



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:08 PM GMT

PDB ID : 1NMP  
Title : Structural genomics, ybgI protein, unknown function  
Authors : Ladner, J.E.; Obmolova, G.; Teplyakov, A.; Khil, P.P.; Camerini-Otero, R.D.;  
Gilliland, G.L.; Structure 2 Function Project (S2F)  
Deposited on : 2003-01-10  
Resolution : 2.20 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

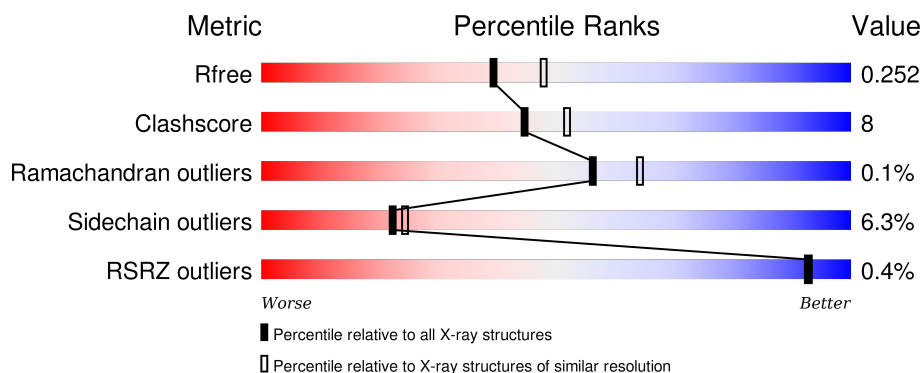
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	247	<div> <div></div> <div>77% 21% .</div> </div>
1	B	247	<div> <div></div> <div>75% 21% ..</div> </div>
1	C	247	<div> <div></div> <div>78% 19% .</div> </div>
1	D	247	<div> <div></div> <div>80% 18% .</div> </div>
1	E	247	<div> <div></div> <div>82% 15% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	247	

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	MG	A	301	-	-	-	X
2	MG	A	302	-	-	-	X
2	MG	B	302	-	-	-	X
2	MG	C	301	-	-	-	X
2	MG	C	302	-	-	-	X
2	MG	D	301	-	-	-	X
2	MG	E	301	-	-	-	X
2	MG	E	302	-	-	-	X
2	MG	F	301	-	-	-	X
2	MG	F	302	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11969 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 Hypothetical protein ybgI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1897	1200	332	359	6			
1	B	247	Total	C	N	O	S	0	0	0
			1897	1200	332	359	6			
1	C	247	Total	C	N	O	S	0	0	0
			1897	1200	332	359	6			
1	D	247	Total	C	N	O	S	0	0	0
			1897	1200	332	359	6			
1	E	247	Total	C	N	O	S	0	0	0
			1897	1200	332	359	6			
1	F	247	Total	C	N	O	S	0	0	0
			1897	1200	332	359	6			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Mg	0	0
			2	2		
2	E	2	Total	Mg	0	0
			2	2		
2	B	1	Total	Mg	0	0
			1	1		
2	C	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		
2	F	2	Total	Mg	0	0
			2	2		

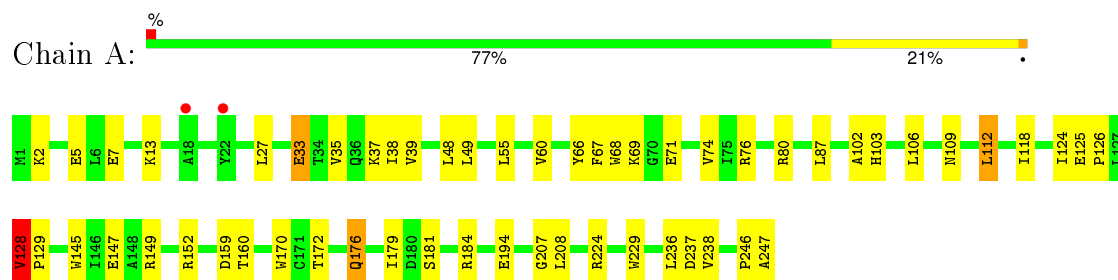
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	78	Total 78	O 78	0	0
3	B	79	Total 79	O 79	0	0
3	C	95	Total 95	O 95	0	0
3	D	87	Total 87	O 87	0	0
3	E	124	Total 124	O 124	0	0
3	F	113	Total 113	O 113	0	0

