



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:54 PM GMT

PDB ID : 4ASU  
Title : F1-ATPase in which all three catalytic sites contain bound nucleotide, with magnesium ion released in the Empty site  
Authors : Rees, D.M.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2012-05-03  
Resolution : 2.60 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

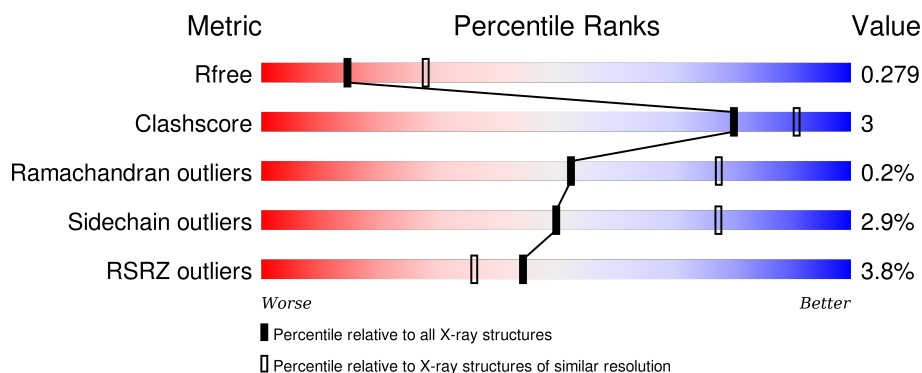
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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>83%</div> <div>12% • 5%</div> </div>
1	B	510	<div> <div>88%</div> <div>6% 6%</div> </div>
1	C	510	<div> <div>88%</div> <div>7% • 5%</div> </div>
2	D	480	<div> <div>86%</div> <div>10% •</div> </div>
2	E	480	<div> <div>85%</div> <div>10% • 5%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	F	480	
3	G	273	
4	H	146	
5	I	50	

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
7	MG	D	601	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24283 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, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	480	Total	C	N	O	S	0	0	0
			3663	2308	648	695	12			
1	C	485	Total	C	N	O	S	0	0	0
			3695	2327	653	703	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, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	458	Total	C	N	O	S	0	0	0
			3472	2201	592	669	10			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	181	Total	C	N	O	S	0	0	0
			1396	881	249	260	6			

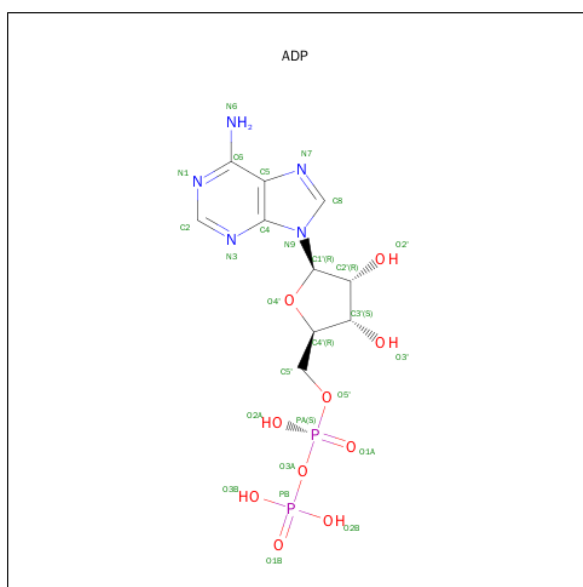
- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	83	Total	C	N	O	0	0	0
			615	392	102	121			

- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	23	Total	C	N	O	S	0	0	0
			183	118	33	31	1			

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- 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

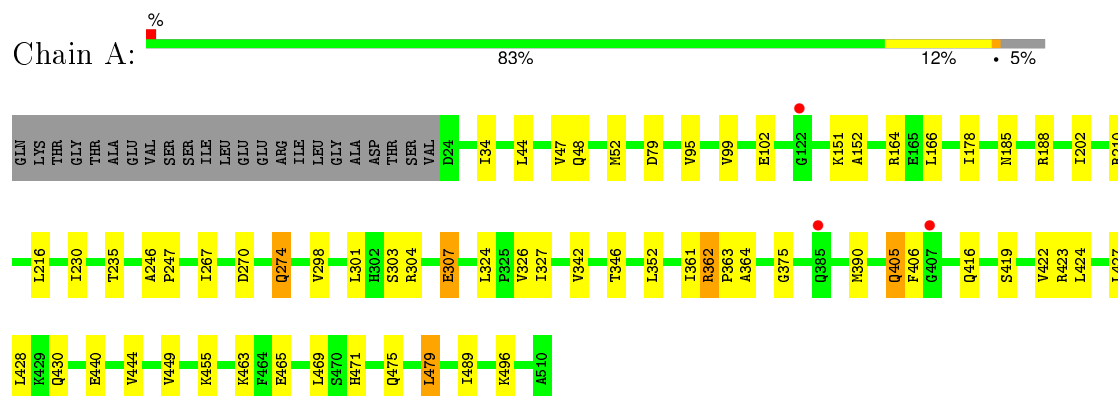
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	52	Total O 52 52	0	0
8	B	70	Total O 70 70	0	0
8	C	50	Total O 50 50	0	0
8	D	28	Total O 28 28	0	0
8	E	24	Total O 24 24	0	0
8	F	54	Total O 54 54	0	0
8	G	19	Total O 19 19	0	0
8	H	10	Total O 10 10	0	0
8	I	1	Total O 1 1	0	0

