Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:31 PM GMT

PDB ID	:	3ZIA
Title	:	The structure of F1-ATPase from Saccharomyces cerevisiae inhibited by its regulatory protein IF1
Authors	:	Robinson, G.C.; Bason, J.V.; Montgomery, M.G.; Fearnley, I.M.; Mueller, D.M.; Leslie, A.G.W.; Walker, J.E.
Deposited on	:	2013-01-07
Resolution	:	2.50 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:

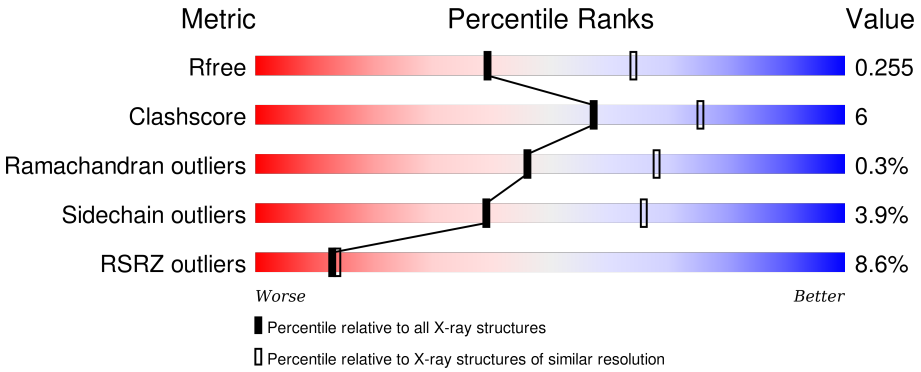
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	510	6% 82% 12% • 5%
1	B	510	6% 81% 12% • 6%
1	C	510	8% 84% 11% • 5%
1	K	510	7% 82% 12% • 5%
1	L	510	% 81% 13% • 6%

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Mol	Chain	Length	Quality of chain
1	M	510	7% 84% 10% • 5%
2	D	478	4% 84% 13% • •
2	E	478	13% 82% 15% • •
2	F	478	2% 88% 9% • •
2	N	478	5% 83% 14% • •
2	O	478	12% 83% 14% • •
2	P	478	4% 88% 9% • •
3	G	278	11% 76% 18% • 5%
3	Q	278	18% 77% 16% • 5%
4	H	138	35% 72% 15% • 10%
4	R	138	36% 72% 16% • 10%
5	I	61	10% 62% 30% • 5%
5	S	61	25% 67% 23% 5% 5%
6	J	63	5% 38% 17% • 43%
6	T	63	8% 38% 17% • 43%

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
10	EDO	L	604	-	-	-	X
10	EDO	O	602	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 51906 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			
1	B	480	Total	C	N	O	S	0	1	0
			3655	2310	648	694	3			
1	C	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			
1	K	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			
1	L	480	Total	C	N	O	S	0	1	0
			3655	2310	648	694	3			
1	M	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	E	468	Total	C	N	O	S	0	0	0
			3536	2243	602	685	6			
2	F	469	Total	C	N	O	S	0	1	0
			3548	2251	603	687	7			
2	N	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	O	468	Total	C	N	O	S	0	0	0
			3536	2243	602	685	6			
2	P	469	Total	C	N	O	S	0	3	0
			3559	2260	603	689	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	265	Total	C	N	O	S	0	0	0
			2057	1291	358	398	10			
3	Q	265	Total	C	N	O	S	0	1	0
			2063	1295	358	400	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	124	Total	C	N	O	S	0	0	0
			937	594	156	185	2			
4	R	124	Total	C	N	O	S	0	0	0
			937	594	156	185	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	58	Total	C	N	O	0	0	0
			450	283	79	88			
5	S	58	Total	C	N	O	0	0	0
			450	283	79	88			

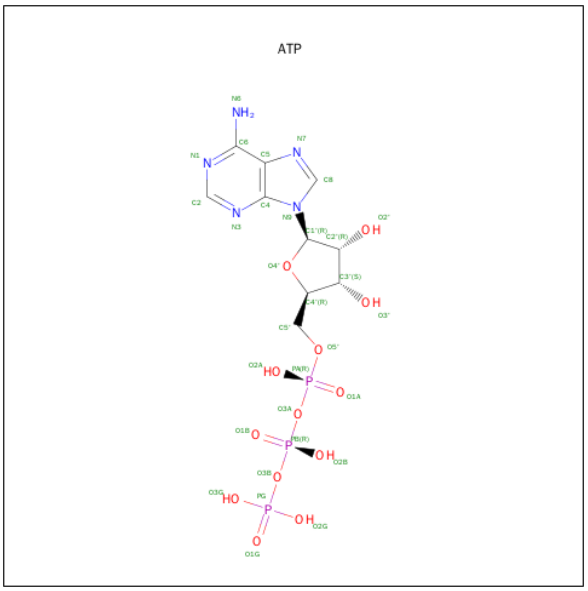
- Molecule 6 is a protein called ATPASE INHIBITOR, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	36	Total	C	N	O	0	0	0
			283	168	55	60			
6	T	36	Total	C	N	O	0	0	0
			283	168	55	60			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	21	ALA	GLU	ENGINEERED MUTATION	UNP P01097
T	21	ALA	GLU	ENGINEERED MUTATION	UNP P01097

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

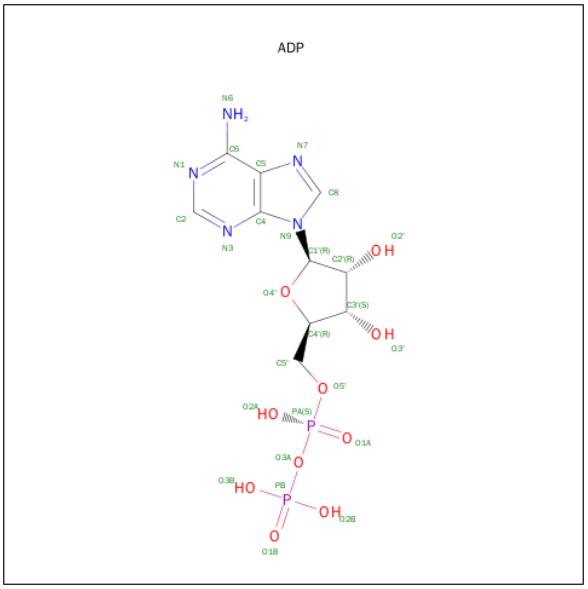


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

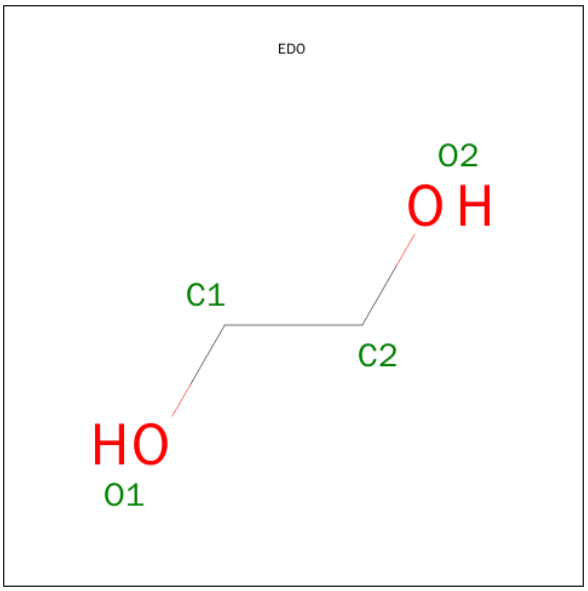
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	P	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		
8	K	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	A	1	Total	Mg	0	0
			1	1		
8	N	1	Total	Mg	0	0
			1	1		
8	L	1	Total	Mg	0	0
			1	1		
8	F	1	Total	Mg	0	0
			1	1		
8	M	1	Total	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	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	E	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		
9	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	O	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	P	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total C O 4 2 2	0	0
10	L	1	Total C O 4 2 2	0	0
10	L	1	Total C O 4 2 2	0	0
10	M	1	Total C O 4 2 2	0	0
10	O	1	Total C O 4 2 2	0	0
10	P	1	Total C O 4 2 2	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	18	Total O 18 18	0	0
11	B	90	Total O 90 90	0	0
11	C	94	Total O 94 94	0	0
11	D	37	Total O 37 37	0	0
11	E	20	Total O 20 20	0	0
11	F	81	Total O 81 81	0	0

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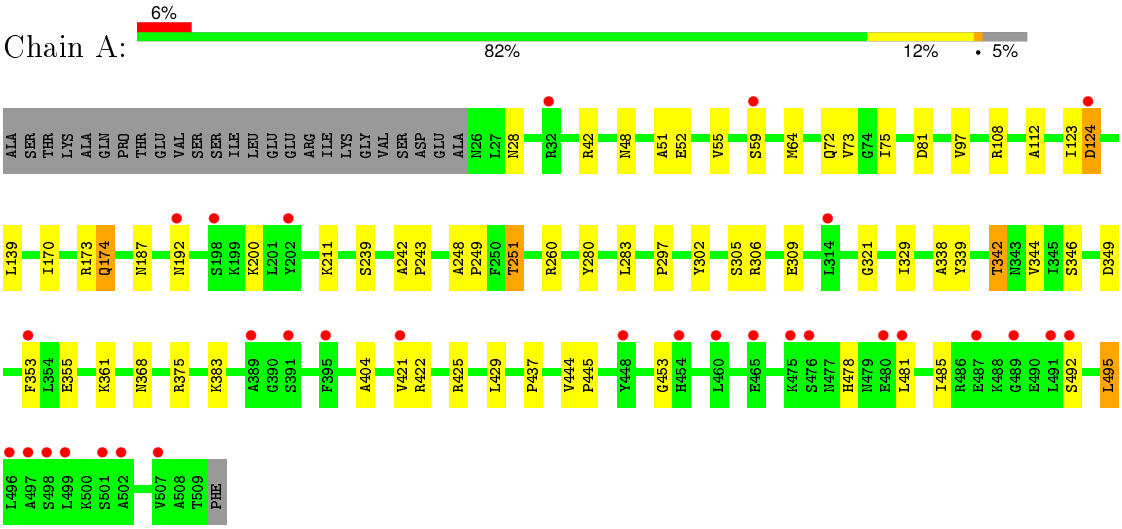
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	G	11	Total O 11 11	0	0
11	H	1	Total O 1 1	0	0
11	I	1	Total O 1 1	0	0
11	K	27	Total O 27 27	0	0
11	L	156	Total O 156 156	0	0
11	M	76	Total O 76 76	0	0
11	N	32	Total O 32 32	0	0
11	O	52	Total O 52 52	0	0
11	P	68	Total O 68 68	0	0
11	Q	8	Total O 8 8	0	0
11	R	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

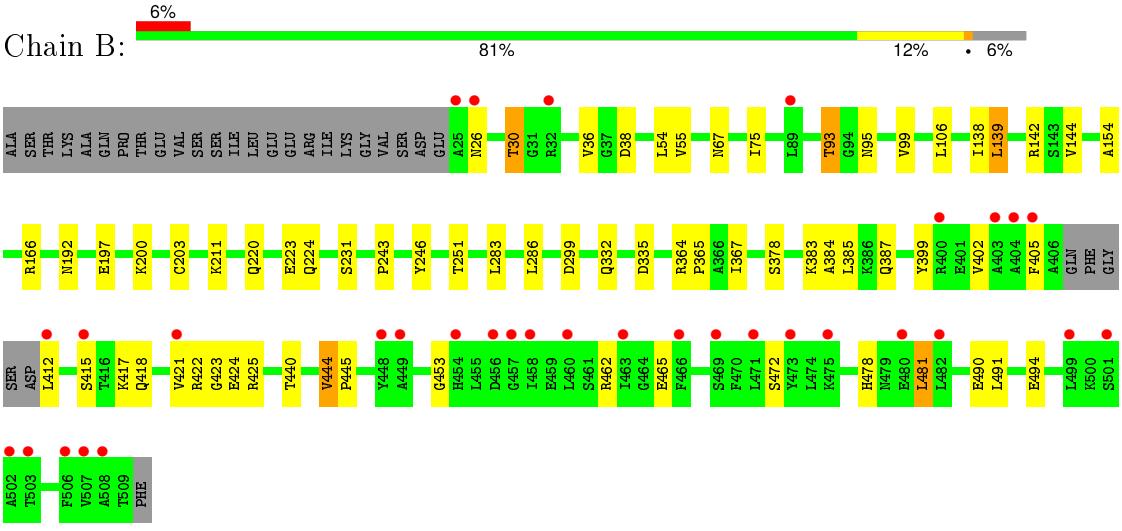
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain A:



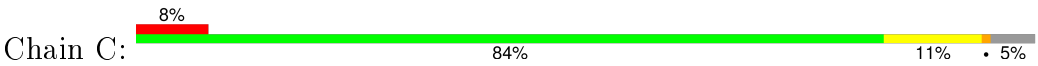
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

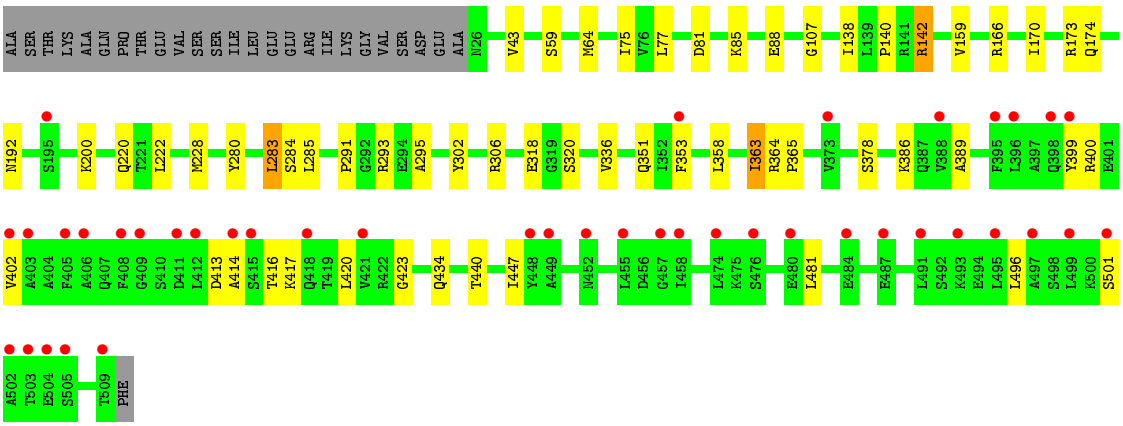
Chain B:



• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

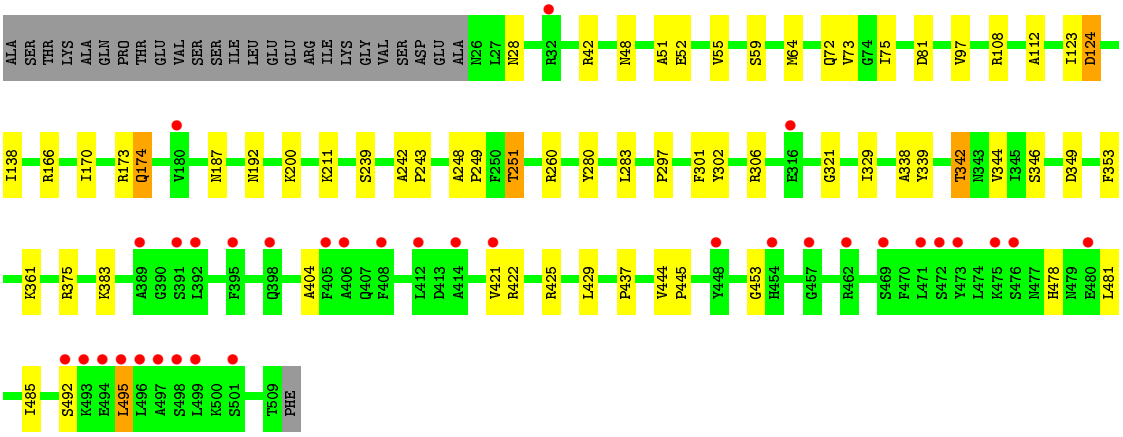
Chain C:





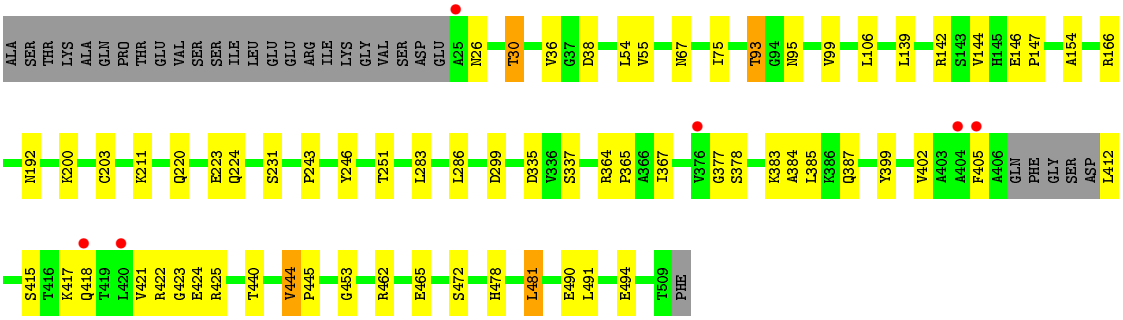
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain K:



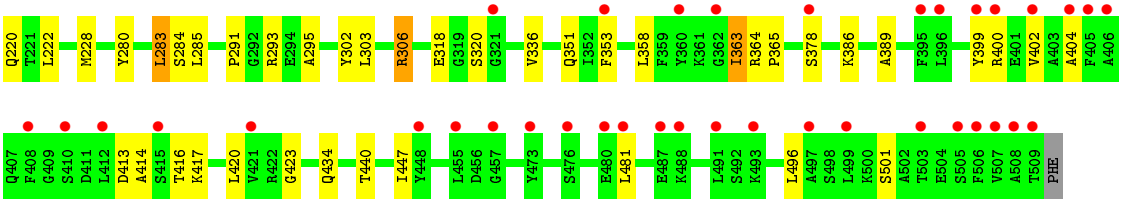
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain L:

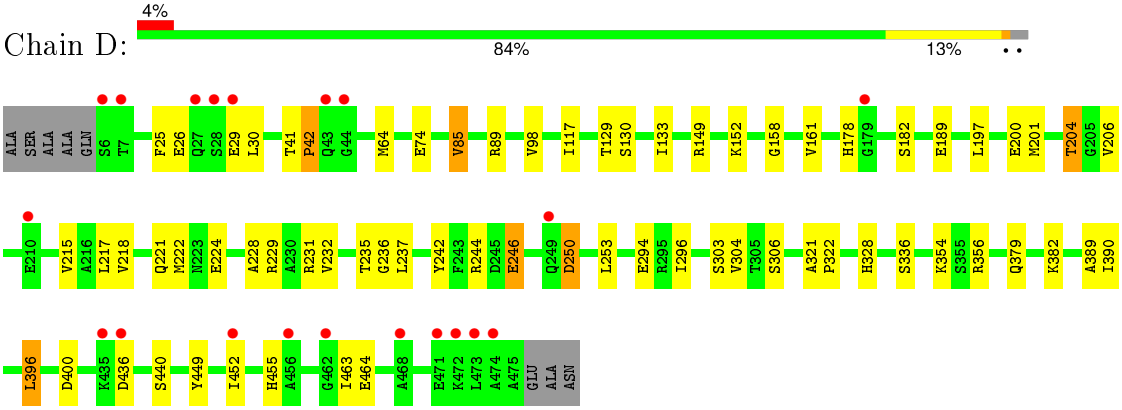


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

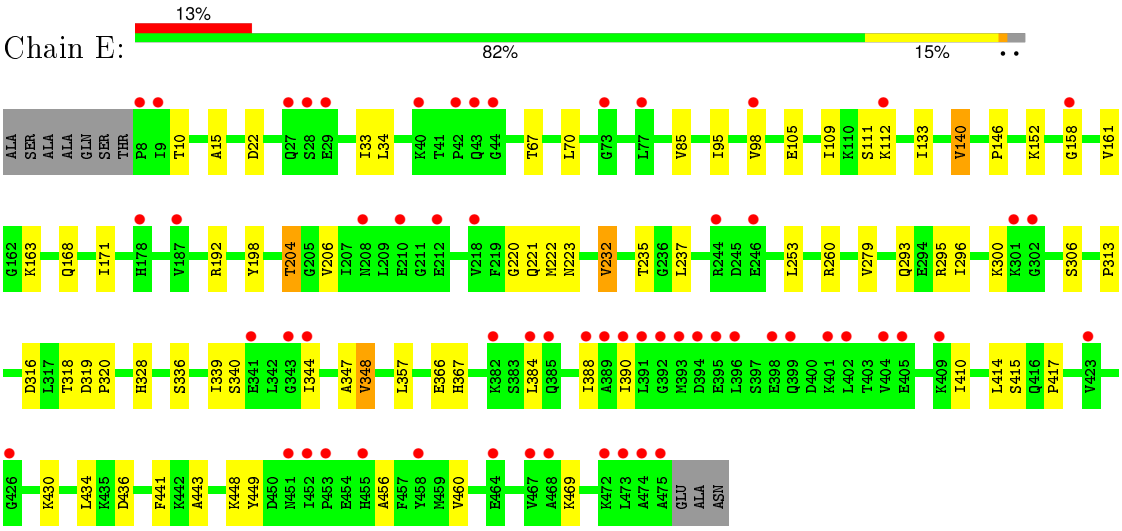
Chain M:



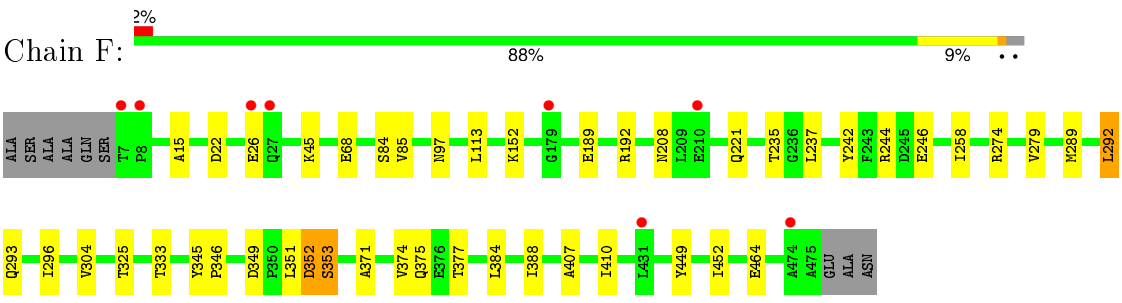
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

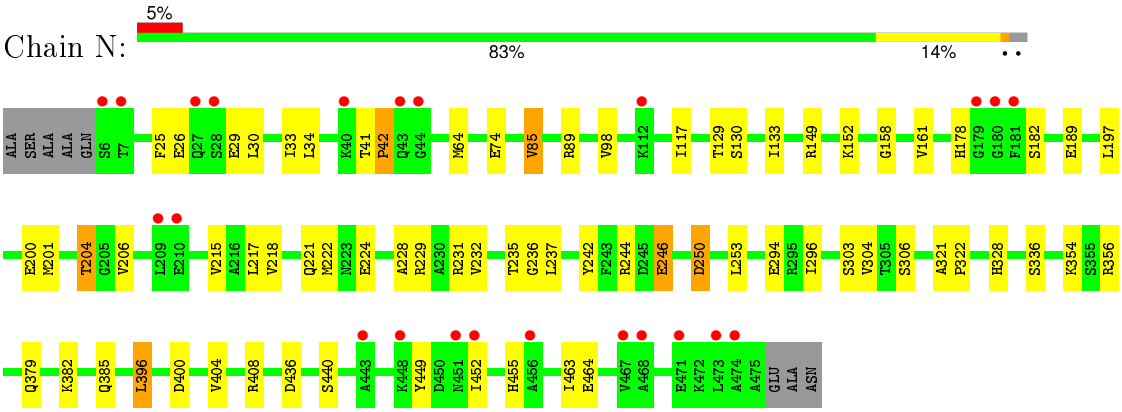


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



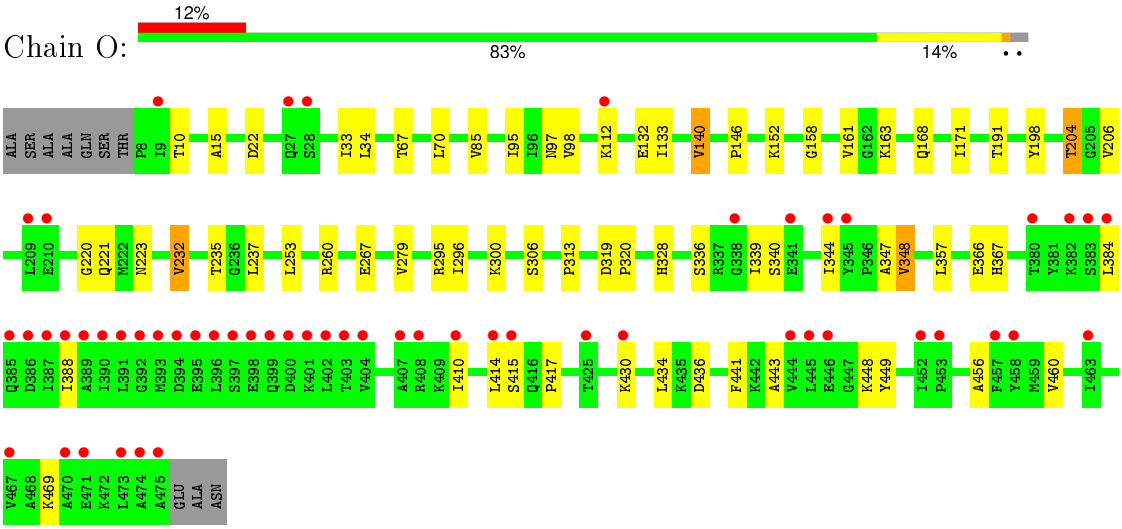
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain N:



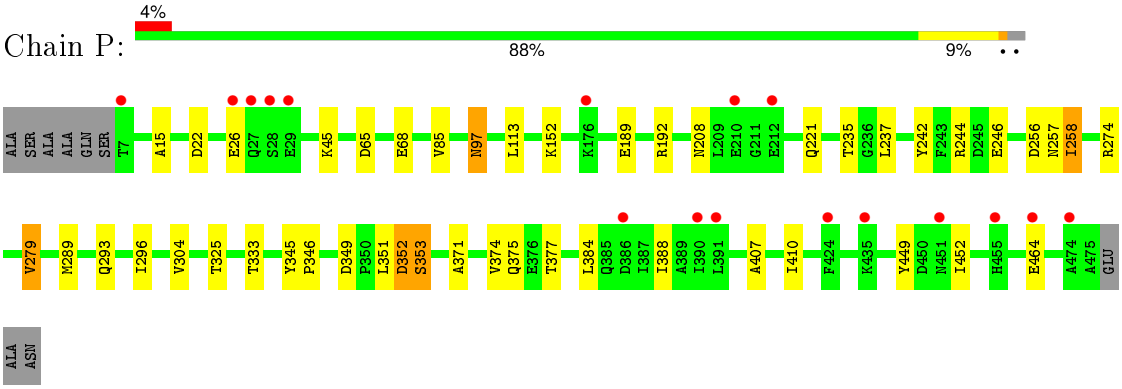
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain O:



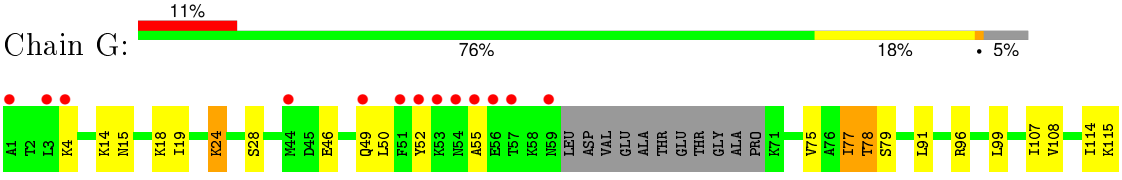
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

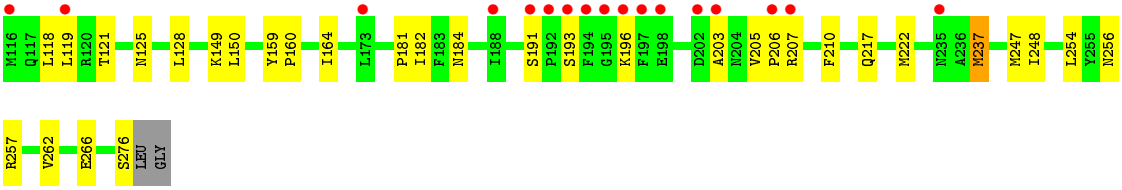
Chain P:



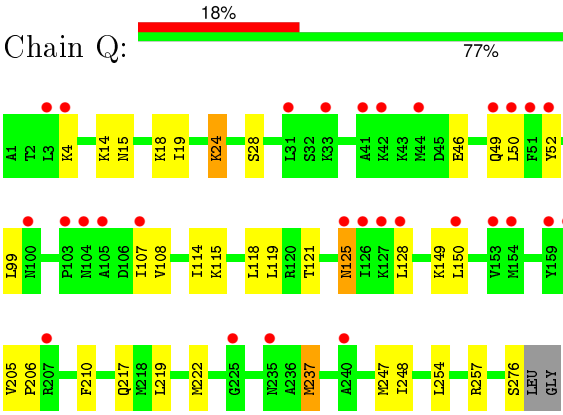
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

Chain G:

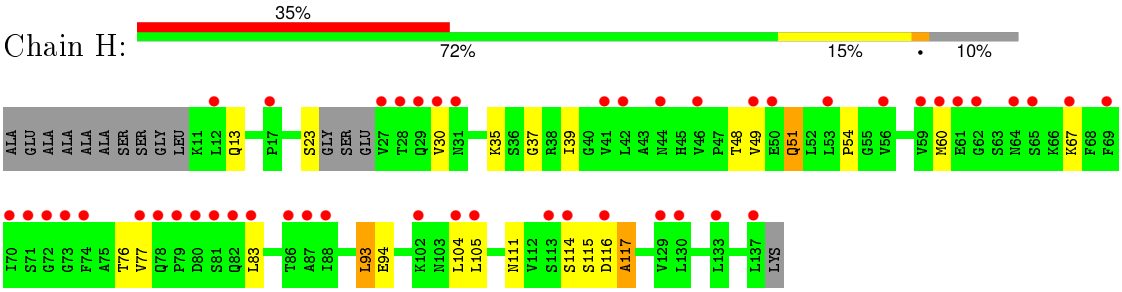




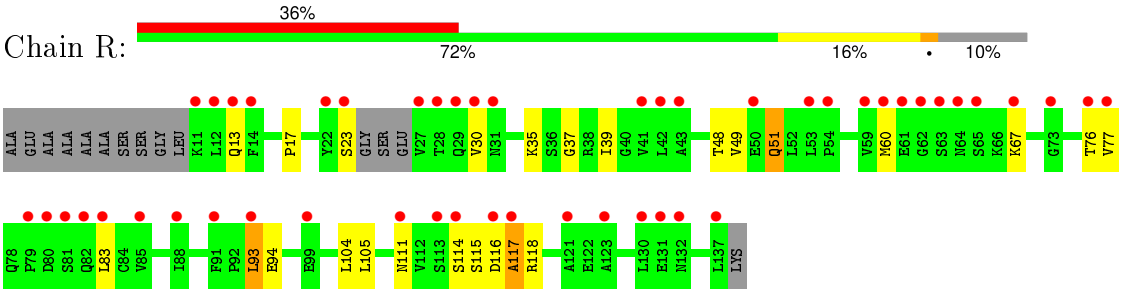
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



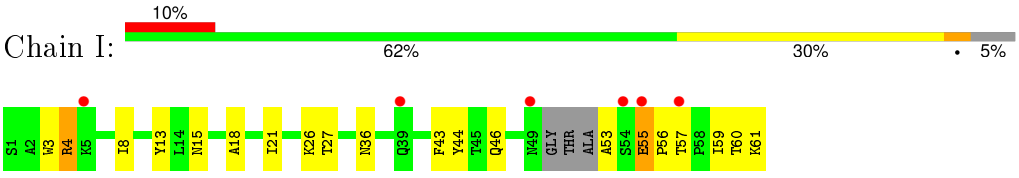
• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL

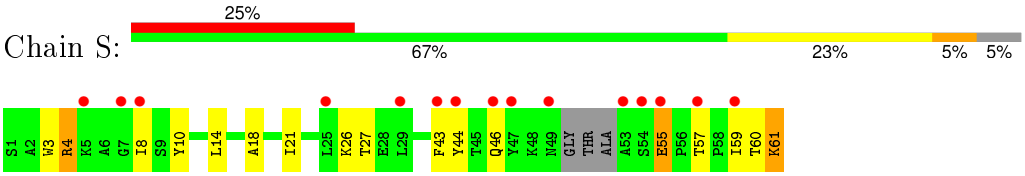


• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL



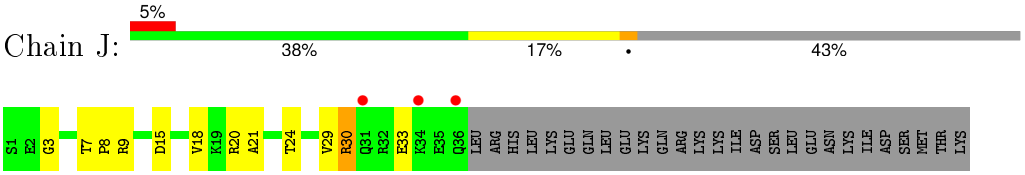
• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

Chain S:



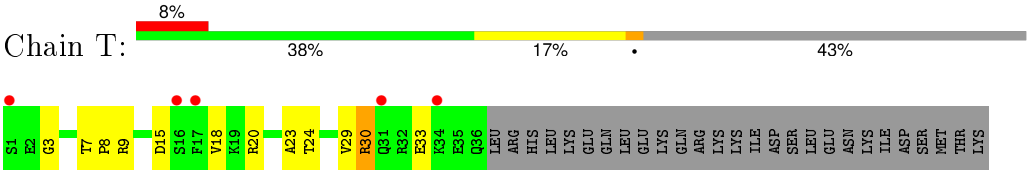
• Molecule 6: ATPASE INHIBITOR, MITOCHONDRIAL

Chain J:



• Molecule 6: ATPASE INHIBITOR, MITOCHONDRIAL

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	118.22Å 187.85Å 181.81Å 90.00° 89.96° 90.00°	Depositor
Resolution (Å)	181.81 – 2.50 40.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (181.81-2.50) 98.3 (40.91-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.224 , 0.262 0.218 , 0.255	Depositor DCC
R_{free} test set	13570 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.0	EDS
Estimated twinning fraction	0.010 for -h,-l,-k 0.004 for -h,l,k 0.079 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 268544 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	51906	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.39	0/3736	0.55	0/5057
1	B	0.50	0/3712	0.62	0/5023
1	C	0.47	0/3736	0.58	0/5057
1	K	0.39	0/3736	0.55	0/5057
1	L	0.53	0/3712	0.63	0/5023
1	M	0.46	0/3736	0.58	0/5057
2	D	0.42	0/3605	0.55	0/4889
2	E	0.42	0/3592	0.58	0/4870
2	F	0.50	0/3607	0.63	0/4891
2	N	0.41	0/3605	0.55	0/4889
2	O	0.45	0/3592	0.59	0/4870
2	P	0.49	0/3624	0.62	0/4914
3	G	0.38	0/2082	0.52	0/2800
3	Q	0.38	0/2091	0.52	0/2812
4	H	0.37	0/950	0.55	0/1288
4	R	0.38	0/950	0.55	0/1288
5	I	0.43	0/457	0.55	0/619
5	S	0.44	0/457	0.55	0/619
6	J	0.42	0/286	0.62	0/379
6	T	0.41	0/286	0.61	0/379
All	All	0.45	0/51552	0.58	0/69781

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 (i)

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	3680	0	3763	45	0
1	B	3655	0	3751	36	0
1	C	3680	0	3763	47	0
1	K	3680	0	3763	42	0
1	L	3655	0	3751	34	0
1	M	3680	0	3763	48	0
2	D	3549	0	3620	45	0
2	E	3536	0	3610	48	0
2	F	3548	0	3624	30	0
2	N	3549	0	3620	46	0
2	O	3536	0	3610	42	0
2	P	3559	0	3641	30	0
3	G	2057	0	2127	38	0
3	Q	2063	0	2133	32	0
4	H	937	0	947	18	0
4	R	937	0	947	22	0
5	I	450	0	452	20	0
5	S	450	0	452	20	0
6	J	283	0	267	11	0
6	T	283	0	267	12	0
7	A	31	0	12	0	0
7	K	31	0	12	0	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
8	K	1	0	0	0	0
8	L	1	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
8	P	1	0	0	0	0
9	B	27	0	12	0	0
9	C	27	0	12	1	0
9	D	27	0	12	0	0
9	E	27	0	12	0	0
9	F	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	27	0	12	0	0
9	M	27	0	12	1	0
9	N	27	0	12	0	0
9	O	27	0	12	0	0
9	P	27	0	12	0	0
10	C	4	0	6	0	0
10	L	8	0	12	0	0
10	M	4	0	6	2	0
10	O	4	0	6	0	0
10	P	4	0	6	1	0
11	A	18	0	0	0	0
11	B	90	0	0	4	0
11	C	94	0	0	1	0
11	D	37	0	0	0	0
11	E	20	0	0	0	0
11	F	81	0	0	3	0
11	G	11	0	0	1	0
11	H	1	0	0	1	0
11	I	1	0	0	1	0
11	K	27	0	0	0	0
11	L	156	0	0	3	0
11	M	76	0	0	0	0
11	N	32	0	0	0	0
11	O	52	0	0	2	0
11	P	68	0	0	0	0
11	Q	8	0	0	0	0
11	R	1	0	0	0	0
All	All	51906	0	52051	617	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 6.