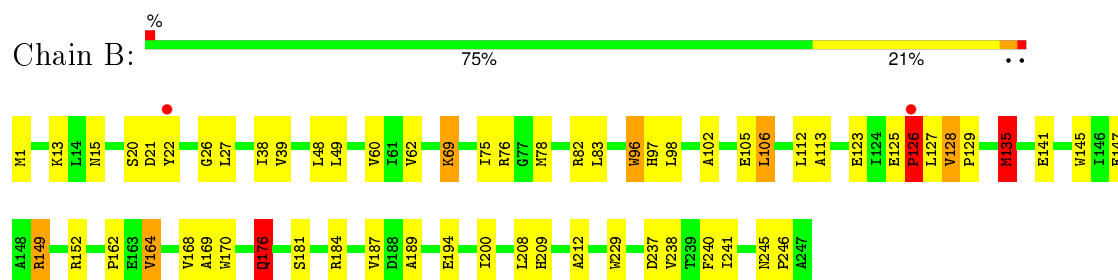
### 3 Residue-property plots

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.

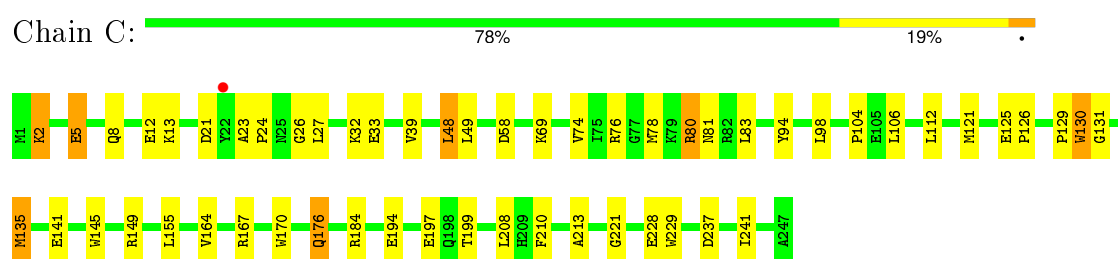
- Molecule 1: Hypothetical protein ybgl



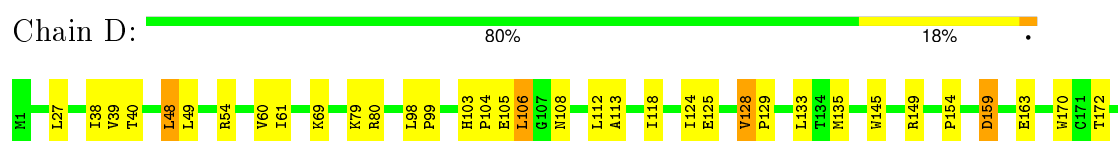
- Molecule 1: Hypothetical protein ybgl



- Molecule 1: Hypothetical protein ybgl



- Molecule 1: Hypothetical protein ybgl





- Molecule 1: Hypothetical protein ybgI

Chain E: 82% 15% •



- Molecule 1: Hypothetical protein ybgI

Chain F: 81% 16% •



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.73 Å   156.73 Å   57.61 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	19.76 – 2.20 19.76 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.9 (19.76-2.20) 85.8 (19.76-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 2.01 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.212 , 0.253 0.212 , 0.252	Depositor DCC
$R_{free}$ test set	3845 reflections (4.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.7	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.7	EDS
Estimated twinning fraction	0.019 for -h,-k,l 0.033 for h,-h-k,-l 0.009 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 141876 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11969	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.02% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	1.24	2/1940 (0.1%)	1.07	6/2641 (0.2%)
1	B	1.27	4/1940 (0.2%)	1.07	4/2641 (0.2%)
1	C	1.16	3/1940 (0.2%)	1.05	1/2641 (0.0%)
1	D	1.15	2/1940 (0.1%)	1.09	8/2641 (0.3%)
1	E	1.16	2/1940 (0.1%)	1.09	9/2641 (0.3%)
1	F	1.17	8/1940 (0.4%)	1.11	3/2641 (0.1%)
All	All	1.19	21/11640 (0.2%)	1.08	31/15846 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	1
All	All	0	2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	128	VAL	CB-CG1	-7.74	1.36	1.52
1	D	128	VAL	CB-CG2	-7.21	1.37	1.52
1	E	228	GLU	CG-CD	6.61	1.61	1.51
1	C	135	MET	SD-CE	6.34	2.13	1.77
1	F	80	ARG	CZ-NH2	6.29	1.41	1.33
1	B	128	VAL	CB-CG1	-6.12	1.40	1.52
1	A	128	VAL	CA-CB	5.98	1.67	1.54
1	B	135	MET	SD-CE	5.93	2.11	1.77
1	F	135	MET	SD-CE	5.87	2.10	1.77
1	B	126	PRO	C-O	5.55	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	213	ALA	CA-CB	5.52	1.64	1.52
1	B	62	VAL	CA-CB	5.51	1.66	1.54
1	F	132	GLU	CG-CD	5.31	1.59	1.51
1	C	228	GLU	CG-CD	5.26	1.59	1.51
1	A	7	GLU	CB-CG	5.20	1.62	1.52
1	D	232	GLU	CG-CD	5.14	1.59	1.51
1	E	232	GLU	CG-CD	5.13	1.59	1.51
1	F	66	TYR	CD2-CE2	5.12	1.47	1.39
1	F	141	GLU	CD-OE1	5.11	1.31	1.25
1	F	176	GLN	CB-CG	-5.10	1.38	1.52
1	F	141	GLU	CD-OE2	5.10	1.31	1.25

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	224	ARG	NE-CZ-NH2	-9.25	115.68	120.30
1	E	224	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	224	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	D	106	LEU	CA-CB-CG	6.45	130.13	115.30
1	D	176	GLN	CB-CA-C	-6.23	97.94	110.40
1	B	212	ALA	N-CA-C	-6.23	94.18	111.00
1	A	80	ARG	NE-CZ-NH1	-6.21	117.20	120.30
1	F	48	LEU	CA-CB-CG	5.99	129.07	115.30
1	D	54	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	80	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	D	224	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	112	LEU	CA-CB-CG	5.68	128.35	115.30
1	A	224	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	D	212	ALA	N-CA-C	-5.55	96.03	111.00
1	B	176	GLN	CB-CA-C	-5.47	99.45	110.40
1	E	133	LEU	CB-CG-CD2	-5.46	101.71	111.00
1	F	167	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	48	LEU	CA-CB-CG	5.44	127.82	115.30
1	E	237	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	204	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	E	220	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	B	237	ASP	CB-CG-OD2	5.29	123.06	118.30
1	E	149	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	D	184	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	E	152	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	C	48	LEU	CA-CB-CG	5.08	126.98	115.30
1	E	76	ARG	NE-CZ-NH2	-5.07	117.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	ALA	N-CA-C	5.04	124.61	111.00
1	A	33	GLU	OE1-CD-OE2	5.04	129.34	123.30
1	E	102	ALA	N-CA-C	5.01	124.54	111.00
1	E	80	ARG	NE-CZ-NH1	-5.01	117.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	22	TYR	Sidechain
1	E	22	TYR	Sidechain

## 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	1897	0	1866	40	0
1	B	1897	0	1866	40	0
1	C	1897	0	1866	36	0
1	D	1897	0	1866	24	0
1	E	1897	0	1866	20	0
1	F	1897	0	1866	28	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	78	0	0	2	0
3	B	79	0	0	1	0
3	C	95	0	0	2	0
3	D	87	0	0	0	0
3	E	124	0	0	0	0
3	F	113	0	0	3	0
All	All	11969	0	11196	178	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 8.

