



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:09 am GMT

PDB ID : 2JDI  
Title : GROUND STATE STRUCTURE OF F1-ATPASE FROM BOVINE HEART MITOCHONDRIA (BOVINE F1-ATPASE CRYSTALLISED IN THE ABSENCE OF AZIDE)  
Authors : Bowler, M.W.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2007-01-09  
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.

---

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

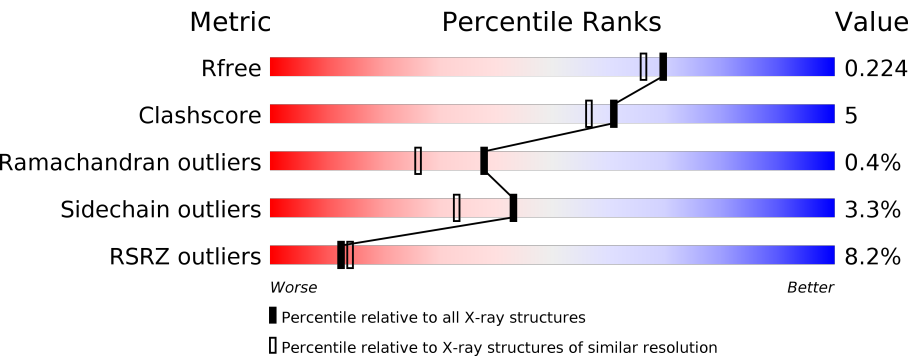
# 1 Overall quality at a glance i

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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (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	510	<div><div>4%</div><div><div></div><div>86%</div><div>9%</div><div>5%</div></div></div>
1	B	510	<div><div>8%</div><div><div></div><div>85%</div><div>9%</div><div>6%</div></div></div>
1	C	510	<div><div>3%</div><div><div></div><div>86%</div><div>8%</div><div>5%</div></div></div>
2	D	482	<div><div>2%</div><div><div></div><div>89%</div><div>7%</div><div></div></div></div>
2	E	482	<div><div>11%</div><div><div></div><div>84%</div><div>9%</div><div>5%</div></div></div>
2	F	482	<div><div>3%</div><div><div></div><div>87%</div><div>8%</div><div></div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	273	<div><div><div></div><div></div><div></div><div></div></div><div>19%52%13%•33%</div></div>
4	H	146	<div><div><div></div><div></div><div></div><div></div></div><div>29%42%15%•40%</div></div>
5	I	50	<div><div><div></div><div></div><div></div><div></div></div><div>12%44%••50%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26426 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 SYNTHASE SUBUNIT ALPHA HEART ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	2	0
			3726	2348	659	707	12			
1	B	480	Total	C	N	O	S	0	0	0
			3663	2308	648	695	12			
1	C	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	SEE REMARK 999	UNP P19483
B	481	GLY	SER	SEE REMARK 999	UNP P19483
C	481	GLY	SER	SEE REMARK 999	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	3	1	0
			3544	2248	601	684	11			
2	E	458	Total	C	N	O	S	5	2	0
			3481	2207	593	671	10			
2	F	466	Total	C	N	O	S	1	2	0
			3538	2246	600	681	11			

- Molecule 3 is a protein called ATP SYNTHASE GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	184	Total	C	N	O	S	0	0	0
			1417	894	252	265	6			

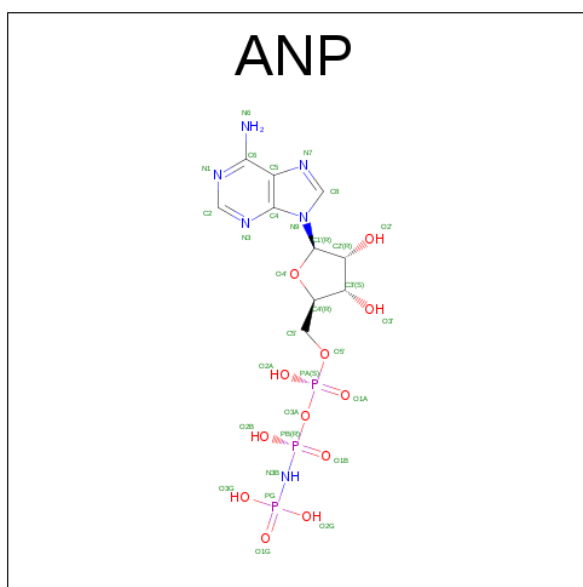
- Molecule 4 is a protein called ATP SYNTHASE DELTA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	88	Total	C	N	O	S	0	0	0
			657	417	108	131	1			

- Molecule 5 is a protein called ATP SYNTHASE EPSILON CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	25	Total	C	N	O	S	0	0	0
			203	130	38	34	1			

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

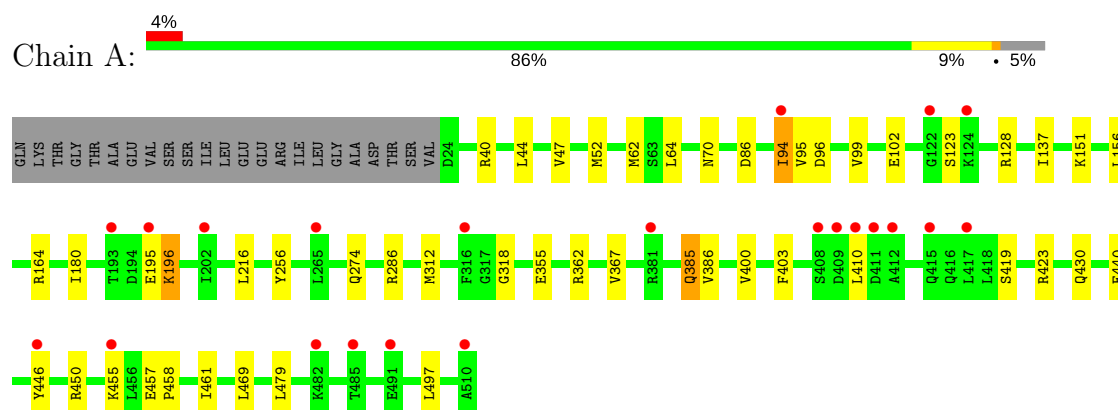
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	354	Total O 354 354	0	0
8	B	348	Total O 348 348	0	0
8	C	367	Total O 367 367	0	0
8	D	389	Total O 389 389	0	0
8	E	267	Total O 267 267	0	0
8	F	436	Total O 436 436	0	0
8	G	114	Total O 114 114	0	0
8	H	31	Total O 31 31	0	0
8	I	16	Total O 16 16	0	0

