



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:48 PM GMT

PDB ID : 1H8E
Title : (ADP.ALF4)2(ADP.SO4) BOVINE F1-ATPASE (ALL THREE CATALYTIC SITES OCCUPIED)
Authors : Menz, R.I.; Walker, J.E.; Leslie, A.G.W.
Deposited on : 2001-02-02
Resolution : 2.00 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 (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

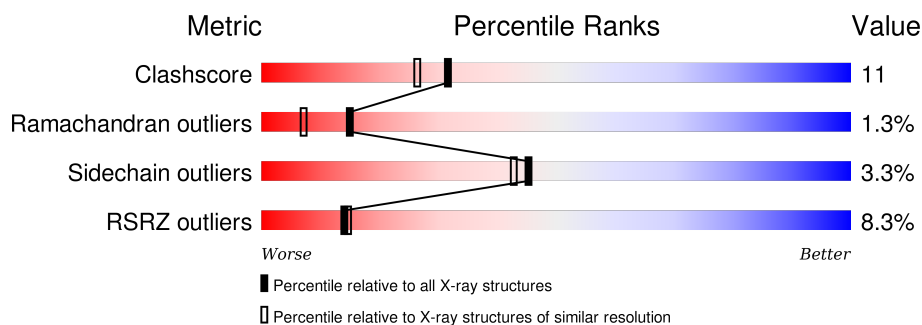
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	A	510	<div> <div>2%</div> <div>79%</div> <div>13%</div> <div>• 5%</div> </div>
1	B	510	<div> <div>5%</div> <div>74%</div> <div>18%</div> <div>• 6%</div> </div>
1	C	510	<div> <div>%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
2	D	482	<div> <div>3%</div> <div>81%</div> <div>14%</div> <div>• •</div> </div>
2	E	482	<div> <div>15%</div> <div>64%</div> <div>27%</div> <div>• 6%</div> </div>
2	F	482	<div> <div>5%</div> <div>79%</div> <div>15%</div> <div>• •</div> </div>
3	G	272	<div> <div>23%</div> <div>48%</div> <div>38%</div> <div>• 10%</div> </div>

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Mol	Chain	Length	Quality of chain
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
8	GOL	B	700	-	-	-	X
9	ALF	D	620	-	-	X	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 26329 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 BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3705	2334	654	705	12			
1	B	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	12			
1	C	488	Total	C	N	O	S	0	0	0
			3718	2341	656	709	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	ENGINEERED	UNP P19483
B	481	GLY	SER	ENGINEERED	UNP P19483
C	481	GLY	SER	ENGINEERED	UNP P19483

- Molecule 2 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

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	454	Total	C	N	O	S	0	0	0
			3447	2186	586	664	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	244	Total	C	N	O	S	0	0	0
			1891	1191	328	364	8			

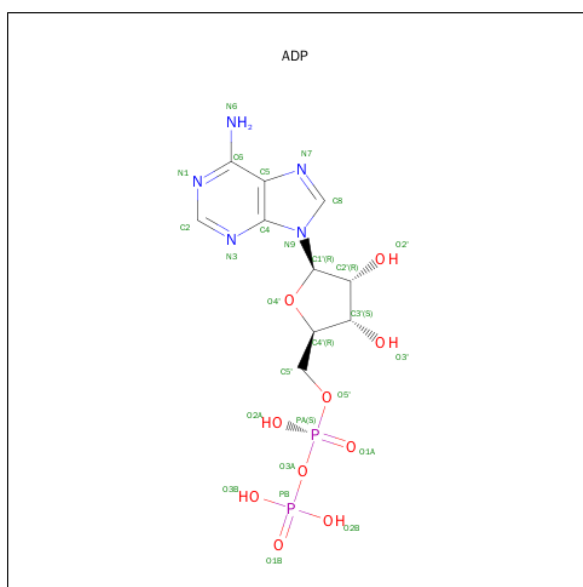
- Molecule 4 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	89	Total	C	N	O	S	0	0	0
			662	420	109	131	2			

- Molecule 5 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	36	Total	C	N	O	S	0	0	0
			281	180	51	49	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).

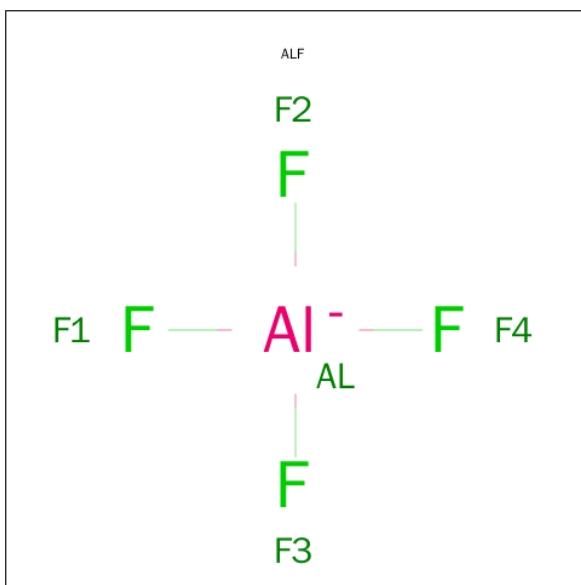
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total Mg 1 1	0	0
7	E	1	Total Mg 1 1	0	0
7	B	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0
7	A	1	Total Mg 1 1	0	0
7	F	1	Total Mg 1 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0

- Molecule 9 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	Al	F	0	0
			5	1	4		
9	F	1	Total	Al	F	0	0
			5	1	4		

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	E	1	Total	O	S	0	0
			5	4	1		

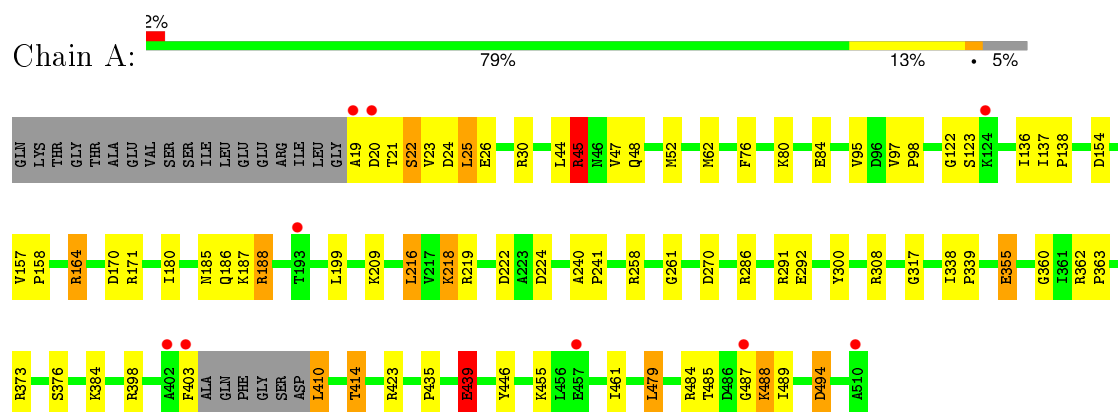
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	310	Total 310	O 310	0	0
11	B	241	Total 241	O 241	0	0
11	C	322	Total 322	O 322	0	0
11	D	310	Total 310	O 310	0	0
11	E	181	Total 181	O 181	0	0
11	F	286	Total 286	O 286	0	0
11	G	39	Total 39	O 39	0	0
11	H	3	Total 3	O 3	0	0
11	I	1	Total 1	O 1	0	0

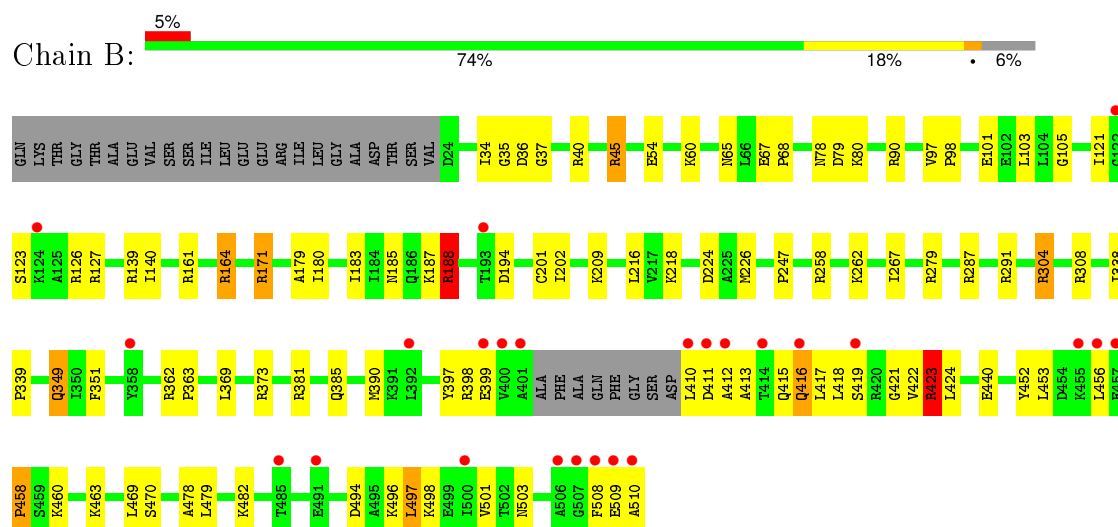
3 Residue-property plots

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

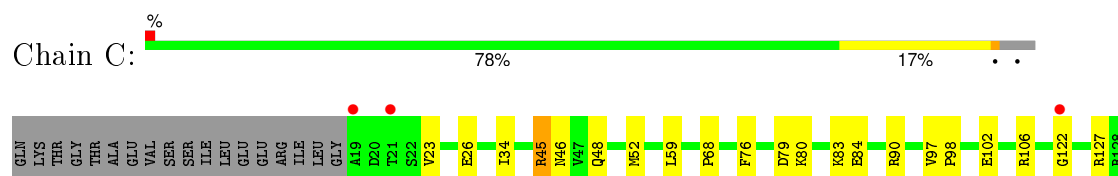
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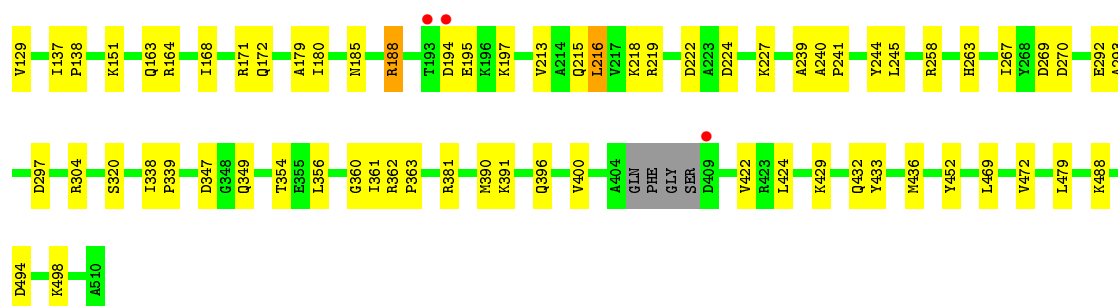


• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

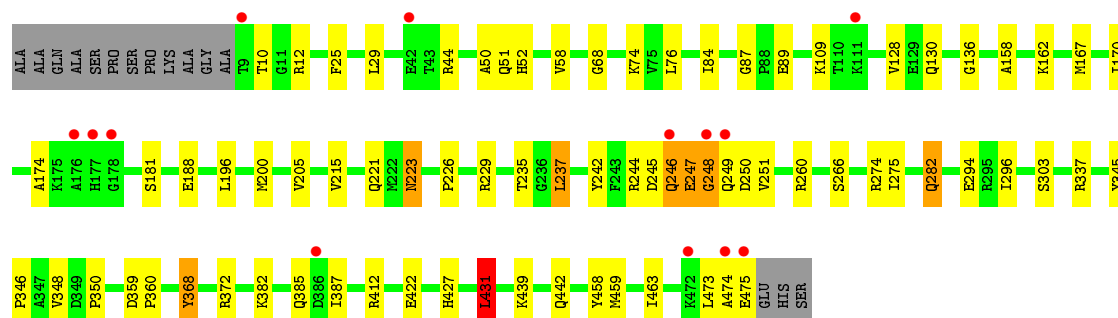
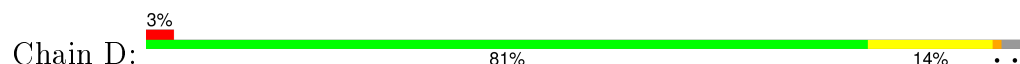


• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

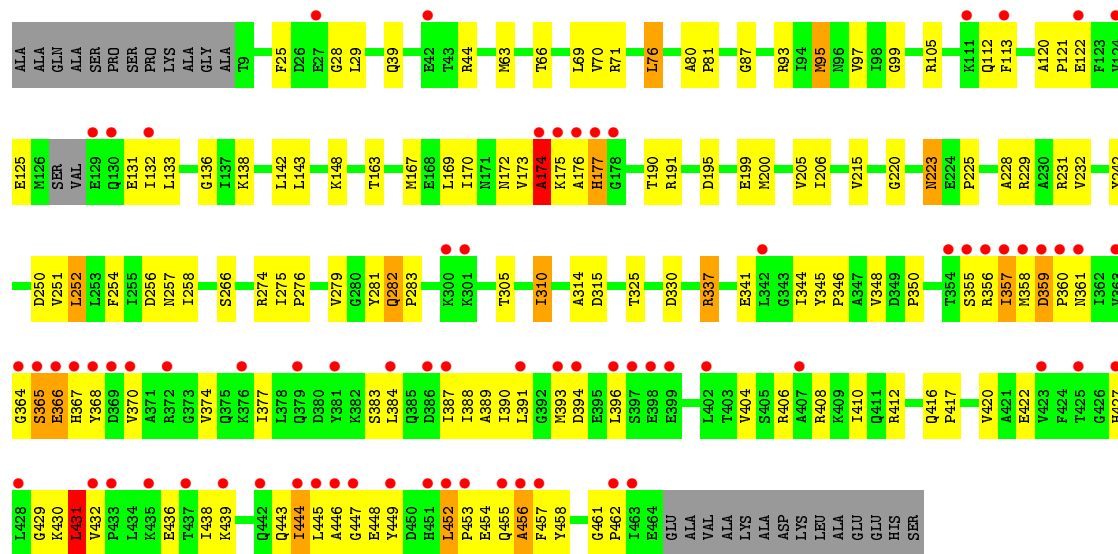




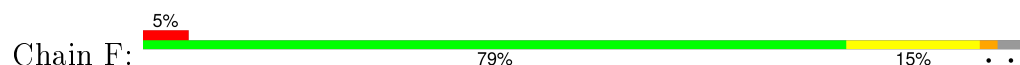
• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

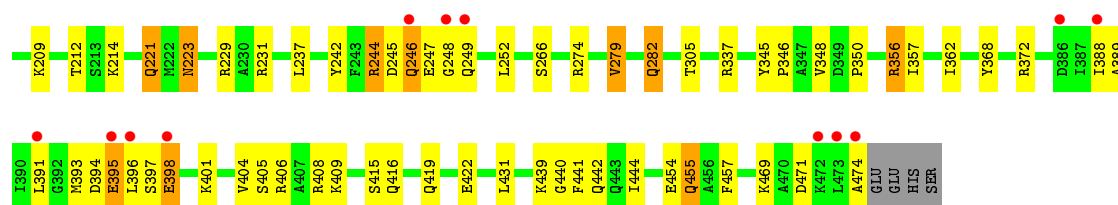


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

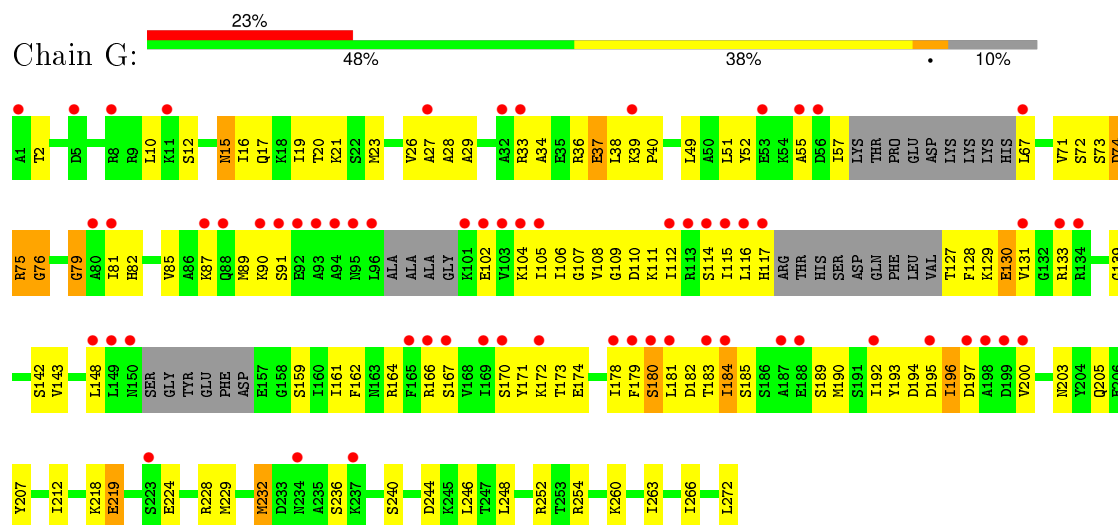


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

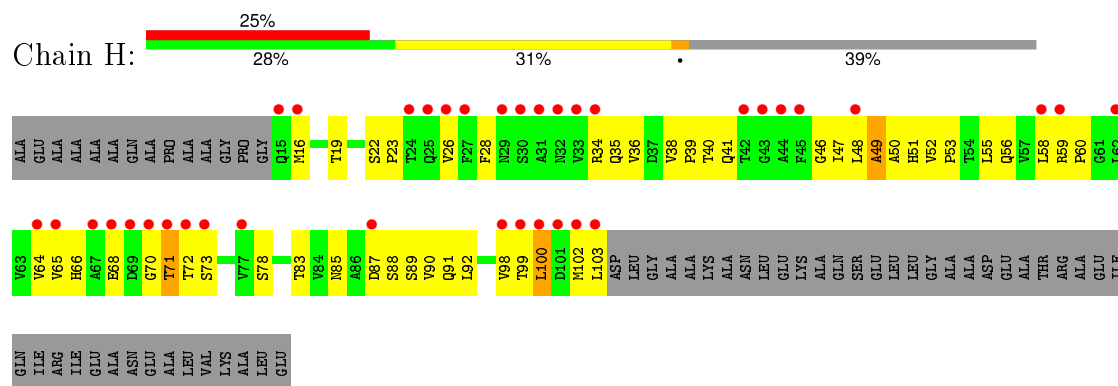




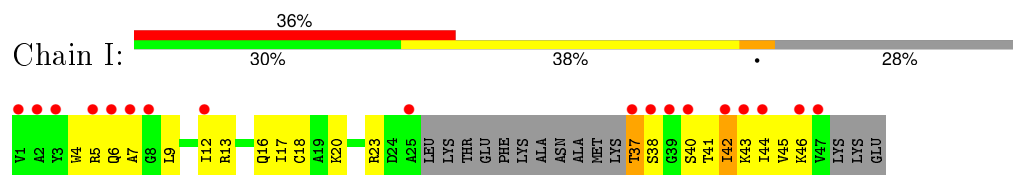
• Molecule 3: BOVINE MITOCHONDRIAL F1-ATPASE



• Molecule 4: BOVINE MITOCHONDRIAL F1-ATPASE



• Molecule 5: BOVINE MITOCHONDRIAL F1-ATPASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	267.70 Å 106.20 Å 138.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	13.50 – 2.00 13.54 – 2.00	Depositor EDS
% Data completeness (in resolution range)	79.6 (13.50-2.00) 79.4 (13.54-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.99 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.264 0.192 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 72.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 209953 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26329	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ALF, GOL, MG, SO4, 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	0.66	1/3754 (0.0%)	1.22	23/5064 (0.5%)
1	B	0.63	0/3704	1.20	23/4995 (0.5%)
1	C	0.69	0/3767	1.24	18/5082 (0.4%)
2	D	0.66	0/3596	1.23	16/4879 (0.3%)
2	E	0.58	0/3503	1.13	18/4752 (0.4%)
2	F	0.65	0/3587	1.20	15/4867 (0.3%)
3	G	0.53	1/1907 (0.1%)	1.06	5/2556 (0.2%)
4	H	0.46	0/674	0.95	0/922
5	I	0.48	0/284	1.10	0/381
All	All	0.63	2/24776 (0.0%)	1.19	118/33498 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	76	GLY	N-CA	-7.01	1.35	1.46
1	A	122	GLY	N-CA	5.52	1.54	1.46

