



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:56 AM GMT

PDB ID : 2OS7  
Title : Caf1M periplasmic chaperone tetramer  
Authors : Knight, S.D.; Zavialov, A.Z.  
Deposited on : 2007-02-05  
Resolution : 2.90 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

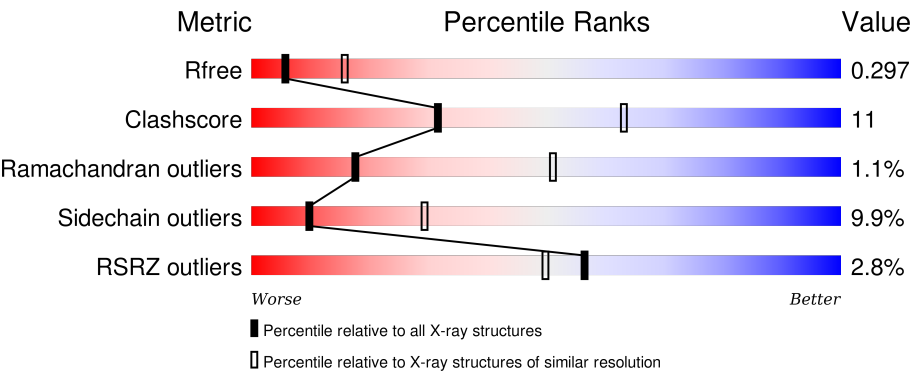
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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 <sub>free</sub>	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	235	<div><div>2%</div><div>67%16%•12%</div></div>
1	B	235	<div><div>2%</div><div>56%23%•17%</div></div>
1	C	235	<div><div>2%</div><div>63%22%•13%</div></div>
1	D	235	<div><div>3%</div><div>55%24%•17%</div></div>
1	E	235	<div><div>4%</div><div>63%21%•14%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	235	<div><div><div>%</div><div><div></div></div><div>54%</div><div>23%</div><div>•</div><div>19%</div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9426 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.

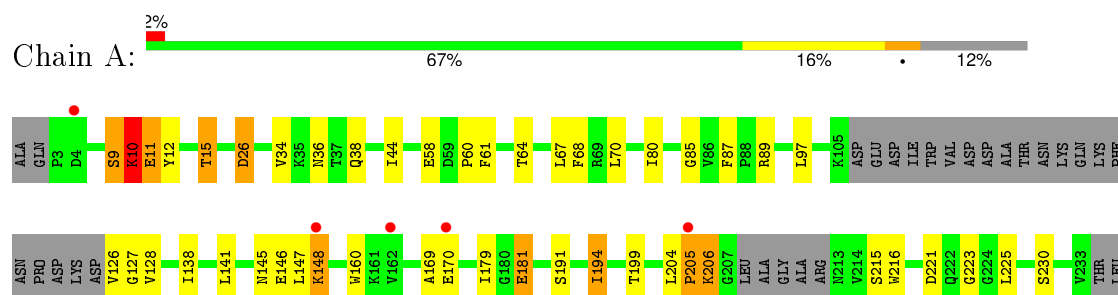
- Molecule 1 is a protein called Chaperone protein caf1M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1628	1053	274	297	4			
1	B	196	Total	C	N	O	S	0	0	0
			1550	1006	263	277	4			
1	C	205	Total	C	N	O	S	0	0	0
			1612	1041	271	296	4			
1	D	195	Total	C	N	O	S	0	0	0
			1523	991	256	272	4			
1	E	202	Total	C	N	O	S	0	0	0
			1603	1035	271	293	4			
1	F	190	Total	C	N	O	S	0	0	0
			1510	982	256	268	4			

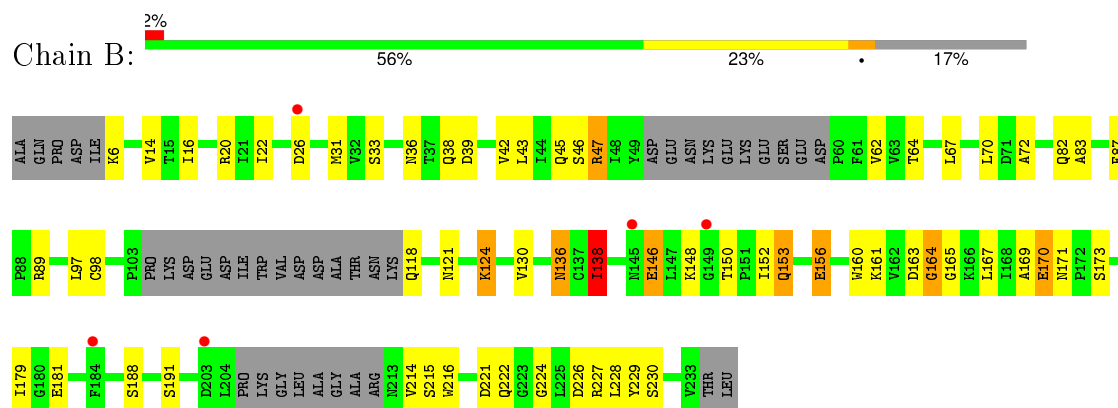
### 3 Residue-property plots [i](#)

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.