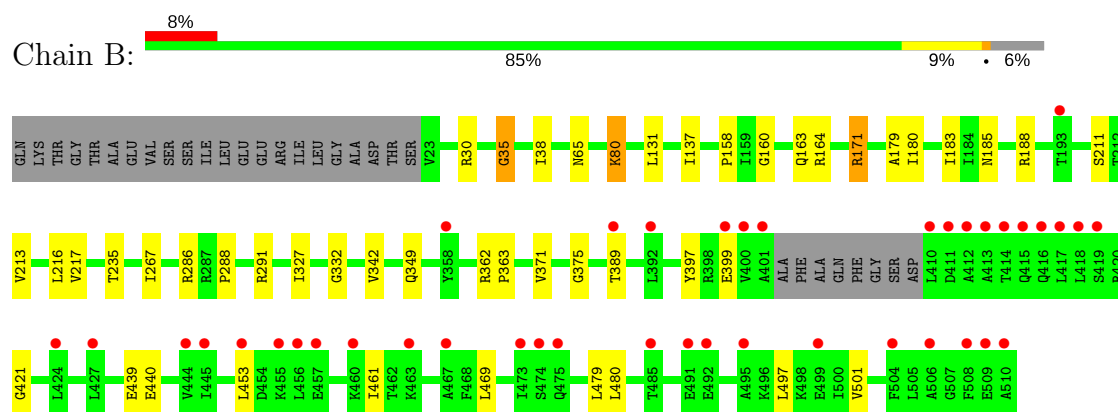
### 3 Residue-property plots

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

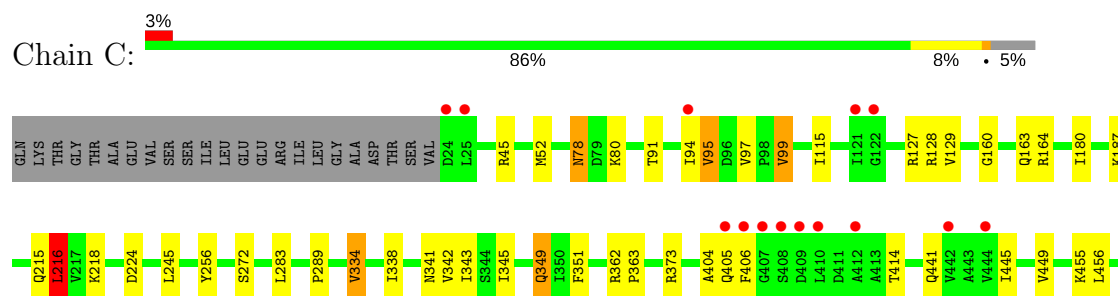
#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM



#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

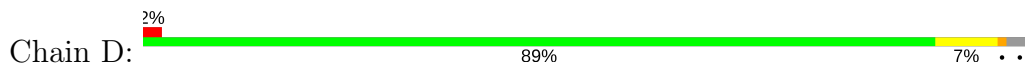


#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

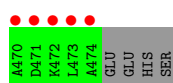
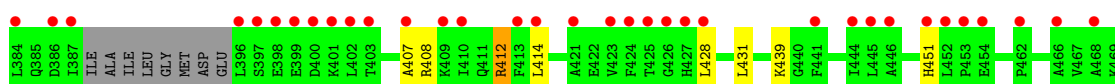
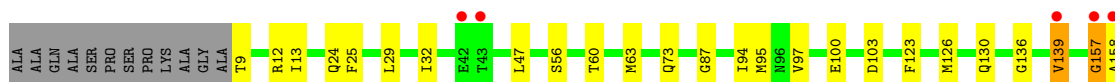
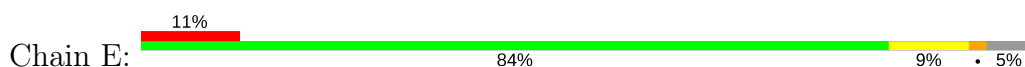




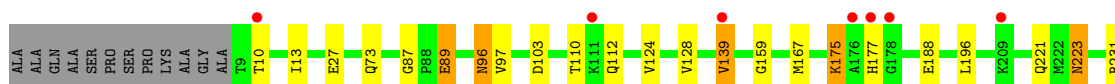
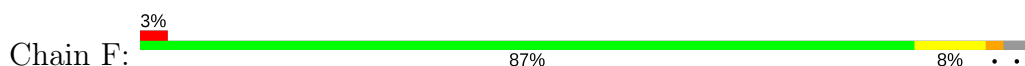
• Molecule 2: ATP SYNTHASE SUBUNIT BETA



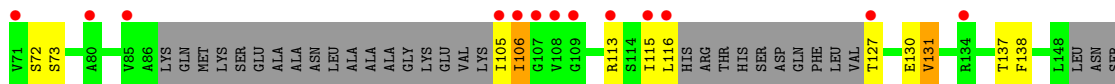
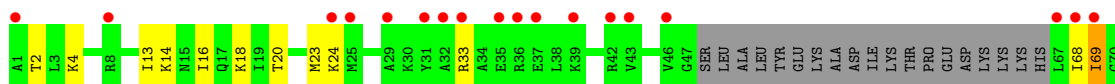
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

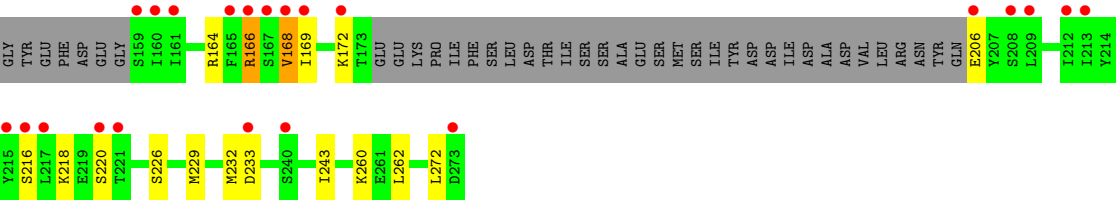


• Molecule 2: ATP SYNTHASE SUBUNIT BETA

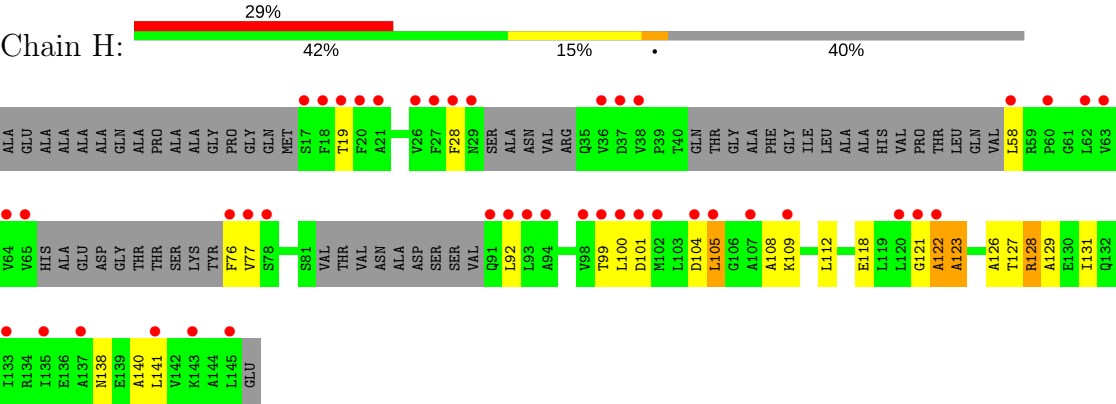


• Molecule 3: ATP SYNTHASE GAMMA CHAIN

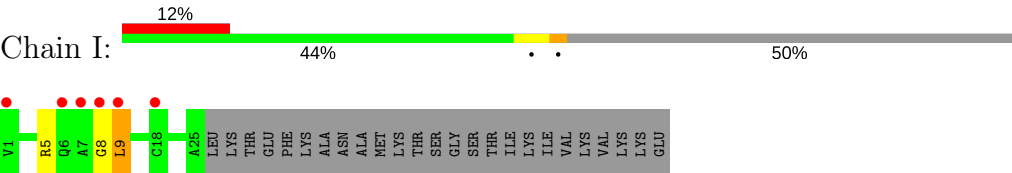




• Molecule 4: ATP SYNTHASE DELTA CHAIN



• Molecule 5: ATP SYNTHASE EPSILON CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.61Å 123.13Å 261.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 23.15 – 1.85	Depositor EDS
% Data completeness (in resolution range)	72.7 (20.00-1.90) 67.6 (23.15-1.85)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.175 , 0.220 0.178 , 0.224	Depositor DCC
$R_{free}$ test set	9778 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	26426	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: MG, ANP