All (178) 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:B:1:MET:CE	1:B:1:MET:SD	2.01	1.49
1:E:135:MET:SD	1:E:135:MET:CE	2.01	1.47
1:D:135:MET:CE	1:D:135:MET:SD	2.03	1.47
1:C:121:MET:CE	1:C:121:MET:SD	2.04	1.44
1:B:135:MET:SD	1:B:135:MET:CE	2.11	1.39
1:F:135:MET:SD	1:F:135:MET:CE	2.10	1.39
1:C:135:MET:CE	1:C:135:MET:SD	2.13	1.36
1:E:246:PRO:HD2	1:F:200:ILE:HG12	1.59	0.83
1:D:128:VAL:O	1:D:128:VAL:HG23	1.78	0.80
1:A:37:LYS:HG3	1:A:237:ASP:OD2	1.83	0.77
1:A:2:LYS:HB2	1:A:2:LYS:NZ	2.02	0.75
1:C:74:VAL:HG12	1:C:76:ARG:HG3	1.69	0.73
1:C:39:VAL:HG13	1:C:241:ILE:HD12	1.70	0.73
1:F:125:GLU:HG3	1:F:128:VAL:HG11	1.72	0.71
1:F:130:TRP:CD1	1:F:131:GLY:N	2.59	0.71
1:F:125:GLU:HG3	1:F:128:VAL:CG1	2.21	0.70
1:C:145:TRP:O	1:C:149:ARG:HG2	1.92	0.69
1:A:38:ILE:HD11	1:A:236:LEU:HD22	1.77	0.66
1:C:8:GLN:O	1:C:12:GLU:HG3	1.95	0.66
1:C:130:TRP:CD1	1:C:131:GLY:N	2.64	0.66
1:A:184:ARG:HH22	1:B:76:ARG:NE	1.95	0.65
1:A:39:VAL:O	1:A:60:VAL:HA	1.98	0.64
1:A:125:GLU:HB2	1:A:128:VAL:HG13	1.80	0.62
1:C:176:GLN:HG3	1:C:194:GLU:O	2.00	0.62
1:B:13:LYS:HE2	1:B:229:TRP:CE2	2.35	0.61
1:B:75:ILE:HD12	1:B:83:LEU:CD1	2.30	0.61
1:A:2:LYS:HB2	1:A:2:LYS:HZ2	1.63	0.61
1:B:75:ILE:HD12	1:B:83:LEU:HD12	1.80	0.61
1:F:129:PRO:HD2	1:F:170:TRP:O	2.02	0.59
1:A:74:VAL:HG12	1:A:76:ARG:HG3	1.84	0.59
1:C:74:VAL:CG1	1:C:76:ARG:HG3	2.33	0.59
1:D:124:ILE:HB	1:D:128:VAL:HG23	1.84	0.58
1:D:240:PHE:C	1:D:241:ILE:HD12	2.24	0.58
1:B:189:ALA:HA	1:B:209:HIS:O	2.05	0.57
1:B:75:ILE:CD1	1:B:83:LEU:HD12	2.34	0.57
1:A:38:ILE:CD1	1:A:236:LEU:HD22	2.34	0.56
1:E:168:VAL:HG22	1:E:189:ALA:HB3	1.86	0.56
1:F:113:ALA:HB2	1:F:170:TRP:CZ2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:GLN:HG3	1:B:194:GLU:O	2.05	0.56
1:E:76:ARG:HB2	1:F:184:ARG:HH12	1.71	0.56
1:D:125:GLU:HB2	1:D:128:VAL:HG22	1.88	0.56
1:A:87:LEU:HA	3:A:322:HOH:O	2.06	0.56
1:F:126:PRO:HB2	3:F:327:HOH:O	2.05	0.56
1:E:138:PRO:HB2	1:E:141:GLU:OE1	2.06	0.56
1:A:160:THR:OG1	1:A:207:GLY:HA2	2.07	0.55
1:A:124:ILE:HB	1:A:128:VAL:HG22	1.89	0.55
