



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2016 – 05:20 PM EDT

PDB ID : 5DN6
Title : ATP synthase from *Paracoccus denitrificans*
Authors : Morales-Rios, E.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2015-09-09
Resolution : 3.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027674
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-20027674

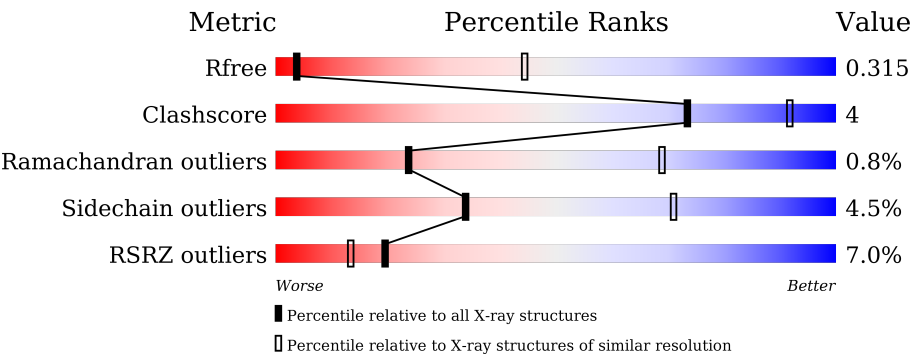
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.98 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	1009 (4.40-3.56)
Clashscore	102246	1033 (4.36-3.60)
Ramachandran outliers	100387	1012 (4.38-3.58)
Sidechain outliers	100360	1002 (4.38-3.58)
RSRZ outliers	91569	1012 (4.40-3.56)

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 ≥ 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	1	20	<div><div></div><div>100%</div></div>
2	2	15	<div><div></div><div>100%</div></div>
3	3	19	<div><div></div><div>100%</div></div>
4	A	511	<div><div></div><div>3%</div><div><div></div><div>85%</div><div></div><div>14%</div><div></div></div><div>..</div></div>
4	B	511	<div><div></div><div>%</div><div><div></div><div>81%</div><div></div><div>14%</div><div></div></div><div>..</div></div>
4	C	511	<div><div></div><div>%</div><div><div></div><div>77%</div><div></div><div>17%</div><div></div></div><div>• 5%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	D	474	 % 88% 10% ..
5	E	474	 3% 86% 12% ..
5	F	474	 2% 82% 14% ..
6	G	290	 4% 77% 11% • 10%
7	H	188	 3% 53% .. 41%
8	I	148	 9% 49% • 49%
9	J	77	 17% 95% ..
9	K	77	 16% 95% ..
9	L	77	 22% 96% .
9	M	77	 22% 96% .
9	N	77	 23% 96% .
9	O	77	 30% 96% .
9	P	77	 27% 96% .
9	Q	77	 29% 96% .
9	R	77	 22% 96% .
9	S	77	 34% 96% .
9	T	77	 19% 95% ..
9	U	77	 16% 95% ..
10	V	78	 100%
11	W	124	 100%
12	X	283	 % 35% 65%
13	Y	54	 100%
14	Z	104	 6% 44% 8% 48%

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 31527 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 Chain A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	1	20	Total	C	N	O	0	0	0
			100	60	20	20			

- Molecule 2 is a protein called Chain B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	2	15	Total	C	N	O	0	0	0
			75	45	15	15			

- Molecule 3 is a protein called Chain C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	3	19	Total	C	N	O	0	0	0
			95	57	19	19			

- Molecule 4 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	505	Total	C	N	O	S	0	0	0
			3811	2395	665	735	16			
4	B	496	Total	C	N	O	S	0	0	0
			3754	2359	657	723	15			
4	C	484	Total	C	N	O	S	0	0	0
			3652	2293	640	703	16			

- Molecule 5 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	470	Total	C	N	O	S	0	0	0
			3508	2211	600	687	10			
5	E	466	Total	C	N	O	S	0	0	0
			3490	2198	596	686	10			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	466	Total	C	N	O	S	0	0	0
			3489	2199	596	684	10			

- Molecule 6 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	260	Total	C	N	O	S	0	0	0
			1978	1227	367	375	9			

- Molecule 7 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	H	110	Total	C	N	O	0	0	0
			544	324	110	110			

- Molecule 8 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	75	Total	C	N	O	0	0	0
			366	216	75	75			

- Molecule 9 is a protein called ATP synthase F0 subcomplex C subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	J	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	K	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	L	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	M	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	N	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	O	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	P	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	Q	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	R	74	Total	C	N	O	0	0	0
			358	210	74	74			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	S	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	T	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	U	74	Total	C	N	O	0	0	0
			358	210	74	74			

- Molecule 10 is a protein called Chain V.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	V	78	Total	C	N	O	0	0	0
			390	234	78	78			

- Molecule 11 is a protein called Chain W.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	W	124	Total	C	N	O	0	0	0
			620	372	124	124			

- Molecule 12 is a protein called ATP synthase subunit a,ATP synthase subunit a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	X	98	Total	C	N	O	0	0	0
			486	291	98	97			

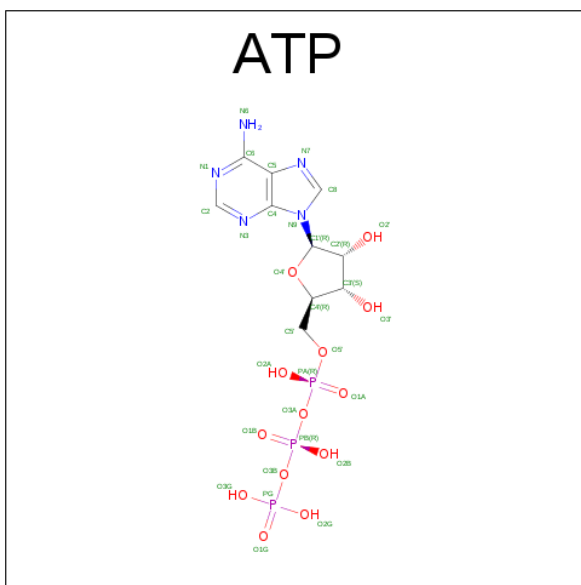
- Molecule 13 is a protein called Chain Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	Y	54	Total	C	N	O	0	0	0
			270	162	54	54			

- Molecule 14 is a protein called Zeta inhibitor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	Z	54	Total	C	N	O	S	0	0	0
			447	274	88	84	1			

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

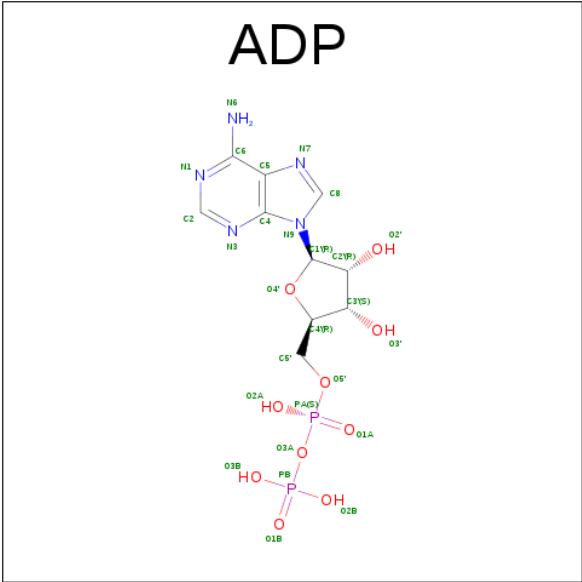


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
15	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
15	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
15	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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 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: Chain A

Chain 1:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Chain B

Chain 2:  100%


There are no outlier residues recorded for this chain.

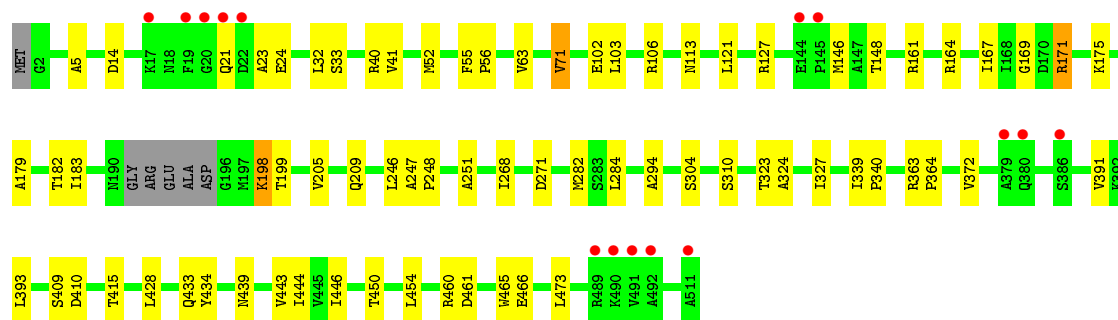
- Molecule 3: Chain C

Chain 3:  100%


There are no outlier residues recorded for this chain.

- Molecule 4: ATP synthase subunit alpha

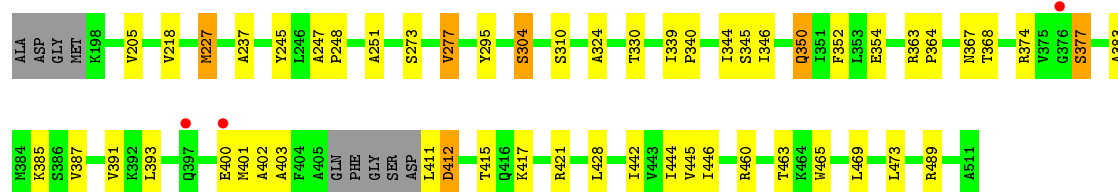
Chain A:  3% 85% 14% ..