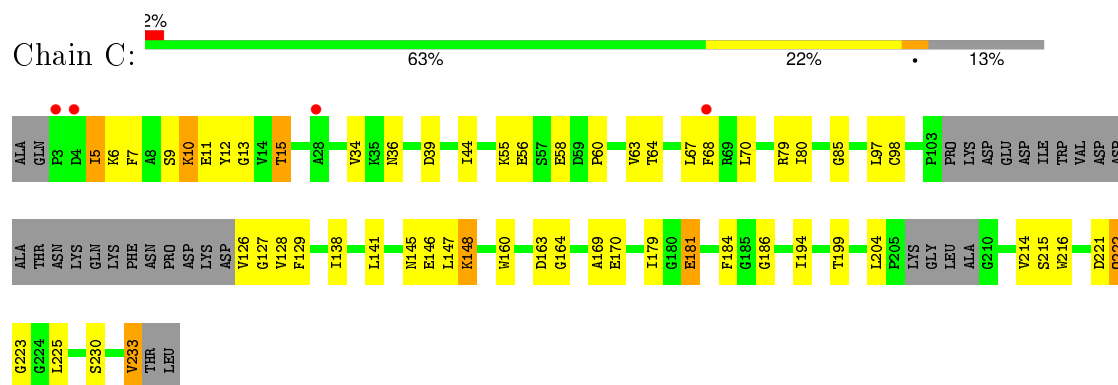
#### • Molecule 1: Chaperone protein caf1M



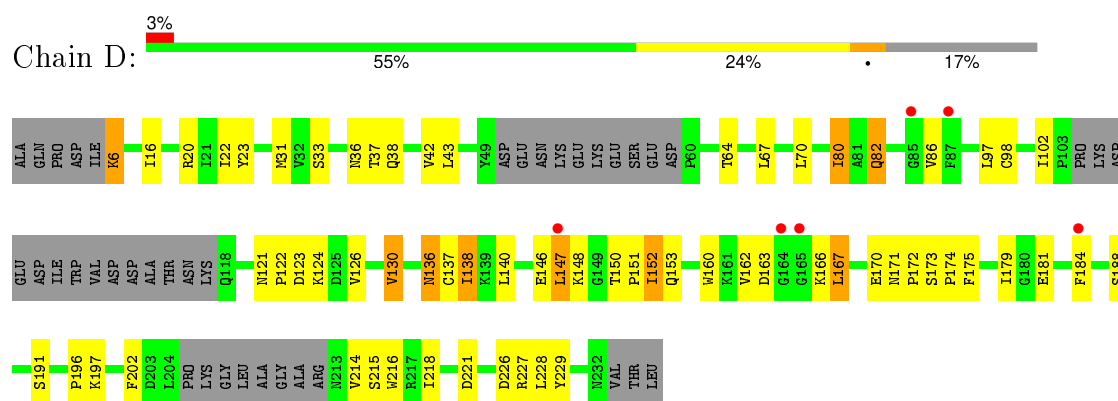
#### • Molecule 1: Chaperone protein caf1M



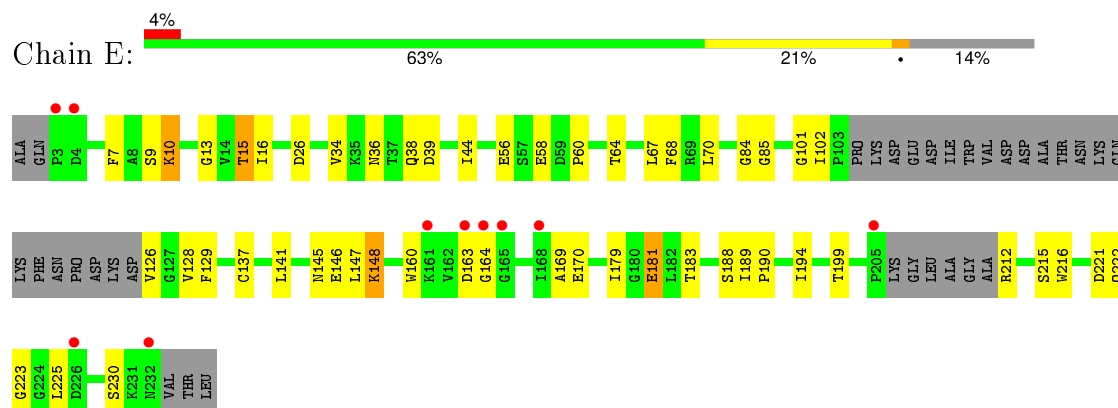
#### • Molecule 1: Chaperone protein caf1M



