Full wwPDB X-ray Structure Validation Report (i)

Aug 17, 2016 – 02:29 PM EDT

PDB ID	:	5FL7
Title	:	Structure of the F1c10 complex from Yarrowia lipolytica ATP synthase
Authors	:	Parey, K.; Bublitz, M.; Meier, T.
Deposited on	:	2015-10-22
Resolution	:	3.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

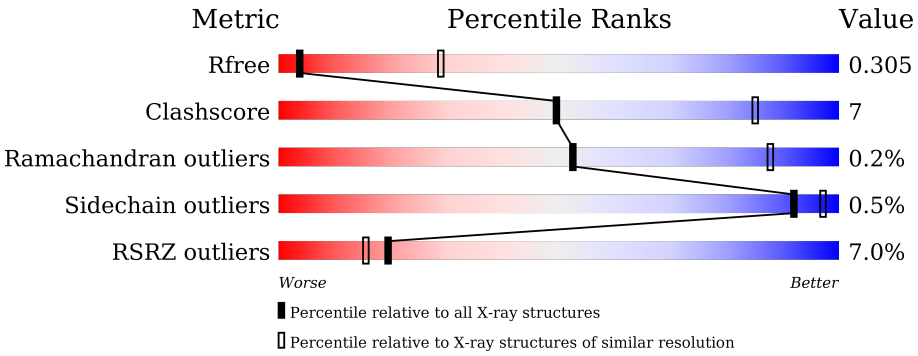
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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 <=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	536	3% 73% 17% 10%
1	B	536	6% 73% 16% 11%
1	C	536	5% 76% 14% 10%
2	D	509	5% 76% 16% 8%
2	E	509	8% 74% 18% 8%
2	F	509	3% 78% 15% 8%

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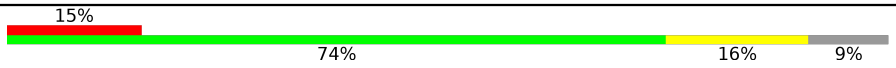
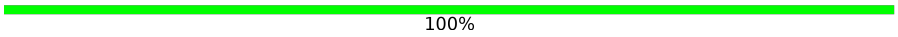
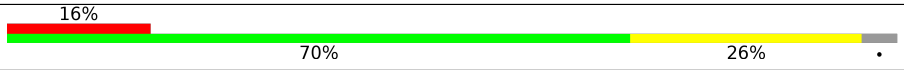
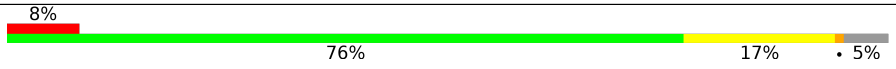
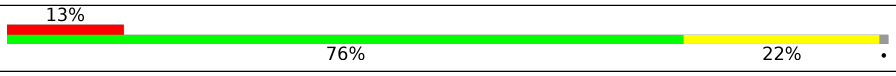
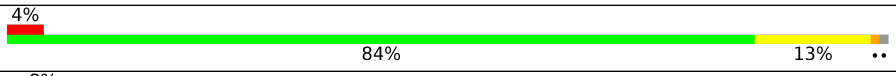
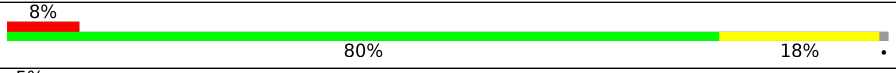
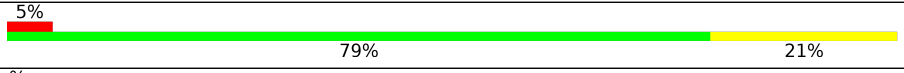
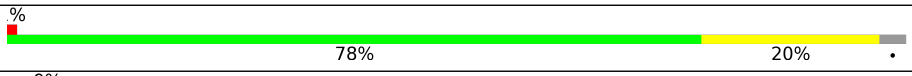
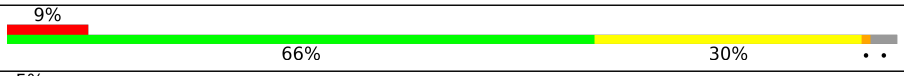
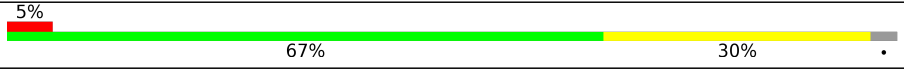
Mol	Chain	Length	Quality of chain
3	G	293	
4	H	137	
5	I	16	
6	K	76	
6	L	76	
6	M	76	
6	N	76	
6	O	76	
6	P	76	
6	Q	76	
6	R	76	
6	S	76	
6	T	76	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 30119 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP SYNTHASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3699	2341	645	704	9			
1	B	479	Total	C	N	O	S	0	0	0
			3653	2310	638	696	9			
1	C	485	Total	C	N	O	S	0	0	0
			3699	2341	645	704	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	470	Total	C	N	O	S	0	0	0
			3535	2226	605	696	8			
2	E	468	Total	C	N	O	S	0	0	0
			3524	2219	603	694	8			
2	F	470	Total	C	N	O	S	0	0	0
			3535	2226	605	696	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	267	Total	C	N	O	S	0	0	0
			2068	1291	357	411	9			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	113	Total	C	N	O	0	0	0
			843	525	135	183			

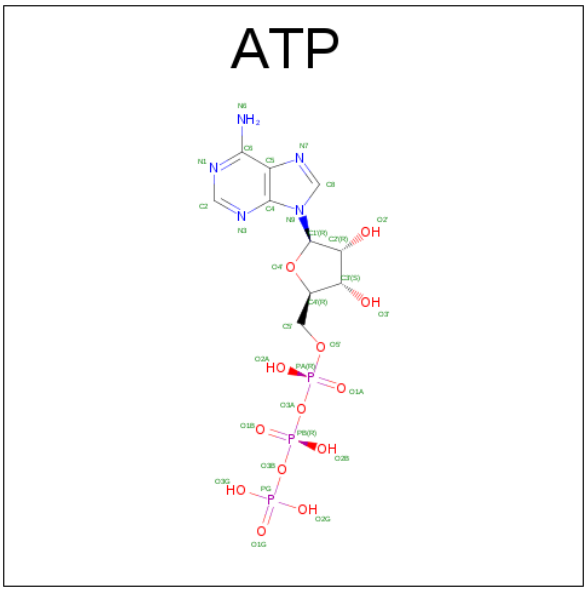
- Molecule 5 is a protein called ATP SYNTHASE EPSILON CHAIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	16	Total	C	N	O	0	0	0
			80	48	16	16			

- Molecule 6 is a protein called ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	K	73	Total	C	N	O	S	0	0	0
			524	353	82	88	1			
6	L	72	Total	C	N	O	S	0	0	0
			512	344	81	86	1			
6	M	75	Total	C	N	O	S	0	0	0
			536	361	84	90	1			
6	N	75	Total	C	N	O	S	0	0	0
			537	361	84	90	2			
6	O	75	Total	C	N	O	S	0	0	0
			537	361	84	91	1			
6	P	75	Total	C	N	O	S	0	0	0
			537	361	84	90	2			
6	Q	76	Total	C	N	O	S	0	0	0
			544	366	85	91	2			
6	R	74	Total	C	N	O	S	0	0	0
			529	356	83	89	1			
6	S	74	Total	C	N	O	S	0	0	0
			529	356	83	89	1			
6	T	74	Total	C	N	O	S	0	0	0
			529	356	83	89	1			

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

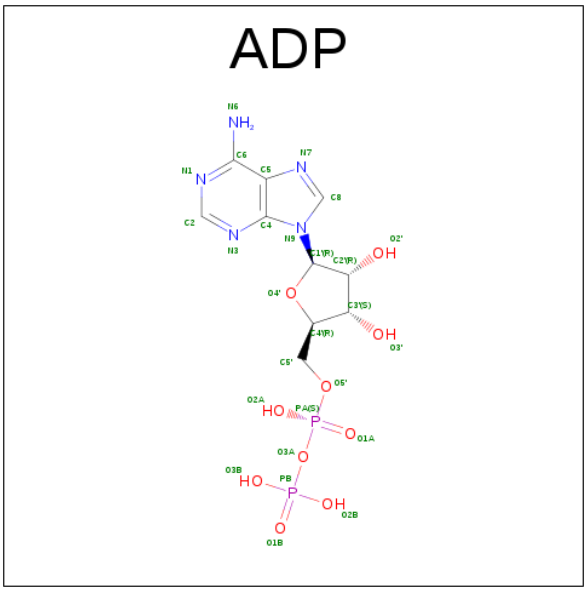


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 10 is water.

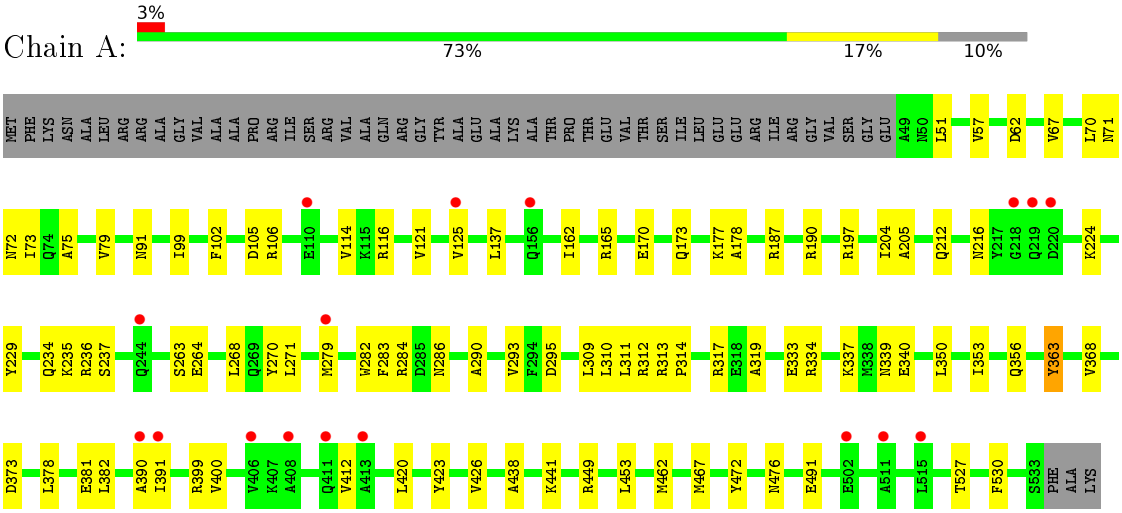
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	3	Total	O	0	0
			3	3		
10	B	3	Total	O	0	0
			3	3		
10	C	3	Total	O	0	0
			3	3		
10	D	4	Total	O	0	0
			4	4		
10	F	4	Total	O	0	0
			4	4		

