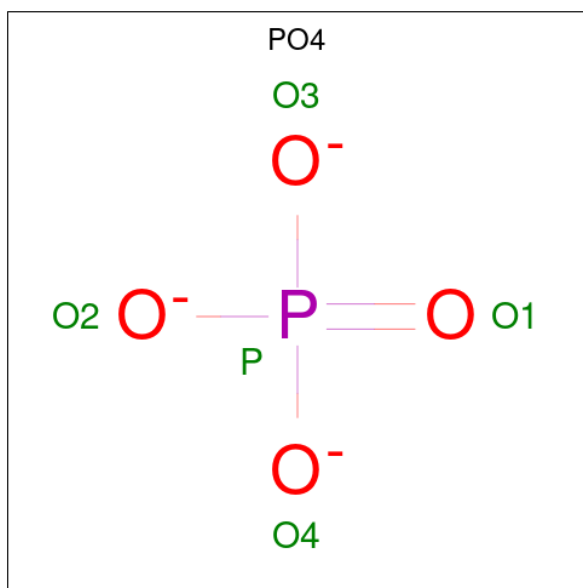
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Q	26	Total	C	N	O	0	0	1
			205	137	36	32			
1	R	26	Total	C	N	O	0	0	1
			180	118	30	32			
1	S	24	Total	C	N	O	0	0	0
			200	135	34	31			
1	T	26	Total	C	N	O	0	0	1
			176	117	31	28			
1	U	24	Total	C	N	O	0	0	0
			203	136	34	33			
1	V	24	Total	C	N	O	0	0	0
			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>).



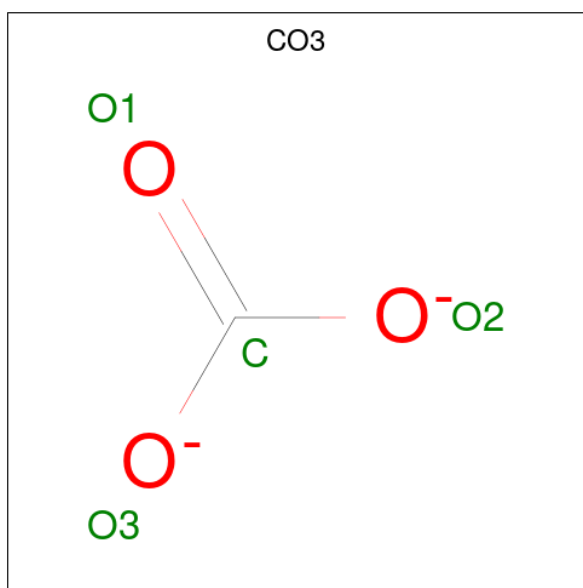
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		

- 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		

*Continued on next page...*



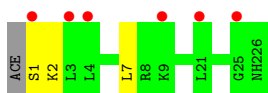
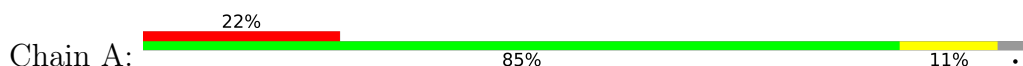
*Continued from previous page...*

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

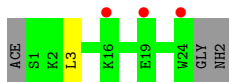
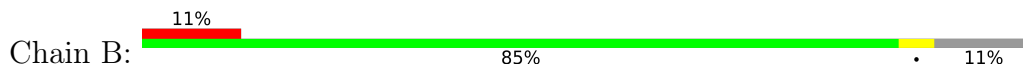
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

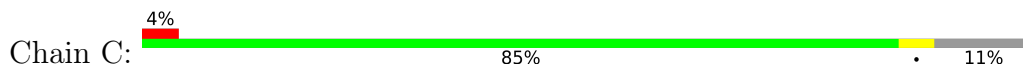
- Molecule 1: alpha-Amyloid peptide alphaAmL



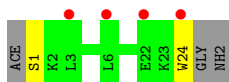
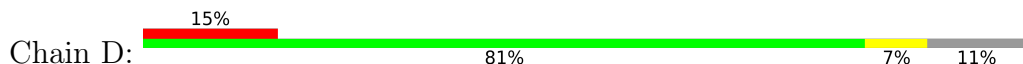
- Molecule 1: alpha-Amyloid peptide alphaAmL



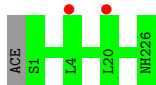
- Molecule 1: alpha-Amyloid peptide alphaAmL



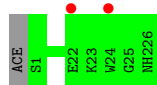
- Molecule 1: alpha-Amyloid peptide alphaAmL



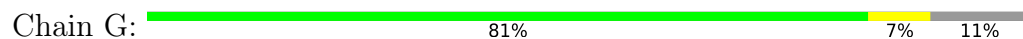
- Molecule 1: alpha-Amyloid peptide alphaAmL



