



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:08 am GMT

PDB ID : 3OX6  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

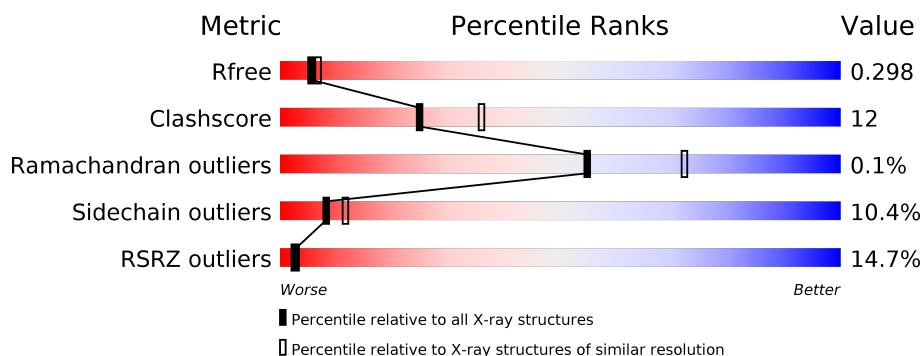
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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 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	153	<div> <div>3%</div> <div>76%</div> <div>20%</div> <div>• •</div> </div>
1	B	153	<div> <div>%</div> <div>76%</div> <div>22%</div> <div>•</div> </div>
1	C	153	<div> <div>12%</div> <div>74%</div> <div>22%</div> <div>•</div> </div>
1	D	153	<div> <div>22%</div> <div>65%</div> <div>25%</div> <div>5% 5%</div> </div>
1	E	153	<div> <div>21%</div> <div>67%</div> <div>10%</div> <div>• 23%</div> </div>
1	F	153	<div> <div>25%</div> <div>76%</div> <div>17%</div> <div>• •</div> </div>

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	CA	F	501	-	-	-	X
3	HEZ	A	604	-	-	-	X
3	HEZ	B	602	-	-	-	X

## 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			

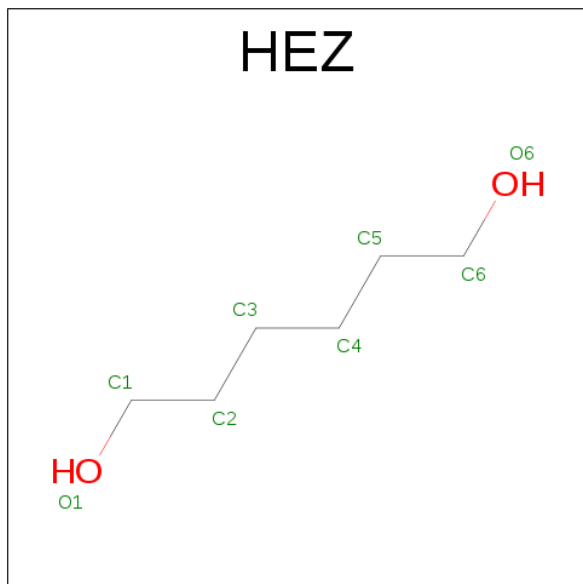
There are 12 discrepancies between the modelled and reference sequences:

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 (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is HEXANE-1,6-DIOL (three-letter code: 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

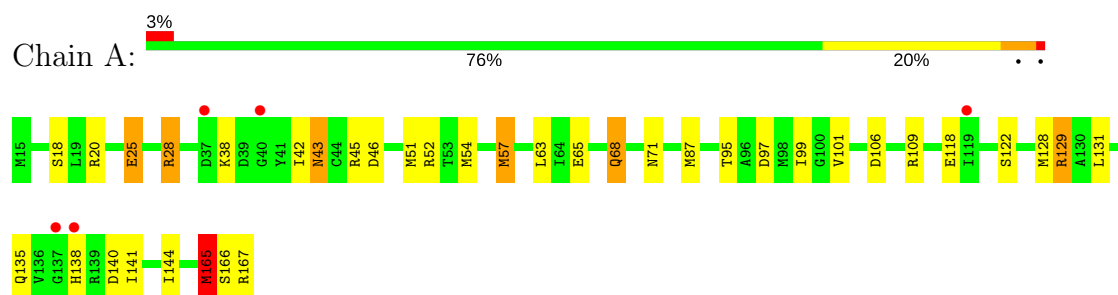
- Molecule 4 is water.