3 Residue-property plots (i)

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

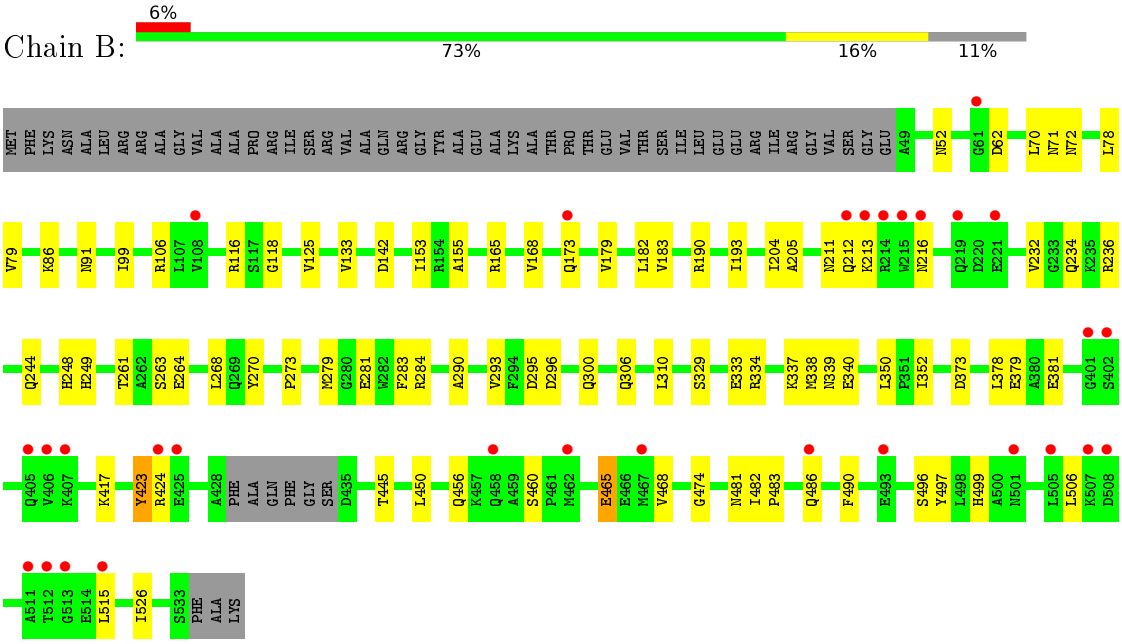
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA

Chain A:



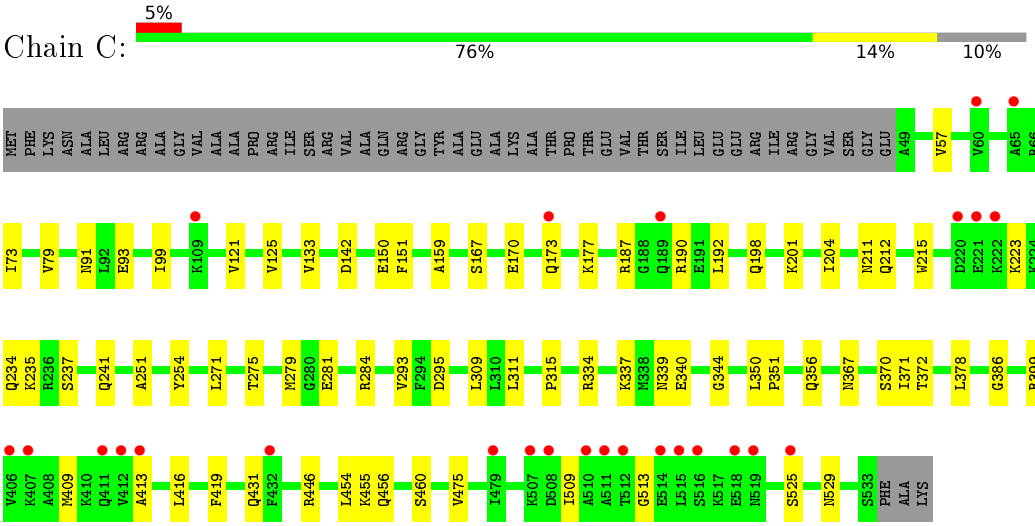
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA

Chain B:



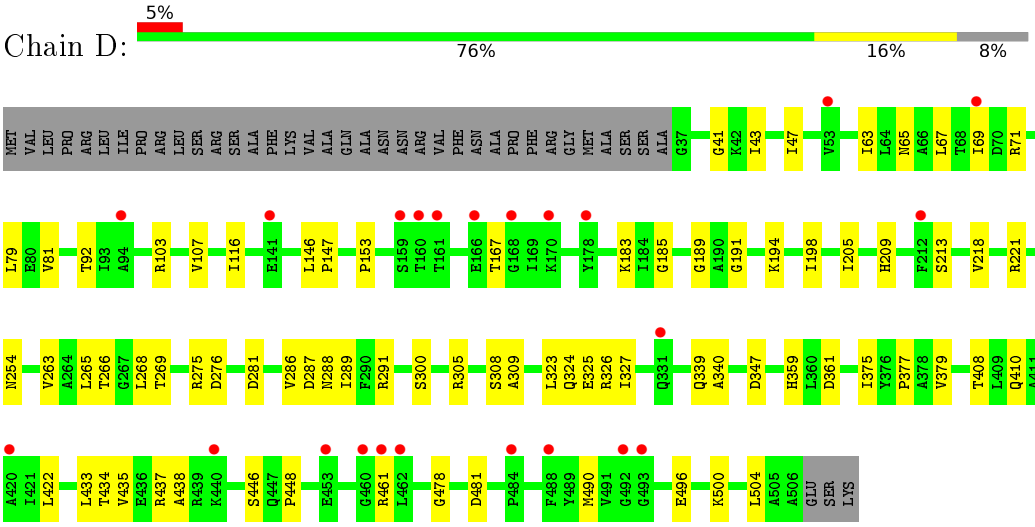
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA

Chain C:



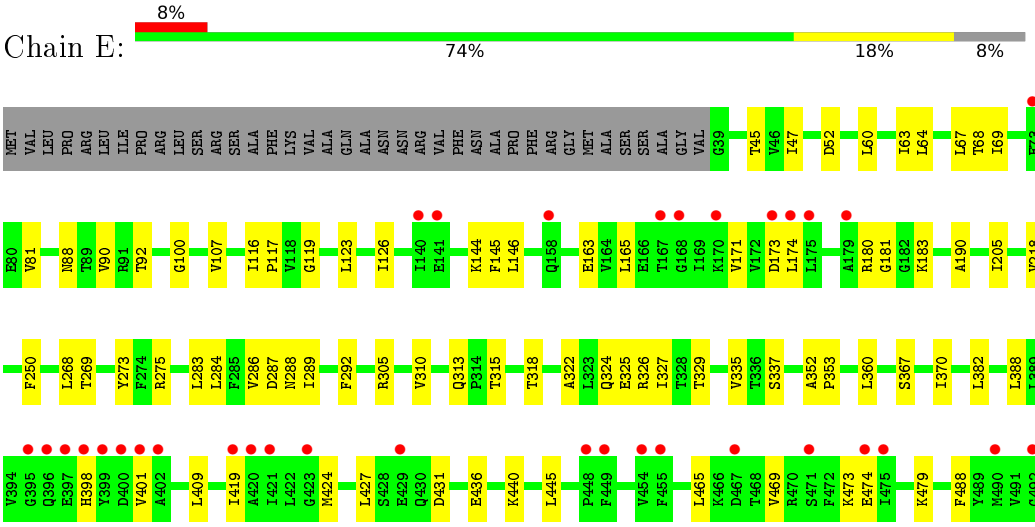
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

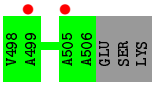
Chain D:



• Molecule 2: ATP SYNTHASE SUBUNIT BETA

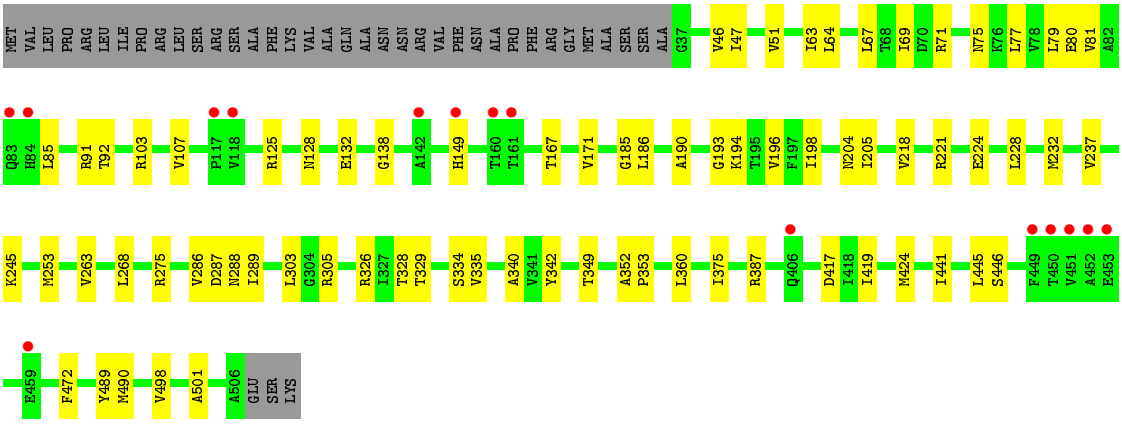
Chain E:





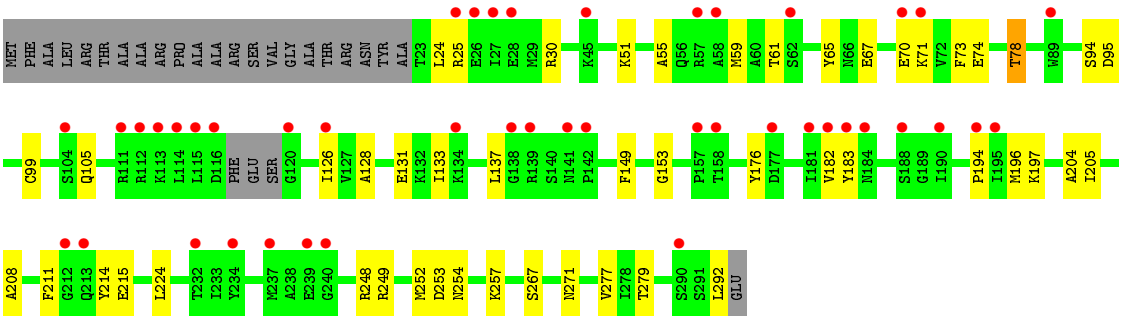
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

Chain F:



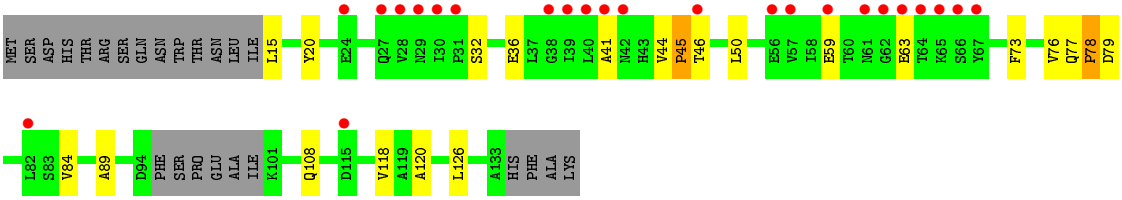
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA CHAIN, MITOCHONDRIAL

Chain G:



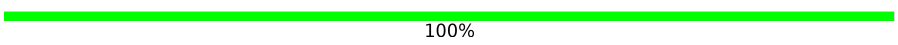
• Molecule 4: ATP SYNTHASE DELTA CHAIN, MITOCHONDRIAL

Chain H:



• Molecule 5: ATP SYNTHASE EPSILON CHAIN, MITOCHONDRIAL

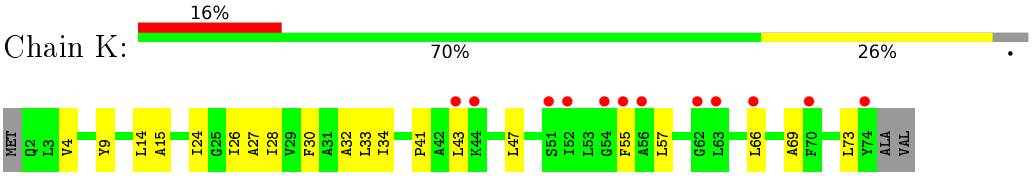
Chain I:



There are no outlier residues recorded for this chain.

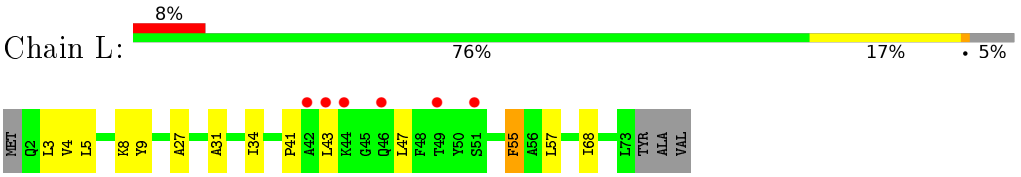
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain K:



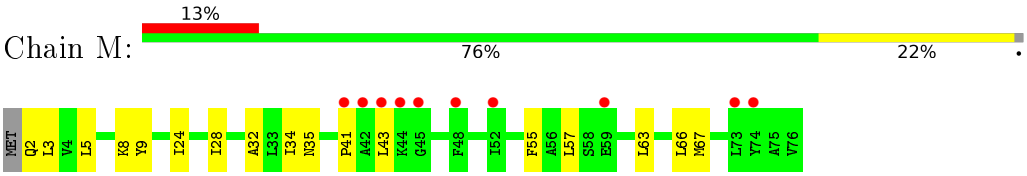
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain L:



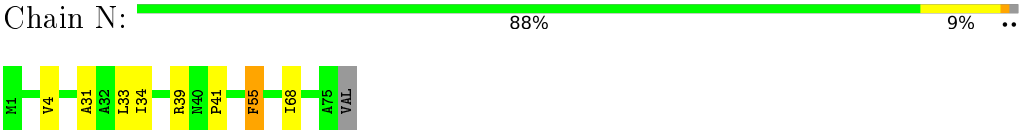
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain M:



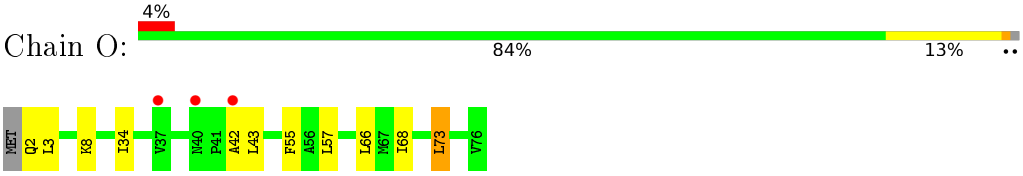
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain N:



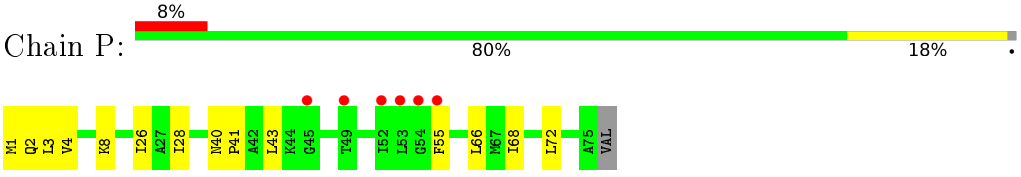
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain O:



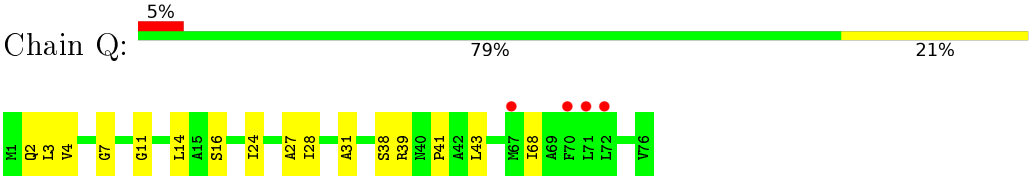
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain P:



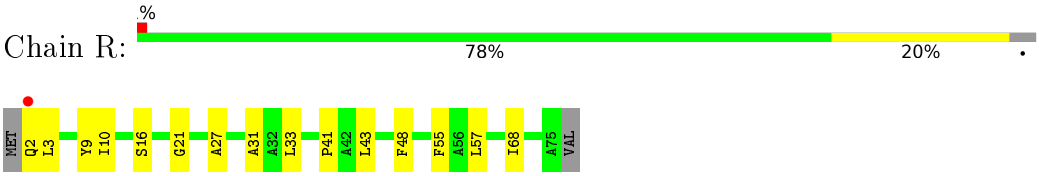
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain Q:



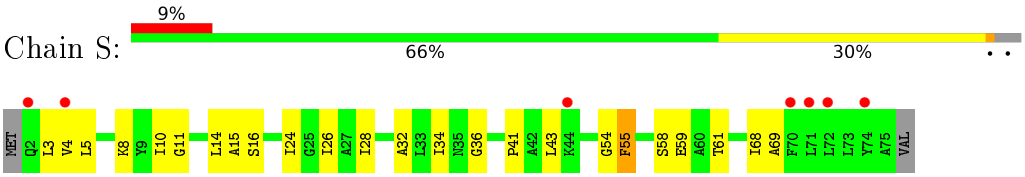
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain R:



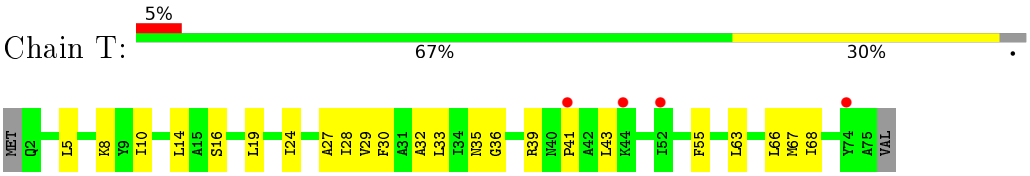
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain S:



• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	169.50Å 182.20Å 193.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 3.50 49.37 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.37-3.50) 100.0 (49.37-3.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.274 , 0.305 0.273 , 0.305	Depositor DCC
R_{free} test set	1894 reflections (2.50%)	DCC
Wilson B-factor (Å^2)	157.5	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 94.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	30119	wwPDB-VP
Average B, all atoms (Å^2)	166.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	#$\|Z\|>5$
1	A	0.24	0/3755	0.41	0/5076
1	B	0.24	0/3706	0.41	0/5009
1	C	0.24	0/3755	0.40	0/5076
2	D	0.24	0/3587	0.40	0/4868
2	E	0.24	0/3576	0.41	0/4853
2	F	0.24	0/3587	0.40	0/4868
3	G	0.23	0/2090	0.38	0/2812
4	H	0.24	0/851	0.43	0/1157
6	K	0.24	0/532	0.36	0/720
6	L	0.24	0/519	0.35	0/702
6	M	0.24	0/544	0.36	0/737
6	N	0.24	0/545	0.35	0/737
6	O	0.25	0/545	0.38	0/737
6	P	0.24	0/545	0.33	0/737
6	Q	0.25	0/552	0.38	0/747
6	R	0.24	0/537	0.35	0/727
6	S	0.25	0/537	0.33	0/727
6	T	0.25	0/537	0.38	0/727
All	All	0.24	0/30300	0.40	0/41017

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3699	0	3781	59	0
1	B	3653	0	3741	52	0
1	C	3699	0	3781	49	0
2	D	3535	0	3562	60	0
2	E	3524	0	3551	58	0
2	F	3535	0	3562	49	0
3	G	2068	0	2099	31	0
4	H	843	0	824	18	0
5	I	80	0	18	0	0
6	K	524	0	565	20	0
6	L	512	0	556	15	0
6	M	536	0	579	15	0
6	N	537	0	582	8	0
6	O	537	0	579	10	0
6	P	537	0	582	15	0
6	Q	544	0	591	15	0
6	R	529	0	570	15	0
6	S	529	0	570	22	0
6	T	529	0	570	22	0
7	A	31	0	12	0	0
7	B	31	0	12	0	0
7	C	31	0	12	2	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
9	D	27	0	12	3	0
9	F	27	0	12	3	0
10	A	3	0	0	0	0
10	B	3	0	0	0	0
10	C	3	0	0	0	0
10	D	4	0	0	0	0
10	F	4	0	0	2	0
All	All	30119	0	30723	432	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 7.

