



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:50 am BST

PDB ID : 6NNV  
Title : PD-L1 IgV domain complex with macro-cyclic peptide  
Authors : Zhao, B.; Perry, E.  
Deposited on : 2019-01-15  
Resolution : 1.92 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

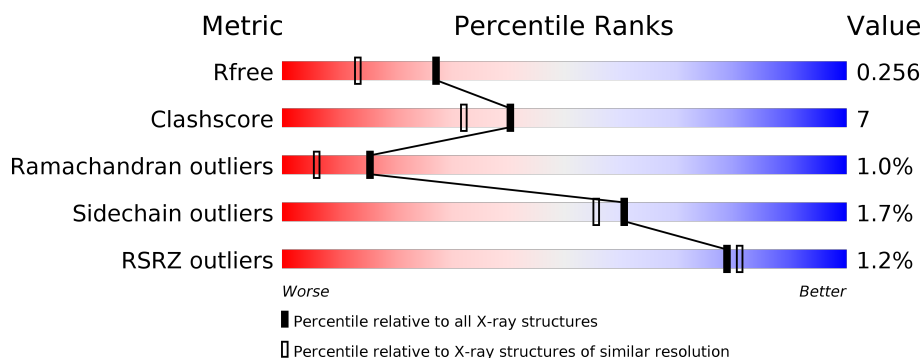
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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.




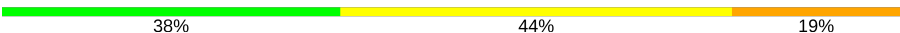
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 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	127	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 80%, yellow 13%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>80%</span> <span>13%</span> <span>6%</span> </div> </div>
1	B	127	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 90%, yellow 5%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>90%</span> <span>5%</span> <span>5%</span> </div> </div>
1	C	127	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 85%, yellow 12%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>85%</span> <span>12%</span> <span>.</span> </div> </div>
1	D	127	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 83%, yellow 13%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>83%</span> <span>13%</span> <span>5%</span> </div> </div>
2	I	16	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 25%, yellow 56%, orange 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>25%</span> <span>56%</span> <span>19%</span> </div> </div>
2	J	16	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, green 38%, yellow 63%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>6%</span> <span>38%</span> <span>63%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
2	K	16	
2	L	16	

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
2	MEA	K	8	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4561 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 Programmed cell death 1 ligand 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	S	0	0	0
			925	594	150	176	5			
1	B	121	Total	C	N	O	S	0	0	0
			935	599	151	180	5			
1	C	123	Total	C	N	O	S	0	0	0
			959	614	159	181	5			
1	D	121	Total	C	N	O	S	0	0	0
			928	594	152	177	5			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	THR	VAL	engineered mutation	UNP Q9NZQ7
A	135	ALA	-	expression tag	UNP Q9NZQ7
A	136	ALA	-	expression tag	UNP Q9NZQ7
A	137	ALA	-	expression tag	UNP Q9NZQ7
A	138	LEU	-	expression tag	UNP Q9NZQ7
A	139	HIS	-	expression tag	UNP Q9NZQ7
A	140	GLU	-	expression tag	UNP Q9NZQ7
A	141	HIS	-	expression tag	UNP Q9NZQ7
A	142	HIS	-	expression tag	UNP Q9NZQ7
A	143	HIS	-	expression tag	UNP Q9NZQ7
A	144	HIS	-	expression tag	UNP Q9NZQ7
B	76	THR	VAL	engineered mutation	UNP Q9NZQ7
B	135	ALA	-	expression tag	UNP Q9NZQ7
B	136	ALA	-	expression tag	UNP Q9NZQ7
B	137	ALA	-	expression tag	UNP Q9NZQ7
B	138	LEU	-	expression tag	UNP Q9NZQ7
B	139	HIS	-	expression tag	UNP Q9NZQ7
B	140	GLU	-	expression tag	UNP Q9NZQ7
B	141	HIS	-	expression tag	UNP Q9NZQ7
B	142	HIS	-	expression tag	UNP Q9NZQ7
B	143	HIS	-	expression tag	UNP Q9NZQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	144	HIS	-	expression tag	UNP Q9NZQ7
C	76	THR	VAL	engineered mutation	UNP Q9NZQ7
C	135	ALA	-	expression tag	UNP Q9NZQ7
C	136	ALA	-	expression tag	UNP Q9NZQ7
C	137	ALA	-	expression tag	UNP Q9NZQ7
C	138	LEU	-	expression tag	UNP Q9NZQ7
C	139	HIS	-	expression tag	UNP Q9NZQ7
C	140	GLU	-	expression tag	UNP Q9NZQ7
C	141	HIS	-	expression tag	UNP Q9NZQ7
C	142	HIS	-	expression tag	UNP Q9NZQ7
C	143	HIS	-	expression tag	UNP Q9NZQ7
C	144	HIS	-	expression tag	UNP Q9NZQ7
D	76	THR	VAL	engineered mutation	UNP Q9NZQ7
D	135	ALA	-	expression tag	UNP Q9NZQ7
D	136	ALA	-	expression tag	UNP Q9NZQ7
D	137	ALA	-	expression tag	UNP Q9NZQ7
D	138	LEU	-	expression tag	UNP Q9NZQ7
D	139	HIS	-	expression tag	UNP Q9NZQ7
D	140	GLU	-	expression tag	UNP Q9NZQ7
D	141	HIS	-	expression tag	UNP Q9NZQ7
D	142	HIS	-	expression tag	UNP Q9NZQ7
D	143	HIS	-	expression tag	UNP Q9NZQ7
D	144	HIS	-	expression tag	UNP Q9NZQ7