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	188	ARG	NE-CZ-NH2	14.29	127.44	120.30
1	C	188	ARG	NE-CZ-NH1	-13.27	113.67	120.30
2	D	260	ARG	NE-CZ-NH1	12.56	126.58	120.30
1	C	258	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	A	188	ARG	CD-NE-CZ	10.81	138.74	123.60
1	A	188	ARG	NE-CZ-NH1	10.73	125.66	120.30
2	F	244	ARG	NE-CZ-NH1	10.29	125.44	120.30
2	D	229	ARG	NE-CZ-NH1	10.29	125.44	120.30
1	A	45	ARG	NE-CZ-NH2	-10.27	115.17	120.30
1	A	45	ARG	NE-CZ-NH1	9.91	125.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	ARG	NE-CZ-NH2	-9.54	115.53	120.30
2	E	105	ARG	CD-NE-CZ	9.49	136.88	123.60
2	D	229	ARG	CD-NE-CZ	9.44	136.82	123.60
1	B	304	ARG	NE-CZ-NH1	-9.32	115.64	120.30
2	E	71	ARG	NE-CZ-NH1	8.63	124.61	120.30
2	D	12	ARG	CD-NE-CZ	8.52	135.52	123.60
3	G	75	ARG	C-N-CA	8.46	140.06	122.30
1	B	258	ARG	CD-NE-CZ	8.22	135.11	123.60
1	B	279	ARG	NE-CZ-NH2	-8.19	116.20	120.30
2	F	274	ARG	NE-CZ-NH1	-8.17	116.21	120.30
1	B	188	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	C	258	ARG	CD-NE-CZ	8.06	134.88	123.60
1	A	45	ARG	CD-NE-CZ	8.00	134.79	123.60
1	C	258	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	B	161	ARG	NE-CZ-NH1	7.62	124.11	120.30
3	G	254	ARG	NE-CZ-NH1	-7.58	116.51	120.30
2	F	406	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	B	126	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	B	258	ARG	NE-CZ-NH1	7.33	123.97	120.30
2	F	337	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	B	291	ARG	NE-CZ-NH2	-7.24	116.68	120.30
2	F	229	ARG	NE-CZ-NH1	7.21	123.91	120.30
2	E	105	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	170	ASP	CB-CG-OD2	7.17	124.76	118.30
2	D	372	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	A	398	ARG	NE-CZ-NH1	-7.12	116.74	120.30
1	B	90	ARG	CD-NE-CZ	6.91	133.27	123.60
2	F	198	HIS	CA-CB-CG	-6.83	101.99	113.60
1	B	45	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	B	308	ARG	NE-CZ-NH2	6.73	123.67	120.30
2	F	274	ARG	NE-CZ-NH2	6.72	123.66	120.30
2	D	431	LEU	CA-CB-CG	6.70	130.72	115.30
2	D	442	GLN	CA-CB-CG	6.67	128.08	113.40
1	C	494	ASP	CB-CG-OD2	6.65	124.29	118.30
1	C	90	ARG	CD-NE-CZ	6.65	132.91	123.60
1	C	297	ASP	CB-CG-OD1	6.50	124.15	118.30
2	F	274	ARG	CA-CB-CG	6.50	127.70	113.40
1	A	479	LEU	CA-CB-CG	6.48	130.20	115.30
2	E	71	ARG	CD-NE-CZ	6.47	132.65	123.60
1	C	106	ARG	NE-CZ-NH2	-6.46	117.07	120.30
2	D	372	ARG	CD-NE-CZ	6.44	132.62	123.60
2	E	76	LEU	CA-CB-CG	6.44	130.10	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	195	ASP	CB-CG-OD1	6.39	124.06	118.30
2	E	274	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	439	GLU	CA-CB-CG	6.33	127.32	113.40
3	G	252	ARG	NE-CZ-NH2	-6.31	117.14	120.30
2	E	174	ALA	N-CA-CB	6.29	118.91	110.10
2	E	281	TYR	CB-CG-CD1	-6.28	117.23	121.00
1	A	270	ASP	CB-CG-OD2	6.26	123.93	118.30
1	B	164	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	C	90	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	40	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	F	231	ARG	NE-CZ-NH2	-6.17	117.22	120.30
2	D	250	ASP	CB-CG-OD1	6.14	123.83	118.30
1	B	279	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	494	ASP	CB-CG-OD1	6.09	123.78	118.30
2	D	359	ASP	CB-CG-OD1	6.05	123.74	118.30
3	G	74	ASP	CB-CG-OD1	6.04	123.74	118.30
1	B	171	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	300	TYR	CA-CB-CG	6.00	124.80	113.40
2	D	12	ARG	NE-CZ-NH2	-5.97	117.31	120.30
2	E	191	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	A	154	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	24	ASP	CB-CG-OD1	5.76	123.48	118.30
2	F	372	ARG	CD-NE-CZ	5.75	131.65	123.60
1	C	106	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	C	45	ARG	NE-CZ-NH2	-5.67	117.47	120.30
2	E	231	ARG	NE-CZ-NH1	-5.67	117.47	120.30
2	E	229	ARG	NE-CZ-NH2	5.65	123.12	120.30
2	F	337	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	244	TYR	CB-CG-CD1	-5.61	117.64	121.00
1	A	171	ARG	NE-CZ-NH1	-5.57	117.51	120.30
2	E	95	MET	CA-CB-CG	5.56	122.75	113.30
1	B	139	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	300	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	C	304	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	B	423	ARG	CD-NE-CZ	5.51	131.31	123.60
1	A	300	TYR	CB-CG-CD1	5.50	124.30	121.00
2	D	260	ARG	NE-CZ-NH2	-5.50	117.55	120.30
2	E	283	PRO	N-CA-CB	5.48	109.87	103.30
1	B	291	ARG	CG-CD-NE	-5.47	100.31	111.80
1	B	291	ARG	NE-CZ-NH1	5.46	123.03	120.30
3	G	252	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	D	337	ARG	NE-CZ-NH1	5.44	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	GLU	OE1-CD-OE2	-5.42	116.80	123.30
1	A	164	ARG	CD-NE-CZ	5.41	131.17	123.60
2	F	406	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	F	237	LEU	CA-CB-CG	5.37	127.64	115.30
1	A	258	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	E	358	MET	N-CA-CB	5.34	120.22	110.60
1	C	216	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	308	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	127	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	F	356	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	A	188	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	373	ARG	NE-CZ-NH1	-5.18	117.71	120.30
2	D	250	ASP	CA-CB-CG	5.18	124.79	113.40
2	D	412	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	219	ARG	NE-CZ-NH1	-5.15	117.73	120.30
1	C	222	ASP	CB-CG-OD1	5.11	122.90	118.30
2	F	368	TYR	CB-CG-CD2	-5.11	117.94	121.00
2	E	431	LEU	CA-CB-CG	5.11	127.05	115.30
2	E	93	ARG	CD-NE-CZ	5.08	130.71	123.60
1	B	349	GLN	CB-CG-CD	5.07	124.78	111.60
2	E	337	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	A	373	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	84	GLU	OE1-CD-OE2	-5.04	117.25	123.30
2	D	368	TYR	CB-CG-CD2	5.03	124.02	121.00

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	3705	0	3809	42	0
1	B	3656	0	3765	66	0
1	C	3718	0	3818	55	0
2	D	3539	0	3592	53	0
2	E	3447	0	3495	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	3530	0	3586	60	0
3	G	1891	0	1971	118	0
4	H	662	0	654	40	0
5	I	281	0	297	23	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	0	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	E	1	0	0	0	0
7	F	1	0	0	0	0
8	A	6	0	8	0	0
8	B	12	0	15	1	0
8	C	6	0	8	1	0
9	D	5	0	0	3	0
9	F	5	0	0	0	0
10	E	5	0	0	0	0
11	A	310	0	0	2	0
11	B	241	0	0	5	0
11	C	322	0	0	6	0
11	D	310	0	0	4	0
11	E	181	0	0	3	0
11	F	286	0	0	3	0
11	G	39	0	0	2	0
11	H	3	0	0	0	0
11	I	1	0	0	0	0
All	All	26329	0	25090	530	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 11.