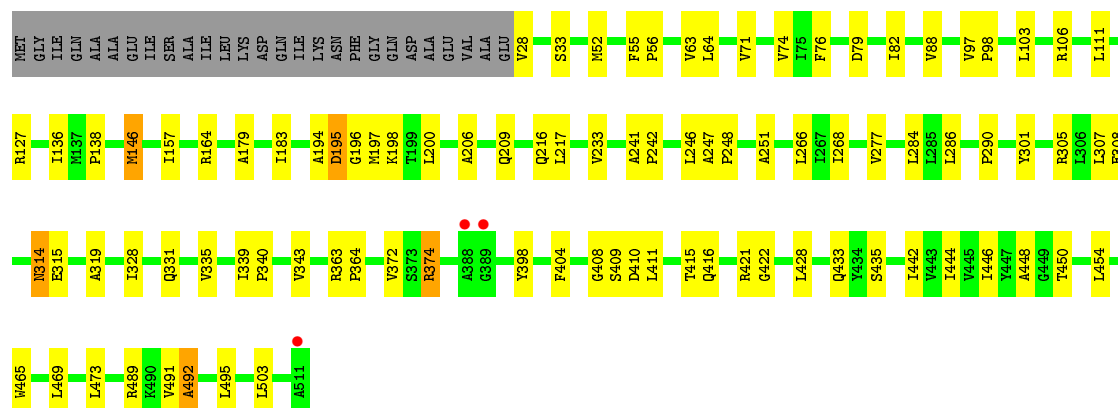
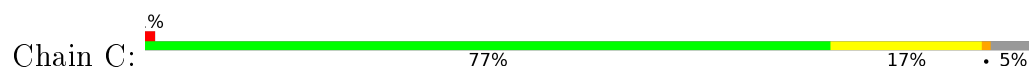
- Molecule 4: ATP synthase subunit alpha

Chain B:  81% 14% . .

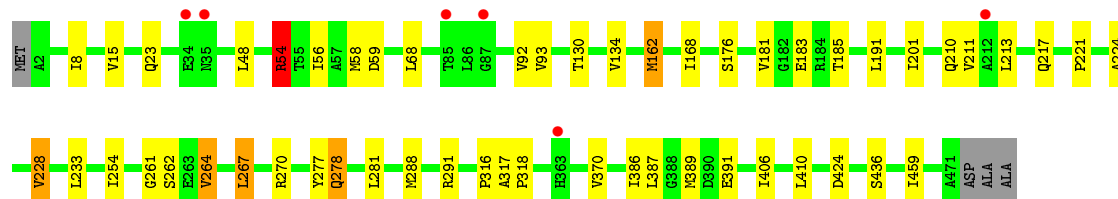
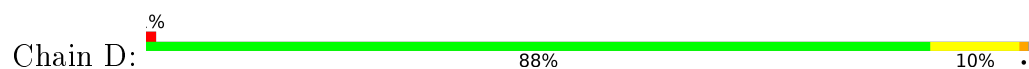




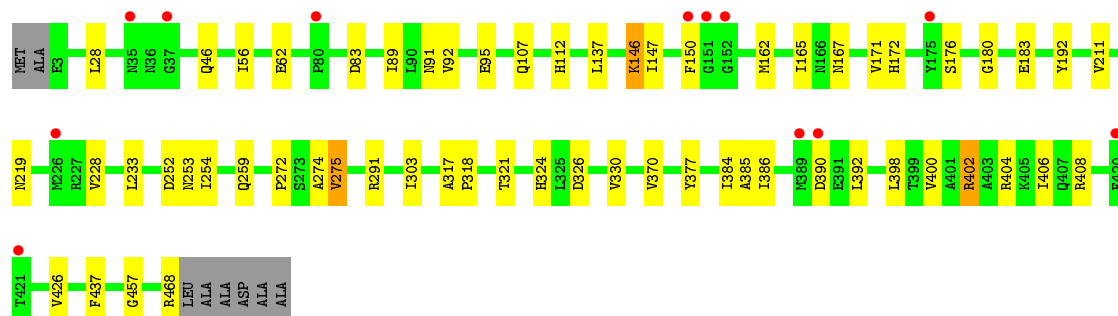
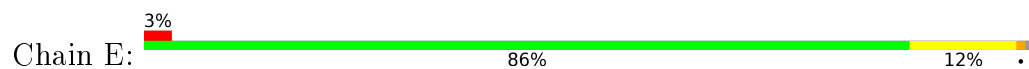
• Molecule 4: ATP synthase subunit alpha



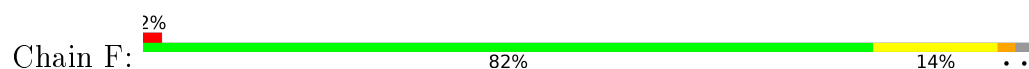
• Molecule 5: ATP synthase subunit beta

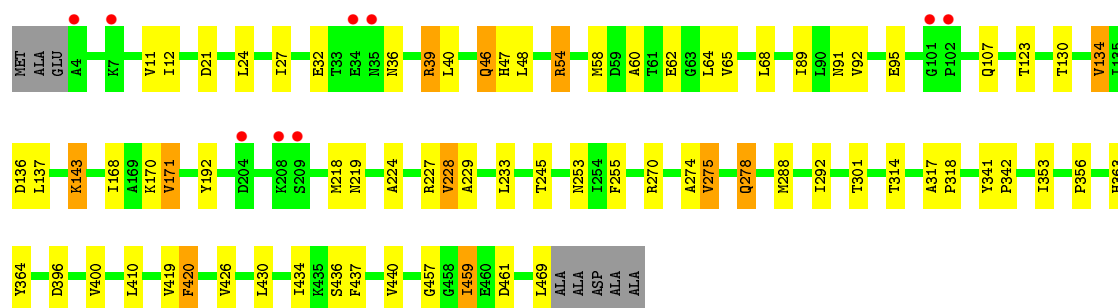


• Molecule 5: ATP synthase subunit beta

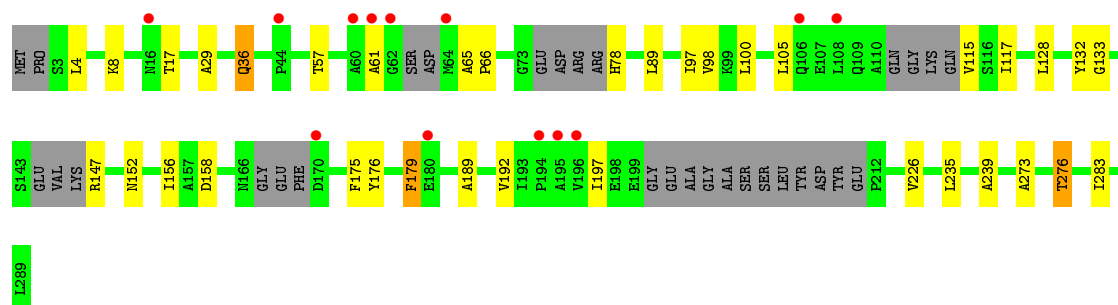
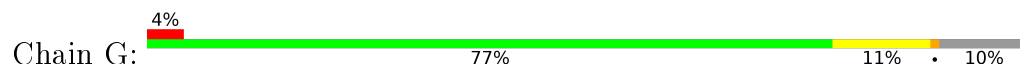


• Molecule 5: ATP synthase subunit beta

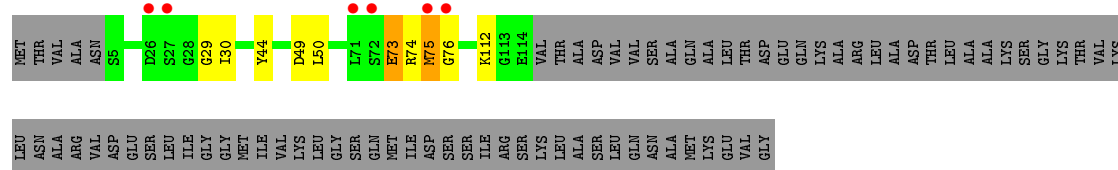




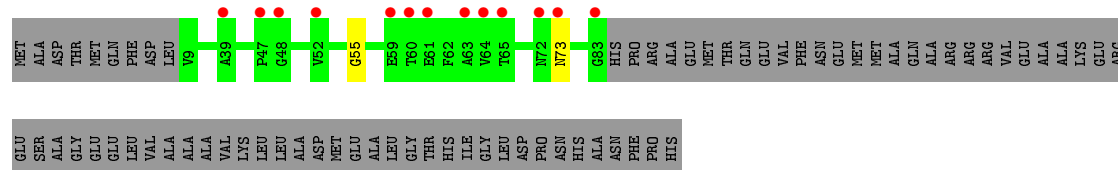
• Molecule 6: ATP synthase gamma chain



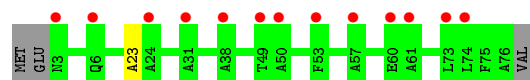
• Molecule 7: ATP synthase subunit delta