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	0.37	0/3783	0.53	0/5102
1	B	0.39	0/3711	0.53	0/5005
1	C	0.39	0/3766	0.56	1/5080 (0.0%)
2	D	1.57	2/3604 (0.1%)	0.64	6/4891 (0.1%)
2	E	0.37	0/3543	0.54	1/4807 (0.0%)
2	F	0.41	0/3601	1.44	2/4887 (0.0%)
3	G	0.35	0/1426	0.49	0/1907
4	H	0.37	0/660	0.63	0/890
5	I	0.31	0/207	0.61	0/279
All	All	0.70	2/24301 (0.0%)	0.76	10/32848 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	275[A]	ILE	CB-CG2	64.47	3.52	1.52
2	D	275[B]	ILE	CB-CG2	64.47	3.52	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	97[A]	VAL	CG1-CB-CG2	-65.79	5.64	110.90
2	F	97[B]	VAL	CG1-CB-CG2	-65.79	5.64	110.90
2	D	275[A]	ILE	CA-CB-CG2	-13.16	84.58	110.90
2	D	275[B]	ILE	CA-CB-CG2	-13.16	84.58	110.90
2	D	275[A]	ILE	CG1-CB-CG2	6.93	126.64	111.40
2	D	275[B]	ILE	CG1-CB-CG2	6.93	126.64	111.40
2	D	275[A]	ILE	CB-CA-C	6.71	125.01	111.60
2	D	275[B]	ILE	CB-CA-C	6.71	125.01	111.60
1	C	216	LEU	CA-CB-CG	6.02	129.14	115.30
2	E	229	ARG	NE-CZ-NH2	-5.06	117.77	120.30

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	3726	0	3832	32	0
1	B	3663	0	3774	30	0
1	C	3715	0	3814	32	0
2	D	3544	0	3603	35	0
2	E	3481	0	3539	39	0
2	F	3538	0	3604	41	0
3	G	1417	0	1501	32	0
4	H	657	0	663	28	0
5	I	203	0	205	2	0
6	A	31	0	13	0	0
6	B	31	0	13	0	0
6	C	31	0	13	0	0
6	D	31	0	13	3	0
6	F	31	0	13	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	A	354	0	0	6	0
8	B	348	0	0	5	0
8	C	367	0	0	11	0
8	D	389	0	0	4	0
8	E	267	0	0	5	0
8	F	436	0	0	8	0
8	G	114	0	0	3	0
8	H	31	0	0	1	0
8	I	16	0	0	0	0
All	All	26426	0	24600	254	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 5.