1:B:13:LYS:HE2	1:B:229:TRP:CZ2	2.42	0.55
1:B:145:TRP:O	1:B:149:ARG:HG2	2.06	0.55
1:C:121:MET:CE	1:C:121:MET:CG	2.84	0.55
1:E:125:GLU:HB2	1:E:128:VAL:HG13	1.89	0.55
1:A:208:LEU:HD12	1:A:208:LEU:C	2.28	0.55
1:F:169:ALA:HB2	1:F:187:VAL:HG11	1.89	0.54
1:F:224:ARG:HD3	3:F:354:HOH:O	2.08	0.54
1:C:32:LYS:HD2	1:C:58:ASP:HB3	1.90	0.54
1:D:145:TRP:O	1:D:149:ARG:HG2	2.08	0.53
1:E:130:TRP:CD1	1:E:131:GLY:N	2.75	0.53
1:D:242:ASP:O	1:D:244:PRO:HD3	2.09	0.53
1:E:74:VAL:HG12	1:E:76:ARG:HG3	1.91	0.53
1:B:39:VAL:O	1:B:60:VAL:HA	2.09	0.52
1:E:176:GLN:HG3	1:E:194:GLU:O	2.10	0.52
1:D:98:LEU:HB2	1:D:99:PRO:HD3	1.92	0.52
1:A:184:ARG:NH2	1:B:76:ARG:NE	2.57	0.52
1:C:237:ASP:C	1:C:237:ASP:OD1	2.49	0.51
1:C:13:LYS:HD3	1:C:229:TRP:CZ2	2.45	0.51
1:D:118:ILE:HG12	1:D:133:LEU:HD23	1.92	0.51
1:A:176:GLN:HG3	1:A:194:GLU:O	2.10	0.51
1:D:38:ILE:HB	1:D:238:VAL:HG13	1.92	0.51
1:D:129:PRO:HD2	1:D:170:TRP:O	2.10	0.51
1:F:147:GLU:HB2	1:F:154:PRO:HD2	1.93	0.51
1:D:195:VAL:HG22	1:D:196:SER:N	2.25	0.51
1:D:128:VAL:CG2	1:D:128:VAL:O	2.51	0.51
1:A:37:LYS:HD3	1:A:55:LEU:O	2.11	0.50
1:A:2:LYS:HG3	1:A:33:GLU:HG2	1.93	0.50
1:A:87:LEU:HD23	3:A:322:HOH:O	2.11	0.50
1:E:176:GLN:HG2	1:E:195:VAL:HA	1.93	0.50
1:A:184:ARG:NH2	1:B:76:ARG:HE	2.10	0.49
1:A:68:TRP:O	1:A:71:GLU:HB3	2.12	0.49
1:F:106:LEU:HD22	1:F:106:LEU:N	2.27	0.49
1:B:21:ASP:OD2	1:B:97:HIS:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:VAL:O	1:A:128:VAL:HG22	2.13	0.49
1:D:113:ALA:HB2	1:D:170:TRP:CZ2	2.48	0.49
1:D:103:HIS:CE1	1:D:105:GLU:HB3	2.48	0.49
1:C:39:VAL:CG1	1:C:241:ILE:HD12	2.39	0.49
1:A:129:PRO:HD2	1:A:170:TRP:O	2.12	0.49
1:E:124:ILE:HB	1:E:128:VAL:HG22	1.93	0.49
1:A:145:TRP:O	1:A:149:ARG:HG2	2.14	0.48
1:A:118:ILE:HG21	1:A:170:TRP:CZ3	2.48	0.48
1:C:199:THR:HG21	1:C:210:PHE:CZ	2.48	0.48
1:C:221:GLY:HA3	3:C:320:HOH:O	2.12	0.48
1:B:125:GLU:HB3	1:B:126:PRO:HD2	1.95	0.48
1:B:69:LYS:HA	1:B:69:LYS:HD3	1.61	0.48
1:A:35:VAL:HG12	1:A:38:ILE:HD11	1.96	0.48
1:C:129:PRO:HD2	1:C:170:TRP:O	2.14	0.48
