



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2016 – 07:35 PM EDT

PDB ID : 4MVL  
Title : Crystal structure of an engineered lipocalin (Anticalin H1GA) in complex with the Alzheimer amyloid peptide Abeta1-40  
Authors : Eichinger, A.; Skerra, A.  
Deposited on : 2013-09-24  
Resolution : 2.30 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.

---

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

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027674  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : rb-20027674

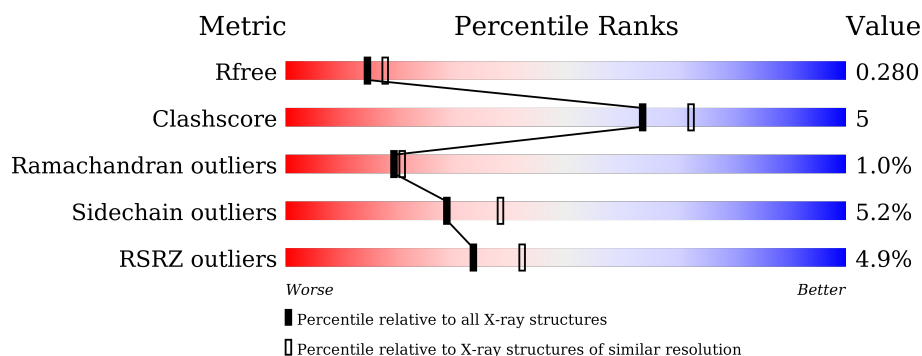
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	188	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	188	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	188	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>•</div> <div>7%</div> </div> </div>
1	D	188	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>••</div> <div>9%</div> </div> </div>
2	E	40	<div> <div></div> <div> <div>28%</div> <div>73%</div> </div> </div>
2	F	40	<div> <div></div> <div> <div>25%</div> <div>•</div> <div>73%</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	G	40	 20% 78%
2	H	40	 23% 78%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5993 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 Neutrophil gelatinase-associated lipocalin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1394	897	234	259	4			
1	B	172	Total	C	N	O	S	0	0	0
			1388	894	233	257	4			
1	C	174	Total	C	N	O	S	0	0	0
			1398	899	235	260	4			
1	D	171	Total	C	N	O	S	0	0	0
			1380	890	232	254	4			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	HIS	GLN	ENGINEERED MUTATION	UNP P80188
A	36	ALA	LEU	ENGINEERED MUTATION	UNP P80188
A	40	VAL	ALA	ENGINEERED MUTATION	UNP P80188
A	41	LEU	ILE	ENGINEERED MUTATION	UNP P80188
A	49	LEU	GLN	ENGINEERED MUTATION	UNP P80188
A	70	GLY	LEU	ENGINEERED MUTATION	UNP P80188
A	72	ASP	ARG	ENGINEERED MUTATION	UNP P80188
A	73	ASP	LYS	ENGINEERED MUTATION	UNP P80188
A	77	LEU	ASP	ENGINEERED MUTATION	UNP P80188
A	79	LYS	TRP	ENGINEERED MUTATION	UNP P80188
A	87	SER	CYS	ENGINEERED MUTATION	UNP P80188
A	96	ARG	ASN	ENGINEERED MUTATION	UNP P80188
A	100	GLU	TYR	ENGINEERED MUTATION	UNP P80188
A	103	GLY	LEU	ENGINEERED MUTATION	UNP P80188
A	106	TRP	TYR	ENGINEERED MUTATION	UNP P80188
A	125	GLU	LYS	ENGINEERED MUTATION	UNP P80188
A	127	ALA	SER	ENGINEERED MUTATION	UNP P80188
A	132	THR	TYR	ENGINEERED MUTATION	UNP P80188
A	134	ASN	LYS	ENGINEERED MUTATION	UNP P80188
A	179	SER	-	EXPRESSION TAG	UNP P80188
A	180	ALA	-	EXPRESSION TAG	UNP P80188