- Molecule 2 is a protein called macrocyclic peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	16	Total 134	C 97	N 17	O 19	S 1	0	0	1
2	J	16	Total 134	C 97	N 17	O 19	S 1	0	0	1
2	K	16	Total 134	C 97	N 17	O 19	S 1	0	0	1
2	L	16	Total 134	C 97	N 17	O 19	S 1	0	0	1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total	O	0	0
			58	58		
3	B	62	Total	O	0	0
			62	62		

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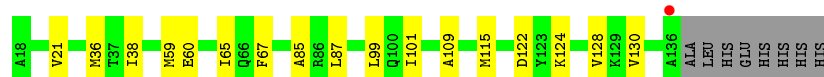
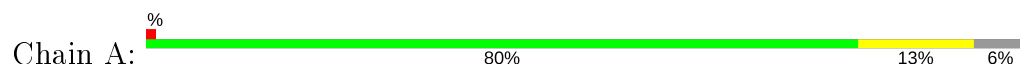
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	63	Total 63	O 63	0	0
3	D	72	Total 72	O 72	0	0
3	I	7	Total 7	O 7	0	0
3	J	7	Total 7	O 7	0	0
3	K	5	Total 5	O 5	0	0
3	L	4	Total 4	O 4	0	0

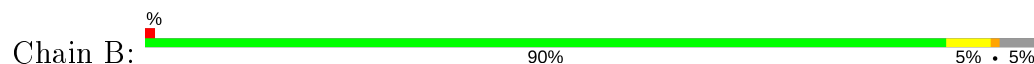
### 3 Residue-property plots [i](#)

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.

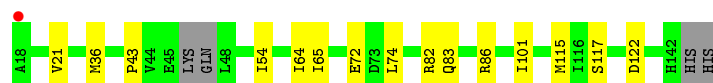
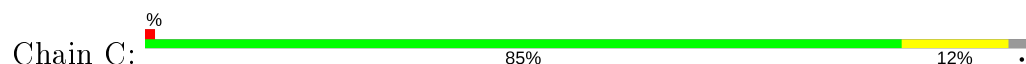
- Molecule 1: Programmed cell death 1 ligand 1



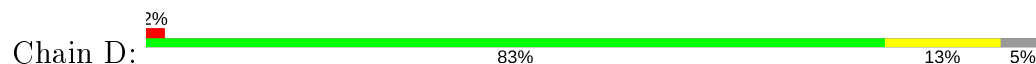
- Molecule 1: Programmed cell death 1 ligand 1