1:B:78:MET:O	1:B:82:ARG:HG3	2.13	0.48
1:A:109:ASN:OD1	1:A:172:THR:HG23	2.13	0.48
1:B:26:GLY:HA2	1:B:96:TRP:CZ2	2.49	0.47
1:C:208:LEU:H	1:C:208:LEU:HD23	1.79	0.47
1:C:2:LYS:HG2	1:C:33:GLU:HG2	1.97	0.47
1:F:176:GLN:H	1:F:176:GLN:CD	2.17	0.47
1:F:176:GLN:HG2	1:F:195:VAL:HA	1.96	0.47
1:A:147:GLU:HA	1:A:152:ARG:O	2.15	0.46
1:A:179:ILE:HD11	1:A:208:LEU:HD11	1.97	0.46
1:F:66:TYR:O	1:F:67:PHE:HB2	2.16	0.46
1:C:130:TRP:C	1:C:130:TRP:CD1	2.89	0.46
1:A:129:PRO:HB2	1:A:170:TRP:CZ2	2.51	0.46
1:F:195:VAL:HG22	1:F:196:SER:N	2.29	0.46
1:A:66:TYR:O	1:A:67:PHE:HB2	2.16	0.46
1:D:124:ILE:HB	1:D:128:VAL:CG2	2.46	0.46
1:E:2:LYS:O	1:E:5:GLU:HB2	2.15	0.46
1:B:38:ILE:HB	1:B:238:VAL:HG22	1.98	0.46
1:B:129:PRO:HD2	1:B:170:TRP:O	2.17	0.45
1:A:106:LEU:HD22	1:A:106:LEU:N	2.31	0.45
1:C:26:GLY:O	1:C:94:TYR:HA	2.16	0.45
1:D:39:VAL:O	1:D:60:VAL:HA	2.16	0.45
1:A:128:VAL:CG2	1:A:128:VAL:O	2.65	0.45
1:B:168:VAL:HG12	1:B:169:ALA:N	2.32	0.45
1:C:2:LYS:O	1:C:5:GLU:N	2.50	0.45
1:E:69:LYS:HA	1:E:69:LYS:HD3	1.76	0.45
1:A:247:ALA:HB2	1:B:200:ILE:HD13	1.98	0.45
1:F:130:TRP:CD1	1:F:130:TRP:C	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ARG:HG3	1:C:81:ASN:N	2.31	0.44
1:D:79:LYS:HB3	1:D:79:LYS:HE3	1.86	0.44
1:F:39:VAL:O	1:F:60:VAL:HA	2.18	0.44
1:A:38:ILE:HB	1:A:238:VAL:HG22	2.00	0.44
1:A:128:VAL:HA	1:A:129:PRO:HD3	1.77	0.44
1:B:240:PHE:C	1:B:241:ILE:HD13	2.38	0.44
1:B:75:ILE:HD11	1:B:83:LEU:HB2	1.99	0.44
1:B:125:GLU:OE2	1:B:181:SER:OG	2.22	0.44
1:D:40:THR:HG22	1:D:61:ILE:HB	2.00	0.43
1:B:147:GLU:HA	1:B:152:ARG:O	2.18	0.43
1:B:162:PRO:HD2	1:B:209:HIS:CD2	2.53	0.43
1:D:159:ASP:OD1	1:D:159:ASP:N	2.51	0.43
1:D:103:HIS:HA	1:D:104:PRO:HD3	1.83	0.43
1:C:167:ARG:HB2	1:C:167:ARG:HE	1.66	0.43
1:C:197:GLU:HB2	1:D:215:HIS:CG	2.53	0.43
1:B:1:MET:CE	1:B:1:MET:CG	2.94	0.43
1:C:78:MET:HE2	1:C:78:MET:HB3	1.90	0.43
1:D:80:ARG:O	1:D:80:ARG:HG2	2.18	0.43
1:B:245:ASN:HA	1:B:246:PRO:HD3	1.82	0.43
1:C:32:LYS:NZ	3:C:391:HOH:O	2.52	0.43
1:E:39:VAL:O	1:E:60:VAL:HA	2.17	0.43
1:B:169:ALA:HB2	1:B:187:VAL:HG11	2.00	0.43
