



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2016 – 11:40 AM EDT

PDB ID : 5G1R  
Title : Open conformation of Francisella tularensis ClpP at 1.9 Å  
Authors : Diaz-Saez, L.; Hunter, W.N.  
Deposited on : 2016-03-29  
Resolution : 1.90 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:

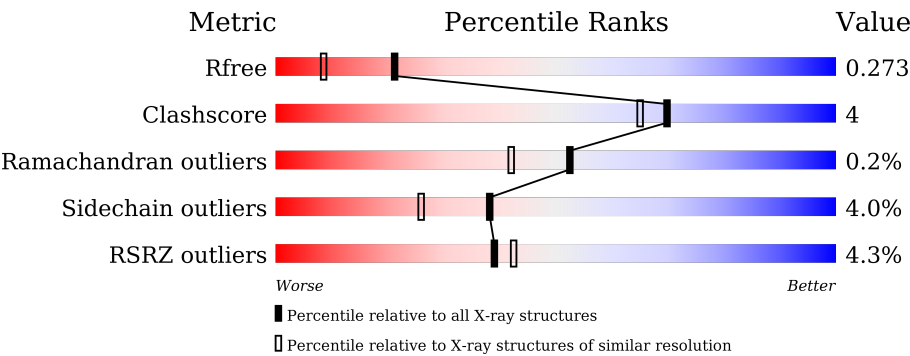
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

# 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 1.90 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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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  $\geq 3$ , 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	201	<div><div>5%</div><div><div></div><div>84%</div><div>12%</div><div>.</div></div></div>
1	B	201	<div><div>3%</div><div><div></div><div>84%</div><div>6%</div><div>.</div><div>8%</div></div></div>
1	C	201	<div><div>8%</div><div><div></div><div>83%</div><div>10%</div><div>.</div><div>5%</div></div></div>
1	D	201	<div><div>3%</div><div><div></div><div>81%</div><div>8%</div><div>.</div><div>8%</div></div></div>
1	E	201	<div><div>4%</div><div><div></div><div>84%</div><div>7%</div><div>.</div><div>6%</div></div></div>
1	F	201	<div><div>2%</div><div><div></div><div>84%</div><div>11%</div><div>.</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	201	 2% 78% 16% ...

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	MPD	F	800	-	-	-	X
3	ACT	A	801	-	-	-	X
3	ACT	C	801	-	-	-	X
3	ACT	F	801	-	-	-	X
3	ACT	G	800	-	-	-	X
4	MRD	C	800	-	-	-	X

## 2 Entry composition

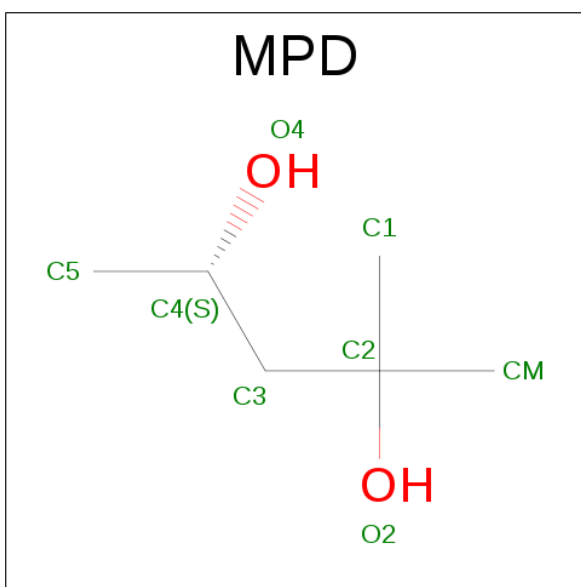
There are 5 unique types of molecules in this entry. The entry contains 11663 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUB-UNIT.