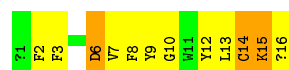
- Molecule 1: Programmed cell death 1 ligand 1



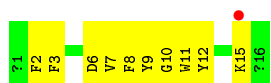
- Molecule 1: Programmed cell death 1 ligand 1



- Molecule 2: macrocyclic peptide



- Molecule 2: macrocyclic peptide



- Molecule 2: macrocyclic peptide



- Molecule 2: macrocyclic peptide





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.84Å 61.68Å 80.89Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	29.10 – 1.92 29.10 – 1.92	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.10-1.92) 96.3 (29.10-1.92)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 1.92Å)	Xtriage
Refinement program	PHENIX (1.14 _3260: ???)	Depositor
R, $R_{free}$	0.215 , 0.253 0.219 , 0.256	Depositor DCC
$R_{free}$ test set	1629 reflections (3.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.6	Xtriage
Anisotropy	0.855	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 27.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.139 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4561	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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 39.78 % 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 3.0147e-04. 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: 9KK, SAR, MEA, ACE, 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	0.27	0/942	0.49	0/1276
1	B	0.27	0/951	0.47	0/1291
1	C	0.28	0/976	0.52	0/1322
1	D	0.30	0/944	0.52	0/1283
2	I	1.08	0/89	1.55	1/116 (0.9%)
2	J	1.07	0/89	1.55	1/116 (0.9%)
2	K	1.07	0/89	1.57	1/116 (0.9%)
2	L	1.06	0/89	1.67	1/116 (0.9%)
All	All	0.41	0/4169	0.66	4/5636 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	6	ASP	CB-CG-OD1	8.65	126.09	118.30
2	I	6	ASP	CB-CG-OD1	8.09	125.58	118.30
2	K	6	ASP	CB-CG-OD1	8.06	125.56	118.30
2	J	6	ASP	CB-CG-OD1	7.64	125.17	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	925	0	908	11	0
1	B	935	0	902	7	0
1	C	959	0	936	12	0
1	D	928	0	890	11	0
2	I	134	0	113	7	0
2	J	134	0	113	5	0
2	K	134	0	112	9	0
2	L	134	0	113	6	0
3	A	58	0	0	1	0
3	B	62	0	0	2	0
3	C	63	0	0	2	0
3	D	72	0	0	0	0
3	I	7	0	0	1	0
3	J	7	0	0	0	0
3	K	5	0	0	0	0
3	L	4	0	0	0	0
All	All	4561	0	4087	60	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 7.