1:A:246:PRO:HD2	1:B:200:ILE:HG12	2.00	0.43
1:F:127:LEU:N	3:F:327:HOH:O	2.05	0.43
1:C:208:LEU:HD23	1:C:208:LEU:N	2.33	0.43
1:A:13:LYS:HD3	1:A:229:TRP:CZ2	2.54	0.42
1:F:168:VAL:HG12	1:F:169:ALA:N	2.33	0.42
1:C:21:ASP:OD1	1:C:98:LEU:HG	2.19	0.42
1:B:123:GLU:O	1:B:123:GLU:HG3	2.20	0.42
1:B:241:ILE:HD13	1:B:241:ILE:N	2.33	0.42
1:B:145:TRP:O	1:B:149:ARG:CG	2.68	0.42
1:C:23:ALA:HB1	1:C:24:PRO:CD	2.50	0.42
1:A:2:LYS:HB2	1:A:2:LYS:HZ3	1.79	0.42
1:F:171:CYS:O	1:F:192:THR:HA	2.19	0.42
1:A:2:LYS:NZ	1:A:2:LYS:CB	2.75	0.42
1:F:40:THR:OG1	1:F:240:PHE:HA	2.19	0.42
1:F:72:SER:HA	1:F:73:PRO:HD3	1.87	0.42
1:C:141:GLU:HG3	1:E:135:MET:SD	2.60	0.41
1:E:76:ARG:HB2	1:F:184:ARG:NH1	2.33	0.41
1:B:164:VAL:HG13	3:B:323:HOH:O	2.19	0.41
1:B:113:ALA:HB2	1:B:170:TRP:CZ2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:LEU:HD22	1:C:106:LEU:N	2.36	0.41
1:E:113:ALA:HB2	1:E:170:TRP:CZ2	2.56	0.41
1:F:189:ALA:HA	1:F:209:HIS:O	2.21	0.41
1:C:164:VAL:HG13	1:C:164:VAL:O	2.20	0.41
1:B:105:GLU:HG2	1:B:106:LEU:HD13	2.02	0.41
1:D:108:ASN:HB3	1:D:172:THR:HG21	2.02	0.41
1:A:102:ALA:O	1:A:103:HIS:C	2.59	0.41
1:E:168:VAL:HG12	1:E:169:ALA:N	2.35	0.41
1:B:98:LEU:HD22	1:B:127:LEU:HD11	2.03	0.41
1:C:125:GLU:HB3	1:C:126:PRO:HD2	2.02	0.41
1:E:147:GLU:HA	1:E:152:ARG:O	2.21	0.41
1:E:149:ARG:HA	1:E:149:ARG:HD2	1.67	0.40
1:F:173:GLY:HA2	1:F:215:HIS:CD2	2.55	0.40
1:F:192:THR:HG23	1:F:193:GLY:N	2.36	0.40
1:B:128:VAL:HG22	1:B:128:VAL:O	2.22	0.40
1:C:129:PRO:HB2	1:C:170:TRP:CZ2	2.56	0.40
1:C:83:LEU:HD23	1:C:83:LEU:HA	1.85	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	245/247 (99%)	231 (94%)	14 (6%)	0	100	100
1	B	245/247 (99%)	236 (96%)	8 (3%)	1 (0%)	39	42
1	C	245/247 (99%)	237 (97%)	8 (3%)	0	100	100
1	D	245/247 (99%)	238 (97%)	7 (3%)	0	100	100
1	E	245/247 (99%)	236 (96%)	9 (4%)	0	100	100
1	F	245/247 (99%)	233 (95%)	11 (4%)	1 (0%)	39	42
All	All	1470/1482 (99%)	1411 (96%)	57 (4%)	2 (0%)	56	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	159	ASP
1	B	126	PRO