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

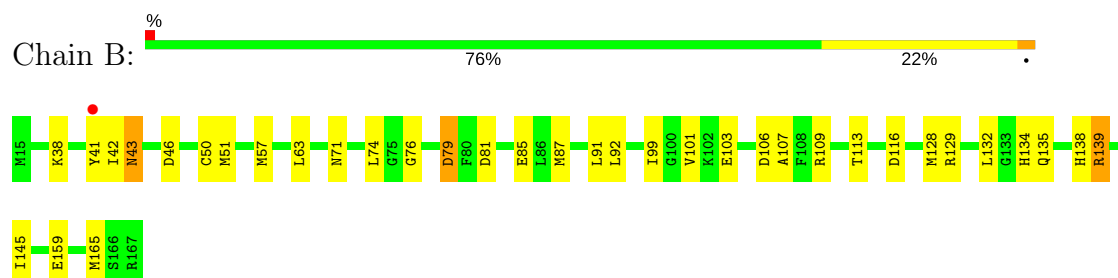
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

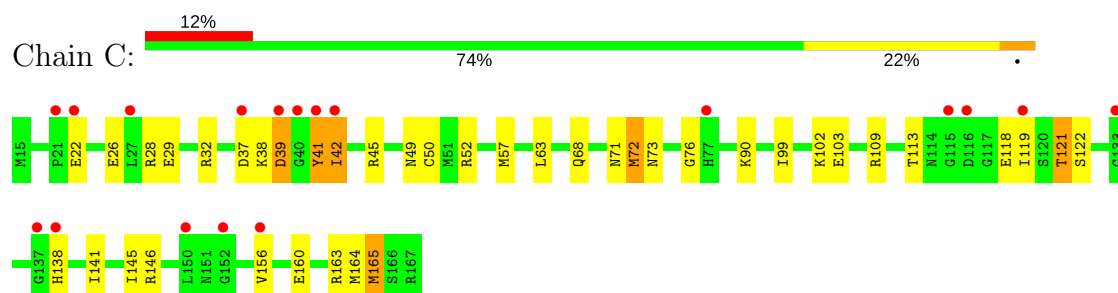
#### • Molecule 1: Calcium-binding protein 1



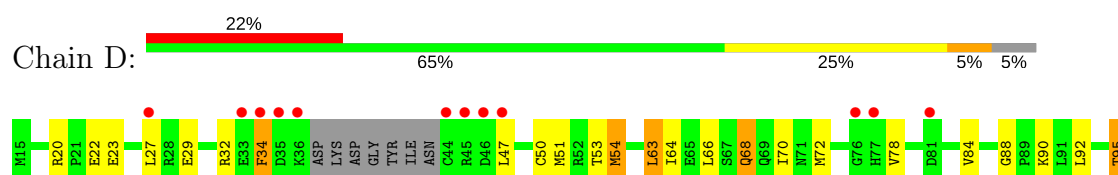
#### • Molecule 1: Calcium-binding protein 1