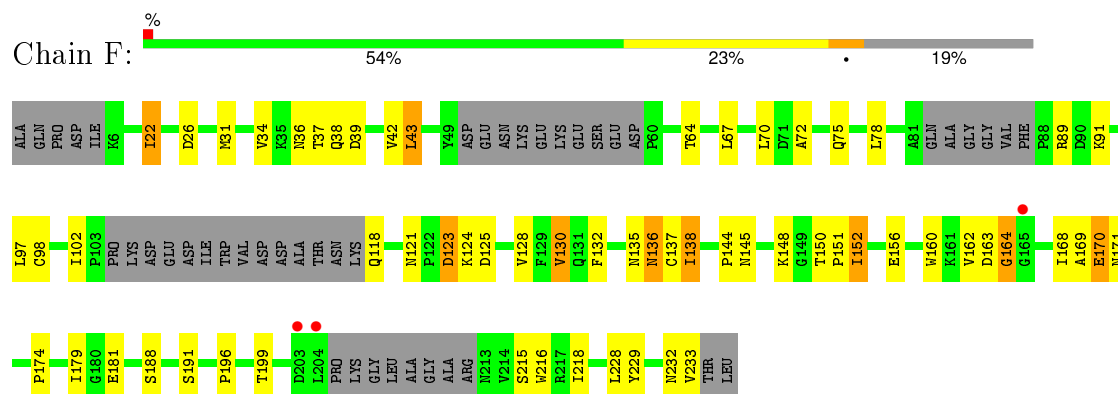
#### • Molecule 1: Chaperone protein caf1M



- Molecule 1: Chaperone protein caf1M



- Molecule 1: Chaperone protein caf1M



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.09 Å   174.27 Å   60.58 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 2.90 37.15 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.90) 99.9 (37.15-2.90)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.90 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.249   ,   0.298 0.247   ,   0.297	Depositor DCC
$R_{free}$ test set	1719 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.5	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 29.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	4 of 33919 reflections (0.012%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9426	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.63% 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	0.88	1/1668 (0.1%)	0.84	0/2259
1	B	0.78	0/1588	0.77	1/2148 (0.0%)
1	C	0.78	1/1651 (0.1%)	0.80	0/2237
1	D	0.74	0/1561	0.79	0/2114
1	E	0.78	0/1642	0.79	0/2224
1	F	0.76	2/1546 (0.1%)	0.81	1/2091 (0.0%)
All	All	0.79	4/9656 (0.0%)	0.80	2/13073 (0.0%)

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	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	GLU	CG-CD	6.69	1.61	1.51
1	F	170	GLU	CB-CG	5.91	1.63	1.52
1	F	170	GLU	CG-CD	5.63	1.60	1.51
1	C	98	CYS	CB-SG	-5.21	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	ILE	CB-CA-C	-5.24	101.12	111.60
1	F	78	LEU	CA-CB-CG	5.03	126.87	115.30



There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	10	LYS	Peptide
1	D	146	GLU	Peptide
1	E	26	ASP	Peptide
1	F	162	VAL	Peptide

## 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	1628	0	1644	31	0
1	B	1550	0	1561	41	0
1	C	1612	0	1617	37	0
1	D	1523	0	1522	45	0
1	E	1603	0	1612	34	0
1	F	1510	0	1532	48	0
All	All	9426	0	9488	202	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 11.