All (60) 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:C:115:MET:HE2	2:K:8:MEA:HB1	1.57	0.86
1:B:115:MET:SD	3:B:253:HOH:O	2.40	0.79
1:C:115:MET:HE2	2:K:8:MEA:CB	2.20	0.71
1:B:21:VAL:HG23	1:B:122:ASP:HB3	1.80	0.62
1:D:115:MET:HE2	2:L:8:MEA:CB	2.29	0.61
2:L:13:LEU:O	2:L:15:LYS:N	2.33	0.61
2:I:13:LEU:O	2:I:15:LYS:N	2.32	0.59
2:I:16:NH2:N	3:I:103:HOH:O	2.36	0.58
1:D:115:MET:HE2	2:L:8:MEA:HB1	1.87	0.57
1:C:54:ILE:HB	1:C:117:SER:HB3	1.88	0.56
1:D:59:MET:SD	1:D:60:GLU:HG3	2.47	0.55
1:D:36:MET:O	1:D:100:GLN:HA	2.07	0.55
1:B:115:MET:HE1	2:I:12:TYR:HB3	1.90	0.54
1:C:115:MET:CE	2:K:8:MEA:CB	2.86	0.54
1:C:72:GLU:OE1	1:C:74:LEU:HD21	2.09	0.52
2:K:2:PHE:HE1	2:K:8:MEA:HC2	1.74	0.52
1:C:64:ILE:O	1:C:65:ILE:HG13	2.10	0.51
1:C:115:MET:CE	2:K:8:MEA:HB1	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ALA:HB2	1:A:101:ILE:HG12	1.94	0.50
1:A:65:ILE:HG21	1:A:87:LEU:HB2	1.94	0.49
1:A:115:MET:HE1	2:J:12:TYR:HB3	1.95	0.48
2:L:9:TYR:HA	2:L:10:SAR:HN1	1.61	0.48
1:C:43:PRO:O	3:C:201:HOH:O	2.20	0.47
1:A:67:PHE:CD2	1:A:87:LEU:HD23	2.49	0.47
1:B:115:MET:HG3	1:B:123:TYR:HB2	1.96	0.47
2:K:9:TYR:HA	2:K:10:SAR:HN1	1.62	0.47
1:B:115:MET:HG3	1:B:123:TYR:CB	2.45	0.46
1:D:36:MET:HE2	1:D:104:VAL:HG22	1.98	0.46
1:B:66:GLN:OE1	1:B:76:THR:HG21	2.15	0.46
1:D:78:HIS:HB3	1:D:81:TYR:HD2	1.81	0.45
1:A:59:MET:SD	1:A:60:GLU:HG3	2.56	0.45
1:C:82:ARG:O	1:C:83:GLN:HB2	2.17	0.45
2:I:2:PHE:HA	2:I:3:MEA:HC1	1.71	0.45
1:A:36:MET:HE1	1:A:128:VAL:HG11	1.99	0.45
2:K:4:9KK:O	2:K:5:SAR:C	2.64	0.45
2:L:8:MEA:HC3	2:L:12:TYR:HE1	1.81	0.45
1:D:82:ARG:O	1:D:83:GLN:HB2	2.16	0.44
2:I:8:MEA:HC3	2:I:12:TYR:HE1	1.81	0.44
1:A:109:ALA:HB2	1:A:130:VAL:HG23	1.99	0.44
1:B:122:ASP:OD1	3:B:201:HOH:O	2.21	0.44
1:C:21:VAL:HG23	1:C:122:ASP:HB3	1.99	0.44
1:D:78:HIS:HB3	1:D:81:TYR:CD2	2.52	0.44
1:A:59:MET:O	1:A:60:GLU:HB2	2.17	0.44
2:L:2:PHE:N	2:L:14:CYS:HB3	2.33	0.44
1:C:86:ARG:NH2	3:C:208:HOH:O	2.50	0.43
2:J:9:TYR:HA	2:J:10:SAR:HN1	1.61	0.43
1:D:65:ILE:HG21	1:D:87:LEU:HB2	1.99	0.43
1:A:21:VAL:HG23	1:A:122:ASP:HB3	2.01	0.43
1:A:38:ILE:HD11	1:A:99:LEU:HD23	2.01	0.43
1:C:36:MET:HE1	1:C:101:ILE:HD12	2.02	0.42
2:J:8:MEA:HD1	2:J:11:TRP:CZ3	2.55	0.42
1:D:57:TRP:CH2	1:D:114:CYS:HB3	2.55	0.42
1:A:124:LYS:NZ	3:A:207:HOH:O	2.42	0.42
1:D:56:TYR:CZ	1:D:58:GLU:HB2	2.56	0.41
2:J:8:MEA:HC3	2:J:12:TYR:HE1	1.84	0.41
2:I:2:PHE:N	2:I:14:CYS:HB3	2.36	0.41
2:K:2:PHE:CE1	2:K:8:MEA:HC2	2.55	0.41
2:I:9:TYR:HA	2:I:10:SAR:HN1	1.71	0.40
2:J:2:PHE:HA	2:J:3:MEA:HC1	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:8:MEA:HC3	2:K:12:TYR:HE1	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	117/127 (92%)	111 (95%)	6 (5%)	0	100	100
1	B	117/127 (92%)	112 (96%)	5 (4%)	0	100	100
1	C	119/127 (94%)	114 (96%)	5 (4%)	0	100	100
1	D	117/127 (92%)	112 (96%)	5 (4%)	0	100	100
2	I	9/16 (56%)	6 (67%)	1 (11%)	2 (22%)	0	0
2	J	9/16 (56%)	8 (89%)	0	1 (11%)	0	0
2	K	9/16 (56%)	7 (78%)	2 (22%)	0	100	100
2	L	9/16 (56%)	7 (78%)	0	2 (22%)	0	0
All	All	506/572 (88%)	477 (94%)	24 (5%)	5 (1%)	15	6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	7	VAL
2	L	14	CYS
2	I	14	CYS
2	I	7	VAL
2	J	7	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/109 (89%)	97 (100%)	0	100	100
1	B	96/109 (88%)	94 (98%)	2 (2%)	53	46
1	C	99/109 (91%)	99 (100%)	0	100	100
1	D	94/109 (86%)	94 (100%)	0	100	100
2	I	9/9 (100%)	7 (78%)	2 (22%)	1	0
2	J	9/9 (100%)	8 (89%)	1 (11%)	6	2
2	K	9/9 (100%)	9 (100%)	0	100	100
2	L	9/9 (100%)	7 (78%)	2 (22%)	1	0
All	All	422/472 (89%)	415 (98%)	7 (2%)	60	55