All (617) 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:O:85:VAL:HG11	2:O:235:THR:HG23	1.30	1.11
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.30	1.09
3:Q:96:ARG:HE	3:Q:121:THR:HG21	1.18	1.08
3:G:96:ARG:HE	3:G:121:THR:HG21	1.18	1.08
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.36	1.07
2:P:85:VAL:HG11	2:P:235:THR:HG23	1.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:422:ARG:HH12	1:K:453:GLY:HA2	1.27	0.98
4:R:93:LEU:HD22	4:R:93:LEU:H	1.26	0.96
4:H:93:LEU:HD22	4:H:93:LEU:H	1.27	0.96
5:S:59:ILE:HG22	5:S:60:THR:H	1.30	0.96
6:T:30:ARG:HG2	6:T:30:ARG:HH11	1.30	0.96
6:J:30:ARG:HG2	6:J:30:ARG:HH11	1.29	0.96
1:A:422:ARG:HH12	1:A:453:GLY:HA2	1.28	0.96
5:I:59:ILE:HG22	5:I:60:THR:H	1.31	0.94
2:O:221:GLN:HG3	2:O:223:ASN:OD1	1.70	0.91
5:S:3:TRP:HB2	5:S:8:ILE:HB	1.52	0.90
5:I:3:TRP:HB2	5:I:8:ILE:HB	1.52	0.90
2:E:221:GLN:HG3	2:E:223:ASN:OD1	1.72	0.89
2:E:319:ASP:OD1	2:E:320:PRO:HD2	1.74	0.87
1:B:387:GLN:HE22	1:B:491:LEU:H	1.21	0.87
1:L:387:GLN:HE22	1:L:491:LEU:H	1.21	0.86
2:P:351:LEU:O	2:P:352:ASP:HB2	1.74	0.86
2:O:319:ASP:OD1	2:O:320:PRO:HD2	1.75	0.85
1:M:142:ARG:HG2	1:M:142:ARG:HH11	1.41	0.85
2:D:201:MET:CE	2:D:217:LEU:HD21	2.07	0.85
2:N:201:MET:CE	2:N:217:LEU:HD21	2.07	0.84
2:F:351:LEU:O	2:F:352:ASP:HB2	1.75	0.84
1:C:142:ARG:HH11	1:C:142:ARG:HG2	1.43	0.84
2:N:41:THR:HB	2:N:42:PRO:HD2	1.60	0.82
2:D:41:THR:HB	2:D:42:PRO:HD2	1.60	0.82
1:M:363:ILE:O	1:M:363:ILE:HG13	1.84	0.78
1:C:363:ILE:HG13	1:C:363:ILE:O	1.85	0.77
3:G:96:ARG:NE	3:G:121:THR:HG21	2.00	0.76
1:A:444:VAL:HG23	1:A:445:PRO:HD3	1.67	0.75
1:M:283:LEU:HD23	1:M:284:SER:N	2.01	0.74
1:K:444:VAL:HG23	1:K:445:PRO:HD3	1.68	0.74
1:M:303:LEU:HA	10:M:602:EDO:H22	1.70	0.73
2:N:201:MET:HE3	2:N:217:LEU:HD21	1.71	0.72
2:O:220:GLY:HA3	2:O:232:VAL:HG11	1.71	0.72
1:A:112:ALA:O	1:A:251:THR:HG21	1.90	0.72
2:P:351:LEU:O	2:P:352:ASP:CB	2.37	0.72
2:E:220:GLY:HA3	2:E:232:VAL:HG11	1.71	0.72
4:H:67:LYS:HB3	4:H:93:LEU:HD21	1.71	0.72
6:J:30:ARG:CG	6:J:30:ARG:HH11	2.01	0.72
1:K:112:ALA:O	1:K:251:THR:HG21	1.90	0.72
2:E:390:ILE:HD11	3:G:24:LYS:HE3	1.71	0.72
4:R:67:LYS:HB3	4:R:93:LEU:HD21	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:96:ARG:NE	3:Q:121:THR:HG21	2.00	0.71
6:T:30:ARG:CG	6:T:30:ARG:HH11	2.01	0.71
2:F:351:LEU:O	2:F:352:ASP:CB	2.38	0.71
1:M:336:VAL:HG11	1:M:353:PHE:CE1	2.26	0.70
1:C:283:LEU:HD23	1:C:284:SER:N	2.06	0.70
2:N:26:GLU:O	2:N:29:GLU:HG3	1.92	0.69
4:H:37:GLY:O	4:H:39:ILE:HG12	1.91	0.69
1:C:336:VAL:HG11	1:C:353:PHE:CE1	2.28	0.69
2:D:26:GLU:O	2:D:29:GLU:HG3	1.93	0.68
2:D:382:LYS:HG2	6:J:7:THR:HG21	1.75	0.68
4:R:37:GLY:O	4:R:39:ILE:HG12	1.92	0.68
2:N:237:LEU:HD13	2:N:296:ILE:HG12	1.75	0.68
1:B:54:LEU:O	1:B:93:THR:HB	1.94	0.68
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.75	0.68
1:L:54:LEU:O	1:L:93:THR:HB	1.94	0.68
4:H:93:LEU:H	4:H:93:LEU:CD2	2.04	0.67
2:F:351:LEU:HD23	11:F:2076:HOH:O	1.93	0.67
4:R:93:LEU:H	4:R:93:LEU:CD2	2.04	0.67
6:J:20:ARG:O	6:J:24:THR:HG23	1.94	0.67
2:N:197:LEU:O	2:N:201:MET:HG2	1.93	0.67
6:T:20:ARG:O	6:T:24:THR:HG23	1.95	0.67
2:N:382:LYS:HG2	6:T:7:THR:HG21	1.77	0.67
2:D:197:LEU:O	2:D:201:MET:HG2	1.94	0.66
1:C:413:ASP:CB	1:C:416:THR:HB	2.25	0.66
1:M:413:ASP:CB	1:M:416:THR:HB	2.25	0.66
1:L:220:GLN:HE21	1:L:224:GLN:HE21	1.42	0.66
2:O:313:PRO:HG2	2:O:319:ASP:OD2	1.96	0.66
1:B:220:GLN:HE21	1:B:224:GLN:HE21	1.43	0.65
1:L:335:ASP:OD2	3:Q:257:ARG:HD3	1.97	0.65
2:E:316:ASP:OD2	3:G:256:ASN:HB3	1.97	0.65
2:D:201:MET:HE3	2:D:217:LEU:HD21	1.78	0.65
1:B:417:LYS:O	1:B:421:VAL:HG23	1.96	0.64
1:L:417:LYS:O	1:L:421:VAL:HG23	1.96	0.64
2:D:201:MET:HE2	2:D:217:LEU:HD21	1.77	0.64
1:K:42:ARG:HD2	1:K:72:GLN:HE22	1.62	0.64
2:E:384:LEU:O	2:E:388:ILE:HG12	1.98	0.64
3:Q:14:LYS:HA	3:Q:248:ILE:HD11	1.79	0.63
4:H:35:LYS:HD2	4:H:51:GLN:NE2	2.12	0.63
4:R:35:LYS:HD2	4:R:51:GLN:NE2	2.12	0.63
4:R:48:THR:H	4:R:77:VAL:HB	1.64	0.63
3:G:14:LYS:HA	3:G:248:ILE:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:384:LEU:O	2:O:388:ILE:HG12	1.99	0.63
1:A:42:ARG:HD2	1:A:72:GLN:HE22	1.64	0.63
2:E:220:GLY:CA	2:E:232:VAL:HG11	2.28	0.63
4:H:48:THR:H	4:H:77:VAL:HB	1.64	0.63
3:Q:24:LYS:HB2	3:Q:237:MET:HB3	1.81	0.62
1:A:52:GLU:O	1:A:97:VAL:HG23	1.99	0.62
1:K:248:ALA:HB3	1:K:249:PRO:HD3	1.81	0.62
1:K:52:GLU:O	1:K:97:VAL:HG23	1.99	0.62
4:R:118:ARG:NH1	5:S:8:ILE:HG13	2.14	0.62
3:G:115:LYS:O	3:G:119:LEU:HB2	2.00	0.62
2:O:220:GLY:CA	2:O:232:VAL:HG11	2.29	0.62
3:G:24:LYS:HB2	3:G:237:MET:HB3	1.82	0.62
2:D:85:VAL:HG22	2:D:117:ILE:HG22	1.81	0.62
1:L:55:VAL:HG21	1:L:75:ILE:HD13	1.82	0.62
1:B:55:VAL:HG21	1:B:75:ILE:HD13	1.82	0.61
5:S:59:ILE:HG22	5:S:60:THR:N	2.09	0.61
4:H:111:ASN:HA	4:H:114:SER:HB3	1.83	0.61
2:E:313:PRO:HG2	2:E:319:ASP:OD2	2.01	0.61
1:A:248:ALA:HB3	1:A:249:PRO:HD3	1.83	0.61
3:Q:78:THR:HG23	3:Q:114:ILE:HB	1.81	0.61
1:C:64:MET:HE1	11:C:2008:HOH:O	1.99	0.61
5:I:59:ILE:HG22	5:I:60:THR:N	2.09	0.61
1:C:413:ASP:O	1:C:416:THR:HB	2.01	0.61
6:J:30:ARG:HG2	6:J:30:ARG:NH1	2.07	0.61
4:R:111:ASN:HA	4:R:114:SER:HB3	1.83	0.61
2:N:85:VAL:HG22	2:N:117:ILE:HG22	1.82	0.61
4:H:93:LEU:HD22	4:H:93:LEU:N	2.10	0.60
3:G:78:THR:HG23	3:G:114:ILE:HB	1.81	0.60
3:Q:115:LYS:O	3:Q:119:LEU:HB2	2.02	0.60
6:T:30:ARG:HG2	6:T:30:ARG:NH1	2.08	0.60
1:M:413:ASP:O	1:M:416:THR:HB	2.02	0.60
2:N:85:VAL:HG13	2:N:235:THR:HG23	1.83	0.60
11:B:2086:HOH:O	2:F:192:ARG:HD3	2.01	0.60
4:R:93:LEU:N	4:R:93:LEU:HD22	2.09	0.60
1:A:444:VAL:CG2	1:A:445:PRO:HD3	2.32	0.60
1:C:413:ASP:HB2	1:C:416:THR:HB	1.83	0.60
3:Q:15:ASN:O	3:Q:19:ILE:HG12	2.02	0.60
2:N:130:SER:O	2:N:356:ARG:NH2	2.35	0.59
1:K:444:VAL:CG2	1:K:445:PRO:HD3	2.32	0.59
2:D:130:SER:O	2:D:356:ARG:NH2	2.35	0.59
3:Q:78:THR:CG2	3:Q:114:ILE:HB	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:93:THR:HG22	1:L:95:ASN:H	1.67	0.59
2:O:410:ILE:HG23	2:O:441:PHE:HE2	1.68	0.59
2:F:371:ALA:O	2:F:375:GLN:HG3	2.03	0.59
1:M:413:ASP:HB2	1:M:416:THR:HB	1.84	0.59
1:M:142:ARG:HH11	1:M:142:ARG:CG	2.13	0.59
3:G:78:THR:CG2	3:G:114:ILE:HB	2.33	0.59
1:A:243:PRO:HG3	1:A:283:LEU:HD21	1.83	0.59
3:G:15:ASN:O	3:G:19:ILE:HG12	2.02	0.59
2:E:410:ILE:HG23	2:E:441:PHE:HE2	1.68	0.59
1:K:243:PRO:HG3	1:K:283:LEU:HD21	1.83	0.59
5:S:59:ILE:CG2	5:S:60:THR:H	2.12	0.59
2:D:85:VAL:HG13	2:D:235:THR:HG23	1.84	0.59
1:M:291:PRO:HB2	1:M:295:ALA:HA	1.85	0.59
2:E:98:VAL:HB	2:E:232:VAL:HG13	1.85	0.58
3:Q:75:VAL:HG22	3:Q:108:VAL:HB	1.85	0.58
3:G:262:VAL:O	3:G:266:GLU:HG3	2.02	0.58
1:C:280:TYR:O	1:C:283:LEU:HD23	2.03	0.58
2:N:85:VAL:CG1	2:N:235:THR:HG23	2.33	0.58
2:D:41:THR:HB	2:D:42:PRO:CD	2.28	0.58
1:L:377:GLY:N	11:L:2148:HOH:O	2.36	0.58
4:R:116:ASP:O	4:R:117:ALA:CB	2.52	0.58
1:C:142:ARG:CG	1:C:142:ARG:HH11	2.14	0.58
2:O:98:VAL:HB	2:O:232:VAL:HG13	1.86	0.58
5:I:59:ILE:CG2	5:I:60:THR:H	2.13	0.58
2:D:85:VAL:CG1	2:D:235:THR:HG23	2.33	0.58
3:G:75:VAL:HB	3:G:164:ILE:HD13	1.85	0.57
5:I:46:GLN:O	5:I:55:GLU:HB2	2.04	0.57
3:Q:78:THR:OG1	3:Q:79:SER:N	2.37	0.57
5:S:46:GLN:O	5:S:55:GLU:HB2	2.04	0.57
4:H:116:ASP:O	4:H:117:ALA:CB	2.52	0.57
2:E:319:ASP:OD1	2:E:320:PRO:CD	2.51	0.57
3:G:78:THR:OG1	3:G:79:SER:N	2.37	0.57
3:Q:75:VAL:HB	3:Q:164:ILE:HD13	1.87	0.57
2:N:41:THR:HB	2:N:42:PRO:CD	2.28	0.57
3:G:75:VAL:HG22	3:G:108:VAL:HB	1.86	0.57
2:N:201:MET:HE2	2:N:217:LEU:HD21	1.85	0.57
1:B:93:THR:HG22	1:B:95:ASN:H	1.69	0.57
1:C:77:LEU:HD12	1:C:81:ASP:HB3	1.85	0.57
1:K:138:ILE:HD13	2:O:191:THR:HG23	1.87	0.56
1:C:291:PRO:HB2	1:C:295:ALA:HA	1.88	0.56
2:O:140:VAL:HG21	2:O:348:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:77:ILE:HG21	3:Q:222:MET:HG2	1.87	0.56
1:B:462:ARG:HD2	1:B:465:GLU:OE1	2.06	0.56
2:E:140:VAL:HG21	2:E:348:VAL:HG11	1.88	0.56
3:G:205:VAL:H	3:G:206:PRO:HD3	1.71	0.56
1:M:173:ARG:HG2	1:M:174:GLN:HG2	1.88	0.56
3:Q:205:VAL:H	3:Q:206:PRO:HD3	1.70	0.56
1:B:138:ILE:HD12	11:B:2027:HOH:O	2.04	0.56
1:B:332:GLN:HB3	2:E:318:THR:HB	1.88	0.56
2:P:371:ALA:O	2:P:375:GLN:HG3	2.05	0.56
1:L:335:ASP:HB2	3:Q:257:ARG:NH1	2.22	0.55
2:P:189:GLU:O	2:P:221:GLN:HB3	2.06	0.55
1:L:462:ARG:HD2	1:L:465:GLU:OE1	2.07	0.55
3:G:77:ILE:HG21	3:G:222:MET:HG2	1.89	0.55
1:C:173:ARG:HG2	1:C:174:GLN:HG2	1.89	0.55
3:Q:205:VAL:N	3:Q:206:PRO:CD	2.70	0.55
11:L:2142:HOH:O	2:P:192:ARG:HD3	2.07	0.55
3:G:205:VAL:N	3:G:206:PRO:CD	2.70	0.55
1:L:211:LYS:HD2	2:O:328:HIS:HA	1.87	0.55
1:A:302:TYR:O	1:A:306:ARG:HB2	2.06	0.55
1:M:77:LEU:HD12	1:M:81:ASP:HB3	1.88	0.55
6:J:3:GLY:CA	6:J:7:THR:HG23	2.38	0.54
2:F:289[B]:MET:CE	2:F:325:THR:HG23	2.37	0.54
3:G:49:GLN:HG2	3:G:52:TYR:HB2	1.88	0.54
2:F:189:GLU:O	2:F:221:GLN:HB3	2.07	0.54
6:T:3:GLY:CA	6:T:7:THR:HG23	2.38	0.54
1:K:42:ARG:HD2	1:K:72:GLN:NE2	2.23	0.54
3:Q:49:GLN:HG2	3:Q:52:TYR:HB2	1.88	0.54
2:O:158:GLY:O	2:O:161:VAL:HG22	2.08	0.54
3:G:108:VAL:HG22	3:G:128:LEU:HB3	1.90	0.54
1:M:170:ILE:HG23	1:M:353:PHE:HD1	1.73	0.54
1:A:42:ARG:HD2	1:A:72:GLN:NE2	2.23	0.54
3:Q:108:VAL:HG22	3:Q:128:LEU:HB3	1.90	0.53
1:M:336:VAL:HG11	1:M:353:PHE:HE1	1.73	0.53
2:E:158:GLY:O	2:E:161:VAL:HG22	2.09	0.53
2:E:133:ILE:HD12	2:E:146:PRO:HB2	1.89	0.53
1:C:222:LEU:HB2	1:C:228:MET:CE	2.38	0.53
1:C:170:ILE:HG23	1:C:353:PHE:HD1	1.73	0.53
2:F:289[B]:MET:CE	2:F:293:GLN:HE21	2.22	0.53
2:D:204:THR:CG2	2:D:206:VAL:HG23	2.38	0.53
3:G:203:ALA:HB1	4:H:35:LYS:NZ	2.24	0.53
2:N:440:SER:HB3	2:N:463:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:302:TYR:O	1:K:306:ARG:HB2	2.07	0.53
2:N:204:THR:CG2	2:N:206:VAL:HG23	2.38	0.53
1:L:399:TYR:OH	1:L:424:GLU:HG3	2.09	0.53
4:R:118:ARG:HH11	5:S:8:ILE:HG13	1.74	0.53
2:O:133:ILE:HD12	2:O:146:PRO:HB2	1.90	0.53
1:C:138:ILE:H	1:C:138:ILE:HD12	1.74	0.53
1:B:399:TYR:OH	1:B:424:GLU:HG3	2.09	0.52
2:P:289[B]:MET:CE	2:P:293:GLN:HE21	2.21	0.52
2:E:33:ILE:O	2:E:34:LEU:HB2	2.09	0.52
4:R:13:GLN:HG2	4:R:23:SER:HA	1.91	0.52
1:M:222:LEU:HB2	1:M:228:MET:CE	2.39	0.52
2:N:396:LEU:HD13	2:N:400:ASP:HB3	1.90	0.52
3:Q:219:LEU:HD21	4:R:17:PRO:HB3	1.92	0.52
2:P:289[B]:MET:CE	2:P:325:THR:HG23	2.40	0.52
1:C:358:LEU:HB3	1:C:363:ILE:HG12	1.92	0.52
1:C:402:VAL:HG12	1:C:420:LEU:HD13	1.92	0.52
2:D:440:SER:HB3	2:D:463:ILE:HB	1.91	0.52
1:M:358:LEU:HB3	1:M:363:ILE:HG12	1.91	0.52
1:A:174:GLN:HG3	2:D:354:LYS:HG3	1.90	0.52
2:D:242:TYR:CD1	2:D:246:GLU:HG3	2.45	0.52
1:C:336:VAL:HG11	1:C:353:PHE:HE1	1.74	0.52
2:P:152:LYS:NZ	2:P:293:GLN:HB3	2.25	0.52
5:I:4:ARG:HD2	5:I:4:ARG:N	2.25	0.52
1:M:402:VAL:HG12	1:M:420:LEU:HD13	1.92	0.52
1:L:220:GLN:HE21	1:L:224:GLN:NE2	2.08	0.52
1:M:389:ALA:HB2	1:M:447:ILE:HG21	1.92	0.52
1:C:283:LEU:HD23	1:C:284:SER:H	1.73	0.51
1:C:389:ALA:HB2	1:C:447:ILE:HG21	1.91	0.51
4:H:13:GLN:HG2	4:H:23:SER:HA	1.92	0.51
2:N:218:VAL:HG21	2:N:236:GLY:HA2	1.91	0.51
4:R:118:ARG:NH1	5:S:8:ILE:HA	2.25	0.51
2:O:456:ALA:HA	2:O:469:LYS:HD3	1.92	0.51
2:N:242:TYR:CD1	2:N:246:GLU:HG3	2.45	0.51
2:O:344:ILE:HG23	2:O:415:SER:HB3	1.92	0.51
1:B:154:ALA:HB1	1:B:367:ILE:HD12	1.93	0.51
2:O:15:ALA:HB3	2:O:22:ASP:HB2	1.93	0.51
2:N:189:GLU:O	2:N:221:GLN:HB3	2.11	0.51
2:O:319:ASP:OD1	2:O:320:PRO:CD	2.54	0.51
1:M:302:TYR:CE1	1:M:306:ARG:HB3	2.46	0.51
4:H:116:ASP:O	4:H:117:ALA:HB3	2.11	0.51
1:B:444:VAL:HG22	1:B:445:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.93	0.51
4:R:116:ASP:O	4:R:117:ALA:HB3	2.10	0.51
1:M:414:ALA:HA	1:M:417:LYS:HE3	1.92	0.51
2:E:456:ALA:HA	2:E:469:LYS:HD3	1.93	0.51
2:F:449:TYR:HD1	2:F:452:ILE:CD1	2.23	0.51
2:O:204:THR:HG23	2:O:206:VAL:HG13	1.92	0.51
1:M:283:LEU:HD23	1:M:284:SER:H	1.76	0.51
1:C:414:ALA:HA	1:C:417:LYS:HE3	1.93	0.51
3:G:207:ARG:HH12	5:I:4:ARG:HH21	1.59	0.51
1:K:404:ALA:HB2	3:Q:18:LYS:HE3	1.92	0.51
5:S:4:ARG:N	5:S:4:ARG:HD2	2.25	0.51
2:E:152:LYS:HE3	2:E:296:ILE:HB	1.94	0.50
2:D:218:VAL:HG21	2:D:236:GLY:HA2	1.92	0.50
2:D:396:LEU:HD13	2:D:400:ASP:HB3	1.91	0.50
1:B:478:HIS:O	1:B:481:LEU:HB2	2.11	0.50
1:L:478:HIS:O	1:L:481:LEU:HB2	2.11	0.50
2:E:344:ILE:HG23	2:E:415:SER:HB3	1.93	0.50
2:F:242:TYR:CE2	2:F:246:GLU:HG3	2.46	0.50
2:F:152:LYS:NZ	2:F:293:GLN:HB3	2.26	0.50
2:P:449:TYR:HD1	2:P:452:ILE:CD1	2.24	0.50
2:F:384:LEU:O	2:F:388:ILE:HG12	2.12	0.50
1:M:404:ALA:HB1	6:T:23:ALA:HB2	1.92	0.50
1:B:220:GLN:HE21	1:B:224:GLN:NE2	2.10	0.50
2:P:242:TYR:CE2	2:P:246:GLU:HG3	2.47	0.50
1:C:364:ARG:HA	1:C:365:PRO:C	2.31	0.50
2:O:340:SER:HB3	2:O:347:ALA:CB	2.42	0.50
1:M:138:ILE:HD12	1:M:138:ILE:H	1.77	0.50
1:K:187:ASN:OD1	1:K:437:PRO:HB2	2.11	0.50
2:F:345:TYR:HA	2:F:346:PRO:C	2.32	0.50
2:O:33:ILE:O	2:O:34:LEU:HB2	2.12	0.49
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.93	0.49
1:L:243:PRO:HG3	1:L:283:LEU:HD21	1.94	0.49
2:D:152:LYS:HD2	2:D:296:ILE:O	2.12	0.49
1:C:413:ASP:HB3	1:C:416:THR:HB	1.94	0.49
2:P:15:ALA:HB3	2:P:22:ASP:HB2	1.92	0.49
1:L:444:VAL:HG22	1:L:445:PRO:HD3	1.94	0.49
1:K:211:LYS:HD3	2:N:328:HIS:HA	1.94	0.49
2:P:384:LEU:O	2:P:388:ILE:HG12	2.13	0.49
1:M:413:ASP:HB3	1:M:416:THR:CB	2.42	0.49
1:M:413:ASP:HB3	1:M:416:THR:HB	1.93	0.49
1:B:421:VAL:O	1:B:425:ARG:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:340:SER:HB3	2:O:347:ALA:HB2	1.94	0.49
1:C:302:TYR:CE1	1:C:306:ARG:HB3	2.48	0.49
1:C:413:ASP:HB3	1:C:416:THR:CB	2.43	0.49
2:F:375:GLN:HG2	11:F:2076:HOH:O	2.11	0.49
1:C:280:TYR:O	1:C:283:LEU:CD2	2.61	0.49
1:A:187:ASN:OD1	1:A:437:PRO:HB2	2.11	0.49
2:N:449:TYR:HD1	2:N:452:ILE:HD12	1.76	0.49
3:Q:99:LEU:HD21	3:Q:107:ILE:HD11	1.95	0.49
1:L:421:VAL:O	1:L:425:ARG:HG2	2.13	0.49
1:M:364:ARG:HA	1:M:365:PRO:C	2.33	0.49
3:G:99:LEU:HD21	3:G:107:ILE:HD11	1.95	0.49
2:D:449:TYR:HD1	2:D:452:ILE:HD12	1.77	0.49
2:E:204:THR:HG23	2:E:206:VAL:HG13	1.94	0.49
2:O:152:LYS:HE3	2:O:296:ILE:HB	1.95	0.49
1:A:28:ASN:HB3	1:A:48:ASN:ND2	2.28	0.49
1:M:142:ARG:HG2	1:M:142:ARG:NH1	2.19	0.49
2:E:140:VAL:HG21	2:E:348:VAL:CG1	2.42	0.49
1:C:222:LEU:CB	1:C:228:MET:HE2	2.43	0.49
2:E:340:SER:HB3	2:E:347:ALA:CB	2.43	0.49
2:P:345:TYR:HA	2:P:346:PRO:C	2.33	0.48
4:R:116:ASP:OD1	4:R:116:ASP:N	2.45	0.48
3:G:75:VAL:HB	3:G:164:ILE:CD1	2.42	0.48
2:O:140:VAL:HG21	2:O:348:VAL:CG1	2.42	0.48
4:H:94:GLU:O	5:I:26:LYS:HD2	2.13	0.48
2:N:178:HIS:HE1	2:N:250:ASP:O	1.96	0.48
4:H:54:PRO:HD3	5:I:13:TYR:OH	2.12	0.48