All (202) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:VAL:HG22	1:F:137:CYS:SG	2.10	0.91
1:C:7:PHE:HB2	1:F:130:VAL:HG22	1.54	0.90
1:C:148:LYS:NZ	1:C:148:LYS:H	1.81	0.78
1:E:225:LEU:HB2	1:F:31:MET:HB2	1.66	0.77
1:D:152:ILE:HD11	1:D:226:ASP:HB2	1.66	0.77
1:C:148:LYS:HZ2	1:C:148:LYS:H	1.35	0.75
1:D:179:ILE:HG22	1:D:191:SER:HB2	1.70	0.74
1:C:126:VAL:CG2	1:F:137:CYS:SG	2.77	0.72
1:D:147:LEU:HD22	1:D:174:PRO:HG2	1.71	0.71
1:E:101:GLY:O	1:E:102:ILE:HG23	1.91	0.71
1:B:160:TRP:HE3	1:B:167:LEU:HD11	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:PHE:HE1	1:C:233:VAL:HG21	1.56	0.70
1:B:171:ASN:OD1	1:B:173:SER:HB3	1.91	0.70
1:F:97:LEU:HB3	1:F:138:ILE:HD12	1.73	0.69
1:B:179:ILE:HG22	1:B:191:SER:HB2	1.74	0.69
1:D:6:LYS:HB2	1:D:6:LYS:NZ	2.07	0.69
1:B:121:ASN:ND2	1:B:124:LYS:HD2	2.07	0.69
1:B:121:ASN:HD22	1:B:124:LYS:HD2	1.59	0.68
1:F:97:LEU:HD23	1:F:138:ILE:HD11	1.76	0.66
1:A:148:LYS:H	1:A:148:LYS:NZ	1.93	0.65
1:D:171:ASN:OD1	1:D:173:SER:OG	2.10	0.65
1:F:38:GLN:OE1	1:F:38:GLN:HA	1.96	0.65
1:F:179:ILE:HG22	1:F:191:SER:HB2	1.78	0.65
1:E:148:LYS:H	1:E:148:LYS:NZ	1.95	0.65
1:B:97:LEU:HD23	1:B:138:ILE:HD11	1.79	0.64
1:C:36:ASN:HB2	1:C:70:LEU:HD23	1.79	0.64
1:E:36:ASN:HB2	1:E:70:LEU:HD23	1.80	0.64
1:A:127:GLY:HA3	1:B:6:LYS:O	1.98	0.64
1:B:45:GLN:HG2	1:B:47:ARG:NH1	2.14	0.63
1:D:152:ILE:HD12	1:D:218:ILE:HD11	1.81	0.62
1:D:122:PRO:O	1:E:10:LYS:HE2	1.99	0.62
1:B:38:GLN:OE1	1:B:38:GLN:HA	1.99	0.62
1:D:97:LEU:HB3	1:D:138:ILE:HD12	1.81	0.62
1:D:152:ILE:HG22	1:D:153:GLN:NE2	2.14	0.62
1:D:171:ASN:ND2	1:D:196:PRO:HA	2.14	0.61
1:B:97:LEU:HB3	1:B:138:ILE:CD1	2.30	0.61
1:F:121:ASN:OD1	1:F:123:ASP:N	2.32	0.61
1:F:97:LEU:HB3	1:F:138:ILE:CD1	2.31	0.60
1:F:160:TRP:HA	1:F:168:ILE:O	2.01	0.60
1:D:130:VAL:HG22	1:E:7:PHE:HB2	1.83	0.59
1:D:97:LEU:HB3	1:D:138:ILE:CD1	2.32	0.59
1:B:160:TRP:CE3	1:B:167:LEU:HD11	2.36	0.59
1:F:91:LYS:O	1:F:144:PRO:HG2	2.03	0.58
1:B:160:TRP:CZ3	1:B:169:ALA:HB2	2.38	0.58
1:D:121:ASN:ND2	1:D:124:LYS:HG2	2.17	0.58
1:A:38:GLN:OE1	1:A:38:GLN:HA	2.04	0.57
1:C:184:PHE:HE1	1:C:233:VAL:CG2	2.16	0.57
1:B:97:LEU:HB3	1:B:138:ILE:HD12	1.86	0.57
1:A:181:GLU:O	1:A:216:TRP:HA	2.05	0.57
1:D:38:GLN:OE1	1:D:38:GLN:HA	2.05	0.57
1:F:148:LYS:NZ	1:F:174:PRO:HG3	2.19	0.57
1:C:80:ILE:HD11	1:C:97:LEU:HD22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:PHE:CE1	1:C:233:VAL:HG21	2.37	0.56
1:A:10:LYS:O	1:A:12:TYR:N	2.40	0.55
1:D:181:GLU:O	1:D:216:TRP:HA	2.06	0.55
1:E:38:GLN:OE1	1:E:38:GLN:HA	2.05	0.55
1:E:170:GLU:HA	1:E:199:THR:HG22	1.88	0.55
1:C:221:ASP:C	1:C:223:GLY:H	2.10	0.55
1:A:148:LYS:H	1:A:148:LYS:HZ2	1.55	0.55
1:D:97:LEU:HD23	1:D:138:ILE:HD11	1.88	0.54
1:A:26:ASP:OD2	1:A:89:ARG:NH1	2.40	0.54
1:A:221:ASP:C	1:A:223:GLY:H	2.11	0.54
1:C:7:PHE:HB2	1:F:130:VAL:CG2	2.34	0.54
1:C:145:ASN:C	1:C:147:LEU:H	2.11	0.53
1:C:5:ILE:H	1:C:5:ILE:HD12	1.72	0.53
1:B:163:ASP:O	1:B:165:GLY:N	2.35	0.53
1:C:225:LEU:HB2	1:D:31:MET:HB2	1.91	0.53
1:A:179:ILE:HD12	1:A:194:ILE:HD11	1.90	0.53
1:C:160:TRP:CZ3	1:C:169:ALA:HB2	2.43	0.53