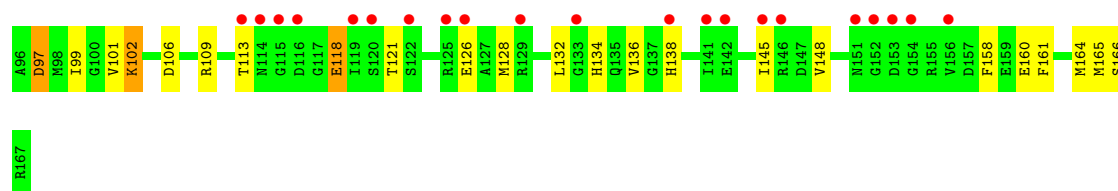


#### • Molecule 1: Calcium-binding protein 1

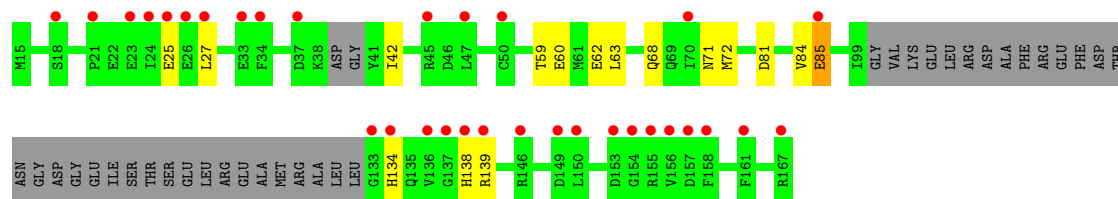


#### • Molecule 1: Calcium-binding protein 1

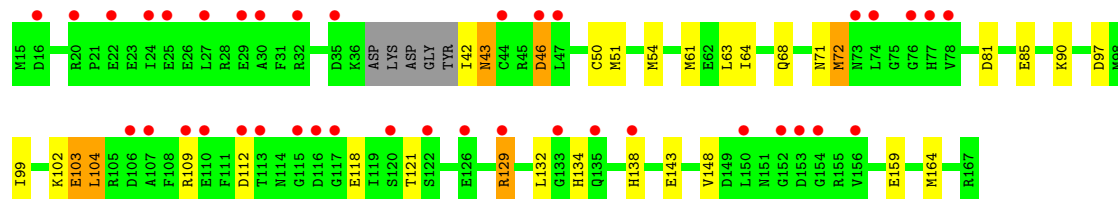
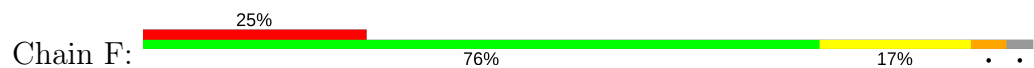




• Molecule 1: Calcium-binding protein 1



• 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, $\alpha$ , $\beta$ , $\gamma$	68.72Å 68.72Å 344.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.40 14.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (15.00-2.40) 99.4 (14.90-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 66.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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	0.81	0/1206	0.85	1/1618 (0.1%)
1	B	0.90	0/1240	0.92	1/1660 (0.1%)
1	C	0.77	0/1229	0.84	1/1648 (0.1%)
1	D	0.66	0/1154	0.76	0/1544
1	E	0.70	1/934 (0.1%)	0.73	0/1248
1	F	0.56	0/1170	0.71	0/1569
All	All	0.75	1/6933 (0.0%)	0.81	3/9287 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	62	GLU	CD-OE2	-5.04	1.20	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	109	ARG	NE-CZ-NH2	5.81	123.21	120.30
1	B	79	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	165	MET	CG-SD-CE	5.22	108.56	100.20

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	1189	0	1101	45	0
1	B	1222	0	1154	44	0
1	C	1205	0	1130	33	0
1	D	1142	0	1065	35	0
1	E	922	0	859	16	0
1	F	1154	0	1064	22	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	162	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 12.