• Molecule 8: ATP synthase epsilon chain

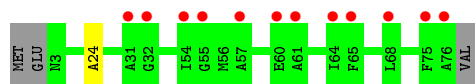


• Molecule 9: ATP synthase F0 subcomplex C subunit



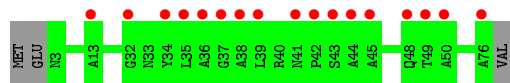
- Molecule 9: ATP synthase F0 subcomplex C subunit

Chain K:  16% 95%



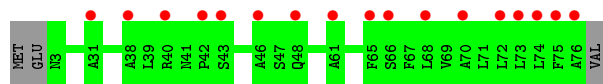
- Molecule 9: ATP synthase F0 subcomplex C subunit

Chain L:  22% 96%



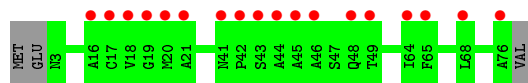
- Molecule 9: ATP synthase F0 subcomplex C subunit

Chain M:  22% 96%



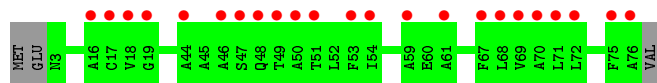
- Molecule 9: ATP synthase F0 subcomplex C subunit

Chain N:  23% 96%



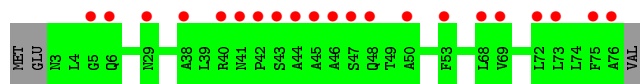
- Molecule 9: ATP synthase F0 subcomplex C subunit

Chain O:  30% 96%



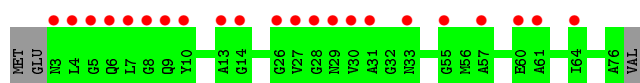
- Molecule 9: ATP synthase F0 subcomplex C subunit

Chain P:  27% 96%

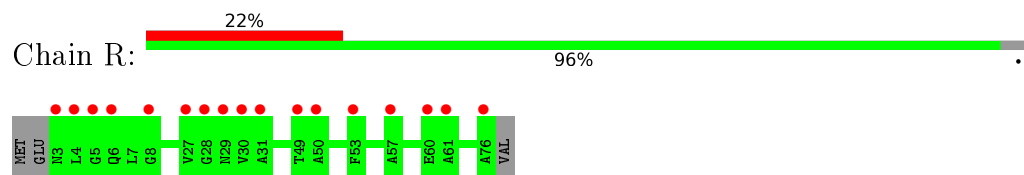


- Molecule 9: ATP synthase F0 subcomplex C subunit

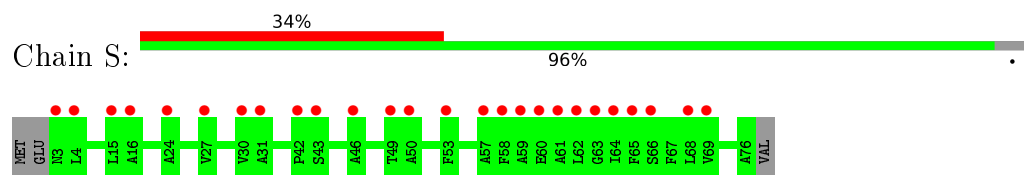
Chain Q:  29% 96%



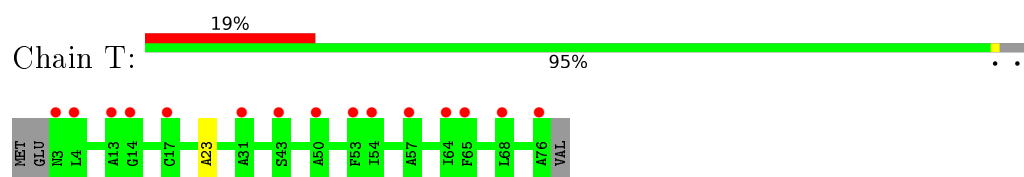
- Molecule 9: ATP synthase F0 subcomplex C subunit



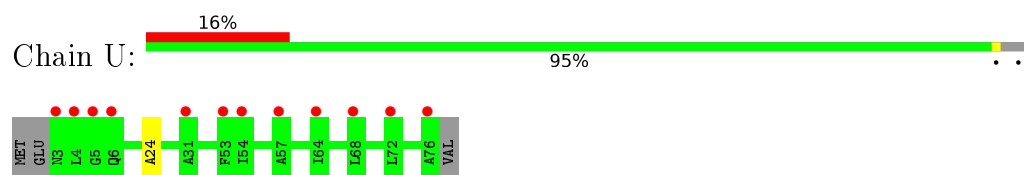
- Molecule 9: ATP synthase F0 subcomplex C subunit



- Molecule 9: ATP synthase F0 subcomplex C subunit



- Molecule 9: ATP synthase F0 subcomplex C subunit



- Molecule 10: Chain V



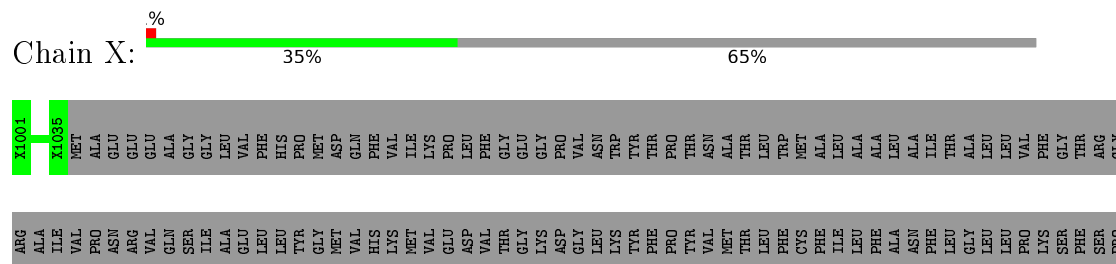
There are no outlier residues recorded for this chain.

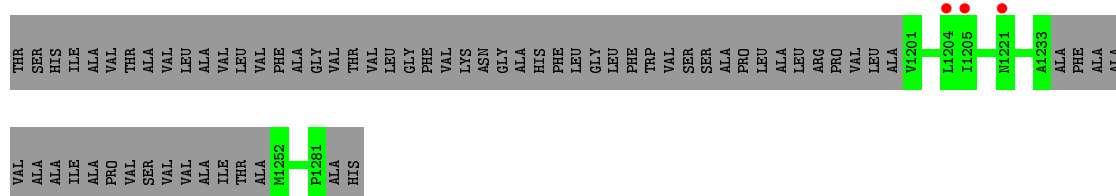
- Molecule 11: Chain W



There are no outlier residues recorded for this chain.

- Molecule 12: ATP synthase subunit a,ATP synthase subunit a



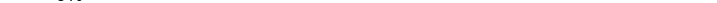


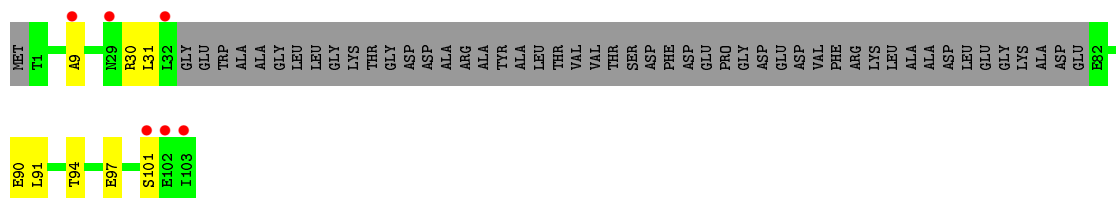
- Molecule 13: Chain Y

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 14: Zeta inhibitor protein

Chain Z: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.00Å 187.94Å 164.72Å 90.00° 97.44° 90.00°	Depositor
Resolution (Å)	36.84 – 3.98 36.84 – 3.98	Depositor EDS
% Data completeness (in resolution range)	98.6 (36.84-3.98) 98.8 (36.84-3.98)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 3.99Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.295 , 0.324 0.292 , 0.315	Depositor DCC
R_{free} test set	2789 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	119.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	31527	wwPDB-VP
Average B, all atoms (Å ²)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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, ATP, 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$
4	A	0.38	1/3864 (0.0%)	0.68	3/5227 (0.1%)
4	B	0.37	0/3805	0.66	2/5146 (0.0%)
4	C	0.36	0/3705	0.68	4/5015 (0.1%)
5	D	0.35	0/3562	0.65	2/4840 (0.0%)
5	E	0.36	1/3544 (0.0%)	0.62	2/4815 (0.0%)
5	F	0.35	0/3543	0.65	0/4814
6	G	0.40	0/1990	0.65	1/2674 (0.0%)
7	H	0.36	0/543	0.52	1/755 (0.1%)
8	I	0.29	0/365	0.55	0/504
9	J	0.43	0/357	0.51	0/491
9	K	0.43	0/357	0.51	0/491
9	L	0.43	0/357	0.52	0/491
9	M	0.43	0/357	0.51	0/491
9	N	0.43	0/357	0.51	0/491
9	O	0.43	0/357	0.51	0/491
9	P	0.43	0/357	0.51	0/491
9	Q	0.43	0/357	0.51	0/491
9	R	0.43	0/357	0.50	0/491
9	S	0.43	0/357	0.51	0/491
9	T	0.43	0/357	0.51	0/491
9	U	0.43	0/357	0.51	0/491
12	X	0.32	0/309	0.50	0/428
14	Z	0.49	0/450	0.69	0/599
All	All	0.38	2/29964 (0.0%)	0.63	15/40709 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	40	ARG	CZ-NH1	7.05	1.42	1.33
5	E	259	GLN	CD-OE1	5.44	1.35	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	106	ARG	NE-CZ-NH2	9.18	124.89	120.30
4	B	139	ARG	NE-CZ-NH2	8.70	124.65	120.30
5	E	402	ARG	NE-CZ-NH2	8.17	124.39	120.30
4	A	40	ARG	NE-CZ-NH2	-7.87	116.37	120.30
4	A	40	ARG	NE-CZ-NH1	7.43	124.02	120.30
5	E	402	ARG	NE-CZ-NH1	-6.40	117.10	120.30
4	C	314	ASN	N-CA-CB	-6.33	99.20	110.60
4	C	106	ARG	NE-CZ-NH1	-6.08	117.26	120.30
4	B	139	ARG	NE-CZ-NH1	-5.84	117.38	120.30
5	D	54	ARG	CG-CD-NE	-5.68	99.86	111.80
4	C	374	ARG	CG-CD-NE	5.49	123.33	111.80
5	D	54	ARG	NE-CZ-NH2	-5.35	117.62	120.30
4	A	171	ARG	NE-CZ-NH2	5.34	122.97	120.30
7	H	49	ASP	CB-CA-C	5.23	120.86	110.40
6	G	179	PHE	CB-CA-C	-5.19	100.03	110.40