All (254) 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)
3:G:68:ILE:HB	3:G:69:ILE:HA	1.29	1.11
4:H:104:ASP:HA	4:H:105:LEU:CB	1.80	1.10
4:H:104:ASP:CA	4:H:105:LEU:HB2	1.82	1.08
1:A:94:ILE:HD11	1:A:128:ARG:HG2	1.31	1.07
4:H:122:ALA:HA	4:H:123:ALA:HB2	1.09	1.05
4:H:122:ALA:HA	4:H:123:ALA:CB	1.82	1.04
2:E:282:GLN:H	2:E:282:GLN:HE21	1.04	1.01
2:F:356:ARG:HD2	8:F:2347:HOH:O	1.64	0.98
4:H:99:THR:HB	4:H:101:ASP:H	1.31	0.93
2:D:282:GLN:H	2:D:282:GLN:HE21	1.01	0.93
4:H:99:THR:HA	4:H:100:LEU:HB2	1.48	0.93
1:A:99:VAL:HG11	1:A:256:TYR:HB2	1.52	0.91
2:D:159:GLY:H	6:D:1480:ANP:HNB1	1.14	0.89
2:F:282:GLN:H	2:F:282:GLN:HE21	0.91	0.87
2:F:282:GLN:N	2:F:282:GLN:HE21	1.73	0.87
1:C:52:MET:SD	8:C:2016:HOH:O	2.32	0.85
2:E:136:GLY:HA3	2:E:431:LEU:HD12	1.57	0.84
8:A:2187:HOH:O	2:D:291:THR:HG22	1.76	0.84
1:C:449:VAL:HB	8:C:2323:HOH:O	1.78	0.83
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.59	0.82
1:C:338:ILE:HG21	8:C:2195:HOH:O	1.81	0.80
4:H:126:ALA:HA	4:H:129:ALA:HB3	1.62	0.80
3:G:20:THR:HG22	3:G:232:MET:HE1	1.63	0.80
2:E:63:MET:HE3	2:E:97:VAL:HG21	1.63	0.79
2:F:282:GLN:H	2:F:282:GLN:NE2	1.76	0.78
1:C:95:VAL:HG22	8:C:2025:HOH:O	1.80	0.78
4:H:104:ASP:HA	4:H:105:LEU:HB2	0.88	0.78
4:H:121:GLY:HA3	4:H:122:ALA:HB3	1.66	0.77
1:A:151:LYS:H	1:A:430:GLN:HE22	1.32	0.76
2:D:97:VAL:HG23	8:D:2198:HOH:O	1.87	0.73
8:A:2213:HOH:O	2:D:275[A]:ILE:HG23	1.88	0.73
1:A:44:LEU:O	1:A:47:VAL:HG22	1.89	0.73
2:F:438:ILE:HG13	8:F:2361:HOH:O	1.87	0.73
1:A:99:VAL:CG1	1:A:256:TYR:HB2	2.19	0.72
1:A:52:MET:HG3	1:A:95:VAL:HG22	1.71	0.71
4:H:99:THR:HB	4:H:101:ASP:N	2.04	0.71
3:G:68:ILE:CB	3:G:69:ILE:HA	2.12	0.71
2:F:223:ASN:H	2:F:223:ASN:HD22	1.37	0.70
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.26	0.70
2:E:158:ALA:HB3	8:E:2134:HOH:O	1.92	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:99:THR:CA	4:H:100:LEU:HB2	2.20	0.69
4:H:122:ALA:CA	4:H:123:ALA:CB	2.66	0.69
2:E:293:GLN:HE22	2:E:308:GLN:HE22	1.40	0.69
1:C:362:ARG:HH12	2:F:372:ARG:CZ	2.06	0.69
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.23	0.69
2:D:282:GLN:H	2:D:282:GLN:NE2	1.85	0.68
1:C:94:ILE:HG22	8:C:2068:HOH:O	1.93	0.68
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.29	0.68
2:F:395:GLU:HB3	8:F:2384:HOH:O	1.94	0.67
1:A:419:SER:O	1:A:423:ARG:HD3	1.93	0.67
2:D:97:VAL:HG22	2:D:232:VAL:HB	1.77	0.67
4:H:127:THR:N	4:H:128:ARG:HB2	2.10	0.66
1:B:217:VAL:HG11	2:E:123:PHE:HZ	1.60	0.66
1:C:160:GLY:H	1:C:163:GLN:NE2	1.92	0.66
4:H:105:LEU:H	4:H:108:ALA:H	1.43	0.65
2:F:249:GLN:OE1	2:F:249:GLN:HA	1.95	0.65
1:B:137:ILE:HG13	2:F:103:ASP:HA	1.79	0.65
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.77	0.65
1:C:272:SER:HA	8:C:2195:HOH:O	1.96	0.65
1:B:35:GLY:O	8:B:2011:HOH:O	2.14	0.64
2:D:85:PRO:HB3	2:D:110:THR:HG21	1.78	0.64
2:F:287:THR:O	2:F:291:THR:HG23	1.97	0.64
1:A:86:ASP:HB3	8:A:2068:HOH:O	1.99	0.63
4:H:126:ALA:HA	4:H:129:ALA:CB	2.28	0.62
1:C:95:VAL:CG2	8:C:2025:HOH:O	2.43	0.62
2:E:157:GLY:HA2	2:E:162:LYS:HE3	1.81	0.62
2:D:275[A]:ILE:HG22	3:G:272:LEU:HD13	1.81	0.62
4:H:127:THR:H	4:H:128:ARG:HB2	1.65	0.61
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.35	0.61
2:F:223:ASN:N	2:F:223:ASN:HD22	1.99	0.60
1:C:95:VAL:O	8:C:2068:HOH:O	2.16	0.60
2:E:223:ASN:H	2:E:223:ASN:HD22	1.48	0.60
3:G:20:THR:HG22	3:G:232:MET:CE	2.32	0.60
1:A:446:TYR:CE1	1:A:450:ARG:HD2	2.35	0.60
2:E:63:MET:HE3	2:E:97:VAL:CG2	2.30	0.60
3:G:168:VAL:HG23	3:G:169:ILE:HD12	1.84	0.59
1:A:99:VAL:CG1	1:A:256:TYR:CB	2.81	0.59
4:H:99:THR:HA	4:H:100:LEU:CB	2.28	0.59
4:H:99:THR:CB	4:H:101:ASP:H	2.12	0.59
2:E:356:ARG:NH2	8:E:2249:HOH:O	2.34	0.58
2:F:96:ASN:HD22	2:F:96:ASN:C	2.06	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:181:SER:HB2	2:E:215:VAL:HG13	1.84	0.58
2:E:282:GLN:H	2:E:282:GLN:NE2	1.87	0.58
1:C:215:GLN:HB3	2:F:356:ARG:HH22	1.69	0.57
2:E:229:ARG:HH22	2:E:267:GLU:CD	2.08	0.57
2:E:377:ILE:HG12	2:E:407:ALA:HB2	1.85	0.57
2:D:159:GLY:N	6:D:1480:ANP:HNB1	1.93	0.57
8:C:2175:HOH:O	2:F:291:THR:HG22	2.04	0.57
3:G:166:ARG:HE	3:G:172:LYS:HB2	1.70	0.57
4:H:127:THR:H	4:H:128:ARG:CB	2.17	0.57
3:G:113:ARG:HD3	3:G:127:THR:HG21	1.87	0.56
1:B:160:GLY:H	1:B:163:GLN:NE2	2.03	0.56
1:B:160:GLY:H	1:B:163:GLN:HE21	1.53	0.56
2:F:139:VAL:HG13	2:F:414:LEU:HD22	1.86	0.56
3:G:73:SER:HA	3:G:131:VAL:CG2	2.36	0.56
2:E:282:GLN:N	2:E:282:GLN:HE21	1.89	0.55
2:E:47:LEU:HB3	2:E:60[B]:THR:CG2	2.37	0.55
2:E:47:LEU:HB3	2:E:60[B]:THR:HG21	1.88	0.55
1:A:446:TYR:CE2	1:A:497:LEU:HB3	2.42	0.55
2:D:287:THR:O	2:D:291:THR:HG23	2.07	0.55
1:B:179:ALA:HB1	1:B:267:ILE:HG12	1.88	0.54
3:G:2:THR:HG22	3:G:4:LYS:H	1.72	0.54
2:F:233:ALA:O	2:F:237:LEU:HD13	2.07	0.54
1:A:40:ARG:HD2	1:A:70:ASN:OD1	2.08	0.54
4:H:122:ALA:HB3	8:H:2007:HOH:O	2.07	0.54
2:E:223:ASN:N	2:E:223:ASN:HD22	2.05	0.54
2:D:205:VAL:CG1	2:D:215:VAL:HG23	2.38	0.54
2:D:390:ILE:HD12	3:G:16:ILE:CD1	2.37	0.54
2:E:258:ILE:HG21	2:E:310:ILE:HD13	1.90	0.54
1:A:423:ARG:HG3	1:A:461:ILE:HD11	1.89	0.54
1:A:355:GLU:HG3	8:A:2131:HOH:O	2.08	0.53
2:D:96:ASN:C	2:D:96:ASN:HD22	2.11	0.53
2:D:188:GLU:O	2:D:221:GLN:HB3	2.08	0.53
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.44	0.53
2:D:390:ILE:HD12	3:G:16:ILE:HD13	1.91	0.53
1:A:156:LEU:HD13	1:A:367:VAL:HG11	1.91	0.52
1:A:102:GLU:HG3	1:A:123:SER:HA	1.91	0.52
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.91	0.52
3:G:229:MET:HB2	8:G:2014:HOH:O	2.09	0.52
1:B:158:PRO:O	1:B:375:GLY:HA3	2.10	0.52
2:F:391:LEU:HB3	2:F:395:GLU:HG3	1.93	0.51
1:B:213:VAL:O	1:B:217:VAL:HG12	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:115:ILE:HG22	3:G:116:LEU:HD12	1.92	0.51
4:H:58:LEU:HD21	4:H:92:LEU:HD11	1.93	0.51
1:C:441:GLN:O	1:C:445:ILE:HG12	2.10	0.51
1:B:183:ILE:HD11	1:B:267:ILE:HD13	1.93	0.50
1:C:218:LYS:HD3	2:F:128:VAL:HG21	1.93	0.50
4:H:127:THR:H	4:H:129:ALA:H	1.59	0.50
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.45	0.50
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.93	0.50
1:C:362:ARG:HA	1:C:363:PRO:C	2.31	0.50