All (432) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:SER:HB2	2:F:253:MET:HB3	1.66	0.77
3:G:208:ALA:HB3	3:G:211:PHE:HB2	1.71	0.73
2:D:189:GLY:O	2:D:194:LYS:NZ	2.22	0.73
1:C:370:SER:HB3	2:D:291:ARG:HH22	1.57	0.70
1:B:450:LEU:HD21	1:B:474:GLY:HA3	1.73	0.70
1:C:309:LEU:HD21	1:C:315:PRO:HB3	1.76	0.67
1:A:236:ARG:NH1	2:D:153:PRO:O	2.28	0.66
2:F:198:ILE:HD11	2:F:340:ALA:HB2	1.76	0.66
6:L:3:LEU:HD21	6:M:3:LEU:HD13	1.77	0.66
6:R:68:ILE:HD12	6:S:16:SER:HB3	1.77	0.66
2:D:183:LYS:HZ1	2:D:324:GLN:HB3	1.61	0.66
2:D:375:ILE:HG23	2:D:446:SER:HB2	1.78	0.65
1:A:177:LYS:NZ	1:A:491:GLU:OE2	2.30	0.65
6:P:4:VAL:HG23	6:Q:2:GLN:HG3	1.79	0.65
1:B:106:ARG:HA	2:E:63:ILE:HB	1.77	0.65
1:A:121:VAL:HG11	1:A:271:LEU:HD21	1.78	0.65
3:G:126:ILE:HD13	3:G:137:LEU:HD23	1.78	0.65
2:E:69:ILE:HG12	2:E:107:VAL:HG22	1.79	0.65
3:G:267:SER:O	3:G:271:ASN:ND2	2.30	0.65
6:S:26:ILE:HD11	6:S:59:GLU:HB2	1.79	0.64
6:K:47:LEU:HD22	6:L:34:ILE:HG23	1.80	0.64
1:B:62:ASP:OD1	2:E:305:ARG:NH2	2.30	0.64
3:G:128:ALA:HB1	3:G:133:ILE:HG23	1.80	0.64
6:L:47:LEU:HD13	6:M:34:ILE:HG23	1.79	0.63
1:A:106:ARG:NH1	2:D:65:ASN:OD1	2.31	0.63
2:D:500:LYS:HE2	2:D:504:LEU:HD11	1.79	0.63
2:F:417:ASP:OD2	3:G:30:ARG:NH2	2.31	0.63
1:C:235:LYS:NZ	1:C:237:SER:OG	2.29	0.62
2:D:198:ILE:HD11	2:D:340:ALA:HB2	1.81	0.62
1:B:70:LEU:O	2:F:103:ARG:NH2	2.33	0.62
1:A:235:LYS:HE3	1:A:237:SER:HB3	1.81	0.62
2:D:347:ASP:HB2	3:G:25:ARG:HH12	1.64	0.62
1:B:456:GLN:NE2	1:B:460:SER:O	2.33	0.62
6:S:26:ILE:HG23	6:S:55:PHE:HB2	1.81	0.62
6:M:43:LEU:HD11	6:N:41:PRO:HB3	1.81	0.61
2:E:67:LEU:HB2	2:E:79:LEU:HB2	1.83	0.61
1:A:197:ARG:NH1	1:A:356:GLN:OE1	2.34	0.61
2:D:408:THR:HG23	2:D:434:THR:HG23	1.81	0.61
2:D:461:ARG:NH1	2:D:496:GLU:OE2	2.34	0.61
2:F:71:ARG:HH21	2:F:77:LEU:HD22	1.65	0.61
1:A:62:ASP:OD1	2:D:305:ARG:NH2	2.33	0.60
1:C:212:GLN:HG3	1:C:225:LEU:HD22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:275:ARG:HD3	2:E:335:VAL:HG23	1.83	0.60
6:R:43:LEU:HD11	6:S:41:PRO:HG3	1.82	0.60
6:P:43:LEU:HD11	6:Q:41:PRO:HG3	1.82	0.60
6:Q:43:LEU:HD11	6:R:41:PRO:HG3	1.82	0.60
6:R:33:LEU:HA	6:S:34:ILE:HG21	1.83	0.60
1:A:235:LYS:NZ	2:D:361:ASP:OD1	2.35	0.59
6:S:68:ILE:HD11	6:T:66:LEU:HD12	1.85	0.59
1:C:121:VAL:HG11	1:C:271:LEU:HD21	1.84	0.59
2:E:419:ILE:HD12	2:E:424:MET:HG2	1.84	0.59
6:K:41:PRO:HG3	6:T:43:LEU:HD11	1.85	0.58
2:D:41:GLY:O	2:D:107:VAL:N	2.35	0.58
1:C:234:GLN:NE2	1:C:295:ASP:OD2	2.37	0.58
1:B:212:GLN:O	1:B:216:ASN:ND2	2.36	0.58
1:C:125:VAL:HG12	1:C:279:MET:HA	1.86	0.58
2:F:194:LYS:HB2	10:F:2001:HOH:O	2.04	0.58
1:A:70:LEU:HD13	1:A:73:ILE:HD12	1.86	0.57
2:D:268:LEU:HD13	2:D:327:ILE:HG12	1.86	0.57
1:C:339:ASN:OD1	1:C:340:GLU:N	2.37	0.57
6:M:28:ILE:HG22	6:N:31:ALA:HB2	1.87	0.57
2:F:125:ARG:NH2	2:F:138:GLY:O	2.37	0.57
1:A:234:GLN:NE2	1:A:295:ASP:OD2	2.38	0.57
1:A:173:GLN:O	1:A:212:GLN:NE2	2.37	0.56
2:D:418:ILE:HG23	2:D:422:LEU:HD12	1.86	0.56
2:E:388:LEU:HD22	2:E:393:VAL:HG11	1.85	0.56
6:K:28:ILE:HB	6:L:27:ALA:HB1	1.86	0.56
2:F:167:THR:O	2:F:204:ASN:ND2	2.39	0.56
6:K:30:PHE:CZ	6:T:29:VAL:HG22	2.40	0.56
1:C:57:VAL:HG22	1:C:67:VAL:HG22	1.88	0.56
1:B:284:ARG:NH1	1:B:338:MET:SD	2.79	0.56
1:C:177:LYS:HD2	1:C:454:LEU:HA	1.88	0.56
1:A:282:TRP:O	1:A:286:ASN:ND2	2.35	0.56
1:C:192:LEU:HB2	1:C:372:THR:HG21	1.88	0.56
6:L:5:LEU:HA	6:L:8:LYS:HD3	1.88	0.56
1:A:263:SER:HB3	2:D:325:GLU:HG3	1.88	0.56
2:D:69:ILE:HG12	2:D:107:VAL:HG22	1.88	0.56
2:F:275:ARG:NH1	2:F:328:THR:O	2.39	0.56
1:A:178:ALA:HB3	1:A:391:ILE:HD12	1.87	0.55
1:B:236:ARG:HG2	1:B:261:THR:HG21	1.88	0.55
2:D:433:LEU:HD21	2:D:437:ARG:HH21	1.71	0.55
2:E:205:ILE:HG13	2:E:283:LEU:HD11	1.89	0.55
3:G:95:ASP:HB3	3:G:131:GLU:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:24:LEU:HD22	3:G:277:VAL:HG21	1.89	0.55
1:B:339:ASN:OD1	1:B:340:GLU:N	2.39	0.55
6:O:43:LEU:HD21	6:P:41:PRO:HB3	1.88	0.55
6:K:43:LEU:HD11	6:L:41:PRO:HG3	1.87	0.55
2:E:401:VAL:HG11	2:E:469:VAL:HG13	1.88	0.54
1:B:293:VAL:HG22	1:B:350:LEU:HB2	1.89	0.54
1:B:78:LEU:HD11	1:B:86:LYS:HB3	1.88	0.54
1:B:62:ASP:HB3	1:B:310:LEU:HD22	1.88	0.54
3:G:249:ARG:O	3:G:253:ASP:N	2.36	0.54
1:A:339:ASN:OD1	1:A:340:GLU:N	2.40	0.54
1:C:133:VAL:HB	1:C:142:ASP:HB3	1.89	0.54
4:H:36:GLU:OE1	6:P:40:ASN:ND2	2.35	0.54
2:D:167:THR:HA	2:D:205:ILE:HD11	1.90	0.54
2:F:80:GLU:OE2	2:F:149:HIS:NE2	2.40	0.54
1:B:179:VAL:HG13	1:B:183:VAL:HG23	1.90	0.54
2:E:63:ILE:HG22	2:E:64:LEU:HG	1.90	0.54
4:H:44:VAL:O	4:H:46:THR:N	2.39	0.54
1:A:399:ARG:HH12	2:E:190:ALA:HB3	1.73	0.54
2:D:183:LYS:HZ1	2:D:359:HIS:HB3	1.73	0.54
1:A:62:ASP:HB3	1:A:310:LEU:HD13	1.90	0.53
1:B:486:GLN:O	1:B:490:PHE:N	2.41	0.53
6:S:68:ILE:HD12	6:T:16:SER:HB3	1.89	0.53
1:A:309:LEU:HD11	1:A:319:ALA:HB1	1.90	0.53
2:E:81:VAL:HA	2:E:92:THR:HG22	1.90	0.53
2:F:193:GLY:HA2	9:F:600:ADP:O1A	2.08	0.53
6:K:66:LEU:HD12	6:T:68:ILE:HD11	1.89	0.53
1:A:293:VAL:HG22	1:A:350:LEU:HB2	1.89	0.53
2:F:194:LYS:N	9:F:600:ADP:O1B	2.40	0.53
4:H:77:GLN:O	4:H:79:ASP:N	2.35	0.53
1:A:91:ASN:HB2	2:E:47:ILE:HG12	1.90	0.53
1:C:159:ALA:HB3	2:D:254:ASN:HD22	1.72	0.53
1:C:93:GLU:O	2:D:103:ARG:NH1	2.40	0.53
1:A:170:GLU:OE2	1:A:337:LYS:NZ	2.42	0.53
1:A:412:VAL:HG12	1:A:472:TYR:HD1	1.74	0.53
1:C:284:ARG:NH1	1:C:334:ARG:O	2.41	0.53
1:A:527:THR:HA	1:A:530:PHE:CE2	2.44	0.53
2:D:448:PRO:HD3	2:D:490:MET:HA	1.91	0.53
2:F:375:ILE:HG23	2:F:446:SER:HB2	1.89	0.53
1:B:244:GLN:O	1:B:248:HIS:N	2.42	0.53
1:B:204:ILE:HD12	1:B:378:LEU:HD11	1.90	0.52
3:G:70:GLU:O	3:G:74:GLU:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:3:LEU:HB3	6:P:2:GLN:HG2	1.90	0.52
2:F:171:VAL:HG12	2:F:445:LEU:HD22	1.92	0.52
6:L:43:LEU:HD11	6:M:41:PRO:HG3	1.91	0.52
1:C:456:GLN:NE2	1:C:460:SER:O	2.31	0.52
2:F:85:LEU:HD21	2:F:91:ARG:HE	1.75	0.52
2:D:300:SER:HB2	2:D:305:ARG:HD2	1.90	0.52
2:E:60:LEU:HD21	2:E:88:ASN:HA	1.91	0.52
6:S:61:THR:HB	6:T:19:LEU:HD21	1.91	0.52
6:S:43:LEU:HD11	6:T:41:PRO:HG3	1.90	0.52
1:B:445:THR:HG23	1:B:481:ASN:HB2	1.91	0.52
1:C:509:ILE:HG23	1:C:513:GLY:HA2	1.91	0.52
6:N:4:VAL:HG23	6:O:2:GLN:HG3	1.91	0.52
2:F:128:ASN:HD21	2:F:132:GLU:HB3	1.74	0.52
6:S:11:GLY:HA2	6:S:14:LEU:HB2	1.91	0.52
1:B:496:SER:O	1:B:499:HIS:ND1	2.36	0.51
1:C:204:ILE:HD12	1:C:378:LEU:HD11	1.91	0.51
4:H:108:GLN:HA	4:H:126:LEU:HD21	1.90	0.51
3:G:214:TYR:HA	4:H:45:PRO:HB2	1.92	0.51
6:S:14:LEU:HD13	6:T:14:LEU:HG	1.91	0.51
6:Q:4:VAL:HG13	6:R:9:TYR:HE2	1.76	0.51
1:B:205:ALA:HB1	1:B:293:VAL:HG11	1.91	0.51
6:R:21:GLY:HA2	6:S:24:ILE:HG13	1.91	0.51
2:E:174:LEU:HA	2:E:398:HIS:HE1	1.74	0.51
2:F:489:TYR:CD1	2:F:490:MET:HG2	2.46	0.51
3:G:182:VAL:HG22	3:G:196:MET:HG2	1.92	0.51
1:A:312:ARG:HH12	3:G:292:LEU:HD12	1.76	0.51
4:H:59:GLU:HB2	4:H:63:GLU:HB2	1.91	0.51
6:K:14:LEU:HD21	6:T:14:LEU:HD13	1.92	0.51
3:G:99:CYS:HA	3:G:248:ARG:HA	1.92	0.51
1:A:79:VAL:HG21	1:A:99:ILE:HD13	1.93	0.51
1:C:79:VAL:HG21	1:C:99:ILE:HD13	1.92	0.51
3:G:105:GLN:HE21	3:G:194:PRO:HG3	1.75	0.51
1:A:284:ARG:NH1	1:A:334:ARG:O	2.44	0.51
3:G:55:ALA:O	3:G:59:MET:N	2.44	0.51
4:H:45:PRO:HA	4:H:76:VAL:HB	1.92	0.51
2:E:268:LEU:HD21	2:E:326:ARG:HB2	1.93	0.50
1:C:173:GLN:O	1:C:211:ASN:ND2	2.44	0.50
1:A:105:ASP:HB3	2:D:63:ILE:HD12	1.94	0.50
2:E:367:SER:HB3	2:E:370:ILE:HG12	1.94	0.50
6:K:9:TYR:CD2	6:T:8:LYS:HG2	2.47	0.50
1:C:281:GLU:OE2	1:C:284:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:268:LEU:HD21	2:F:326:ARG:HB2	1.93	0.50
4:H:41:ALA:HB3	6:O:42:ALA:HB2	1.94	0.50
1:A:381:GLU:OE2	2:D:410:GLN:NE2	2.44	0.50
1:A:472:TYR:O	1:A:476:ASN:ND2	2.37	0.50
1:C:215:TRP:CD1	1:C:223:LYS:HB3	2.47	0.50
2:D:286:VAL:HG11	2:D:289:ILE:HD13	1.94	0.50
1:A:317:ARG:HH11	1:A:363:TYR:HB2	1.77	0.50
1:C:241:GLN:HE22	2:F:387:ARG:HE	1.60	0.50
1:B:190:ARG:O	1:B:373:ASP:N	2.45	0.50
1:B:263:SER:HB3	2:E:325:GLU:HG3	1.94	0.50
3:G:254:ASN:HA	3:G:257:LYS:HG2	1.93	0.50
1:A:204:ILE:HD12	1:A:378:LEU:HD11	1.92	0.49
1:A:67:VAL:HG21	1:A:114:VAL:HG21	1.94	0.49
1:B:283:PHE:HB2	1:B:290:ALA:HB2	1.94	0.49
6:K:30:PHE:HA	6:K:33:LEU:HB3	1.94	0.49
1:B:72:ASN:O	1:B:116:ARG:NH1	2.45	0.49
1:C:201:LYS:N	7:C:600:ATP:O1B	2.39	0.49
4:H:20:TYR:OH	4:H:84:VAL:O	2.24	0.49
6:T:32:ALA:O	6:T:36:GLY:N	2.46	0.49
1:A:283:PHE:HB2	1:A:290:ALA:HB2	1.94	0.49
2:E:67:LEU:HD12	2:E:92:THR:HG21	1.94	0.49
6:K:73:LEU:HD11	6:T:68:ILE:HG23	1.93	0.49
6:Q:28:ILE:HG22	6:R:31:ALA:HB2	1.95	0.49
1:C:150:GLU:HG2	1:C:151:PHE:CD2	2.47	0.49
2:D:412:TYR:HE1	2:D:435:VAL:HG13	1.77	0.49
2:D:194:LYS:NZ	9:D:600:ADP:O2B	2.33	0.49
1:A:75:ALA:HB3	2:E:100:GLY:H	1.78	0.49
1:C:198:GLN:HA	7:C:600:ATP:O3B	2.12	0.49
2:F:190:ALA:HB2	2:F:342:TYR:HE1	1.78	0.49
1:B:165:ARG:NH2	1:B:333:GLU:O	2.45	0.49
2:F:69:ILE:HG12	2:F:107:VAL:HG22	1.93	0.49
2:D:67:LEU:HB2	2:D:79:LEU:HB2	1.94	0.49
2:E:163:GLU:OE2	2:E:180:ARG:NH1	2.46	0.49
2:F:352:ALA:HB3	2:F:353:PRO:HD3	1.95	0.49
6:K:32:ALA:HB1	6:L:34:ILE:HB	1.94	0.49
2:D:116:ILE:HG21	2:D:266:THR:HG23	1.94	0.49
1:A:57:VAL:HG22	1:A:67:VAL:HG22	1.95	0.49
2:E:45:THR:HB	2:E:52:ASP:HB2	1.95	0.49
2:F:67:LEU:HB2	2:F:79:LEU:HB2	1.94	0.49
3:G:67:GLU:HB2	3:G:71:LYS:HB2	1.94	0.49
6:T:30:PHE:HA	6:T:33:LEU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ALA:HA	1:A:441:LYS:HE2	1.95	0.48
2:F:81:VAL:HA	2:F:92:THR:HG22	1.95	0.48
6:L:4:VAL:HG13	6:M:9:TYR:HE2	1.77	0.48
1:C:251:ALA:HA	1:C:254:TYR:CE2	2.48	0.48
6:S:5:LEU:HA	6:S:8:LYS:HD3	1.95	0.48
1:C:446:ARG:NH2	1:C:475:VAL:O	2.47	0.48
6:R:3:LEU:HD21	6:S:3:LEU:HD13	1.96	0.48
1:A:423:TYR:HA	1:A:426:VAL:HG12	1.96	0.48
2:E:352:ALA:HB3	2:E:353:PRO:HD3	1.95	0.48
3:G:70:GLU:HA	3:G:73:PHE:HB3	1.95	0.48
6:K:26:ILE:HG23	6:K:55:PHE:HB2	1.96	0.48
6:L:68:ILE:HD11	6:M:66:LEU:HD12	1.96	0.48
2:E:68:THR:HB	2:E:76:LYS:HE2	1.96	0.48
2:F:419:ILE:HG23	2:F:424:MET:HG2	1.96	0.48
6:T:63:LEU:O	6:T:67:MET:N	2.47	0.48
2:E:436:GLU:O	2:E:440:LYS:HG2	2.14	0.47
1:B:52:ASN:HA	1:B:71:ASN:HB2	1.96	0.47
2:E:171:VAL:HG22	2:E:445:LEU:HD22	1.95	0.47
6:O:3:LEU:HD21	6:P:3:LEU:HD13	1.96	0.47
1:A:420:LEU:HA	1:A:423:TYR:HB3	1.96	0.47
