



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:04 AM UTC

PDB ID : 3OX6 / pdb_00003ox6
Title : Crystal Structure of the calcium sensor calcium-binding protein 1 (CaBP1)
Authors : Findeisen, F.; Minor, D.L.
Deposited on : 2010-09-21
Resolution : 2.40 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

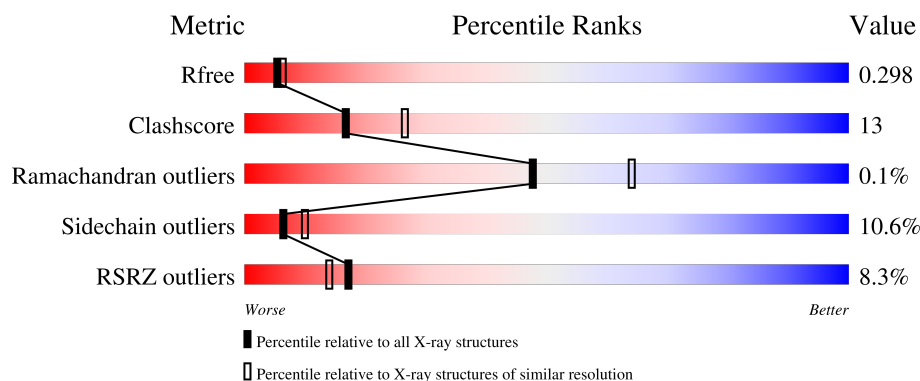
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	153	74% 22% 5%
1	B	153	75% 23% .
1	C	153	4% 71% 25% 5%
1	D	153	8% 66% 23% 7% 5%
1	E	153	16% 65% 10% . 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	153	16% 74% 19% ...

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6985 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 Calcium-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	1	0
			1189	730	204	242	13			
1	B	153	Total	C	N	O	S	0	1	0
			1222	751	210	247	14			
1	C	153	Total	C	N	O	S	0	3	0
			1205	744	203	242	16			
1	D	146	Total	C	N	O	S	0	0	0
			1142	701	196	232	13			
1	E	118	Total	C	N	O	S	0	1	0
			922	569	158	182	13			
1	F	148	Total	C	N	O	S	0	1	0
			1154	711	194	236	13			

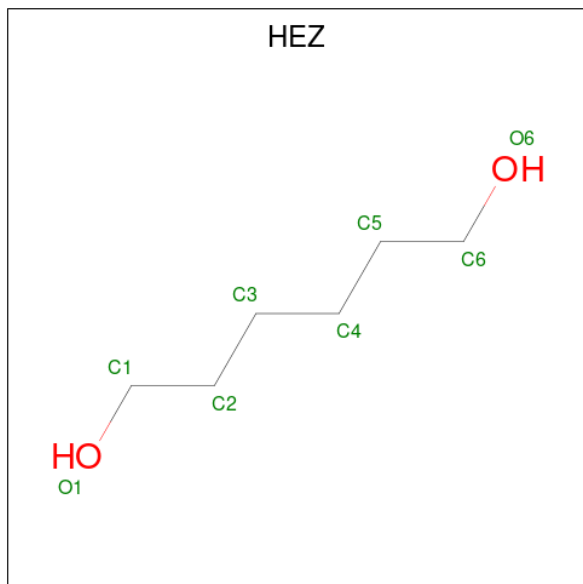
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	expression tag	UNP Q9NZU7
A	130	ALA	LYS	engineered mutation	UNP Q9NZU7
B	15	MET	-	expression tag	UNP Q9NZU7
B	130	ALA	LYS	engineered mutation	UNP Q9NZU7
C	15	MET	-	expression tag	UNP Q9NZU7
C	130	ALA	LYS	engineered mutation	UNP Q9NZU7
D	15	MET	-	expression tag	UNP Q9NZU7
D	130	ALA	LYS	engineered mutation	UNP Q9NZU7
E	15	MET	-	expression tag	UNP Q9NZU7
E	130	ALA	LYS	engineered mutation	UNP Q9NZU7
F	15	MET	-	expression tag	UNP Q9NZU7
F	130	ALA	LYS	engineered mutation	UNP Q9NZU7

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is HEXANE-1,6-DIOL (CCD ID: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0