1:B:98:CYS:HA	1:B:136:ASN:O	2.09	0.53
1:C:138:ILE:HG21	1:D:16:ILE:HG21	1.90	0.53
1:C:179:ILE:HD12	1:C:194:ILE:HD11	1.90	0.53
1:E:145:ASN:C	1:E:147:LEU:H	2.13	0.52
1:B:170:GLU:HG3	1:B:171:ASN:N	2.25	0.52
1:E:60:PRO:HB3	1:E:85:GLY:HA3	1.91	0.52
1:F:215:SER:HB3	1:F:228:LEU:HD11	1.91	0.51
1:B:226:ASP:CG	1:B:227:ARG:H	2.14	0.51
1:E:179:ILE:HD12	1:E:194:ILE:HD11	1.93	0.51
1:E:181:GLU:O	1:E:216:TRP:HA	2.10	0.51
1:A:205:PRO:C	1:A:206:LYS:HD2	2.30	0.51
1:C:129:PHE:O	1:F:132:PHE:HA	2.11	0.50
1:A:145:ASN:C	1:A:147:LEU:H	2.14	0.50
1:B:150:THR:H	1:B:153:GLN:HG3	1.76	0.50
1:B:39:ASP:HA	1:B:72:ALA:HB1	1.93	0.50
1:F:181:GLU:O	1:F:216:TRP:HA	2.11	0.50
1:B:215:SER:HA	1:B:229:TYR:O	2.11	0.50
1:C:170:GLU:HA	1:C:199:THR:HG22	1.93	0.50
1:B:62:VAL:HG11	1:C:186:GLY:HA3	1.93	0.50
1:D:20:ARG:NH2	1:D:221:ASP:OD2	2.45	0.50
1:F:26:ASP:OD2	1:F:89:ARG:NH1	2.45	0.49
1:A:60:PRO:HB3	1:A:85:GLY:HA3	1.93	0.49
1:E:101:GLY:O	1:E:102:ILE:CG2	2.60	0.49
1:C:60:PRO:HB3	1:C:85:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PHE:HE2	1:A:87:PHE:CE1	2.31	0.48
1:A:36:ASN:HB2	1:A:70:LEU:HD23	1.94	0.48
1:A:126:VAL:O	1:B:6:LYS:HB2	2.13	0.48
1:B:87:PHE:H	1:B:89:ARG:HH21	1.60	0.48
1:A:44:ILE:HD11	1:B:14:VAL:HG13	1.96	0.48
1:A:138:ILE:HG21	1:B:16:ILE:HG21	1.95	0.48
1:E:221:ASP:C	1:E:223:GLY:H	2.16	0.48
1:D:147:LEU:HD22	1:D:174:PRO:CG	2.41	0.48
1:A:10:LYS:H	1:A:10:LYS:HE3	1.79	0.48
1:A:10:LYS:O	1:A:11:GLU:C	2.52	0.48
1:B:215:SER:HB3	1:B:228:LEU:HD11	1.96	0.48
1:C:63:VAL:HA	1:C:79:ARG:O	2.14	0.48
1:F:156:GLU:HG3	1:F:229:TYR:CD2	2.49	0.47
1:F:98:CYS:HA	1:F:136:ASN:O	2.14	0.47
1:B:156:GLU:HB2	1:B:229:TYR:CE2	2.50	0.47
1:D:23:TYR:HB2	1:D:140:LEU:HD11	1.96	0.47
1:D:173:SER:O	1:D:196:PRO:HB2	2.14	0.47
1:F:97:LEU:O	1:F:137:CYS:HA	2.15	0.47
1:D:150:THR:HB	1:D:151:PRO:HD2	1.97	0.47
1:F:152:ILE:HA	1:F:218:ILE:HD11	1.96	0.47
1:F:163:ASP:O	1:F:164:GLY:C	2.52	0.47
1:E:189:ILE:O	1:F:75:GLN:NE2	2.44	0.47
1:B:181:GLU:O	1:B:216:TRP:HA	2.15	0.47
1:A:126:VAL:O	1:B:6:LYS:N	2.48	0.47
1:C:44:ILE:HG22	1:C:68:PHE:HB3	1.97	0.46
1:C:55:LYS:NZ	1:F:125:ASP:OD1	2.44	0.46
1:D:152:ILE:HD11	1:D:226:ASP:CB	2.40	0.46
1:B:226:ASP:CG	1:B:227:ARG:N	2.68	0.46
1:D:184:PHE:CD1	1:D:214:VAL:HG22	2.51	0.46
1:F:39:ASP:HA	1:F:72:ALA:HB1	1.98	0.46
1:F:215:SER:HA	1:F:229:TYR:O	2.15	0.46
1:D:167:LEU:HB3	1:D:202:PHE:HB2	1.98	0.46
1:A:44:ILE:HG22	1:A:68:PHE:HB3	1.98	0.45
1:B:89:ARG:HB3	1:B:146:GLU:OE1	2.16	0.45
1:D:226:ASP:CG	1:D:227:ARG:H	2.20	0.45
1:F:150:THR:HB	1:F:151:PRO:HD2	1.98	0.45
1:E:148:LYS:H	1:E:148:LYS:HZ2	1.63	0.45
1:C:9:SER:O	1:C:12:TYR:N	2.50	0.45
1:C:163:ASP:O	1:C:164:GLY:C	2.54	0.45
1:C:6:LYS:HE3	1:F:124:LYS:O	2.17	0.45
1:A:15:THR:O	1:A:15:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ASN:HB2	1:B:70:LEU:HD23	1.99	0.45
1:A:80:ILE:HD11	1:A:97:LEU:HD22	1.99	0.44
1:D:98:CYS:HA	1:D:136:ASN:O	2.16	0.44
1:E:16:ILE:HG21	1:F:138:ILE:HD11	1.99	0.44
1:D:175:PHE:N	1:D:196:PRO:HB3	2.33	0.44
1:C:181:GLU:O	1:C:216:TRP:HA	2.17	0.44