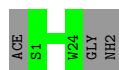
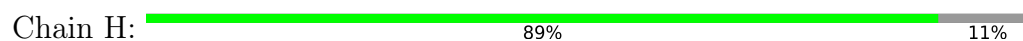
- Molecule 1: alpha-Amyloid peptide alphaAmL



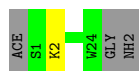
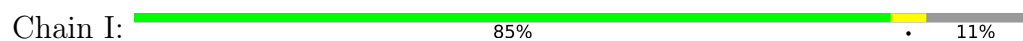
- Molecule 1: alpha-Amyloid peptide alphaAmL



- Molecule 1: alpha-Amyloid peptide alphaAmL



- Molecule 1: alpha-Amyloid peptide alphaAmL



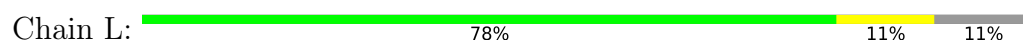
- Molecule 1: alpha-Amyloid peptide alphaAmL



- Molecule 1: alpha-Amyloid peptide alphaAmL



- Molecule 1: alpha-Amyloid peptide alphaAmL




- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain M:  93%



- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain N:  85% 11%




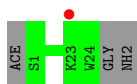
- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain O:  93%



- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain P:  4% 89% 11%




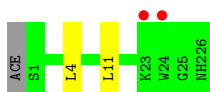
- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain Q:  96%




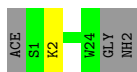
- Molecule 1: alpha-Amyloid peptide alphaAmL

Chain R:  7% 89% 7%

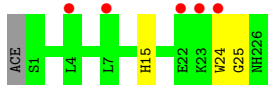
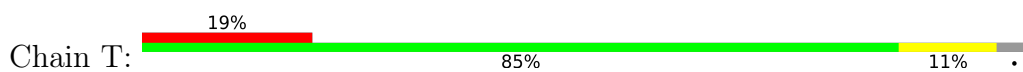


- Molecule 1: alpha-Amyloid peptide alphaAmL

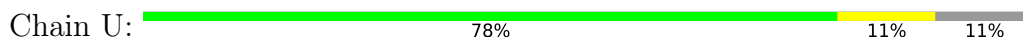
Chain S:  85% 11%



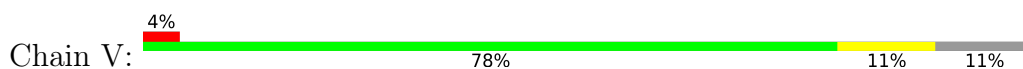
- Molecule 1: alpha-Amyloid peptide alphaAmL



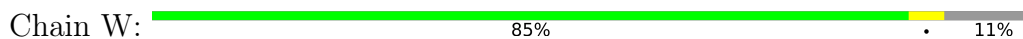
- Molecule 1: alpha-Amyloid peptide alphaAmL



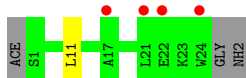
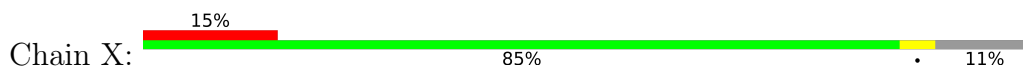
- Molecule 1: alpha-Amyloid peptide alphaAmL



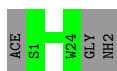
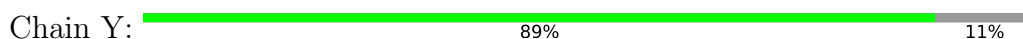
- Molecule 1: alpha-Amyloid peptide alphaAmL



- Molecule 1: alpha-Amyloid peptide alphaAmL



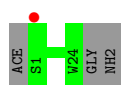
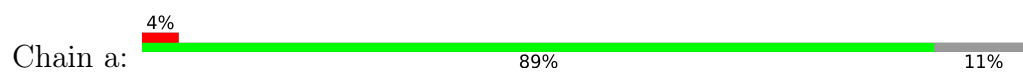
- Molecule 1: alpha-Amyloid peptide alphaAmL



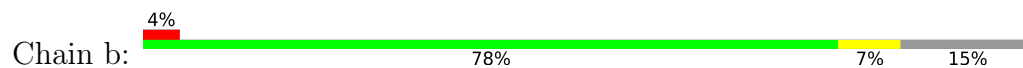
- Molecule 1: alpha-Amyloid peptide alphaAmL