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	TRP	-	EXPRESSION TAG	UNP P80188
A	182	SER	-	EXPRESSION TAG	UNP P80188
A	183	HIS	-	EXPRESSION TAG	UNP P80188
A	184	PRO	-	EXPRESSION TAG	UNP P80188
A	185	GLN	-	EXPRESSION TAG	UNP P80188
A	186	PHE	-	EXPRESSION TAG	UNP P80188
A	187	GLU	-	EXPRESSION TAG	UNP P80188
A	188	LYS	-	EXPRESSION TAG	UNP P80188
B	28	HIS	GLN	ENGINEERED MUTATION	UNP P80188
B	36	ALA	LEU	ENGINEERED MUTATION	UNP P80188
B	40	VAL	ALA	ENGINEERED MUTATION	UNP P80188
B	41	LEU	ILE	ENGINEERED MUTATION	UNP P80188
B	49	LEU	GLN	ENGINEERED MUTATION	UNP P80188
B	70	GLY	LEU	ENGINEERED MUTATION	UNP P80188
B	72	ASP	ARG	ENGINEERED MUTATION	UNP P80188
B	73	ASP	LYS	ENGINEERED MUTATION	UNP P80188
B	77	LEU	ASP	ENGINEERED MUTATION	UNP P80188
B	79	LYS	TRP	ENGINEERED MUTATION	UNP P80188
B	87	SER	CYS	ENGINEERED MUTATION	UNP P80188
B	96	ARG	ASN	ENGINEERED MUTATION	UNP P80188
B	100	GLU	TYR	ENGINEERED MUTATION	UNP P80188
B	103	GLY	LEU	ENGINEERED MUTATION	UNP P80188
B	106	TRP	TYR	ENGINEERED MUTATION	UNP P80188
B	125	GLU	LYS	ENGINEERED MUTATION	UNP P80188
B	127	ALA	SER	ENGINEERED MUTATION	UNP P80188
B	132	THR	TYR	ENGINEERED MUTATION	UNP P80188
B	134	ASN	LYS	ENGINEERED MUTATION	UNP P80188
B	179	SER	-	EXPRESSION TAG	UNP P80188
B	180	ALA	-	EXPRESSION TAG	UNP P80188
B	181	TRP	-	EXPRESSION TAG	UNP P80188
B	182	SER	-	EXPRESSION TAG	UNP P80188
B	183	HIS	-	EXPRESSION TAG	UNP P80188
B	184	PRO	-	EXPRESSION TAG	UNP P80188
B	185	GLN	-	EXPRESSION TAG	UNP P80188
B	186	PHE	-	EXPRESSION TAG	UNP P80188
B	187	GLU	-	EXPRESSION TAG	UNP P80188
B	188	LYS	-	EXPRESSION TAG	UNP P80188
C	28	HIS	GLN	ENGINEERED MUTATION	UNP P80188
C	36	ALA	LEU	ENGINEERED MUTATION	UNP P80188
C	40	VAL	ALA	ENGINEERED MUTATION	UNP P80188
C	41	LEU	ILE	ENGINEERED MUTATION	UNP P80188
C	49	LEU	GLN	ENGINEERED MUTATION	UNP P80188