All (530) 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:130:GLN:HB3	2:F:357:ILE:HD11	1.27	1.12
3:G:130:GLU:HG3	5:I:41:THR:HG22	1.30	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:75:ARG:HG2	3:G:76:GLY:H	1.25	1.01
2:D:382:LYS:HA	2:D:385:GLN:HE21	1.27	0.98
2:D:282:GLN:H	2:D:282:GLN:HE21	1.01	0.95
2:F:136:GLY:HA3	2:F:431:LEU:HD12	1.47	0.94
2:F:282:GLN:H	2:F:282:GLN:HE21	0.99	0.93
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.52	0.92
1:C:381:ARG:HH11	1:C:488:LYS:HZ3	1.19	0.90
2:E:282:GLN:HE21	2:E:282:GLN:H	1.21	0.89
2:E:97:VAL:HB	2:E:232:VAL:HG12	1.55	0.87
2:E:133:LEU:HD11	2:E:252:LEU:HD21	1.56	0.86
1:B:34:ILE:HD11	1:B:79:ASP:HB2	1.58	0.86
2:F:136:GLY:HA3	2:F:431:LEU:CD1	2.07	0.83
1:C:381:ARG:HH11	1:C:488:LYS:NZ	1.76	0.83
2:D:387:ILE:HG13	3:G:16:ILE:HD13	1.59	0.82
2:F:10:THR:HG22	2:F:76:LEU:HD22	1.61	0.81
1:C:390:MET:HE3	1:C:424:LEU:HD22	1.64	0.79
2:E:138:LYS:HD2	2:E:432:VAL:HG21	1.65	0.79
2:F:131:GLU:HG2	2:F:148:LYS:HD2	1.66	0.78
3:G:197:ASP:H	3:G:200:VAL:HG12	1.47	0.78
2:E:455:GLN:C	2:E:457:PHE:H	1.87	0.78
2:F:394:ASP:HB3	3:G:79:GLY:HA3	1.66	0.76
3:G:76:GLY:HA3	3:G:228:ARG:NH2	2.00	0.76
2:E:169:LEU:O	2:E:173:VAL:HG22	1.83	0.76
1:B:65:ASN:ND2	2:F:17:ILE:HD13	1.99	0.76
2:F:388:ILE:HD11	2:F:396:LEU:HD22	1.67	0.76
2:F:282:GLN:N	2:F:282:GLN:HE21	1.82	0.76
2:D:136:GLY:HA3	2:D:431:LEU:HD13	1.69	0.75
3:G:76:GLY:HA3	3:G:228:ARG:HH21	1.49	0.75
3:G:197:ASP:H	3:G:200:VAL:CG1	2.00	0.75
2:E:148:LYS:HE2	2:E:250:ASP:HB3	1.68	0.75
3:G:129:LYS:HE2	5:I:43:LYS:HG2	1.67	0.75
3:G:192:ILE:HG22	4:H:53:PRO:HG2	1.68	0.75
1:C:215:GLN:HG3	2:F:356:ARG:HH22	1.51	0.75
1:C:185:ASN:OD1	1:C:188:ARG:NH1	2.21	0.74
3:G:179:PHE:O	3:G:181:LEU:N	2.21	0.73
1:A:423:ARG:HG2	1:A:461:ILE:HD11	1.71	0.73
3:G:87:LYS:HA	3:G:90:LYS:HE2	1.68	0.73
1:B:508:PHE:CZ	1:B:510:ALA:HB3	2.24	0.72
1:A:376:SER:HB3	1:A:384:LYS:HD3	1.70	0.72
1:B:78:ASN:HD21	1:B:80:LYS:HE2	1.53	0.72
2:D:223:ASN:HD22	2:D:223:ASN:H	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:220:GLY:HA3	2:E:232:VAL:HG11	1.72	0.71
3:G:167:SER:OG	3:G:170:SER:HB3	1.91	0.71
1:A:286:ARG:NH2	3:G:272:LEU:HD13	2.05	0.70
3:G:75:ARG:CG	3:G:76:GLY:H	1.98	0.70
3:G:51:LEU:HD13	4:H:55:LEU:HD21	1.73	0.70
3:G:166:ARG:NH2	3:G:172:LYS:HD3	2.06	0.70
1:B:479:LEU:HA	1:B:482:LYS:HD2	1.72	0.70
1:C:354:THR:HG23	11:C:2111:HOH:O	1.91	0.69
3:G:82:HIS:CD2	3:G:111:LYS:HG2	2.27	0.69
2:E:174:ALA:HB2	11:E:2078:HOH:O	1.91	0.69
2:F:245:ASP:C	2:F:247:GLU:H	1.96	0.69
1:A:487:GLY:O	1:A:488:LYS:HB2	1.93	0.69
2:D:382:LYS:HA	2:D:385:GLN:NE2	2.05	0.69
1:B:37:GLY:O	11:B:2005:HOH:O	2.10	0.69
3:G:39:LYS:HB2	3:G:40:PRO:HD3	1.73	0.68
5:I:5:ARG:C	5:I:7:ALA:H	1.95	0.68
2:D:282:GLN:H	2:D:282:GLN:NE2	1.84	0.68
4:H:48:LEU:HD13	4:H:49:ALA:N	2.08	0.68
4:H:48:LEU:O	4:H:50:ALA:N	2.27	0.68
1:A:180:ILE:CD1	1:A:216:LEU:HD21	2.23	0.68
4:H:34:ARG:HE	4:H:66:HIS:HB3	1.59	0.68
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.59	0.68
2:F:188:GLU:H	2:F:221:GLN:NE2	1.92	0.67
4:H:22:SER:HB2	4:H:23:PRO:HD2	1.76	0.67
1:B:381:ARG:O	1:B:385:GLN:HG3	1.95	0.67
1:B:460:LYS:HZ2	1:B:510:ALA:HB1	1.60	0.66
2:E:228:ALA:O	2:E:232:VAL:HG13	1.95	0.66
1:C:171:ARG:HD2	11:C:2114:HOH:O	1.95	0.66
2:E:172:ASN:ND2	2:E:431:LEU:HD13	2.10	0.66
2:E:410:ILE:HG13	2:E:444:ILE:HG21	1.78	0.66
3:G:106:ILE:HD11	3:G:148:LEU:HD13	1.76	0.66
4:H:58:LEU:HD11	4:H:92:LEU:HD11	1.78	0.66
3:G:127:THR:OG1	5:I:45:VAL:HB	1.95	0.65
3:G:71:VAL:HA	3:G:108:VAL:HG22	1.78	0.65
2:D:473:LEU:C	2:D:475:GLU:H	1.99	0.65
2:E:388:ILE:HG23	2:E:393:MET:HB2	1.78	0.65
2:E:200:MET:SD	2:E:205:VAL:HG21	2.37	0.65
3:G:87:LYS:O	3:G:90:LYS:HG2	1.96	0.64
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.78	0.64
2:E:131:GLU:HG2	2:E:132:ILE:H	1.61	0.64
3:G:207:TYR:HA	5:I:12:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:39:LYS:N	3:G:40:PRO:HD2	2.13	0.64
2:E:348:VAL:O	2:E:350:PRO:HD3	1.97	0.64
4:H:85:ASN:HD21	4:H:91:GLN:HE22	1.43	0.64
3:G:75:ARG:HG2	3:G:76:GLY:N	2.06	0.63
4:H:48:LEU:C	4:H:50:ALA:H	2.02	0.63
2:E:455:GLN:C	2:E:457:PHE:N	2.51	0.63
1:C:218:LYS:HD2	2:F:128:VAL:HG21	1.81	0.63
3:G:130:GLU:HG3	5:I:41:THR:CG2	2.20	0.63
1:B:418:LEU:O	1:B:422:VAL:HG23	1.99	0.63
2:E:310:ILE:HD13	2:E:325:THR:HG21	1.80	0.63
1:A:185:ASN:OD1	1:A:435:PRO:HB2	1.99	0.63
1:B:412:ALA:HA	1:B:415:GLN:HB3	1.80	0.63
2:E:220:GLY:CA	2:E:232:VAL:HG11	2.29	0.62
2:E:360:PRO:HD3	2:E:368:TYR:CD1	2.34	0.62
1:C:338:ILE:HB	1:C:339:PRO:HD3	1.80	0.62
2:E:452:LEU:HD11	2:E:456:ALA:HB3	1.82	0.62
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.35	0.62
2:F:223:ASN:H	2:F:223:ASN:HD22	1.47	0.62
3:G:82:HIS:CG	3:G:111:LYS:HG2	2.34	0.62
4:H:65:VAL:O	4:H:72:THR:HG23	2.00	0.62
3:G:85:VAL:HG13	3:G:161:ILE:HG22	1.81	0.62
1:C:452:TYR:OH	1:C:498:LYS:HG3	2.00	0.62
1:B:65:ASN:HD22	2:F:17:ILE:HD13	1.62	0.61
3:G:49:LEU:HD21	3:G:212:ILE:HD12	1.80	0.61
2:D:25:PHE:HB2	2:D:29:LEU:HD23	1.81	0.61
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.81	0.61
2:E:370:VAL:HG21	2:E:438:ILE:HG23	1.81	0.61
1:B:497:LEU:O	1:B:501:VAL:HG23	2.01	0.61
1:B:478:ALA:O	1:B:482:LYS:HG3	2.01	0.61
2:F:171:ASN:HA	2:F:175:LYS:HD2	1.82	0.61
2:D:458:TYR:CE2	2:D:459:MET:HG2	2.37	0.60
2:D:244:ARG:O	2:D:248:GLY:HA2	2.00	0.60
1:C:23:VAL:O	1:C:23:VAL:HG12	2.02	0.60
1:A:187:LYS:NZ	1:A:224:ASP:HB3	2.17	0.60
4:H:85:ASN:HD21	4:H:91:GLN:NE2	1.98	0.60
4:H:65:VAL:C	4:H:72:THR:HG23	2.22	0.60
1:C:362:ARG:HA	1:C:363:PRO:C	2.22	0.60
1:C:129:VAL:HG21	1:C:245:LEU:HD11	1.84	0.60
2:E:143:LEU:HD12	2:E:350:PRO:HB3	1.84	0.59
1:A:360:GLY:HA2	1:A:362:ARG:NH1	2.17	0.59
3:G:23:MET:SD	3:G:232:MET:HE3	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:282:GLN:H	2:F:282:GLN:NE2	1.84	0.59
3:G:111:LYS:O	3:G:115:ILE:HG13	2.03	0.59
2:E:447:GLY:C	2:E:449:TYR:H	2.03	0.59
2:E:148:LYS:CE	2:E:250:ASP:HB3	2.32	0.59
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.85	0.59
3:G:21:LYS:HG2	3:G:236:SER:HB2	1.85	0.58
2:E:170:ILE:CG2	2:E:215:VAL:HG21	2.34	0.58
2:D:387:ILE:HG13	3:G:16:ILE:CD1	2.30	0.58
2:E:330:ASP:HA	2:E:356:ARG:HD2	1.83	0.58
3:G:82:HIS:HB3	3:G:115:ILE:CD1	2.33	0.58
1:C:45:ARG:NH2	1:C:68:PRO:O	2.35	0.58
3:G:105:ILE:HG22	3:G:106:ILE:N	2.18	0.58
4:H:47:ILE:HG21	4:H:90:VAL:HG21	1.85	0.58
1:B:416:GLN:HG2	1:B:417:LEU:N	2.18	0.58
2:D:245:ASP:C	2:D:247:GLU:H	2.07	0.58
3:G:128:PHE:HE2	5:I:44:ILE:HD13	1.69	0.58
2:E:136:GLY:HA3	2:E:431:LEU:HD12	1.85	0.58
1:B:183:ILE:HD11	1:B:267:ILE:HD12	1.86	0.58
1:B:463:LYS:NZ	1:B:510:ALA:HB2	2.18	0.58
1:B:78:ASN:ND2	1:B:80:LYS:HE2	2.19	0.58
2:E:377:ILE:HG21	2:E:410:ILE:HD12	1.85	0.58
2:F:252:LEU:HD23	2:F:305:THR:HB	1.86	0.58
1:B:187:LYS:HE3	1:B:224:ASP:HB3	1.85	0.58
2:E:443:GLN:O	2:E:444:ILE:C	2.42	0.57
1:B:509:GLU:O	1:B:510:ALA:C	2.43	0.57
3:G:39:LYS:HB2	3:G:40:PRO:CD	2.34	0.57
5:I:5:ARG:O	5:I:6:GLN:HB3	2.04	0.57
4:H:36:VAL:O	4:H:46:GLY:HA2	2.04	0.57
2:E:388:ILE:HG23	2:E:393:MET:CB	2.34	0.57
1:A:19:ALA:O	1:A:22:SER:HB3	2.04	0.57
1:A:23:VAL:HG21	1:A:30:ARG:NH2	2.20	0.57
3:G:164:ARG:HA	3:G:219:GLU:HG2	1.87	0.57
2:F:266:SER:HB3	2:F:282:GLN:HE22	1.69	0.56
2:E:173:VAL:HG23	11:E:2076:HOH:O	2.04	0.56
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.34	0.56
2:E:366:GLU:HG3	2:E:367:HIS:H	1.71	0.56
2:E:112:GLN:C	2:E:113:PHE:CD2	2.79	0.56
1:C:194:ASP:OD2	1:C:197:LYS:HG3	2.06	0.56
1:B:390:MET:HE2	1:B:424:LEU:HD22	1.88	0.56
3:G:180:SER:O	3:G:181:LEU:C	2.44	0.56
1:C:263:HIS:HD2	1:C:320:SER:OG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:LYS:NZ	2:E:356:ARG:HH12	2.04	0.55
4:H:40:THR:HG23	4:H:56:GLN:HB3	1.88	0.55
2:F:174:ALA:O	2:F:177:HIS:HB3	2.07	0.55
3:G:75:ARG:CG	3:G:76:GLY:N	2.65	0.55
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.42	0.55
3:G:207:TYR:HA	5:I:12:ILE:CD1	2.37	0.55
3:G:164:ARG:HD3	3:G:174:GLU:OE2	2.07	0.55
3:G:164:ARG:NH1	3:G:174:GLU:OE2	2.40	0.55
1:B:479:LEU:HD23	1:B:496:LYS:HD3	1.88	0.55
2:E:444:ILE:O	2:E:445:LEU:C	2.45	0.55
