



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:19 am GMT

PDB ID : 3EZQ  
Title : Crystal Structure of the Fas/FADD Death Domain Complex  
Authors : Schwarzenbacher, R.; Robinson, H.; Stec, B.; Riedl, S.J.  
Deposited on : 2008-10-23  
Resolution : 2.73 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

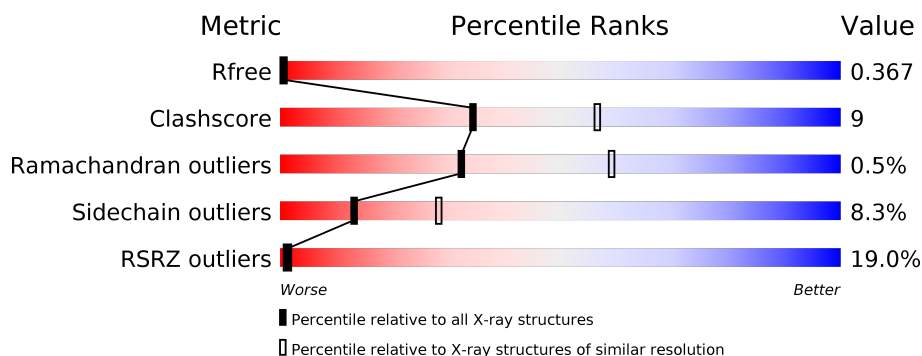
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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))
$R_{free}$	100719	3342 (2.78-2.70)
Clashscore	112137	3731 (2.78-2.70)
Ramachandran outliers	110173	3670 (2.78-2.70)
Sidechain outliers	110143	3671 (2.78-2.70)
RSRZ outliers	101464	3362 (2.78-2.70)

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	115	<div> <div>13%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	C	115	<div> <div>17%</div> <div>80%</div> <div>16%</div> <div>.</div> </div>
1	E	115	<div> <div>13%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	G	115	<div> <div>17%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	I	115	<div> <div>16%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	K	115	<div> <div>13%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	M	115	
1	O	115	
2	B	122	
2	D	122	
2	F	122	
2	H	122	
2	J	122	
2	L	122	
2	N	122	
2	P	122	

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	SO4	K	13	-	-	X	-
4	NA	B	21	-	-	-	X
4	NA	E	14	-	-	-	X
4	NA	K	16	-	-	-	X
4	NA	M	17	-	-	-	X
4	NA	P	18	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13933 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 Tumor necrosis factor receptor superfamily member 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	S	0	0	0
			916	571	159	184	2			
1	C	115	Total	C	N	O	S	0	0	0
			916	571	159	184	2			
1	E	115	Total	C	N	O	S	0	0	0
			916	571	159	184	2			
1	G	115	Total	C	N	O	S	0	0	0
			916	571	159	184	2			
1	I	115	Total	C	N	O	S	0	0	0
			916	571	159	184	2			
1	K	115	Total	C	N	O	S	0	0	0
			916	571	159	184	2			
1	M	115	Total	C	N	O	S	0	0	0
			916	571	159	184	2			
1	O	115	Total	C	N	O	S	0	0	0
			916	571	159	184	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	336	LEU	-	EXPRESSION TAG	UNP P25445
A	337	GLU	-	EXPRESSION TAG	UNP P25445
C	336	LEU	-	EXPRESSION TAG	UNP P25445
C	337	GLU	-	EXPRESSION TAG	UNP P25445
E	336	LEU	-	EXPRESSION TAG	UNP P25445
E	337	GLU	-	EXPRESSION TAG	UNP P25445
G	336	LEU	-	EXPRESSION TAG	UNP P25445
G	337	GLU	-	EXPRESSION TAG	UNP P25445
I	336	LEU	-	EXPRESSION TAG	UNP P25445
I	337	GLU	-	EXPRESSION TAG	UNP P25445
K	336	LEU	-	EXPRESSION TAG	UNP P25445
K	337	GLU	-	EXPRESSION TAG	UNP P25445
M	336	LEU	-	EXPRESSION TAG	UNP P25445

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Chain	Residue	Modelled	Actual	Comment	Reference
M	337	GLU	-	EXPRESSION TAG	UNP P25445
O	336	LEU	-	EXPRESSION TAG	UNP P25445
O	337	GLU	-	EXPRESSION TAG	UNP P25445

- Molecule 2 is a protein called Protein FADD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			795	483	154	154	4			
2	D	99	Total	C	N	O	S	0	0	0
			795	483	154	154	4			
2	F	99	Total	C	N	O	S	0	0	0
			795	483	154	154	4			
2	H	99	Total	C	N	O	S	0	0	0
			795	483	154	154	4			
2	J	99	Total	C	N	O	S	0	0	0
			795	483	154	154	4			
2	L	99	Total	C	N	O	S	0	0	0
			795	483	154	154	4			
2	N	99	Total	C	N	O	S	0	0	0
			795	483	154	154	4			
2	P	99	Total	C	N	O	S	0	0	0
			795	483	154	154	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	209	HIS	-	EXPRESSION TAG	UNP Q13158
B	210	HIS	-	EXPRESSION TAG	UNP Q13158
B	211	HIS	-	EXPRESSION TAG	UNP Q13158
B	212	HIS	-	EXPRESSION TAG	UNP Q13158
B	213	HIS	-	EXPRESSION TAG	UNP Q13158
B	214	HIS	-	EXPRESSION TAG	UNP Q13158
D	209	HIS	-	EXPRESSION TAG	UNP Q13158
D	210	HIS	-	EXPRESSION TAG	UNP Q13158
D	211	HIS	-	EXPRESSION TAG	UNP Q13158
D	212	HIS	-	EXPRESSION TAG	UNP Q13158
D	213	HIS	-	EXPRESSION TAG	UNP Q13158
D	214	HIS	-	EXPRESSION TAG	UNP Q13158
F	209	HIS	-	EXPRESSION TAG	UNP Q13158
F	210	HIS	-	EXPRESSION TAG	UNP Q13158
F	211	HIS	-	EXPRESSION TAG	UNP Q13158

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Chain	Residue	Modelled	Actual	Comment	Reference
F	212	HIS	-	EXPRESSION TAG	UNP Q13158
F	213	HIS	-	EXPRESSION TAG	UNP Q13158
F	214	HIS	-	EXPRESSION TAG	UNP Q13158
H	209	HIS	-	EXPRESSION TAG	UNP Q13158
H	210	HIS	-	EXPRESSION TAG	UNP Q13158
H	211	HIS	-	EXPRESSION TAG	UNP Q13158
H	212	HIS	-	EXPRESSION TAG	UNP Q13158
H	213	HIS	-	EXPRESSION TAG	UNP Q13158
H	214	HIS	-	EXPRESSION TAG	UNP Q13158
J	209	HIS	-	EXPRESSION TAG	UNP Q13158
J	210	HIS	-	EXPRESSION TAG	UNP Q13158
J	211	HIS	-	EXPRESSION TAG	UNP Q13158
J	212	HIS	-	EXPRESSION TAG	UNP Q13158
J	213	HIS	-	EXPRESSION TAG	UNP Q13158
J	214	HIS	-	EXPRESSION TAG	UNP Q13158
L	209	HIS	-	EXPRESSION TAG	UNP Q13158
L	210	HIS	-	EXPRESSION TAG	UNP Q13158
L	211	HIS	-	EXPRESSION TAG	UNP Q13158
L	212	HIS	-	EXPRESSION TAG	UNP Q13158
L	213	HIS	-	EXPRESSION TAG	UNP Q13158
L	214	HIS	-	EXPRESSION TAG	UNP Q13158
N	209	HIS	-	EXPRESSION TAG	UNP Q13158
N	210	HIS	-	EXPRESSION TAG	UNP Q13158
N	211	HIS	-	EXPRESSION TAG	UNP Q13158
N	212	HIS	-	EXPRESSION TAG	UNP Q13158
N	213	HIS	-	EXPRESSION TAG	UNP Q13158
N	214	HIS	-	EXPRESSION TAG	UNP Q13158
P	209	HIS	-	EXPRESSION TAG	UNP Q13158
P	210	HIS	-	EXPRESSION TAG	UNP Q13158
P	211	HIS	-	EXPRESSION TAG	UNP Q13158
P	212	HIS	-	EXPRESSION TAG	UNP Q13158
P	213	HIS	-	EXPRESSION TAG	UNP Q13158
P	214	HIS	-	EXPRESSION TAG	UNP Q13158

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total Na 1 1	0	0
4	J	1	Total Na 1 1	0	0
4	K	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0
4	H	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0
4	M	1	Total Na 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	7	Total O 7 7	0	0
5	B	2	Total O 2 2	0	0
5	C	8	Total O 8 8	0	0
5	D	4	Total O 4 4	0	0
5	E	9	Total O 9 9	0	0
5	F	4	Total O 4 4	0	0
5	G	11	Total O 11 11	0	0
5	H	8	Total O 8 8	0	0
5	I	84	Total O 84 84	0	0
5	J	8	Total O 8 8	0	0
5	K	6	Total O 6 6	0	0
5	L	7	Total O 7 7	0	0