4:H:116:ASP:OD1	4:H:116:ASP:N	2.46	0.48
2:N:244:ARG:HD3	2:N:304:VAL:HG23	1.95	0.48
1:A:478:HIS:HB3	1:A:481:LEU:HG	1.94	0.48
1:B:299:ASP:HA	11:B:2075:HOH:O	2.13	0.48
1:L:154:ALA:HB1	1:L:367:ILE:HD12	1.96	0.48
5:I:4:ARG:HD2	5:I:4:ARG:H	1.79	0.48
2:N:25:PHE:HB2	2:N:30:LEU:HD23	1.96	0.48
1:C:363:ILE:CG1	1:C:363:ILE:O	2.60	0.48
2:P:152:LYS:HZ1	2:P:293:GLN:HB3	1.78	0.48
3:Q:75:VAL:HB	3:Q:164:ILE:CD1	2.43	0.48
11:H:2001:HOH:O	5:I:13:TYR:HE2	1.97	0.48
1:B:243:PRO:HG3	1:B:283:LEU:HD21	1.95	0.48
1:K:478:HIS:HB3	1:K:481:LEU:HG	1.94	0.48
2:P:333:THR:HA	2:P:353:SER:HB3	1.94	0.48
3:G:184:ASN:HA	3:G:210:PHE:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:LEU:HB2	1:C:228:MET:HE2	1.94	0.48
1:B:335:ASP:HB2	3:G:257:ARG:NH1	2.28	0.48
3:G:119:LEU:HD11	5:I:53:ALA:HB1	1.95	0.48
2:E:340:SER:HB3	2:E:347:ALA:HB2	1.96	0.48
2:D:25:PHE:HB2	2:D:30:LEU:HD23	1.96	0.48
1:K:28:ASN:HB3	1:K:48:ASN:ND2	2.29	0.48
2:D:189:GLU:O	2:D:221:GLN:HB3	2.14	0.48
1:K:174:GLN:HG3	2:N:354:LYS:HG3	1.95	0.48
2:F:333:THR:HA	2:F:353:SER:HB3	1.95	0.48
1:A:239:SER:HB3	2:D:294:GLU:HG3	1.96	0.48
1:M:336:VAL:HG11	1:M:353:PHE:CZ	2.48	0.47
5:S:4:ARG:H	5:S:4:ARG:HD2	1.79	0.47
1:M:280:TYR:O	1:M:283:LEU:CD2	2.62	0.47
1:M:306:ARG:HE	10:M:602:EDO:H21	1.78	0.47
2:N:152:LYS:HD2	2:N:296:ILE:O	2.14	0.47
2:D:64:MET:CE	2:D:228:ALA:HA	2.43	0.47
5:I:15:ASN:ND2	11:I:2001:HOH:O	2.27	0.47
3:Q:184:ASN:HA	3:Q:210:PHE:CD1	2.49	0.47
1:A:444:VAL:HG23	1:A:445:PRO:CD	2.42	0.47
1:M:280:TYR:O	1:M:283:LEU:HD23	2.15	0.47
2:F:289[B]:MET:HE3	2:F:293:GLN:HE21	1.79	0.47
2:N:64:MET:CE	2:N:228:ALA:HA	2.44	0.47
1:K:421:VAL:O	1:K:425:ARG:HD2	2.15	0.47
5:S:61:LYS:HE3	5:S:61:LYS:HB3	1.60	0.47
1:B:211:LYS:HD2	2:E:328:HIS:HA	1.96	0.47
2:N:224:GLU:O	2:N:229:ARG:HD3	2.15	0.47
2:P:65:ASP:HB2	10:P:603:EDO:H21	1.96	0.47
3:Q:91:LEU:HD23	3:Q:114:ILE:HD13	1.96	0.47
2:F:152:LYS:HZ1	2:F:293:GLN:HB3	1.79	0.47
2:D:200:GLU:O	2:D:204:THR:HB	2.15	0.47
2:N:200:GLU:O	2:N:204:THR:HB	2.15	0.47
2:O:339:ILE:HG22	2:O:340:SER:H	1.79	0.47
2:N:64:MET:HE1	2:N:228:ALA:HA	1.97	0.47
4:R:30:VAL:HG21	4:R:83:LEU:CD2	2.45	0.47
1:K:301:PHE:HB3	2:O:267:GLU:OE2	2.15	0.47
4:H:30:VAL:HG21	4:H:83:LEU:CD2	2.45	0.47
1:K:239:SER:HB3	2:N:294:GLU:HG3	1.96	0.47
2:D:178:HIS:HE1	2:D:250:ASP:O	1.97	0.47
2:E:336:SER:HB3	2:E:339:ILE:HG12	1.97	0.47
1:C:192:ASN:HA	1:C:200:LYS:HG2	1.96	0.47
1:A:280:TYR:CE2	1:A:297:PRO:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:222:LEU:CB	1:M:228:MET:HE2	2.45	0.46
1:A:64:MET:SD	1:A:97:VAL:HG21	2.55	0.46
3:G:205:VAL:H	3:G:206:PRO:CD	2.28	0.46
1:K:55:VAL:HG21	1:K:75:ILE:HD13	1.96	0.46
1:M:192:ASN:HA	1:M:200:LYS:HG2	1.97	0.46
2:N:385:GLN:OE1	6:T:7:THR:HG22	2.15	0.46
5:S:4:ARG:N	5:S:4:ARG:CD	2.79	0.46
2:D:64:MET:HE1	2:D:231:ARG:HB2	1.97	0.46
2:O:417:PRO:HG2	2:O:430:LYS:HG2	1.98	0.46
1:A:421:VAL:O	1:A:425:ARG:HD2	2.16	0.46
1:A:346:SER:CB	2:E:260:ARG:HH22	2.29	0.46
1:A:55:VAL:HG21	1:A:75:ILE:HD13	1.97	0.46
1:K:444:VAL:HG23	1:K:445:PRO:CD	2.43	0.46
1:B:384:ALA:HA	1:B:387:GLN:HE21	1.81	0.46
2:F:349:ASP:OD1	2:F:351:LEU:O	2.34	0.46
1:C:336:VAL:HG11	1:C:353:PHE:CZ	2.49	0.46
1:K:108:ARG:NH1	1:K:123:ILE:HD13	2.31	0.46
4:R:118:ARG:HH12	5:S:8:ILE:HA	1.80	0.46
2:P:289[B]:MET:HE3	2:P:293:GLN:HE21	1.81	0.46
3:G:91:LEU:HD23	3:G:114:ILE:HD13	1.97	0.46
2:E:339:ILE:HG22	2:E:340:SER:H	1.81	0.46
1:M:43:VAL:HG21	1:M:75:ILE:HD12	1.98	0.46
2:D:244:ARG:HD3	2:D:304:VAL:HG23	1.98	0.46
1:A:108:ARG:NH1	1:A:123:ILE:HD13	2.31	0.46
3:G:125:ASN:N	3:G:125:ASN:HD22	2.14	0.46
3:Q:205:VAL:H	3:Q:206:PRO:CD	2.28	0.46
6:T:15:ASP:HB2	6:T:18:VAL:H	1.81	0.46
3:Q:125:ASN:HD22	3:Q:125:ASN:N	2.13	0.46
1:L:384:ALA:HA	1:L:387:GLN:HE21	1.81	0.46
2:D:224:GLU:O	2:D:229:ARG:HD3	2.16	0.46
1:B:197:GLU:HB2	11:B:2049:HOH:O	2.16	0.45
1:A:192:ASN:HA	1:A:200:LYS:HG2	1.98	0.45
2:O:336:SER:HB3	2:O:339:ILE:HG12	1.98	0.45
1:A:139:LEU:HD22	2:E:105:GLU:HB2	1.97	0.45
2:E:67:THR:HB	2:E:70:LEU:HD12	1.98	0.45
1:K:64:MET:SD	1:K:97:VAL:HG21	2.56	0.45
2:N:253:LEU:O	2:N:306:SER:HA	2.15	0.45
2:E:417:PRO:HG2	2:E:430:LYS:HG2	1.99	0.45
1:L:402:VAL:O	1:L:405:PHE:CD1	2.69	0.45
1:A:329:ILE:HD11	1:A:344:VAL:HG21	1.98	0.45
2:F:377:THR:HG22	2:F:407:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:15:ASP:HB2	6:J:18:VAL:H	1.82	0.45
1:K:124:ASP:N	1:K:124:ASP:OD1	2.49	0.45
2:E:168:GLN:HA	2:E:171:ILE:HD12	1.98	0.45
1:K:280:TYR:CE2	1:K:297:PRO:HG2	2.51	0.45
1:K:361:LYS:HG3	2:N:379:GLN:HG2	1.98	0.45
1:C:43:VAL:HG21	1:C:75:ILE:HD12	1.99	0.45
1:B:402:VAL:O	1:B:405:PHE:CD1	2.69	0.45
6:J:29:VAL:O	6:J:33:GLU:HG3	2.15	0.45
2:P:349:ASP:OD1	2:P:351:LEU:O	2.35	0.45
1:M:222:LEU:HB2	1:M:228:MET:HE2	1.98	0.45
6:T:29:VAL:O	6:T:33:GLU:HG3	2.15	0.45
1:L:93:THR:HG22	1:L:95:ASN:N	2.31	0.45
1:A:139:LEU:CD2	2:E:105:GLU:HB2	2.47	0.45
2:D:389:ALA:HB2	6:J:21:ALA:HB2	1.98	0.45
3:Q:46:GLU:O	3:Q:50:LEU:HB2	2.17	0.45
2:O:443:ALA:HB1	2:O:449:TYR:HE2	1.82	0.45
1:C:107:GLY:HA2	1:C:228:MET:O	2.17	0.44
2:P:152:LYS:NZ	2:P:293:GLN:O	2.50	0.44
1:K:192:ASN:HA	1:K:200:LYS:HG2	1.99	0.44
1:A:124:ASP:OD1	1:A:124:ASP:N	2.49	0.44
2:O:237:LEU:HD21	2:O:295:ARG:HB2	1.99	0.44
1:B:93:THR:HG22	1:B:95:ASN:N	2.32	0.44
2:P:244:ARG:HD3	2:P:304:VAL:HG23	1.99	0.44
2:P:279:VAL:O	2:P:279:VAL:HG12	2.17	0.44
5:I:4:ARG:N	5:I:4:ARG:CD	2.78	0.44
1:M:417:LYS:HA	1:M:420:LEU:HB3	2.00	0.44
1:L:364:ARG:HA	1:L:365:PRO:C	2.37	0.44
1:B:364:ARG:HA	1:B:365:PRO:C	2.37	0.44
2:E:443:ALA:HB1	2:E:449:TYR:HE2	1.82	0.44
2:D:64:MET:HE1	2:D:228:ALA:HA	2.00	0.44
2:P:237:LEU:HD13	2:P:296:ILE:HG12	1.99	0.44
2:P:377:THR:HG22	2:P:407:ALA:HB2	1.99	0.44
1:C:417:LYS:HA	1:C:420:LEU:HB3	2.00	0.44
2:F:244:ARG:HD3	2:F:304:VAL:HG23	1.99	0.44
2:F:292:LEU:HD12	2:F:292:LEU:C	2.38	0.44
2:N:64:MET:HE1	2:N:231:ARG:HB2	1.99	0.44
1:A:309:GLU:HG3	2:E:223:ASN:HB3	2.00	0.44
5:S:55:GLU:OE1	5:S:55:GLU:N	2.51	0.44
1:C:378:SER:HB2	1:C:386:LYS:HD2	2.00	0.44
2:E:237:LEU:HD21	2:E:295:ARG:HB2	1.99	0.44
2:O:67:THR:HB	2:O:70:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ASP:CB	1:C:416:THR:CB	2.95	0.44
1:L:26:ASN:O	1:L:30:THR:HB	2.17	0.44
2:O:168:GLN:HA	2:O:171:ILE:HD12	2.00	0.44
1:L:383:LYS:HD3	1:L:490:GLU:HG3	2.00	0.44
1:B:383:LYS:HD3	1:B:490:GLU:HG3	2.00	0.44
4:R:94:GLU:O	5:S:26:LYS:HD2	2.18	0.44
2:O:97:ASN:HB2	11:O:2010:HOH:O	2.18	0.43
3:G:182:ILE:HD11	3:G:217:GLN:HG3	2.00	0.43
1:B:422:ARG:HE	1:B:453:GLY:HA2	1.83	0.43
5:I:18:ALA:HA	5:I:21:ILE:HD12	2.00	0.43
1:A:422:ARG:NH1	1:A:453:GLY:HA2	2.11	0.43
4:R:118:ARG:HD2	5:S:8:ILE:HD11	2.00	0.43
1:K:51:ALA:O	1:K:52:GLU:HB2	2.18	0.43
5:I:55:GLU:OE1	5:I:55:GLU:N	2.51	0.43
1:B:335:ASP:OD2	3:G:257:ARG:HD3	2.18	0.43
1:A:73:VAL:HG12	1:A:75:ILE:HG13	1.99	0.43
3:G:46:GLU:O	3:G:50:LEU:HB2	2.18	0.43
1:K:329:ILE:HD11	1:K:344:VAL:HG21	2.00	0.43
1:A:361:LYS:HG3	2:D:379:GLN:HG2	2.00	0.43
1:C:413:ASP:HB3	1:C:416:THR:OG1	2.18	0.43
2:E:140:VAL:HG13	2:E:414:LEU:HB3	2.00	0.43
1:L:440:THR:O	1:L:444:VAL:HG13	2.17	0.43
1:L:402:VAL:HA	1:L:405:PHE:CD1	2.52	0.43
1:B:402:VAL:HA	1:B:405:PHE:CD1	2.52	0.43
1:C:142:ARG:NH1	1:C:142:ARG:CG	2.75	0.43
1:K:444:VAL:HG21	1:K:485:ILE:HG21	2.00	0.43
1:A:173:ARG:C	1:A:174:GLN:HG2	2.38	0.43
2:O:300:LYS:HD3	2:O:300:LYS:HA	1.74	0.43
1:C:140:PRO:HB3	1:C:318:GLU:HG3	2.00	0.43
2:F:84:SER:HB3	11:F:2015:HOH:O	2.19	0.43
1:M:413:ASP:HB3	1:M:416:THR:OG1	2.18	0.43
2:D:390:ILE:HD13	3:G:19:ILE:HG13	1.99	0.43
2:F:152:LYS:NZ	2:F:293:GLN:O	2.52	0.43
1:B:440:THR:O	1:B:444:VAL:HG13	2.18	0.43
2:E:300:LYS:HA	2:E:300:LYS:HD3	1.75	0.43
2:N:98:VAL:HG23	2:N:232:VAL:HA	2.01	0.43
1:M:140:PRO:HB3	1:M:318:GLU:HG3	2.01	0.43
3:Q:182:ILE:HD11	3:Q:217:GLN:HG3	2.01	0.43
1:K:422:ARG:NH1	1:K:453:GLY:HA2	2.10	0.43
5:S:18:ALA:HA	5:S:21:ILE:HD12	2.00	0.43
1:A:211:LYS:HD3	2:D:328:HIS:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:338:ALA:O	1:K:342:THR:HB	2.18	0.43
1:A:492:SER:HB2	1:A:495:LEU:H	1.84	0.43
1:L:422:ARG:HE	1:L:453:GLY:HA2	1.84	0.43
2:D:41:THR:CB	2:D:42:PRO:HD2	2.40	0.43
1:A:444:VAL:HG21	1:A:485:ILE:HG21	2.01	0.43
2:D:253:LEU:O	2:D:306:SER:HA	2.18	0.43
2:O:95:ILE:HD11	2:O:198:TYR:CD1	2.54	0.43
1:M:285:LEU:HD21	1:M:291:PRO:HB3	2.01	0.43
2:N:26:GLU:O	2:N:29:GLU:CG	2.66	0.42
2:D:222:MET:HA	2:D:229:ARG:HD2	2.01	0.42
1:A:404:ALA:HB2	3:G:18:LYS:HE3	2.01	0.42
1:K:346:SER:CB	2:O:260:ARG:HH22	2.32	0.42
2:O:367:HIS:CE1	2:O:434:LEU:HD11	2.54	0.42
2:O:140:VAL:HG13	2:O:414:LEU:HB3	2.01	0.42
2:F:374:VAL:HG13	2:F:410:ILE:HG21	2.01	0.42
2:D:98:VAL:HG23	2:D:232:VAL:HA	2.01	0.42
1:K:170:ILE:HG23	1:K:353:PHE:HD1	1.84	0.42
3:G:149:LYS:HE2	5:I:44:TYR:CZ	2.53	0.42
1:C:399:TYR:CG	1:C:423:GLY:HA3	2.54	0.42
1:M:107:GLY:HA2	1:M:228:MET:O	2.20	0.42
1:M:399:TYR:CG	1:M:423:GLY:HA3	2.55	0.42
1:M:378:SER:HB2	1:M:386:LYS:HD2	2.01	0.42
1:C:402:VAL:O	1:C:402:VAL:HG12	2.19	0.42
1:M:402:VAL:O	1:M:402:VAL:HG12	2.19	0.42
3:Q:55:ALA:O	3:Q:191:SER:HB2	2.20	0.42
2:E:367:HIS:CE1	2:E:434:LEU:HD11	2.55	0.42
1:M:142:ARG:NH1	1:M:142:ARG:CG	2.74	0.42
2:E:152:LYS:HE2	2:E:293:GLN:HB3	2.02	0.42
2:N:321:ALA:HB3	2:N:322:PRO:CD	2.49	0.42
1:M:434:GLN:OE1	9:M:600:ADP:H2'	2.19	0.42
1:K:492:SER:HB2	1:K:495:LEU:H	1.84	0.42
1:K:173:ARG:C	1:K:174:GLN:HG2	2.39	0.42
1:B:26:ASN:O	1:B:30:THR:HB	2.19	0.42
2:P:258:ILE:O	2:P:258:ILE:HD13	2.20	0.42
1:K:73:VAL:HG12	1:K:75:ILE:HG13	2.01	0.42
2:N:158:GLY:O	2:N:161:VAL:HG22	2.19	0.42
1:L:99:VAL:HG21	1:L:251:THR:HB	2.02	0.42
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.50	0.42
2:P:97:ASN:HD22	2:P:97:ASN:C	2.23	0.42
6:J:30:ARG:CG	6:J:30:ARG:NH1	2.70	0.42
1:A:51:ALA:O	1:A:52:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ASP:OD1	2:E:192:ARG:NE	2.42	0.42
2:D:182:SER:O	2:D:215:VAL:HA	2.20	0.42
1:M:400:ARG:HA	1:M:400:ARG:HD2	1.88	0.42
5:I:43:PHE:CD2	5:I:59:ILE:O	2.74	0.41
2:D:26:GLU:O	2:D:29:GLU:CG	2.67	0.41
6:T:7:THR:HA	6:T:8:PRO:HD3	1.92	0.41
2:O:253:LEU:O	2:O:306:SER:HA	2.20	0.41
2:E:95:ILE:HD11	2:E:198:TYR:CD1	2.55	0.41
1:K:260:ARG:O	1:K:321:GLY:HA3	2.20	0.41
2:N:242:TYR:CE1	2:N:246:GLU:HG3	2.55	0.41
2:F:449:TYR:HD1	2:F:452:ILE:HD12	1.85	0.41
2:N:449:TYR:CD1	2:N:452:ILE:HD12	2.54	0.41
3:G:159:TYR:HA	3:G:160:PRO:HD3	1.94	0.41
1:A:170:ILE:HG23	1:A:353:PHE:HD1	1.85	0.41
2:D:242:TYR:CE1	2:D:246:GLU:HG3	2.55	0.41
2:N:222:MET:HA	2:N:229:ARG:HD2	2.02	0.41
2:O:300:LYS:HG2	11:O:2015:HOH:O	2.20	0.41
1:L:38:ASP:HB3	1:L:286:LEU:HD22	2.02	0.41
4:R:49:VAL:HG22	4:R:76:THR:HG23	2.02	0.41
1:A:260:ARG:O	1:A:321:GLY:HA3	2.20	0.41
1:A:355:GLU:OE2	1:A:368:ASN:ND2	2.48	0.41
1:C:400:ARG:HA	1:C:400:ARG:HD2	1.88	0.41
1:K:242:ALA:N	1:K:243:PRO:CD	2.83	0.41
2:P:449:TYR:HD1	2:P:452:ILE:HD12	1.85	0.41
1:K:346:SER:HB2	2:O:260:ARG:HH22	1.85	0.41
2:P:374:VAL:HG13	2:P:410:ILE:HG21	2.03	0.41
1:A:338:ALA:O	1:A:342:THR:HB	2.20	0.41
1:L:192:ASN:HA	1:L:200:LYS:HG2	2.03	0.41
3:G:55:ALA:O	3:G:191:SER:HB2	2.20	0.41
11:G:2007:HOH:O	5:I:36:ASN:HB3	2.21	0.41
1:M:413:ASP:CB	1:M:416:THR:CB	2.95	0.41
1:L:299:ASP:HA	11:L:2125:HOH:O	2.21	0.41
4:H:49:VAL:HG22	4:H:76:THR:HG23	2.03	0.41
2:E:98:VAL:HB	2:E:232:VAL:CG1	2.50	0.41
2:F:449:TYR:CD1	2:F:452:ILE:HD12	2.56	0.41
2:D:449:TYR:CD1	2:D:452:ILE:HD12	2.55	0.41
1:B:192:ASN:HA	1:B:200:LYS:HG2	2.03	0.41
4:R:35:LYS:HD2	4:R:51:GLN:HE22	1.84	0.41
1:A:242:ALA:N	1:A:243:PRO:CD	2.83	0.41
1:C:434:GLN:OE1	9:C:600:ADP:H2'	2.20	0.41
1:C:285:LEU:HD21	1:C:291:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:449:TYR:CD1	2:P:452:ILE:HD12	2.56	0.41
1:L:203:CYS:O	1:L:231:SER:HA	2.21	0.41
1:K:349:ASP:O	1:K:375:ARG:HB2	2.21	0.41
5:S:43:PHE:CD2	5:S:59:ILE:O	2.74	0.41
2:E:221:GLN:H	2:E:221:GLN:HG2	1.66	0.41
4:H:111:ASN:O	4:H:114:SER:HB3	2.21	0.41
2:F:449:TYR:HD1	2:F:452:ILE:HD11	1.85	0.41
2:F:237:LEU:HD13	2:F:296:ILE:HG12	2.02	0.41
3:G:193:SER:HB3	3:G:196:LYS:HE2	2.02	0.41
2:N:33:ILE:O	2:N:34:LEU:HB2	2.21	0.41
6:J:7:THR:HA	6:J:8:PRO:HD3	1.92	0.40
1:B:399:TYR:CD1	1:B:423:GLY:HA3	2.57	0.40
1:A:349:ASP:O	1:A:375:ARG:HB2	2.22	0.40
2:P:256:ASP:HA	2:P:257:ASN:HA	1.88	0.40
1:B:203:CYS:O	1:B:231:SER:HA	2.22	0.40
5:I:55:GLU:HA	5:I:56:PRO:HD3	1.96	0.40
3:Q:193:SER:HB3	3:Q:196:LYS:HE2	2.02	0.40
5:S:10:TYR:CE2	5:S:14:LEU:HD11	2.56	0.40
1:B:99:VAL:HG21	1:B:251:THR:HB	2.04	0.40
1:L:146:GLU:HA	1:L:147:PRO:HD3	1.95	0.40
1:C:85:LYS:O	1:C:88:GLU:HB3	2.20	0.40
2:N:404:VAL:O	2:N:408:ARG:HG3	2.22	0.40
1:L:399:TYR:CD1	1:L:423:GLY:HA3	2.57	0.40
1:M:363:ILE:CG1	1:M:363:ILE:O	2.59	0.40
2:O:98:VAL:HB	2:O:232:VAL:CG1	2.50	0.40
2:E:109:ILE:HG22	2:E:111:SER:HB2	2.03	0.40
2:E:253:LEU:O	2:E:306:SER:HA	2.22	0.40
2:N:182:SER:O	2:N:215:VAL:HA	2.21	0.40
1:A:305:SER:HB2	2:E:222:MET:HB3	2.03	0.40
2:D:158:GLY:O	2:D:161:VAL:HG22	2.21	0.40
1:B:139:LEU:HD12	1:B:139:LEU:HA	1.89	0.40
6:T:30:ARG:NH1	6:T:30:ARG:CG	2.70	0.40
2:N:396:LEU:CD1	2:N:400:ASP:HB3	2.50	0.40
1:C:399:TYR:CD1	1:C:423:GLY:HA3	2.57	0.40
3:Q:191:SER:OG	3:Q:194:PHE:HB2	2.22	0.40
3:Q:149:LYS:HE2	5:S:44:TYR:CZ	2.57	0.40
1:B:38:ASP:HB3	1:B:286:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	482/510 (94%)	462 (96%)	19 (4%)	1 (0%)	52 75
1	B	477/510 (94%)	464 (97%)	13 (3%)	0	100 100
1	C	482/510 (94%)	460 (95%)	22 (5%)	0	100 100
1	K	482/510 (94%)	460 (95%)	21 (4%)	1 (0%)	52 75
1	L	477/510 (94%)	463 (97%)	14 (3%)	0	100 100
1	M	482/510 (94%)	460 (95%)	22 (5%)	0	100 100
2	D	468/478 (98%)	449 (96%)	18 (4%)	1 (0%)	52 75
2	E	466/478 (98%)	444 (95%)	20 (4%)	2 (0%)	39 61
2	F	468/478 (98%)	445 (95%)	21 (4%)	2 (0%)	39 61
2	N	468/478 (98%)	449 (96%)	18 (4%)	1 (0%)	52 75
2	O	466/478 (98%)	445 (96%)	19 (4%)	2 (0%)	39 61
2	P	470/478 (98%)	446 (95%)	22 (5%)	2 (0%)	39 61
3	G	261/278 (94%)	251 (96%)	10 (4%)	0	100 100
3	Q	262/278 (94%)	252 (96%)	10 (4%)	0	100 100
4	H	120/138 (87%)	104 (87%)	14 (12%)	2 (2%)	11 19
4	R	120/138 (87%)	104 (87%)	14 (12%)	2 (2%)	11 19
5	I	54/61 (88%)	51 (94%)	2 (4%)	1 (2%)	10 16
5	S	54/61 (88%)	51 (94%)	2 (4%)	1 (2%)	10 16
6	J	34/63 (54%)	33 (97%)	1 (3%)	0	100 100
6	T	34/63 (54%)	33 (97%)	1 (3%)	0	100 100
All	All	6627/7008 (95%)	6326 (96%)	283 (4%)	18 (0%)	46 68