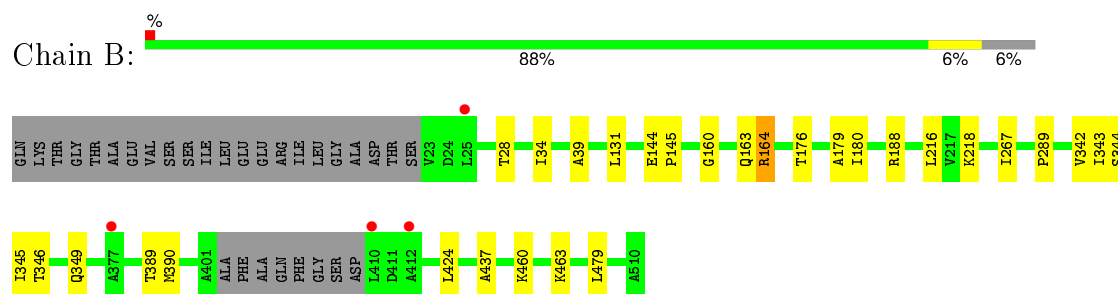
### 3 Residue-property plots [i](#)

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.

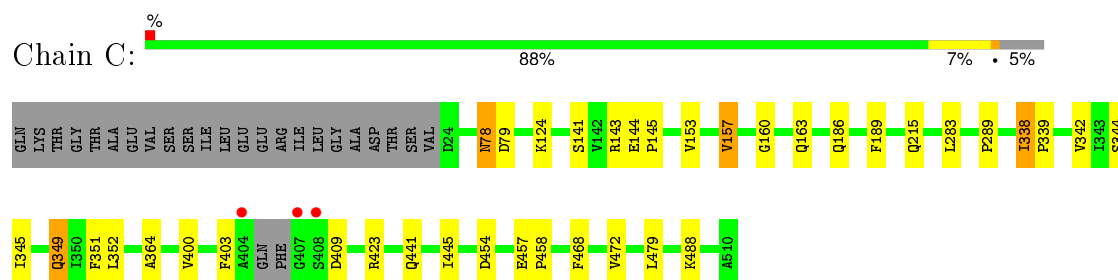
#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



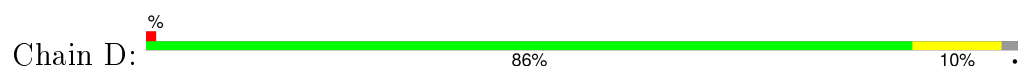
#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