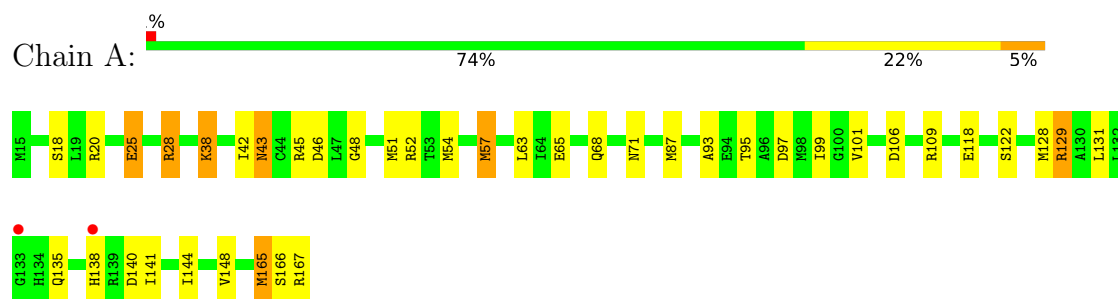
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total 22	O 22	0	0
4	B	32	Total 32	O 32	0	0
4	C	29	Total 29	O 29	0	0
4	D	13	Total 13	O 13	0	0
4	E	9	Total 9	O 9	0	0
4	F	3	Total 3	O 3	0	0

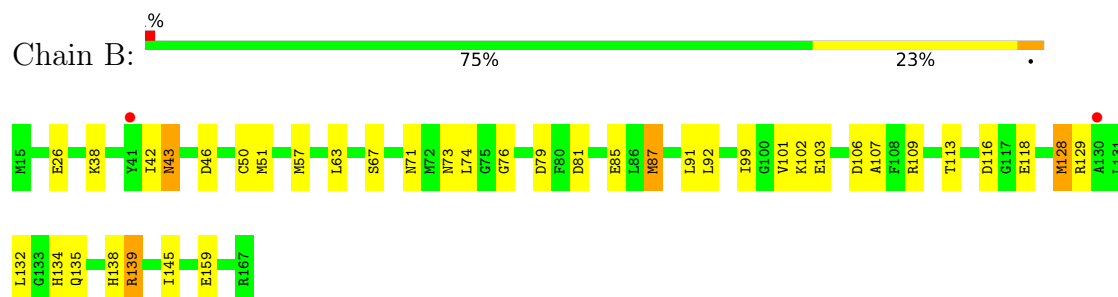
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