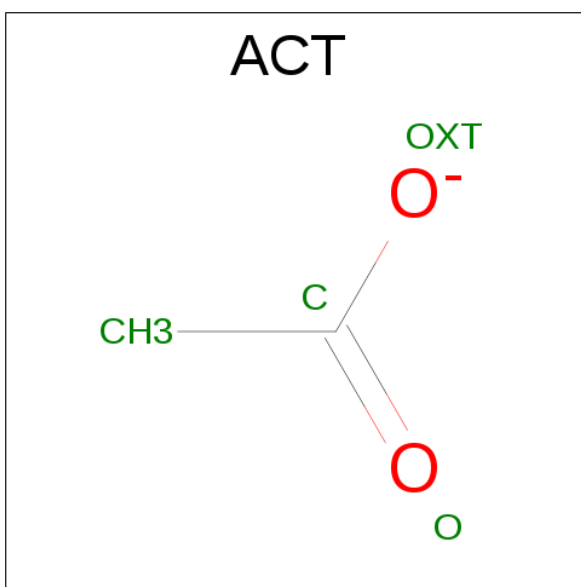
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	10	0
			1539	977	263	289	10			
1	B	184	Total	C	N	O	S	0	5	0
			1459	927	253	271	8			
1	C	190	Total	C	N	O	S	5	3	0
			1493	948	253	284	8			
1	D	184	Total	C	N	O	S	3	5	0
			1455	923	249	274	9			
1	E	189	Total	C	N	O	S	5	3	0
			1476	939	249	280	8			
1	F	192	Total	C	N	O	S	0	7	0
			1527	967	264	287	9			
1	G	194	Total	C	N	O	S	0	13	0
			1561	990	269	293	9			

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



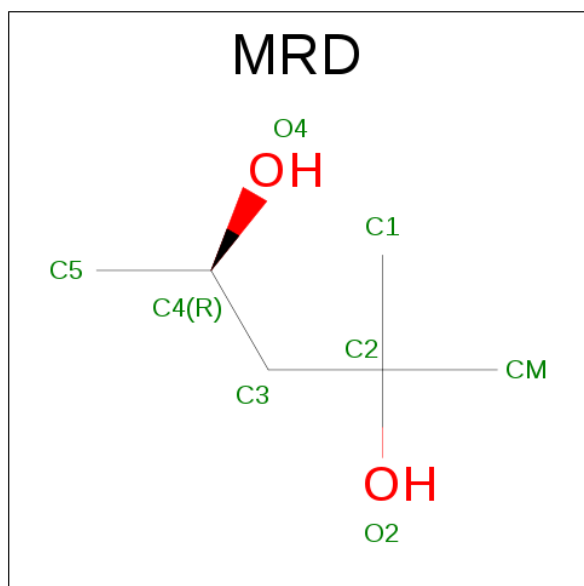
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	194	Total	O	0	0
			194	194		

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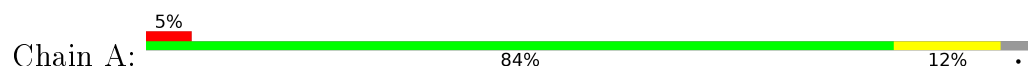
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	172	Total 172	O 172	0	0
5	C	87	Total 87	O 87	0	0
5	D	99	Total 99	O 99	0	0
5	E	147	Total 147	O 147	0	0
5	F	224	Total 224	O 224	0	0
5	G	162	Total 162	O 162	0	0

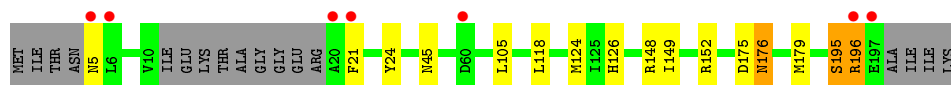
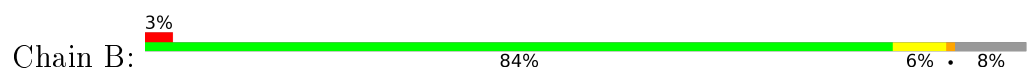
### 3 Residue-property plots [i](#)