1:B:34:ILE:HD11	1:B:79:ASP:CB	2.35	0.54
2:D:458:TYR:CZ	2:D:459:MET:HG2	2.43	0.54
2:E:200:MET:HB3	2:E:206:ILE:HG13	1.89	0.54
4:H:70:GLY:O	4:H:71:THR:C	2.45	0.54
2:E:447:GLY:C	2:E:449:TYR:N	2.61	0.54
3:G:74:ASP:OD1	3:G:110:ASP:N	2.37	0.54
1:C:179:ALA:HB1	1:C:267:ILE:HG12	1.88	0.54
4:H:64:VAL:HG12	4:H:72:THR:CG2	2.36	0.54
1:B:410:LEU:HG	1:B:411:ASP:H	1.73	0.54
2:E:355:SER:C	2:E:357:ILE:H	2.10	0.54
2:D:44:ARG:HD3	11:D:2020:HOH:O	2.08	0.54
1:C:172:GLN:HG3	1:C:172:GLN:O	2.07	0.54
3:G:128:PHE:CE2	5:I:44:ILE:HD13	2.43	0.53
2:E:370:VAL:HG21	2:E:438:ILE:CG2	2.38	0.53
2:F:398:GLU:HA	2:F:401:LYS:HB2	1.90	0.53
3:G:15:ASN:OD1	3:G:16:ILE:N	2.41	0.53
5:I:13:ARG:NH1	5:I:16:GLN:NE2	2.56	0.53
4:H:78:SER:HB2	5:I:18:CYS:C	2.29	0.53
3:G:51:LEU:CD1	4:H:55:LEU:HD21	2.37	0.53
1:C:240:ALA:N	1:C:241:PRO:CD	2.71	0.53
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.90	0.53
2:E:408:ARG:NH1	2:E:454:GLU:OE2	2.41	0.53
5:I:5:ARG:C	5:I:7:ALA:N	2.61	0.53
4:H:48:LEU:C	4:H:50:ALA:N	2.61	0.53
3:G:139:GLY:O	3:G:143:VAL:HG23	2.08	0.53
1:B:78:ASN:HD21	1:B:80:LYS:CE	2.20	0.53
3:G:179:PHE:C	3:G:181:LEU:N	2.61	0.53
4:H:59:ARG:HG2	4:H:60:PRO:HD2	1.91	0.53
1:A:52:MET:HG3	1:A:95:VAL:CG2	2.39	0.53
3:G:67:LEU:HD12	3:G:104:LYS:O	2.07	0.53
2:E:429:GLY:C	2:E:430:LYS:HG2	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:404:VAL:O	2:E:408:ARG:HG3	2.10	0.52
2:E:452:LEU:HD12	2:E:457:PHE:CE1	2.43	0.52
1:B:105:GLY:HA2	1:B:226:MET:O	2.09	0.52
2:F:25:PHE:HB2	2:F:29:LEU:HD23	1.90	0.52
2:E:374:VAL:HG13	2:E:410:ILE:HG21	1.92	0.52
1:A:218:LYS:HG3	2:D:128:VAL:HG21	1.91	0.52
2:F:245:ASP:C	2:F:247:GLU:N	2.62	0.52
2:E:337:ARG:O	2:E:341:GLU:HG2	2.10	0.52
3:G:76:GLY:HA3	3:G:228:ARG:CZ	2.39	0.52
3:G:82:HIS:HB3	3:G:115:ILE:HD11	1.92	0.52
2:F:393:MET:SD	2:F:404:VAL:HG11	2.49	0.52
1:B:362:ARG:HA	1:B:363:PRO:C	2.30	0.52
1:A:487:GLY:O	1:A:488:LYS:CB	2.58	0.51
1:B:209:LYS:NZ	2:E:356:ARG:NH1	2.58	0.51
1:B:97:VAL:HB	1:B:98:PRO:HD2	1.92	0.51
1:B:351:PHE:HE1	1:B:369:LEU:O	1.92	0.51
2:E:412:ARG:HB3	2:E:458:TYR:HA	1.92	0.51
1:C:381:ARG:HD3	1:C:488:LYS:NZ	2.25	0.51
2:E:252:LEU:HD22	2:E:305:THR:HB	1.90	0.51
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.43	0.51
4:H:51:HIS:ND1	4:H:52:VAL:O	2.36	0.51
1:B:479:LEU:HA	1:B:482:LYS:CD	2.41	0.51
1:A:362:ARG:HA	1:A:363:PRO:C	2.30	0.51
1:B:45:ARG:NH2	1:B:68:PRO:O	2.33	0.51
2:F:357:ILE:HD13	2:F:362:ILE:HD13	1.93	0.51
2:E:25:PHE:HB2	2:E:29:LEU:HD23	1.93	0.51
2:D:89:GLU:HG2	2:D:109:LYS:O	2.10	0.51
1:B:463:LYS:HD3	1:B:510:ALA:CB	2.41	0.51
2:E:360:PRO:HD3	2:E:368:TYR:CE1	2.46	0.51
1:C:129:VAL:HG23	8:C:602:GOL:H12	1.93	0.51
3:G:116:LEU:O	3:G:117:HIS:C	2.49	0.51
1:A:136:ILE:HD13	2:E:190:THR:HG23	1.93	0.51
3:G:167:SER:HG	3:G:170:SER:HB3	1.76	0.50
2:F:357:ILE:CD1	2:F:362:ILE:HG21	2.40	0.50
2:E:355:SER:C	2:E:357:ILE:N	2.65	0.50
5:I:20:LYS:O	5:I:23:ARG:HB2	2.11	0.50
2:E:416:GLN:HG3	2:E:417:PRO:HD2	1.93	0.50
2:F:223:ASN:N	2:F:223:ASN:HD22	2.07	0.50
3:G:85:VAL:HG12	3:G:89:MET:HE2	1.94	0.50
2:D:249:GLN:O	2:D:251:VAL:HG23	2.11	0.50
1:B:209:LYS:HZ2	2:E:356:ARG:HH12	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:28:ALA:HA	3:G:229:MET:CE	2.42	0.50
2:E:447:GLY:O	2:E:449:TYR:N	2.45	0.50
2:F:245:ASP:O	2:F:247:GLU:N	2.45	0.50
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.94	0.50
3:G:17:GLN:OE1	3:G:240:SER:N	2.44	0.50
4:H:64:VAL:HG12	4:H:72:THR:HG21	1.92	0.50
1:B:410:LEU:HG	1:B:411:ASP:N	2.27	0.50
2:F:454:GLU:HG3	11:F:2277:HOH:O	2.12	0.50
3:G:26:VAL:O	3:G:29:ALA:N	2.44	0.50
1:C:356:LEU:HB3	1:C:361:ILE:HB	1.94	0.50
3:G:52:TYR:CD2	3:G:57:ILE:HD12	2.46	0.49
1:C:168:ILE:HD11	1:C:339:PRO:HB3	1.94	0.49
1:A:25:LEU:N	1:A:25:LEU:HD23	2.27	0.49
1:B:440:GLU:HB3	1:B:469:LEU:HD11	1.93	0.49
1:A:157:VAL:N	1:A:158:PRO:CD	2.74	0.49
3:G:115:ILE:O	3:G:115:ILE:HG22	2.13	0.49
4:H:35:GLN:HB3	4:H:66:HIS:CD2	2.47	0.49
2:E:410:ILE:CG1	2:E:444:ILE:HG21	2.42	0.49
3:G:105:ILE:CG2	3:G:106:ILE:N	2.75	0.49
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.47	0.49
2:E:455:GLN:O	2:E:457:PHE:N	2.46	0.49
3:G:244:ASP:O	3:G:248:LEU:HG	2.11	0.49
1:C:171:ARG:NH1	11:C:2112:HOH:O	2.45	0.49
4:H:99:THR:O	4:H:102:MET:HG2	2.13	0.49
1:A:186:GLN:HG3	1:A:199:LEU:HD23	1.95	0.49
2:E:223:ASN:H	2:E:223:ASN:HD22	1.60	0.49
2:F:455:GLN:O	2:F:469:LYS:HE2	2.13	0.49
1:B:54:GLU:HG2	1:B:60:LYS:CD	2.43	0.49
1:A:414:THR:HG21	2:E:389:ALA:HB1	1.94	0.49
4:H:85:ASN:ND2	4:H:91:GLN:HE22	2.11	0.48
1:A:291:ARG:HG2	1:A:292:GLU:HG3	1.95	0.48
3:G:133:ARG:HG2	11:G:2013:HOH:O	2.13	0.48
2:D:196:LEU:O	2:D:200:MET:HG3	2.13	0.48
3:G:184:ILE:O	3:G:184:ILE:HD13	2.14	0.48
5:I:13:ARG:HH11	5:I:16:GLN:NE2	2.10	0.48
2:F:419:GLN:O	2:F:422:GLU:HG3	2.13	0.48
5:I:37:THR:HG22	5:I:38:SER:H	1.78	0.48
3:G:37:GLU:OE2	3:G:218:LYS:NZ	2.46	0.48
1:B:463:LYS:HD3	1:B:510:ALA:HB2	1.95	0.48
3:G:181:LEU:HD23	3:G:184:ILE:H	1.79	0.48
4:H:35:GLN:HB3	4:H:66:HIS:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:357:ILE:HD12	2:F:362:ILE:HG21	1.95	0.48
2:E:449:TYR:HB3	2:E:452:LEU:HB3	1.95	0.48
3:G:81:ILE:HG22	3:G:82:HIS:N	2.28	0.48
5:I:5:ARG:O	5:I:6:GLN:CB	2.59	0.48
2:E:439:LYS:HE2	2:E:443:GLN:NE2	2.28	0.48
2:D:158:ALA:HA	9:D:620:ALF:F1	2.03	0.48
2:E:276:PRO:HD2	3:G:266:ILE:HD11	1.96	0.48
3:G:181:LEU:HD23	3:G:184:ILE:N	2.29	0.47
2:E:359:ASP:OD1	2:E:360:PRO:HD2	2.14	0.47
3:G:162:PHE:O	3:G:173:THR:HA	2.14	0.47
2:E:63:MET:HE3	2:E:97:VAL:HG21	1.95	0.47
2:E:97:VAL:HB	2:E:232:VAL:CG1	2.37	0.47
3:G:179:PHE:O	3:G:180:SER:C	2.52	0.47
3:G:185:SER:CB	3:G:205:GLN:HE21	2.27	0.47
3:G:129:LYS:O	3:G:130:GLU:CB	2.62	0.47
3:G:203:ASN:OD1	5:I:5:ARG:NH2	2.43	0.47
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.96	0.47
2:E:388:ILE:HG12	2:E:396:LEU:HD11	1.97	0.47
4:H:40:THR:CG2	4:H:56:GLN:HB3	2.45	0.47
1:C:224:ASP:O	1:C:227:LYS:HE2	2.14	0.47
1:C:97:VAL:HB	1:C:98:PRO:HD2	1.97	0.47
1:B:185:ASN:O	1:B:188:ARG:HD2	2.14	0.47
2:E:95:MET:HG3	2:E:99:GLY:HA2	1.95	0.47
3:G:189:SER:O	3:G:192:ILE:HD12	2.14	0.47
3:G:36:ARG:O	3:G:39:LYS:HG3	2.14	0.47
2:E:394:ASP:C	2:E:396:LEU:H	2.18	0.47
1:C:26:GLU:HB3	1:C:46:ASN:ND2	2.30	0.47
5:I:4:TRP:HB2	5:I:9:LEU:HB2	1.96	0.47
9:D:620:ALF:F4	11:D:2121:HOH:O	2.10	0.47
2:F:388:ILE:O	2:F:389:ALA:C	2.53	0.47
1:A:216:LEU:HD22	1:A:216:LEU:O	2.14	0.47
1:B:453:LEU:O	1:B:456:LEU:HB2	2.15	0.47
2:D:360:PRO:HD3	2:D:368:TYR:CD1	2.50	0.47
2:E:364:GLY:O	2:E:365:SER:C	2.52	0.47
4:H:40:THR:HG22	4:H:41:GLN:N	2.30	0.46
1:C:137:ILE:HB	1:C:138:PRO:HD3	1.97	0.46
4:H:98:VAL:HG21	4:H:103:LEU:HD21	1.96	0.46
1:A:338:ILE:N	1:A:339:PRO:CD	2.78	0.46
1:A:240:ALA:N	1:A:241:PRO:HD2	2.30	0.46
2:E:148:LYS:HE3	2:E:305:THR:OG1	2.15	0.46
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:107:GLY:HA3	3:G:112:ILE:HG21	1.98	0.46
4:H:87:ASP:O	4:H:89:SER:N	2.48	0.46
2:F:391:LEU:HD13	2:F:395:GLU:HG2	1.98	0.46
3:G:75:ARG:O	3:G:82:HIS:HE1	1.98	0.46
1:B:509:GLU:OE1	1:B:509:GLU:HA	2.15	0.46
2:E:314:ALA:O	2:E:315:ASP:HB2	2.15	0.46
3:G:76:GLY:CA	3:G:228:ARG:HH21	2.24	0.46
1:C:381:ARG:NH1	1:C:488:LYS:NZ	2.56	0.46
3:G:131:VAL:C	3:G:133:ARG:H	2.20	0.46
3:G:81:ILE:HG13	3:G:224:GLU:HA	1.96	0.46
3:G:33:ARG:O	3:G:36:ARG:N	2.46	0.46
1:C:80:LYS:HE3	2:F:33:LEU:HD12	1.98	0.46
5:I:44:ILE:HG21	5:I:46:LYS:HE2	1.98	0.46
3:G:181:LEU:CD2	3:G:183:THR:HB	2.46	0.46
2:F:188:GLU:O	2:F:221:GLN:HB3	2.15	0.46
2:D:249:GLN:HA	2:D:249:GLN:OE1	2.16	0.46
1:B:397:TYR:O	1:B:399:GLU:N	2.49	0.46
2:E:422:GLU:HG2	2:E:427:HIS:O	2.16	0.46
2:E:461:GLY:HA3	2:E:462:PRO:HD3	1.81	0.45
2:E:416:GLN:NE2	2:E:432:VAL:HG23	2.32	0.45
2:D:223:ASN:N	2:D:223:ASN:HD22	2.07	0.45
2:D:348:VAL:O	2:D:350:PRO:HD3	2.16	0.45
2:E:266:SER:HB2	2:E:282:GLN:NE2	2.32	0.45
3:G:15:ASN:OD1	3:G:15:ASN:C	2.55	0.45
2:E:443:GLN:O	2:E:446:ALA:N	2.49	0.45
2:D:52:HIS:CD2	2:D:58:VAL:HG12	2.51	0.45
1:C:469:LEU:HD12	1:C:472:VAL:CG2	2.46	0.45
4:H:19:THR:HA	4:H:28:PHE:O	2.17	0.45
2:F:249:GLN:OE1	2:F:249:GLN:HA	2.16	0.45