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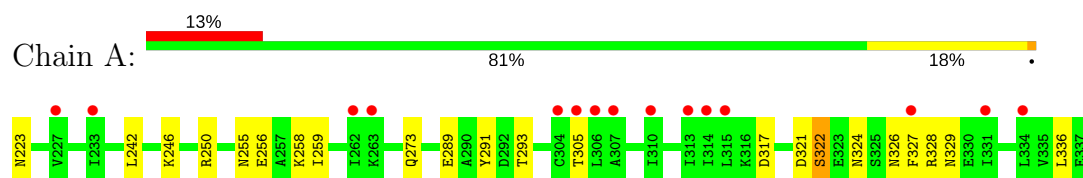
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	9	Total	O	0	0
			9	9		
5	N	3	Total	O	0	0
			3	3		
5	O	5	Total	O	0	0
			5	5		
5	P	2	Total	O	0	0
			2	2		

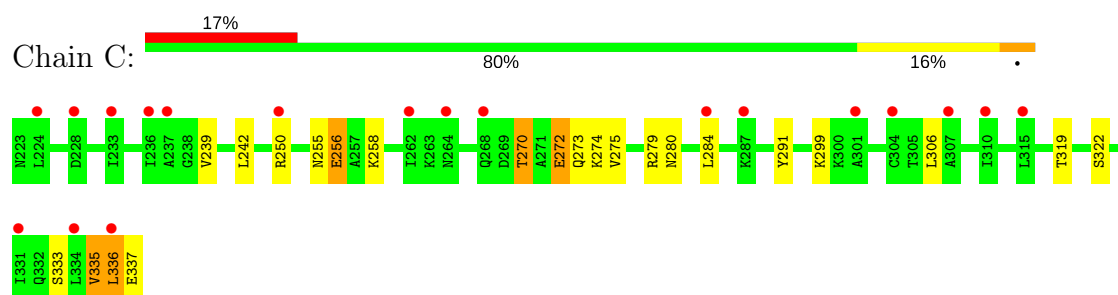
### 3 Residue-property plots [i](#)

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.

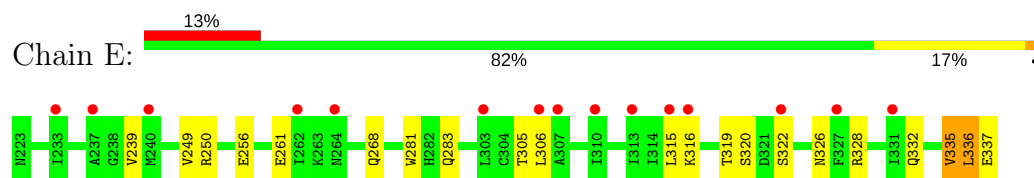
- Molecule 1: Tumor necrosis factor receptor superfamily member 6



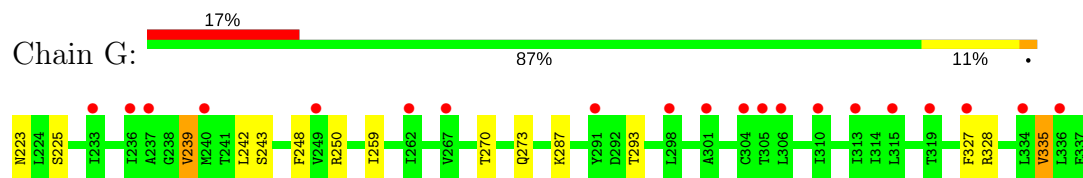
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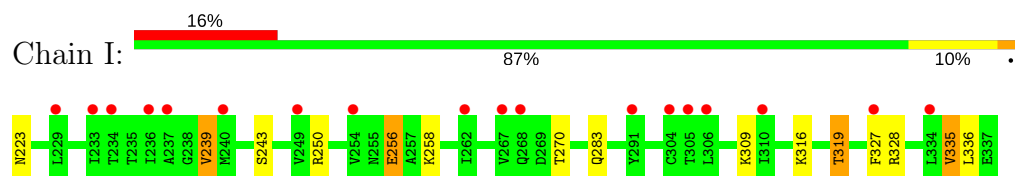
- Molecule 1: Tumor necrosis factor receptor superfamily member 6



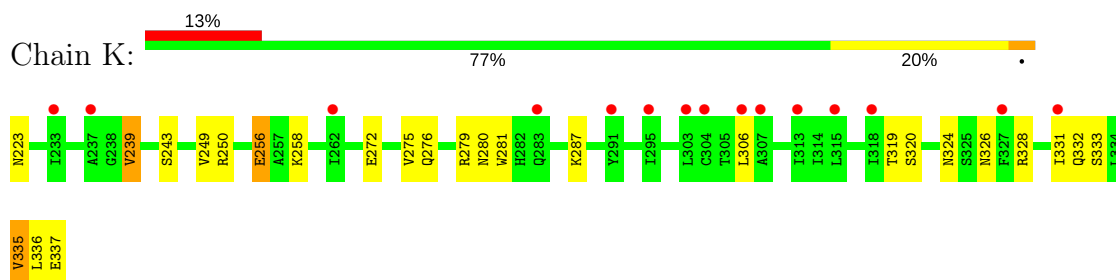
- Molecule 1: Tumor necrosis factor receptor superfamily member 6



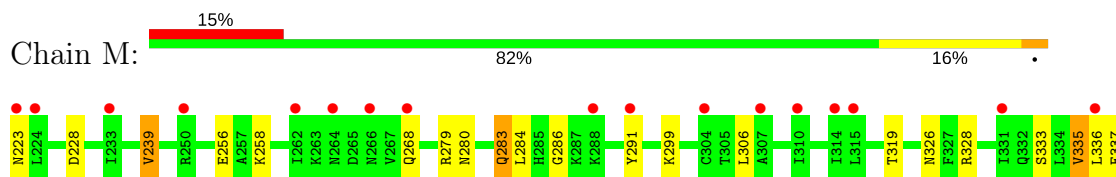
- Molecule 1: Tumor necrosis factor receptor superfamily member 6



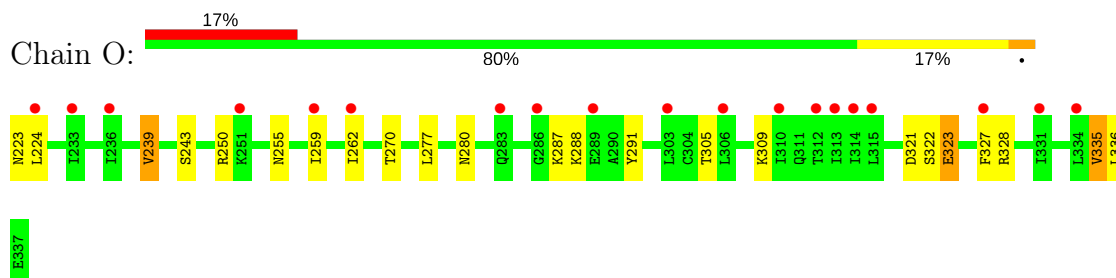
- Molecule 1: Tumor necrosis factor receptor superfamily member 6



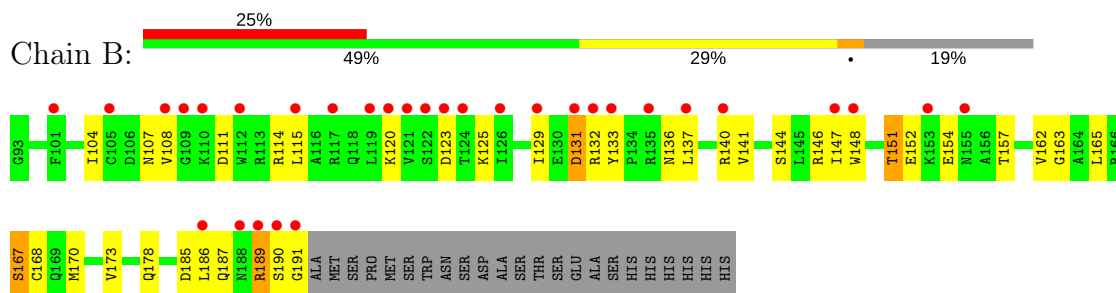
- Molecule 1: Tumor necrosis factor receptor superfamily member 6



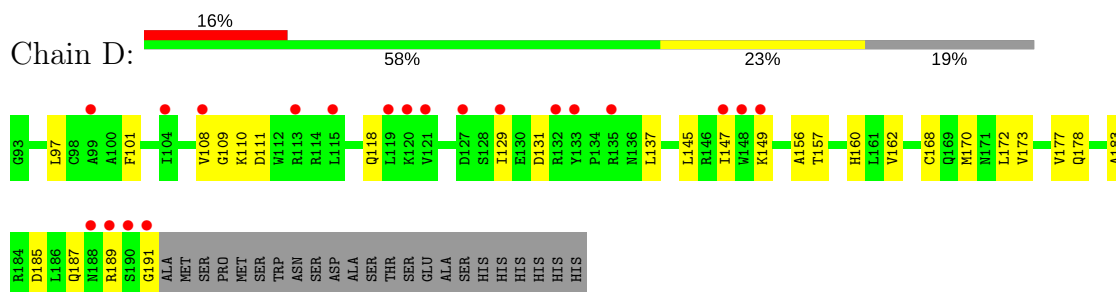
- Molecule 1: Tumor necrosis factor receptor superfamily member 6