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

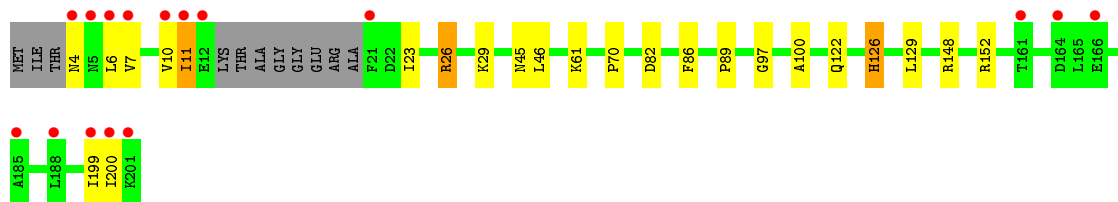
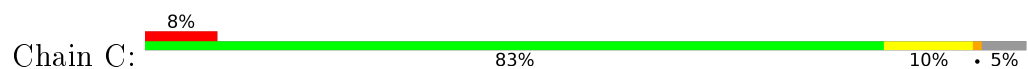
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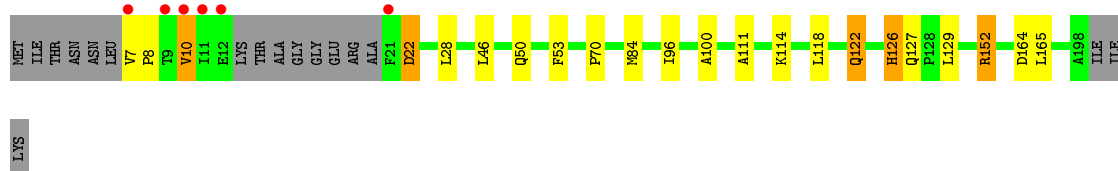
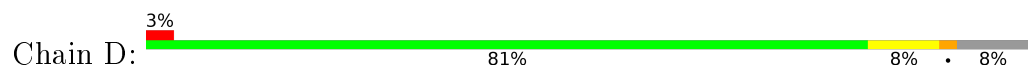
#### • Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT



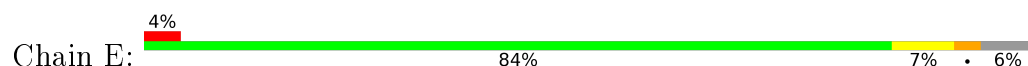
#### • Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT



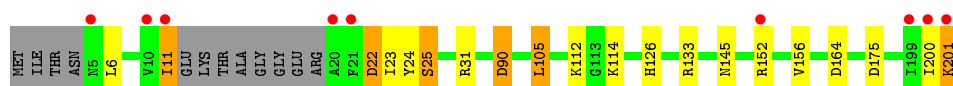
#### • Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT



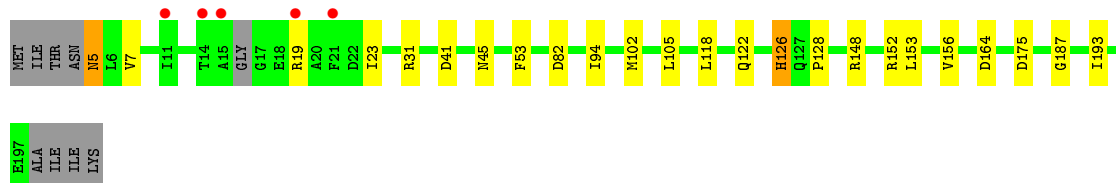
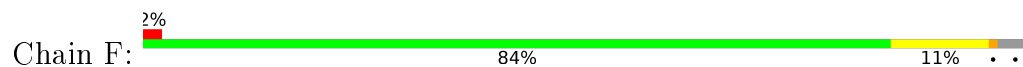
#### • Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT



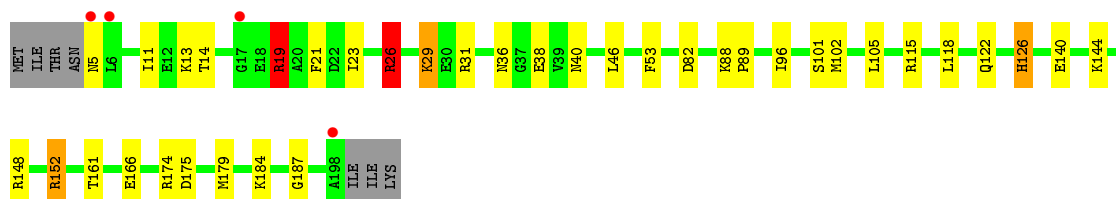
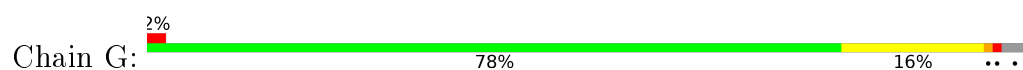




● Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT



● Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.94Å 128.17Å 98.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.26 – 1.90 47.04 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (98.26-1.90) 100.0 (47.04-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.14 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.201 , 0.269 0.208 , 0.273	Depositor DCC
$R_{free}$ test set	5861 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.7	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11663	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, MPD, ACT