1:B:423:TYR:CE1	1:B:424:ARG:HG3	2.49	0.47
1:B:379:GLU:HG3	1:B:381:GLU:H	1.79	0.47
2:D:268:LEU:HD21	2:D:326:ARG:HB2	1.97	0.47
6:Q:68:ILE:HD12	6:R:16:SER:HB3	1.97	0.47
1:A:190:ARG:O	1:A:373:ASP:N	2.46	0.47
1:A:353:ILE:HD11	1:A:368:VAL:HG21	1.97	0.47
2:E:173:ASP:HB3	2:E:465:LEU:HD13	1.96	0.47
6:K:28:ILE:HG22	6:L:31:ALA:HB2	1.96	0.47
6:L:4:VAL:HG23	6:M:2:GLN:HG3	1.97	0.47
6:O:68:ILE:HD11	6:P:66:LEU:HD12	1.97	0.47
1:A:165:ARG:NH2	1:A:333:GLU:O	2.47	0.47
2:D:191:GLY:HA2	9:D:600:ADP:H5'1	1.97	0.47
1:A:125:VAL:HG12	1:A:279:MET:HA	1.97	0.46
2:D:43:ILE:HD11	2:D:69:ILE:HD13	1.97	0.46
2:E:390:ASP:OD1	2:E:391:ILE:N	2.48	0.46
2:E:81:VAL:HG13	2:E:90:VAL:HG13	1.96	0.46
6:S:4:VAL:HG22	6:T:5:LEU:HB2	1.97	0.46
1:A:382:LEU:HB2	1:A:390:ALA:HB1	1.96	0.46
1:C:167:SER:OG	2:D:230:ARG:NE	2.48	0.46
2:D:116:ILE:HD11	2:D:269:THR:HB	1.97	0.46
2:F:286:VAL:HG11	2:F:289:ILE:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:441:ILE:HG23	2:F:472:PHE:HE2	1.79	0.46
2:D:433:LEU:HG	2:D:437:ARG:HE	1.81	0.46
2:F:221:ARG:NH1	2:F:224:GLU:OE2	2.47	0.46
2:F:63:ILE:HG22	2:F:64:LEU:HG	1.97	0.46
3:G:215:GLU:OE2	6:N:39:ARG:NH1	2.48	0.46
1:A:264:GLU:HB3	1:A:268:LEU:HD12	1.96	0.46
2:E:183:LYS:HB3	2:E:360:LEU:HD23	1.97	0.46
6:K:9:TYR:HD2	6:T:8:LYS:HG2	1.79	0.46
3:G:61:THR:HG23	4:H:15:LEU:O	2.16	0.46
2:D:67:LEU:HD12	2:D:92:THR:HG21	1.98	0.46
6:M:63:LEU:O	6:M:67:MET:N	2.48	0.46
1:A:449:ARG:O	1:A:453:LEU:N	2.45	0.46
1:B:79:VAL:HG21	1:B:99:ILE:HD13	1.97	0.46
6:M:32:ALA:HA	6:M:35:ASN:HB3	1.98	0.46
2:E:318:THR:O	2:E:322:ALA:N	2.44	0.46
3:G:224:LEU:HA	4:H:73:PHE:HE2	1.81	0.46
6:S:28:ILE:HB	6:T:27:ALA:HB1	1.98	0.46
6:T:35:ASN:O	6:T:39:ARG:HG2	2.17	0.46
1:C:271:LEU:HG	1:C:275:THR:HG23	1.97	0.45
1:C:293:VAL:HG22	1:C:350:LEU:HB2	1.98	0.45
1:B:482:ILE:HD12	1:B:483:PRO:HD2	1.98	0.45
2:D:287:ASP:HA	2:D:288:ASN:HA	1.56	0.45
2:E:123:LEU:HD23	2:E:247:THR:HB	1.98	0.45
2:E:287:ASP:HA	2:E:288:ASN:HA	1.55	0.45
6:Q:3:LEU:HB3	6:R:2:GLN:HB3	1.97	0.45
1:A:162:ILE:O	2:E:226:ASN:ND2	2.49	0.45
6:K:34:ILE:HG21	6:T:33:LEU:HA	1.99	0.45
1:B:468:VAL:HG11	1:B:515:LEU:HD11	1.99	0.45
1:C:192:LEU:HA	1:C:351:PRO:HD2	1.99	0.45
2:D:183:LYS:NZ	2:D:324:GLN:HB3	2.30	0.45
1:A:170:GLU:HB2	1:A:187:ARG:HB2	1.97	0.45
1:A:216:ASN:HA	1:A:224:LYS:HD3	1.98	0.45
2:E:117:PRO:HA	2:E:144:LYS:HA	1.98	0.45
2:D:185:GLY:HA2	2:D:339:GLN:O	2.16	0.45
2:D:71:ARG:NH1	2:D:77:LEU:HB2	2.31	0.45
1:B:116:ARG:HH21	1:B:118:GLY:HA2	1.81	0.45
1:C:356:GLN:HB3	2:F:349:THR:HG22	1.99	0.45
2:E:116:ILE:HD11	2:E:269:THR:HB	1.98	0.45
2:D:218:VAL:HG22	2:D:263:VAL:HG13	1.99	0.45
2:D:308:SER:OG	2:D:309:ALA:N	2.50	0.45
2:D:437:ARG:HH12	2:D:478:GLY:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:329:THR:HG23	2:F:334:SER:HA	1.99	0.45
6:K:57:LEU:HD13	6:L:55:PHE:CE1	2.52	0.45
6:S:10:ILE:HB	6:T:10:ILE:HG12	1.99	0.45
2:F:186:LEU:HB2	2:F:340:ALA:HA	1.99	0.44
6:N:33:LEU:HA	6:O:34:ILE:HG21	1.99	0.44
4:H:36:GLU:N	6:Q:39:ARG:O	2.51	0.44
1:A:70:LEU:HB3	1:A:73:ILE:HB	1.99	0.44
6:Q:7:GLY:HA2	6:R:10:ILE:HD11	1.98	0.44
1:B:173:GLN:O	1:B:211:ASN:ND2	2.50	0.44
1:A:399:ARG:NH1	2:E:190:ALA:HB3	2.32	0.44
1:B:465:GLU:HB3	1:B:506:LEU:HB3	2.00	0.44
2:E:181:GLY:HA3	2:E:329:THR:OG1	2.17	0.44
2:E:145:PHE:HD2	2:E:146:LEU:HG	1.82	0.44
6:M:5:LEU:HA	6:M:8:LYS:HD3	1.99	0.44
6:S:15:ALA:HB3	6:S:69:ALA:HB2	1.99	0.44
2:E:218:VAL:HG11	2:E:292:PHE:HB2	2.00	0.44
2:E:286:VAL:HG11	2:E:289:ILE:HD13	2.00	0.44
2:E:313:GLN:OE1	2:E:313:GLN:N	2.43	0.44
1:B:279:MET:HB3	1:B:279:MET:HE2	1.93	0.44
1:C:70:LEU:HD13	1:C:73:ILE:HD12	2.00	0.44
2:F:303:LEU:HD12	2:F:305:ARG:HH12	1.83	0.44
3:G:65:TYR:HD1	4:H:15:LEU:HD12	1.82	0.44
1:C:337:LYS:NZ	1:C:344:GLY:O	2.42	0.44
1:C:419:PHE:CE2	1:C:475:VAL:HG23	2.53	0.44
1:C:190:ARG:HH22	2:D:221:ARG:HB3	1.82	0.44
2:D:408:THR:HG22	2:D:438:ALA:HB2	2.00	0.44
6:R:27:ALA:O	6:R:31:ALA:N	2.46	0.44
2:F:218:VAL:HG22	2:F:263:VAL:HG13	1.98	0.44
1:A:72:ASN:O	1:A:116:ARG:NH1	2.50	0.43
1:B:125:VAL:HG21	1:B:153:ILE:HG13	1.98	0.43
2:D:275:ARG:NH1	2:D:276:ASP:OD1	2.51	0.43
2:E:310:VAL:H	3:G:279:THR:HG22	1.82	0.43
4:H:36:GLU:O	6:P:40:ASN:ND2	2.51	0.43
6:K:15:ALA:HB3	6:K:69:ALA:HB2	2.00	0.43
1:C:413:ALA:HA	1:C:416:LEU:HB3	2.01	0.43
2:F:221:ARG:NH1	10:F:2003:HOH:O	2.50	0.43
3:G:183:TYR:HE1	3:G:197:LYS:HB2	1.83	0.43
1:A:51:LEU:O	1:A:71:ASN:ND2	2.48	0.43
2:D:69:ILE:HD12	2:D:77:LEU:HD23	2.01	0.43
2:E:382:LEU:HD21	2:E:409:LEU:HB2	2.00	0.43
3:G:67:GLU:HB2	3:G:71:LYS:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:24:ILE:O	6:K:28:ILE:HG13	2.19	0.43
6:M:24:ILE:O	6:M:28:ILE:HG13	2.18	0.43
1:A:205:ALA:HB1	1:A:293:VAL:HG11	1.99	0.43
1:B:232:VAL:HG11	1:B:300:GLN:HB2	1.99	0.43
1:C:170:GLU:OE2	1:C:337:LYS:NZ	2.44	0.43
1:C:431:GLN:OE1	1:C:431:GLN:N	2.52	0.43
6:K:4:VAL:HG13	6:L:9:TYR:HE2	1.84	0.43
6:P:43:LEU:HD12	6:Q:38:SER:HA	1.99	0.43
1:C:399:ARG:HE	9:D:600:ADP:H5'2	1.84	0.42
2:E:126:ILE:HG23	2:E:250:PHE:HD2	1.83	0.42
2:F:167:THR:HA	2:F:205:ILE:HD11	2.00	0.42
4:H:15:LEU:HD22	4:H:89:ALA:HB2	2.01	0.42
6:R:33:LEU:HD21	6:R:48:PHE:HE1	1.83	0.42
1:C:367:ASN:O	1:C:371:ILE:HG13	2.19	0.42
2:F:275:ARG:HD3	2:F:335:VAL:HG23	2.00	0.42
6:L:57:LEU:HD13	6:M:55:PHE:CZ	2.54	0.42
1:B:281:GLU:HG3	1:B:284:ARG:HE	1.85	0.42
1:A:102:PHE:CE2	1:A:137:LEU:HD21	2.53	0.42
1:B:155:ALA:O	1:B:334:ARG:NH1	2.52	0.42
2:D:71:ARG:HH12	2:D:77:LEU:HB2	1.84	0.42
1:A:177:LYS:HB3	1:A:177:LYS:HE2	1.84	0.42
1:B:497:TYR:HE2	1:B:526:ILE:HD11	1.84	0.42
3:G:94:SER:HB2	3:G:153:GLY:HA3	2.02	0.42
6:T:24:ILE:O	6:T:28:ILE:HG13	2.20	0.42
1:C:409:MET:O	1:C:413:ALA:N	2.46	0.42
6:P:8:LYS:HB3	6:P:72:LEU:O	2.20	0.42
1:B:295:ASP:HA	1:B:296:ASP:HA	1.79	0.42
1:B:91:ASN:HB3	2:F:47:ILE:HG23	2.01	0.42
6:N:68:ILE:HD11	6:O:66:LEU:HD12	2.01	0.42
1:C:91:ASN:HB2	2:D:47:ILE:HG12	2.01	0.42
2:D:265:LEU:HD23	2:D:323:LEU:HD13	2.01	0.42
2:F:69:ILE:HB	2:F:77:LEU:HB3	2.01	0.42
6:S:58:SER:O	6:S:61:THR:OG1	2.36	0.42
6:K:27:ALA:HA	6:K:30:PHE:CE2	2.54	0.42
6:Q:11:GLY:HA2	6:Q:14:LEU:HD12	2.02	0.42
1:A:462:MET:HB2	1:A:467:MET:HE3	2.02	0.41
1:B:232:VAL:HG21	1:B:273:PRO:HG3	2.01	0.41
1:B:306:GLN:NE2	2:E:315:THR:HG22	2.34	0.41
2:E:174:LEU:HA	2:E:398:HIS:CE1	2.54	0.41
2:E:327:ILE:HG21	2:E:337:SER:HB2	2.02	0.41
2:E:183:LYS:HB2	2:E:360:LEU:HA	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:473:LYS:HB3	2:E:473:LYS:HE2	1.87	0.41
6:M:32:ALA:HB1	6:N:34:ILE:HB	2.02	0.41
1:C:525:SER:O	1:C:529:ASN:ND2	2.54	0.41
2:E:183:LYS:HE2	2:E:324:GLN:HB3	2.02	0.41
3:G:73:PHE:HZ	3:G:205:ILE:HG12	1.85	0.41
2:D:81:VAL:HA	2:D:92:THR:HG22	2.02	0.41
6:O:8:LYS:HE2	6:O:73:LEU:HA	2.02	0.41
1:A:229:TYR:OH	1:A:295:ASP:OD2	2.34	0.41
2:F:237:VAL:HG13	2:F:245:LYS:HB3	2.02	0.41
6:P:26:ILE:HG23	6:P:55:PHE:HB2	2.02	0.41
6:P:68:ILE:HD12	6:Q:16:SER:HB3	2.02	0.41
2:E:427:LEU:HD22	2:E:431:ASP:HB3	2.02	0.41
2:F:185:GLY:HA3	2:F:360:LEU:HD13	2.02	0.41
2:D:478:GLY:HA2	2:D:481:ASP:HB2	2.01	0.41
2:F:498:VAL:HA	2:F:501:ALA:HB3	2.01	0.41
2:F:69:ILE:HD11	2:F:79:LEU:HD11	2.01	0.41
1:C:229:TYR:OH	1:C:295:ASP:OD2	2.26	0.41
2:D:412:TYR:CE1	2:D:435:VAL:HG13	2.56	0.41
6:P:28:ILE:HG22	6:Q:31:ALA:HB2	2.01	0.41
1:B:193:ILE:HB	1:B:352:ILE:HG12	2.03	0.41
1:C:91:ASN:HD21	1:C:311:LEU:HB3	1.85	0.41
1:B:70:LEU:HD22	1:B:116:ARG:HG3	2.03	0.41
1:B:168:VAL:HG12	1:B:337:LYS:HB3	2.02	0.41
1:B:295:ASP:HB2	1:B:352:ILE:HD12	2.03	0.41
2:E:488:PHE:HE1	2:E:497:VAL:HG11	1.86	0.41
4:H:32:SER:HA	4:H:50:LEU:HA	2.02	0.41
6:S:32:ALA:O	6:S:36:GLY:N	2.54	0.41
1:A:313:ARG:HA	1:A:314:PRO:HD3	1.98	0.41
1:B:213:LYS:NZ	1:B:249:HIS:HB3	2.36	0.41
2:D:209:HIS:NE2	2:D:281:ASP:O	2.40	0.41
2:D:377:PRO:HB2	2:D:379:VAL:HG23	2.03	0.41
2:E:268:LEU:HD13	2:E:284:LEU:HD22	2.02	0.41
4:H:45:PRO:HG3	4:H:78:PRO:HD3	2.02	0.41
6:O:57:LEU:HD13	6:P:55:PHE:CE2	2.55	0.41
1:A:91:ASN:HD21	1:A:311:LEU:HD22	1.86	0.41
1:B:182:LEU:HD22	1:B:417:LYS:HB2	2.03	0.41
1:C:187:ARG:NH2	1:C:225:LEU:HB2	2.36	0.41
2:E:119:GLY:HA2	2:E:273:TYR:CE2	2.56	0.41
2:E:165:LEU:HB2	2:E:180:ARG:HB2	2.03	0.41
2:F:228:LEU:O	2:F:232:MET:HG2	2.21	0.41
2:F:194:LYS:HE3	2:F:342:TYR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:78:THR:HB	3:G:204:ALA:O	2.21	0.41
6:M:57:LEU:HD13	6:N:55:PHE:CE2	2.56	0.41
6:S:54:GLY:HA2	6:T:30:PHE:CD1	2.56	0.41
1:B:133:VAL:HB	1:B:142:ASP:HB3	2.03	0.40
2:F:245:LYS:HE2	2:F:245:LYS:HB2	1.93	0.40
3:G:51:LYS:O	3:G:55:ALA:N	2.53	0.40
6:P:28:ILE:HB	6:Q:27:ALA:HB1	2.02	0.40
6:Q:24:ILE:O	6:Q:28:ILE:HG13	2.21	0.40
6:R:33:LEU:HD21	6:R:48:PHE:CE1	2.56	0.40
2:D:146:LEU:HA	2:D:147:PRO:HD3	1.96	0.40
2:F:46:VAL:HG22	2:F:51:VAL:HG13	2.03	0.40
3:G:248:ARG:O	3:G:252:MET:HG2	2.21	0.40
4:H:32:SER:HA	4:H:50:LEU:HD23	2.02	0.40
6:R:57:LEU:HB2	6:S:26:ILE:HG21	2.02	0.40
1:C:386:GLY:O	1:C:455:LYS:HE2	2.20	0.40
2:E:474:GLU:O	2:E:479:LYS:HB2	2.21	0.40
2:F:196:VAL:HG23	9:F:600:ADP:O1A	2.22	0.40
1:B:264:GLU:HB3	1:B:268:LEU:HD12	2.03	0.40
2:D:213:SER:HB2	2:D:246:VAL:HG23	2.03	0.40
2:E:145:PHE:CD2	2:E:146:LEU:HG	2.57	0.40
2:F:287:ASP:HA	2:F:288:ASN:HA	1.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	483/536 (90%)	456 (94%)	26 (5%)	1 (0%)	52 88
1	B	475/536 (89%)	454 (96%)	21 (4%)	0	100 100
1	C	483/536 (90%)	456 (94%)	27 (6%)	0	100 100
2	D	468/509 (92%)	448 (96%)	20 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	E	466/509 (92%)	443 (95%)	23 (5%)	0	100 100
2	F	468/509 (92%)	439 (94%)	28 (6%)	1 (0%)	52 88
3	G	263/293 (90%)	242 (92%)	21 (8%)	0	100 100
4	H	109/137 (80%)	92 (84%)	13 (12%)	4 (4%)	4 36
6	K	71/76 (93%)	71 (100%)	0	0	100 100
6	L	70/76 (92%)	67 (96%)	3 (4%)	0	100 100
6	M	73/76 (96%)	71 (97%)	2 (3%)	0	100 100
6	N	73/76 (96%)	71 (97%)	2 (3%)	0	100 100
6	O	73/76 (96%)	73 (100%)	0	0	100 100
6	P	73/76 (96%)	72 (99%)	1 (1%)	0	100 100
6	Q	74/76 (97%)	71 (96%)	3 (4%)	0	100 100
6	R	72/76 (95%)	72 (100%)	0	0	100 100
6	S	72/76 (95%)	70 (97%)	2 (3%)	0	100 100
6	T	72/76 (95%)	71 (99%)	1 (1%)	0	100 100
All	All	3938/4325 (91%)	3739 (95%)	193 (5%)	6 (0%)	52 88