1:E:183:THR:HG22	1:E:188:SER:HA	1.99	0.44
1:B:26:ASP:HA	1:B:82:GLN:OE1	2.17	0.44
1:B:82:GLN:O	1:B:83:ALA:C	2.56	0.44
1:C:127:GLY:O	1:F:135:ASN:N	2.41	0.44
1:E:10:LYS:CD	1:E:10:LYS:H	2.31	0.44
1:F:232:ASN:C	1:F:233:VAL:CG2	2.86	0.44
1:D:6:LYS:HB2	1:D:6:LYS:HZ3	1.82	0.44
1:C:55:LYS:HG3	1:F:118:GLN:O	2.17	0.44
1:F:169:ALA:O	1:F:199:THR:HA	2.17	0.44
1:D:215:SER:HA	1:D:229:TYR:O	2.17	0.44
1:D:226:ASP:CG	1:D:227:ARG:N	2.72	0.43
1:B:46:SER:O	1:B:47:ARG:HD2	2.17	0.43
1:D:126:VAL:HG22	1:E:137:CYS:SG	2.57	0.43
1:C:222:GLN:CD	1:C:222:GLN:H	2.22	0.43
1:E:13:GLY:O	1:F:36:ASN:HA	2.19	0.43
1:A:10:LYS:C	1:A:12:TYR:N	2.71	0.43
1:E:38:GLN:CA	1:E:38:GLN:OE1	2.67	0.43
1:D:172:PRO:O	1:D:197:LYS:HG2	2.19	0.43
1:E:16:ILE:HD12	1:F:138:ILE:HG13	2.00	0.43
1:D:152:ILE:CG2	1:D:153:GLN:NE2	2.81	0.43
1:E:9:SER:O	1:E:10:LYS:C	2.56	0.43
1:F:43:LEU:HA	1:F:43:LEU:HD22	1.92	0.43
1:D:36:ASN:HB2	1:D:70:LEU:HD23	2.00	0.43
1:D:137:CYS:SG	1:E:126:VAL:HG22	2.59	0.43
1:F:148:LYS:HZ3	1:F:174:PRO:HG3	1.83	0.43
1:D:160:TRP:HE3	1:D:167:LEU:HD11	1.84	0.43
1:A:170:GLU:HA	1:A:199:THR:HG22	2.01	0.43
1:D:97:LEU:O	1:D:137:CYS:HA	2.19	0.43
1:B:39:ASP:OD1	1:B:39:ASP:C	2.58	0.43
1:E:160:TRP:CZ3	1:E:169:ALA:HB2	2.54	0.43
1:F:171:ASN:ND2	1:F:196:PRO:HA	2.34	0.43
1:D:215:SER:HB3	1:D:228:LEU:HD11	2.00	0.42
1:C:204:LEU:HD23	1:C:204:LEU:HA	1.81	0.42
1:E:163:ASP:O	1:E:164:GLY:C	2.58	0.42
1:F:97:LEU:HD23	1:F:138:ILE:CD1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TRP:CZ3	1:A:169:ALA:HB2	2.53	0.42
1:B:20:ARG:NH2	1:B:221:ASP:OD2	2.52	0.42
1:A:179:ILE:HG22	1:A:191:SER:HB2	2.01	0.42
1:B:214:VAL:O	1:B:230:SER:HA	2.19	0.42
1:C:13:GLY:HA2	1:D:37:THR:OG1	2.20	0.42
1:F:232:ASN:C	1:F:233:VAL:HG23	2.40	0.42
1:B:222:GLN:C	1:B:224:GLY:H	2.23	0.42
1:E:222:GLN:HA	1:F:22:ILE:HG13	2.01	0.42
1:A:38:GLN:OE1	1:A:38:GLN:CA	2.64	0.42
1:E:15:THR:O	1:F:34:VAL:HA	2.20	0.42
1:D:184:PHE:HD1	1:D:214:VAL:HG22	1.86	0.41
1:E:13:GLY:HA2	1:F:37:THR:OG1	2.19	0.41
1:A:9:SER:O	1:A:10:LYS:C	2.59	0.41
1:B:163:ASP:HB3	1:B:164:GLY:H	1.46	0.41
1:C:12:TYR:CE2	1:F:128:VAL:HG21	2.55	0.41
1:E:16:ILE:CD1	1:F:138:ILE:HG13	2.51	0.41
1:D:80:ILE:HD11	1:D:97:LEU:HD22	2.02	0.41
1:F:170:GLU:HG3	1:F:171:ASN:N	2.35	0.41
1:D:137:CYS:SG	1:E:126:VAL:CG2	3.09	0.41
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.75	0.41
1:D:82:GLN:H	1:D:82:GLN:HG3	1.73	0.41
1:E:44:ILE:HG22	1:E:68:PHE:HB3	2.01	0.40
1:C:214:VAL:HG23	1:C:233:VAL:HG22	2.04	0.40
1:E:10:LYS:H	1:E:10:LYS:HD2	1.87	0.40
1:A:225:LEU:HB2	1:B:31:MET:HB2	2.03	0.40
1:F:36:ASN:HB2	1:F:70:LEU:HD23	2.02	0.40
1:C:15:THR:HG22	1:C:15:THR:O	2.20	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	200/235 (85%)	184 (92%)	13 (6%)	3 (2%)	13	42
1	B	188/235 (80%)	172 (92%)	14 (7%)	2 (1%)	17	51
1	C	199/235 (85%)	180 (90%)	16 (8%)	3 (2%)	13	42
1	D	187/235 (80%)	169 (90%)	17 (9%)	1 (0%)	34	71
1	E	196/235 (83%)	180 (92%)	13 (7%)	3 (2%)	13	42
1	F	180/235 (77%)	166 (92%)	13 (7%)	1 (1%)	30	67
All	All	1150/1410 (82%)	1051 (91%)	86 (8%)	13 (1%)	17	51