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	0.92	0/1602	1.03	7/2157 (0.3%)
1	B	0.86	0/1502	0.90	1/2023 (0.0%)
1	C	1.05	1/1524 (0.1%)	1.03	5/2054 (0.2%)
1	D	0.83	0/1496	1.04	5/2015 (0.2%)
1	E	0.93	1/1511 (0.1%)	1.40	10/2036 (0.5%)
1	F	0.95	1/1576 (0.1%)	1.08	8/2120 (0.4%)
1	G	0.95	0/1635	1.02	9/2201 (0.4%)
All	All	0.93	3/10846 (0.0%)	1.08	45/14606 (0.3%)

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	C	0	1
1	D	0	1
1	E	1	0
All	All	1	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	152	ARG	CG-CD	-24.25	0.91	1.51
1	E	201	LYS	CA-CB	-20.44	1.08	1.53
1	F	187	GLY	C-O	-5.08	1.15	1.23

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	201	LYS	CB-CA-C	-43.34	23.72	110.40
1	C	152	ARG	CB-CG-CD	16.08	153.40	111.60
1	D	10	VAL	N-CA-CB	-14.70	79.16	111.50
1	D	10	VAL	CA-CB-CG2	11.86	128.69	110.90
1	E	201	LYS	CA-CB-CG	11.46	138.62	113.40
1	E	201	LYS	N-CA-CB	-11.16	90.51	110.60
1	A	148	ARG	NE-CZ-NH2	-9.71	115.45	120.30
1	G	115	ARG	NE-CZ-NH1	8.91	124.75	120.30
1	F	164	ASP	CB-CG-OD2	-7.76	111.31	118.30
1	F	148	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	F	164	ASP	CB-CG-OD1	7.31	124.88	118.30
1	C	152	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	F	148	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	E	90	ASP	CB-CG-OD1	7.01	124.61	118.30
1	G	31	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	G	148	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	A	148	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	E	175	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	G	19	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	164	ASP	CB-CA-C	-6.47	97.46	110.40
1	E	31	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	E	90	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	D	10	VAL	CB-CA-C	6.15	123.08	111.40
1	G	19	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	G	26[A]	ARG	NE-CZ-NH1	-6.13	117.24	120.30
1	G	26[B]	ARG	NE-CZ-NH1	-6.13	117.24	120.30
1	C	26	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	F	175	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	C	148	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	22	ASP	CB-CG-OD1	5.73	123.46	118.30
1	F	82	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	D	84	MET	CG-SD-CE	-5.70	91.09	100.20
1	D	10	VAL	CA-CB-CG1	-5.69	102.36	110.90
1	G	148	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	B	175	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	E	175	ASP	CB-CG-OD1	5.46	123.21	118.30
1	F	31	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	C	152	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	124	MET	CG-SD-CE	-5.33	91.67	100.20
1	F	41	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	115	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	G	175	ASP	CB-CG-OD1	5.27	123.04	118.30
1	E	105[A]	LEU	CA-CB-CG	5.26	127.40	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	105[B]	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	82	ASP	CB-CG-OD2	-5.16	113.66	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	201	LYS	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	195	SER	Peptide
1	C	4	ASN	Peptide
1	D	8	PRO	Peptide

## 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	1539	0	1558	17	1
1	B	1459	0	1473	13	0
1	C	1493	0	1505	12	0
1	D	1455	0	1468	12	0
1	E	1476	0	1488	10	0
1	F	1527	0	1547	23	0
1	G	1561	0	1579	31	0
2	A	8	0	14	0	0
2	E	8	0	14	1	0
2	F	8	0	14	2	0
3	A	4	0	3	0	0
3	B	8	0	6	0	0
3	C	4	0	3	0	0
3	D	4	0	3	0	0
3	F	4	0	3	0	0
3	G	4	0	3	0	0
4	B	8	0	14	0	0
4	C	8	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	194	0	0	4	0
5	B	172	0	0	0	0
5	C	87	0	0	1	0
5	D	99	0	0	0	0
5	E	147	0	0	0	0
5	F	224	0	0	1	1
5	G	162	0	0	1	0
All	All	11663	0	10709	96	1

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 4.