### 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	197/197 (100%)	186 (94%)	11 (6%)	26	29
1	B	197/197 (100%)	180 (91%)	17 (9%)	13	12
1	C	197/197 (100%)	184 (93%)	13 (7%)	21	22
1	D	197/197 (100%)	186 (94%)	11 (6%)	26	29
1	E	197/197 (100%)	184 (93%)	13 (7%)	21	22
1	F	197/197 (100%)	187 (95%)	10 (5%)	29	34
All	All	1182/1182 (100%)	1107 (94%)	75 (6%)	22	24

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	27	LEU
1	A	48	LEU
1	A	49	LEU
1	A	69	LYS
1	A	112	LEU
1	A	126	PRO
1	A	128	VAL
1	A	159	ASP
1	A	176	GLN
1	A	181	SER
1	B	15	ASN
1	B	20	SER
1	B	27	LEU
1	B	48	LEU

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Mol	Chain	Res	Type
1	B	49	LEU
1	B	69	LYS
1	B	96	TRP
1	B	106	LEU
1	B	112	LEU
1	B	126	PRO
1	B	135	MET
1	B	141	GLU
1	B	149	ARG
1	B	164	VAL
1	B	176	GLN
1	B	184	ARG
1	B	208	LEU
1	C	2	LYS
1	C	5	GLU
1	C	27	LEU
1	C	48	LEU
1	C	49	LEU
1	C	69	LYS
1	C	80	ARG
1	C	104	PRO
1	C	112	LEU
1	C	130	TRP
1	C	155	LEU
1	C	176	GLN
1	C	184	ARG
1	D	27	LEU
1	D	48	LEU
1	D	49	LEU
1	D	69	LYS
1	D	106	LEU
1	D	112	LEU
1	D	154	PRO
1	D	159	ASP
1	D	163	GLU
1	D	176	GLN
1	D	208	LEU
1	E	20	SER
1	E	27	LEU
1	E	34	THR
1	E	39	VAL
1	E	48	LEU