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	75	ASN
4	H	120	ALA
4	H	45	PRO
1	A	400	VAL
4	H	78	PRO
4	H	118	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
1	A	391/429 (91%)	389 (100%)	2 (0%)	92 97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	387/429 (90%)	383 (99%)	4 (1%)	82 93
1	C	391/429 (91%)	391 (100%)	0	100 100
2	D	377/409 (92%)	377 (100%)	0	100 100
2	E	376/409 (92%)	376 (100%)	0	100 100
2	F	377/409 (92%)	377 (100%)	0	100 100
3	G	224/242 (93%)	221 (99%)	3 (1%)	76 91
4	H	92/114 (81%)	92 (100%)	0	100 100
6	K	50/52 (96%)	50 (100%)	0	100 100
6	L	49/52 (94%)	48 (98%)	1 (2%)	63 87
6	M	51/52 (98%)	51 (100%)	0	100 100
6	N	51/52 (98%)	50 (98%)	1 (2%)	63 87
6	O	51/52 (98%)	49 (96%)	2 (4%)	39 76
6	P	51/52 (98%)	50 (98%)	1 (2%)	63 87
6	Q	52/52 (100%)	52 (100%)	0	100 100
6	R	50/52 (96%)	49 (98%)	1 (2%)	63 87
6	S	50/52 (96%)	49 (98%)	1 (2%)	63 87
6	T	50/52 (96%)	49 (98%)	1 (2%)	63 87
All	All	3120/3390 (92%)	3103 (100%)	17 (0%)	92 97