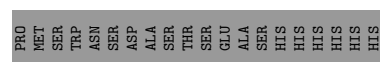
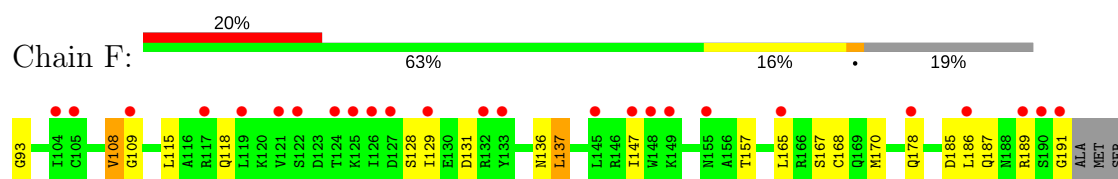
- Molecule 2: Protein FADD



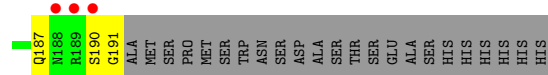
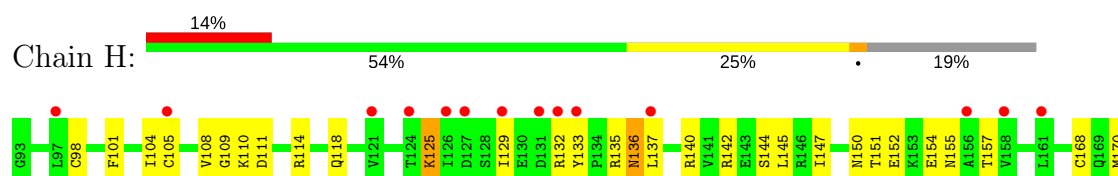
- Molecule 2: Protein FADD



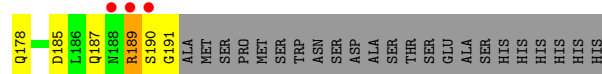
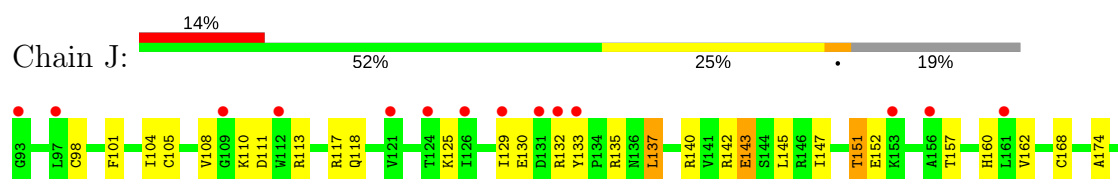
- Molecule 2: Protein FADD



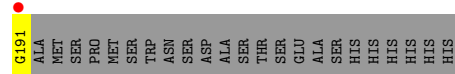
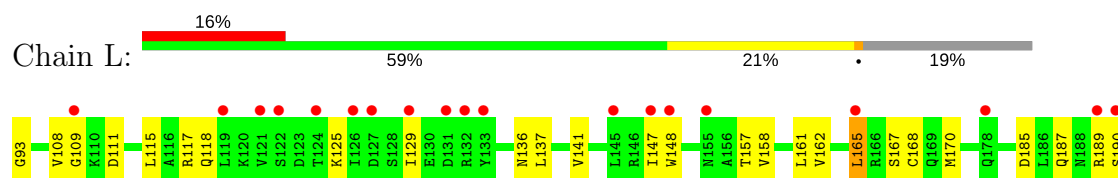
• Molecule 2: Protein FADD



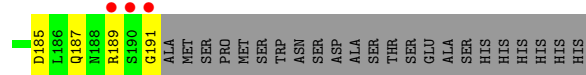
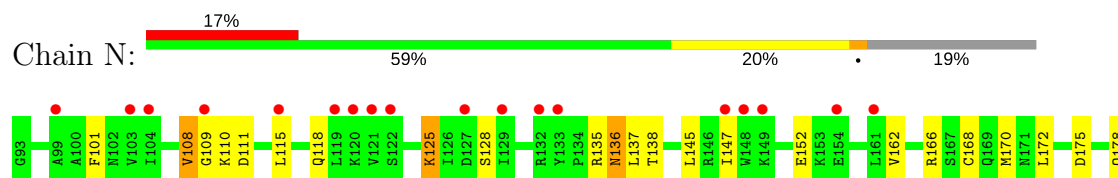
• Molecule 2: Protein FADD



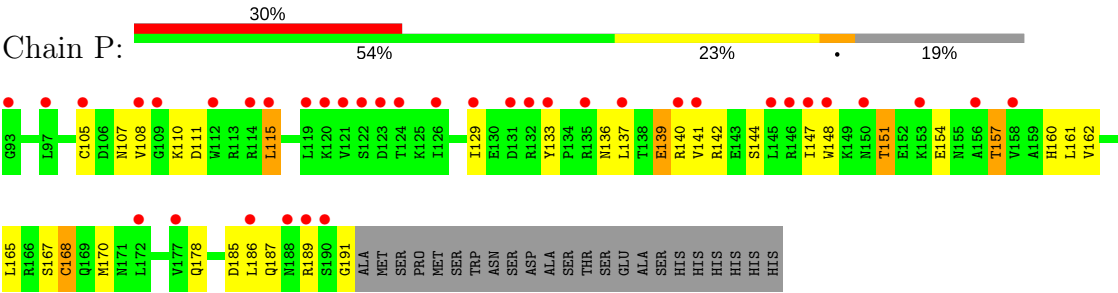
• Molecule 2: Protein FADD



• Molecule 2: Protein FADD



• Molecule 2: Protein FADD



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.22Å 126.22Å 299.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.73 29.71 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-2.73) 98.8 (29.71-2.73)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.234 , 0.278 0.339 , 0.367	Depositor DCC
$R_{free}$ test set	3544 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.2	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.499 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13933	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	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 45.65 % 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 1.2821e-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: NA, SO4

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	0.61	0/923	0.68	0/1241
1	C	0.71	1/923 (0.1%)	0.70	0/1241
1	E	0.67	0/923	0.67	0/1241
1	G	0.73	0/923	0.74	0/1241
1	I	0.70	0/923	0.74	0/1241
1	K	0.64	0/923	0.71	0/1241
1	M	0.72	1/923 (0.1%)	0.72	0/1241
1	O	0.61	0/923	0.66	0/1241
2	B	0.57	0/802	0.61	0/1080
2	D	0.54	1/802 (0.1%)	0.61	0/1080
2	F	0.49	0/802	0.62	0/1080
2	H	0.57	1/802 (0.1%)	0.66	0/1080
2	J	0.55	1/802 (0.1%)	0.65	0/1080
2	L	0.51	0/802	0.59	0/1080
2	N	0.50	0/802	0.63	0/1080
2	P	0.58	2/802 (0.2%)	0.58	0/1080
All	All	0.62	7/13800 (0.1%)	0.66	0/18568

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	279	ARG	NE-CZ	5.70	1.40	1.33
1	M	228	ASP	CG-OD1	5.59	1.38	1.25
2	J	98	CYS	CB-SG	-5.55	1.72	1.81
2	H	98	CYS	CB-SG	-5.33	1.73	1.81
2	D	131	ASP	CG-OD2	5.29	1.37	1.25
2	P	154	GLU	CD-OE1	5.28	1.31	1.25
2	P	154	GLU	CD-OE2	5.02	1.31	1.25

There are no bond angle outliers.