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Mol	Chain	Res	Type
1	E	49	LEU
1	E	69	LYS
1	E	112	LEU
1	E	126	PRO
1	E	128	VAL
1	E	130	TRP
1	E	176	GLN
1	E	208	LEU
1	F	27	LEU
1	F	48	LEU
1	F	49	LEU
1	F	69	LYS
1	F	80	ARG
1	F	112	LEU
1	F	125	GLU
1	F	126	PRO
1	F	130	TRP
1	F	176	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	166	GLN
1	B	36	GLN
1	B	166	GLN
1	C	36	GLN
1	C	166	GLN
1	D	36	GLN
1	D	206	GLN
1	E	36	GLN
1	E	166	GLN
1	E	233	ASN
1	F	166	GLN

### 5.3.3 RNA ⓘ

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](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	247/247 (100%)	-0.40	2 (0%) 87 87	7, 14, 23, 29	0
1	B	247/247 (100%)	-0.39	2 (0%) 87 87	7, 14, 24, 28	0
1	C	247/247 (100%)	-0.55	1 (0%) 93 93	5, 12, 22, 28	0
1	D	247/247 (100%)	-0.52	0 100 100	5, 12, 23, 27	0
1	E	247/247 (100%)	-0.57	1 (0%) 93 93	4, 11, 21, 28	0
1	F	247/247 (100%)	-0.63	0 100 100	5, 11, 20, 26	0
All	All	1482/1482 (100%)	-0.51	6 (0%) 93 93	4, 12, 22, 29	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	18	ALA	2.7
1	B	126	PRO	2.4
1	A	18	ALA	2.3
1	B	22	TYR	2.2
1	A	22	TYR	2.2
1	C	22	TYR	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	MG	C	301	1/1	0.69	0.49	43.36	58,58,58,58	0
2	MG	E	301	1/1	0.91	0.44	29.97	49,49,49,49	0
2	MG	F	301	1/1	0.85	0.35	24.91	55,55,55,55	0
2	MG	A	301	1/1	0.74	0.35	13.44	55,55,55,55	0
2	MG	D	301	1/1	0.73	0.33	12.24	48,48,48,48	0
2	MG	B	302	1/1	0.61	0.28	9.82	41,41,41,41	0
2	MG	C	302	1/1	0.93	0.20	9.17	27,27,27,27	0
2	MG	E	302	1/1	0.96	0.24	7.53	30,30,30,30	0
2	MG	A	302	1/1	0.93	0.15	5.31	24,24,24,24	0
2	MG	F	302	1/1	0.94	0.14	4.46	23,23,23,23	0
2	MG	D	302	1/1	0.95	0.06	-1.98	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.