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	1	100	0	23	0	0
2	2	75	0	17	0	0
3	3	95	0	21	0	0
4	A	3811	0	3875	29	0
4	B	3754	0	3822	38	0
4	C	3652	0	3709	48	0
5	D	3508	0	3532	32	0
5	E	3490	0	3513	32	0
5	F	3489	0	3517	45	0
6	G	1978	0	2035	22	0
7	H	544	0	277	3	0
8	I	366	0	176	0	0
9	J	358	0	209	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	358	0	209	1	0
9	L	358	0	209	0	0
9	M	358	0	209	0	0
9	N	358	0	209	0	0
9	O	358	0	209	0	0
9	P	358	0	209	0	0
9	Q	358	0	209	0	0
9	R	358	0	209	0	0
9	S	358	0	209	0	0
9	T	358	0	209	1	0
9	U	358	0	209	1	0
10	V	390	0	80	0	0
11	W	620	0	127	0	0
12	X	486	0	181	0	0
13	Y	270	0	58	0	0
14	Z	447	0	449	4	0
15	A	31	0	12	0	0
15	C	31	0	12	0	0
15	D	31	0	12	0	0
15	F	31	0	12	0	0
16	A	1	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	D	1	0	0	0	0
16	F	1	0	0	0	0
17	B	27	0	12	0	0
All	All	31527	0	27980	242	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 4.