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	TYR
1	A	363	TYR
1	B	234	GLN
1	B	270	TYR
1	B	423	TYR
1	B	465	GLU
3	G	78	THR
3	G	149	PHE
3	G	176	TYR
6	L	55	PHE
6	N	55	PHE
6	O	55	PHE
6	O	73	LEU
6	P	1	MET

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Mol	Chain	Res	Type
6	R	55	PHE
6	S	55	PHE
6	T	55	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	203	GLN
6	S	46	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	ATP	A	600	8	26,33,33	0.97	1 (3%)	26,52,52	1.66	1 (3%)
7	ATP	B	600	8	26,33,33	0.97	1 (3%)	26,52,52	1.63	1 (3%)
7	ATP	C	600	8	26,33,33	0.96	1 (3%)	26,52,52	1.65	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	ADP	D	600	8	24,29,29	0.99	1 (4%)	23,45,45	1.74	1 (4%)
9	ADP	F	600	8	24,29,29	0.99	1 (4%)	23,45,45	1.71	1 (4%)

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
7	ATP	A	600	8	-	0/18/38/38	0/3/3/3
7	ATP	B	600	8	-	0/18/38/38	0/3/3/3
7	ATP	C	600	8	-	0/18/38/38	0/3/3/3
9	ADP	D	600	8	-	0/12/32/32	0/3/3/3
9	ADP	F	600	8	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	600	ADP	C5-C4	3.11	1.47	1.40
7	C	600	ATP	C5-C4	3.11	1.47	1.40
9	F	600	ADP	C5-C4	3.12	1.47	1.40
7	B	600	ATP	C5-C4	3.15	1.47	1.40
7	A	600	ATP	C5-C4	3.16	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	600	ADP	N3-C2-N1	-6.63	123.66	128.87
7	A	600	ATP	N3-C2-N1	-6.59	123.70	128.87
7	B	600	ATP	N3-C2-N1	-6.55	123.72	128.87
7	C	600	ATP	N3-C2-N1	-6.55	123.73	128.87
9	F	600	ADP	N3-C2-N1	-6.51	123.76	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	600	ATP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	600	ADP	3	0
9	F	600	ADP	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, 95^{th} 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	485/536 (90%)	0.11	17 (3%) 48 38	116, 153, 209, 224	0
1	B	479/536 (89%)	0.26	30 (6%) 23 18	104, 156, 234, 261	0
1	C	485/536 (90%)	0.21	28 (5%) 26 21	108, 150, 222, 280	0
2	D	470/509 (92%)	0.28	26 (5%) 29 22	108, 158, 195, 215	0
2	E	468/509 (91%)	0.34	42 (8%) 12 10	117, 160, 210, 248	0
2	F	470/509 (92%)	0.07	15 (3%) 51 42	113, 152, 192, 213	0
3	G	267/293 (91%)	0.70	44 (16%) 2 3	109, 185, 224, 241	0
4	H	113/137 (82%)	0.92	24 (21%) 1 1	161, 207, 255, 277	0
5	I	0/16	-	-	-	-
6	K	73/76 (96%)	0.45	12 (16%) 2 3	148, 184, 206, 218	0
6	L	72/76 (94%)	0.10	6 (8%) 14 12	154, 180, 213, 224	0
6	M	75/76 (98%)	0.17	10 (13%) 4 5	152, 179, 200, 213	0
6	N	75/76 (98%)	-0.31	0 100 100	140, 157, 188, 194	0
6	O	75/76 (98%)	0.15	3 (4%) 42 33	132, 158, 186, 192	0
6	P	75/76 (98%)	0.13	6 (8%) 15 12	132, 160, 200, 205	0
6	Q	76/76 (100%)	0.18	4 (5%) 30 23	150, 177, 198, 204	0
6	R	74/76 (97%)	-0.17	1 (1%) 78 68	162, 182, 197, 213	0
6	S	74/76 (97%)	0.15	7 (9%) 10 10	164, 179, 203, 217	0
6	T	74/76 (97%)	0.10	4 (5%) 29 23	163, 182, 205, 210	0
All	All	3980/4341 (91%)	0.24	279 (7%) 19 15	104, 163, 216, 280	0