All (162) 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:HG2	1:A:87:MET:HE1	1.20	1.12
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:B:51:MET:CE	1:B:87:MET:HE1	1.95	0.96
1:A:51:MET:CG	1:A:87:MET:HE1	1.99	0.93
1:B:51:MET:HE3	1:B:87:MET:HE1	1.50	0.91
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ARG:HH11	1:B:139:ARG:HG2	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:HG3	1:A:28:ARG:HH11	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:A:43:ASN:C	1:A:43:ASN:HD22	1.95	0.69
1:B:43:ASN:ND2	1:B:46:ASP:H	1.91	0.69
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:A:57[A]:MET:HE2	1:A:57[A]:MET:HA	1.79	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:C:39:ASP:N	1:C:39:ASP:OD1	2.33	0.61
1:B:132:LEU:HD13	1:C:68:GLN:HG3	1.82	0.61
1:F:43:ASN:H	1:F:43:ASN:HD22	1.48	0.61
1:C:72[B]:MET:HG3	1:C:73:ASN:N	2.16	0.61
1:C:57[A]:MET:HG2	1:D:101:VAL:HG21	1.82	0.60
1:C:42:ILE:H	1:C:71:ASN:HD21	1.48	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
1:C:102:LYS:HZ2	1:C:102:LYS:HB2	1.68	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: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
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:A:95:THR:O	1:A:99:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:51:MET:HE3	1:B:87:MET:CE	2.34	0.52
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:39:ASP:C	1:C:41:TYR:H	2.12	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:A:51:MET:CE	1:A:87:MET:HE1	2.41	0.51
1:D:166:SER:O	1:E:59:THR:HG22	2.11	0.51
1:A:128:MET:CE	1:F:64:ILE:HG21	2.41	0.51
1:D:20:ARG:N	1:D:23:GLU:OE1	2.34	0.51
1:A:57[B]:MET:HE1	1:B:101:VAL:HG13	1.93	0.50
1:B:43:ASN:C	1:B:43:ASN:HD22	2.14	0.50
1:C:156:VAL:HA	1:C:160:GLU:OE1	2.12	0.50
1:C:164:MET:HB3	1:C:165:MET:HE3	1.94	0.49
1:B:134:HIS:HD2	1:B:135:GLN:O	1.95	0.49
1:C:28:ARG:O	1:C:32:ARG:HG3	2.12	0.49
1:A:51:MET:SD	1:A:87:MET:HE1	2.53	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: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:B:51:MET:HE2	1:B:87:MET:HE1	1.88	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:68:GLN:O	1:D:72:MET:HB2	2.14	0.47
1:D:47:LEU:O	1:D:51:MET:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ILE:HB	1:C:156:VAL:HB	1.97	0.47
1:B:87:MET:HE3	1:B:87:MET:HA	1.96	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:A:57[B]:MET:HE2	1:B:101:VAL:CG1	2.45	0.46
1:B:91:LEU:HD21	3:B:602:HEZ:C5	2.41	0.46
1:A:128:MET:HE1	1:F:64:ILE:HG21	1.97	0.46
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:A:57[B]:MET:HE2	1:B:101:VAL:HG11	1.99	0.45
1:D:166:SER:C	1:E:59:THR:HG22	2.36	0.45
1:A:51:MET:CE	1:A:87:MET:CE	2.95	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:D:72:MET:SD	1:E:134:HIS:CG	3.10	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:B:132:LEU:CD1	1:C:68:GLN:HG3	2.47	0.42
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:D:22:GLU:H	1:D:22:GLU:CD	2.21	0.42
1:F:148:VAL:CG2	1:F:164:MET:HG3	2.49	0.42
1:F:43:ASN:N	1:F:43:ASN:HD22	2.07	0.42
1:D:97:ASP:N	1:D:97:ASP:OD2	2.50	0.42
1:B:79:ASP:HB2	4:B:175:HOH:O	2.19	0.42
1:D:63:LEU:HA	1:D:63:LEU:HD12	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:B:57[B]:MET:HB3	1:B:57[B]:MET:HE2	1.76	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:HA	1:B:145:ILE:HD13	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ALA:HB1	3:B:601:HEZ:H32	2.02	0.41
1:B:99:ILE:CG2	1:B:103:GLU:HB3	2.50	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:F:104:LEU:HA	1:F:104:LEU:HD12	1.91	0.41
1:A:165:MET:CE	1:F:61:MET:CE	2.98	0.41
1:F:81:ASP:O	1:F:85:GLU:HG2	2.21	0.41
1:A:57[B]:MET:HE3	1:B:101:VAL:HG22	2.02	0.41
1:B:51:MET:CE	1:B:87:MET:CE	2.83	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:A:57[A]:MET:HA	1:A:57[A]:MET:CE	2.47	0.40
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:A:165:MET:HE2	1:F:61:MET:CE	2.51	0.40
1:C:121:THR:HG23	1:C:145:ILE:HG13	2.04	0.40
1:A:43:ASN:C	1:A:43:ASN:ND2	2.69	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:141:ILE:HD13	1:A:144:ILE:HD12	2.02	0.40
1:B:43:ASN:HD21	1:B:46:ASP:CG	2.25	0.40
1:C:39:ASP:C	1:C:41:TYR:N	2.75	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	152/153 (99%)	149 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	25	37
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%)	55	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	88	GLY

### 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	124/134 (92%)	109 (88%)	15 (12%)	6	7
1	B	131/134 (98%)	119 (91%)	12 (9%)	11	16
1	C	128/134 (96%)	112 (88%)	16 (12%)	5	6
1	D	120/134 (90%)	106 (88%)	14 (12%)	6	8
1	E	97/134 (72%)	92 (95%)	5 (5%)	27	43
1	F	121/134 (90%)	106 (88%)	15 (12%)	5	6
All	All	721/804 (90%)	644 (89%)	77 (11%)	8	10