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	107	GLN
1	B	115	MET
2	I	6	ASP
2	I	15	LYS
2	J	15	LYS
2	L	13	LEU
2	L	15	LYS

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

20 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	MEA	I	8	2	11,12,13	0.85	0	13,14,16	1.40	1 (7%)
2	MEA	J	8	2	11,12,13	0.88	0	13,14,16	1.62	1 (7%)
2	9KK	L	4	2	7,8,9	1.04	1 (14%)	5,8,10	1.44	1 (20%)
2	SAR	J	10	2	4,4,5	1.11	0	1,3,5	2.35	1 (100%)
2	MEA	K	3	2	11,12,13	1.45	2 (18%)	13,14,16	3.31	4 (30%)
2	SAR	I	5	2	4,4,5	1.52	1 (25%)	1,3,5	1.91	0
2	9KK	J	4	2	7,8,9	1.02	1 (14%)	5,8,10	1.26	1 (20%)
2	SAR	K	5	2	4,4,5	1.20	0	1,3,5	2.12	1 (100%)
2	MEA	L	8	2	11,12,13	0.83	0	13,14,16	0.92	1 (7%)
2	MEA	I	3	2	11,12,13	1.45	1 (9%)	13,14,16	2.47	5 (38%)
2	SAR	L	10	2	4,4,5	0.98	0	1,3,5	2.15	1 (100%)
2	SAR	I	10	2	4,4,5	0.94	0	1,3,5	2.22	1 (100%)
2	SAR	K	10	2	4,4,5	1.09	0	1,3,5	2.09	1 (100%)
2	9KK	I	4	2	7,8,9	1.10	1 (14%)	5,8,10	1.32	1 (20%)
2	SAR	J	5	2	4,4,5	1.50	1 (25%)	1,3,5	1.86	0
2	MEA	K	8	2	11,12,13	0.87	0	13,14,16	1.34	1 (7%)
2	SAR	L	5	2	4,4,5	1.47	1 (25%)	1,3,5	1.38	0
2	MEA	L	3	2	11,12,13	1.51	1 (9%)	13,14,16	2.45	5 (38%)
2	MEA	J	3	2	11,12,13	1.47	1 (9%)	13,14,16	2.43	4 (30%)
2	9KK	K	4	2	7,8,9	1.68	1 (14%)	5,8,10	1.74	1 (20%)