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.76	0.50
2:F:244:ARG:O	2:F:248:GLY:HA2	2.10	0.50
1:B:171:ARG:HD3	8:E:2234:HOH:O	2.10	0.50
2:E:13:ILE:HD12	2:E:73:GLN:HB3	1.94	0.50
2:E:293:GLN:HA	2:E:293:GLN:HE21	1.77	0.50
2:D:275[A]:ILE:CG2	3:G:272:LEU:HD13	2.41	0.50
2:D:85:PRO:HB3	2:D:110:THR:CG2	2.41	0.49
5:I:5:ARG:HA	5:I:9:LEU:H	1.76	0.49
2:E:408:ARG:O	2:E:412:ARG:NE	2.45	0.49
2:D:130:GLN:HE22	2:D:356:ARG:HD2	1.77	0.49
1:A:286:ARG:HG2	2:D:275[A]:ILE:HG21	1.94	0.49
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.39	0.49
2:D:414:LEU:HD23	2:D:441:PHE:CZ	2.48	0.49
2:F:159:GLY:HA2	6:F:1479:ANP:HNB1	1.77	0.48
1:B:30:ARG:HB3	8:B:2062:HOH:O	2.13	0.48
2:D:61:ILE:HD13	8:D:2057:HOH:O	2.12	0.48
1:B:349:GLN:NE2	8:B:2298:HOH:O	2.31	0.48
2:E:229:ARG:NH2	2:E:267:GLU:OE1	2.39	0.48
1:B:497:LEU:O	1:B:501:VAL:HG23	2.14	0.48
2:D:200:MET:HE1	2:D:217:LEU:HD21	1.96	0.47
3:G:137:THR:HG22	3:G:138:PHE:N	2.29	0.47
3:G:68:ILE:HB	3:G:69:ILE:CA	2.21	0.47
1:A:62:MET:CE	1:A:64:LEU:HD21	2.45	0.47
3:G:164:ARG:HH12	3:G:172:LYS:HE2	1.79	0.47
2:F:188:GLU:O	2:F:221:GLN:HB3	2.14	0.47
1:B:332:GLY:HA2	8:B:2283:HOH:O	2.13	0.47
2:F:454:GLU:HG2	8:F:2388:HOH:O	2.13	0.47
4:H:128:ARG:H	4:H:131:ILE:HD12	1.80	0.47
3:G:24:LYS:HG3	3:G:233:ASP:HB2	1.97	0.47
2:E:47:LEU:CB	2:E:60[B]:THR:HG21	2.45	0.46
2:F:223:ASN:H	2:F:223:ASN:ND2	2.11	0.46
3:G:260:LYS:HD2	8:G:2043:HOH:O	2.14	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:69:ILE:HG21	3:G:106:ILE:HD12	1.98	0.46
1:C:78:ASN:HD22	1:C:80:LYS:H	1.61	0.46
2:F:139:VAL:CG1	2:F:414:LEU:HD22	2.46	0.46
1:A:362:ARG:NH1	8:A:2283:HOH:O	2.48	0.46
3:G:14:LYS:O	3:G:18:LYS:HE3	2.14	0.46
3:G:23:MET:SD	3:G:232:MET:HE2	2.55	0.46
2:D:89:GLU:H	2:D:89:GLU:CD	2.19	0.46
1:A:457:GLU:HA	1:A:458:PRO:HD2	1.79	0.46
1:A:440:GLU:HB3	1:A:469:LEU:HD11	1.98	0.45
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.99	0.45
1:B:362:ARG:HA	1:B:363:PRO:C	2.36	0.45
2:D:205:VAL:CG1	2:D:215:VAL:CG2	2.95	0.45
2:D:275[A]:ILE:CG2	2:D:275[A]:ILE:H	2.28	0.45
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.80	0.45
1:C:115:ILE:O	2:F:124:VAL:HG13	2.16	0.45
2:F:13:ILE:HD12	2:F:73:GLN:HB3	1.97	0.45
2:F:175:LYS:C	2:F:177:HIS:H	2.18	0.45
2:E:25:PHE:HB2	2:E:29:LEU:HD12	1.97	0.45
1:A:400:VAL:HG13	1:A:403:PHE:CE1	2.52	0.45
4:H:121:GLY:CA	4:H:122:ALA:HB3	2.40	0.45
2:E:9:THR:N	8:E:2001:HOH:O	2.49	0.45
1:A:286:ARG:CZ	2:D:275[A]:ILE:HG21	2.47	0.45
1:C:94:ILE:HD11	8:C:2023:HOH:O	2.16	0.45
2:E:94:ILE:HG12	2:E:217:LEU:HD12	1.98	0.45
3:G:69:ILE:HG13	3:G:106:ILE:HG13	1.99	0.45
2:F:231:ARG:NH1	8:F:2250:HOH:O	2.50	0.44
1:B:211:SER:HA	2:E:126:MET:HE2	1.98	0.44
2:D:13:ILE:HD12	2:D:73:GLN:HB3	1.99	0.44
3:G:73:SER:HA	3:G:131:VAL:HG23	1.98	0.44
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.98	0.44
3:G:106:ILE:HG22	3:G:127:THR:N	2.31	0.44
2:F:455:GLN:H	2:F:455:GLN:CD	2.20	0.44
1:A:128:ARG:NE	8:A:2105:HOH:O	2.48	0.44
1:B:371:VAL:HG21	8:F:2436:HOH:O	2.17	0.44
1:A:385:GLN:HG3	1:A:386:VAL:HG13	1.99	0.44
2:E:139:VAL:HG13	2:E:414:LEU:HB3	1.98	0.44
2:D:242:TYR:CD1	2:D:246:GLN:HG3	2.53	0.44
1:A:62:MET:HE2	1:A:64:LEU:HD21	2.00	0.44
1:C:99:VAL:HG21	1:C:127:ARG:HB2	1.99	0.44
1:C:342:VAL:HA	1:C:345:ILE:HD12	2.00	0.44
1:C:404:ALA:O	1:C:406:PHE:N	2.51	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:GLU:HG2	8:F:2013:HOH:O	2.18	0.44
1:C:128:ARG:NH1	8:C:2101:HOH:O	2.51	0.43
2:E:12:ARG:NH2	2:E:24:GLN:OE1	2.49	0.43
1:C:52:MET:O	1:C:91:THR:HB	2.17	0.43
1:B:440:GLU:HB3	1:B:469:LEU:HD11	2.00	0.43
1:C:129:VAL:HG21	1:C:245:LEU:HD11	2.01	0.43
3:G:216:SER:O	3:G:220:SER:HB2	2.18	0.43
1:A:195:GLU:O	1:A:196:LYS:HB2	2.19	0.43
2:E:25:PHE:O	2:E:56:SER:HB3	2.19	0.43
2:E:95:MET:HA	2:E:100:GLU:O	2.18	0.43
2:F:291:THR:HG21	8:F:2161:HOH:O	2.17	0.43
1:C:160:GLY:H	1:C:163:GLN:HE21	1.61	0.43
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.49	0.43
2:E:256:ASP:HA	2:E:257[A]:ASN:HA	1.67	0.43
1:C:187:LYS:HE2	1:C:224:ASP:HB3	2.00	0.43
1:B:327:ILE:HD11	1:B:342:VAL:HG21	2.02	0.42
1:A:312:MET:O	1:A:318:GLY:HA2	2.19	0.42
2:F:249:GLN:CA	2:F:249:GLN:OE1	2.66	0.42
2:D:367:HIS:CE1	2:D:434:LEU:HD11	2.54	0.42
2:F:188:GLU:H	2:F:221:GLN:NE2	2.18	0.42
3:G:69:ILE:HD11	3:G:105:ILE:N	2.34	0.42
4:H:19:THR:HA	4:H:28:PHE:O	2.18	0.42
5:I:8:GLY:HA3	5:I:9:LEU:CD1	2.50	0.42
1:A:94:ILE:CD1	1:A:96:ASP:HB3	2.49	0.42
1:B:180:ILE:HG13	1:B:216:LEU:HD21	2.02	0.42
3:G:166:ARG:HH21	3:G:172:LYS:HB2	1.85	0.42
1:C:343:ILE:HG23	1:C:349:GLN:NE2	2.34	0.42
1:C:373:ARG:HA	6:D:1480:ANP:O3'	2.20	0.42
3:G:69:ILE:O	3:G:69:ILE:HG23	2.20	0.42
3:G:13:ILE:HG22	3:G:243:ILE:HG13	2.02	0.42
1:B:286:ARG:HA	2:E:275:ILE:HD12	2.01	0.41
1:C:414:THR:HG21	8:D:2367:HOH:O	2.19	0.41
4:H:138:ASN:HA	4:H:141:LEU:HD12	2.00	0.41
1:B:235:THR:HG22	8:B:2182:HOH:O	2.20	0.41
4:H:58:LEU:HD13	4:H:77:VAL:HG11	2.02	0.41
2:F:167:MET:CE	2:F:196:LEU:HD13	2.50	0.41
2:F:89:GLU:HG3	2:F:110:THR:HA	2.02	0.41
1:C:99:VAL:HG13	1:C:256:TYR:HB2	2.02	0.41
2:E:260:ARG:HD2	8:E:2086:HOH:O	2.20	0.41
2:F:387:ILE:H	2:F:387:ILE:HG13	1.70	0.41
1:B:288:PRO:HB3	2:F:276:PRO:HG3	2.03	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:76:PHE:CZ	4:H:140:ALA:O	2.73	0.41
1:A:137:ILE:HD11	2:E:103:ASP:HA	2.04	0.40
1:B:439:GLU:HG3	1:B:480:LEU:HB3	2.02	0.40
3:G:226:SER:HB2	8:G:2075:HOH:O	2.21	0.40
1:A:151:LYS:H	1:A:430:GLN:NE2	2.10	0.40
1:B:80:LYS:HA	2:E:32:ILE:HB	2.02	0.40
2:D:9:THR:N	8:D:2001:HOH:O	2.54	0.40
1:B:453:LEU:HB3	1:B:461:ILE:HD12	2.04	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	487/510 (96%)	475 (98%)	11 (2%)	1 (0%)	51	41
1	B	476/510 (93%)	463 (97%)	12 (2%)	1 (0%)	51	41
1	C	485/510 (95%)	474 (98%)	10 (2%)	1 (0%)	51	41
2	D	466/482 (97%)	450 (97%)	16 (3%)	0	100	100
2	E	456/482 (95%)	442 (97%)	12 (3%)	2 (0%)	38	26
2	F	466/482 (97%)	453 (97%)	12 (3%)	1 (0%)	51	41
3	G	172/273 (63%)	163 (95%)	8 (5%)	1 (1%)	28	16
4	H	78/146 (53%)	65 (83%)	9 (12%)	4 (5%)	2	0
5	I	23/50 (46%)	22 (96%)	1 (4%)	0	100	100
All	All	3109/3445 (90%)	3007 (97%)	91 (3%)	11 (0%)	38	26