All (242) 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)
5:F:278:GLN:H	5:F:278:GLN:HE21	1.24	0.83
5:D:386:ILE:HD11	6:G:17:THR:HG22	1.59	0.82
5:E:176:SER:HB2	5:E:211:VAL:HG12	1.62	0.80
14:Z:31:LEU:HD23	14:Z:91:LEU:HD22	1.64	0.80
5:D:48:LEU:HD21	5:D:54:ARG:HG3	1.67	0.77
4:A:433:GLN:HG2	4:A:434:TYR:CE2	2.21	0.76
6:G:179:PHE:CE1	6:G:239:ALA:HB3	2.21	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:97:ILE:HD11	6:G:176:TYR:HA	1.68	0.74
5:F:91:ASN:HD21	5:F:95:GLU:HB2	1.52	0.73
7:H:73:GLU:O	7:H:75:MET:N	2.22	0.72
4:C:146:MET:HE3	4:C:266:LEU:HD13	1.76	0.68
4:C:206:ALA:HB1	4:C:209:GLN:OE1	1.93	0.68
4:C:76:PHE:HE2	4:C:246:LEU:HD22	1.58	0.67
5:F:278:GLN:N	5:F:278:GLN:HE21	1.92	0.67
6:G:105:LEU:HD13	6:G:115:VAL:HG11	1.78	0.66
4:B:411:LEU:HD23	4:B:415:THR:HB	1.78	0.65
4:A:5:ALA:HB1	4:A:32:LEU:HD13	1.79	0.64
5:D:48:LEU:HD11	5:D:54:ARG:HG2	1.79	0.64
5:E:165:ILE:HD13	5:E:211:VAL:HG11	1.79	0.64
5:F:170:LYS:O	5:F:171:VAL:HG22	1.98	0.62
5:F:92:VAL:HB	5:F:228:VAL:HG13	1.82	0.61
4:B:247:ALA:HB3	4:B:248:PRO:HD3	1.80	0.61
4:A:391:VAL:HG21	4:A:446:ILE:HG23	1.83	0.61
4:A:179:ALA:HB1	4:A:268:ILE:HD13	1.82	0.61
5:F:32:GLU:OE2	5:F:39:ARG:NH1	2.34	0.60
5:D:162:MET:SD	5:D:191:LEU:HD13	2.42	0.60
4:C:404:PHE:HA	14:Z:9:ALA:HB1	1.84	0.60
4:C:301:TYR:CE1	4:C:305:ARG:HG3	2.37	0.59
5:D:386:ILE:HD11	6:G:17:THR:CG2	2.31	0.59
5:D:176:SER:HB2	5:D:211:VAL:HG22	1.84	0.59
5:F:46:GLN:HG2	5:F:54:ARG:HB2	1.83	0.59
4:B:428:LEU:HD22	4:B:445:VAL:CG2	2.33	0.59
6:G:36:GLN:HA	6:G:36:GLN:HE21	1.68	0.58
5:D:181:VAL:HG13	5:D:228:VAL:HG13	1.84	0.58
4:B:51:GLU:OE2	4:B:90:ARG:HB2	2.03	0.58
5:E:146:LYS:HG2	5:E:324:HIS:O	2.04	0.58
5:F:48:LEU:HD21	5:F:54:ARG:HG3	1.85	0.58
6:G:117:ILE:HD13	6:G:128:LEU:HD23	1.84	0.58
5:E:404:ARG:O	5:E:408:ARG:HG2	2.03	0.58
6:G:179:PHE:HE1	6:G:239:ALA:HB3	1.63	0.58
4:C:64:LEU:HD12	4:C:286:LEU:HD11	1.86	0.57
4:A:247:ALA:HB3	4:A:248:PRO:HD3	1.86	0.57
4:A:391:VAL:HG21	4:A:446:ILE:CG2	2.35	0.56
4:C:179:ALA:HB1	4:C:268:ILE:HD13	1.86	0.56
4:B:465:TRP:CH2	4:B:469:LEU:HD13	2.41	0.56
5:F:363:HIS:CD2	5:F:430:LEU:HD11	2.41	0.56
4:B:391:VAL:HG21	4:B:446:ILE:CG2	2.35	0.56
4:A:102:GLU:O	4:A:106:ARG:NH1	2.37	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:60:ALA:HB1	5:F:62:GLU:OE1	2.06	0.56
5:E:384:ILE:HG12	5:E:392:LEU:HD11	1.88	0.55
5:D:254:ILE:HD11	5:D:288:MET:SD	2.46	0.55
6:G:4:LEU:HD23	6:G:8:LYS:HD2	1.88	0.55
4:A:161:ARG:NH1	4:A:198:LYS:O	2.33	0.55
5:E:233:LEU:HD21	5:E:291:ARG:HB2	1.88	0.55
5:F:134:VAL:HG13	5:F:410:LEU:HD22	1.88	0.55
4:B:295:TYR:CZ	4:B:339:ILE:HD11	2.42	0.55
5:F:48:LEU:HD11	5:F:54:ARG:HG2	1.88	0.54
6:G:57:THR:HG21	6:G:197:ILE:HG23	1.90	0.54
4:B:97:VAL:HB	4:B:98:PRO:HD2	1.90	0.54
5:E:89:ILE:HD11	5:E:192:TYR:CD1	2.42	0.54
5:D:317:ALA:HB3	5:D:318:PRO:CD	2.37	0.54
4:C:444:ILE:HG21	4:C:473:LEU:HD11	1.90	0.54
5:F:317:ALA:HB3	5:F:318:PRO:CD	2.38	0.54
5:E:147:ILE:HD13	5:E:303:ILE:CD1	2.38	0.54
5:E:28:LEU:HD13	5:E:112:HIS:CD2	2.43	0.53
4:A:41:VAL:HB	4:A:71:VAL:HG12	1.90	0.53
4:B:383:ALA:HB2	4:B:489:ARG:O	2.08	0.53
4:B:391:VAL:HG21	4:B:446:ILE:HG23	1.90	0.53
4:B:151:LYS:HG2	4:B:442:ILE:HG23	1.90	0.53
5:D:15:VAL:HG21	5:D:267:LEU:HB2	1.91	0.53
5:E:171:VAL:HG23	5:E:172:HIS:CD2	2.44	0.53
5:F:136:ASP:HB3	5:F:430:LEU:HD13	1.91	0.52
5:F:426:VAL:HG11	5:F:457:GLY:HA3	1.91	0.52
4:C:183:ILE:HD11	4:C:268:ILE:HD12	1.92	0.52
5:D:201:ILE:CD1	5:D:213:LEU:HD11	2.40	0.51
6:G:147:ARG:NH1	6:G:235:LEU:HD22	2.26	0.51
4:A:439:ASN:O	4:A:443:VAL:HG23	2.11	0.51
4:C:196:GLY:O	4:C:198:LYS:N	2.43	0.51
4:C:284:LEU:HD21	4:C:290:PRO:HB3	1.92	0.51
4:C:307:LEU:O	4:C:308:GLU:CB	2.57	0.51
4:A:148:THR:HA	4:A:182:THR:HG23	1.93	0.51
4:A:55:PHE:HB3	4:A:56:PRO:HD2	1.92	0.51
4:C:465:TRP:CH2	4:C:469:LEU:HD22	2.46	0.51
5:D:261:GLY:HA3	5:D:278:GLN:HE22	1.76	0.50
5:D:387:LEU:HD13	5:D:391:GLU:HG2	1.94	0.50
5:F:65:VAL:HB	5:F:68:LEU:HD13	1.92	0.50
4:C:421:ARG:NH2	4:C:450:THR:O	2.45	0.50
5:E:180:GLY:HA3	5:E:183:GLU:HG2	1.94	0.50
4:B:168:ILE:HD11	4:B:330:THR:CG2	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:167:ASN:O	5:E:171:VAL:HG22	2.11	0.50
6:G:97:ILE:CD1	6:G:176:TYR:HA	2.40	0.49
5:F:419:VAL:HG23	5:F:420:PHE:CE1	2.48	0.49
5:D:134:VAL:HG22	5:D:410:LEU:HB3	1.93	0.49
14:Z:90:GLU:O	14:Z:94:THR:OG1	2.23	0.49
4:C:454:LEU:HD21	4:C:465:TRP:CH2	2.46	0.49
5:D:317:ALA:HB3	5:D:318:PRO:HD3	1.94	0.49
6:G:273:ALA:HA	6:G:276:THR:OG1	2.13	0.49
4:C:138:PRO:O	4:C:314:ASN:HB2	2.13	0.49
5:D:201:ILE:HD11	5:D:213:LEU:HD11	1.93	0.49
4:C:146:MET:CE	4:C:266:LEU:HD13	2.42	0.49
5:F:27:ILE:HD12	5:F:46:GLN:HA	1.94	0.49
5:F:440:VAL:HG23	5:F:459:ILE:HD11	1.94	0.48
6:G:179:PHE:CZ	6:G:239:ALA:HB3	2.48	0.48
4:B:63:VAL:HG13	4:B:71:VAL:CG1	2.43	0.48
5:F:317:ALA:HB3	5:F:318:PRO:HD3	1.95	0.48
5:D:92:VAL:HG13	5:D:93:VAL:HG13	1.95	0.48
4:A:428:LEU:HD12	4:A:466:GLU:OE1	2.14	0.48
4:B:38:ILE:HD11	4:B:74:VAL:HG13	1.95	0.48
5:F:363:HIS:CD2	5:F:434:ILE:HD11	2.49	0.48
4:B:411:LEU:HD23	4:B:415:THR:CB	2.42	0.48
4:B:387:VAL:O	4:B:391:VAL:HG23	2.14	0.48
5:F:143:LYS:O	5:F:301:THR:OG1	2.27	0.48
4:B:55:PHE:CD2	4:B:82:ILE:HD11	2.48	0.47
5:E:385:ALA:HB3	5:E:386:ILE:HD12	1.96	0.47
4:B:310:SER:OG	4:B:324:ALA:HB2	2.14	0.47
4:B:142:VAL:HG11	4:B:160:GLY:HA3	1.96	0.47
4:A:169:GLY:O	4:A:175:LYS:HE2	2.15	0.47
4:A:363:ARG:HA	4:A:364:PRO:C	2.34	0.47
4:A:183:ILE:HD11	4:A:268:ILE:HD12	1.97	0.47
4:A:433:GLN:CG	4:A:434:TYR:CE2	2.96	0.47
4:C:55:PHE:HB3	4:C:56:PRO:HD2	1.97	0.47
5:F:288:MET:CE	5:F:292:ILE:HD11	2.45	0.47
5:E:386:ILE:HG21	6:G:29:ALA:HB3	1.97	0.47
4:C:301:TYR:CZ	5:D:221:PRO:HA	2.50	0.46
5:D:386:ILE:HG22	6:G:89:LEU:HD11	1.96	0.46
5:E:150:PHE:HD2	5:E:330:VAL:HG22	1.81	0.46
5:F:143:LYS:O	5:F:301:THR:HG23	2.15	0.46
5:F:58:MET:CE	5:F:224:ALA:HA	2.46	0.46
4:C:448:ALA:HB2	4:C:503:LEU:HD21	1.97	0.46
5:D:130:THR:HA	5:D:168:ILE:HD11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:398:LEU:HD21	5:E:402:ARG:NH2	2.30	0.46
5:F:396:ASP:O	5:F:400:VAL:HG23	2.16	0.46
7:H:73:GLU:O	7:H:76:GLY:N	2.49	0.46
4:C:442:ILE:O	4:C:446:ILE:HG12	2.15	0.46
5:F:130:THR:HA	5:F:168:ILE:HD11	1.97	0.46
4:A:454:LEU:HD21	4:A:465:TRP:CE3	2.51	0.46
4:B:205:VAL:CG2	4:B:251:ALA:CB	2.94	0.46
5:E:91:ASN:OD1	5:E:95:GLU:N	2.49	0.46
4:C:328:ILE:HD11	4:C:343:VAL:HG21	1.97	0.46
5:D:277:TYR:HE2	5:D:317:ALA:HB2	1.81	0.46
5:F:436:SER:CA	5:F:459:ILE:HD12	2.46	0.46
4:C:28:VAL:HG13	4:C:88:VAL:O	2.16	0.45
5:E:147:ILE:HD13	5:E:303:ILE:HD13	1.98	0.45
4:A:167:ILE:HG22	4:A:175:LYS:HB2	1.99	0.45
4:B:102:GLU:HG3	4:B:123:ALA:HA	1.97	0.45
4:C:216:GLN:HE22	5:F:123:THR:HA	1.81	0.45
4:C:247:ALA:HB3	4:C:248:PRO:HD3	1.99	0.45
4:B:363:ARG:HA	4:B:364:PRO:C	2.37	0.45
4:C:79:ASP:HA	4:C:82:ILE:HD12	1.98	0.45
5:D:233:LEU:HD11	5:D:291:ARG:NE	2.31	0.45
4:B:273:SER:O	4:B:277:VAL:HG13	2.16	0.45
4:C:146:MET:HE1	4:C:200:LEU:HD21	1.99	0.45
5:E:377:TYR:CE1	5:E:400:VAL:HG13	2.51	0.45
4:A:444:ILE:HG21	4:A:473:LEU:HD11	1.99	0.45
4:B:428:LEU:HD22	4:B:445:VAL:HG22	2.00	0.45
5:E:137:LEU:HD22	5:E:437:PHE:CD2	2.52	0.45
5:D:277:TYR:CE1	5:D:316:PRO:HG2	2.52	0.44
5:E:272:PRO:HD2	6:G:283:ILE:HD13	1.99	0.44
4:A:391:VAL:HG22	4:A:450:THR:CG2	2.47	0.44
6:G:175:PHE:CE1	6:G:189:ALA:HB2	2.52	0.44
5:F:11:VAL:O	5:F:12:ILE:HD13	2.17	0.44
5:F:229:ALA:HB1	5:F:288:MET:HE3	2.00	0.44
4:C:146:MET:HE1	4:C:266:LEU:HD22	2.00	0.44
5:F:40:LEU:HD23	5:F:64:LEU:HD21	1.99	0.44
6:G:36:GLN:HA	6:G:36:GLN:NE2	2.32	0.44
4:C:398:TYR:CD1	4:C:422:GLY:HA3	2.53	0.44
4:C:97:VAL:HB	4:C:98:PRO:HD2	1.99	0.44
4:C:404:PHE:CA	14:Z:9:ALA:HB1	2.47	0.44
4:B:218:VAL:HG13	4:B:227:MET:CE	2.48	0.44
4:B:65:ASN:N	4:B:65:ASN:HD22	2.15	0.44
4:C:339:ILE:HB	4:C:340:PRO:HD3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:363:ARG:HA	4:C:364:PRO:C	2.38	0.44
5:F:274:ALA:O	5:F:275:VAL:HG12	2.17	0.44
4:B:304:SER:HB3	5:F:218:MET:HB2	1.98	0.44
4:B:354:GLU:CD	4:B:367:ASN:HD22	2.22	0.43
4:B:158:PRO:HG2	4:B:377:SER:HA	2.00	0.43
4:C:63:VAL:HG13	4:C:71:VAL:HG13	2.00	0.43
5:E:254:ILE:HG21	5:E:321:THR:HG21	2.00	0.43
4:C:331:GLN:HB3	5:F:314:THR:HG22	2.00	0.43
4:C:315:GLU:HA	4:C:319:ALA:HB2	2.00	0.43
5:E:384:ILE:CG1	5:E:392:LEU:HD11	2.47	0.43
6:G:98:VAL:HG13	6:G:128:LEU:HD11	2.00	0.43
4:B:63:VAL:HG13	4:B:71:VAL:HG13	2.00	0.43
9:T:23:ALA:HA	9:U:24:ALA:CB	2.48	0.43
4:A:205:VAL:HG22	4:A:251:ALA:CB	2.48	0.43
4:C:63:VAL:HG13	4:C:71:VAL:CG1	2.48	0.43
5:F:48:LEU:HD21	5:F:54:ARG:CG	2.49	0.43
4:A:271:ASP:HB2	4:A:327:ILE:O	2.19	0.43
4:B:218:VAL:HG13	4:B:227:MET:HE3	2.01	0.43
5:F:89:ILE:HD11	5:F:192:TYR:CD1	2.53	0.43
4:B:401:MET:O	4:B:403:ALA:N	2.51	0.43
4:B:444:ILE:HG21	4:B:473:LEU:HD11	2.01	0.43
6:G:192:VAL:CG2	6:G:226:VAL:HG13	2.49	0.43
4:A:310:SER:OG	4:A:324:ALA:HB2	2.18	0.43
4:B:340:PRO:O	4:B:344:ILE:HG13	2.19	0.43
5:E:317:ALA:HB3	5:E:318:PRO:CD	2.49	0.43
5:D:370:VAL:HG13	5:D:406:ILE:HG21	2.01	0.43
4:A:454:LEU:HD21	4:A:465:TRP:CZ3	2.53	0.42
4:B:339:ILE:H	4:B:339:ILE:HD12	1.83	0.42
5:E:317:ALA:HB3	5:E:318:PRO:HD3	2.01	0.42
5:D:436:SER:HB3	5:D:459:ILE:HB	2.00	0.42
5:E:165:ILE:HG21	5:E:211:VAL:HG13	2.01	0.42
9:J:23:ALA:HA	9:K:24:ALA:CB	2.48	0.42
5:F:137:LEU:HD22	5:F:437:PHE:CD2	2.53	0.42
4:C:411:LEU:O	4:C:416:GLN:NE2	2.51	0.42
4:C:194:ALA:C	4:C:196:GLY:N	2.73	0.42
5:D:8:ILE:HD12	5:D:68:LEU:HB2	2.02	0.42
5:E:426:VAL:HG21	5:E:457:GLY:HA3	2.00	0.42
4:A:284:LEU:HD11	4:A:294:ALA:O	2.20	0.42
4:B:30:GLN:O	4:B:31:VAL:HB	2.19	0.42
5:D:58:MET:CE	5:D:224:ALA:HA	2.50	0.42
4:B:350:GLN:HG3	4:B:352:PHE:CZ	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:241:ALA:HB3	4:C:242:PRO:HD3	2.01	0.41
5:E:162:MET:HA	5:E:165:ILE:HD12	2.02	0.41
5:E:275:VAL:HG12	5:E:275:VAL:O	2.20	0.41
5:F:341:TYR:HA	5:F:342:PRO:C	2.40	0.41
4:B:156:MET:CE	4:B:368:THR:HG21	2.51	0.41
5:D:277:TYR:HD2	5:D:281:LEU:HD12	1.85	0.41
5:F:356:PRO:HD3	5:F:364:TYR:CE1	2.55	0.41
4:C:233:VAL:HG21	4:C:251:ALA:HB2	2.02	0.41
4:C:136:ILE:HD13	5:D:185:THR:HG23	2.02	0.41
5:D:233:LEU:HD11	5:D:291:ARG:CZ	2.51	0.41
5:E:252:ASP:HA	5:E:253:ASN:HA	1.93	0.41
5:F:92:VAL:HG21	5:F:227:ARG:HB2	2.03	0.41
5:F:436:SER:HB3	5:F:459:ILE:HD12	2.03	0.41
4:A:63:VAL:HG13	4:A:71:VAL:HG22	2.01	0.41
4:A:63:VAL:HG13	4:A:71:VAL:CG2	2.50	0.41
4:C:301:TYR:CE1	4:C:305:ARG:CG	3.04	0.41
4:C:491:VAL:O	4:C:492:ALA:HB2	2.21	0.41
5:D:183:GLU:H	5:D:217:GLN:NE2	2.19	0.41
5:E:370:VAL:HG13	5:E:406:ILE:HG21	2.02	0.41
4:C:428:LEU:HD11	4:C:454:LEU:HD11	2.03	0.41
6:G:105:LEU:CD1	6:G:115:VAL:HG11	2.49	0.41
5:E:165:ILE:CD1	5:E:211:VAL:HG11	2.48	0.40
7:H:44:TYR:O	7:H:50:LEU:CB	2.69	0.40
5:D:15:VAL:CG2	5:D:264:VAL:HG23	2.51	0.40
5:F:253:ASN:OD1	5:F:255:PHE:HB3	2.21	0.40
4:C:206:ALA:CB	4:C:209:GLN:OE1	2.66	0.40
4:C:489:ARG:HG3	4:C:495:LEU:HD22	2.02	0.40
4:A:339:ILE:N	4:A:340:PRO:CD	2.85	0.40
4:C:33:SER:HB2	5:F:47:HIS:O	2.22	0.40
5:F:356:PRO:HD3	5:F:364:TYR:CD1	2.56	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	
4	A	501/511 (98%)	470 (94%)	24 (5%)	7 (1%)	14	59
4	B	490/511 (96%)	459 (94%)	26 (5%)	5 (1%)	19	65
4	C	482/511 (94%)	463 (96%)	15 (3%)	4 (1%)	24	69
5	D	468/474 (99%)	448 (96%)	19 (4%)	1 (0%)	52	86
5	E	464/474 (98%)	439 (95%)	22 (5%)	3 (1%)	30	73
5	F	464/474 (98%)	439 (95%)	23 (5%)	2 (0%)	39	79
6	G	246/290 (85%)	233 (95%)	8 (3%)	5 (2%)	9	53
7	H	108/188 (57%)	90 (83%)	12 (11%)	6 (6%)	2	29
8	I	73/148 (49%)	66 (90%)	5 (7%)	2 (3%)	6	47
9	J	72/77 (94%)	72 (100%)	0	0	100	100
9	K	72/77 (94%)	72 (100%)	0	0	100	100
9	L	72/77 (94%)	72 (100%)	0	0	100	100
9	M	72/77 (94%)	72 (100%)	0	0	100	100
9	N	72/77 (94%)	72 (100%)	0	0	100	100
9	O	72/77 (94%)	72 (100%)	0	0	100	100
9	P	72/77 (94%)	72 (100%)	0	0	100	100
9	Q	72/77 (94%)	72 (100%)	0	0	100	100
9	R	72/77 (94%)	72 (100%)	0	0	100	100
9	S	72/77 (94%)	72 (100%)	0	0	100	100
9	T	72/77 (94%)	72 (100%)	0	0	100	100
9	U	72/77 (94%)	72 (100%)	0	0	100	100
12	X	59/283 (21%)	58 (98%)	1 (2%)	0	100	100
14	Z	50/104 (48%)	47 (94%)	2 (4%)	1 (2%)	9	53
All	All	4269/4892 (87%)	4076 (96%)	157 (4%)	36 (1%)	24	69