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	916	0	939	16	0
1	C	916	0	939	17	0
1	E	916	0	939	14	0
1	G	916	0	939	13	0
1	I	916	0	939	17	0
1	K	916	0	939	21	0
1	M	916	0	939	15	0
1	O	916	0	939	26	0
2	B	795	0	793	24	0
2	D	795	0	793	17	0
2	F	795	0	793	20	0
2	H	795	0	793	20	0
2	J	795	0	793	26	0
2	L	795	0	793	23	0
2	N	795	0	793	19	0
2	P	795	0	793	29	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
3	E	10	0	0	0	0
3	G	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	10	0	0	2	0
3	M	10	0	0	1	0
3	O	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	7	0	0	1	0
5	B	2	0	0	0	0
5	C	8	0	0	1	0
5	D	4	0	0	0	0
5	E	9	0	0	0	0
5	F	4	0	0	0	0
5	G	11	0	0	0	0
5	H	8	0	0	1	0
5	I	84	0	0	4	0
5	J	8	0	0	0	0
5	K	6	0	0	0	0
5	L	7	0	0	1	0
5	M	9	0	0	1	0
5	N	3	0	0	0	0
5	O	5	0	0	0	0
5	P	2	0	0	3	0
All	All	13933	0	13856	261	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (261) 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)
2:L:109:GLY:HA2	2:L:137:LEU:HD21	1.37	1.04
2:B:115:LEU:HD11	2:B:165:LEU:HD23	1.42	1.01
1:K:328:ARG:HE	1:K:332:GLN:HE22	1.13	0.95
2:F:109:GLY:HA2	2:F:137:LEU:HD21	1.47	0.91
1:A:289:GLU:O	1:A:293:THR:HG22	1.73	0.89
1:K:258:LYS:HG2	1:K:280:ASN:ND2	1.86	0.89
2:F:108:VAL:HG13	2:F:170:MET:HE1	1.59	0.84
1:A:328:ARG:HG3	1:C:335:VAL:HG13	1.60	0.83
1:K:258:LYS:HG2	1:K:280:ASN:HD21	1.44	0.80
2:H:108:VAL:HG22	2:H:170:MET:HE1	1.64	0.80
1:K:328:ARG:NE	1:K:332:GLN:HE22	1.78	0.79
2:P:162:VAL:HG11	2:P:178:GLN:HE21	1.47	0.79
1:K:328:ARG:HE	1:K:332:GLN:NE2	1.79	0.79
2:D:162:VAL:HG11	2:D:178:GLN:HE21	1.51	0.75
1:I:223:ASN:HB2	2:J:135:ARG:CZ	2.17	0.74
2:L:129:ILE:HD11	2:L:147:ILE:HD12	1.69	0.74
1:K:250:ARG:CZ	1:K:256:GLU:OE2	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:328:ARG:HG3	1:O:335:VAL:HG13	1.70	0.73
1:G:223:ASN:HB2	2:H:135:ARG:CZ	2.18	0.73
2:F:115:LEU:HD11	2:F:165:LEU:HD12	1.70	0.73
2:J:137:LEU:HG	2:J:140:ARG:NH2	2.04	0.72
2:H:151:THR:HG22	2:H:152:GLU:OE1	1.90	0.72
2:L:108:VAL:HG23	2:L:109:GLY:H	1.55	0.71
2:H:136:ASN:HB2	5:H:19:HOH:O	1.90	0.71
2:B:115:LEU:CD1	2:B:165:LEU:HD23	2.20	0.71
1:M:291:TYR:HB3	2:N:172:LEU:HD12	1.74	0.70
2:F:93:GLY:N	5:I:175:HOH:O	2.24	0.70
1:O:309:LYS:NZ	2:P:189:ARG:HB3	2.07	0.69
1:G:248:PHE:CZ	1:G:293:THR:HG22	2.27	0.68
5:I:106:HOH:O	2:N:136:ASN:ND2	2.27	0.68
2:F:129:ILE:HD11	2:F:147:ILE:HD12	1.77	0.67
2:H:108:VAL:HG13	2:H:170:MET:CE	2.25	0.67
1:G:248:PHE:CE1	1:G:293:THR:HG22	2.30	0.66
2:P:115:LEU:HD11	2:P:165:LEU:HD23	1.78	0.65
1:A:322:SER:O	1:C:299:LYS:NZ	2.29	0.65
2:B:129:ILE:HD11	2:B:147:ILE:HD12	1.78	0.65
2:N:101:PHE:CD1	2:N:145:LEU:HD13	2.32	0.65
1:I:309:LYS:HZ2	2:J:189:ARG:HB3	1.62	0.65
1:O:323:GLU:OE2	1:O:323:GLU:HA	1.96	0.64
2:J:151:THR:HG23	2:J:152:GLU:OE2	1.97	0.64
2:D:157:THR:HG23	2:D:160:HIS:H	1.62	0.63
1:C:291:TYR:HB3	2:D:172:LEU:HD12	1.79	0.63
2:B:162:VAL:HG11	2:B:178:GLN:HE21	1.61	0.63
2:B:115:LEU:HD11	2:B:165:LEU:CD2	2.26	0.63
2:P:148:TRP:O	2:P:151:THR:HG22	1.99	0.62
1:G:223:ASN:HB2	2:H:135:ARG:NE	2.14	0.62
2:B:178:GLN:NE2	5:I:97:HOH:O	2.31	0.62
1:G:239:VAL:HG13	1:G:239:VAL:O	2.00	0.62
2:N:175:ASP:CG	1:O:323:GLU:HG2	2.20	0.62
2:N:162:VAL:HG11	2:N:178:GLN:HE21	1.64	0.62
2:H:132:ARG:HD3	2:H:133:TYR:CE1	2.35	0.61
2:P:129:ILE:HD11	2:P:147:ILE:HD12	1.80	0.61
1:A:291:TYR:OH	2:B:107:ASN:HB3	2.01	0.61
1:E:239:VAL:HA	2:F:187:GLN:HE22	1.64	0.61
1:A:255:ASN:OD1	1:A:258:LYS:HG3	2.00	0.61
2:L:115:LEU:HD11	2:L:165:LEU:HD12	1.83	0.60
2:J:151:THR:CG2	2:J:152:GLU:OE2	2.49	0.60
2:D:108:VAL:HG22	2:D:170:MET:HE1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:VAL:HG13	2:B:170:MET:CE	2.31	0.60
2:B:148:TRP:O	2:B:151:THR:HG22	2.02	0.60
2:D:118:GLN:HG3	2:D:168:CYS:SG	2.42	0.60
2:L:109:GLY:HA2	2:L:137:LEU:CD2	2.24	0.60
2:J:118:GLN:HG3	2:J:168:CYS:SG	2.42	0.59
2:L:108:VAL:HG21	2:L:141:VAL:HG11	1.84	0.59
1:M:279:ARG:O	1:M:283:GLN:HG3	2.02	0.59
1:C:270:THR:HG23	5:C:199:HOH:O	2.02	0.59
1:O:239:VAL:O	1:O:239:VAL:HG13	2.01	0.59
1:I:336:LEU:O	2:J:185:ASP:OD2	2.21	0.59
2:P:115:LEU:HD12	2:P:168:CYS:SG	2.44	0.58
2:H:118:GLN:HG3	2:H:168:CYS:SG	2.43	0.58
2:L:108:VAL:HG23	2:L:141:VAL:HG21	1.85	0.58
1:O:309:LYS:NZ	2:P:189:ARG:CD	2.67	0.57
2:F:118:GLN:HG3	2:F:168:CYS:SG	2.44	0.57
2:N:118:GLN:HG3	2:N:168:CYS:SG	2.44	0.57
2:P:189:ARG:HB2	5:P:217:HOH:O	2.04	0.57
2:D:108:VAL:HG13	2:D:170:MET:HE3	1.85	0.57
2:L:129:ILE:HD11	2:L:147:ILE:CD1	2.35	0.57
2:L:115:LEU:CD1	2:L:165:LEU:HD12	2.35	0.57
1:O:323:GLU:OE2	1:O:323:GLU:CA	2.53	0.57
2:H:108:VAL:HG13	2:H:170:MET:HE3	1.88	0.56
1:I:250:ARG:NE	1:I:256:GLU:OE1	2.38	0.56
1:M:306:LEU:HD13	1:O:327:PHE:CE2	2.41	0.56
2:F:109:GLY:C	2:F:137:LEU:HD11	2.26	0.55
1:O:309:LYS:NZ	2:P:189:ARG:HD2	2.22	0.55
1:A:327:PHE:CE2	1:C:306:LEU:HD13	2.42	0.55
2:J:187:GLN:O	2:J:191:GLY:N	2.38	0.55
2:N:137:LEU:HD12	2:N:137:LEU:H	1.71	0.55
2:N:125:LYS:HG2	2:N:147:ILE:HD13	1.88	0.55
2:P:189:ARG:CB	5:P:217:HOH:O	2.54	0.55
2:L:109:GLY:C	2:L:137:LEU:HD11	2.27	0.55
2:B:108:VAL:HG13	2:B:170:MET:HE3	1.88	0.55
1:I:239:VAL:O	1:I:239:VAL:HG13	2.06	0.55
1:O:305:THR:HB	2:P:186:LEU:HD13	1.88	0.54
2:D:187:GLN:O	2:D:191:GLY:N	2.39	0.54
1:O:291:TYR:OH	2:P:107:ASN:HB3	2.07	0.54
2:F:129:ILE:HD11	2:F:147:ILE:CD1	2.37	0.54
1:O:335:VAL:O	1:O:335:VAL:HG13	2.06	0.54
1:A:317:ASP:OD1	1:A:324:ASN:ND2	2.40	0.53
1:O:309:LYS:HZ2	2:P:189:ARG:HB3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:309:LYS:HZ2	2:P:189:ARG:HD2	1.72	0.53
2:H:187:GLN:O	2:H:191:GLY:N	2.39	0.53
1:K:239:VAL:HG13	1:K:239:VAL:O	2.09	0.53
2:F:109:GLY:HA2	2:F:137:LEU:CD2	2.32	0.53
1:A:250:ARG:HG3	1:A:259:ILE:HD11	1.91	0.53
1:A:223:ASN:HB3	2:B:136:ASN:HD21	1.74	0.53
1:M:326:ASN:HB2	3:M:12:SO4:S	2.49	0.53
1:E:239:VAL:HA	2:F:187:GLN:NE2	2.24	0.52
1:O:250:ARG:HG3	1:O:259:ILE:HD11	1.92	0.52
2:H:108:VAL:HG13	2:H:170:MET:HE1	1.90	0.52
2:L:187:GLN:O	2:L:191:GLY:N	2.42	0.52
2:N:108:VAL:HG13	2:N:170:MET:HE3	1.91	0.52
2:L:108:VAL:CG2	2:L:141:VAL:HG11	2.39	0.52
2:B:125:LYS:HG2	2:B:147:ILE:HD13	1.92	0.52
2:B:187:GLN:O	2:B:191:GLY:N	2.40	0.52
2:D:97:LEU:HD11	2:D:156:ALA:O	2.10	0.52
1:K:336:LEU:O	2:L:185:ASP:OD2	2.28	0.52
1:M:336:LEU:O	2:N:185:ASP:OD2	2.28	0.52
2:F:115:LEU:CD1	2:F:165:LEU:HD12	2.39	0.51
1:I:327:PHE:CE2	1:K:306:LEU:HD13	2.45	0.51
1:O:336:LEU:O	2:P:185:ASP:OD2	2.29	0.51
2:P:129:ILE:HD11	2:P:147:ILE:CD1	2.40	0.51
1:C:250:ARG:HE	1:C:256:GLU:HG3	1.75	0.51
1:K:326:ASN:HB2	3:K:13:SO4:S	2.51	0.51
1:K:249:VAL:HG12	1:K:281:TRP:HB2	1.93	0.51
1:G:239:VAL:CG1	1:G:239:VAL:O	2.59	0.51
2:H:101:PHE:CD1	2:H:145:LEU:HD13	2.46	0.51
2:P:187:GLN:O	2:P:191:GLY:N	2.41	0.51
1:O:262:ILE:HD12	1:O:277:LEU:HD23	1.92	0.51
2:P:115:LEU:HD11	2:P:165:LEU:CD2	2.41	0.51
2:F:187:GLN:O	2:F:191:GLY:N	2.42	0.51