3:G:180:SER:O	3:G:182:ASP:N	2.50	0.45
3:G:181:LEU:O	3:G:184:ILE:HG22	2.17	0.45
3:G:73:SER:HA	3:G:131:VAL:HB	1.98	0.45
1:B:287:ARG:NE	11:B:2149:HOH:O	2.48	0.45
2:D:10:THR:OG1	2:D:76:LEU:HD23	2.16	0.45
2:E:345:TYR:HA	2:E:346:PRO:C	2.36	0.45
1:C:338:ILE:N	1:C:339:PRO:CD	2.79	0.45
1:A:23:VAL:HG12	1:A:25:LEU:CD2	2.47	0.45
2:D:167:MET:HE1	2:D:196:LEU:HD13	1.99	0.45
1:B:101:GLU:OE2	1:B:262:LYS:NZ	2.47	0.45
2:F:348:VAL:O	2:F:350:PRO:HD3	2.17	0.45
2:D:246:GLN:O	2:D:247:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:196:LEU:O	2:D:196:LEU:HD12	2.17	0.44
2:F:212:THR:O	2:F:214:LYS:HE2	2.17	0.44
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.52	0.44
1:A:187:LYS:HZ2	1:A:224:ASP:HB3	1.82	0.44
3:G:20:THR:HA	3:G:23:MET:CE	2.48	0.44
1:B:209:LYS:HZ1	2:E:356:ARG:NH1	2.15	0.44
1:C:239:ALA:HB1	1:C:241:PRO:HD2	1.99	0.44
1:A:44:LEU:HB3	1:A:47:VAL:HB	1.99	0.44
2:D:345:TYR:HA	2:D:346:PRO:C	2.37	0.44
3:G:39:LYS:N	3:G:40:PRO:CD	2.79	0.44
1:B:390:MET:CE	1:B:424:LEU:HD22	2.47	0.44
3:G:52:TYR:HD2	3:G:57:ILE:HD12	1.81	0.44
2:E:374:VAL:O	2:E:377:ILE:HG22	2.17	0.44
2:F:223:ASN:H	2:F:223:ASN:ND2	2.15	0.44
2:D:245:ASP:C	2:D:247:GLU:N	2.71	0.44
2:D:130:GLN:NE2	11:D:2088:HOH:O	2.50	0.44
4:H:38:VAL:HG13	4:H:39:PRO:HD2	1.99	0.44
1:C:102:GLU:HG2	1:C:122:GLY:O	2.17	0.44
1:B:140:ILE:HD12	11:B:2077:HOH:O	2.18	0.44
2:E:39:GLN:NE2	2:E:76:LEU:HG	2.32	0.44
2:F:388:ILE:CD1	2:F:396:LEU:HD22	2.44	0.44
2:E:360:PRO:HG3	2:E:368:TYR:CD2	2.53	0.44
3:G:85:VAL:HG12	3:G:89:MET:CE	2.48	0.44
2:D:205:VAL:HG12	2:D:215:VAL:HG23	1.99	0.44
2:E:452:LEU:HA	2:E:453:PRO:HD3	1.87	0.44
3:G:39:LYS:CB	3:G:40:PRO:CD	2.95	0.44
2:E:66:THR:HB	2:E:69:LEU:HD12	2.00	0.44
2:F:188:GLU:H	2:F:221:GLN:HE22	1.66	0.43
1:C:83:LYS:NZ	2:F:29:LEU:O	2.50	0.43
1:C:269:ASP:HA	1:C:270:ASP:HA	1.74	0.43
1:A:137:ILE:N	1:A:138:PRO:HD2	2.33	0.43
2:E:416:GLN:NE2	2:E:430:LYS:O	2.49	0.43
1:A:410:LEU:HD23	1:A:410:LEU:N	2.33	0.43
2:E:452:LEU:CD1	2:E:456:ALA:HB3	2.48	0.43
1:B:496:LYS:NZ	11:B:2232:HOH:O	2.50	0.43
2:E:359:ASP:OD2	2:E:361:ASN:HB2	2.18	0.43
8:B:700:GOL:H11	11:F:2286:HOH:O	2.18	0.43
1:C:396:GLN:O	1:C:400:VAL:HG23	2.19	0.43
2:E:384:LEU:O	2:E:387:ILE:HG23	2.19	0.43
3:G:72:SER:OG	3:G:82:HIS:HD2	2.01	0.43
2:E:275:ILE:HA	2:E:276:PRO:HD3	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:164:ARG:NH2	3:G:166:ARG:NE	2.67	0.43
4:H:16:MET:HB3	4:H:49:ALA:HA	1.99	0.43
11:B:2153:HOH:O	3:G:263:ILE:HG21	2.18	0.43
1:B:338:ILE:HB	1:B:339:PRO:HD3	2.01	0.43
2:D:84:ILE:HG21	2:D:235:THR:HG23	2.00	0.43
2:E:366:GLU:O	2:E:370:VAL:HG23	2.18	0.43
3:G:193:TYR:HB3	3:G:196:ILE:HD11	1.99	0.43
1:B:35:GLY:O	1:B:36:ASP:HB2	2.19	0.43
4:H:26:VAL:O	4:H:26:VAL:HG13	2.19	0.43
2:F:471:ASP:O	2:F:474:ALA:N	2.52	0.43
2:F:345:TYR:HA	2:F:346:PRO:C	2.39	0.43
1:C:188:ARG:HH11	1:C:188:ARG:HG2	1.84	0.43
2:F:174:ALA:O	2:F:177:HIS:N	2.51	0.43
1:A:218:LYS:HE2	1:A:222:ASP:OD2	2.18	0.43
2:D:422:GLU:HG2	2:D:427:HIS:O	2.18	0.43
1:B:463:LYS:CE	1:B:510:ALA:HB2	2.48	0.42
2:F:408:ARG:NE	2:F:454:GLU:OE2	2.42	0.42
1:C:137:ILE:HG12	11:D:2065:HOH:O	2.19	0.42
11:C:2191:HOH:O	2:D:226:PRO:HG3	2.18	0.42
3:G:178:ILE:CD1	3:G:212:ILE:HG21	2.50	0.42
3:G:28:ALA:HA	3:G:229:MET:HE2	2.00	0.42
2:E:120:ALA:HB1	2:E:121:PRO:HD2	2.00	0.42
2:E:256:ASP:HA	2:E:257:ASN:HA	1.85	0.42
1:C:52:MET:HE1	1:C:76:PHE:HD1	1.84	0.42
2:D:50:ALA:C	2:D:51:GLN:HG3	2.39	0.42
2:F:408:ARG:HE	2:F:454:GLU:CD	2.22	0.42
2:F:415:SER:O	2:F:416:GLN:HB2	2.19	0.42
4:H:41:GLN:OE1	4:H:59:ARG:HG3	2.19	0.42
2:E:252:LEU:HD12	2:E:254:PHE:CZ	2.54	0.42
1:B:482:LYS:NZ	1:B:496:LYS:NZ	2.67	0.42
2:E:142:LEU:HD11	2:E:370:VAL:HG12	2.02	0.42
2:D:247:GLU:O	2:D:249:GLN:NE2	2.52	0.42
3:G:26:VAL:O	3:G:27:ALA:C	2.57	0.42
1:C:48:GLN:HB3	2:D:68:GLY:HA2	2.02	0.42
1:A:209:LYS:HB2	2:D:294:GLU:OE1	2.20	0.42
2:D:188:GLU:O	2:D:221:GLN:HB3	2.19	0.42
5:I:4:TRP:O	5:I:7:ALA:HB3	2.20	0.42
2:D:205:VAL:CG1	2:D:215:VAL:HG23	2.50	0.42
2:D:245:ASP:O	2:D:247:GLU:N	2.53	0.42
2:D:463:ILE:HD12	2:D:463:ILE:HA	1.83	0.42
3:G:128:PHE:HA	5:I:43:LYS:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:81:ILE:HD13	3:G:171:TYR:CZ	2.55	0.42
3:G:87:LYS:HA	3:G:90:LYS:CE	2.43	0.42
3:G:33:ARG:O	3:G:34:ALA:C	2.58	0.42
1:A:26:GLU:HA	1:A:45:ARG:HB2	2.00	0.42
2:D:170:ILE:O	2:D:174:ALA:HB3	2.20	0.42
3:G:76:GLY:HA3	3:G:228:ARG:NE	2.33	0.42
4:H:38:VAL:HA	4:H:39:PRO:HD3	1.86	0.42
1:A:62:MET:HE3	1:A:76:PHE:HZ	1.84	0.42
1:B:103:LEU:HD12	1:B:121:ILE:HG21	2.02	0.42
1:C:381:ARG:HD3	1:C:488:LYS:HZ3	1.85	0.42
3:G:74:ASP:OD1	3:G:109:GLY:HA2	2.19	0.42
1:B:287:ARG:HH11	1:B:287:ARG:HD2	1.62	0.42
2:E:199:GLU:OE2	2:E:420:VAL:HB	2.20	0.42
1:A:403:PHE:CE1	2:E:390:ILE:HD11	2.55	0.42
2:F:440:GLY:O	2:F:444:ILE:HG13	2.19	0.42
5:I:5:ARG:O	5:I:7:ALA:N	2.51	0.41
4:H:83:THR:HB	4:H:91:GLN:HE21	1.85	0.41
1:C:360:GLY:O	1:C:429:LYS:HE2	2.20	0.41
1:C:292:GLU:O	1:C:293:ALA:HB3	2.20	0.41
1:A:261:GLY:HA2	1:A:317:GLY:O	2.21	0.41
1:B:460:LYS:NZ	1:B:510:ALA:HB1	2.29	0.41
1:A:439:GLU:CG	1:A:484:ARG:HB2	2.49	0.41
2:F:405:SER:O	2:F:409:LYS:HG3	2.20	0.41
1:C:390:MET:CE	1:C:424:LEU:HD13	2.50	0.41
2:E:199:GLU:OE2	2:E:420:VAL:O	2.39	0.41
4:H:100:LEU:H	4:H:100:LEU:HG	1.75	0.41
1:C:391:LYS:NZ	11:C:2240:HOH:O	2.52	0.41
2:D:162:LYS:CE	9:D:620:ALF:F4	2.58	0.41
2:F:409:LYS:HD3	2:F:457:PHE:CE1	2.56	0.41
3:G:181:LEU:HD23	3:G:184:ILE:HB	2.03	0.41
3:G:51:LEU:O	3:G:55:ALA:HB3	2.20	0.41
1:B:180:ILE:HD12	1:B:216:LEU:HD21	2.02	0.41
2:F:246:GLN:O	2:F:247:GLU:HG2	2.21	0.41
2:E:406:ARG:NE	2:E:445:LEU:O	2.53	0.41
1:C:213:VAL:O	1:C:216:LEU:HB3	2.21	0.41
4:H:64:VAL:HG12	4:H:72:THR:HG22	2.03	0.41
2:E:113:PHE:CD2	2:E:113:PHE:N	2.89	0.41
1:C:151:LYS:HE2	1:C:436:MET:SD	2.60	0.41
1:B:304:ARG:HH11	1:B:304:ARG:HD3	1.59	0.41
1:B:201:CYS:C	1:B:202:ILE:HG13	2.40	0.41
3:G:10:LEU:HD13	3:G:246:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:57:ILE:HG22	3:G:184:ILE:HD12	2.02	0.41
2:F:221:GLN:NE2	2:F:221:GLN:HA	2.31	0.41
1:C:171:ARG:HG2	11:C:2209:HOH:O	2.21	0.41
2:D:84:ILE:HD13	2:D:235:THR:HG23	2.02	0.41
1:B:452:TYR:OH	1:B:498:LYS:HG3	2.21	0.41
1:A:446:TYR:OH	1:A:494:ASP:OD1	2.34	0.41
3:G:178:ILE:HD12	3:G:212:ILE:HG21	2.03	0.41
1:B:67:GLU:HB3	1:B:68:PRO:HD2	2.02	0.41
1:C:137:ILE:N	1:C:138:PRO:CD	2.84	0.41
1:A:484:ARG:NH2	11:A:2287:HOH:O	2.54	0.41
1:A:355:GLU:HB3	11:A:2220:HOH:O	2.20	0.41
2:E:122:GLU:HB2	2:E:125:GLU:HG3	2.01	0.41
1:C:163:GLN:HG3	1:C:347:ASP:HB2	2.03	0.41
2:F:442:GLN:NE2	11:F:2272:HOH:O	2.52	0.41
2:D:282:GLN:N	2:D:282:GLN:HE21	1.86	0.40
2:E:394:ASP:C	2:E:396:LEU:N	2.75	0.40
2:D:275:ILE:HG21	2:D:275:ILE:HD13	1.89	0.40
1:B:503:ASN:HD22	1:B:503:ASN:HA	1.61	0.40
3:G:21:LYS:HE2	3:G:236:SER:HB2	2.04	0.40
2:F:142:LEU:HD22	2:F:441:PHE:CD1	2.57	0.40
1:A:48:GLN:HG2	2:E:70:VAL:CG2	2.51	0.40
3:G:260:LYS:HE3	3:G:260:LYS:HB2	1.61	0.40
1:B:508:PHE:CE2	1:B:510:ALA:HB3	2.56	0.40
3:G:36:ARG:C	3:G:38:LEU:H	2.23	0.40
1:C:432:GLN:O	1:C:433:TYR:HB2	2.21	0.40
1:B:423:ARG:HH21	1:B:458:PRO:HD3	1.85	0.40
1:C:195:GLU:O	1:C:195:GLU:HG3	2.21	0.40
3:G:19:ILE:HG22	3:G:23:MET:CE	2.51	0.40
3:G:67:LEU:HA	3:G:104:LYS:O	2.20	0.40
2:E:391:LEU:HD11	3:G:26:VAL:HA	2.03	0.40
2:D:167:MET:HB3	2:D:167:MET:HE2	1.89	0.40
2:E:173:VAL:O	11:E:2078:HOH:O	2.22	0.40
3:G:67:LEU:N	11:G:2007:HOH:O	2.54	0.40
1:A:439:GLU:HG3	1:A:484:ARG:HB2	2.04	0.40
2:E:163:THR:O	2:E:167:MET:HG3	2.22	0.40
2:F:244:ARG:O	2:F:248:GLY:HA2	2.21	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	482/510 (94%)	466 (97%)	12 (2%)	4 (1%)	24	15
1	B	475/510 (93%)	456 (96%)	15 (3%)	4 (1%)	24	15
1	C	484/510 (95%)	475 (98%)	9 (2%)	0	100	100
2	D	465/482 (96%)	448 (96%)	13 (3%)	4 (1%)	21	13
2	E	450/482 (93%)	407 (90%)	31 (7%)	12 (3%)	6	2
2	F	464/482 (96%)	437 (94%)	22 (5%)	5 (1%)	17	9
3	G	234/272 (86%)	197 (84%)	29 (12%)	8 (3%)	5	1
4	H	87/146 (60%)	79 (91%)	5 (6%)	3 (3%)	5	1
5	I	32/50 (64%)	28 (88%)	2 (6%)	2 (6%)	2	0
All	All	3173/3444 (92%)	2993 (94%)	138 (4%)	42 (1%)	15	7