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	23	ALA
4	A	199	THR
4	B	402	ALA
4	C	197	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	C	492	ALA
5	E	274	ALA
5	F	143	LYS
6	G	66	PRO
6	G	132	TYR
7	H	73	GLU
7	H	74	ARG
7	H	75	MET
14	Z	101	SER
4	A	24	GLU
4	A	171	ARG
4	B	80	ARG
4	B	237	ALA
4	B	412	ASP
5	F	171	VAL
6	G	61	ALA
7	H	30	ILE
7	H	112	LYS
8	I	55	GLY
8	I	73	ASN
4	A	21	GLN
4	A	121	LEU
4	A	409	SER
6	G	133	GLY
4	C	195	ASP
6	G	65	ALA
4	B	31	VAL
4	C	408	GLY
5	D	23	GLN
5	E	390	ASP
7	H	29	GLY
5	E	275	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	396/401 (99%)	375 (95%)	21 (5%)	28	67
4	B	391/401 (98%)	369 (94%)	22 (6%)	26	65
4	C	379/401 (94%)	360 (95%)	19 (5%)	30	68
5	D	371/375 (99%)	358 (96%)	13 (4%)	43	77
5	E	372/375 (99%)	361 (97%)	11 (3%)	48	79
5	F	372/375 (99%)	352 (95%)	20 (5%)	27	67
6	G	203/227 (89%)	196 (97%)	7 (3%)	44	77
14	Z	45/81 (56%)	43 (96%)	2 (4%)	35	71
All	All	2529/2636 (96%)	2414 (96%)	115 (4%)	34	71