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	LYS
1	C	405	GLN
4	H	105	LEU
4	H	123	ALA
1	B	35	GLY
4	H	128	ARG
3	G	72	SER
4	H	122	ALA
2	E	279	VAL
2	F	279	VAL
2	E	157	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	395/412 (96%)	388 (98%)	7 (2%)	64	60
1	B	389/412 (94%)	379 (97%)	10 (3%)	51	43
1	C	393/412 (95%)	379 (96%)	14 (4%)	40	29
2	D	378/386 (98%)	367 (97%)	11 (3%)	48	39
2	E	372/386 (96%)	357 (96%)	15 (4%)	36	25
2	F	378/386 (98%)	364 (96%)	14 (4%)	39	28
3	G	154/231 (67%)	144 (94%)	10 (6%)	20	9
4	H	70/109 (64%)	67 (96%)	3 (4%)	33	22
5	I	19/41 (46%)	18 (95%)	1 (5%)	26	15
All	All	2548/2775 (92%)	2463 (97%)	85 (3%)	43	33

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ILE
1	A	164	ARG
1	A	274	GLN
1	A	385	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	410	LEU
1	A	455	LYS
1	A	479	LEU
1	B	38	ILE
1	B	65	ASN
1	B	80	LYS
1	B	131	LEU
1	B	164	ARG
1	B	171	ARG
1	B	291	ARG
1	B	389	THR
1	B	399	GLU
1	B	479	LEU
1	C	45	ARG
1	C	78	ASN
1	C	95	VAL
1	C	97	VAL
1	C	99	VAL
1	C	164	ARG
1	C	216	LEU
1	C	334	VAL
1	C	341	ASN
1	C	349	GLN
1	C	455	LYS
1	C	456	LEU
1	C	479	LEU
1	C	505	LEU
2	D	96	ASN
2	D	237	LEU
2	D	246	GLN
2	D	247	GLU
2	D	249	GLN
2	D	275[A]	ILE
2	D	275[B]	ILE
2	D	282	GLN
2	D	341	GLU
2	D	393	MET
2	D	400	ASP
2	E	130	GLN
2	E	139	VAL
2	E	163	THR
2	E	215	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	223	ASN
2	E	257[A]	ASN
2	E	257[B]	ASN
2	E	282	GLN
2	E	293	GLN
2	E	301	LYS
2	E	310	ILE
2	E	412	ARG
2	E	428	LEU
2	E	439	LYS
2	E	451	HIS
2	F	10	THR
2	F	89	GLU
2	F	96	ASN
2	F	112	GLN
2	F	139	VAL
2	F	175	LYS
2	F	223	ASN
2	F	247	GLU
2	F	249	GLN
2	F	274	ARG
2	F	282	GLN
2	F	387	ILE
2	F	420	VAL
2	F	455	GLN
3	G	33	ARG
3	G	69	ILE
3	G	106	ILE
3	G	130	GLU
3	G	131	VAL
3	G	166	ARG
3	G	168	VAL
3	G	206	GLU
3	G	218	LYS
3	G	262	LEU
4	H	109	LYS
4	H	112	LEU
4	H	118	GLU
5	I	9	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	GLN
1	A	396	GLN
1	A	430	GLN
1	A	477	GLN
1	B	65	ASN
1	B	163	GLN
1	B	208	GLN
1	B	471	HIS
1	B	503	ASN
1	C	48	GLN
1	C	78	ASN
1	C	163	GLN
1	C	263	HIS
1	C	341	ASN
1	C	349	GLN
1	C	476	HIS
2	D	73	GLN
2	D	96	ASN
2	D	112	GLN
2	D	130	GLN
2	D	194	ASN
2	D	221	GLN
2	D	282	GLN
2	E	130	GLN
2	E	194	ASN
2	E	223	ASN
2	E	249	GLN
2	E	282	GLN
2	E	293	GLN
2	E	379	GLN
2	F	51	GLN
2	F	73	GLN
2	F	96	ASN
2	F	112	GLN
2	F	194	ASN
2	F	198	HIS
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	379	GLN
2	F	443	GLN
3	G	15	ASN
3	G	211	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	H	91	GLN
5	I	16	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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$
6	ANP	A	1511	7	29,33,33	2.02	7 (24%)	28,52,52	2.38	7 (25%)
6	ANP	B	1511	7	29,33,33	1.98	8 (27%)	28,52,52	2.13	5 (17%)
6	ANP	C	1511	7	29,33,33	2.07	7 (24%)	28,52,52	2.22	4 (14%)
6	ANP	D	1480	7	29,33,33	2.03	7 (24%)	28,52,52	2.38	5 (17%)
6	ANP	F	1479	7	29,33,33	2.00	8 (27%)	28,52,52	2.26	5 (17%)