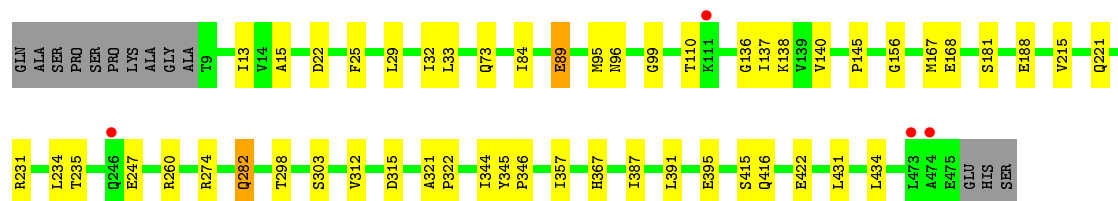


#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

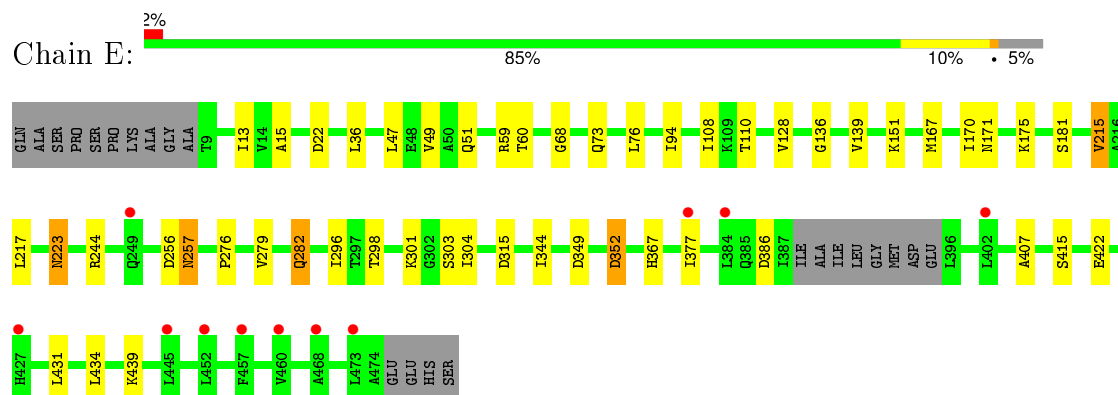


#### • Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

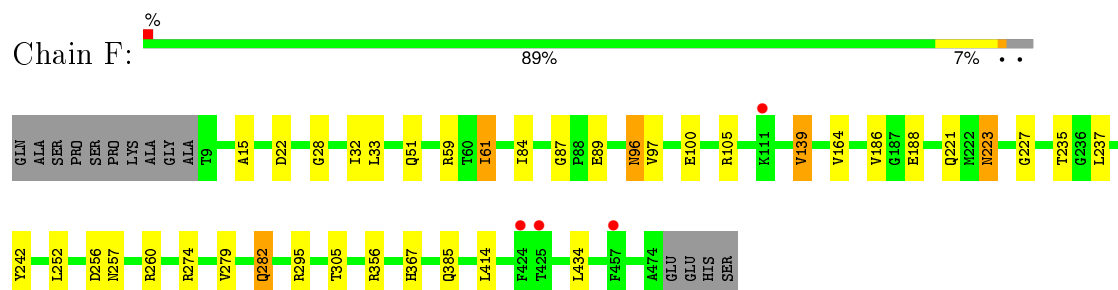




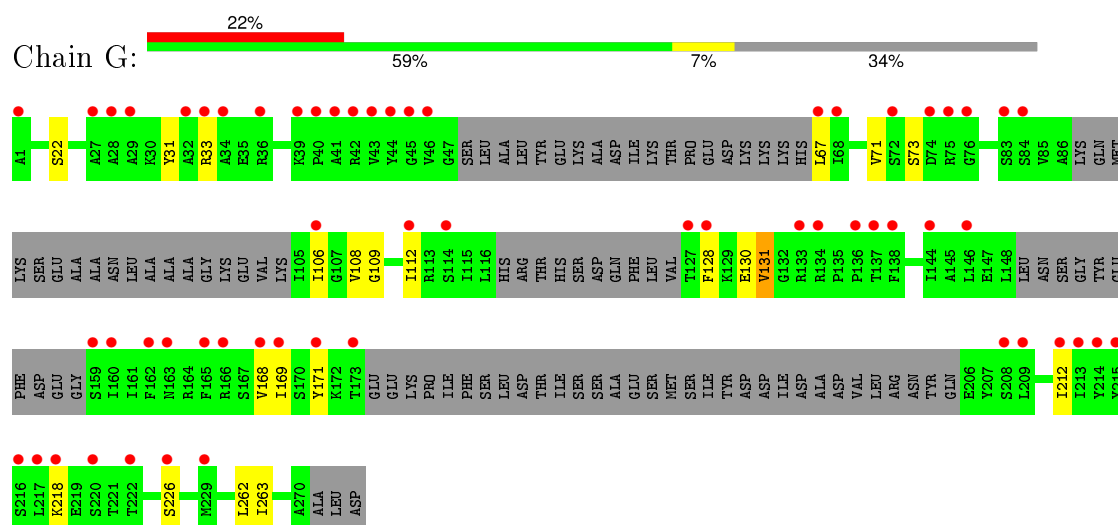
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

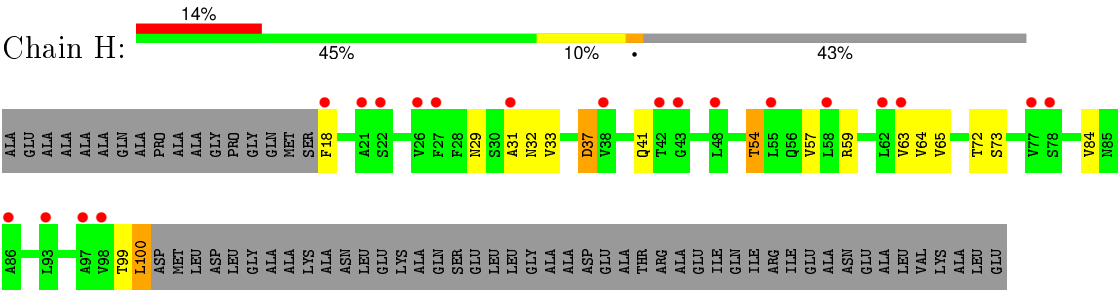


• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

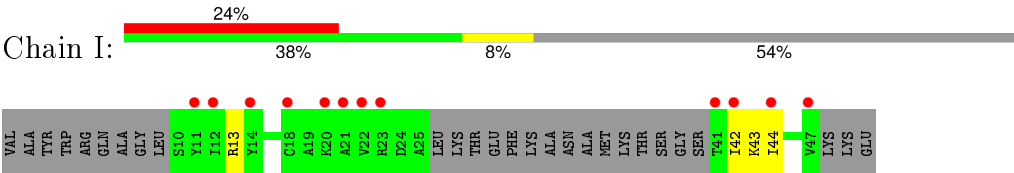


• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL





• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.27Å 135.11Å 266.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.50 – 2.60 59.73 – 2.59	Depositor EDS
% Data completeness (in resolution range)	78.0 (63.50-2.60) 78.0 (59.73-2.59)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, $R_{free}$	0.245 , 0.289 0.237 , 0.279	Depositor DCC
$R_{free}$ test set	4562 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 30.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 92050 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	24283	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP

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	0.30	0/3766	0.47	0/5080
1	B	0.30	0/3711	0.46	0/5005
1	C	0.30	0/3744	0.47	0/5049
2	D	0.31	0/3596	0.47	0/4879
2	E	0.31	0/3528	0.47	0/4786
2	F	0.31	0/3587	0.47	0/4867
3	G	0.28	0/1405	0.43	0/1878
4	H	0.37	0/627	0.50	0/860
5	I	0.28	0/183	0.41	0/243
All	All	0.31	0/24147	0.47	0/32647

There are no bond length outliers.

There are no bond angle outliers.

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	3715	0	3814	34	0
1	B	3663	0	3774	16	0
1	C	3695	0	3796	21	0
2	D	3539	0	3592	29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3472	0	3526	26	0
2	F	3530	0	3586	26	0
3	G	1396	0	1481	9	0
4	H	615	0	608	10	0
5	I	183	0	201	1	0
6	A	27	0	12	0	0
6	B	27	0	12	0	0
6	C	27	0	12	0	0
6	D	27	0	12	0	0
6	E	27	0	12	0	0
6	F	27	0	12	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	52	0	0	0	0
8	B	70	0	0	1	0
8	C	50	0	0	0	0
8	D	28	0	0	0	0
8	E	24	0	0	0	0
8	F	54	0	0	1	0
8	G	19	0	0	1	0
8	H	10	0	0	0	0
8	I	1	0	0	0	0
All	All	24283	0	24450	164	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 3.