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	70	GLY	LEU	ENGINEERED MUTATION	UNP P80188
C	72	ASP	ARG	ENGINEERED MUTATION	UNP P80188
C	73	ASP	LYS	ENGINEERED MUTATION	UNP P80188
C	77	LEU	ASP	ENGINEERED MUTATION	UNP P80188
C	79	LYS	TRP	ENGINEERED MUTATION	UNP P80188
C	87	SER	CYS	ENGINEERED MUTATION	UNP P80188
C	96	ARG	ASN	ENGINEERED MUTATION	UNP P80188
C	100	GLU	TYR	ENGINEERED MUTATION	UNP P80188
C	103	GLY	LEU	ENGINEERED MUTATION	UNP P80188
C	106	TRP	TYR	ENGINEERED MUTATION	UNP P80188
C	125	GLU	LYS	ENGINEERED MUTATION	UNP P80188
C	127	ALA	SER	ENGINEERED MUTATION	UNP P80188
C	132	THR	TYR	ENGINEERED MUTATION	UNP P80188
C	134	ASN	LYS	ENGINEERED MUTATION	UNP P80188
C	179	SER	-	EXPRESSION TAG	UNP P80188
C	180	ALA	-	EXPRESSION TAG	UNP P80188
C	181	TRP	-	EXPRESSION TAG	UNP P80188
C	182	SER	-	EXPRESSION TAG	UNP P80188
C	183	HIS	-	EXPRESSION TAG	UNP P80188
C	184	PRO	-	EXPRESSION TAG	UNP P80188
C	185	GLN	-	EXPRESSION TAG	UNP P80188
C	186	PHE	-	EXPRESSION TAG	UNP P80188
C	187	GLU	-	EXPRESSION TAG	UNP P80188
C	188	LYS	-	EXPRESSION TAG	UNP P80188
D	28	HIS	GLN	ENGINEERED MUTATION	UNP P80188
D	36	ALA	LEU	ENGINEERED MUTATION	UNP P80188
D	40	VAL	ALA	ENGINEERED MUTATION	UNP P80188
D	41	LEU	ILE	ENGINEERED MUTATION	UNP P80188
D	49	LEU	GLN	ENGINEERED MUTATION	UNP P80188
D	70	GLY	LEU	ENGINEERED MUTATION	UNP P80188
D	72	ASP	ARG	ENGINEERED MUTATION	UNP P80188
D	73	ASP	LYS	ENGINEERED MUTATION	UNP P80188
D	77	LEU	ASP	ENGINEERED MUTATION	UNP P80188
D	79	LYS	TRP	ENGINEERED MUTATION	UNP P80188
D	87	SER	CYS	ENGINEERED MUTATION	UNP P80188
D	96	ARG	ASN	ENGINEERED MUTATION	UNP P80188
D	100	GLU	TYR	ENGINEERED MUTATION	UNP P80188
D	103	GLY	LEU	ENGINEERED MUTATION	UNP P80188
D	106	TRP	TYR	ENGINEERED MUTATION	UNP P80188
D	125	GLU	LYS	ENGINEERED MUTATION	UNP P80188
D	127	ALA	SER	ENGINEERED MUTATION	UNP P80188
D	132	THR	TYR	ENGINEERED MUTATION	UNP P80188

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	134	ASN	LYS	ENGINEERED MUTATION	UNP P80188
D	179	SER	-	EXPRESSION TAG	UNP P80188
D	180	ALA	-	EXPRESSION TAG	UNP P80188
D	181	TRP	-	EXPRESSION TAG	UNP P80188
D	182	SER	-	EXPRESSION TAG	UNP P80188
D	183	HIS	-	EXPRESSION TAG	UNP P80188
D	184	PRO	-	EXPRESSION TAG	UNP P80188
D	185	GLN	-	EXPRESSION TAG	UNP P80188
D	186	PHE	-	EXPRESSION TAG	UNP P80188
D	187	GLU	-	EXPRESSION TAG	UNP P80188
D	188	LYS	-	EXPRESSION TAG	UNP P80188

- Molecule 2 is a protein called Beta-amyloid protein 40.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	0	0	0
			84	55	12	17			
2	F	11	Total	C	N	O	0	0	0
			84	55	12	17			
2	G	9	Total	C	N	O	0	0	0
			68	45	9	14			
2	H	9	Total	C	N	O	0	0	0
			68	45	9	14			

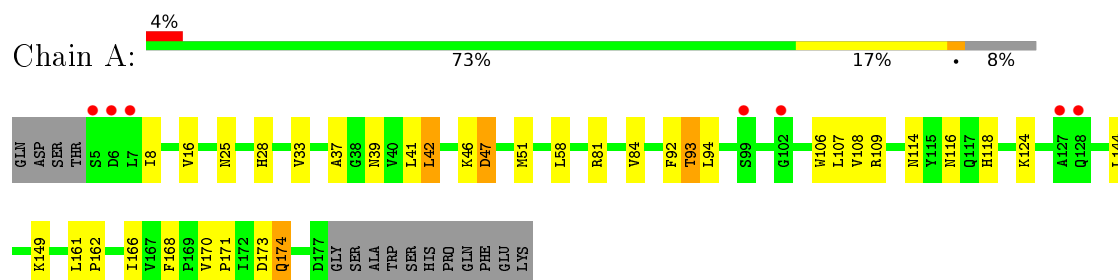
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	26	Total	O	0	0
			26	26		
3	C	28	Total	O	0	0
			28	28		
3	D	34	Total	O	0	0
			34	34		
3	G	1	Total	O	0	0
			1	1		
3	H	7	Total	O	0	0
			7	7		