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
6	ANP	A	1511	7	-	0/13/38/38	0/3/3/3
6	ANP	B	1511	7	-	0/13/38/38	0/3/3/3
6	ANP	C	1511	7	-	0/13/38/38	0/3/3/3
6	ANP	D	1480	7	-	0/13/38/38	0/3/3/3
6	ANP	F	1479	7	-	1/13/38/38	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1480	ANP	PB-O2B	-2.54	1.49	1.56
6	F	1479	ANP	PG-O2G	-2.49	1.49	1.56
6	A	1511	ANP	PG-O2G	-2.33	1.50	1.56
6	F	1479	ANP	PB-O2B	-2.23	1.50	1.56
6	A	1511	ANP	PB-O2B	-2.21	1.50	1.56
6	B	1511	ANP	PB-O2B	-2.17	1.50	1.56
6	C	1511	ANP	PG-O3G	-2.14	1.50	1.56
6	C	1511	ANP	PB-O2B	-2.12	1.50	1.56
6	D	1480	ANP	PG-O2G	-2.11	1.50	1.56
6	B	1511	ANP	PG-O2G	-2.05	1.51	1.56
6	F	1479	ANP	PG-O3G	-2.03	1.51	1.56
6	B	1511	ANP	PG-O3G	-2.02	1.51	1.56
6	B	1511	ANP	C5-C4	3.13	1.47	1.40
6	A	1511	ANP	C5-C4	3.19	1.47	1.40
6	F	1479	ANP	C5-C4	3.19	1.47	1.40
6	C	1511	ANP	C5-C4	3.19	1.47	1.40
6	D	1480	ANP	C5-C4	3.31	1.48	1.40
6	F	1479	ANP	PB-N3B	3.57	1.72	1.63
6	F	1479	ANP	PG-N3B	3.64	1.73	1.63
6	D	1480	ANP	PB-N3B	3.64	1.73	1.63
6	D	1480	ANP	PG-N3B	3.89	1.73	1.63
6	A	1511	ANP	PG-N3B	3.90	1.73	1.63
6	F	1479	ANP	PG-O1G	3.97	1.50	1.46
6	A	1511	ANP	PB-N3B	4.06	1.74	1.63
6	B	1511	ANP	PG-N3B	4.06	1.74	1.63
6	C	1511	ANP	PG-N3B	4.33	1.74	1.63
6	B	1511	ANP	PB-N3B	4.35	1.74	1.63
6	C	1511	ANP	PB-N3B	4.35	1.74	1.63
6	B	1511	ANP	PB-O1B	4.36	1.51	1.46
6	C	1511	ANP	PG-O1G	4.73	1.51	1.46
6	B	1511	ANP	PG-O1G	4.74	1.51	1.46
6	D	1480	ANP	PG-O1G	4.77	1.51	1.46
6	A	1511	ANP	PB-O1B	4.84	1.51	1.46
6	A	1511	ANP	PG-O1G	5.03	1.51	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1480	ANP	PB-O1B	5.15	1.52	1.46
6	C	1511	ANP	PB-O1B	5.21	1.52	1.46
6	F	1479	ANP	PB-O1B	6.01	1.52	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1480	ANP	O1G-PG-N3B	-8.95	98.41	111.79
6	C	1511	ANP	O1G-PG-N3B	-7.73	100.22	111.79
6	F	1479	ANP	O1G-PG-N3B	-7.52	100.54	111.79
6	A	1511	ANP	O1G-PG-N3B	-7.43	100.67	111.79
6	A	1511	ANP	N3-C2-N1	-6.76	122.97	128.86
6	B	1511	ANP	N3-C2-N1	-6.56	123.14	128.86
6	B	1511	ANP	O1G-PG-N3B	-6.45	102.15	111.79
6	C	1511	ANP	N3-C2-N1	-6.36	123.32	128.86
6	D	1480	ANP	N3-C2-N1	-6.35	123.33	128.86
6	F	1479	ANP	N3-C2-N1	-6.33	123.34	128.86
6	A	1511	ANP	O1B-PB-N3B	-3.14	107.10	111.79
6	B	1511	ANP	C4-C5-N7	-2.98	106.53	109.41
6	F	1479	ANP	O3A-PB-N3B	-2.96	98.37	106.59
6	A	1511	ANP	C4-C5-N7	-2.75	106.75	109.41
6	F	1479	ANP	C4-C5-N7	-2.60	106.90	109.41
6	C	1511	ANP	C4-C5-N7	-2.57	106.93	109.41
6	D	1480	ANP	C4-C5-N7	-2.41	107.08	109.41
6	A	1511	ANP	PA-O3A-PB	-2.06	125.11	132.38
6	B	1511	ANP	PA-O3A-PB	-2.02	125.27	132.38
6	A	1511	ANP	C2-N1-C6	2.07	122.39	118.77
6	D	1480	ANP	C2-N1-C6	2.28	122.75	118.77
6	D	1480	ANP	O2B-PB-O1B	2.52	115.11	109.87
6	C	1511	ANP	O2B-PB-O1B	2.95	116.00	109.87
6	B	1511	ANP	O2B-PB-O1B	3.37	116.88	109.87
6	F	1479	ANP	O2B-PB-O1B	3.40	116.94	109.87
6	A	1511	ANP	O2B-PB-O1B	4.17	118.54	109.87

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	1479	ANP	O1B-PB-N3B-PG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1480	ANP	3	0
6	F	1479	ANP	1	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	487/510 (95%)	-0.02	22 (4%)	34 37	5, 15, 36, 66	3 (0%)
1	B	480/510 (94%)	0.12	41 (8%)	11 13	5, 14, 48, 78	1 (0%)
1	C	487/510 (95%)	-0.16	16 (3%)	47 50	8, 15, 32, 70	0
2	D	467/482 (96%)	-0.22	11 (2%)	59 63	6, 14, 34, 71	1 (0%)
2	E	458/482 (95%)	0.44	54 (11%)	5 5	7, 18, 60, 81	2 (0%)
2	F	466/482 (96%)	-0.17	13 (2%)	53 57	8, 14, 38, 59	1 (0%)
3	G	184/273 (67%)	1.48	53 (28%)	1 0	5, 32, 48, 54	1 (0%)
4	H	88/146 (60%)	2.50	43 (48%)	0 0	2, 20, 42, 50	0
5	I	25/50 (50%)	1.63	6 (24%)	1 1	2, 7, 32, 34	0
All	All	3142/3445 (91%)	0.17	259 (8%)	12 14	2, 15, 45, 81	9 (0%)