All (164) 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)
2:F:282:GLN:H	2:F:282:GLN:HE21	1.05	0.93
2:D:282:GLN:HE21	2:D:282:GLN:H	1.00	0.92
2:D:282:GLN:NE2	2:D:282:GLN:H	1.73	0.86
2:E:282:GLN:H	2:E:282:GLN:HE21	1.22	0.86
2:D:282:GLN:HE21	2:D:282:GLN:N	1.82	0.77
1:C:153:VAL:HA	1:C:157:VAL:HG23	1.67	0.77
2:F:223:ASN:H	2:F:223:ASN:HD22	1.37	0.71
1:A:210:ARG:HG3	1:A:235:THR:HG21	1.78	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:276:PRO:HB2	3:G:262:LEU:HD21	1.78	0.65
3:G:108:VAL:HA	3:G:128:PHE:HB2	1.79	0.64
1:C:78:ASN:HD22	1:C:79:ASP:H	1.46	0.63
2:F:282:GLN:H	2:F:282:GLN:NE2	1.88	0.63
3:G:171:TYR:OH	3:G:226:SER:HB2	1.98	0.62
2:F:61:ILE:HD11	2:F:227:GLY:HA2	1.82	0.62
1:A:52:MET:HG2	1:A:95:VAL:HG22	1.82	0.61
2:E:244:ARG:HD3	2:E:304:ILE:HG13	1.83	0.61
1:C:160:GLY:H	1:C:163:GLN:NE2	1.99	0.60
1:A:362:ARG:HA	1:A:363:PRO:C	2.21	0.60
2:D:367:HIS:HE1	2:D:434:LEU:HD11	1.66	0.59
4:H:18:PHE:N	4:H:31:ALA:O	2.36	0.59
4:H:18:PHE:HB3	4:H:31:ALA:HB3	1.85	0.58
4:H:31:ALA:HA	4:H:32:ASN:CB	2.34	0.58
2:D:188:GLU:O	2:D:221:GLN:HB3	2.03	0.58
2:F:237:LEU:HD21	2:F:295:ARG:HB3	1.86	0.57
1:B:160:GLY:H	1:B:163:GLN:NE2	2.03	0.57
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.86	0.57
2:E:282:GLN:H	2:E:282:GLN:NE2	1.98	0.56
1:A:479:LEU:HG	1:A:496:LYS:HD3	1.88	0.56
1:C:215:GLN:HG2	2:F:356:ARG:HH12	1.71	0.55
2:E:13:ILE:HD12	2:E:73:GLN:HB3	1.88	0.55
1:A:471:HIS:CE1	1:A:475:GLN:HG3	2.42	0.55
1:C:338:ILE:HB	1:C:339:PRO:HD3	1.89	0.55
2:F:96:ASN:HD22	2:F:96:ASN:C	2.11	0.55
1:A:267:ILE:HG13	1:A:324:LEU:HB2	1.90	0.54
2:E:94:ILE:HG12	2:E:217:LEU:HD12	1.90	0.54
4:H:54:THR:H	4:H:84:VAL:HG13	1.72	0.54
1:B:218:LYS:HD2	2:E:128:VAL:HB	1.89	0.53
2:F:188:GLU:O	2:F:221:GLN:HB3	2.08	0.53
2:E:51:GLN:HB2	2:E:59:ARG:HB3	1.90	0.53
1:A:44:LEU:HB3	1:A:47:VAL:HG13	1.91	0.53
1:C:349:GLN:HG3	1:C:351:PHE:HE2	1.74	0.52
1:C:344:SER:HB2	2:D:260:ARG:HH22	1.74	0.52
1:A:44:LEU:O	1:A:47:VAL:HG22	2.08	0.52
2:E:377:ILE:HG12	2:E:407:ALA:HB2	1.92	0.52
2:E:223:ASN:H	2:E:223:ASN:HD22	1.58	0.52
1:A:444:VAL:HG21	1:A:465:GLU:HG3	1.91	0.51
2:F:51:GLN:HB2	2:F:59:ARG:HB3	1.93	0.51
2:F:367:HIS:CE1	2:F:434:LEU:HD11	2.46	0.51
1:C:78:ASN:HD22	1:C:79:ASP:N	2.08	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:95:MET:HE3	2:D:99:GLY:HA2	1.94	0.50
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.94	0.50
1:A:405:GLN:HG2	2:D:387:ILE:HD11	1.94	0.49
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.94	0.49
2:F:139:VAL:HG12	2:F:414:LEU:HD22	1.95	0.49
1:A:327:ILE:HD11	1:A:342:VAL:HG21	1.95	0.49
2:D:298:THR:HG23	2:D:303:SER:HA	1.94	0.49
1:C:186:GLN:HA	1:C:189:PHE:HD2	1.78	0.48
2:D:138:LYS:HE3	2:D:416:GLN:HB3	1.95	0.48
2:F:186:VAL:HG12	2:F:260:ARG:HB2	1.95	0.48
1:A:152:ALA:HA	1:A:428:LEU:HD22	1.95	0.48
2:E:171:ASN:O	2:E:175:LYS:HB2	2.14	0.48
1:A:151:LYS:H	1:A:430:GLN:HE22	1.60	0.48
1:B:160:GLY:H	1:B:163:GLN:HE21	1.60	0.48
2:D:344:ILE:HG23	2:D:415:SER:HB2	1.96	0.48
2:D:89:GLU:HG3	2:D:110:THR:HB	1.95	0.48
3:G:71:VAL:HA	3:G:108:VAL:HG13	1.95	0.48
4:H:31:ALA:HA	4:H:32:ASN:HB3	1.95	0.47
4:H:99:THR:HA	4:H:100:LEU:HA	1.59	0.47
1:A:301:LEU:HA	1:A:304:ARG:HH21	1.79	0.47
1:C:349:GLN:HG3	1:C:351:PHE:CE2	2.50	0.47
2:D:221:GLN:HA	2:D:221:GLN:HE21	1.80	0.47
2:E:256:ASP:HA	2:E:257:ASN:HA	1.67	0.47
2:E:49:VAL:HA	2:E:60:THR:HG22	1.97	0.47
3:G:73:SER:HA	3:G:131:VAL:HG23	1.97	0.47
8:G:2006:HOH:O	5:I:44:ILE:HA	2.15	0.47
2:F:252:LEU:HD23	2:F:305:THR:HB	1.96	0.46
1:B:289:PRO:HG2	3:G:263:ILE:HG12	1.97	0.46
1:A:424:LEU:HA	1:A:427:LEU:HD12	1.97	0.46
1:A:390:MET:HG3	1:A:424:LEU:HD22	1.97	0.46
2:E:223:ASN:N	2:E:223:ASN:HD22	2.13	0.46
1:C:441:GLN:O	1:C:445:ILE:HG12	2.15	0.46
2:D:345:TYR:HA	2:D:346:PRO:C	2.36	0.46
1:C:400:VAL:HA	1:C:403:PHE:HB3	1.98	0.46
2:D:391:LEU:HB3	2:D:395:GLU:HG3	1.98	0.46
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.98	0.46
1:A:151:LYS:H	1:A:430:GLN:NE2	2.14	0.46
2:D:156:GLY:H	2:D:312:VAL:HG23	1.80	0.46
1:C:457:GLU:HA	1:C:458:PRO:HD3	1.87	0.45
1:A:361:ILE:O	1:A:364:ALA:HA	2.16	0.45
1:B:34:ILE:HD13	1:B:39:ALA:HB2	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLN:HB3	1:A:274:GLN:HE21	1.66	0.45
1:A:270:ASP:HB2	1:A:326:VAL:O	2.16	0.45
2:D:84:ILE:HG21	2:D:235:THR:HG23	1.98	0.45