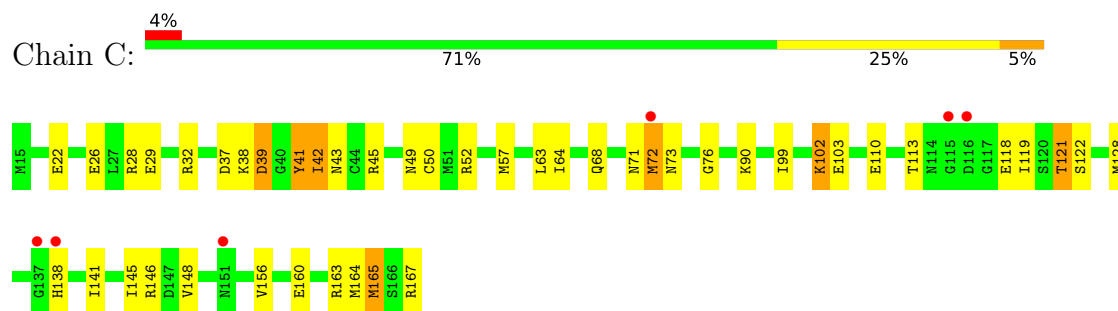
• Molecule 1: Calcium-binding protein 1



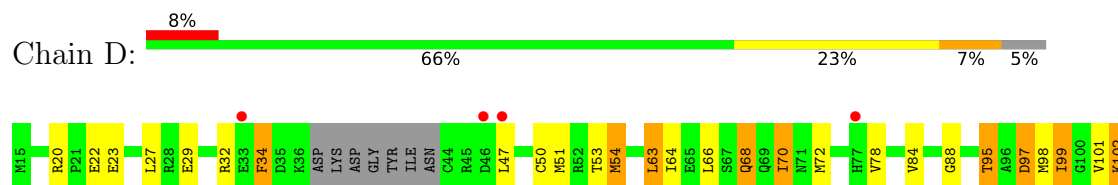
• Molecule 1: Calcium-binding protein 1



• Molecule 1: Calcium-binding protein 1

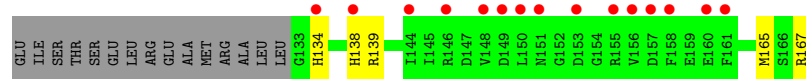


• Molecule 1: Calcium-binding protein 1

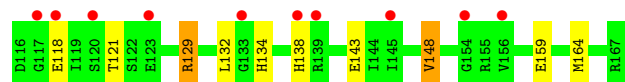
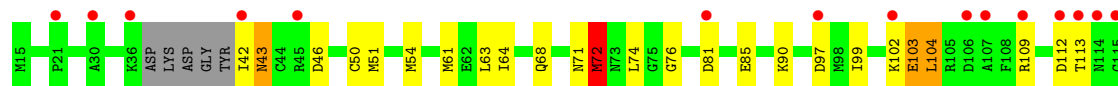
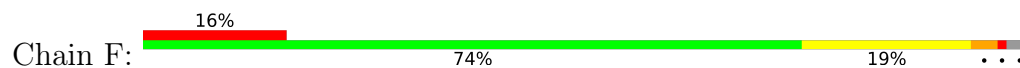




• Molecule 1: Calcium-binding protein 1



• Molecule 1: Calcium-binding protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	68.72Å 68.72Å 344.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (15.00-2.40) 98.9 (15.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.252 , 0.295 0.254 , 0.298	Depositor DCC
R_{free} test set	1944 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6985	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CA, HEZ

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	1.01	0/1206	1.08	2/1618 (0.1%)
1	B	1.12	1/1240 (0.1%)	1.14	3/1660 (0.2%)
1	C	0.93	0/1229	1.08	1/1648 (0.1%)
1	D	0.80	0/1154	1.08	1/1544 (0.1%)
1	E	0.81	0/934	1.03	1/1248 (0.1%)
1	F	0.69	0/1170	1.02	3/1569 (0.2%)
All	All	0.91	1/6933 (0.0%)	1.07	11/9287 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	MET	SD-CE	-6.26	1.64	1.79

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	113	THR	N-CA-C	10.79	123.12	111.36
1	D	99	ILE	N-CA-C	8.19	118.99	110.72
1	B	67	SER	CB-CA-C	-6.36	100.64	110.81
1	F	72	MET	N-CA-C	5.81	120.53	112.45
1	A	93	ALA	N-CA-C	-5.58	105.68	112.88
1	E	42	ILE	N-CA-C	5.44	116.61	109.21
1	B	26	GLU	N-CA-C	5.38	118.06	111.82
1	C	43	ASN	N-CA-CB	-5.33	102.49	110.17
1	F	113	THR	CB-CA-C	-5.27	101.89	110.85
1	B	73	ASN	N-CA-C	5.15	116.89	111.28
1	A	48	GLY	N-CA-C	-5.01	106.68	112.50

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	1189	0	1101	48	0
1	B	1222	0	1154	40	0
1	C	1205	0	1130	37	0
1	D	1142	0	1065	37	0
1	E	922	0	859	18	0
1	F	1154	0	1064	24	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
3	A	16	0	28	0	0
3	B	16	0	28	7	0
4	A	22	0	0	2	0
4	B	32	0	0	1	0
4	C	29	0	0	3	0
4	D	13	0	0	2	0
4	E	9	0	0	1	0
4	F	3	0	0	0	0
All	All	6985	0	6429	170	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 13.