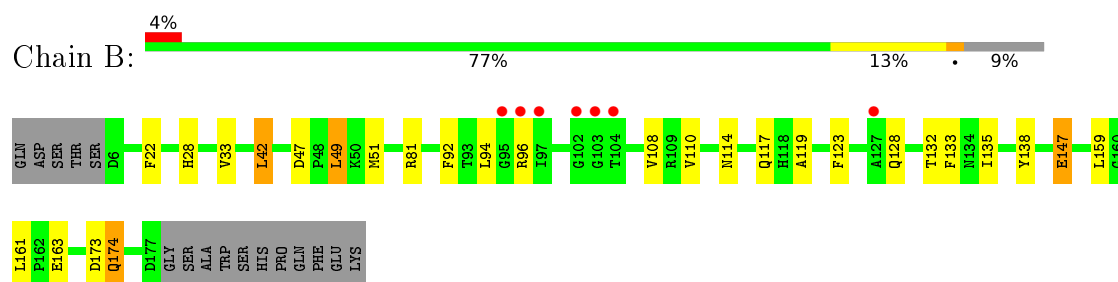
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

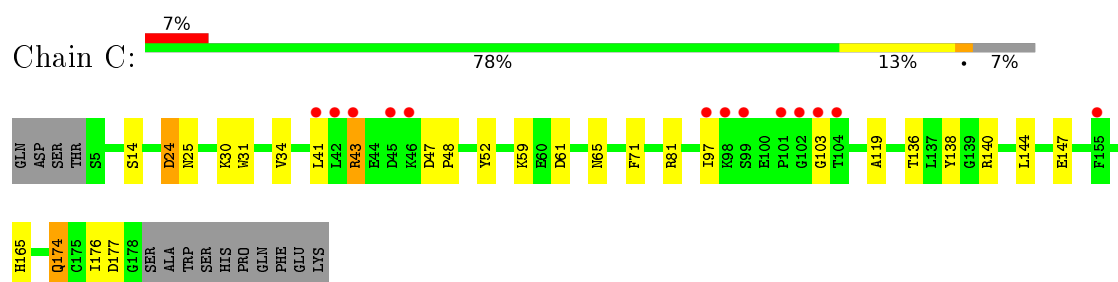
- Molecule 1: Neutrophil gelatinase-associated lipocalin



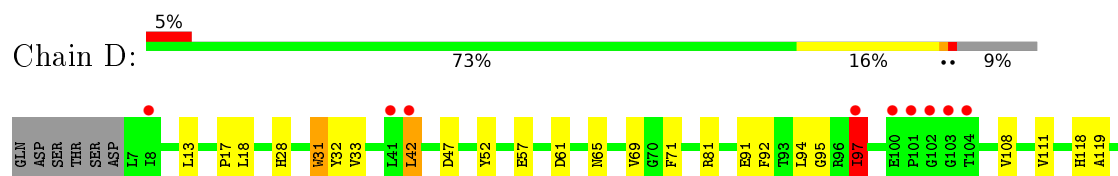
- Molecule 1: Neutrophil gelatinase-associated lipocalin