2:N:175:ASP:OD2	1:O:323:GLU:HG2	2.10	0.50
1:I:223:ASN:HB2	2:J:135:ARG:NE	2.26	0.50
2:H:137:LEU:HD12	2:H:140:ARG:HH22	1.75	0.50
2:N:125:LYS:CG	2:N:147:ILE:HD13	2.42	0.50
2:P:133:TYR:O	2:P:140:ARG:HD3	2.11	0.50
2:J:113:ARG:NH1	2:J:130:GLU:OE1	2.45	0.50
1:A:305:THR:HB	2:B:186:LEU:HD13	1.92	0.50
2:B:129:ILE:HD11	2:B:147:ILE:CD1	2.41	0.50
2:F:108:VAL:HG22	2:F:170:MET:CE	2.42	0.50
2:L:118:GLN:HG3	2:L:168:CYS:SG	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:239:VAL:O	1:O:239:VAL:CG1	2.59	0.50
1:M:239:VAL:HG13	1:M:239:VAL:O	2.12	0.49
1:A:326:ASN:HA	1:A:329:ASN:HD22	1.76	0.49
1:C:242:LEU:HD12	1:C:274:LYS:HG3	1.94	0.49
1:C:337:GLU:OE1	2:D:178:GLN:HG2	2.11	0.49
1:K:337:GLU:HG3	2:L:158:VAL:HG23	1.94	0.49
2:N:108:VAL:HG12	2:N:109:GLY:N	2.28	0.49
2:N:187:GLN:O	2:N:191:GLY:N	2.41	0.49
1:A:336:LEU:O	2:B:185:ASP:OD2	2.30	0.49
2:B:132:ARG:HG2	2:B:133:TYR:CE2	2.47	0.49
2:D:101:PHE:CD1	2:D:145:LEU:HD13	2.46	0.49
2:H:132:ARG:HD3	2:H:133:TYR:CZ	2.48	0.49
1:I:256:GLU:OE2	1:I:256:GLU:HA	2.12	0.49
2:J:125:LYS:HG2	2:J:147:ILE:HD13	1.95	0.49
1:I:335:VAL:HG13	1:K:328:ARG:HG3	1.93	0.49
1:I:328:ARG:HG3	1:K:335:VAL:HG13	1.95	0.49
1:O:309:LYS:HZ1	2:P:189:ARG:HB3	1.76	0.49
2:J:137:LEU:CG	2:J:140:ARG:NH2	2.76	0.48
1:A:246:LYS:NZ	5:A:64:HOH:O	2.45	0.48
1:I:309:LYS:HZ2	2:J:189:ARG:CD	2.27	0.48
1:E:305:THR:HB	2:F:186:LEU:HD13	1.96	0.48
1:E:328:ARG:HG3	1:G:335:VAL:HG13	1.95	0.48
1:M:335:VAL:HG13	1:O:328:ARG:HG3	1.96	0.48
1:E:336:LEU:O	2:F:185:ASP:OD2	2.31	0.47
1:C:272:GLU:HA	1:C:275:VAL:HG22	1.94	0.47
2:J:101:PHE:CD1	2:J:145:LEU:HD13	2.50	0.47
2:J:105:CYS:SG	2:J:142:ARG:HB2	2.54	0.47
2:L:158:VAL:O	2:L:162:VAL:HG23	2.14	0.47
1:C:280:ASN:O	1:C:284:LEU:HG	2.14	0.47
2:D:129:ILE:HD11	2:D:147:ILE:HD12	1.97	0.47
1:K:239:VAL:CG1	1:K:239:VAL:O	2.62	0.47
2:L:108:VAL:CG2	2:L:141:VAL:HG21	2.44	0.47
2:H:105:CYS:SG	2:H:142:ARG:HB2	2.55	0.47
1:K:272:GLU:OE1	1:K:272:GLU:HA	2.14	0.47
1:C:336:LEU:O	2:D:185:ASP:OD2	2.33	0.47
2:J:104:ILE:HG23	2:J:108:VAL:CG2	2.44	0.47
1:M:223:ASN:HB2	2:N:135:ARG:HE	1.80	0.47
2:F:108:VAL:HG22	2:F:170:MET:HE1	1.97	0.47
1:I:239:VAL:CG1	1:I:239:VAL:O	2.62	0.47
1:A:242:LEU:HD11	1:A:273:GLN:HE21	1.79	0.46
2:L:108:VAL:HG12	2:L:170:MET:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:LEU:HD21	1:C:273:GLN:OE1	2.16	0.46
1:I:309:LYS:NZ	2:J:189:ARG:HB3	2.29	0.46
2:H:109:GLY:HA2	2:H:137:LEU:HD23	1.97	0.46
2:P:157:THR:CG2	2:P:160:HIS:ND1	2.79	0.46
1:E:306:LEU:HD13	1:G:327:PHE:CE2	2.51	0.46
1:M:337:GLU:OE1	2:N:178:GLN:HG2	2.15	0.46
1:E:315:LEU:O	1:E:319:THR:HG22	2.16	0.46
2:B:165:LEU:HD13	2:B:173:VAL:HG12	1.98	0.46
2:D:137:LEU:H	2:D:137:LEU:HD12	1.81	0.46
1:G:250:ARG:HG3	1:G:259:ILE:HD11	1.98	0.45
2:J:104:ILE:HG23	2:J:108:VAL:HG21	1.98	0.45
2:H:125:LYS:HG2	2:H:147:ILE:HD13	1.98	0.45
2:L:115:LEU:HD11	2:L:165:LEU:CD1	2.46	0.45
2:H:152:GLU:HB3	2:H:155:ASN:HB2	1.99	0.45
1:C:255:ASN:OD1	1:C:258:LYS:HG3	2.16	0.45
1:M:299:LYS:NZ	1:O:322:SER:O	2.47	0.45
1:E:316:LYS:O	1:E:319:THR:HG22	2.17	0.44
1:E:328:ARG:HH21	1:E:332:GLN:HE22	1.65	0.44
5:I:106:HOH:O	2:N:138:THR:HG23	2.18	0.44
2:P:133:TYR:CG	2:P:139:GLU:HG3	2.53	0.44
1:E:335:VAL:HG13	1:G:328:ARG:HG3	1.98	0.44
1:E:337:GLU:OE1	2:F:178:GLN:HG2	2.18	0.44
2:B:131:ASP:OD2	2:B:132:ARG:N	2.51	0.44
2:J:162:VAL:HG11	2:J:178:GLN:HE21	1.83	0.44
1:O:223:ASN:HB3	5:P:61:HOH:O	2.18	0.44
2:B:137:LEU:O	2:B:141:VAL:HG23	2.17	0.44
2:F:128:SER:O	2:F:131:ASP:OD2	2.36	0.43
2:H:104:ILE:HG23	2:H:108:VAL:CG2	2.48	0.43
1:A:328:ARG:HG3	1:C:335:VAL:CG1	2.42	0.43
1:I:335:VAL:O	1:I:335:VAL:HG13	2.18	0.43
1:G:242:LEU:HD21	1:G:273:GLN:NE2	2.34	0.43
2:D:108:VAL:HG13	2:D:170:MET:CE	2.47	0.43
2:J:129:ILE:HD11	2:J:147:ILE:HD12	2.00	0.43
1:M:258:LYS:CD	1:M:280:ASN:HD21	2.32	0.43
1:C:242:LEU:CD1	1:C:274:LYS:HG3	2.49	0.43
1:O:224:LEU:HB2	2:P:136:ASN:HD22	1.84	0.43
1:I:258:LYS:HA	1:I:258:LYS:HD3	1.89	0.42
2:J:137:LEU:HG	2:J:140:ARG:HH22	1.81	0.42
1:E:249:VAL:HG12	1:E:281:TRP:HB2	2.02	0.42
2:L:108:VAL:HG21	2:L:141:VAL:CG1	2.48	0.42
1:E:328:ARG:HE	1:E:332:GLN:NE2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:328:ARG:NE	1:K:332:GLN:NE2	2.52	0.42
2:D:108:VAL:HG12	2:D:109:GLY:N	2.35	0.42
2:H:129:ILE:HD11	2:H:147:ILE:HD12	2.01	0.42
2:P:133:TYR:HB3	2:P:139:GLU:CG	2.50	0.42
2:J:132:ARG:HG2	2:J:133:TYR:CE2	2.55	0.42
2:J:133:TYR:HE1	2:J:143:GLU:HG3	1.85	0.42
1:O:309:LYS:HZ2	2:P:189:ARG:CD	2.31	0.42
2:F:108:VAL:HG12	2:F:109:GLY:N	2.35	0.41
1:K:275:VAL:O	1:K:279:ARG:HG3	2.20	0.41
1:G:335:VAL:O	1:G:335:VAL:HG13	2.20	0.41
1:A:289:GLU:O	1:A:293:THR:CG2	2.56	0.41
1:K:324:ASN:ND2	3:K:13:SO4:O3	2.45	0.41
1:K:249:VAL:HG12	1:K:281:TRP:CB	2.50	0.41
2:P:129:ILE:HG22	2:P:140:ARG:HG2	2.01	0.41
2:P:157:THR:HG23	2:P:160:HIS:ND1	2.34	0.41
1:C:239:VAL:HB	2:D:183:ALA:HB1	2.01	0.41
1:O:309:LYS:HZ3	2:P:189:ARG:CD	2.33	0.41
2:B:189:ARG:HD3	2:B:189:ARG:C	2.41	0.41
1:M:280:ASN:O	1:M:284:LEU:HG	2.21	0.41
2:D:173:VAL:O	2:D:177:VAL:HG23	2.21	0.41
1:I:309:LYS:HZ2	2:J:189:ARG:HD2	1.86	0.41
1:G:248:PHE:CE1	1:G:293:THR:CG2	3.00	0.41
1:M:239:VAL:O	1:M:239:VAL:CG1	2.67	0.41
2:N:162:VAL:HG11	2:N:178:GLN:NE2	2.33	0.41
2:L:93:GLY:N	5:L:90:HOH:O	2.54	0.40
2:J:162:VAL:HG13	2:J:174:ALA:HB1	2.03	0.40
2:B:137:LEU:HG	2:B:140:ARG:NH2	2.37	0.40
1:C:335:VAL:HG13	1:C:335:VAL:O	2.21	0.40
1:E:250:ARG:HD2	1:E:256:GLU:OE2	2.21	0.40
1:K:331:ILE:HA	1:K:331:ILE:HD13	1.93	0.40
2:L:148:TRP:CH2	2:L:161:LEU:HG	2.56	0.40
1:M:286:GLY:N	5:M:222:HOH:O	2.29	0.40
2:N:162:VAL:O	2:N:166:ARG:HG3	2.21	0.40
2:B:104:ILE:HG23	2:B:108:VAL:CG2	2.51	0.40
2:J:189:ARG:C	2:J:189:ARG:HD3	2.42	0.40
2:L:108:VAL:HG23	2:L:109:GLY:N	2.28	0.40
2:B:163:GLY:O	2:B:167:SER:OG	2.38	0.40
1:I:316:LYS:O	1:I:319:THR:HG22	2.20	0.40
2:P:137:LEU:O	2:P:141:VAL:HG23	2.21	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	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	20	44
1	C	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	20	44
1	E	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
1	G	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
1	I	113/115 (98%)	108 (96%)	4 (4%)	1 (1%)	20	44
1	K	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	20	44
1	M	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	20	44
1	O	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
2	B	97/122 (80%)	92 (95%)	5 (5%)	0	100	100
2	D	97/122 (80%)	92 (95%)	5 (5%)	0	100	100
2	F	97/122 (80%)	93 (96%)	3 (3%)	1 (1%)	18	40
2	H	97/122 (80%)	92 (95%)	5 (5%)	0	100	100
2	J	97/122 (80%)	93 (96%)	4 (4%)	0	100	100
2	L	97/122 (80%)	92 (95%)	5 (5%)	0	100	100
2	N	97/122 (80%)	93 (96%)	3 (3%)	1 (1%)	18	40
2	P	97/122 (80%)	93 (96%)	3 (3%)	1 (1%)	18	40
All	All	1680/1896 (89%)	1592 (95%)	80 (5%)	8 (0%)	32	59