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	488	LYS
1	B	413	ALA
2	E	176	ALA
2	E	444	ILE
2	F	246	GLN
3	G	79	GLY
3	G	102	GLU
3	G	180	SER
3	G	194	ASP
3	G	195	ASP
4	H	49	ALA
1	B	194	ASP
1	B	398	ARG
2	D	246	GLN
2	D	248	GLY
2	E	28	GLY

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Mol	Chain	Res	Type
2	E	174	ALA
2	E	365	SER
2	E	366	GLU
2	F	28	GLY
2	F	175	LYS
2	F	398	GLU
3	G	130	GLU
3	G	196	ILE
2	E	448	GLU
4	H	71	THR
1	A	20	ASP
1	A	22	SER
2	D	474	ALA
2	E	175	LYS
2	E	357	ILE
4	H	88	SER
5	I	40	SER
2	D	247	GLU
2	E	177	HIS
3	G	37	GLU
2	E	456	ALA
5	I	42	ILE
1	B	458	PRO
2	E	279	VAL
1	A	489	ILE
2	F	279	VAL

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%)	376 (96%)	17 (4%)	35	30
1	B	388/412 (94%)	376 (97%)	12 (3%)	47	46
1	C	394/412 (96%)	388 (98%)	6 (2%)	72	75
2	D	377/386 (98%)	368 (98%)	9 (2%)	57	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	368/386 (95%)	353 (96%)	15 (4%)	37	32
2	F	376/386 (97%)	365 (97%)	11 (3%)	50	49
3	G	207/230 (90%)	196 (95%)	11 (5%)	28	22
4	H	75/109 (69%)	72 (96%)	3 (4%)	38	33
5	I	29/41 (71%)	26 (90%)	3 (10%)	9	5
All	All	2607/2774 (94%)	2520 (97%)	87 (3%)	45	43

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	25	LEU
1	A	45	ARG
1	A	80	LYS
1	A	123	SER
1	A	164	ARG
1	A	188	ARG
1	A	216	LEU
1	A	218	LYS
1	A	355	GLU
1	A	410	LEU
1	A	414	THR
1	A	439	GLU
1	A	455	LYS
1	A	479	LEU
1	A	485	THR
1	A	494	ASP
1	B	123	SER
1	B	164	ARG
1	B	171	ARG
1	B	188	ARG
1	B	218	LYS
1	B	247	PRO
1	B	349	GLN
1	B	416	GLN
1	B	419	SER
1	B	423	ARG
1	B	470	SER
1	B	497	LEU
1	C	59	LEU

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Mol	Chain	Res	Type
1	C	164	ARG
1	C	219	ARG
1	C	349	GLN
1	C	422	VAL
1	C	479	LEU
2	D	74	LYS
2	D	223	ASN
2	D	237	LEU
2	D	266	SER
2	D	274	ARG
2	D	282	GLN
2	D	303	SER
2	D	431	LEU
2	D	439	LYS
2	E	44	ARG
2	E	177	HIS
2	E	223	ASN
2	E	225	PRO
2	E	251	VAL
2	E	252	LEU
2	E	258	ILE
2	E	282	GLN
2	E	310	ILE
2	E	344	ILE
2	E	359	ASP
2	E	383	SER
2	E	431	LEU
2	E	436	GLU
2	E	452	LEU
2	F	95	MET
2	F	127	SER
2	F	209	LYS
2	F	221	GLN
2	F	223	ASN
2	F	279	VAL
2	F	282	GLN
2	F	395	GLU
2	F	397	SER
2	F	439	LYS
2	F	455	GLN
3	G	2	THR
3	G	12	SER

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Mol	Chain	Res	Type
3	G	15	ASN
3	G	91	SER
3	G	114	SER
3	G	142	SER
3	G	159	SER
3	G	184	ILE
3	G	190	MET
3	G	219	GLU
3	G	232	MET
4	H	68	GLU
4	H	73	SER
4	H	100	LEU
5	I	17	ILE
5	I	37	THR
5	I	42	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	ASN
1	A	471	HIS
1	B	48	GLN
1	B	65	ASN
1	B	78	ASN
1	B	260	ASN
1	B	349	GLN
1	B	503	ASN
1	C	48	GLN
1	C	260	ASN
1	C	263	HIS
1	C	349	GLN
1	C	416	GLN
2	D	130	GLN
2	D	194	ASN
2	D	221	GLN
2	D	223	ASN
2	D	282	GLN
2	D	385	GLN
2	E	39	GLN
2	E	194	ASN
2	E	223	ASN
2	E	263	GLN

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Mol	Chain	Res	Type
2	E	282	GLN
2	E	361	ASN
2	F	39	GLN
2	F	194	ASN
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	442	GLN
3	G	82	HIS
3	G	88	GLN
3	G	205	GLN
4	H	91	GLN
5	I	16	GLN

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 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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	1.15	1 (4%)	27,45,45	0.86	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	A	602	-	5,5,5	0.42	0	5,5,5	0.49	0
6	ADP	B	600	7	22,29,29	0.96	1 (4%)	27,45,45	1.03	1 (3%)
8	GOL	B	602	-	5,5,5	1.09	0	5,5,5	1.86	3 (60%)
8	GOL	B	700	-	5,5,5	0.35	0	5,5,5	0.45	0
6	ADP	C	600	7	22,29,29	1.17	3 (13%)	27,45,45	1.28	3 (11%)
8	GOL	C	602	-	5,5,5	0.37	0	5,5,5	0.81	0
6	ADP	D	600	9,7	22,29,29	1.17	3 (13%)	27,45,45	0.88	1 (3%)
9	ALF	D	620	11,2,7,6	0,4,4	0.00	-	0,6,6	0.00	-
6	ADP	E	600	7	22,29,29	0.96	0	27,45,45	0.70	0
10	SO4	E	630	-	4,4,4	0.94	0	6,6,6	0.50	0
6	ADP	F	600	9,7	22,29,29	1.04	2 (9%)	27,45,45	1.15	3 (11%)
9	ALF	F	620	11,7,6	0,4,4	0.00	-	0,6,6	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	A	600	7	-	0/12/32/32	0/3/3/3
8	GOL	A	602	-	-	0/4/4/4	0/0/0/0
6	ADP	B	600	7	-	0/12/32/32	0/3/3/3
8	GOL	B	602	-	-	0/4/4/4	0/0/0/0
8	GOL	B	700	-	-	0/4/4/4	0/0/0/0
6	ADP	C	600	7	-	0/12/32/32	0/3/3/3
8	GOL	C	602	-	-	0/4/4/4	0/0/0/0
6	ADP	D	600	9,7	-	0/12/32/32	0/3/3/3
9	ALF	D	620	11,2,7,6	-	0/0/0/0	0/0/0/0
6	ADP	E	600	7	-	0/12/32/32	0/3/3/3
10	SO4	E	630	-	-	0/0/0/0	0/0/0/0
6	ADP	F	600	9,7	-	0/12/32/32	0/3/3/3
9	ALF	F	620	11,7,6	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	600	ADP	PB-O2B	-2.91	1.44	1.54
6	F	600	ADP	PB-O2B	-2.59	1.45	1.54
6	C	600	ADP	PA-O2A	-2.54	1.44	1.54
6	D	600	ADP	PB-O2B	-2.49	1.45	1.54
6	F	600	ADP	PA-O1A	-2.33	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	600	ADP	PB-O3B	-2.17	1.46	1.54
6	A	600	ADP	PB-O3B	-2.12	1.47	1.54
6	D	600	ADP	PB-O3B	-2.01	1.47	1.54
6	C	600	ADP	C2-N1	2.08	1.37	1.33
6	D	600	ADP	O4'-C1'	2.76	1.44	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	600	ADP	C1'-N9-C4	-3.38	121.84	126.94
6	F	600	ADP	C2'-C1'-N9	-3.02	109.67	114.29
6	B	600	ADP	C2'-C1'-N9	-2.47	110.52	114.29
6	D	600	ADP	C2'-C1'-N9	-2.29	110.79	114.29
6	F	600	ADP	O4'-C4'-C3'	-2.02	101.07	105.15
6	C	600	ADP	O2A-PA-O3A	2.03	114.32	105.09
8	B	602	GOL	O2-C2-C3	2.05	118.06	108.65
8	B	602	GOL	O2-C2-C1	2.26	119.03	108.65
6	C	600	ADP	C4-C5-N7	2.41	111.70	109.48
6	F	600	ADP	O3B-PB-O2B	2.45	116.72	107.38
6	A	600	ADP	O3B-PB-O1B	2.74	119.41	110.58
8	B	602	GOL	C3-C2-C1	2.81	122.12	111.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	700	GOL	1	0
8	C	602	GOL	1	0
9	D	620	ALF	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	486/510 (95%)	-0.27	9 (1%) 70 70	24, 36, 57, 99	0
1	B	479/510 (93%)	-0.01	25 (5%) 31 33	24, 38, 71, 113	0
1	C	488/510 (95%)	-0.33	6 (1%) 81 81	22, 34, 53, 82	0
2	D	467/482 (96%)	-0.34	13 (2%) 56 57	24, 34, 57, 83	0
2	E	454/482 (94%)	0.58	72 (15%) 3 3	24, 47, 105, 120	0
2	F	466/482 (96%)	-0.17	23 (4%) 33 35	23, 34, 65, 88	0
3	G	244/272 (89%)	1.36	63 (25%) 1 1	28, 66, 95, 115	0
4	H	89/146 (60%)	1.94	37 (41%) 0 1	51, 73, 110, 122	0
5	I	36/50 (72%)	3.07	18 (50%) 0 1	58, 87, 113, 119	0
All	All	3209/3444 (93%)	0.10	266 (8%) 14 15	22, 38, 86, 122	0