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	117	ALA

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Mol	Chain	Res	Type
5	I	57	THR
4	R	117	ALA
5	S	57	THR
2	F	352	ASP
4	H	115	SER
2	P	352	ASP
4	R	115	SER
2	O	448	LYS
2	E	448	LYS
1	K	339	TYR
2	O	279	VAL
1	A	339	TYR
2	E	279	VAL
2	D	42	PRO
2	N	42	PRO
2	F	279	VAL
2	P	279	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	390/412 (95%)	381 (98%)	9 (2%)	58	83
1	B	387/412 (94%)	367 (95%)	20 (5%)	29	51
1	C	390/412 (95%)	376 (96%)	14 (4%)	42	69
1	K	390/412 (95%)	380 (97%)	10 (3%)	54	81
1	L	387/412 (94%)	366 (95%)	21 (5%)	27	49
1	M	390/412 (95%)	375 (96%)	15 (4%)	40	67
2	D	380/384 (99%)	365 (96%)	15 (4%)	39	66
2	E	378/384 (98%)	367 (97%)	11 (3%)	50	77
2	F	380/384 (99%)	369 (97%)	11 (3%)	50	77
2	N	380/384 (99%)	365 (96%)	15 (4%)	39	66
2	O	378/384 (98%)	366 (97%)	12 (3%)	46	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	P	382/384 (100%)	372 (97%)	10 (3%)	54 81
3	G	227/236 (96%)	215 (95%)	12 (5%)	28 50
3	Q	228/236 (97%)	215 (94%)	13 (6%)	25 46
4	H	105/112 (94%)	100 (95%)	5 (5%)	31 55
4	R	105/112 (94%)	100 (95%)	5 (5%)	31 55
5	I	47/48 (98%)	43 (92%)	4 (8%)	13 25
5	S	47/48 (98%)	43 (92%)	4 (8%)	13 25
6	J	30/57 (53%)	28 (93%)	2 (7%)	20 37
6	T	30/57 (53%)	28 (93%)	2 (7%)	20 37
All	All	5431/5682 (96%)	5221 (96%)	210 (4%)	39 66

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	SER
1	A	81	ASP
1	A	124	ASP
1	A	174	GLN
1	A	251	THR
1	A	342	THR
1	A	383	LYS
1	A	429	LEU
1	A	495	LEU
1	B	30	THR
1	B	36	VAL
1	B	67	ASN
1	B	93	THR
1	B	106	LEU
1	B	139	LEU
1	B	142	ARG
1	B	144	VAL
1	B	166	ARG
1	B	223	GLU
1	B	246	TYR
1	B	378	SER
1	B	385	LEU
1	B	412	LEU
1	B	415	SER
1	B	418	GLN

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Mol	Chain	Res	Type
1	B	444	VAL
1	B	472	SER
1	B	481	LEU
1	B	494	GLU
1	C	59	SER
1	C	142	ARG
1	C	159	VAL
1	C	166	ARG
1	C	220	GLN
1	C	283	LEU
1	C	293	ARG
1	C	320	SER
1	C	351	GLN
1	C	363	ILE
1	C	440	THR
1	C	481	LEU
1	C	496	LEU
1	C	501	SER
2	D	74	GLU
2	D	85	VAL
2	D	89	ARG
2	D	129	THR
2	D	133	ILE
2	D	149	ARG
2	D	204	THR
2	D	246	GLU
2	D	250	ASP
2	D	303	SER
2	D	336	SER
2	D	396	LEU
2	D	436	ASP
2	D	455	HIS
2	D	464	GLU
2	E	10	THR
2	E	112	LYS
2	E	140	VAL
2	E	163	LYS
2	E	204	THR
2	E	232	VAL
2	E	348	VAL
2	E	357	LEU
2	E	366	GLU

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Mol	Chain	Res	Type
2	E	436	ASP
2	E	460	VAL
2	F	26	GLU
2	F	45	LYS
2	F	68	GLU
2	F	97	ASN
2	F	113	LEU
2	F	208	ASN
2	F	258	ILE
2	F	274	ARG
2	F	292	LEU
2	F	353	SER
2	F	464	GLU
3	G	4	LYS
3	G	24	LYS
3	G	28	SER
3	G	77	ILE
3	G	78	THR
3	G	118	LEU
3	G	150	LEU
3	G	181	PRO
3	G	237	MET
3	G	247	MET
3	G	254	LEU
3	G	276	SER
4	H	51	GLN
4	H	60	MET
4	H	93	LEU
4	H	104	LEU
4	H	105	LEU
5	I	4	ARG
5	I	27	THR
5	I	55	GLU
5	I	61	LYS
6	J	9	ARG
6	J	30	ARG
1	K	59	SER
1	K	81	ASP
1	K	124	ASP
1	K	166	ARG
1	K	174	GLN
1	K	251	THR

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Mol	Chain	Res	Type
1	K	342	THR
1	K	383	LYS
1	K	429	LEU
1	K	495	LEU
1	L	30	THR
1	L	36	VAL
1	L	67	ASN
1	L	93	THR
1	L	106	LEU
1	L	139	LEU
1	L	142	ARG
1	L	144	VAL
1	L	166	ARG
1	L	223	GLU
1	L	246	TYR
1	L	337	SER
1	L	378	SER
1	L	385	LEU
1	L	412	LEU
1	L	415	SER
1	L	418	GLN
1	L	444	VAL
1	L	472	SER
1	L	481	LEU
1	L	494	GLU
1	M	59	SER
1	M	142	ARG
1	M	159	VAL
1	M	166	ARG
1	M	220	GLN
1	M	283	LEU
1	M	293	ARG
1	M	306	ARG
1	M	320	SER
1	M	351	GLN
1	M	363	ILE
1	M	440	THR
1	M	481	LEU
1	M	496	LEU
1	M	501	SER
2	N	74	GLU
2	N	85	VAL

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Mol	Chain	Res	Type
2	N	89	ARG
2	N	129	THR
2	N	133	ILE
2	N	149	ARG
2	N	204	THR
2	N	246	GLU
2	N	250	ASP
2	N	303	SER
2	N	336	SER
2	N	396	LEU
2	N	436	ASP
2	N	455	HIS
2	N	464	GLU
2	O	10	THR
2	O	112	LYS
2	O	132	GLU
2	O	140	VAL
2	O	163	LYS
2	O	204	THR
2	O	232	VAL
2	O	348	VAL
2	O	357	LEU
2	O	366	GLU
2	O	436	ASP
2	O	460	VAL
2	P	26	GLU
2	P	45	LYS
2	P	68	GLU
2	P	97	ASN
2	P	113	LEU
2	P	208	ASN
2	P	258	ILE
2	P	274	ARG
2	P	353	SER
2	P	464	GLU
3	Q	4	LYS
3	Q	24	LYS
3	Q	28	SER
3	Q	77	ILE
3	Q	78	THR
3	Q	118	LEU
3	Q	125	ASN

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Mol	Chain	Res	Type
3	Q	150	LEU
3	Q	181	PRO
3	Q	237	MET
3	Q	247	MET
3	Q	254	LEU
3	Q	276	SER
4	R	51	GLN
4	R	60	MET
4	R	93	LEU
4	R	104	LEU
4	R	105	LEU
5	S	4	ARG
5	S	27	THR
5	S	55	GLU
5	S	61	LYS
6	T	9	ARG
6	T	30	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	149	GLN
1	A	174	GLN
1	A	220	GLN
1	A	262	ASN
1	A	265	HIS
1	A	407	GLN
1	B	95	ASN
1	B	145	HIS
1	B	224	GLN
1	B	387	GLN
1	B	418	GLN
1	C	220	GLN
2	D	178	HIS
2	D	195	ASN
2	D	367	HIS
2	E	168	GLN
2	E	221	GLN
2	F	52	GLN
2	F	97	ASN
2	F	208	ASN