All (77) 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

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Mol	Chain	Res	Type
1	A	57[A]	MET
1	A	57[B]	MET
1	A	63	LEU
1	A	68	GLN
1	A	97	ASP
1	A	118	GLU
1	A	122	SER
1	A	129	ARG
1	A	138	HIS
1	A	165	MET
1	B	41	TYR
1	B	43	ASN
1	B	50	CYS
1	B	63	LEU
1	B	74	LEU
1	B	113	THR
1	B	128	MET
1	B	129	ARG
1	B	138	HIS
1	B	139	ARG
1	B	159	GLU
1	B	165	MET
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
1	C	113	THR
1	C	118	GLU
1	C	121	THR
1	C	122	SER
1	C	146	ARG
1	C	165	MET
1	D	34	PHE
1	D	53	THR
1	D	54	MET
1	D	63	LEU

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Mol	Chain	Res	Type
1	D	68	GLN
1	D	90	LYS
1	D	92	LEU
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	D	138	HIS
1	E	25	GLU
1	E	63	LEU
1	E	85	GLU
1	E	138	HIS
1	E	139	ARG
1	F	43	ASN
1	F	46	ASP
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	159	GLU

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	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

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Mol	Chain	Res	Type
1	E	68	GLN
1	E	69	GLN
1	E	71	ASN
1	F	43	ASN
1	F	68	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 carbohydrates 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	A	603	-	7,7,7	0.42	0	6,6,6	0.32	0
3	HEZ	A	604	-	7,7,7	0.31	0	6,6,6	0.63	0
3	HEZ	B	601	-	7,7,7	0.30	0	6,6,6	0.55	0
3	HEZ	B	602	-	7,7,7	0.43	0	6,6,6	0.43	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	A	603	-	-	0/5/5/5	0/0/0/0
3	HEZ	A	604	-	-	0/5/5/5	0/0/0/0
3	HEZ	B	601	-	-	0/5/5/5	0/0/0/0
3	HEZ	B	602	-	-	0/5/5/5	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	HEZ	4	0
3	B	602	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, 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	153/153 (100%)	0.18	5 (3%)	47 45	41, 73, 116, 139	0
1	B	153/153 (100%)	0.03	1 (0%)	87 86	44, 64, 88, 96	0
1	C	153/153 (100%)	0.40	18 (11%)	5 4	46, 85, 121, 146	0
1	D	146/153 (95%)	1.14	33 (22%)	1 1	62, 104, 147, 175	0
1	E	118/153 (77%)	1.36	32 (27%)	1 1	69, 101, 157, 193	0
1	F	148/153 (96%)	1.38	39 (26%)	1 1	73, 119, 163, 189	0
All	All	871/918 (94%)	0.72	128 (14%)	3 2	41, 88, 148, 193	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	113	THR	10.1
1	C	138	HIS	7.5
1	D	146	ARG	7.4
1	F	117	GLY	6.8
1	F	138	HIS	6.6
1	E	138	HIS	6.5
1	D	138	HIS	6.0
1	D	145	ILE	6.0
1	E	136	VAL	5.8
1	D	46	ASP	5.6
1	E	146	ARG	5.6
1	E	150	LEU	5.2
1	E	155	ARG	5.2
1	F	153	ASP	4.8
1	F	76	GLY	4.7
1	F	35	ASP	4.7
1	F	122	SER	4.6
1	E	33	GLU	4.6
1	E	137	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	126	GLU	4.4
1	C	119	ILE	4.4
1	E	134	HIS	4.4
1	E	156	VAL	4.4
1	D	33	GLU	4.3
1	E	24	ILE	4.2
1	D	156	VAL	4.2
1	F	106	ASP	4.1
1	F	129	ARG	4.1
1	D	44	CYS	4.1
1	E	18	SER	4.1
1	D	133	GLY	4.1
1	E	25	GLU	4.0
1	F	109	ARG	3.9
1	D	115	GLY	3.8
1	E	133	GLY	3.8
1	C	156	VAL	3.8
1	A	138	HIS	3.8
1	D	122	SER	3.7
1	F	154	GLY	3.7
1	B	41	TYR	3.6
1	F	77	HIS	3.6
1	F	20	ARG	3.5
1	F	116	ASP	3.5
1	E	154	GLY	3.5
1	F	32	ARG	3.5
1	E	158	PHE	3.4
1	C	27	LEU	3.4
1	F	156	VAL	3.4
1	A	137	GLY	3.4
1	F	46	ASP	3.4
1	E	50[A]	CYS	3.4
1	E	161	PHE	3.4
1	D	27	LEU	3.3
1	E	37	ASP	3.3
1	E	149	ASP	3.3
1	F	44	CYS	3.2
1	E	21	PRO	3.2
1	D	120	SER	3.2
1	F	107	ALA	3.2
1	D	45	ARG	3.2
1	C	133	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	142	GLU	3.2
1	C	77	HIS	3.1
1	D	152	GLY	3.1
1	C	40	GLY	3.1
1	F	110	GLU	3.1
1	D	36	LYS	3.1
1	E	45	ARG	3.1
1	E	157	ASP	2.9
1	A	119	ILE	2.9
1	C	41	TYR	2.9
1	A	40	GLY	2.9
1	D	77	HIS	2.9
1	F	25	GLU	2.9
1	D	34	PHE	2.9
1	E	27	LEU	2.8
1	F	30	ALA	2.8
1	E	153	ASP	2.8
1	C	115	GLY	2.8
1	F	22	GLU	2.8
1	F	74	LEU	2.8
1	F	152	GLY	2.7
1	D	153	ASP	2.7
1	D	141	ILE	2.7
1	F	126	GLU	2.6
1	D	76	GLY	2.6
1	C	37	ASP	2.6
1	E	23	GLU	2.6
1	D	119	ILE	2.6
1	D	35	ASP	2.6
1	D	81	ASP	2.6
1	D	116	ASP	2.6
1	E	167	ARG	2.5
1	C	21	PRO	2.5
1	C	152	GLY	2.5
1	D	129	ARG	2.5
1	E	26	GLU	2.5
1	E	85	GLU	2.5
1	E	47	LEU	2.4
1	D	125	ARG	2.4
1	F	78	VAL	2.4
1	C	116	ASP	2.4
1	F	27	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	37	ASP	2.4
1	F	112	ASP	2.4
1	C	137	GLY	2.3
1	C	39	ASP	2.3
1	C	42	ILE	2.3
1	F	16	ASP	2.3
1	F	29	GLU	2.3
1	F	47	LEU	2.2
1	E	70	ILE	2.2
1	F	150	LEU	2.2
1	F	24	ILE	2.1
1	F	115	GLY	2.1
1	F	135	GLN	2.1
1	D	113	THR	2.1
1	D	114	ASN	2.1
1	D	151	ASN	2.1
1	D	47	LEU	2.0
1	C	22	GLU	2.0
1	F	73	ASN	2.0
1	C	150	LEU	2.0
1	D	154	GLY	2.0
1	F	133	GLY	2.0
1	E	34	PHE	2.0
1	E	139	ARG	2.0
1	F	120	SER	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 ⓘ