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	273	ASP	11.7
1	B	412	ALA	9.6
2	E	402	LEU	9.0
1	C	407	GLY	8.5
4	H	63	VAL	7.9
1	C	406	PHE	7.7
4	H	27	PHE	7.7
4	H	105	LEU	7.7
4	H	18	PHE	7.7
2	E	424	PHE	7.4
2	E	451	HIS	7.4
2	E	384	LEU	7.4
2	F	474	ALA	6.9
4	H	64	VAL	6.8
5	I	8	GLY	6.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	E	423	VAL	6.7
4	H	65	VAL	6.7
2	E	383	SER	6.6
3	G	85	VAL	6.5
1	B	400	VAL	6.5
2	E	398	GLU	6.4
2	D	475	GLU	6.4
1	C	409	ASP	6.1
3	G	1	ALA	6.0
4	H	145	LEU	6.0
1	B	414	THR	5.7
2	E	470	ALA	5.7
1	B	455	LYS	5.7
5	I	7	ALA	5.6
2	E	400	ASP	5.5
4	H	26	VAL	5.5
2	F	176	ALA	5.4
3	G	25	MET	5.4
1	B	413	ALA	5.4
3	G	169	ILE	5.3
1	B	416	GLN	5.3
4	H	62	LEU	5.2
3	G	106	ILE	5.2
2	E	472	LYS	5.2
3	G	159	SER	5.2
1	B	358	TYR	5.2
2	E	410	ILE	5.2
5	I	1	VAL	5.1
4	H	36	VAL	5.1
4	H	28	PHE	5.1
2	E	468	ALA	5.0
1	B	417	LEU	4.9
3	G	217	LEU	4.9
3	G	172	LYS	4.9
2	E	399	GLU	4.9
1	B	411	ASP	4.9
1	B	506	ALA	4.9
2	E	474	ALA	4.9
3	G	160	ILE	4.9
3	G	116	LEU	4.9
2	E	414	LEU	4.8
4	H	17	SER	4.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	G	32	ALA	4.7
2	D	248	GLY	4.7
2	E	473	LEU	4.7
1	B	510	ALA	4.6
3	G	29	ALA	4.6
2	E	413	PHE	4.5
4	H	107	ALA	4.5
2	E	159	GLY	4.5
1	A	410	LEU	4.5
3	G	36	ARG	4.4
4	H	100	LEU	4.4
4	H	99	THR	4.4
4	H	102	MET	4.3
1	B	419	SER	4.3
3	G	209	LEU	4.3
2	E	441	PHE	4.2
3	G	46	VAL	4.2
2	E	379	GLN	4.2
3	G	208	SER	4.2
1	C	24	ASP	4.2
3	G	168	VAL	4.2
2	E	42	GLU	4.1
4	H	122	ALA	4.1
2	F	248	GLY	4.1
1	A	193	THR	4.1
2	E	425	THR	4.1
2	D	249	GLN	4.0
3	G	67	LEU	4.0
1	B	474	SER	4.0
1	A	408	SER	4.0
1	B	460	LYS	4.0
4	H	76	PHE	3.9
3	G	167	SER	3.9
3	G	68	ILE	3.9
1	C	122	GLY	3.9
1	C	412	ALA	3.9
3	G	43	VAL	3.8
1	C	405	GLN	3.8
4	H	120	LEU	3.8
4	H	37	ASP	3.8
2	E	139	VAL	3.8
4	H	29	ASN	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	410	LEU	3.8
1	B	427	LEU	3.7
2	D	275[A]	ILE	3.7
3	G	221	THR	3.7
3	G	108	VAL	3.7
2	F	473	LEU	3.7
3	G	69	ILE	3.6
1	B	392	LEU	3.6
1	B	457	GLU	3.6
2	E	396	LEU	3.6
1	A	122	GLY	3.6
3	G	39	LYS	3.6
4	H	91	GLN	3.6
2	F	178	GLY	3.6
3	G	105	ILE	3.5
4	H	92	LEU	3.5
1	B	492	GLU	3.5
1	B	473	ILE	3.5
1	A	417	LEU	3.5
2	E	401	LYS	3.5
1	A	94	ILE	3.5
2	E	452	LEU	3.5
1	B	418	LEU	3.4
2	E	386	ASP	3.4
2	D	474	ALA	3.4
1	B	444	VAL	3.4
2	D	9	THR	3.4
1	B	509	GLU	3.4
2	E	471	ASP	3.4
2	E	444	ILE	3.3
2	E	427	HIS	3.3
2	E	446	ALA	3.3
1	B	475	GLN	3.3
2	E	43	THR	3.3
1	B	504	PHE	3.2
1	B	467	ALA	3.2
3	G	127	THR	3.2
4	H	19	THR	3.2
4	H	135	ILE	3.2
2	E	407	ALA	3.2
5	I	6	GLN	3.2
2	E	428	LEU	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	H	141	LEU	3.1
1	B	495	ALA	3.1
1	B	508	PHE	3.1
2	D	472	LYS	3.1
3	G	115	ILE	3.1
4	H	98	VAL	3.1
1	B	399	GLU	3.1
3	G	213	ILE	3.1
1	A	381	ARG	3.1
5	I	9	LEU	3.0
1	A	455	LYS	3.0
3	G	33	ARG	3.0
3	G	31	TYR	3.0
4	H	137	ALA	3.0
1	B	445	ILE	2.9
3	G	220	SER	2.9
3	G	206	GLU	2.9
1	A	491	GLU	2.9
3	G	134	ARG	2.8
2	F	426	GLY	2.8
2	E	454	GLU	2.8
1	A	412	ALA	2.8
3	G	215	TYR	2.8
1	B	415	GLN	2.8
3	G	161	ILE	2.8
4	H	20	PHE	2.8
2	E	409	LYS	2.7
2	E	360	PRO	2.7
4	H	38	VAL	2.7
3	G	24	LYS	2.7
3	G	107	GLY	2.7
2	E	387	ILE	2.7
1	A	510	ALA	2.7
3	G	71	VAL	2.7
1	A	202	ILE	2.6
3	G	216	SER	2.6
3	G	240	SER	2.6
2	E	397	SER	2.6
1	B	424	LEU	2.6
4	H	21	ALA	2.6
4	H	104	ASP	2.6
2	D	399	GLU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	482	LYS	2.6
2	F	209	LYS	2.6
4	H	133	ILE	2.6
2	E	157	GLY	2.6
1	A	316	PHE	2.5
3	G	8	ARG	2.5
2	F	398	GLU	2.5
4	H	121	GLY	2.5
2	E	363	VAL	2.5
2	E	341	GLU	2.5
3	G	109	GLY	2.5
4	H	109	LYS	2.5
3	G	35	GLU	2.5
1	A	409	ASP	2.5
1	B	453	LEU	2.5
2	E	158	ALA	2.5
2	E	453	PRO	2.5
2	F	111	LYS	2.5
3	G	233	ASP	2.5
3	G	212	ILE	2.5
1	B	401	ALA	2.5
1	C	410	LEU	2.5
2	F	139	VAL	2.4
1	B	463	LYS	2.4
2	F	413	PHE	2.4
2	E	466	ALA	2.4
1	C	408	SER	2.4
2	E	345	TYR	2.4
1	A	411	ASP	2.4
2	E	374	VAL	2.4
1	A	446	TYR	2.3
1	C	510	ALA	2.3
1	B	193	THR	2.3
2	F	177	HIS	2.3
1	C	94	ILE	2.3
1	B	491	GLU	2.3
5	I	18	CYS	2.3
4	H	78	SER	2.3
2	E	462	PRO	2.3
2	D	402	LEU	2.3
3	G	165	PHE	2.3
4	H	143	LYS	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	G	166	ARG	2.2
2	E	445	LEU	2.2
4	H	93	LEU	2.2
1	A	195	GLU	2.2
4	H	60	PRO	2.2
2	F	10	THR	2.2
3	G	80	ALA	2.2
1	C	444	VAL	2.2
2	D	28	GLY	2.2
4	H	101	ASP	2.2
2	E	421	ALA	2.2
1	A	415	GLN	2.2
1	B	499	GLU	2.2
1	A	485	THR	2.2
2	E	381	TYR	2.2
3	G	42	ARG	2.2
1	A	265	LEU	2.2
1	B	456	LEU	2.2
1	B	389	THR	2.2
1	C	468	PHE	2.2
3	G	113	ARG	2.1
1	B	485	THR	2.1
1	C	25	LEU	2.1
2	D	246	GLN	2.1
2	E	403	THR	2.1
4	H	94	ALA	2.1
3	G	37	GLU	2.1
2	E	351	LEU	2.1
1	A	124	LYS	2.1
4	H	77	VAL	2.0
1	C	442	VAL	2.0
2	E	426	GLY	2.0
1	C	121	ILE	2.0
4	H	58	LEU	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 [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( $\text{\AA}^2$ )	Q<0.9
7	MG	D	1481	1/1	0.99	0.10	0.43	14,14,14,14	0
7	MG	F	1480	1/1	0.98	0.10	0.24	13,13,13,13	0
6	ANP	F	1479	31/31	0.98	0.08	-0.42	8,12,18,21	0
6	ANP	A	1511	31/31	0.98	0.08	-0.43	8,12,19,21	0
6	ANP	C	1511	31/31	0.99	0.07	-0.79	8,12,17,25	0
6	ANP	B	1511	31/31	0.98	0.07	-0.79	8,15,24,33	0
6	ANP	D	1480	31/31	0.99	0.07	-0.82	6,10,14,16	0
7	MG	C	1512	1/1	0.99	0.07	-	13,13,13,13	0
7	MG	B	1512	1/1	0.98	0.06	-	15,15,15,15	0
7	MG	A	1512	1/1	0.99	0.10	-	16,16,16,16	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.