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	MEA	I	8	2	-	0/5/8/10	0/1/1/1
2	MEA	J	8	2	-	0/5/8/10	0/1/1/1
2	9KK	L	4	2	-	3/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAR	J	10	2	-	1/1/2/3	-
2	MEA	K	3	2	-	0/5/8/10	0/1/1/1
2	SAR	I	5	2	-	1/1/2/3	-
2	9KK	J	4	2	-	2/5/8/10	-
2	SAR	K	5	2	-	1/1/2/3	-
2	MEA	L	8	2	-	0/5/8/10	0/1/1/1
2	MEA	I	3	2	-	1/5/8/10	0/1/1/1
2	SAR	L	10	2	-	1/1/2/3	-
2	SAR	I	10	2	-	1/1/2/3	-
2	SAR	K	10	2	-	1/1/2/3	-
2	9KK	I	4	2	-	2/5/8/10	-
2	SAR	J	5	2	-	1/1/2/3	-
2	MEA	K	8	2	-	1/5/8/10	0/1/1/1
2	SAR	L	5	2	-	1/1/2/3	-
2	MEA	L	3	2	-	0/5/8/10	0/1/1/1
2	MEA	J	3	2	-	0/5/8/10	0/1/1/1
2	9KK	K	4	2	-	4/5/8/10	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	4	9KK	CA-N	3.85	1.54	1.47
2	L	3	MEA	CA-N	3.79	1.54	1.47
2	I	3	MEA	CA-N	3.54	1.53	1.47
2	J	3	MEA	CA-N	3.51	1.53	1.47
2	K	3	MEA	CA-N	3.09	1.52	1.47
2	I	5	SAR	CA-N	2.57	1.49	1.46
2	J	5	SAR	CA-N	2.54	1.49	1.46
2	L	5	SAR	CA-N	2.44	1.49	1.46
2	I	4	9KK	CA-N	2.13	1.51	1.47
2	K	3	MEA	CB-CA	2.11	1.59	1.54
2	L	4	9KK	CA-N	2.07	1.51	1.47
2	J	4	9KK	CA-N	2.04	1.51	1.47

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	3	MEA	CB-CA-C	7.36	125.60	111.65
2	K	3	MEA	O-C-CA	-6.15	108.67	124.78
2	J	8	MEA	CG-CB-CA	5.20	121.08	113.63
2	J	3	MEA	CB-CA-C	5.17	121.45	111.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	3	MEA	CB-CA-N	-5.02	102.88	110.65
2	I	3	MEA	CB-CA-C	4.99	121.11	111.65
2	L	3	MEA	O-C-CA	-4.78	112.25	124.78
2	I	3	MEA	O-C-CA	-4.75	112.33	124.78
2	L	3	MEA	CB-CA-C	4.56	120.28	111.65
2	J	3	MEA	O-C-CA	-4.53	112.92	124.78
2	K	8	MEA	CG-CB-CA	4.16	119.58	113.63
2	L	3	MEA	CG-CB-CA	-4.08	107.80	113.63
2	K	3	MEA	C1-N-CA	4.03	126.19	113.64
2	I	8	MEA	CG-CB-CA	4.01	119.36	113.63
2	I	3	MEA	CG-CB-CA	-3.66	108.39	113.63
2	J	3	MEA	CG-CB-CA	-3.55	108.56	113.63
2	J	3	MEA	C1-N-CA	3.41	124.25	113.64
2	I	3	MEA	C1-N-CA	3.36	124.10	113.64
2	L	3	MEA	C1-N-CA	3.34	124.04	113.64
2	K	4	9KK	O-C-CA	-3.25	116.27	124.78
2	L	4	9KK	O-C-CA	-2.94	117.08	124.78
2	I	4	9KK	O-C-CA	-2.75	117.58	124.78
2	J	4	9KK	O-C-CA	-2.63	117.87	124.78
2	L	8	MEA	CG-CB-CA	2.36	117.00	113.63
2	J	10	SAR	O-C-CA	-2.35	118.61	125.42
2	I	3	MEA	CB-CA-N	-2.32	107.05	110.65
2	L	3	MEA	CB-CA-N	-2.24	107.18	110.65
2	I	10	SAR	O-C-CA	-2.22	118.99	125.42
2	L	10	SAR	O-C-CA	-2.15	119.21	125.42
2	K	5	SAR	O-C-CA	-2.12	119.28	125.42
2	K	10	SAR	O-C-CA	-2.09	119.36	125.42

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	10	SAR	C-CA-N-CN
2	I	5	SAR	C-CA-N-CN
2	K	5	SAR	C-CA-N-CN
2	I	3	MEA	O-C-CA-CB
2	L	10	SAR	C-CA-N-CN
2	I	10	SAR	C-CA-N-CN
2	K	10	SAR	C-CA-N-CN
2	J	5	SAR	C-CA-N-CN
2	K	8	MEA	O-C-CA-CB
2	L	5	SAR	C-CA-N-CN