2:F:96:ASN:HD21	2:F:100:GLU:H	1.65	0.45
4:H:65:VAL:HB	4:H:73:SER:HB2	1.97	0.45
1:C:141:SER:HB2	1:C:143:ARG:HH21	1.82	0.45
2:F:223:ASN:N	2:F:223:ASN:HD22	2.04	0.45
1:B:144:GLU:HA	1:B:145:PRO:HD3	1.88	0.44
2:F:84:ILE:HG21	2:F:235:THR:HG23	1.97	0.44
1:B:460:LYS:HE2	1:B:463:LYS:HD2	2.00	0.44
2:F:256:ASP:HA	2:F:257:ASN:HA	1.79	0.44
1:C:160:GLY:H	1:C:163:GLN:HE21	1.64	0.44
1:B:163:GLN:HG2	1:B:164:ARG:N	2.33	0.44
1:A:48:GLN:HB3	2:E:68:GLY:HA2	1.99	0.44
2:D:145:PRO:HB2	2:D:357:ILE:HD11	2.00	0.44
2:D:221:GLN:HA	2:D:221:GLN:NE2	2.33	0.44
1:A:185:ASN:OD1	1:A:188:ARG:NH1	2.51	0.44
1:A:352:LEU:HA	1:A:364:ALA:O	2.18	0.43
4:H:37:ASP:HB2	4:H:64:VAL:HB	2.00	0.43
3:G:168:VAL:HG23	3:G:169:ILE:HG13	2.00	0.43
2:D:231:ARG:HD3	2:D:234:LEU:HD12	1.98	0.43
1:A:34:ILE:HD11	1:A:79:ASP:HB2	1.99	0.43
1:A:298:VAL:O	1:A:301:LEU:HB3	2.18	0.43
3:G:109:GLY:O	3:G:112:ILE:HG22	2.18	0.43
1:A:246:ALA:HB3	1:A:247:PRO:HD3	1.99	0.43
1:B:344:SER:HB2	8:B:2056:HOH:O	2.18	0.43
1:B:176:THR:O	1:B:180:ILE:HG12	2.18	0.43
2:D:13:ILE:HD12	2:D:73:GLN:HB3	2.01	0.43
2:E:108:ILE:HG22	2:E:110:THR:HG23	2.01	0.43
1:C:423:ARG:HD3	1:C:454:ASP:HA	2.00	0.43
2:E:36:LEU:HB2	2:E:47:LEU:HB2	2.00	0.43
2:D:136:GLY:HA3	2:D:431:LEU:HG	2.01	0.43
1:B:188:ARG:HH21	1:B:437:ALA:HB2	1.82	0.43
2:F:221:GLN:HA	2:F:221:GLN:HE21	1.84	0.42
1:C:144:GLU:HA	1:C:145:PRO:HD3	1.90	0.42
2:E:344:ILE:HG23	2:E:415:SER:HB3	2.00	0.42
2:F:32:ILE:HG22	2:F:33:LEU:HG	2.01	0.42
1:B:390:MET:HG3	1:B:424:LEU:HD13	2.00	0.42
4:H:41:GLN:HA	4:H:59:ARG:HH11	1.84	0.42
2:E:349:ASP:HB3	2:E:352:ASP:HB2	2.01	0.42
2:F:164:VAL:HG23	6:F:600:ADP:O2A	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:LEU:HD21	1:C:289:PRO:HB3	2.00	0.42
2:E:298:THR:HG23	2:E:303:SER:HB3	2.02	0.42
2:E:151:LYS:HE3	2:E:296:ILE:HB	2.02	0.42
2:E:167:MET:HA	2:E:170:ILE:HD12	2.02	0.42
2:F:87:GLY:HA2	2:F:242:TYR:CE1	2.55	0.42
1:A:419:SER:O	1:A:423:ARG:HD3	2.20	0.42
2:D:137:ILE:HG23	2:D:140:VAL:HB	2.01	0.42
2:D:25:PHE:HB2	2:D:29:LEU:HD12	2.02	0.42
1:B:343:ILE:HG12	1:B:349:GLN:HG2	2.00	0.42
1:A:406:PHE:HD1	3:G:22:SER:HG	1.68	0.41
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.50	0.41
2:D:367:HIS:CE1	2:D:434:LEU:HD11	2.52	0.41
1:A:178:ILE:HD11	1:A:352:LEU:HD21	2.02	0.41
2:F:32:ILE:O	2:F:33:LEU:HB2	2.20	0.41
1:A:166:LEU:HB2	1:A:346:THR:HG21	2.01	0.41
4:H:31:ALA:HB1	4:H:32:ASN:C	2.41	0.41
1:C:342:VAL:HA	1:C:345:ILE:HD12	2.03	0.41
1:B:342:VAL:HA	1:B:345:ILE:HD12	2.03	0.41
1:B:164:ARG:HB3	1:B:346:THR:HG22	2.02	0.41
2:E:136:GLY:HA3	2:E:431:LEU:HD12	2.03	0.41
1:C:352:LEU:HA	1:C:364:ALA:O	2.20	0.41
1:A:440:GLU:HB3	1:A:469:LEU:HD11	2.03	0.41
2:F:367:HIS:HE1	2:F:434:LEU:HD11	1.86	0.41
2:D:32:ILE:O	2:D:33:LEU:HB2	2.21	0.41
2:F:105:ARG:HD3	8:F:2013:HOH:O	2.21	0.41
2:E:181:SER:HB2	2:E:215:VAL:HG13	2.03	0.41
1:A:202:ILE:HG23	1:A:230:ILE:HG13	2.01	0.41
1:C:468:PHE:O	1:C:472:VAL:HG23	2.21	0.41
2:F:96:ASN:ND2	2:F:100:GLU:H	2.19	0.40
2:E:367:HIS:HE1	2:E:434:LEU:HD11	1.85	0.40
1:A:422:VAL:HG23	1:A:423:ARG:HD2	2.03	0.40
2:D:15:ALA:HB3	2:D:22:ASP:HB2	2.03	0.40
1:A:303:SER:O	1:A:307:GLU:HB2	2.22	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	485/510 (95%)	470 (97%)	14 (3%)	1 (0%)	52	77
1	B	476/510 (93%)	465 (98%)	11 (2%)	0	100	100
1	C	481/510 (94%)	472 (98%)	8 (2%)	1 (0%)	52	77
2	D	465/480 (97%)	439 (94%)	26 (6%)	0	100	100
2	E	454/480 (95%)	436 (96%)	17 (4%)	1 (0%)	52	77
2	F	464/480 (97%)	440 (95%)	22 (5%)	2 (0%)	39	65
3	G	169/273 (62%)	162 (96%)	5 (3%)	2 (1%)	16	33
4	H	81/146 (56%)	74 (91%)	7 (9%)	0	100	100
5	I	19/50 (38%)	19 (100%)	0	0	100	100
All	All	3094/3439 (90%)	2977 (96%)	110 (4%)	7 (0%)	52	77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	GLY
3	G	130	GLU
1	C	409	ASP
2	F	279	VAL
3	G	106	ILE
2	E	279	VAL
2	F	28	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	393/412 (95%)	379 (96%)	14 (4%)	42	71
1	B	389/412 (94%)	383 (98%)	6 (2%)	72	90
1	C	391/412 (95%)	384 (98%)	7 (2%)	66	87
2	D	377/386 (98%)	368 (98%)	9 (2%)	57	82
2	E	370/386 (96%)	358 (97%)	12 (3%)	46	74
2	F	376/386 (97%)	367 (98%)	9 (2%)	57	82
3	G	152/231 (66%)	146 (96%)	6 (4%)	39	68
4	H	69/109 (63%)	61 (88%)	8 (12%)	7	12
5	I	20/41 (49%)	17 (85%)	3 (15%)	3	6
All	All	2537/2775 (91%)	2463 (97%)	74 (3%)	50	77