All (279) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	GLN	9.8
3	G	116	ASP	8.5

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Mol	Chain	Res	Type	RSRZ
4	H	61	ASN	8.4
1	C	515	LEU	7.3
2	E	396	GLN	6.9
6	M	44	LYS	6.4
2	F	453	GLU	6.1
2	F	450	THR	6.0
1	C	516	SER	5.6
1	A	515	LEU	5.6
4	H	27	GLN	5.5
3	G	26	GLU	5.5
6	L	43	LEU	5.3
1	C	220	ASP	5.3
6	K	52	ILE	5.1
4	H	62	GLY	5.1
4	H	66	SER	4.9
1	B	219	GLN	4.9
2	E	419	ILE	4.9
3	G	139	ARG	4.9
1	C	413	ALA	4.8
1	C	510	ALA	4.7
6	K	55	PHE	4.6
1	B	511	ALA	4.5
2	E	399	TYR	4.5
1	C	221	GLU	4.5
6	M	45	GLY	4.5
2	D	492	GLY	4.5
2	D	160	THR	4.4
2	E	455	PHE	4.3
2	E	471	SER	4.3
6	K	74	TYR	4.3
1	B	216	ASN	4.2
2	E	398	HIS	4.2
6	K	51	SER	4.2
1	C	173	GLN	4.2
3	G	194	PRO	4.2
1	C	511	ALA	4.1
1	B	405	GLN	4.1
1	A	218	GLY	4.1
1	C	405	GLN	4.1
6	O	40	ASN	4.0
1	B	507	LYS	4.0
2	E	390	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	161	THR	4.0
6	Q	67	MET	4.0
2	E	490	MET	4.0
4	H	56	GLU	4.0
2	E	174	LEU	3.9
6	P	52	ILE	3.9
4	H	67	TYR	3.9
3	G	188	SER	3.8
4	H	64	THR	3.8
6	M	43	LEU	3.8
3	G	240	GLY	3.8
2	E	429	GLU	3.8
3	G	28	GLU	3.8
2	E	392	ASP	3.7
2	E	449	PHE	3.7
4	H	65	LYS	3.6
3	G	112	ARG	3.6
6	Q	71	LEU	3.6
2	E	73	GLU	3.6
2	E	400	ASP	3.5
6	Q	70	PHE	3.5
6	K	54	GLY	3.5
6	S	74	TYR	3.5
4	H	39	ILE	3.5
6	L	44	LYS	3.5
2	E	173	ASP	3.5
6	S	44	LYS	3.5
6	K	56	ALA	3.4
4	H	28	VAL	3.4
1	C	406	VAL	3.4
2	D	168	GLY	3.4
3	G	115	LEU	3.4
3	G	27	ILE	3.4
2	E	496	GLU	3.4
2	E	475	ILE	3.4
6	S	72	LEU	3.3
2	D	420	ALA	3.3
1	B	212	GLN	3.3
1	B	215	TRP	3.3
1	B	402	SER	3.3
2	D	453	GLU	3.3
2	E	493	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
6	K	66	LEU	3.3
2	E	448	PRO	3.3
1	C	189	GLN	3.2
3	G	120	GLY	3.2
2	E	420	ALA	3.2
2	D	440	LYS	3.2
6	K	70	PHE	3.2
2	F	452	ALA	3.2
6	O	42	ALA	3.2
6	S	4	VAL	3.2
6	P	49	THR	3.2
2	F	451	VAL	3.1
4	H	41	ALA	3.1
4	H	29	ASN	3.1
2	F	459	GLU	3.1
2	E	423	GLY	3.1
1	B	467	MET	3.1
2	D	53	VAL	3.1
3	G	142	PRO	3.1
6	P	45	GLY	3.0
6	K	44	LYS	3.0
1	A	408	ALA	3.0
2	F	449	PHE	3.0
1	B	406	VAL	3.0
3	G	183	TYR	3.0
2	D	460	GLY	3.0
2	E	421	ILE	3.0
1	B	108	VAL	3.0
3	G	141	ASN	3.0
2	F	149	HIS	3.0
1	B	512	THR	3.0
2	F	160	THR	2.9
1	B	462	MET	2.9
1	C	519	ASN	2.9
6	M	74	TYR	2.9
2	E	140	ILE	2.9
2	D	461	ARG	2.9
2	D	159	SER	2.9
2	D	170	LYS	2.9
6	P	53	LEU	2.8
3	G	71	LYS	2.8
2	E	167	THR	2.8

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Mol	Chain	Res	Type	RSRZ
6	M	59	GLU	2.8
1	A	244	GLN	2.8
6	S	2	GLN	2.8
2	E	391	ILE	2.8
2	D	462	LEU	2.8
1	B	401	GLY	2.8
1	C	512	THR	2.8
2	E	402	ALA	2.8
4	H	38	GLY	2.8
2	E	401	VAL	2.8
2	F	142	ALA	2.8
3	G	184	ASN	2.8
2	E	141	GLU	2.7
2	F	117	PRO	2.7
1	C	60	VAL	2.7
3	G	126	ILE	2.7
6	L	51	SER	2.7
1	B	515	LEU	2.7
2	E	454	VAL	2.7
2	D	493	GLY	2.7
1	C	508	ASP	2.7
3	G	25	ARG	2.7
3	G	158	THR	2.7
3	G	58	ALA	2.7
3	G	111	ARG	2.6
2	E	158	GLN	2.6
3	G	239	GLU	2.6
1	A	411	GLN	2.6
2	D	75	ASN	2.6
2	E	395	GLY	2.6
3	G	213	GLN	2.6
2	D	141	GLU	2.6
3	G	195	ILE	2.6
6	K	62	GLY	2.6
2	F	118	VAL	2.6
2	E	467	ASP	2.6
3	G	138	GLY	2.6
1	C	407	LYS	2.6
1	B	508	ASP	2.6
3	G	157	PRO	2.6
2	E	175	LEU	2.6
2	D	94	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
6	M	52	ILE	2.6
1	B	221	GLU	2.6
4	H	24	GLU	2.6
4	H	82	LEU	2.6
1	A	390	ALA	2.5
1	B	61	GLY	2.5
1	C	479	ILE	2.5
2	D	178	TYR	2.5
2	D	488	PHE	2.5
6	O	37	VAL	2.5
4	H	42	ASN	2.5
2	E	393	VAL	2.5
3	G	113	LYS	2.5
1	C	507	LYS	2.5
6	P	54	GLY	2.5
3	G	177	ASP	2.5
3	G	181	ILE	2.5
1	B	458	GLN	2.5
2	E	168	GLY	2.5
2	D	419	ILE	2.5
1	B	425	GLU	2.5
2	D	212	PHE	2.5
1	B	486	GLN	2.5
1	A	413	ALA	2.5
6	T	44	LYS	2.5
6	K	63	LEU	2.4
2	E	492	GLY	2.4
6	S	71	LEU	2.4
3	G	234	TYR	2.4
4	H	30	ILE	2.4
6	T	52	ILE	2.4
1	B	501	ASN	2.4
6	P	55	PHE	2.4
3	G	89	TRP	2.4
2	E	505	ALA	2.4
1	B	173	GLN	2.4
2	F	83	GLN	2.4
1	A	110	GLU	2.4
1	C	109	LYS	2.4
3	G	104	SER	2.4
1	B	505	LEU	2.4
4	H	115	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
6	M	73	LEU	2.3
1	A	220	ASP	2.3
6	L	46	GLN	2.3
2	D	418	ILE	2.3
1	C	518	GLU	2.3
1	C	432	PHE	2.3
1	A	406	VAL	2.3
3	G	182	VAL	2.3
1	B	513	GLY	2.3
6	M	48	PHE	2.3
3	G	114	LEU	2.3
1	A	502	GLU	2.3
4	H	46	THR	2.3
1	C	412	VAL	2.3
1	C	525	SER	2.3
6	T	74	TYR	2.3
1	C	514	GLU	2.3
6	S	70	PHE	2.3
3	G	237	MET	2.3
3	G	70	GLU	2.3
6	L	49	THR	2.3
1	B	214	ARG	2.2
6	K	43	LEU	2.2
1	B	407	LYS	2.2
1	C	401	GLY	2.2
3	G	62	SER	2.2
3	G	290	SER	2.2
1	C	222	LYS	2.2
3	G	45	LYS	2.2
1	B	493	GLU	2.2
1	A	391	ILE	2.2
2	E	179	ALA	2.2
6	Q	72	LEU	2.2
2	F	161	THR	2.2
2	E	474	GLU	2.2
2	D	69	ILE	2.2
2	E	397	GLU	2.1
1	A	511	ALA	2.1
4	H	31	PRO	2.1
1	A	156	GLN	2.1
2	E	170	LYS	2.1
4	H	40	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
6	T	41	PRO	2.1
1	A	125	VAL	2.1
6	L	42	ALA	2.1
3	G	232	THR	2.1
4	H	57	VAL	2.1
2	F	84	HIS	2.1
4	H	59	GLU	2.1
3	G	190	ILE	2.1
4	H	63	GLU	2.1
1	B	424	ARG	2.1
1	C	411	GLN	2.1
1	A	279	MET	2.0
2	F	406	GLN	2.0
6	R	2	GLN	2.0
1	C	65	ALA	2.0
2	E	499	ALA	2.0
1	B	213	LYS	2.0
2	D	331	GLN	2.0
6	M	42	ALA	2.0
3	G	57	ARG	2.0
2	D	484	PRO	2.0
2	D	166	GLU	2.0
3	G	212	GLY	2.0
3	G	134	LYS	2.0
6	M	41	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	ADP	F	600	27/27	0.92	0.30	-0.11	159,176,182,186	0
7	ATP	B	600	31/31	0.89	0.29	-0.23	149,182,193,201	0
7	ATP	C	600	31/31	0.92	0.26	-0.23	149,159,174,183	0
7	ATP	A	600	31/31	0.92	0.24	-0.48	146,160,172,197	0
9	ADP	D	600	27/27	0.96	0.26	-0.56	159,164,170,173	0
8	MG	F	601	1/1	0.93	0.13	-3.14	189,189,189,189	0
8	MG	D	601	1/1	0.83	0.17	-	183,183,183,183	0
8	MG	A	601	1/1	0.96	0.20	-	173,173,173,173	0
8	MG	B	601	1/1	0.98	0.18	-	154,154,154,154	0
8	MG	C	601	1/1	0.90	0.22	-	171,171,171,171	0

6.5 Other polymers (i)

There are no such residues in this entry.