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Mol	Chain	Res	Type
3	G	90	GLN
3	G	125	ASN
4	H	103	ASN
5	I	19	GLN
5	I	36	ASN
6	J	36	GLN
1	K	72	GLN
1	K	149	GLN
1	K	174	GLN
1	K	220	GLN
1	K	262	ASN
1	K	265	HIS
1	K	407	GLN
1	L	95	ASN
1	L	224	GLN
1	L	387	GLN
1	L	418	GLN
1	M	220	GLN
2	N	178	HIS
2	N	195	ASN
2	N	367	HIS
2	O	168	GLN
2	O	221	GLN
2	P	52	GLN
2	P	97	ASN
2	P	208	ASN
3	Q	90	GLN
3	Q	125	ASN
4	R	51	GLN
5	S	19	GLN
5	S	36	ASN
6	T	36	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 28 ligands modelled in this entry, 10 are monoatomic - leaving 18 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	24,33,33	1.19	3 (12%)	31,52,52	1.99	2 (6%)
9	ADP	B	600	8	22,29,29	1.41	3 (13%)	27,45,45	2.12	5 (18%)
9	ADP	C	600	8	22,29,29	1.22	2 (9%)	27,45,45	2.28	6 (22%)
10	EDO	C	603	-	3,3,3	0.35	0	2,2,2	0.53	0
9	ADP	D	600	8	22,29,29	1.40	3 (13%)	27,45,45	2.25	3 (11%)
9	ADP	E	600	-	22,29,29	1.38	3 (13%)	27,45,45	2.22	3 (11%)
9	ADP	F	600	8	22,29,29	1.22	2 (9%)	27,45,45	2.40	3 (11%)
7	ATP	K	600	8	24,33,33	1.10	2 (8%)	31,52,52	2.00	2 (6%)
9	ADP	L	600	8	22,29,29	1.21	2 (9%)	27,45,45	2.07	5 (18%)
10	EDO	L	602	-	3,3,3	0.59	0	2,2,2	0.16	0
10	EDO	L	604	-	3,3,3	0.53	0	2,2,2	0.34	0
9	ADP	M	600	8	22,29,29	1.20	2 (9%)	27,45,45	2.25	5 (18%)
10	EDO	M	602	-	3,3,3	0.39	0	2,2,2	0.39	0
9	ADP	N	600	8	22,29,29	1.35	3 (13%)	27,45,45	2.31	3 (11%)
9	ADP	O	600	-	22,29,29	1.51	3 (13%)	27,45,45	2.18	3 (11%)
10	EDO	O	602	-	3,3,3	0.47	0	2,2,2	0.49	0
9	ADP	P	600	8	22,29,29	1.29	2 (9%)	27,45,45	2.39	4 (14%)
10	EDO	P	603	-	3,3,3	0.69	0	2,2,2	0.38	0

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
9	ADP	B	600	8	-	0/12/32/32	0/3/3/3
9	ADP	C	600	8	-	0/12/32/32	0/3/3/3
10	EDO	C	603	-	-	0/1/1/1	0/0/0/0
9	ADP	D	600	8	-	0/12/32/32	0/3/3/3
9	ADP	E	600	-	-	0/12/32/32	0/3/3/3
9	ADP	F	600	8	-	0/12/32/32	0/3/3/3
7	ATP	K	600	8	-	0/18/38/38	0/3/3/3
9	ADP	L	600	8	-	0/12/32/32	0/3/3/3
10	EDO	L	602	-	-	0/1/1/1	0/0/0/0
10	EDO	L	604	-	-	0/1/1/1	0/0/0/0
9	ADP	M	600	8	-	0/12/32/32	0/3/3/3
10	EDO	M	602	-	-	0/1/1/1	0/0/0/0
9	ADP	N	600	8	-	0/12/32/32	0/3/3/3
9	ADP	O	600	-	-	0/12/32/32	0/3/3/3
10	EDO	O	602	-	-	0/1/1/1	0/0/0/0
9	ADP	P	600	8	-	0/12/32/32	0/3/3/3
10	EDO	P	603	-	-	0/1/1/1	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	600	ADP	PB-O2B	2.03	1.62	1.54
9	C	600	ADP	PB-O1B	2.06	1.57	1.51
9	N	600	ADP	PB-O2B	2.08	1.62	1.54
7	A	600	ATP	PG-O2G	2.09	1.62	1.54
9	P	600	ADP	PB-O2B	2.13	1.62	1.54
7	K	600	ATP	PG-O3G	2.14	1.62	1.54
9	M	600	ADP	PB-O1B	2.18	1.58	1.51
9	D	600	ADP	PB-O2B	2.20	1.62	1.54
7	A	600	ATP	PG-O3G	2.21	1.62	1.54
9	B	600	ADP	PB-O2B	2.26	1.62	1.54
9	F	600	ADP	PB-O2B	2.28	1.62	1.54
7	K	600	ATP	O4'-C1'	2.36	1.44	1.41
9	O	600	ADP	PB-O2B	2.54	1.63	1.54
9	L	600	ADP	O4'-C1'	2.82	1.44	1.41
9	N	600	ADP	PB-O1B	2.88	1.60	1.51
9	L	600	ADP	PB-O1B	2.90	1.60	1.51
9	D	600	ADP	PB-O1B	3.09	1.61	1.51
9	E	600	ADP	PB-O1B	3.12	1.61	1.51
9	F	600	ADP	O4'-C1'	3.18	1.45	1.41
9	B	600	ADP	O4'-C1'	3.22	1.45	1.41
7	A	600	ATP	O4'-C1'	3.36	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	600	ADP	O4'-C1'	3.55	1.45	1.41
9	O	600	ADP	PB-O1B	3.57	1.62	1.51
9	M	600	ADP	O4'-C1'	3.64	1.45	1.41
9	B	600	ADP	PB-O1B	3.88	1.63	1.51
9	P	600	ADP	O4'-C1'	3.89	1.46	1.41
9	N	600	ADP	O4'-C1'	3.89	1.46	1.41
9	D	600	ADP	O4'-C1'	4.10	1.46	1.41
9	E	600	ADP	O4'-C1'	4.13	1.46	1.41
9	O	600	ADP	O4'-C1'	4.28	1.46	1.41

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	600	ADP	N3-C2-N1	-10.27	121.03	128.89
9	F	600	ADP	N3-C2-N1	-10.25	121.04	128.89
9	P	600	ADP	N3-C2-N1	-10.10	121.16	128.89
9	D	600	ADP	N3-C2-N1	-9.74	121.44	128.89
9	M	600	ADP	N3-C2-N1	-9.67	121.49	128.89
9	C	600	ADP	N3-C2-N1	-9.57	121.56	128.89
7	K	600	ATP	N3-C2-N1	-9.44	121.66	128.89
7	A	600	ATP	N3-C2-N1	-9.39	121.70	128.89
9	E	600	ADP	N3-C2-N1	-9.35	121.73	128.89
9	O	600	ADP	N3-C2-N1	-8.99	122.01	128.89
9	B	600	ADP	N3-C2-N1	-8.45	122.42	128.89
9	L	600	ADP	N3-C2-N1	-8.40	122.46	128.89
9	P	600	ADP	C2'-C1'-N9	-4.32	107.69	114.29
9	F	600	ADP	C2'-C1'-N9	-4.24	107.81	114.29
9	O	600	ADP	PA-O3A-PB	-3.48	121.02	132.67
9	E	600	ADP	PA-O3A-PB	-3.45	121.09	132.67
9	B	600	ADP	PA-O3A-PB	-3.27	121.69	132.67
9	D	600	ADP	PA-O3A-PB	-3.13	122.17	132.67
9	C	600	ADP	PA-O3A-PB	-3.12	122.20	132.67
9	O	600	ADP	C2'-C1'-N9	-3.12	109.53	114.29
9	L	600	ADP	PA-O3A-PB	-3.11	122.25	132.67
9	E	600	ADP	C2'-C1'-N9	-2.99	109.73	114.29
9	M	600	ADP	PA-O3A-PB	-2.87	123.06	132.67
9	P	600	ADP	PA-O3A-PB	-2.85	123.11	132.67
9	N	600	ADP	PA-O3A-PB	-2.81	123.23	132.67
9	C	600	ADP	C4-C5-N7	-2.80	106.91	109.48
9	L	600	ADP	O3A-PA-O5'	-2.69	95.80	102.94
9	L	600	ADP	C4-C5-N7	-2.68	107.01	109.48
9	M	600	ADP	C4-C5-N7	-2.64	107.05	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	600	ADP	O3A-PA-O5'	-2.61	96.00	102.94
9	F	600	ADP	PA-O3A-PB	-2.50	124.27	132.67
9	B	600	ADP	C4-C5-N7	-2.49	107.19	109.48
9	C	600	ADP	C4'-O4'-C1'	-2.45	107.02	109.72
9	C	600	ADP	O3A-PA-O5'	-2.44	96.47	102.94
9	D	600	ADP	C2'-C1'-N9	-2.38	110.65	114.29
9	N	600	ADP	C2'-C1'-N9	-2.33	110.73	114.29
9	M	600	ADP	C4'-O4'-C1'	-2.29	107.20	109.72
7	A	600	ATP	C4-C5-N7	-2.27	107.39	109.48
7	K	600	ATP	C4-C5-N7	-2.20	107.45	109.48
9	P	600	ADP	C4'-O4'-C1'	-2.05	107.46	109.72
9	C	600	ADP	O3B-PB-O3A	2.40	116.00	105.09
9	M	600	ADP	O3B-PB-O3A	2.43	116.13	105.09
9	L	600	ADP	O3B-PB-O3A	2.76	117.60	105.09
9	B	600	ADP	O3B-PB-O3A	3.03	118.86	105.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	600	ADP	1	0
9	M	600	ADP	1	0
10	M	602	EDO	2	0
10	P	603	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	484/510 (94%)	0.46	31 (6%) 23 25	34, 67, 108, 119	0
1	B	480/510 (94%)	0.22	33 (6%) 20 22	18, 42, 84, 104	0
1	C	484/510 (94%)	0.24	42 (8%) 13 13	22, 40, 112, 138	0
1	K	484/510 (94%)	0.50	34 (7%) 19 22	32, 60, 110, 119	0
1	L	480/510 (94%)	-0.13	6 (1%) 79 82	15, 31, 70, 100	0
1	M	484/510 (94%)	0.35	38 (7%) 15 17	23, 48, 116, 138	0
2	D	470/478 (98%)	0.27	20 (4%) 39 44	32, 55, 77, 100	0
2	E	468/478 (97%)	0.76	60 (12%) 5 5	34, 65, 118, 133	0
2	F	469/478 (98%)	-0.05	8 (1%) 73 76	19, 38, 64, 76	0
2	N	470/478 (98%)	0.35	23 (4%) 33 38	34, 60, 82, 103	0
2	O	468/478 (97%)	0.64	55 (11%) 6 6	20, 50, 119, 135	0
2	P	469/478 (98%)	0.13	17 (3%) 46 51	20, 43, 72, 79	0
3	G	265/278 (95%)	0.77	30 (11%) 7 7	36, 70, 120, 129	0
3	Q	265/278 (95%)	1.12	49 (18%) 2 2	30, 83, 122, 128	0
4	H	124/138 (89%)	1.88	48 (38%) 0 0	97, 110, 128, 133	0
4	R	124/138 (89%)	1.74	49 (39%) 0 0	96, 111, 127, 132	0
5	I	58/61 (95%)	1.07	6 (10%) 9 9	64, 84, 115, 117	0
5	S	58/61 (95%)	1.17	15 (25%) 1 1	65, 86, 121, 123	0
6	J	36/63 (57%)	0.69	3 (8%) 14 15	70, 84, 109, 110	0
6	T	36/63 (57%)	0.88	5 (13%) 4 4	76, 87, 112, 113	0
All	All	6676/7008 (95%)	0.44	572 (8%) 13 14	15, 57, 113, 138	0