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	GLU
1	C	256	GLU
1	K	256	GLU
1	M	256	GLU
1	I	256	GLU
2	F	108	VAL

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Mol	Chain	Res	Type
2	N	108	VAL
2	P	108	VAL

### 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	105/105 (100%)	103 (98%)	2 (2%)	62	85
1	C	105/105 (100%)	98 (93%)	7 (7%)	19	40
1	E	105/105 (100%)	97 (92%)	8 (8%)	15	33
1	G	105/105 (100%)	99 (94%)	6 (6%)	24	49
1	I	105/105 (100%)	99 (94%)	6 (6%)	24	49
1	K	105/105 (100%)	96 (91%)	9 (9%)	12	26
1	M	105/105 (100%)	99 (94%)	6 (6%)	24	49
1	O	105/105 (100%)	95 (90%)	10 (10%)	10	22
2	B	87/107 (81%)	72 (83%)	15 (17%)	2	5
2	D	87/107 (81%)	83 (95%)	4 (5%)	31	59
2	F	87/107 (81%)	82 (94%)	5 (6%)	24	49
2	H	87/107 (81%)	77 (88%)	10 (12%)	6	14
2	J	87/107 (81%)	77 (88%)	10 (12%)	6	14
2	L	87/107 (81%)	78 (90%)	9 (10%)	8	18
2	N	87/107 (81%)	79 (91%)	8 (9%)	11	23
2	P	87/107 (81%)	74 (85%)	13 (15%)	3	7
All	All	1536/1696 (91%)	1408 (92%)	128 (8%)	13	28

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	ASP
1	A	322	SER

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Mol	Chain	Res	Type
2	B	111	ASP
2	B	114	ARG
2	B	120	LYS
2	B	123	ASP
2	B	131	ASP
2	B	144	SER
2	B	146	ARG
2	B	151	THR
2	B	152	GLU
2	B	154	GLU
2	B	157	THR
2	B	167	SER
2	B	168	CYS
2	B	189	ARG
2	B	190	SER
1	C	270	THR
1	C	272	GLU
1	C	319	THR
1	C	322	SER
1	C	333	SER
1	C	335	VAL
1	C	336	LEU
2	D	110	LYS
2	D	111	ASP
2	D	149	LYS
2	D	189	ARG
1	E	261	GLU
1	E	268	GLN
1	E	283	GLN
1	E	320	SER
1	E	322	SER
1	E	326	ASN
1	E	335	VAL
1	E	336	LEU
2	F	136	ASN
2	F	137	LEU
2	F	157	THR
2	F	167	SER
2	F	189	ARG
1	G	225	SER
1	G	239	VAL
1	G	243	SER

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Mol	Chain	Res	Type
1	G	270	THR
1	G	287	LYS
1	G	335	VAL
2	H	110	LYS
2	H	111	ASP
2	H	114	ARG
2	H	125	LYS
2	H	136	ASN
2	H	144	SER
2	H	150	ASN
2	H	154	GLU
2	H	157	THR
2	H	190	SER
1	I	239	VAL
1	I	243	SER
1	I	270	THR
1	I	283	GLN
1	I	319	THR
1	I	335	VAL
2	J	110	LYS
2	J	111	ASP
2	J	117	ARG
2	J	137	LEU
2	J	143	GLU
2	J	151	THR
2	J	157	THR
2	J	160	HIS
2	J	189	ARG
2	J	190	SER
1	K	223	ASN
1	K	239	VAL
1	K	243	SER
1	K	276	GLN
1	K	287	LYS
1	K	319	THR
1	K	320	SER
1	K	333	SER
1	K	335	VAL
2	L	111	ASP
2	L	117	ARG
2	L	125	LYS
2	L	136	ASN