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	PRO
1	E	146	GLU
1	B	164	GLY
1	C	146	GLU
1	D	86	VAL
1	F	164	GLY
1	A	10	LYS
1	A	146	GLU
1	C	11	GLU
1	C	222	GLN
1	E	84	GLY
1	E	190	PRO
1	B	152	ILE

### 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	180/204 (88%)	164 (91%)	16 (9%)	12	35
1	B	170/204 (83%)	151 (89%)	19 (11%)	7	22
1	C	177/204 (87%)	161 (91%)	16 (9%)	12	34
1	D	165/204 (81%)	142 (86%)	23 (14%)	4	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	177/204 (87%)	161 (91%)	16 (9%)	12	34
1	F	167/204 (82%)	154 (92%)	13 (8%)	16	41
All	All	1036/1224 (85%)	933 (90%)	103 (10%)	10	29

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	10	LYS
1	A	15	THR
1	A	26	ASP
1	A	34	VAL
1	A	58	GLU
1	A	64	THR
1	A	67	LEU
1	A	128	VAL
1	A	141	LEU
1	A	148	LYS
1	A	181	GLU
1	A	194	ILE
1	A	206	LYS
1	A	215	SER
1	A	230	SER
1	B	22	ILE
1	B	33	SER
1	B	42	VAL
1	B	43	LEU
1	B	47	ARG
1	B	64	THR
1	B	67	LEU
1	B	118	GLN
1	B	124	LYS
1	B	130	VAL
1	B	136	ASN
1	B	138	ILE
1	B	146	GLU
1	B	148	LYS
1	B	153	GLN
1	B	156	GLU
1	B	161	LYS
1	B	170	GLU