- Molecule 1: Neutrophil gelatinase-associated lipocalin



- Molecule 1: Neutrophil gelatinase-associated lipocalin







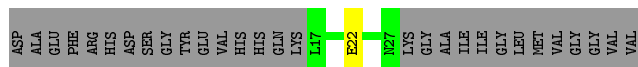
- Molecule 2: Beta-amyloid protein 40

Chain E: 28% 73%



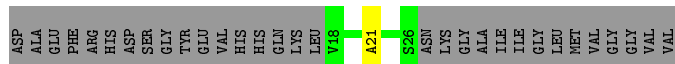
- Molecule 2: Beta-amyloid protein 40

Chain F: 25% 73%



- Molecule 2: Beta-amyloid protein 40

Chain G: 20% 78%



- Molecule 2: Beta-amyloid protein 40

Chain H: 23% 78%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.30Å 79.18Å 142.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.30 – 2.30 39.65 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (71.30-2.30) 97.7 (39.65-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.88 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.219 , 0.279 0.219 , 0.280	Depositor DCC
$R_{free}$ test set	1995 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 13.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.457 for k,h,-l	Xtriage
Reported twinning fraction	0.516 for H, K, L 0.484 for K, H, -L	Depositor
Outliers	0 of 39910 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	5993	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.44	1/1429 (0.1%)	0.53	0/1936
1	B	0.44	0/1423	0.57	0/1928
1	C	0.42	0/1433	0.52	0/1941
1	D	0.44	1/1415 (0.1%)	0.53	0/1917
2	E	0.39	0/85	0.61	0/114
2	F	0.41	0/85	0.59	0/114
2	G	0.44	0/69	0.51	0/92
2	H	0.40	0/69	0.54	0/92
All	All	0.43	2/6008 (0.0%)	0.54	0/8134

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	31	TRP	CD2-CE2	5.16	1.47	1.41
1	A	106	TRP	CD2-CE2	5.04	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1394	0	1382	16	0
1	B	1388	0	1377	15	0
1	C	1398	0	1385	16	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1380	0	1373	15	0
2	E	84	0	75	0	0
2	F	84	0	75	1	0
2	G	68	0	58	1	0
2	H	68	0	58	0	0
3	A	33	0	0	0	0
3	B	26	0	0	1	0
3	C	28	0	0	0	0
3	D	34	0	0	0	0
3	G	1	0	0	0	0
3	H	7	0	0	0	0
All	All	5993	0	5783	61	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 5.