All (170) 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:A:51:MET:HE3	1:A:87:MET:HE1	1.31	1.11
1:B:51:MET:HE3	1:B:87:MET:HE1	1.10	1.08
1:B:51:MET:HE3	1:B:87:MET:CE	1.88	1.03
1:A:43:ASN:ND2	1:A:46:ASP:H	1.60	1.00
1:C:138:HIS:HB3	4:C:192:HOH:O	1.63	0.99
1:A:51:MET:HG2	1:A:87:MET:CE	1.95	0.97
1:A:128:MET:HE2	1:F:64:ILE:HG21	1.49	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:LEU:O	1:D:70:ILE:HD12	1.72	0.88
1:A:43:ASN:HD21	1:A:46:ASP:H	1.21	0.86
1:A:51:MET:CE	1:A:87:MET:HE1	2.04	0.85
1:A:51:MET:HG2	1:A:87:MET:HE2	1.59	0.83
1:B:51:MET:CE	1:B:87:MET:HE1	2.03	0.82
1:A:51:MET:HG2	1:A:87:MET:HE1	1.61	0.81
1:D:132:LEU:HD13	1:E:68:GLN:HG3	1.62	0.81
1:D:29:GLU:HG3	1:D:32:ARG:HH22	1.47	0.78
1:A:51:MET:HE3	1:A:87:MET:CE	2.13	0.77
1:A:95:THR:HB	4:A:178:HOH:O	1.86	0.76
1:D:121:THR:HG22	1:D:145:ILE:HG13	1.68	0.75
1:A:106:ASP:OD1	1:A:109:ARG:NH1	2.20	0.74
1:A:43:ASN:HD22	1:A:43:ASN:C	1.95	0.74
1:B:139:ARG:HG2	1:B:139:ARG:HH11	1.52	0.74
1:A:42:ILE:H	1:A:71:ASN:HD21	1.38	0.71
1:B:91:LEU:HD21	3:B:602:HEZ:H51	1.70	0.71
1:A:28:ARG:HH11	1:A:28:ARG:HG3	1.56	0.70
1:E:68:GLN:NE2	1:E:72:MET:HG3	2.07	0.70
1:A:101:VAL:HG21	1:B:57[A]:MET:CG	2.21	0.70
1:C:103:GLU:HB2	4:C:3:HOH:O	1.92	0.70
1:B:43:ASN:ND2	1:B:46:ASP:H	1.91	0.69
1:B:87:MET:HE3	1:B:87:MET:HA	1.77	0.67
1:E:42:ILE:H	1:E:71:ASN:HD21	1.39	0.67
1:A:101:VAL:HG21	1:B:57[A]:MET:HG3	1.77	0.67
1:B:139:ARG:HG2	1:B:139:ARG:NH1	2.10	0.66
1:B:81:ASP:O	1:B:85:GLU:HG2	1.97	0.64
1:C:72[B]:MET:HG3	1:C:73:ASN:H	1.64	0.63
1:F:42:ILE:HG22	1:F:71:ASN:HD21	1.62	0.63
1:B:43:ASN:HD21	1:B:46:ASP:H	1.46	0.62
1:F:43:ASN:ND2	1:F:43:ASN:H	1.98	0.62
1:E:68:GLN:HE22	1:E:72:MET:HG3	1.65	0.62
1:B:132:LEU:HD13	1:C:68:GLN:HG3	1.82	0.61
1:C:39:ASP:N	1:C:39:ASP:OD1	2.33	0.61
1:F:43:ASN:H	1:F:43:ASN:HD22	1.48	0.61
1:C:102:LYS:HB2	1:C:102:LYS:HZ2	1.65	0.61
1:C:72[B]:MET:HG3	1:C:73:ASN:N	2.16	0.61
1:C:42:ILE:H	1:C:71:ASN:HD21	1.48	0.60
1:C:57[A]:MET:HG2	1:D:101:VAL:HG21	1.82	0.60
1:B:103:GLU:OE2	3:B:601:HEZ:O6	2.20	0.59
1:D:128:MET:HB3	1:D:136:VAL:HG21	1.84	0.59
1:D:51:MET:O	1:D:54:MET:HG3	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:MET:CG	1:A:87:MET:HE1	2.30	0.58
1:C:160:GLU:O	1:C:163:ARG:HG2	2.03	0.58
1:B:139:ARG:HH11	1:B:139:ARG:CG	2.18	0.57
1:A:57[B]:MET:HE1	1:B:101:VAL:HG13	1.87	0.57
1:C:39:ASP:C	1:C:41:TYR:H	2.12	0.56
1:F:43:ASN:HD21	1:F:46:ASP:HB2	1.70	0.56
1:A:28:ARG:HG3	1:A:28:ARG:NH1	2.20	0.56
1:B:134:HIS:NE2	1:C:68:GLN:NE2	2.52	0.56
1:A:43:ASN:HD21	1:A:46:ASP:N	1.97	0.56
1:D:132:LEU:CD1	1:E:68:GLN:HG3	2.34	0.56