All (266) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	71	THR	17.3
5	I	47	VAL	10.8
1	A	402	ALA	10.0
5	I	7	ALA	10.0
1	A	19	ALA	8.1
1	B	410	LEU	7.9
2	F	474	ALA	7.7
2	E	445	LEU	7.6
3	G	94	ALA	7.4
2	E	402	LEU	7.3
2	E	356	ARG	7.2
2	E	176	ALA	7.2
3	G	180	SER	7.2
4	H	70	GLY	7.0
3	G	181	LEU	6.8

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Mol	Chain	Res	Type	RSRZ
1	C	409	ASP	6.7
2	E	456	ALA	6.7
2	E	452	LEU	6.7
5	I	1	VAL	6.4
4	H	72	THR	6.3
1	B	400	VAL	6.1
5	I	38	SER	6.1
4	H	68	GLU	6.0
4	H	69	ASP	5.9
2	E	177	HIS	5.9
2	E	178	GLY	5.9
4	H	43	GLY	5.6
2	E	444	ILE	5.6
3	G	165	PHE	5.6
2	F	246	GLN	5.5
5	I	46	LYS	5.5
2	E	366	GLU	5.4
3	G	117	HIS	5.4
3	G	116	LEU	5.3
4	H	100	LEU	5.2
4	H	42	THR	5.2
2	E	129	GLU	5.1
2	F	178	GLY	5.1
1	A	20	ASP	5.1
2	E	446	ALA	5.0
3	G	169	ILE	5.0
2	E	364	GLY	5.0
2	E	357	ILE	5.0
2	F	248	GLY	4.9
1	B	358	TYR	4.9
4	H	32	ASN	4.7
4	H	34	ARG	4.7
5	I	25	ALA	4.7
3	G	183	THR	4.6
2	E	451	HIS	4.6
1	C	193	THR	4.6
3	G	101	LYS	4.5
3	G	92	GLU	4.4
2	E	174	ALA	4.4
4	H	101	ASP	4.3
5	I	6	GLN	4.3
2	D	176	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
2	F	174	ALA	4.3
2	E	301	LYS	4.3
2	E	435	LYS	4.2
3	G	198	ALA	4.2
3	G	188	GLU	4.1
5	I	8	GLY	4.1
1	B	193	THR	4.1
3	G	115	ILE	4.0
3	G	199	ASP	4.0
2	F	175	LYS	4.0
5	I	37	THR	4.0
5	I	3	TYR	4.0
4	H	15	GLN	4.0
3	G	87	LYS	3.9
5	I	39	GLY	3.9
3	G	113	ARG	3.8
1	B	510	ALA	3.8
1	B	401	ALA	3.8
3	G	170	SER	3.8
3	G	148	LEU	3.8
2	E	360	PRO	3.7
3	G	8	ARG	3.7
4	H	73	SER	3.7
3	G	103	VAL	3.7
2	E	393	MET	3.7
2	F	391	LEU	3.7
3	G	90	LYS	3.7
3	G	55	ALA	3.7
2	E	368	TYR	3.6
3	G	1	ALA	3.6
4	H	33	VAL	3.6
1	B	506	ALA	3.6
3	G	149	LEU	3.6
3	G	133	ARG	3.6
4	H	65	VAL	3.5
2	D	248	GLY	3.5
2	E	369	ASP	3.5
3	G	134	ARG	3.5
2	E	453	PRO	3.5
1	B	507	GLY	3.5
2	E	365	SER	3.5
1	B	414	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	457	GLU	3.5
1	B	455	LYS	3.4
2	E	394	ASP	3.4
2	E	130	GLN	3.4
2	E	361	ASN	3.4
3	G	102	GLU	3.4
5	I	44	ILE	3.4
2	E	122	GLU	3.4
3	G	104	LYS	3.4
3	G	197	ASP	3.4
2	D	475	GLU	3.4
4	H	24	THR	3.3
2	E	427	HIS	3.3
2	E	363	VAL	3.3
4	H	62	LEU	3.3
3	G	80	ALA	3.3
3	G	179	PHE	3.3
2	F	249	GLN	3.3
2	E	27	GLU	3.3
2	F	398	GLU	3.3
1	B	416	GLN	3.2
2	E	124	VAL	3.2
2	E	457	PHE	3.2
2	E	396	LEU	3.2
2	E	367	HIS	3.2
2	E	379	GLN	3.2
2	E	175	LYS	3.2
3	G	114	SER	3.2
3	G	11	LYS	3.2
1	A	193	THR	3.2
2	E	449	TYR	3.2
4	H	103	LEU	3.2
2	E	391	LEU	3.1
3	G	53	GLU	3.1
1	B	485	THR	3.1
4	H	87	ASP	3.1
2	E	376	LYS	3.1
2	D	249	GLN	3.1
2	F	177	HIS	3.1
2	E	399	GLU	3.1
2	E	342	LEU	3.1
3	G	39	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	411	ASP	3.1
3	G	150	ASN	3.0
1	B	509	GLU	3.0
4	H	26	VAL	3.0
2	D	111	LYS	3.0
2	F	27	GLU	3.0
2	D	246	GLN	3.0
5	I	5	ARG	3.0
1	A	510	ALA	3.0
2	E	398	GLU	3.0
3	G	192	ILE	3.0
4	H	30	SER	3.0
3	G	88	GLN	3.0
3	G	172	LYS	3.0
2	D	386	ASP	2.9
4	H	31	ALA	2.9
5	I	2	ALA	2.9
2	E	387	ILE	2.9
5	I	42	ILE	2.9
2	E	428	LEU	2.9
1	B	392	LEU	2.9
4	H	77	VAL	2.9
3	G	33	ARG	2.9
3	G	178	ILE	2.9
3	G	237	LYS	2.8
3	G	56	ASP	2.8
4	H	48	LEU	2.8
2	E	437	THR	2.8
3	G	195	ASP	2.8
2	E	113	PHE	2.8
1	C	21	THR	2.8
5	I	40	SER	2.7
2	D	178	GLY	2.7
2	E	447	GLY	2.7
2	E	355	SER	2.7
3	G	93	ALA	2.7
5	I	43	LYS	2.7
2	F	388	ILE	2.7
2	E	439	LYS	2.7
1	C	194	ASP	2.7
2	E	111	LYS	2.7
3	G	105	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
3	G	27	ALA	2.7
2	E	397	SER	2.7
3	G	67	LEU	2.6
2	F	395	GLU	2.6
2	E	300	LYS	2.6
3	G	166	ARG	2.6
2	E	354	THR	2.6
1	A	403	PHE	2.6
2	E	463	ILE	2.6
2	E	455	GLN	2.6
3	G	187	ALA	2.6
1	B	124	LYS	2.5
2	E	425	THR	2.5
4	H	16	MET	2.5
2	E	370	VAL	2.5
5	I	12	ILE	2.5
1	B	419	SER	2.5
1	B	412	ALA	2.5
4	H	67	ALA	2.5
4	H	58	LEU	2.5
2	F	111	LYS	2.5
2	F	386	ASP	2.5
3	G	81	ILE	2.5
1	B	456	LEU	2.5
2	E	372	ARG	2.5
2	E	384	LEU	2.5
4	H	64	VAL	2.5
4	H	27	PHE	2.5
3	G	184	ILE	2.5
2	E	358	MET	2.4
3	G	95	ASN	2.4
1	C	19	ALA	2.4
2	D	42	GLU	2.4
2	E	359	ASP	2.4
2	E	433	PRO	2.4
2	D	9	THR	2.4
2	E	381	TYR	2.4
1	A	487	GLY	2.4
1	A	124	LYS	2.4
4	H	59	ARG	2.4
2	F	9	THR	2.4
4	H	99	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	472	LYS	2.4
4	H	102	MET	2.3
4	H	98	VAL	2.3
1	B	500	ILE	2.3
1	B	399	GLU	2.3
1	B	491	GLU	2.3
2	F	473	LEU	2.3
3	G	96	LEU	2.3
4	H	29	ASN	2.3
3	G	131	VAL	2.3
2	F	396	LEU	2.3
2	E	442	GLN	2.2
3	G	5	ASP	2.2
3	G	112	ILE	2.2
3	G	234	ASN	2.2
1	B	122	GLY	2.2
2	F	12	ARG	2.2
4	H	25	GLN	2.2
4	H	45	PHE	2.2
2	E	423	VAL	2.2
2	E	42	GLU	2.2
3	G	200	VAL	2.2
2	D	474	ALA	2.2
2	E	407	ALA	2.2
2	F	176	ALA	2.2
1	C	122	GLY	2.2
1	B	508	PHE	2.2
4	H	44	ALA	2.1
2	E	132	ILE	2.1
2	E	386	ASP	2.1
3	G	91	SER	2.1
3	G	32	ALA	2.1
2	E	432	VAL	2.1
2	D	177	HIS	2.1
2	D	472	LYS	2.1
3	G	167	SER	2.0
3	G	223	SER	2.0
1	A	457	GLU	2.0
2	F	202	GLU	2.0
2	E	462	PRO	2.0
2	F	28	GLY	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(Å ²)	Q<0.9
9	ALF	D	620	5/5	0.94	0.17	6.43	37,37,40,41	0
8	GOL	B	700	6/6	0.64	0.25	6.13	67,71,72,73	0
10	SO4	E	630	5/5	0.97	0.13	1.76	36,40,41,44	0
9	ALF	F	620	5/5	0.98	0.10	0.63	33,33,34,35	0
7	MG	D	601	1/1	0.98	0.09	0.23	30,30,30,30	0
8	GOL	A	602	6/6	0.92	0.10	-0.03	42,42,44,46	0
6	ADP	B	600	27/27	0.97	0.09	-0.41	30,39,42,45	0
8	GOL	C	602	6/6	0.96	0.07	-0.64	33,34,36,37	0
6	ADP	E	600	27/27	0.96	0.09	-0.68	35,42,46,47	0
6	ADP	D	600	27/27	0.99	0.07	-0.87	24,27,30,31	0
6	ADP	F	600	27/27	0.99	0.07	-0.88	24,30,34,36	0
6	ADP	C	600	27/27	0.98	0.07	-0.88	25,29,31,33	0
8	GOL	B	602	6/6	0.98	0.06	-1.28	31,35,36,39	0
6	ADP	A	600	27/27	0.99	0.07	-1.34	25,34,37,44	0
7	MG	F	601	1/1	0.96	0.07	-2.76	28,28,28,28	0
7	MG	E	601	1/1	0.98	0.05	-3.09	42,42,42,42	0
7	MG	A	601	1/1	0.99	0.04	-	33,33,33,33	0
7	MG	C	601	1/1	0.97	0.07	-	30,30,30,30	0
7	MG	B	601	1/1	0.98	0.03	-	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.