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Mol	Chain	Res	Type
2	L	157	THR
2	L	165	LEU
2	L	167	SER
2	L	189	ARG
2	L	190	SER
1	M	239	VAL
1	M	268	GLN
1	M	283	GLN
1	M	319	THR
1	M	333	SER
1	M	335	VAL
2	N	110	LYS
2	N	111	ASP
2	N	115	LEU
2	N	125	LYS
2	N	128	SER
2	N	136	ASN
2	N	152	GLU
2	N	189	ARG
1	O	239	VAL
1	O	243	SER
1	O	255	ASN
1	O	270	THR
1	O	280	ASN
1	O	287	LYS
1	O	288	LYS
1	O	321	ASP
1	O	323	GLU
1	O	335	VAL
2	P	105	CYS
2	P	110	LYS
2	P	111	ASP
2	P	115	LEU
2	P	139	GLU
2	P	142	ARG
2	P	144	SER
2	P	151	THR
2	P	157	THR
2	P	161	LEU
2	P	167	SER
2	P	168	CYS
2	P	170	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
1	A	324	ASN
1	A	329	ASN
1	A	332	GLN
2	B	136	ASN
2	B	178	GLN
1	C	252	ASN
1	C	280	ASN
2	D	160	HIS
2	D	178	GLN
1	E	280	ASN
1	E	332	GLN
1	G	273	GLN
1	K	252	ASN
1	K	280	ASN
1	K	332	GLN
2	L	155	ASN
1	M	252	ASN
1	M	280	ASN
1	M	311	GLN
2	N	107	ASN
2	N	178	GLN
1	O	280	ASN
1	O	332	GLN
2	P	136	ASN
2	P	178	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	A	10	-	4,4,4	0.21	0	6,6,6	0.21	0
3	SO4	C	7	-	4,4,4	0.16	0	6,6,6	0.47	0
3	SO4	E	1	-	4,4,4	0.23	0	6,6,6	0.49	0
3	SO4	E	11	-	4,4,4	0.16	0	6,6,6	0.12	0
3	SO4	G	2	-	4,4,4	0.09	0	6,6,6	0.48	0
3	SO4	I	6	-	4,4,4	0.10	0	6,6,6	0.40	0
3	SO4	J	8	-	4,4,4	0.17	0	6,6,6	0.19	0
3	SO4	K	13	-	4,4,4	0.16	0	6,6,6	0.35	0
3	SO4	K	3	-	4,4,4	0.21	0	6,6,6	0.66	0
3	SO4	M	12	-	4,4,4	0.21	0	6,6,6	0.12	0
3	SO4	M	9	-	4,4,4	0.17	0	6,6,6	0.34	0
3	SO4	O	4	-	4,4,4	0.14	0	6,6,6	0.31	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
3	SO4	A	10	-	-	0/0/0/0	0/0/0/0
3	SO4	C	7	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1	-	-	0/0/0/0	0/0/0/0
3	SO4	E	11	-	-	0/0/0/0	0/0/0/0
3	SO4	G	2	-	-	0/0/0/0	0/0/0/0
3	SO4	I	6	-	-	0/0/0/0	0/0/0/0
3	SO4	J	8	-	-	0/0/0/0	0/0/0/0
3	SO4	K	13	-	-	0/0/0/0	0/0/0/0
3	SO4	K	3	-	-	0/0/0/0	0/0/0/0
3	SO4	M	12	-	-	0/0/0/0	0/0/0/0
3	SO4	M	9	-	-	0/0/0/0	0/0/0/0
3	SO4	O	4	-	-	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	13	SO4	2	0
3	M	12	SO4	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	115/115 (100%)	1.05	15 (13%) 4 3	72, 85, 99, 103	0
1	C	115/115 (100%)	1.11	19 (16%) 2 1	72, 85, 99, 103	0
1	E	115/115 (100%)	1.01	15 (13%) 4 3	72, 85, 99, 103	0
1	G	115/115 (100%)	1.25	20 (17%) 2 1	72, 85, 99, 104	0
1	I	115/115 (100%)	1.24	18 (15%) 2 2	72, 85, 99, 104	0
1	K	115/115 (100%)	1.02	15 (13%) 4 3	72, 85, 99, 103	0
1	M	115/115 (100%)	1.10	17 (14%) 3 2	72, 85, 99, 103	0
1	O	115/115 (100%)	1.09	19 (16%) 2 1	72, 85, 99, 103	0
2	B	99/122 (81%)	1.95	31 (31%) 0 0	77, 89, 95, 108	0
2	D	99/122 (81%)	1.27	20 (20%) 1 1	76, 89, 95, 108	0
2	F	99/122 (81%)	1.37	25 (25%) 1 0	76, 89, 95, 108	0
2	H	99/122 (81%)	1.20	17 (17%) 2 1	77, 89, 96, 108	0
2	J	99/122 (81%)	1.18	17 (17%) 2 1	77, 89, 96, 108	0
2	L	99/122 (81%)	1.30	20 (20%) 1 1	76, 89, 95, 108	0
2	N	99/122 (81%)	1.31	21 (21%) 1 1	77, 89, 95, 108	0
2	P	99/122 (81%)	1.95	37 (37%) 0 0	77, 89, 95, 108	0
All	All	1712/1896 (90%)	1.26	326 (19%) 1 1	72, 88, 99, 108	0

All (326) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	129	ILE	12.4
2	B	129	ILE	11.1
2	F	129	ILE	10.3
2	J	129	ILE	8.8
2	N	129	ILE	8.8