1:D:78:VAL:HA	4:D:173:HOH:O	2.04	0.56
1:D:134:HIS:NE2	1:E:68:GLN:NE2	2.54	0.56
1:A:165:MET:CE	1:F:61:MET:HE2	2.37	0.55
3:B:601:HEZ:O6	3:B:602:HEZ:H61	2.06	0.55
1:D:27:LEU:HD13	1:D:84:VAL:HG22	1.88	0.55
1:B:43:ASN:C	1:B:43:ASN:HD22	2.14	0.55
1:A:95:THR:O	1:A:99:ILE:HG13	2.07	0.55
1:A:165:MET:HE2	1:F:61:MET:CE	2.37	0.55
1:A:68:GLN:HG3	1:F:134:HIS:HE1	1.72	0.55
1:B:42:ILE:H	1:B:71:ASN:HD21	1.54	0.54
1:C:57[B]:MET:HG3	1:D:101:VAL:HG21	1.88	0.54
1:A:65:GLU:O	1:A:68:GLN:OE1	2.26	0.54
1:F:109:ARG:HA	1:F:112:ASP:HB3	1.89	0.54
1:A:57[A]:MET:HA	1:A:57[A]:MET:HE2	1.88	0.54
1:C:26:GLU:OE1	1:D:102:LYS:HE2	2.08	0.53
1:F:68:GLN:O	1:F:72:MET:HB3	2.08	0.53
1:A:20:ARG:HD3	1:A:131:LEU:HD23	1.91	0.53
1:A:57[B]:MET:CE	1:B:101:VAL:HG13	2.39	0.53
1:E:81:ASP:O	1:E:85:GLU:HG2	2.08	0.53
1:C:102:LYS:HB2	1:C:102:LYS:NZ	2.24	0.53
1:E:68:GLN:NE2	1:E:72:MET:CG	2.72	0.53
1:E:42:ILE:N	1:E:71:ASN:HD21	2.06	0.52
1:F:51:MET:O	1:F:54:MET:HG3	2.10	0.52
1:C:38:LYS:NZ	1:C:76:GLY:O	2.27	0.52
1:D:106:ASP:OD1	1:D:109:ARG:NH1	2.42	0.52
1:C:52:ARG:HD3	1:D:158:PHE:CE2	2.45	0.51
1:D:98:MET:HE2	1:E:167:ARG:HD3	1.93	0.51
1:D:166:SER:O	1:E:59:THR:HG22	2.11	0.51
1:D:20:ARG:N	1:D:23:GLU:OE1	2.34	0.51
1:C:156:VAL:HA	1:C:160:GLU:OE1	2.12	0.50
1:A:38:LYS:HZ2	1:A:38:LYS:HB3	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:SER:C	1:E:59:THR:HG22	2.36	0.49
1:A:51:MET:SD	1:A:87:MET:HE1	2.53	0.49
1:B:134:HIS:HD2	1:B:135:GLN:O	1.95	0.49
1:B:57[B]:MET:HE2	1:C:167:ARG:O	2.13	0.49
1:C:28:ARG:O	1:C:32:ARG:HG3	2.12	0.49
1:D:22:GLU:H	1:D:22:GLU:CD	2.21	0.48
1:B:107:ALA:CB	3:B:601:HEZ:H32	2.43	0.48
1:D:95:THR:HG22	1:D:165:MET:O	2.14	0.48
1:A:129:ARG:NH2	1:A:135:GLN:OE1	2.47	0.48
1:A:165:MET:HE2	1:F:61:MET:HE3	1.95	0.48
1:A:101:VAL:HG11	1:B:57[B]:MET:HG2	1.96	0.48
1:D:64:ILE:O	1:D:68:GLN:HB2	2.13	0.48
1:C:72[B]:MET:CG	1:C:73:ASN:N	2.76	0.47
1:C:90:LYS:NZ	4:C:183:HOH:O	2.47	0.47
1:D:148:VAL:CG2	1:E:60:GLU:HG2	2.43	0.47
1:D:47:LEU:O	1:D:51:MET:HG3	2.14	0.47
1:D:68:GLN:O	1:D:72:MET:HB2	2.14	0.47
1:C:119:ILE:HB	1:C:156:VAL:HB	1.97	0.47
1:A:167:ARG:HH11	1:A:167:ARG:HG2	1.80	0.47
1:B:106:ASP:OD1	1:B:109:ARG:NH1	2.44	0.47
1:B:91:LEU:HD21	3:B:602:HEZ:C5	2.41	0.46
1:A:43:ASN:ND2	1:A:43:ASN:C	2.69	0.45
1:D:161:PHE:O	1:D:164:MET:HB2	2.16	0.45
1:A:51:MET:O	1:A:54:MET:HG3	2.17	0.45
1:D:134:HIS:NE2	1:E:72:MET:HG3	2.31	0.45
1:B:43:ASN:HD21	1:B:46:ASP:CG	2.25	0.45
1:A:45:ARG:NH2	1:B:116:ASP:O	2.50	0.45
1:A:57[B]:MET:CE	1:B:101:VAL:CG1	2.96	0.44
1:F:64:ILE:O	1:F:68:GLN:HG2	2.17	0.44
1:D:68:GLN:HG3	1:E:134:HIS:NE2	2.33	0.44