All (96) 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:196[B]:ARG:HG3	1:B:196[B]:ARG:HH11	0.99	1.07
1:G:140[B]:GLU:OE1	5:G:2095:HOH:O	1.79	1.00
1:D:152[B]:ARG:HG2	1:D:152[B]:ARG:HH11	1.35	0.92
1:B:196[B]:ARG:NH1	1:B:196[B]:ARG:HG3	1.75	0.85
1:A:152[A]:ARG:HH11	1:A:152[A]:ARG:HG2	1.53	0.72
1:B:196[B]:ARG:CG	1:B:196[B]:ARG:HH11	1.88	0.70
1:G:140[A]:GLU:OE2	1:G:144[A]:LYS:NZ	2.26	0.66
1:D:152[B]:ARG:HG2	1:D:152[B]:ARG:NH1	2.10	0.63
1:G:19:ARG:HE	1:G:19:ARG:HA	1.63	0.62
1:F:7:VAL:HG13	1:F:23:ILE:HG22	1.82	0.62
1:A:15:ALA:N	1:A:16:GLY:HA3	2.17	0.60
1:G:152[A]:ARG:HG2	1:G:152[A]:ARG:HH11	1.68	0.59
1:E:105[B]:LEU:HD11	1:E:156:VAL:HG12	1.85	0.58
1:C:70:PRO:HA	1:C:100:ALA:HB3	1.86	0.58
2:E:800:MPD:HM2	2:E:800:MPD:H52	1.88	0.56
1:A:133[A]:ARG:NH1	5:A:2126:HOH:O	2.38	0.56
1:E:105[B]:LEU:HD11	1:E:156:VAL:CG1	2.36	0.56
1:F:23:ILE:HD11	1:G:53:PHE:CB	2.36	0.56
1:A:135:GLN:HE22	1:G:174:ARG:HH22	1.54	0.54
4:C:800:MRD:O2	4:C:800:MRD:O4	2.21	0.54
1:A:24:TYR:OH	1:B:45:ASN:ND2	2.34	0.53
1:G:38[A]:GLU:CD	1:G:40:ASN:HD22	2.12	0.53
1:B:196[B]:ARG:CG	1:B:196[B]:ARG:NH1	2.53	0.53
1:A:53:PHE:CB	1:G:23:ILE:HD11	2.38	0.53
1:G:21:PHE:CE2	1:G:26[A]:ARG:HD2	2.44	0.53
1:F:7:VAL:HG22	1:G:46[A]:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:THR:HG23	1:A:16:GLY:CA	2.39	0.52
1:F:152[A]:ARG:NH1	1:F:152[A]:ARG:HG3	2.24	0.52
1:A:152[A]:ARG:HH11	1:A:152[A]:ARG:CG	2.24	0.50
1:D:96:ILE:HG22	1:D:118:LEU:HD12	1.94	0.50
1:E:23:ILE:HD11	1:F:53:PHE:CB	2.42	0.50
1:G:122[A]:GLN:NE2	1:G:179:MET:SD	2.83	0.50
1:E:22:ASP:OD2	1:E:25:SER:OG	2.30	0.49
1:F:5:ASN:HD21	1:G:36:ASN:HD22	1.58	0.49
1:D:126:HIS:CD2	1:D:127:GLN:O	2.65	0.49
1:F:7:VAL:CG1	1:F:23:ILE:HG22	2.42	0.49
1:G:96:ILE:HG22	1:G:118:LEU:HD12	1.93	0.49
1:C:199:ILE:H	1:C:199:ILE:HD12	1.77	0.49
1:F:105[A]:LEU:HD11	1:F:156:VAL:HG11	1.95	0.49
1:A:14:THR:HG23	1:A:16:GLY:HA2	1.95	0.48
1:A:105[B]:LEU:HD11	1:A:156:VAL:CG1	2.43	0.48
1:C:10:VAL:HG12	1:C:11:ILE:HG22	1.95	0.48
1:E:6:LEU:HD22	1:F:7:VAL:HG21	1.94	0.48
1:G:152[A]:ARG:CG	1:G:152[A]:ARG:HH11	2.27	0.47
1:E:23:ILE:HD11	1:F:53:PHE:HB2	1.95	0.47
1:G:102[A]:MET:HE3	1:G:105[A]:LEU:HB3	1.97	0.47
1:D:122:GLN:OE1	1:E:145:ASN:ND2	2.40	0.47
1:G:26[A]:ARG:HE	1:G:26[A]:ARG:CA	2.26	0.47
1:A:152[A]:ARG:HG2	1:A:152[A]:ARG:NH1	2.26	0.46
1:B:24:TYR:OH	1:C:45:ASN:ND2	2.43	0.46
1:B:195:SER:HA	1:C:86:PHE:CD1	2.51	0.46
1:E:11:ILE:HG21	1:F:19:ARG:HD3	1.98	0.46
1:D:126:HIS:CD2	1:D:126:HIS:C	2.89	0.46
1:G:101:SER:HG	1:G:126:HIS:CE1	2.34	0.46
1:G:102[B]:MET:SD	1:G:105[B]:LEU:HD23	2.56	0.45
1:A:135:GLN:NE2	1:G:174:ARG:HH12	2.13	0.45
5:A:2116:HOH:O	1:B:152[B]:ARG:NH2	2.49	0.45
1:A:11:ILE:HD12	1:B:21[B]:PHE:CE1	2.52	0.45
1:F:152[A]:ARG:HH11	1:F:152[A]:ARG:HG3	1.82	0.45
1:D:164:ASP:O	1:D:165:LEU:C	2.54	0.44
5:F:2011:HOH:O	1:G:13:LYS:CB	2.65	0.44
1:C:200:ILE:HG23	1:C:200:ILE:O	2.18	0.44
1:G:96:ILE:HG22	1:G:118:LEU:CD1	2.48	0.44
1:A:46[B]:LEU:HD11	1:G:11:ILE:HG22	1.98	0.44
1:D:70:PRO:HA	1:D:100:ALA:HB3	2.01	0.43
1:F:126:HIS:C	1:F:126:HIS:CD2	2.92	0.43
1:F:23:ILE:HD11	1:G:53:PHE:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:TYR:OH	1:F:45:ASN:ND2	2.49	0.42
1:F:105[B]:LEU:HD13	1:F:153:LEU:HD22	2.01	0.42
5:A:2178:HOH:O	1:B:148:ARG:NH1	2.45	0.42
1:A:122[B]:GLN:HE22	1:B:149:ILE:HD11	1.85	0.42
1:B:118:LEU:HD13	1:C:82:ASP:HB3	2.01	0.42
1:F:118:LEU:HD13	1:G:82:ASP:HB3	2.00	0.42
1:F:94:ILE:HG12	2:F:800:MPD:H12	2.01	0.42
1:B:124:MET:HA	1:B:176:ASN:O	2.20	0.42
1:C:7:VAL:HG23	1:C:7:VAL:O	2.19	0.42
1:C:23:ILE:HD11	1:D:53:PHE:CB	2.50	0.42
1:A:53:PHE:CE1	1:G:26[B]:ARG:HG2	2.55	0.42
1:D:7:VAL:HG11	1:D:22:ASP:OD2	2.20	0.41
1:E:90:ASP:OD2	1:E:114:LYS:NZ	2.41	0.41
1:G:21:PHE:HE2	1:G:26[A]:ARG:HD2	1.85	0.41
1:C:46[A]:LEU:HD12	1:C:46[A]:LEU:HA	1.89	0.41
1:F:23:ILE:HD11	1:G:53:PHE:HB2	2.01	0.41
1:G:88:LYS:N	1:G:89:PRO:CD	2.84	0.41
1:C:126:HIS:HE1	5:C:2010:HOH:O	2.03	0.41
1:F:193:ILE:HD13	2:F:800:MPD:H52	2.03	0.41
1:D:28:LEU:HD13	1:D:50:GLN:HE21	1.86	0.41
1:F:5:ASN:HD22	1:F:5:ASN:N	2.19	0.41
1:G:161:THR:HA	1:G:187:GLY:O	2.21	0.40
1:D:111:ALA:O	1:D:114:LYS:N	2.49	0.40
1:A:142:HIS:HD2	5:A:2050:HOH:O	2.03	0.40
1:G:102[B]:MET:CE	1:G:105[B]:LEU:HD23	2.51	0.40
1:C:61:LYS:O	1:C:89:PRO:HB3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLU:OE2	5:F:2177:HOH:O[3_555]	2.14	0.06