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	VAL
1	A	102	GLU
1	A	164	ARG
1	A	216	LEU
1	A	274	GLN
1	A	307	GLU
1	A	362	ARG
1	A	405	GLN
1	A	416	GLN
1	A	449	VAL
1	A	455	LYS
1	A	463	LYS
1	A	479	LEU
1	A	489	ILE
1	B	28	THR
1	B	131	LEU
1	B	164	ARG
1	B	216	LEU
1	B	389	THR
1	B	479	LEU
1	C	78	ASN
1	C	124	LYS
1	C	157	VAL
1	C	338	ILE
1	C	349	GLN
1	C	479	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	488	LYS
2	D	89	GLU
2	D	96	ASN
2	D	167	MET
2	D	168	GLU
2	D	247	GLU
2	D	274	ARG
2	D	282	GLN
2	D	315	ASP
2	D	422	GLU
2	E	76	LEU
2	E	139	VAL
2	E	215	VAL
2	E	223	ASN
2	E	257	ASN
2	E	282	GLN
2	E	301	LYS
2	E	315	ASP
2	E	352	ASP
2	E	386	ASP
2	E	422	GLU
2	E	439	LYS
2	F	61	ILE
2	F	89	GLU
2	F	96	ASN
2	F	97	VAL
2	F	139	VAL
2	F	223	ASN
2	F	274	ARG
2	F	282	GLN
2	F	385	GLN
3	G	31	TYR
3	G	33	ARG
3	G	67	LEU
3	G	131	VAL
3	G	212	ILE
3	G	218	LYS
4	H	29	ASN
4	H	33	VAL
4	H	37	ASP
4	H	54	THR
4	H	57	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	H	63	VAL
4	H	72	THR
4	H	100	LEU
5	I	13	ARG
5	I	42	ILE
5	I	43	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	GLN
1	A	302	HIS
1	A	396	GLN
1	A	405	GLN
1	A	430	GLN
1	A	471	HIS
1	B	163	GLN
1	B	208	GLN
1	B	260	ASN
1	B	503	ASN
1	C	78	ASN
1	C	163	GLN
1	C	263	HIS
1	C	341	ASN
1	C	349	GLN
2	D	73	GLN
2	D	194	ASN
2	D	221	GLN
2	D	282	GLN
2	D	367	HIS
2	D	419	GLN
2	E	39	GLN
2	E	223	ASN
2	E	249	GLN
2	E	282	GLN
2	E	308	GLN
2	E	367	HIS
2	E	375	GLN
2	E	379	GLN
2	F	51	GLN
2	F	73	GLN
2	F	96	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	F	112	GLN
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	328	HIS
2	F	367	HIS
3	G	211	ASN
4	H	29	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	ADP	A	600	7	22,29,29	1.06	1 (4%)	27,45,45	1.90	4 (14%)
6	ADP	B	600	7	22,29,29	1.05	1 (4%)	27,45,45	1.92	3 (11%)
6	ADP	C	600	7	22,29,29	1.03	1 (4%)	27,45,45	1.89	4 (14%)
6	ADP	D	600	7	22,29,29	1.07	1 (4%)	27,45,45	1.93	4 (14%)
6	ADP	E	600	-	22,29,29	1.06	1 (4%)	27,45,45	1.92	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	ADP	F	600	7	22,29,29	1.05	1 (4%)	27,45,45	1.94	4 (14%)