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Mol	Chain	Res	Type	RSRZ
2	D	129	ILE	8.4
2	H	129	ILE	8.0
2	L	129	ILE	8.0
2	P	121	VAL	7.3
2	N	190	SER	7.3
2	H	190	SER	7.0
2	B	133	TYR	6.8
2	B	190	SER	6.5
2	D	190	SER	6.4
2	B	121	VAL	6.4
2	B	124	THR	5.9
2	B	131	ASP	5.8
2	P	126	ILE	5.6
2	D	147	ILE	5.4
2	L	148	TRP	5.4
2	B	126	ILE	5.4
2	B	119	LEU	5.4
2	N	147	ILE	5.2
2	B	189	ARG	5.2
2	P	190	SER	5.2
2	P	133	TYR	5.2
2	J	121	VAL	5.2
2	P	119	LEU	5.2
2	N	132	ARG	4.9
2	H	189	ARG	4.9
2	P	131	ASP	4.9
2	L	191	GLY	4.8
2	F	148	TRP	4.7
2	B	122	SER	4.7
2	J	189	ARG	4.5
2	D	191	GLY	4.5
2	N	191	GLY	4.4
2	J	190	SER	4.4
2	P	122	SER	4.4
2	P	189	ARG	4.3
2	D	121	VAL	4.2
2	N	121	VAL	4.2
2	F	190	SER	4.2
2	B	137	LEU	4.2
2	N	148	TRP	4.1
2	P	148	TRP	4.1
2	D	189	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
2	H	121	VAL	4.0
2	P	108	VAL	4.0
2	P	150	ASN	4.0
2	B	108	VAL	4.0
2	L	190	SER	3.9
2	P	135	ARG	3.9
2	L	127	ASP	3.9
2	B	148	TRP	3.9
2	B	109	GLY	3.8
2	P	145	LEU	3.8
2	L	132	ARG	3.8
2	N	119	LEU	3.8
2	B	132	ARG	3.8
1	C	264	ASN	3.7
2	J	124	THR	3.7
2	D	104	ILE	3.7
2	F	165	LEU	3.7
2	F	124	THR	3.7
2	H	124	THR	3.7
1	M	264	ASN	3.7
2	B	112	TRP	3.6
2	F	189	ARG	3.6
2	F	132	ARG	3.6
2	P	153	LYS	3.6
2	B	123	ASP	3.6
2	H	126	ILE	3.6
2	L	147	ILE	3.6
2	P	147	ILE	3.6
2	P	120	LYS	3.6
2	F	191	GLY	3.5
1	I	327	PHE	3.5
1	G	327	PHE	3.5
2	J	132	ARG	3.5
2	L	189	ARG	3.5
2	J	188	ASN	3.5
1	C	224	LEU	3.5
2	B	115	LEU	3.5
2	H	133	TYR	3.4
2	P	132	ARG	3.4
2	L	131	ASP	3.4
2	F	127	ASP	3.4
2	B	117	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	188	ASN	3.4
1	A	306	LEU	3.4
2	L	126	ILE	3.3
2	J	153	LYS	3.3
2	L	124	THR	3.3
1	M	262	ILE	3.3
1	C	268	GLN	3.3
2	N	104	ILE	3.3
1	A	327	PHE	3.3
1	E	262	ILE	3.3
2	B	135	ARG	3.3
1	C	233	ILE	3.2
1	O	331	ILE	3.2
2	D	148	TRP	3.2
2	H	132	ARG	3.2
2	P	140	ARG	3.2
2	D	132	ARG	3.2
2	B	153	LYS	3.2
2	P	112	TRP	3.2
1	A	331	ILE	3.2
2	H	156	ALA	3.2
2	F	155	ASN	3.2
1	A	313	ILE	3.1
2	D	119	LEU	3.1
2	P	188	ASN	3.1
1	E	322	SER	3.1
1	E	313	ILE	3.1
1	E	315	LEU	3.1
2	F	145	LEU	3.1
2	B	140	ARG	3.1
2	F	119	LEU	3.1
1	O	327	PHE	3.0
1	C	237	ALA	3.0
1	M	288	LYS	3.0
2	B	147	ILE	3.0
2	H	161	LEU	3.0
2	L	119	LEU	3.0
1	I	268	GLN	3.0
2	P	124	THR	3.0
1	E	310	ILE	3.0
2	F	126	ILE	3.0
1	O	283	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	121	VAL	3.0
1	M	224	LEU	2.9
1	A	263	LYS	2.9
1	O	313	ILE	2.9
2	J	126	ILE	2.9
2	H	97	LEU	2.9
2	P	137	LEU	2.9
1	E	327	PHE	2.9
1	M	268	GLN	2.9
2	D	99	ALA	2.9
1	A	233	ILE	2.8
2	L	122	SER	2.8
2	N	122	SER	2.8
1	M	336	LEU	2.8
2	P	115	LEU	2.8
2	P	109	GLY	2.8
1	M	250	ARG	2.8
2	F	147	ILE	2.8
2	H	188	ASN	2.8
1	O	251	LYS	2.8
2	D	120	LYS	2.8
1	A	314	ILE	2.8
2	J	131	ASP	2.8
2	L	121	VAL	2.8
1	E	331	ILE	2.8
1	K	233	ILE	2.8
2	P	141	VAL	2.7
1	O	262	ILE	2.7
1	E	237	ALA	2.7
1	K	315	LEU	2.7
2	N	99	ALA	2.7
2	B	105	CYS	2.7
1	O	306	LEU	2.7
2	L	133	TYR	2.7
1	C	262	ILE	2.7
1	K	262	ILE	2.7
1	O	233	ILE	2.7
1	A	227	VAL	2.7
1	G	315	LEU	2.7
2	N	115	LEU	2.7
2	P	123	ASP	2.7
1	E	306	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	291	TYR	2.6
2	J	112	TRP	2.6
2	B	120	LYS	2.6
1	I	240	MET	2.6
2	B	186	LEU	2.6
1	G	237	ALA	2.6
1	M	304	CYS	2.6
1	I	236	ILE	2.6
2	P	114	ARG	2.6
2	D	133	TYR	2.6
2	D	135	ARG	2.6
2	D	108	VAL	2.6
1	O	312	THR	2.5
2	L	155	ASN	2.5
1	G	267	VAL	2.5
2	L	165	LEU	2.5
1	G	233	ILE	2.5
1	K	331	ILE	2.5
1	M	307	ALA	2.5
1	G	306	LEU	2.5
1	O	286	GLY	2.5
2	J	93	GLY	2.5
2	N	103	VAL	2.5
1	A	307	ALA	2.5
1	C	304	CYS	2.5
2	P	105	CYS	2.5
1	O	224	LEU	2.5
2	J	97	LEU	2.5
2	P	158	VAL	2.5
1	I	304	CYS	2.5
1	G	310	ILE	2.5
1	K	327	PHE	2.5
1	K	318	ILE	2.5
1	A	334	LEU	2.5
1	G	240	MET	2.5
1	M	331	ILE	2.4
2	F	122	SER	2.4
2	H	131	ASP	2.4
1	E	307	ALA	2.4
1	K	295	ILE	2.4
1	K	306	LEU	2.4
1	G	334	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	336	LEU	2.4
1	I	233	ILE	2.4
2	F	104	ILE	2.4
1	K	291	TYR	2.4
2	F	133	TYR	2.4
2	F	105	CYS	2.4
1	K	307	ALA	2.4
1	C	228	ASP	2.4
1	G	236	ILE	2.4
1	G	313	ILE	2.4
1	M	266	ASN	2.4
2	D	149	LYS	2.4
1	O	315	LEU	2.4
2	D	188	ASN	2.4
2	F	125	LYS	2.4
1	K	283	GLN	2.3
1	A	315	LEU	2.3
2	B	110	LYS	2.3
2	B	191	GLY	2.3
1	M	233	ILE	2.3
2	N	154	GLU	2.3
2	H	105	CYS	2.3
1	E	233	ILE	2.3
2	N	109	GLY	2.3
1	O	334	LEU	2.3
1	I	237	ALA	2.3
1	M	291	TYR	2.3
1	A	310	ILE	2.3
1	G	262	ILE	2.3
2	P	146	ARG	2.3
1	G	301	ALA	2.3
1	I	291	TYR	2.3
1	O	314	ILE	2.3
2	F	149	LYS	2.3
2	N	120	LYS	2.3
2	P	93	GLY	2.2
1	A	305	THR	2.2
1	I	305	THR	2.2
1	K	313	ILE	2.2
1	O	289	GLU	2.2
2	J	161	LEU	2.2
2	D	127	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	P	186	LEU	2.2
2	J	109	GLY	2.2
2	N	133	TYR	2.2
2	B	155	ASN	2.2
1	I	306	LEU	2.2
1	G	319	THR	2.2
1	C	310	ILE	2.2
1	G	249	VAL	2.2
1	C	315	LEU	2.2
1	I	229	LEU	2.2
2	L	145	LEU	2.2
1	C	307	ALA	2.2
1	C	331	ILE	2.2
1	I	267	VAL	2.2
2	F	117	ARG	2.2
1	O	236	ILE	2.2
1	O	310	ILE	2.2
1	M	315	LEU	2.2
2	L	109	GLY	2.2
1	M	223	ASN	2.1
2	J	133	TYR	2.1
1	C	334	LEU	2.1
1	I	334	LEU	2.1
1	M	314	ILE	2.1
2	N	161	LEU	2.1
2	P	97	LEU	2.1
2	B	101	PHE	2.1
1	I	254	VAL	2.1
1	C	287	LYS	2.1
2	D	113	ARG	2.1
1	C	250	ARG	2.1
1	I	249	VAL	2.1
2	N	189	ARG	2.1
1	O	259	ILE	2.1
1	O	303	LEU	2.1
1	K	237	ALA	2.1
2	H	127	ASP	2.1
1	C	284	LEU	2.1
1	A	262	ILE	2.1
2	J	156	ALA	2.1
1	E	240	MET	2.1
1	G	305	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	234	THR	2.1
2	H	137	LEU	2.1
1	I	262	ILE	2.1
1	I	310	ILE	2.1
2	H	158	VAL	2.1
2	L	178	GLN	2.1
1	E	316	LYS	2.0
2	F	178	GLN	2.0
2	P	172	LEU	2.0
1	G	304	CYS	2.0
1	K	304	CYS	2.0
2	D	115	LEU	2.0
2	P	177	VAL	2.0
1	C	236	ILE	2.0
1	M	310	ILE	2.0
1	C	301	ALA	2.0
2	P	156	ALA	2.0
1	C	336	LEU	2.0
1	E	303	LEU	2.0
1	G	298	LEU	2.0
1	K	303	LEU	2.0
1	E	264	ASN	2.0
2	N	149	LYS	2.0
2	F	109	GLY	2.0
2	N	127	ASP	2.0
1	A	304	CYS	2.0
2	F	186	LEU	2.0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.



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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NA	K	16	1/1	0.95	0.49	11.50	62,62,62,62	0
4	NA	M	17	1/1	0.97	0.39	4.63	64,64,64,64	0
4	NA	P	18	1/1	0.33	0.39	4.03	88,88,88,88	0
4	NA	B	21	1/1	0.70	0.36	3.77	84,84,84,84	0
4	NA	E	14	1/1	0.93	0.44	3.61	63,63,63,63	0
4	NA	A	15	1/1	0.96	0.35	1.96	62,62,62,62	0
4	NA	H	20	1/1	0.78	0.32	0.50	77,77,77,77	0
4	NA	J	19	1/1	0.79	0.29	0.17	76,76,76,76	0
3	SO4	M	12	5/5	0.91	0.22	-0.38	117,117,117,118	0
3	SO4	K	3	5/5	0.95	0.19	-0.87	92,95,97,99	0
3	SO4	I	6	5/5	0.92	0.20	-1.38	91,94,96,97	0
3	SO4	E	1	5/5	0.96	0.15	-1.65	95,96,99,101	0
3	SO4	M	9	5/5	0.87	0.17	-1.67	111,111,114,116	0
3	SO4	K	13	5/5	0.93	0.15	-1.98	109,109,110,110	0
3	SO4	A	10	5/5	0.91	0.16	-	114,114,117,117	0
3	SO4	E	11	5/5	0.85	0.21	-	135,135,135,136	0
3	SO4	J	8	5/5	0.93	0.17	-	127,127,128,128	0
3	SO4	C	7	5/5	0.84	0.24	-	120,120,121,124	0
3	SO4	G	2	5/5	0.89	0.21	-	95,95,97,98	0
3	SO4	O	4	5/5	0.88	0.19	-	116,117,119,120	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.