1:C:128:MET:HE3	1:C:128:MET:HA	1.99	0.44
1:D:72:MET:SD	1:E:134:HIS:CG	3.10	0.44
1:C:164:MET:HB3	1:C:165:MET:HE3	1.99	0.44
1:A:57[A]:MET:HA	1:A:57[A]:MET:CE	2.47	0.44
1:B:38:LYS:HE3	1:B:76:GLY:O	2.18	0.44
1:F:99:ILE:O	1:F:103:GLU:HB3	2.18	0.43
1:E:27:LEU:HD13	1:E:84:VAL:HG22	2.00	0.43
1:A:129:ARG:NH2	1:A:135:GLN:CD	2.76	0.43
1:F:74:LEU:C	1:F:76:GLY:H	2.26	0.43
1:C:39:ASP:C	1:C:41:TYR:N	2.75	0.43
1:B:132:LEU:CD1	1:C:68:GLN:HG3	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:THR:O	1:D:99:ILE:HG13	2.19	0.42
1:A:166:SER:HA	4:A:178:HOH:O	2.18	0.42
1:B:128:MET:HE2	1:C:64:ILE:HG21	2.00	0.42
1:F:43:ASN:HD22	1:F:43:ASN:N	2.07	0.42
1:F:148:VAL:CG2	1:F:164:MET:HG3	2.49	0.42
1:D:97:ASP:OD2	1:D:97:ASP:N	2.50	0.42
1:B:79:ASP:HB2	4:B:175:HOH:O	2.19	0.42
1:D:63:LEU:HD12	1:D:63:LEU:HA	1.90	0.42
1:C:99:ILE:CG2	1:C:103:GLU:HB3	2.50	0.42
1:D:160:GLU:HA	4:D:169:HOH:O	2.18	0.42
1:C:45:ARG:NE	1:D:118:GLU:OE1	2.52	0.42
1:C:42:ILE:H	1:C:71:ASN:ND2	2.16	0.42
1:F:129:ARG:HA	1:F:134:HIS:O	2.20	0.42
1:B:145:ILE:HD13	1:B:145:ILE:HA	1.94	0.42
1:D:22:GLU:CD	1:D:22:GLU:N	2.77	0.42
1:A:52:ARG:HE	1:A:57[A]:MET:CE	2.33	0.42
4:E:175:HOH:O	1:F:102:LYS:CB	2.67	0.42
1:A:25:GLU:O	1:A:28:ARG:HB2	2.20	0.41
1:B:38:LYS:CE	1:B:76:GLY:O	2.68	0.41
1:B:99:ILE:CG2	1:B:103:GLU:HB3	2.50	0.41
1:B:107:ALA:HB1	3:B:601:HEZ:H32	2.02	0.41
1:E:165:MET:HE2	1:E:165:MET:HB2	1.96	0.41
1:B:134:HIS:CD2	1:B:135:GLN:O	2.73	0.41
1:C:26:GLU:HA	1:C:29:GLU:HG3	2.02	0.41
1:F:148:VAL:HG21	1:F:164:MET:HG3	2.02	0.41
1:A:101:VAL:HG21	1:B:57[A]:MET:HG2	2.01	0.41
1:A:140:ASP:O	1:A:144:ILE:HG13	2.20	0.41
1:A:165:MET:CE	1:F:61:MET:CE	2.98	0.41
1:F:104:LEU:HD12	1:F:104:LEU:HA	1.91	0.41
1:F:81:ASP:O	1:F:85:GLU:HG2	2.21	0.41
1:C:121:THR:HG22	1:C:141:ILE:HG22	2.03	0.41
1:D:34:PHE:HB2	1:D:50:CYS:SG	2.61	0.41
1:B:92:LEU:O	3:B:602:HEZ:H11	2.20	0.40
1:C:57[A]:MET:HG2	1:D:101:VAL:CG2	2.51	0.40
1:C:121:THR:HG23	1:C:145:ILE:HG13	2.04	0.40
1:C:49:ASN:OD1	1:C:52:ARG:NH1	2.52	0.40
1:F:132:LEU:HB3	1:F:134:HIS:CE1	2.56	0.40
1:A:52:ARG:HE	1:A:57[A]:MET:HE2	1.86	0.40
1:A:141:ILE:HD13	1:A:144:ILE:HD12	2.02	0.40
1:C:41:TYR:CD1	1:C:41:TYR:C	2.99	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	152/153 (99%)	149 (98%)	3 (2%)	0	100	100
1	B	152/153 (99%)	149 (98%)	3 (2%)	0	100	100
1	C	154/153 (101%)	149 (97%)	5 (3%)	0	100	100
1	D	142/153 (93%)	138 (97%)	3 (2%)	1 (1%)	18	28
1	E	113/153 (74%)	111 (98%)	2 (2%)	0	100	100
1	F	145/153 (95%)	142 (98%)	3 (2%)	0	100	100
All	All	858/918 (94%)	838 (98%)	19 (2%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	88	GLY