All (61) 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:D:42:LEU:HD21	1:D:167:VAL:HG21	1.72	0.71
1:C:97:ILE:HG21	1:C:103:GLY:HA3	1.76	0.68
1:B:173:ASP:O	1:B:174:GLN:HB2	1.96	0.66
1:B:114:ASN:HD21	1:B:117:GLN:HG2	1.65	0.61
1:D:57:GLU:HB3	1:D:65:ASN:HB3	1.85	0.59
1:A:41:LEU:HG	1:A:42:LEU:H	1.68	0.58
1:D:33:VAL:HG21	1:D:52:TYR:CZ	2.39	0.58
1:B:133:PHE:CE2	1:B:161:LEU:HD11	2.40	0.57
1:B:133:PHE:HE2	1:B:161:LEU:HD11	1.69	0.56
1:B:92:PHE:HB2	1:B:108:VAL:HB	1.86	0.56
1:A:84:VAL:HB	1:A:93:THR:HG22	1.86	0.55
1:A:92:PHE:HB2	1:A:108:VAL:HB	1.89	0.55
1:A:33:VAL:O	1:A:51:MET:HG3	2.09	0.53
1:D:32:TYR:HE1	1:D:176:ILE:HD13	1.75	0.52
1:C:34:VAL:HG11	1:C:144:LEU:HB2	1.92	0.51
1:B:42:LEU:HD13	1:B:49:LEU:HD13	1.91	0.51
1:C:43:ARG:H	1:C:43:ARG:HD2	1.75	0.51
1:C:41:LEU:HB2	1:C:165:HIS:CE1	2.46	0.51
1:B:119:ALA:HB3	1:B:138:TYR:HB2	1.92	0.50
1:A:114:ASN:C	1:A:116:ASN:H	2.14	0.50
1:A:8:ILE:H	1:A:39:ASN:HB2	1.77	0.49
1:D:32:TYR:CE1	1:D:176:ILE:HD13	2.48	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ASP:HB3	1:C:48:PRO:HD3	1.94	0.48
1:D:92:PHE:HB2	1:D:108:VAL:HB	1.95	0.48
1:C:25:ASN:N	1:C:25:ASN:OD1	2.47	0.48
1:B:114:ASN:HD21	1:B:117:GLN:CG	2.27	0.47
1:C:34:VAL:O	1:C:34:VAL:HG12	2.15	0.47
1:D:17:PRO:HG2	1:D:111:VAL:HG13	1.96	0.47
1:D:13:LEU:H	1:D:13:LEU:HD12	1.80	0.46
1:B:147:GLU:HB3	3:B:202:HOH:O	2.15	0.46
1:C:71:PHE:CD1	1:C:174:GLN:HG2	2.51	0.46
1:C:30:LYS:NZ	1:C:177:ASP:HB2	2.30	0.46
1:C:119:ALA:HB3	1:C:138:TYR:HB2	1.98	0.45
1:C:59:LYS:HE2	1:C:65:ASN:HB2	1.99	0.45
1:D:71:PHE:CG	1:D:174:GLN:HG2	2.51	0.45
1:A:107:LEU:HB3	1:A:124:LYS:HB3	1.99	0.44
1:B:132:THR:HG22	1:B:133:PHE:N	2.32	0.44
1:D:52:TYR:HB2	1:D:69:VAL:O	2.17	0.44
1:A:37:ALA:HB2	1:A:166:ILE:HG23	2.00	0.44
1:D:31:TRP:CE3	1:D:138:TYR:HB3	2.52	0.44
1:A:114:ASN:HB2	1:A:118:HIS:H	1.82	0.43
1:C:147:GLU:HG3	1:D:140:ARG:O	2.18	0.43
1:D:95:GLY:O	1:D:97:ILE:HG13	2.18	0.43
1:A:28:HIS:HD2	1:A:58:LEU:H	1.66	0.43
1:B:173:ASP:O	1:B:174:GLN:CB	2.66	0.43
1:B:33:VAL:O	1:B:51:MET:HG3	2.19	0.43
1:C:31:TRP:CZ3	1:C:140:ARG:HG2	2.54	0.42
1:B:135:ILE:HD11	1:B:159:LEU:HD22	2.01	0.42
1:A:149:LYS:HE3	1:A:168:PHE:CE2	2.54	0.42
1:B:22:PHE:CE1	1:B:110:VAL:HG21	2.54	0.42
1:B:123:PHE:CD1	2:F:22:GLU:HA	2.54	0.42
1:D:91:GLU:HA	1:D:108:VAL:O	2.19	0.42
1:A:16:VAL:O	1:A:109:ARG:NH1	2.52	0.42
1:C:136:THR:HG22	2:G:21:ALA:HB1	2.01	0.42
1:A:174:GLN:HB2	1:A:174:GLN:HE21	1.65	0.41
1:A:161:LEU:HA	1:A:162:PRO:HD3	1.86	0.41
1:D:119:ALA:HB3	1:D:138:TYR:HB2	2.01	0.41
1:A:170:VAL:HA	1:A:171:PRO:HD3	1.96	0.41
1:C:34:VAL:CG1	1:C:144:LEU:HB2	2.51	0.41
1:C:52:TYR:HA	1:C:176:ILE:HG21	2.04	0.41
1:A:46:LYS:O	1:A:47:ASP:CB	2.69	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	171/188 (91%)	153 (90%)	17 (10%)	1 (1%)	30	36
1	B	170/188 (90%)	156 (92%)	12 (7%)	2 (1%)	16	16
1	C	172/188 (92%)	157 (91%)	13 (8%)	2 (1%)	16	16
1	D	169/188 (90%)	154 (91%)	13 (8%)	2 (1%)	16	16
2	E	9/40 (22%)	6 (67%)	3 (33%)	0	100	100
2	F	9/40 (22%)	6 (67%)	3 (33%)	0	100	100
2	G	7/40 (18%)	5 (71%)	2 (29%)	0	100	100
2	H	7/40 (18%)	5 (71%)	2 (29%)	0	100	100
All	All	714/912 (78%)	642 (90%)	65 (9%)	7 (1%)	19	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	D	97	ILE
1	C	174	GLN
1	D	128	GLN
1	B	128	GLN
1	B	174	GLN
1	C	24	ASP