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Mol	Chain	Res	Type	Atoms
2	K	4	9KK	C-CA-CB-CG
2	I	4	9KK	N-CA-CB-CG
2	K	4	9KK	N-CA-CB-CG
2	J	4	9KK	CA-CB-CG-CD
2	L	4	9KK	CA-CB-CG-CD
2	I	4	9KK	CA-CB-CG-CD
2	L	4	9KK	CE-CD-CG-CB
2	K	4	9KK	CA-CB-CG-CD
2	L	4	9KK	N-CA-CB-CG
2	J	4	9KK	CE-CD-CG-CB
2	K	4	9KK	CE-CD-CG-CB

There are no ring outliers.

12 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	8	MEA	1	0
2	J	8	MEA	2	0
2	J	10	SAR	1	0
2	K	5	SAR	1	0
2	L	8	MEA	3	0
2	I	3	MEA	1	0
2	L	10	SAR	1	0
2	I	10	SAR	1	0
2	K	10	SAR	1	0
2	K	8	MEA	7	0
2	J	3	MEA	1	0
2	K	4	9KK	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	44:VAL	C	47:GLU	N	6.24

## 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	119/127 (93%)	-0.10	1 (0%) 86 87	15, 23, 38, 52	0
1	B	121/127 (95%)	-0.19	1 (0%) 86 87	12, 22, 33, 48	0
1	C	123/127 (96%)	-0.00	1 (0%) 86 87	16, 22, 39, 46	0
1	D	121/127 (95%)	-0.02	2 (1%) 70 72	16, 23, 41, 46	0
2	I	9/16 (56%)	0.38	0 100 100	11, 17, 26, 34	0
2	J	9/16 (56%)	0.56	1 (11%) 5 6	11, 21, 30, 41	0
2	K	9/16 (56%)	0.24	0 100 100	14, 19, 26, 31	0
2	L	9/16 (56%)	0.45	0 100 100	15, 21, 30, 41	0
All	All	520/572 (90%)	-0.05	6 (1%) 79 81	11, 23, 39, 52	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	ALA	3.5
1	C	18	ALA	3.0
2	J	15	LYS	2.3
1	B	139	HIS	2.2
1	D	24	PRO	2.1
1	D	138	LEU	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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( $\text{\AA}^2$ )	Q<0.9
2	9KK	K	4	9/10	0.82	0.25	21,27,33,37	0
2	9KK	L	4	9/10	0.84	0.18	22,26,32,32	0
2	MEA	L	3	12/13	0.86	0.12	23,33,37,37	0
2	9KK	J	4	9/10	0.87	0.16	27,29,33,34	0
2	9KK	I	4	9/10	0.87	0.17	23,28,34,36	0
2	MEA	K	3	12/13	0.88	0.12	20,24,31,33	0
2	MEA	K	8	12/13	0.88	0.13	7,13,17,21	0
2	MEA	I	3	12/13	0.89	0.12	23,26,32,34	0
2	SAR	I	10	5/6	0.89	0.11	14,15,16,17	0
2	MEA	L	8	12/13	0.89	0.13	7,14,21,22	0
2	SAR	L	5	5/6	0.90	0.16	23,23,28,29	0
2	MEA	J	3	12/13	0.90	0.10	24,27,28,28	0
2	MEA	J	8	12/13	0.90	0.12	14,16,21,22	0
2	MEA	I	8	12/13	0.91	0.11	10,16,22,23	0
2	SAR	K	10	5/6	0.91	0.10	19,20,20,21	0
2	SAR	J	5	5/6	0.92	0.11	21,23,24,24	0
2	SAR	L	10	5/6	0.93	0.11	16,16,17,19	0
2	SAR	K	5	5/6	0.94	0.09	12,16,17,19	0
2	SAR	I	5	5/6	0.96	0.08	18,19,20,21	0
2	SAR	J	10	5/6	0.96	0.07	15,15,19,19	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.