## 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	201/201 (100%)	197 (98%)	4 (2%)	0	100	100
1	B	185/201 (92%)	179 (97%)	4 (2%)	2 (1%)	17	6
1	C	189/201 (94%)	180 (95%)	7 (4%)	2 (1%)	17	6
1	D	185/201 (92%)	179 (97%)	6 (3%)	0	100	100
1	E	188/201 (94%)	181 (96%)	7 (4%)	0	100	100
1	F	195/201 (97%)	190 (97%)	5 (3%)	0	100	100
1	G	205/201 (102%)	201 (98%)	4 (2%)	0	100	100
All	All	1348/1407 (96%)	1307 (97%)	37 (3%)	4 (0%)	52	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	196[A]	ARG
1	B	196[B]	ARG
1	C	11	ILE
1	C	97	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	170/168 (101%)	167 (98%)	3 (2%)	66	61
1	B	160/168 (95%)	155 (97%)	5 (3%)	47	37
1	C	164/168 (98%)	158 (96%)	6 (4%)	41	29
1	D	160/168 (95%)	151 (94%)	9 (6%)	26	14
1	E	161/168 (96%)	151 (94%)	10 (6%)	23	11
1	F	168/168 (100%)	163 (97%)	5 (3%)	48	38
1	G	173/168 (103%)	161 (93%)	12 (7%)	19	8
All	All	1156/1176 (98%)	1106 (96%)	50 (4%)	38	23