### 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	156/169 (92%)	148 (95%)	8 (5%)	29	39
1	B	155/169 (92%)	146 (94%)	9 (6%)	25	33
1	C	156/169 (92%)	151 (97%)	5 (3%)	46	62
1	D	154/169 (91%)	142 (92%)	12 (8%)	16	19
2	E	9/31 (29%)	9 (100%)	0	100	100
2	F	9/31 (29%)	9 (100%)	0	100	100
2	G	7/31 (23%)	7 (100%)	0	100	100
2	H	7/31 (23%)	7 (100%)	0	100	100
All	All	653/800 (82%)	619 (95%)	34 (5%)	29	38

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	42	LEU
1	A	81	ARG
1	A	93	THR
1	A	94	LEU
1	A	144	LEU
1	A	173	ASP
1	A	174	GLN
1	B	28	HIS
1	B	42	LEU
1	B	47	ASP
1	B	49	LEU
1	B	81	ARG
1	B	94	LEU
1	B	96	ARG
1	B	147	GLU
1	B	163	GLU
1	C	14	SER
1	C	24	ASP
1	C	43	ARG
1	C	61	ASP
1	C	81	ARG
1	D	18	LEU
1	D	28	HIS
1	D	42	LEU
1	D	47	ASP
1	D	61	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	81	ARG
1	D	94	LEU
1	D	97	ILE
1	D	118	HIS
1	D	126	VAL
1	D	154	ARG
1	D	172	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	116	ASN
1	A	174	GLN
1	C	88	GLN
1	D	26	GLN

### 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 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 ⓘ

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	173/188 (92%)	0.01	7 (4%)	42	51	15, 20, 43, 51	0
1	B	172/188 (91%)	0.12	7 (4%)	41	50	15, 24, 52, 67	0
1	C	174/188 (92%)	0.30	13 (7%)	17	24	17, 26, 52, 59	0
1	D	171/188 (90%)	0.09	9 (5%)	30	39	16, 23, 51, 61	0
2	E	11/40 (27%)	-0.15	0	100	100	18, 19, 25, 29	0
2	F	11/40 (27%)	0.05	0	100	100	23, 25, 37, 40	0
2	G	9/40 (22%)	-0.00	0	100	100	27, 28, 34, 34	0
2	H	9/40 (22%)	-0.31	0	100	100	20, 21, 22, 22	0
All	All	730/912 (80%)	0.12	36 (4%)	33	42	15, 23, 51, 67	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	42	LEU	6.7
1	A	99	SER	6.5
1	D	97	ILE	5.2
1	D	101	PRO	5.0
1	C	103	GLY	4.9
1	B	103	GLY	4.8
1	D	103	GLY	4.8
1	C	98	LYS	4.8
1	B	102	GLY	4.2
1	C	97	ILE	4.2
1	C	102	GLY	4.2
1	D	102	GLY	4.1
1	B	95	GLY	4.1
1	C	41	LEU	3.6
1	D	42	LEU	3.6
1	B	127	ALA	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	96	ARG	3.3
1	A	5	SER	3.0
1	A	128	GLN	3.0
1	C	99	SER	3.0
1	B	97	ILE	2.8
1	C	104	THR	2.7
1	C	46	LYS	2.7
1	C	43	ARG	2.6
1	D	104	THR	2.6
1	D	41	LEU	2.6
1	B	104	THR	2.6
1	A	102	GLY	2.4
1	D	100	GLU	2.2
1	C	155	PHE	2.2
1	C	101	PRO	2.2
1	A	7	LEU	2.1
1	D	8	ILE	2.1
1	A	6	ASP	2.0
1	C	45	ASP	2.0
1	A	127	ALA	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.