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
3	HEZ	A	604	8/8	0.63	0.28	4.25	102,105,110,114	0
3	HEZ	B	602	8/8	0.75	0.26	2.97	81,83,85,86	0
3	HEZ	A	603	8/8	0.83	0.20	1.17	83,88,93,95	0
3	HEZ	B	601	8/8	0.85	0.17	0.90	75,78,80,83	0
2	CA	F	501	1/1	0.80	0.46	0.37	182,182,182,182	0
2	CA	A	501	1/1	0.86	0.22	0.16	84,84,84,84	0
2	CA	C	502	1/1	0.96	0.18	-0.69	114,114,114,114	0
2	CA	A	502	1/1	0.91	0.17	-0.69	111,111,111,111	0
2	CA	B	502	1/1	0.96	0.14	-0.80	79,79,79,79	0
2	CA	B	501	1/1	0.96	0.14	-0.92	84,84,84,84	0
2	CA	C	501	1/1	0.82	0.17	-1.13	136,136,136,136	0
2	CA	F	502	1/1	0.71	0.14	-1.19	172,172,172,172	0
2	CA	D	502	1/1	0.76	0.05	-2.34	140,140,140,140	0
2	CA	E	502	1/1	0.87	0.12	-2.52	252,252,252,252	0
2	CA	D	501	1/1	0.61	0.08	-3.26	131,131,131,131	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.