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	14	ASP
4	A	33	SER
4	A	52	MET
4	A	71	VAL
4	A	103	LEU
4	A	113	ASN
4	A	127	ARG
4	A	146	MET
4	A	164	ARG
4	A	198	LYS
4	A	209	GLN
4	A	246	LEU
4	A	282	MET
4	A	304	SER
4	A	323	THR
4	A	372	VAL
4	A	393	LEU
4	A	410	ASP
4	A	415	THR
4	A	460	ARG
4	A	461	ASP
4	B	30	GLN
4	B	74	VAL
4	B	89	LYS
4	B	127	ARG
4	B	146	MET
4	B	227	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	245	TYR
4	B	277	VAL
4	B	304	SER
4	B	345	SER
4	B	346	ILE
4	B	350	GLN
4	B	374	ARG
4	B	377	SER
4	B	385	LYS
4	B	393	LEU
4	B	400	GLU
4	B	412	ASP
4	B	417	LYS
4	B	421	ARG
4	B	460	ARG
4	B	463	THR
4	C	52	MET
4	C	74	VAL
4	C	103	LEU
4	C	111	LEU
4	C	127	ARG
4	C	146	MET
4	C	157	ILE
4	C	164	ARG
4	C	195	ASP
4	C	217	LEU
4	C	277	VAL
4	C	335	VAL
4	C	372	VAL
4	C	374	ARG
4	C	409	SER
4	C	410	ASP
4	C	415	THR
4	C	433	GLN
4	C	435	SER
5	D	54	ARG
5	D	56	ILE
5	D	59	ASP
5	D	162	MET
5	D	210	GLN
5	D	228	VAL
5	D	262	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	D	264	VAL
5	D	267	LEU
5	D	270	ARG
5	D	278	GLN
5	D	389	MET
5	D	424	ASP
5	E	46	GLN
5	E	56	ILE
5	E	62	GLU
5	E	83	ASP
5	E	92	VAL
5	E	107	GLN
5	E	146	LYS
5	E	219	ASN
5	E	228	VAL
5	E	326	ASP
5	E	468	ARG
5	F	21	ASP
5	F	24	LEU
5	F	36	ASN
5	F	39	ARG
5	F	46	GLN
5	F	54	ARG
5	F	107	GLN
5	F	134	VAL
5	F	219	ASN
5	F	228	VAL
5	F	233	LEU
5	F	245	THR
5	F	270	ARG
5	F	275	VAL
5	F	278	GLN
5	F	353	ILE
5	F	420	PHE
5	F	459	ILE
5	F	461	ASP
5	F	469	LEU
6	G	36	GLN
6	G	78	HIS
6	G	100	LEU
6	G	152	ASN
6	G	156	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	G	158	ASP
6	G	276	THR
14	Z	30	ARG
14	Z	97	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	261	ASN
4	A	380	GLN
4	A	475	ASN
4	B	65	ASN
4	C	48	GLN
4	C	216	GLN
4	C	261	ASN
5	D	217	GLN
5	D	278	GLN
5	D	375	GLN
5	E	107	GLN
5	E	189	ASN
5	E	217	GLN
5	E	219	ASN
5	E	407	GLN
5	F	36	ASN
5	F	46	GLN
5	F	91	ASN
5	F	189	ASN
5	F	217	GLN
5	F	278	GLN
6	G	138	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
15	ATP	A	600	16	26,33,33	1.07	2 (7%)	26,52,52	1.80	2 (7%)
17	ADP	B	600	16	24,29,29	1.07	2 (8%)	23,45,45	1.96	1 (4%)
15	ATP	C	600	16	26,33,33	0.99	1 (3%)	26,52,52	1.79	1 (3%)
15	ATP	D	600	16	26,33,33	1.01	1 (3%)	26,52,52	1.96	3 (11%)
15	ATP	F	600	16	26,33,33	1.03	1 (3%)	26,52,52	1.71	2 (7%)

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
15	ATP	A	600	16	-	0/18/38/38	0/3/3/3
17	ADP	B	600	16	-	0/12/32/32	0/3/3/3
15	ATP	C	600	16	-	0/18/38/38	0/3/3/3
15	ATP	D	600	16	-	0/18/38/38	0/3/3/3
15	ATP	F	600	16	-	0/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	600	ATP	C2-N3	2.03	1.35	1.32
17	B	600	ADP	C2-N3	2.04	1.35	1.32
15	D	600	ATP	C5-C4	3.12	1.47	1.40
15	C	600	ATP	C5-C4	3.19	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	600	ADP	C5-C4	3.24	1.47	1.40
15	F	600	ATP	C5-C4	3.26	1.47	1.40
15	A	600	ATP	C5-C4	3.42	1.48	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	600	ADP	N3-C2-N1	-7.95	122.63	128.87
15	D	600	ATP	N3-C2-N1	-7.86	122.70	128.87
15	C	600	ATP	N3-C2-N1	-7.52	122.96	128.87
15	A	600	ATP	N3-C2-N1	-7.26	123.17	128.87
15	F	600	ATP	N3-C2-N1	-7.08	123.31	128.87
15	D	600	ATP	C1'-N9-C4	-2.11	124.45	126.81
15	A	600	ATP	N6-C6-N1	2.13	122.08	118.52
15	F	600	ATP	C4'-O4'-C1'	2.49	112.28	109.64
15	D	600	ATP	O4'-C1'-N9	2.71	113.22	108.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	0/20	-	-	-	-
2	2	0/15	-	-	-	-
3	3	0/19	-	-	-	-
4	A	505/511 (98%)	-0.20	15 (2%) 54 41	73, 123, 205, 249	0
4	B	496/511 (97%)	-0.26	4 (0%) 87 82	59, 112, 185, 216	0
4	C	484/511 (94%)	-0.30	3 (0%) 90 86	67, 107, 159, 206	0
5	D	470/474 (99%)	-0.23	6 (1%) 79 70	73, 107, 156, 186	0
5	E	466/474 (98%)	-0.08	12 (2%) 59 47	72, 131, 203, 247	0
5	F	466/474 (98%)	-0.23	9 (1%) 70 59	58, 100, 153, 189	0
6	G	260/290 (89%)	0.08	13 (5%) 32 24	80, 143, 203, 224	0
7	H	110/188 (58%)	-0.21	6 (5%) 29 21	110, 152, 185, 215	0
8	I	75/148 (50%)	0.71	13 (17%) 2 3	167, 207, 238, 241	0
9	J	74/77 (96%)	1.10	13 (17%) 2 3	217, 279, 383, 417	0
9	K	74/77 (96%)	0.87	12 (16%) 3 3	182, 295, 402, 415	0
9	L	74/77 (96%)	0.87	17 (22%) 1 2	224, 296, 463, 488	0
9	M	74/77 (96%)	0.89	17 (22%) 1 2	209, 279, 409, 418	0
9	N	74/77 (96%)	0.96	18 (24%) 1 1	214, 273, 401, 421	0
9	O	74/77 (96%)	0.92	23 (31%) 1 1	220, 287, 352, 363	0
9	P	74/77 (96%)	1.39	21 (28%) 1 1	222, 304, 397, 443	0
9	Q	74/77 (96%)	1.32	22 (29%) 1 1	266, 349, 427, 451	0
9	R	74/77 (96%)	0.92	17 (22%) 1 2	200, 315, 439, 449	0
9	S	74/77 (96%)	1.71	26 (35%) 0 1	239, 320, 445, 471	0
9	T	74/77 (96%)	0.91	15 (20%) 1 2	260, 317, 430, 437	0
9	U	74/77 (96%)	0.56	12 (16%) 3 3	231, 279, 431, 447	0
10	V	0/78	-	-	-	-

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
11	W	0/124	-	-	-	-
12	X	63/283 (22%)	-0.47	3 (4%) 34 25	147, 201, 252, 268	0
13	Y	0/54	-	-	-	-
14	Z	54/104 (51%)	0.47	6 (11%) 7 6	135, 172, 218, 248	0
All	All	4337/5202 (83%)	0.08	303 (6%) 19 13	58, 131, 361, 488	0