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	88	LYS
1	A	126	HIS
1	B	5	ASN
1	B	105	LEU
1	B	126	HIS
1	B	176	ASN
1	B	179	MET
1	C	6	LEU
1	C	26	ARG
1	C	29	LYS
1	C	122	GLN
1	C	126	HIS
1	C	129	LEU
1	D	10	VAL
1	D	22	ASP
1	D	46[A]	LEU
1	D	46[B]	LEU
1	D	122	GLN
1	D	126	HIS
1	D	129	LEU
1	D	152[A]	ARG
1	D	152[B]	ARG
1	E	11	ILE
1	E	22	ASP
1	E	25	SER
1	E	112	LYS
1	E	126	HIS
1	E	133	ARG
1	E	152	ARG
1	E	164	ASP
1	E	200	ILE
1	E	201	LYS
1	F	5	ASN
1	F	122[A]	GLN
1	F	122[B]	GLN
1	F	126	HIS
1	F	128	PRO
1	G	5	ASN
1	G	14	THR
1	G	19	ARG
1	G	26[A]	ARG

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Mol	Chain	Res	Type
1	G	26[B]	ARG
1	G	29	LYS
1	G	126	HIS
1	G	152[A]	ARG
1	G	152[B]	ARG
1	G	166	GLU
1	G	184[A]	LYS
1	G	184[B]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	142	HIS
1	B	5	ASN
1	B	45	ASN
1	B	122	GLN
1	B	176	ASN
1	C	45	ASN
1	C	126	HIS
1	C	159	HIS
1	D	45	ASN
1	D	126	HIS
1	D	127	GLN
1	D	145	ASN
1	E	45	ASN
1	E	154	ASN
1	F	5	ASN
1	F	42	HIS
1	F	45	ASN
1	F	126	HIS
1	G	145	ASN
1	G	159	HIS

### 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](#)

12 ligands are modelled in this entry.

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	$\# Z  > 2$
2	MPD	A	800	-	6,7,7	0.22	0	6,10,10	0.28	0
3	ACT	A	801	-	0,3,3	0.00	-	0,3,3	0.00	-
4	MRD	B	800	-	6,7,7	0.62	0	6,10,10	0.43	0
3	ACT	B	801	-	0,3,3	0.00	-	0,3,3	0.00	-
3	ACT	B	802	-	0,3,3	0.00	-	0,3,3	0.00	-
4	MRD	C	800	-	6,7,7	0.54	0	6,10,10	0.56	0
3	ACT	C	801	-	0,3,3	0.00	-	0,3,3	0.00	-
3	ACT	D	800	-	0,3,3	0.00	-	0,3,3	0.00	-
2	MPD	E	800	-	6,7,7	0.30	0	6,10,10	0.50	0
2	MPD	F	800	-	6,7,7	0.47	0	6,10,10	1.11	0
3	ACT	F	801	-	0,3,3	0.00	-	0,3,3	0.00	-
3	ACT	G	800	-	0,3,3	0.00	-	0,3,3	0.00	-