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	ADP	A	600	7	-	0/12/32/32	0/3/3/3
6	ADP	B	600	7	-	0/12/32/32	0/3/3/3
6	ADP	C	600	7	-	0/12/32/32	0/3/3/3
6	ADP	D	600	7	-	0/12/32/32	0/3/3/3
6	ADP	E	600	-	-	0/12/32/32	0/3/3/3
6	ADP	F	600	7	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	600	ADP	C5-C4	3.21	1.47	1.40
6	D	600	ADP	C5-C4	3.23	1.47	1.40
6	F	600	ADP	C5-C4	3.24	1.47	1.40
6	E	600	ADP	C5-C4	3.25	1.47	1.40
6	A	600	ADP	C5-C4	3.26	1.47	1.40
6	B	600	ADP	C5-C4	3.29	1.47	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	600	ADP	N3-C2-N1	-7.44	123.20	128.89
6	B	600	ADP	N3-C2-N1	-7.37	123.25	128.89
6	A	600	ADP	N3-C2-N1	-7.25	123.34	128.89
6	D	600	ADP	N3-C2-N1	-7.19	123.39	128.89
6	E	600	ADP	N3-C2-N1	-7.13	123.44	128.89
6	F	600	ADP	N3-C2-N1	-7.10	123.46	128.89
6	F	600	ADP	C2'-C1'-N9	-4.17	107.92	114.29
6	D	600	ADP	C2'-C1'-N9	-3.79	108.51	114.29
6	E	600	ADP	PA-O3A-PB	-3.45	121.09	132.67
6	B	600	ADP	PA-O3A-PB	-3.17	122.04	132.67
6	A	600	ADP	C4-C5-N7	-3.15	106.58	109.48
6	B	600	ADP	C4-C5-N7	-3.15	106.58	109.48
6	D	600	ADP	C4-C5-N7	-3.04	106.69	109.48
6	E	600	ADP	C4-C5-N7	-3.02	106.70	109.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	600	ADP	C4-C5-N7	-2.99	106.72	109.48
6	C	600	ADP	C4-C5-N7	-2.91	106.80	109.48
6	D	600	ADP	PA-O3A-PB	-2.89	122.98	132.67
6	A	600	ADP	PA-O3A-PB	-2.86	123.08	132.67
6	C	600	ADP	PA-O3A-PB	-2.84	123.15	132.67
6	E	600	ADP	C2'-C1'-N9	-2.82	109.98	114.29
6	F	600	ADP	PA-O3A-PB	-2.77	123.39	132.67
6	A	600	ADP	C2'-C1'-N9	-2.03	111.19	114.29
6	C	600	ADP	O3B-PB-O2B	2.02	115.07	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	600	ADP	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%)	-0.06	3 (0%) 90 88	29, 49, 69, 97	0
1	B	480/510 (94%)	-0.20	4 (0%) 87 85	26, 43, 74, 111	0
1	C	485/510 (95%)	-0.20	3 (0%) 90 88	26, 39, 64, 97	0
2	D	467/480 (97%)	-0.15	4 (0%) 85 83	29, 48, 80, 127	0
2	E	458/480 (95%)	-0.00	11 (2%) 62 56	29, 53, 93, 114	0
2	F	466/480 (97%)	-0.17	4 (0%) 85 83	25, 42, 74, 103	0
3	G	181/273 (66%)	1.48	59 (32%) 1 0	33, 70, 102, 138	0
4	H	83/146 (56%)	1.26	20 (24%) 1 0	55, 75, 97, 113	0
5	I	23/50 (46%)	2.11	12 (52%) 0 0	86, 113, 121, 124	0
All	All	3130/3439 (91%)	0.02	120 (3%) 44 36	25, 47, 86, 138	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	67	LEU	5.8
3	G	83	SER	5.5
3	G	212	ILE	5.2
3	G	68	ILE	5.0
5	I	47	VAL	5.0
5	I	14	TYR	4.9
4	H	98	VAL	4.5
3	G	138	PHE	4.2
3	G	43	VAL	4.2
1	C	404	ALA	4.2
3	G	106	ILE	4.1
3	G	75	ARG	4.1
3	G	134	ARG	4.0
4	H	97	ALA	3.9
5	I	12	ILE	3.9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
5	I	44	ILE	3.9
5	I	22	VAL	3.8
2	D	111	LYS	3.8
4	H	21	ALA	3.6
1	C	407	GLY	3.6
4	H	77	VAL	3.6
2	D	474	ALA	3.6
2	E	457	PHE	3.6
3	G	137	THR	3.5
3	G	171	TYR	3.5
4	H	31	ALA	3.4
4	H	62	LEU	3.4
3	G	159	SER	3.3
3	G	114	SER	3.3
4	H	27	PHE	3.2
3	G	40	PRO	3.2
1	A	385	GLN	3.1
3	G	42	ARG	3.1
3	G	46	VAL	3.1
3	G	136	PRO	3.1
3	G	112	ILE	3.0
4	H	55	LEU	3.0
5	I	21	ALA	3.0
3	G	220	SER	3.0
3	G	33	ARG	3.0
2	E	445	LEU	3.0
3	G	128	PHE	2.9
3	G	165	PHE	2.9
4	H	43	GLY	2.9
2	E	377	ILE	2.8
3	G	209	LEU	2.8
4	H	18	PHE	2.8
3	G	214	TYR	2.8
3	G	36	ARG	2.8
3	G	160	ILE	2.7
3	G	45	GLY	2.7
3	G	72	SER	2.7
3	G	28	ALA	2.7
1	A	407	GLY	2.7
3	G	41	ALA	2.7
4	H	78	SER	2.7
3	G	39	LYS	2.7