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	124/134 (92%)	109 (88%)	15 (12%)	5	7
1	B	131/134 (98%)	119 (91%)	12 (9%)	8	14
1	C	128/134 (96%)	109 (85%)	19 (15%)	3	4
1	D	120/134 (90%)	108 (90%)	12 (10%)	7	11
1	E	97/134 (72%)	91 (94%)	6 (6%)	16	29
1	F	121/134 (90%)	106 (88%)	15 (12%)	4	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	721/804 (90%)	642 (89%)	79 (11%)	6 9

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	25	GLU
1	A	28	ARG
1	A	38	LYS
1	A	43	ASN
1	A	57[A]	MET
1	A	57[B]	MET
1	A	63	LEU
1	A	97	ASP
1	A	118	GLU
1	A	122	SER
1	A	129	ARG
1	A	138	HIS
1	A	148	VAL
1	A	165	MET
1	B	43	ASN
1	B	50	CYS
1	B	63	LEU
1	B	74	LEU
1	B	102	LYS
1	B	113	THR
1	B	118	GLU
1	B	128	MET
1	B	129	ARG
1	B	138	HIS
1	B	139	ARG
1	B	159	GLU
1	C	22	GLU
1	C	37	ASP
1	C	39	ASP
1	C	41	TYR
1	C	42	ILE
1	C	50[A]	CYS
1	C	50[B]	CYS
1	C	63	LEU
1	C	72[A]	MET
1	C	72[B]	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	102	LYS
1	C	110	GLU
1	C	113	THR
1	C	118	GLU
1	C	121	THR
1	C	122	SER
1	C	146	ARG
1	C	148	VAL
1	C	165	MET
1	D	34	PHE
1	D	53	THR
1	D	54	MET
1	D	63	LEU
1	D	68	GLN
1	D	70	ILE
1	D	95	THR
1	D	97	ASP
1	D	102	LYS
1	D	113	THR
1	D	118	GLU
1	D	126	GLU
1	E	25	GLU
1	E	63	LEU
1	E	78	VAL
1	E	85	GLU
1	E	138	HIS
1	E	139	ARG
1	F	43	ASN
1	F	50	CYS
1	F	63	LEU
1	F	72	MET
1	F	90	LYS
1	F	97	ASP
1	F	103	GLU
1	F	104	LEU
1	F	118	GLU
1	F	121	THR
1	F	129	ARG
1	F	138	HIS
1	F	143	GLU
1	F	148	VAL
1	F	159	GLU