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Mol	Chain	Res	Type
1	B	188	SER
1	C	5	ILE
1	C	10	LYS
1	C	15	THR
1	C	34	VAL
1	C	39	ASP
1	C	56	GLU
1	C	58	GLU
1	C	64	THR
1	C	67	LEU
1	C	128	VAL
1	C	141	LEU
1	C	148	LYS
1	C	181	GLU
1	C	215	SER
1	C	230	SER
1	C	233	VAL
1	D	6	LYS
1	D	22	ILE
1	D	33	SER
1	D	42	VAL
1	D	43	LEU
1	D	64	THR
1	D	67	LEU
1	D	80	ILE
1	D	82	GLN
1	D	102	ILE
1	D	123	ASP
1	D	130	VAL
1	D	136	ASN
1	D	138	ILE
1	D	147	LEU
1	D	148	LYS
1	D	152	ILE
1	D	162	VAL
1	D	163	ASP
1	D	166	LYS
1	D	167	LEU
1	D	170	GLU
1	D	188	SER
1	E	10	LYS
1	E	15	THR

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Mol	Chain	Res	Type
1	E	34	VAL
1	E	39	ASP
1	E	56	GLU
1	E	58	GLU
1	E	64	THR
1	E	67	LEU
1	E	128	VAL
1	E	129	PHE
1	E	141	LEU
1	E	148	LYS
1	E	181	GLU
1	E	212	ARG
1	E	215	SER
1	E	230	SER
1	F	22	ILE
1	F	42	VAL
1	F	43	LEU
1	F	64	THR
1	F	67	LEU
1	F	102	ILE
1	F	123	ASP
1	F	130	VAL
1	F	136	ASN
1	F	138	ILE
1	F	145	ASN
1	F	152	ILE
1	F	188	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	178	ASN
1	A	213	ASN
1	B	121	ASN
1	B	153	GLN
1	C	145	ASN
1	C	178	ASN
1	C	213	ASN
1	C	222	GLN
1	D	82	GLN
1	D	121	ASN

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Mol	Chain	Res	Type
1	D	153	GLN
1	D	178	ASN
1	E	145	ASN
1	E	213	ASN

### 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 [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	206/235 (87%)	0.12	5 (2%) 62 57	35, 44, 52, 60	0
1	B	196/235 (83%)	0.14	5 (2%) 59 54	34, 45, 53, 64	0
1	C	205/235 (87%)	0.14	4 (1%) 68 64	35, 44, 52, 67	0
1	D	195/235 (82%)	0.27	6 (3%) 52 45	40, 46, 58, 68	0
1	E	202/235 (85%)	0.32	10 (4%) 32 26	34, 44, 51, 65	0
1	F	190/235 (80%)	0.18	3 (1%) 74 72	40, 45, 52, 56	0
All	All	1194/1410 (84%)	0.20	33 (2%) 56 50	34, 45, 53, 68	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	PRO	4.9
1	F	203	ASP	4.7
1	E	3	PRO	4.0
1	E	165	GLY	4.0
1	D	85	GLY	3.8
1	B	203	ASP	3.5
1	B	26	ASP	3.5
1	A	205	PRO	3.4
1	D	147	LEU	3.3
1	F	165	GLY	3.3
1	D	165	GLY	3.1
1	E	168	ILE	3.0
1	F	204	LEU	3.0
1	D	184	PHE	2.8
1	D	164	GLY	2.8
1	E	226	ASP	2.6
1	C	28	ALA	2.6
1	B	184	PHE	2.4
1	E	161	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	205	PRO	2.3
1	E	4	ASP	2.3
1	E	164	GLY	2.3
1	B	149	GLY	2.3
1	A	4	ASP	2.2
1	A	148	LYS	2.3
1	D	87	PHE	2.2
1	E	232	ASN	2.2
1	E	163	ASP	2.2
1	A	170	GLU	2.2
1	A	162	VAL	2.1
1	B	145	ASN	2.1
1	C	4	ASP	2.0
1	C	68	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.