All (572) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	389	ALA	10.5
2	O	396	LEU	9.4
2	O	386	ASP	8.9
2	O	387	ILE	8.6
2	O	404	VAL	8.5
2	O	391	LEU	8.1
2	D	6	SER	7.8
4	R	12	LEU	7.5
4	R	42	LEU	7.5
1	C	408	PHE	7.4
2	O	390	ILE	7.2
1	M	405	PHE	6.9
2	E	467	VAL	6.8
1	M	402	VAL	6.6
1	B	405	PHE	6.6
1	C	402	VAL	6.4
2	O	403	THR	6.3
1	C	406	ALA	6.3
2	O	467	VAL	6.0
2	E	402	LEU	6.0
2	E	392	GLY	5.9
1	B	25	ALA	5.9
3	Q	128	LEU	5.8
1	C	409	GLY	5.7
5	S	49	ASN	5.7
3	G	195	GLY	5.6
1	A	499	LEU	5.6
4	H	77	VAL	5.6
3	Q	105	ALA	5.6
3	Q	153	VAL	5.5
5	S	57	THR	5.5
2	O	395	GLU	5.4
2	E	389	ALA	5.4
1	C	457	GLY	5.4
1	M	195	SER	5.3
2	O	470	ALA	5.3
1	B	499	LEU	5.3
3	G	53	LYS	5.3
2	N	27	GLN	5.3
2	O	385	GLN	5.2
1	K	497	ALA	5.0
1	K	412	LEU	5.0
2	E	468	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
3	G	192	PRO	5.0
1	K	473	TYR	5.0
2	D	7	THR	4.9
2	N	6	SER	4.9
4	R	62	GLY	4.9
1	B	457	GLY	4.9
2	O	384	LEU	4.9
3	Q	202	ASP	4.9
2	O	474	ALA	4.9
5	I	49	ASN	4.8
2	E	475	ALA	4.8
4	R	28	THR	4.8
2	O	473	LEU	4.8
2	O	27	GLN	4.8
4	H	64	ASN	4.8
1	M	509	THR	4.8
3	G	197	PHE	4.7
5	S	54	SER	4.7
2	E	393	MET	4.7
2	E	43	GLN	4.7
4	R	27	VAL	4.7
1	M	415	SER	4.7
2	O	392	GLY	4.7
3	G	1	ALA	4.7
3	G	52	TYR	4.7
2	F	179	GLY	4.6
2	E	29	GLU	4.6
5	S	7	GLY	4.6
1	C	395	PHE	4.6
1	M	353	PHE	4.6
3	Q	50	LEU	4.6
4	R	82	GLN	4.5
5	S	55	GLU	4.5
2	O	402	LEU	4.5
3	Q	127	LYS	4.5
4	H	41	VAL	4.4
2	N	474	ALA	4.4
4	R	59	VAL	4.4
2	E	474	ALA	4.3
2	F	7	THR	4.3
2	N	473	LEU	4.3
2	E	27	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
3	G	206	PRO	4.2
2	O	393	MET	4.2
2	E	28	SER	4.2
3	Q	197	PHE	4.2
4	R	60	MET	4.1
1	C	448	TYR	4.1
2	O	382	LYS	4.1
2	O	397	SER	4.1
1	K	391	SER	4.1
4	H	42	LEU	4.1
3	Q	192	PRO	4.1
2	O	407	ALA	4.1
2	E	9	ILE	4.0
2	E	398	GLU	4.0
5	I	57	THR	4.0
1	K	395	PHE	4.0
4	H	46	VAL	4.0
2	E	473	LEU	4.0
1	M	473	TYR	4.0
3	Q	172	SER	4.0
1	B	460	LEU	4.0
4	R	63	SER	4.0
2	P	28	SER	3.9
4	H	79	PRO	3.9
1	A	502	ALA	3.9
2	E	394	ASP	3.9
2	O	388	ILE	3.9
2	O	457	PHE	3.9
1	C	509	THR	3.9
2	O	394	ASP	3.9
3	G	51	PHE	3.9
3	Q	49	GLN	3.9
2	O	383	SER	3.9
1	C	399	TYR	3.8
2	D	473	LEU	3.8
1	C	414	ALA	3.8
1	A	507	VAL	3.8
2	E	8	PRO	3.8
3	Q	104	ASN	3.8
1	K	32	ARG	3.8
4	H	133	LEU	3.8
1	A	497	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	195	SER	3.8
2	E	390	ILE	3.8
2	O	344	ILE	3.8
3	G	202	ASP	3.8
2	O	445	LEU	3.8
1	M	503	THR	3.7
3	Q	154	MET	3.7
4	H	12	LEU	3.7
4	R	43	ALA	3.7
1	M	448	TYR	3.7
4	H	73	GLY	3.7
5	I	55	GLU	3.7
1	B	506	PHE	3.7
2	P	7	THR	3.7
4	H	30	VAL	3.7
1	B	503	THR	3.7
4	H	28	THR	3.7
4	H	80	ASP	3.7
4	R	137	LEU	3.7
1	L	404	ALA	3.6
1	M	457	GLY	3.6
1	M	476	SER	3.6
3	Q	126	ILE	3.6
3	G	203	ALA	3.6
2	E	452	ILE	3.6
5	S	47	TYR	3.6
4	R	61	GLU	3.6
1	K	392	LEU	3.6
1	C	449	ALA	3.6
2	O	401	LYS	3.6
3	Q	161	LYS	3.6
2	O	400	ASP	3.6
1	A	501	SER	3.6
3	Q	173	LEU	3.6
4	H	82	GLN	3.5
3	G	55	ALA	3.5
1	A	395	PHE	3.5
2	N	467	VAL	3.5
5	I	5	LYS	3.5
3	Q	51	PHE	3.5
1	M	508	ALA	3.5
1	M	408	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
4	H	113	SER	3.5
2	N	7	THR	3.5
2	O	338	GLY	3.5
1	A	481	LEU	3.5
2	E	112	LYS	3.4
4	H	29	GLN	3.4
2	E	472	LYS	3.4
1	B	26	ASN	3.4
2	O	410	ILE	3.4
1	B	507	VAL	3.4
2	O	430	LYS	3.4
2	O	425	THR	3.4
1	B	412	LEU	3.3
4	H	56	VAL	3.3
1	K	494	GLU	3.3
1	C	499	LEU	3.3
2	E	401	LYS	3.3
1	A	448	TYR	3.3
1	M	410	SER	3.3
4	H	116	ASP	3.3
5	S	8	ILE	3.3
1	B	404	ALA	3.3
4	H	44	ASN	3.3
2	E	391	LEU	3.3
2	F	27	GLN	3.3
4	H	27	VAL	3.3
1	M	497	ALA	3.3
1	A	389	ALA	3.2
3	Q	195	GLY	3.2
1	A	202	TYR	3.2
1	A	465	GLU	3.2
1	B	454	HIS	3.2
1	B	463	ILE	3.2
1	C	458	ILE	3.2
4	H	59	VAL	3.2
6	T	31	GLN	3.2
3	Q	100	ASN	3.2
1	C	501	SER	3.2
2	D	28	SER	3.2
4	R	65	SER	3.2
4	R	93	LEU	3.2
1	C	353	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
3	Q	203	ALA	3.2
2	P	27	GLN	3.2
1	B	456	ASP	3.1
4	H	61	GLU	3.1
1	K	421	VAL	3.1
2	D	435	LYS	3.1
1	B	469	SER	3.1
1	K	492	SER	3.1
4	R	13	GLN	3.1
4	R	99	GLU	3.1
2	D	43	GLN	3.1
1	C	411	ASP	3.1
1	L	405	PHE	3.1
1	K	476	SER	3.1
3	Q	160	PRO	3.1
4	R	83	LEU	3.1
1	K	457	GLY	3.1
1	K	406	ALA	3.0
3	Q	171	SER	3.0
1	A	124	ASP	3.0
4	R	41	VAL	3.0
1	C	418	GLN	3.0
1	C	491	LEU	3.0
1	L	420	LEU	3.0
2	O	415	SER	3.0
2	N	452	ILE	3.0
4	H	62	GLY	3.0
1	M	480	GLU	3.0
3	Q	159	TYR	3.0
3	Q	107	ILE	3.0
4	R	116	ASP	3.0
1	A	496	LEU	3.0
1	M	505	SER	3.0
1	A	454	HIS	3.0
4	R	31	ASN	3.0
4	H	72	GLY	2.9
1	K	414	ALA	2.9
2	O	444	VAL	2.9
2	N	28	SER	2.9
4	H	114	SER	2.9
2	E	409	LYS	2.9
4	H	49	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	210	GLU	2.9
2	P	464	GLU	2.9
1	B	403	ALA	2.9
2	N	451	ASN	2.9
1	M	399	TYR	2.9
2	E	388	ILE	2.9
4	R	114	SER	2.9
1	C	484	GLU	2.9
4	R	22	TYR	2.9
1	K	501	SER	2.9
1	M	378	SER	2.9
1	C	412	LEU	2.9
1	K	475	LYS	2.9
3	Q	59	ASN	2.9
1	K	454	HIS	2.9
3	Q	103	PRO	2.9
2	D	210	GLU	2.8
1	M	481	LEU	2.8
2	E	451	ASN	2.8
6	J	31	GLN	2.8
1	B	502	ALA	2.8
1	A	421	VAL	2.8
4	H	53	LEU	2.8
3	Q	165	PHE	2.8
1	M	406	ALA	2.8
2	E	399	GLN	2.8
5	S	46	GLN	2.8
2	E	396	LEU	2.8
4	H	74	PHE	2.8
1	A	489	GLY	2.8
2	E	158	GLY	2.8
2	D	456	ALA	2.8
2	E	178	HIS	2.8
1	K	495	LEU	2.8
2	O	458	TYR	2.8
4	H	130	LEU	2.8
4	R	30	VAL	2.8
6	T	17	PHE	2.8
1	K	389	ALA	2.8
1	K	480	GLU	2.8
2	E	42	PRO	2.8
4	R	54	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	O	9	ILE	2.7
1	K	316	GLU	2.7
3	G	194	PHE	2.7
1	A	476	SER	2.7
2	N	43	GLN	2.7
3	Q	56	GLU	2.7
2	P	435	LYS	2.7
1	M	506	PHE	2.7
4	H	17	PRO	2.7
2	N	210	GLU	2.7
4	R	23	SER	2.7
4	R	79	PRO	2.7
1	C	398	GLN	2.7
1	K	496	LEU	2.7
2	E	301	LYS	2.7
2	P	391	LEU	2.7
2	E	395	GLU	2.7
4	R	14	PHE	2.7
1	K	448	TYR	2.7
2	P	210	GLU	2.7
4	H	60	MET	2.7
1	B	466	PHE	2.7
4	R	91	PHE	2.7
1	B	473	TYR	2.7
4	R	11	LYS	2.7
5	S	44	TYR	2.7
4	R	88	ILE	2.6
1	B	482	LEU	2.6
2	E	302	GLY	2.6
3	G	49	GLN	2.6
4	R	131	GLU	2.6
1	C	495	LEU	2.6
4	H	83	LEU	2.6
4	H	81	SER	2.6
4	R	113	SER	2.6
1	B	421	VAL	2.6
2	N	468	ALA	2.6
4	R	77	VAL	2.6
2	O	28	SER	2.6
4	R	80	ASP	2.6
1	K	405	PHE	2.6
1	M	404	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
3	Q	240	ALA	2.6
4	H	129	VAL	2.6
1	C	503	THR	2.6
4	H	86	THR	2.6
1	C	502	ALA	2.6
3	G	3	LEU	2.6
3	G	44	MET	2.6
2	D	468	ALA	2.6
2	O	475	ALA	2.6
2	P	424	PHE	2.6
1	K	499	LEU	2.6
4	H	137	LEU	2.6
3	G	56	GLU	2.6
2	E	455	HIS	2.6
2	O	380	THR	2.5
4	R	132	ASN	2.5
1	M	491	LEU	2.5
2	D	29	GLU	2.5
1	C	474	LEU	2.5
1	A	480	GLU	2.5
2	D	436	ASP	2.5
1	B	415	SER	2.5
1	C	476	SER	2.5
1	K	472	SER	2.5
5	S	5	LYS	2.5
1	C	421	VAL	2.5
2	E	453	PRO	2.5
2	O	398	GLU	2.5
2	E	344	ILE	2.5
4	H	88	ILE	2.5
3	G	235	ASN	2.5
2	D	27	GLN	2.5
2	E	244	ARG	2.5
2	E	405	GLU	2.5
4	H	50	GLU	2.5
1	K	180	VAL	2.5
3	Q	196	LYS	2.5
1	B	89	LEU	2.5
3	G	57	THR	2.5
2	O	399	GLN	2.5
3	Q	74	ILE	2.5
2	D	462	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	212	GLU	2.5
2	O	210	GLU	2.5
2	P	212	GLU	2.5
1	M	488	LYS	2.4
4	R	130	LEU	2.4
1	M	400	ARG	2.4
2	N	112	LYS	2.4
1	K	462	ARG	2.4
2	F	210	GLU	2.4
2	P	26	GLU	2.4
2	N	44	GLY	2.4
4	H	65	SER	2.4
1	C	480	GLU	2.4
2	P	386	ASP	2.4
1	M	507	VAL	2.4
1	A	460	LEU	2.4
2	N	180	GLY	2.4
3	Q	150	LEU	2.4
4	H	31	ASN	2.4
1	K	408	PHE	2.4
1	C	373	VAL	2.4
1	K	471	LEU	2.4
2	N	209	LEU	2.4
1	A	492	SER	2.4
4	H	71	SER	2.4
5	S	43	PHE	2.4
1	M	321	GLY	2.4
2	N	179	GLY	2.4
3	G	54	ASN	2.4
4	H	67	LYS	2.4
4	R	67	LYS	2.4
2	F	474	ALA	2.4
2	P	474	ALA	2.4
1	C	487	GLU	2.4
2	N	448	LYS	2.4
4	H	70	ILE	2.4
6	J	34	LYS	2.3
2	D	452	ILE	2.3
4	R	64	ASN	2.3
2	D	471	GLU	2.3
3	Q	198	GLU	2.3
1	B	449	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
4	R	123	ALA	2.3
4	H	69	PHE	2.3
1	M	493	LYS	2.3
1	M	421	VAL	2.3
2	E	423	VAL	2.3
2	P	455	HIS	2.3
2	O	463	ILE	2.3
4	R	121	ALA	2.3
3	Q	4	LYS	2.3
3	Q	183	PHE	2.3
5	S	29	LEU	2.3
1	C	388	VAL	2.3
2	E	404	VAL	2.3
2	E	341	GLU	2.3
3	Q	235	ASN	2.3
2	O	452	ILE	2.3
2	F	26	GLU	2.3
4	R	50	GLU	2.3
2	E	458	TYR	2.3
2	E	246	GLU	2.3
3	G	198	GLU	2.3
4	R	29	GLN	2.3
1	C	396	LEU	2.3
1	C	493	LYS	2.3
4	H	105	LEU	2.3
3	Q	201	THR	2.3
1	B	400	ARG	2.3
2	O	209	LEU	2.2
3	Q	3	LEU	2.2
1	C	504	GLU	2.2
1	A	475	LYS	2.2
3	G	4	LYS	2.2
3	Q	42	LYS	2.2
1	C	452	ASN	2.2
3	G	191	SER	2.2
1	A	314	LEU	2.2
1	M	455	LEU	2.2
2	E	464	GLU	2.2
3	Q	179	GLU	2.2
2	D	472	LYS	2.2
2	E	187	VAL	2.2
4	H	102	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	O	453	PRO	2.2
1	K	493	LYS	2.2
2	O	112	LYS	2.2
2	D	474	ALA	2.2
2	N	456	ALA	2.2
2	P	451	ASN	2.2
1	A	198	SER	2.2
3	Q	33	LYS	2.2
1	M	412	LEU	2.2
2	E	218	VAL	2.2
4	H	87	ALA	2.2
5	S	53	ALA	2.2
3	Q	44	MET	2.2
1	M	362	GLY	2.2
2	D	44	GLY	2.2
2	E	385	GLN	2.2
1	A	491	LEU	2.2
2	O	341	GLU	2.2
4	H	104	LEU	2.2
4	R	53	LEU	2.2
4	R	76	THR	2.2
3	G	59	ASN	2.2
1	A	498	SER	2.2
1	K	498	SER	2.2
1	A	487	GLU	2.2
2	P	29	GLU	2.2
1	M	396	LEU	2.2
1	M	499	LEU	2.2
2	N	40	LYS	2.2
3	G	173	LEU	2.2
3	Q	31	LEU	2.2
5	S	25	LEU	2.2
2	E	98	VAL	2.1
1	K	398	GLN	2.1
1	M	360	TYR	2.1
3	Q	52	TYR	2.1
6	T	1	SER	2.1
2	P	176	LYS	2.1
2	O	408	ARG	2.1
3	Q	207	ARG	2.1
2	F	431	LEU	2.1
1	M	487	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	475	LYS	2.1
4	R	117	ALA	2.1
3	G	116	MET	2.1
1	K	469	SER	2.1
1	L	376	VAL	2.1
2	P	390	ILE	2.1
2	N	471	GLU	2.1
1	L	418	GLN	2.1
2	E	44	GLY	2.1
2	E	73	GLY	2.1
4	R	73	GLY	2.1
4	R	81	SER	2.1
1	B	508	ALA	2.1
2	O	446	GLU	2.1
5	S	59	ILE	2.1
1	A	192	ASN	2.1
4	R	111	ASN	2.1
5	I	39	GLN	2.1
1	A	353	PHE	2.1
2	E	384	LEU	2.1
2	E	426	GLY	2.1
1	C	505	SER	2.1
1	C	403	ALA	2.1
3	Q	41	ALA	2.1
4	R	85	VAL	2.1
6	T	34	LYS	2.1
2	D	249	GLN	2.1
6	J	36	GLN	2.1
1	B	458	ILE	2.1
1	A	32	ARG	2.1
1	C	405	PHE	2.1
5	I	54	SER	2.1
2	E	40	LYS	2.1
2	N	443	ALA	2.1
3	Q	125	ASN	2.1
1	B	471	LEU	2.1
1	M	395	PHE	2.1
2	O	414	LEU	2.1
3	Q	73	LEU	2.1
4	H	78	GLN	2.0
1	C	497	ALA	2.0
1	L	25	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
3	G	188	ILE	2.0
3	Q	182	ILE	2.0
2	E	77	LEU	2.0
2	F	8	PRO	2.0
3	G	119	LEU	2.0
1	A	391	SER	2.0
1	B	501	SER	2.0
6	T	16	SER	2.0
2	E	382	LYS	2.0
2	D	179	GLY	2.0
2	E	343	GLY	2.0
1	A	59	SER	2.0
1	C	415	SER	2.0
2	O	345	TYR	2.0
3	G	193	SER	2.0
1	B	480	GLU	2.0
3	G	207	ARG	2.0
2	E	208	ASN	2.0
3	G	196	LYS	2.0
3	Q	225	GLY	2.0
1	B	32	ARG	2.0
2	O	471	GLU	2.0
1	C	455	LEU	2.0
1	B	448	TYR	2.0
2	N	181	PHE	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
10	EDO	L	604	4/4	0.86	0.26	4.13	46,47,51,51	0
10	EDO	O	602	4/4	0.86	0.29	3.99	46,47,49,53	0
10	EDO	C	603	4/4	0.98	0.20	1.99	33,35,36,39	0
10	EDO	P	603	4/4	0.90	0.18	1.12	31,42,47,50	0
10	EDO	M	602	4/4	0.98	0.20	1.08	32,39,42,45	0
8	MG	F	601	1/1	0.98	0.20	0.50	24,24,24,24	0
8	MG	P	601	1/1	0.95	0.22	0.48	25,25,25,25	0
10	EDO	L	602	4/4	0.96	0.12	0.11	28,28,31,32	0
9	ADP	F	600	27/27	0.98	0.17	0.01	24,29,32,39	0
9	ADP	C	600	27/27	0.96	0.16	-0.04	28,53,65,65	0
9	ADP	B	600	27/27	0.97	0.14	-0.28	29,48,55,57	0
9	ADP	D	600	27/27	0.98	0.16	-0.34	33,46,55,58	0
7	ATP	K	600	31/31	0.96	0.19	-0.42	38,54,59,60	4
9	ADP	L	600	27/27	0.98	0.14	-0.51	18,32,41,43	0
9	ADP	N	600	27/27	0.96	0.15	-0.60	37,46,55,57	0
8	MG	D	601	1/1	0.99	0.18	-0.64	35,35,35,35	0
9	ADP	O	600	27/27	0.91	0.17	-0.76	74,90,91,92	0
9	ADP	P	600	27/27	0.99	0.16	-0.82	22,33,36,41	0
7	ATP	A	600	31/31	0.96	0.16	-0.95	45,53,57,58	4
9	ADP	E	600	27/27	0.89	0.15	-0.99	86,90,92,93	0
9	ADP	M	600	27/27	0.96	0.13	-1.19	36,65,72,73	0
8	MG	N	601	1/1	0.99	0.15	-2.08	40,40,40,40	0
8	MG	C	601	1/1	0.99	0.16	-	27,27,27,27	0
8	MG	M	601	1/1	0.98	0.15	-	34,34,34,34	0
8	MG	L	601	1/1	0.92	0.20	-	24,24,24,24	0
8	MG	B	601	1/1	0.93	0.15	-	40,40,40,40	0
8	MG	A	601	1/1	0.92	0.18	-	50,50,50,50	0
8	MG	K	601	1/1	0.95	0.19	-	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.