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

Mol	Chain	Res	Type
1	A	43	ASN
1	A	71	ASN
1	A	73	ASN
1	B	43	ASN
1	B	71	ASN
1	C	68	GLN
1	C	71	ASN
1	D	68	GLN
1	E	68	GLN
1	E	69	GLN
1	E	71	ASN
1	F	43	ASN
1	F	69	GLN
1	F	71	ASN
1	F	134	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 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	HEZ	B	602	-	7,7,7	0.43	0	6,6,6	0.43	0
3	HEZ	A	604	-	7,7,7	0.30	0	6,6,6	0.64	0
3	HEZ	B	601	-	7,7,7	0.30	0	6,6,6	0.55	0
3	HEZ	A	603	-	7,7,7	0.42	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	HEZ	B	602	-	-	4/5/5/5	-
3	HEZ	A	604	-	-	3/5/5/5	-
3	HEZ	B	601	-	-	5/5/5/5	-
3	HEZ	A	603	-	-	3/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	HEZ	C3-C4-C5-C6
3	B	601	HEZ	C3-C4-C5-C6
3	B	601	HEZ	C1-C2-C3-C4
3	A	603	HEZ	C4-C5-C6-O6
3	B	602	HEZ	O1-C1-C2-C3
3	B	602	HEZ	C4-C5-C6-O6
3	A	604	HEZ	O1-C1-C2-C3
3	B	601	HEZ	O1-C1-C2-C3
3	A	603	HEZ	O1-C1-C2-C3
3	B	601	HEZ	C4-C5-C6-O6
3	A	604	HEZ	C2-C3-C4-C5
3	A	603	HEZ	C2-C3-C4-C5
3	A	604	HEZ	C4-C5-C6-O6
3	B	602	HEZ	C2-C3-C4-C5
3	B	601	HEZ	C2-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	HEZ	4	0
3	B	601	HEZ	4	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, 95th 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 ²)	Q<0.9
1	A	153/153 (100%)	0.19	2 (1%) 75 71	35, 73, 116, 139	1 (0%)
1	B	153/153 (100%)	-0.03	2 (1%) 75 71	29, 64, 88, 96	1 (0%)
1	C	153/153 (100%)	0.30	6 (3%) 43 39	34, 84, 121, 146	3 (1%)
1	D	146/153 (95%)	0.87	13 (8%) 15 12	62, 104, 147, 175	0
1	E	118/153 (77%)	1.19	24 (20%) 3 2	55, 101, 157, 193	1 (0%)
1	F	148/153 (96%)	1.09	25 (16%) 4 3	73, 119, 163, 189	1 (0%)
All	All	871/918 (94%)	0.57	72 (8%) 17 14	29, 88, 148, 193	7 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	113	THR	5.7
1	F	138	HIS	4.6
1	C	137	GLY	4.3
1	F	106	ASP	4.2
1	D	145	ILE	4.0
1	D	146	ARG	3.8
1	E	158	PHE	3.5
1	A	133	GLY	3.5
1	D	46	ASP	3.4
1	F	117	GLY	3.4
1	F	139	ARG	3.4
1	F	107	ALA	3.3
1	D	141	ILE	3.3
1	E	150	LEU	3.1
1	E	37	ASP	3.1
1	F	109	ARG	3.1
1	E	134	HIS	3.1
1	E	18	SER	3.1
1	F	112	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	77	HIS	2.9
1	E	155	ARG	2.9
1	E	149	ASP	2.8
1	E	35	ASP	2.8
1	A	138	HIS	2.8
1	E	25	GLU	2.8
1	E	36	LYS	2.7
1	F	123	GLU	2.7
1	D	156	VAL	2.6
1	D	120	SER	2.6
1	F	120	SER	2.6
1	B	41	TYR	2.5
1	E	46	ASP	2.5
1	D	148	VAL	2.5
1	E	151	ASN	2.5
1	F	21	PRO	2.5
1	E	83	PHE	2.5
1	E	138	HIS	2.4
1	B	130	ALA	2.4
1	D	133	GLY	2.3
1	F	115	GLY	2.3
1	C	138	HIS	2.3
1	F	114	ASN	2.3
1	F	30	ALA	2.3
1	D	47	LEU	2.3
1	E	157	ASP	2.3
1	F	102	LYS	2.3
1	F	45	ARG	2.3
1	E	33	GLU	2.3
1	E	144	ILE	2.3
1	C	115	GLY	2.2
1	F	36	LYS	2.2
1	F	42	ILE	2.2
1	E	160	GLU	2.1
1	C	116	ASP	2.1
1	C	72[A]	MET	2.1
1	C	151	ASN	2.1
1	E	22	GLU	2.1
1	D	106	ASP	2.1
1	E	153	ASP	2.1
1	E	156	VAL	2.1
1	D	150	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	33	GLU	2.1
1	F	145	ILE	2.1
1	F	81	ASP	2.1
1	E	148	VAL	2.0
1	E	146	ARG	2.0
1	E	161	PHE	2.0
1	F	156	VAL	2.0
1	F	118	GLU	2.0
1	F	133	GLY	2.0
1	F	154	GLY	2.0
1	F	97	ASP	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	E	502	1/1	0.61	0.17	252,252,252,252	0
3	HEZ	A	604	8/8	0.66	0.15	102,105,110,114	0
2	CA	F	501	1/1	0.71	0.30	182,182,182,182	0
2	CA	D	501	1/1	0.84	0.12	131,131,131,131	0
3	HEZ	B	602	8/8	0.84	0.11	81,83,85,86	0
2	CA	F	502	1/1	0.86	0.13	172,172,172,172	0
3	HEZ	B	601	8/8	0.90	0.08	75,78,80,83	0
2	CA	C	501	1/1	0.92	0.13	136,136,136,136	0
3	HEZ	A	603	8/8	0.93	0.10	83,88,93,95	0
2	CA	A	501	1/1	0.95	0.11	84,84,84,84	0
2	CA	C	502	1/1	0.95	0.11	114,114,114,114	0
2	CA	D	502	1/1	0.96	0.05	140,140,140,140	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	B	502	1/1	0.97	0.10	79,79,79,79	0
2	CA	A	502	1/1	0.97	0.12	111,111,111,111	0
2	CA	B	501	1/1	0.98	0.10	84,84,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.