All (303) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	P	76	ALA	9.3
9	S	3	ASN	7.6
9	N	43	SER	7.5
9	K	61	ALA	7.3
9	P	68	LEU	7.0
9	N	42	PRO	6.8
9	R	61	ALA	6.8
9	S	16	ALA	6.7
5	E	390	ASP	6.5
5	F	35	ASN	6.4
9	P	75	PHE	6.4
9	Q	61	ALA	6.3
9	R	27	VAL	6.2
9	Q	27	VAL	6.1
9	L	49	THR	6.0
9	Q	5	GLY	6.0
9	L	35	LEU	6.0
9	S	61	ALA	6.0
9	N	44	ALA	5.9
9	Q	6	GLN	5.9
9	S	65	PHE	5.9
9	T	76	ALA	5.8
9	T	31	ALA	5.7
9	S	57	ALA	5.7
9	O	68	LEU	5.6
9	M	43	SER	5.6
9	J	61	ALA	5.6
9	U	54	ILE	5.5
4	A	491	VAL	5.4
9	K	75	PHE	5.4
9	S	64	ILE	5.4
5	D	35	ASN	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	A	490	LYS	5.3
9	U	3	ASN	5.2
9	N	45	ALA	5.1
9	N	48	GLN	5.0
9	P	43	SER	5.0
9	K	64	ILE	4.9
9	P	38	ALA	4.8
9	L	38	ALA	4.8
9	N	19	GLY	4.8
9	P	72	LEU	4.7
9	P	50	ALA	4.7
9	J	31	ALA	4.7
9	T	43	SER	4.6
14	Z	32	LEU	4.6
9	Q	3	ASN	4.6
8	I	60	THR	4.6
9	L	43	SER	4.5
9	J	57	ALA	4.4
9	U	68	LEU	4.4
9	K	60	GLU	4.4
8	I	65	THR	4.3
9	N	65	PHE	4.3
9	T	68	LEU	4.2
9	R	28	GLY	4.1
9	O	69	VAL	4.1
9	P	44	ALA	4.1
6	G	180	GLU	4.1
9	J	49	THR	4.1
9	J	53	PHE	4.1
9	K	76	ALA	4.0
9	M	76	ALA	4.0
9	S	15	LEU	4.0
9	N	64	ILE	4.0
9	R	50	ALA	4.0
9	L	48	GLN	4.0
9	N	41	ASN	4.0
9	O	44	ALA	4.0
4	A	19	PHE	3.9
9	S	43	SER	3.9
4	A	380	GLN	3.9
9	S	46	ALA	3.9
9	U	53	PHE	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	H	75	MET	3.8
9	R	6	GLN	3.8
9	L	44	ALA	3.8
9	S	68	LEU	3.8
9	R	57	ALA	3.8
9	S	53	PHE	3.7
9	N	18	VAL	3.7
9	P	40	ARG	3.7
6	G	61	ALA	3.7
9	Q	64	ILE	3.6
5	E	151	GLY	3.6
9	Q	57	ALA	3.6
9	S	50	ALA	3.5
9	S	60	GLU	3.5
9	S	31	ALA	3.5
6	G	170	ASP	3.5
8	I	52	VAL	3.5
9	J	74	LEU	3.4
9	R	3	ASN	3.4
9	K	55	GLY	3.4
9	Q	8	GLY	3.4
9	K	68	LEU	3.4
9	J	60	GLU	3.4
6	G	16	ASN	3.4
9	M	74	LEU	3.4
9	U	31	ALA	3.4
9	Q	30	VAL	3.4
9	L	42	PRO	3.4
9	T	57	ALA	3.4
9	O	76	ALA	3.4
9	J	24	ALA	3.4
6	G	62	GLY	3.3
9	J	6	GLN	3.3
5	E	389	MET	3.3
5	E	420	PHE	3.3
9	K	31	ALA	3.3
9	N	17	CYS	3.3
9	P	41	ASN	3.3
4	A	386	SER	3.3
9	U	76	ALA	3.3
8	I	73	ASN	3.3
5	E	150	PHE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	K	65	PHE	3.2
9	Q	13	ALA	3.2
9	P	42	PRO	3.2
9	M	65	PHE	3.2
4	A	145	PRO	3.2
9	O	50	ALA	3.2
9	O	70	ALA	3.2
8	I	64	VAL	3.1
9	O	48	GLN	3.1
7	H	27	SER	3.1
9	O	16	ALA	3.1
14	Z	102	GLU	3.1
5	F	204	ASP	3.1
9	P	47	SER	3.1
9	J	38	ALA	3.0
9	S	30	VAL	3.0
4	B	397	GLN	3.0
9	L	45	ALA	3.0
9	T	17	CYS	3.0
5	E	80	PRO	3.0
4	A	492	ALA	3.0
5	D	212	ALA	3.0
12	X	1205	ILE	3.0
9	P	29	ASN	3.0
9	Q	33	ASN	3.0
9	O	51	THR	3.0
9	R	5	GLY	3.0
9	N	76	ALA	2.9
9	P	53	PHE	2.9
6	G	196	VAL	2.9
9	S	49	THR	2.9
14	Z	103	ILE	2.9
9	O	47	SER	2.9
6	G	108	LEU	2.9
9	P	6	GLN	2.9
9	P	69	VAL	2.9
5	F	208	LYS	2.9
5	F	102	PRO	2.9
9	L	36	ALA	2.9
9	T	14	GLY	2.8
9	Q	9	GLN	2.8
9	O	17	CYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	N	46	ALA	2.8
6	G	195	ALA	2.8
9	R	31	ALA	2.8
4	A	379	ALA	2.8
8	I	47	PRO	2.8
9	Q	31	ALA	2.8
9	O	71	LEU	2.8
9	O	49	THR	2.8
9	R	53	PHE	2.8
9	N	21	ALA	2.7
9	O	53	PHE	2.7
9	T	50	ALA	2.7
9	U	6	GLN	2.7
9	M	73	LEU	2.7
9	R	49	THR	2.7
9	L	76	ALA	2.7
5	E	37	GLY	2.7
8	I	63	ALA	2.7
9	S	58	PHE	2.7
8	I	59	GLU	2.7
9	U	57	ALA	2.6
9	J	3	ASN	2.6
9	Q	29	ASN	2.6
7	H	71	LEU	2.6
9	S	27	VAL	2.6
9	T	53	PHE	2.6
9	R	8	GLY	2.6
9	Q	14	GLY	2.6
9	M	75	PHE	2.6
8	I	61	GLU	2.6
9	O	72	LEU	2.6
9	Q	4	LEU	2.6
9	Q	7	LEU	2.5
5	D	85	THR	2.5
6	G	194	PRO	2.5
5	D	87	GLY	2.5
4	B	400	GLU	2.5
14	Z	29	ASN	2.5
9	M	72	LEU	2.5
9	O	18	VAL	2.5
9	K	57	ALA	2.5
5	F	34	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	F	4	ALA	2.5
9	Q	28	GLY	2.5
9	O	75	PHE	2.5
9	S	63	GLY	2.5
9	T	13	ALA	2.5
9	T	64	ILE	2.5
9	M	48	GLN	2.5
5	E	421	THR	2.4
5	F	101	GLY	2.4
9	M	42	PRO	2.4
9	Q	10	TYR	2.4
9	M	70	ALA	2.4
8	I	72	ASN	2.4
9	Q	26	GLY	2.4
9	R	30	VAL	2.4
9	J	73	LEU	2.4
4	C	388	ALA	2.4
9	O	46	ALA	2.4
9	P	5	GLY	2.4
9	M	61	ALA	2.4
9	O	59	ALA	2.4
9	O	54	ILE	2.3
4	A	20	GLY	2.3
8	I	48	GLY	2.3
6	G	64	MET	2.3
9	U	5	GLY	2.3
9	Q	60	GLU	2.3
5	D	34	GLU	2.3
9	S	66	SER	2.3
4	A	489	ARG	2.3
9	L	37	GLY	2.3
5	E	35	ASN	2.3
9	S	62	LEU	2.3
4	A	21	GLN	2.3
5	E	226	MET	2.3
9	R	29	ASN	2.3
9	Q	55	GLY	2.3
9	M	68	LEU	2.3
14	Z	101	SER	2.3
4	A	22	ASP	2.3
9	U	4	LEU	2.3
9	R	60	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	U	72	LEU	2.3
5	E	152	GLY	2.2
9	J	50	ALA	2.2
9	M	46	ALA	2.2
12	X	1221	ASN	2.2
4	B	172	GLN	2.2
9	S	4	LEU	2.2
9	T	54	ILE	2.2
9	T	4	LEU	2.2
9	O	61	ALA	2.2
4	A	144	GLU	2.2
9	K	32	GLY	2.2
9	N	68	LEU	2.2
9	L	13	ALA	2.2
9	L	41	ASN	2.2
9	M	66	SER	2.2
7	H	26	ASP	2.2
12	X	1204	LEU	2.2
9	T	3	ASN	2.2
5	F	209	SER	2.2
9	S	69	VAL	2.2
4	A	511	ALA	2.2
9	N	49	THR	2.2
9	S	59	ALA	2.2
9	S	24	ALA	2.2
9	K	54	ILE	2.1
7	H	72	SER	2.1
6	G	106	GLN	2.1
9	O	19	GLY	2.1
9	P	48	GLN	2.1
9	M	38	ALA	2.1
9	O	67	PHE	2.1
5	D	363	HIS	2.1
9	P	46	ALA	2.1
9	U	64	ILE	2.1
4	A	17	LYS	2.1
8	I	83	GLY	2.1
8	I	39	ALA	2.1
9	L	50	ALA	2.1
4	B	376	GLY	2.1
4	C	389	GLY	2.1
9	T	65	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	L	34	TYR	2.1
14	Z	9	ALA	2.1
9	L	32	GLY	2.1
9	R	4	LEU	2.1
9	N	20	MET	2.1
5	E	175	TYR	2.1
6	G	60	ALA	2.1
7	H	76	GLY	2.0
9	M	31	ALA	2.0
9	S	42	PRO	2.0
9	M	40	ARG	2.0
9	P	73	LEU	2.0
5	F	7	LYS	2.0
6	G	44	PRO	2.0
9	P	45	ALA	2.0
9	R	76	ALA	2.0
9	L	39	LEU	2.0
4	C	511	ALA	2.0
9	N	16	ALA	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
15	ATP	A	600	31/31	0.92	0.29	0.31	96,98,105,106	0
15	ATP	D	600	31/31	0.93	0.26	0.25	90,96,152,153	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
15	ATP	F	600	31/31	0.92	0.25	-0.20	69,74,109,110	0
17	ADP	B	600	27/27	0.86	0.25	-0.40	155,165,171,173	0
15	ATP	C	600	31/31	0.93	0.19	-0.50	103,110,115,118	0
16	MG	F	601	1/1	0.96	0.29	-	35,35,35,35	0
16	MG	B	601	1/1	0.93	0.20	-	72,72,72,72	0
16	MG	C	601	1/1	0.99	0.35	-	48,48,48,48	0
16	MG	A	601	1/1	0.97	0.41	-	78,78,78,78	0
16	MG	D	601	1/1	0.96	0.28	-	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.