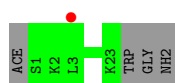
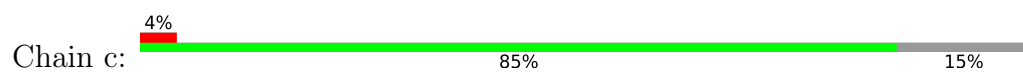
- Molecule 1: alpha-Amyloid peptide alphaAmL



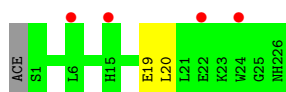
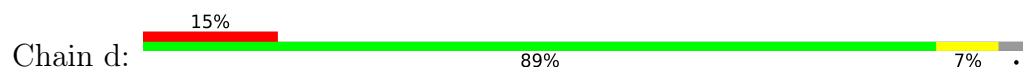
- Molecule 1: alpha-Amyloid peptide alphaAmL



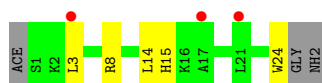
- Molecule 1: alpha-Amyloid peptide alphaAmL



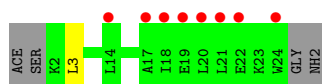
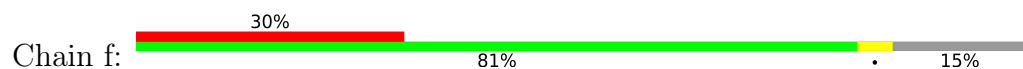
- Molecule 1: alpha-Amyloid peptide alphaAmL



- Molecule 1: alpha-Amyloid peptide alphaAmL



- Molecule 1: alpha-Amyloid peptide alphaAmL



## 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)	Xtrriage
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	Xtrriage
Anisotropy	0.347	Xtrriage
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>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.447 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6078	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage'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, NH2, PO4, MPD

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
All	All	724/864 (84%)	662 (91%)	61 (8%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	25	GLY

### 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	A	20/22 (91%)	17 (85%)	3 (15%)	3	5
1	B	10/22 (46%)	9 (90%)	1 (10%)	7	15
1	C	20/22 (91%)	19 (95%)	1 (5%)	24	46
1	D	17/22 (77%)	15 (88%)	2 (12%)	5	10
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%)	8	17
1	H	15/22 (68%)	15 (100%)	0	100	100
1	I	20/22 (91%)	19 (95%)	1 (5%)	24	46
1	J	14/22 (64%)	14 (100%)	0	100	100
1	K	20/22 (91%)	19 (95%)	1 (5%)	24	46
1	L	18/22 (82%)	15 (83%)	3 (17%)	2	4
1	M	19/22 (86%)	18 (95%)	1 (5%)	22	43
1	N	15/22 (68%)	14 (93%)	1 (7%)	16	31
1	O	20/22 (91%)	19 (95%)	1 (5%)	24	46
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	7
1	S	21/22 (96%)	20 (95%)	1 (5%)	25	48
1	T	14/22 (64%)	12 (86%)	2 (14%)	3	6
1	U	22/22 (100%)	19 (86%)	3 (14%)	3	7
1	V	17/22 (77%)	14 (82%)	3 (18%)	2	3
1	W	21/22 (96%)	20 (95%)	1 (5%)	25	48
1	X	15/22 (68%)	14 (93%)	1 (7%)	16	31
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	7
1	c	16/22 (73%)	16 (100%)	0	100	100
1	d	17/22 (77%)	15 (88%)	2 (12%)	5	10
1	e	16/22 (73%)	11 (69%)	5 (31%)	0	0
1	f	14/22 (64%)	13 (93%)	1 (7%)	14	28

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	551/704 (78%)	511 (93%)	40 (7%)	14	27

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	21	LEU
1	e	8	ARG
1	X	11	LEU
1	d	19	GLU
1	e	15	HIS

Sometimes 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 [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](#)

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	0.30	0	9,10,10	0.68	0
4	CO3	Q	101	-	2,3,3	0.39	0	2,3,3	0.34	0
3	PO4	E	101	-	4,4,4	0.98	0	6,6,6	0.51	0
3	PO4	I	101	-	4,4,4	1.06	0	6,6,6	0.63	0
3	PO4	M	101	-	4,4,4	0.92	0	6,6,6	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	A	101	-	-	0/5/5/5	-

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](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	25/27 (92%)	0.82	6 (24%) 0 0	49, 59, 106, 311	0
1	B	24/27 (88%)	0.65	3 (12%) 3 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 0	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

*Continued on next page...*

Continued from previous page...

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%)	3 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

The worst 5 of 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

## 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 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PO4	M	101	5/5	0.90	0.12	52,54,55,56	0
2	MPD	A	101	8/8	0.95	0.09	5,26,36,39	0

Continued on next page...

*Continued from previous page...*

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

## 6.5 Other polymers [i](#)

There are no such residues in this entry.