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
2	MPD	A	800	-	-	0/5/5/5	0/0/0/0
3	ACT	A	801	-	-	0/0/0/0	0/0/0/0
4	MRD	B	800	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	B	801	-	-	0/0/0/0	0/0/0/0
3	ACT	B	802	-	-	0/0/0/0	0/0/0/0
4	MRD	C	800	-	-	0/5/5/5	0/0/0/0
3	ACT	C	801	-	-	0/0/0/0	0/0/0/0
3	ACT	D	800	-	-	0/0/0/0	0/0/0/0
2	MPD	E	800	-	-	0/5/5/5	0/0/0/0
2	MPD	F	800	-	-	0/5/5/5	0/0/0/0
3	ACT	F	801	-	-	0/0/0/0	0/0/0/0
3	ACT	G	800	-	-	0/0/0/0	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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	800	MRD	1	0
2	E	800	MPD	1	0
2	F	800	MPD	2	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	193/201 (96%)	0.06	10 (5%) 31 34	7, 12, 35, 87	0
1	B	184/201 (91%)	0.14	7 (3%) 44 48	8, 17, 35, 71	0
1	C	190/201 (94%)	0.59	16 (8%) 14 15	16, 24, 51, 75	1 (0%)
1	D	184/201 (91%)	0.65	6 (3%) 50 53	17, 25, 46, 67	1 (0%)
1	E	189/201 (94%)	0.20	9 (4%) 34 37	12, 21, 42, 106	1 (0%)
1	F	192/201 (95%)	-0.06	5 (2%) 59 63	8, 13, 34, 53	0
1	G	194/201 (96%)	0.05	4 (2%) 67 70	7, 11, 33, 63	0
All	All	1326/1407 (94%)	0.23	57 (4%) 39 42	7, 18, 42, 106	3 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	11	ILE	11.0
1	A	15	ALA	6.6
1	D	11	ILE	6.5
1	D	10	VAL	6.3
1	E	200	ILE	6.1
1	A	17	GLY	6.0
1	E	201	LYS	5.7
1	F	15	ALA	5.5
1	D	9	THR	5.3
1	D	21	PHE	5.1
1	C	5	ASN	5.0
1	B	6	LEU	5.0
1	A	16	GLY	4.6
1	E	11	ILE	4.6
1	A	198	ALA	4.4
1	E	199	ILE	4.3
1	G	5	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	20	ALA	4.1
1	A	197	GLU	4.1
1	A	13	LYS	3.9
1	C	4	ASN	3.7
1	E	5	ASN	3.7
1	C	199	ILE	3.7
1	B	21[A]	PHE	3.4
1	C	21	PHE	3.4
1	C	200	ILE	3.3
1	F	14	THR	3.2
1	B	197	GLU	3.2
1	E	21	PHE	3.2
1	C	6	LEU	3.0
1	C	12	GLU	3.0
1	C	164	ASP	2.9
1	B	196[A]	ARG	2.9
1	F	11	ILE	2.9
1	A	11	ILE	2.9
1	D	7	VAL	2.8
1	B	5	ASN	2.7
1	G	17	GLY	2.7
1	D	12	GLU	2.6
1	C	166	GLU	2.6
1	A	18[A]	GLU	2.5
1	A	14	THR	2.4
1	F	19	ARG	2.4
1	C	201	LYS	2.4
1	C	161	THR	2.4
1	E	20	ALA	2.4
1	G	198	ALA	2.3
1	C	7	VAL	2.2
1	C	185	ALA	2.2
1	E	10	VAL	2.2
1	G	6	LEU	2.2
1	F	21	PHE	2.2
1	E	152	ARG	2.1
1	C	188	LEU	2.1
1	B	60	ASP	2.1
1	C	10	VAL	2.1
1	A	12	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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	ACT	F	801	4/4	0.80	0.19	6.67	24,30,31,33	0
4	MRD	C	800	8/8	0.74	0.28	6.47	39,43,56,57	0
2	MPD	F	800	8/8	0.77	0.24	6.15	43,44,49,54	0
3	ACT	A	801	4/4	0.83	0.17	4.98	27,31,33,34	0
3	ACT	G	800	4/4	0.91	0.14	4.44	21,23,29,30	0
3	ACT	C	801	4/4	0.80	0.23	3.69	45,45,47,48	0
4	MRD	B	800	8/8	0.79	0.27	1.09	58,61,68,68	0
2	MPD	A	800	8/8	0.86	0.14	0.79	36,38,39,42	0
2	MPD	E	800	8/8	0.68	0.26	0.73	42,47,52,52	0
3	ACT	B	801	4/4	0.96	0.11	-0.18	23,26,27,28	0
3	ACT	D	800	4/4	0.90	0.12	-1.24	36,37,37,39	0
3	ACT	B	802	4/4	0.89	0.17	-	34,37,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.