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	246	GLN	2.6
1	B	412	ALA	2.6
3	G	27	ALA	2.6
4	H	22	SER	2.6
5	I	11	TYR	2.6
2	F	425	THR	2.6
4	H	63	VAL	2.6
3	G	173	THR	2.6
3	G	215	TYR	2.6
3	G	216	SER	2.6
5	I	42	ILE	2.6
2	E	452	LEU	2.5
3	G	163	ASN	2.5
3	G	166	ARG	2.5
5	I	20	LYS	2.5
3	G	44	TYR	2.5
3	G	144	ILE	2.5
4	H	93	LEU	2.5
4	H	42	THR	2.5
2	F	424	PHE	2.5
2	E	402	LEU	2.5
3	G	226	SER	2.4
3	G	229	MET	2.4
5	I	41	THR	2.4
3	G	74	ASP	2.4
3	G	222	THR	2.4
1	B	25	LEU	2.4
5	I	23	ARG	2.3
3	G	162	PHE	2.3
2	F	111	LYS	2.3
1	B	377	ALA	2.3
2	E	427	HIS	2.3
3	G	169	ILE	2.2
2	F	457	PHE	2.2
3	G	133	ARG	2.2
3	G	1	ALA	2.2
3	G	76	GLY	2.2
4	H	38	VAL	2.2
3	G	146	LEU	2.2
4	H	48	LEU	2.2
3	G	217	LEU	2.2
3	G	208	SER	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	G	29	ALA	2.2
2	E	460	VAL	2.2
3	G	34	ALA	2.2
2	E	384	LEU	2.2
2	E	473	LEU	2.2
3	G	32	ALA	2.1
3	G	218	LYS	2.1
1	B	410	LEU	2.1
4	H	58	LEU	2.1
1	A	122	GLY	2.1
2	D	473	LEU	2.1
3	G	127	THR	2.1
3	G	84	SER	2.1
3	G	213	ILE	2.1
3	G	168	VAL	2.1
5	I	18	CYS	2.1
4	H	86	ALA	2.1
1	C	408	SER	2.1
2	E	249	GLN	2.1
2	E	468	ALA	2.0
4	H	26	VAL	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
7	MG	D	601	1/1	0.95	0.22	4.83	48,48,48,48	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	ADP	C	600	27/27	0.96	0.16	0.05	28,34,37,38	0
6	ADP	D	600	27/27	0.96	0.16	-0.06	32,42,47,49	0
6	ADP	B	600	27/27	0.97	0.14	-0.57	37,41,45,46	0
6	ADP	F	600	27/27	0.97	0.14	-0.82	34,40,43,44	0
6	ADP	A	600	27/27	0.97	0.13	-1.39	33,41,47,48	0
6	ADP	E	600	27/27	0.94	0.12	-1.45	64,69,72,73	0
7	MG	C	601	1/1	0.97	0.10	-	34,34,34,34	0
7	MG	F	601	1/1	0.91	0.17	-	32,32,32,32	0
7	MG	B	601	1/1	0.93	0.10	-	45,45,45,45	0
7	MG	A	601	1/1	0.92	0.10	-	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.