Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:34 AM GMT

PDB ID	:	3EYA
Title	:	Structural basis for membrane binding and catalytic activation of the peripheral membrane enzyme pyruvate oxidase from Escherichia coli
Authors	:	Neumann, P.; Weidner, A.; Pech, A.; Stubbs, M.T.; Tittmann, K.
Deposited on	:	2008-10-20
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:

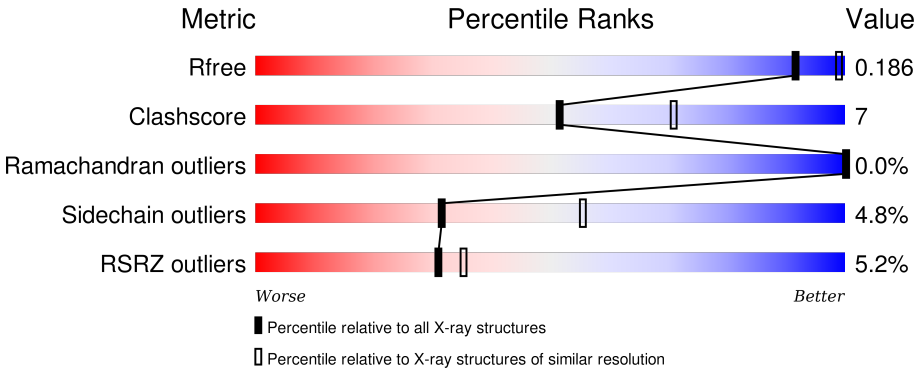
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	549	4% 81% 12% • •
1	B	549	5% 82% 11% • 5%
1	C	549	6% 82% 11% • 5%
1	D	549	4% 81% 12% • 5%
1	E	549	6% 82% 10% • 5%

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Mol	Chain	Length	Quality of chain
1	F	549	5% 82% 11% • 5%
1	G	549	7% 82% 11% • 5%
1	H	549	4% 82% 11% • 5%
1	I	549	5% 81% 12% • 5%
1	J	549	6% 83% 9% • 5%
1	K	549	5% 83% 10% • 5%
1	L	549	2% 80% 13% • 5%

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
5	PO4	A	615	-	-	-	X
5	PO4	A	616	-	-	X	X
5	PO4	A	618	-	-	X	-
5	PO4	A	619	-	-	X	-
5	PO4	B	615	-	-	-	X
5	PO4	B	616	-	-	-	X
5	PO4	C	615	-	-	-	X
5	PO4	D	616	-	-	-	X
5	PO4	D	620	-	-	-	X
5	PO4	F	615	-	-	-	X
5	PO4	H	614	-	-	-	X
5	PO4	L	615	-	-	-	X

2 Entry composition (i)

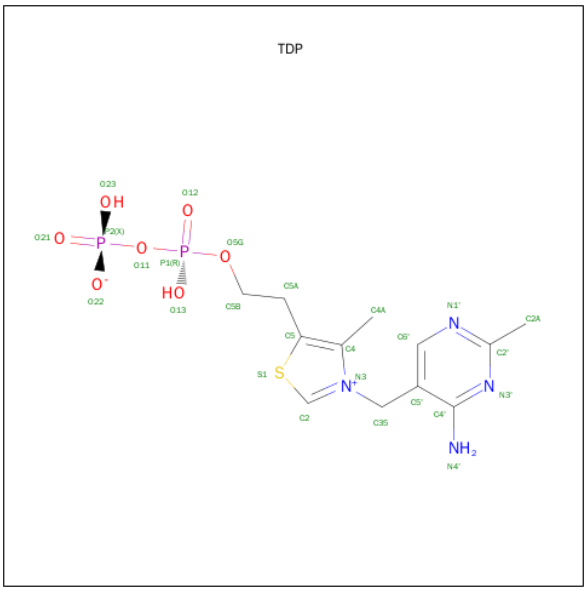
There are 6 unique types of molecules in this entry. The entry contains 50360 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyruvate dehydrogenase [cytochrome].

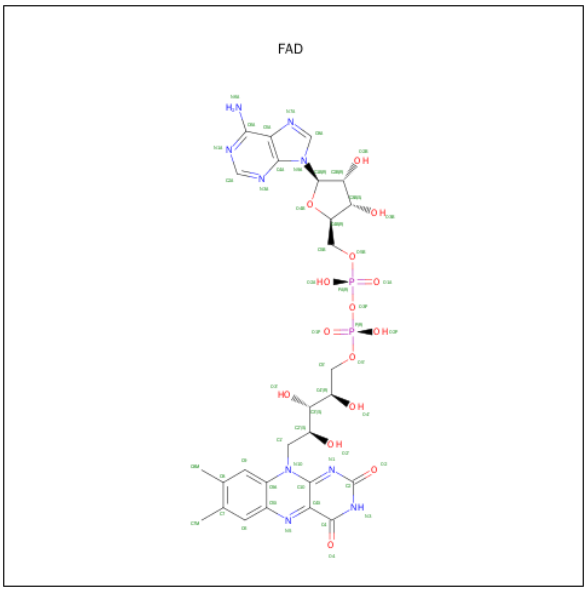
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	12	0
			4066	2579	708	752	27			
1	B	524	Total	C	N	O	S	0	5	0
			3999	2529	694	749	27			
1	C	522	Total	C	N	O	S	0	6	0
			4001	2530	697	748	26			
1	D	520	Total	C	N	O	S	0	6	0
			3977	2516	693	741	27			
1	E	522	Total	C	N	O	S	0	3	0
			3975	2513	693	743	26			
1	F	521	Total	C	N	O	S	0	3	0
			3969	2510	693	739	27			
1	G	519	Total	C	N	O	S	0	2	0
			3939	2490	684	738	27			
1	H	522	Total	C	N	O	S	0	4	0
			3973	2515	688	743	27			
1	I	523	Total	C	N	O	S	0	2	0
			3978	2516	694	741	27			
1	J	522	Total	C	N	O	S	0	6	0
			3993	2527	696	743	27			
1	K	523	Total	C	N	O	S	0	5	0
			4005	2533	702	743	27			
1	L	523	Total	C	N	O	S	0	8	0
			4016	2541	704	744	27			

- Molecule 2 is THIAMIN DIPHOSPHATE (three-letter code: TDP) (formula: $C_{12}H_{18}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	E	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	F	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	G	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	H	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	I	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	J	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	K	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	L	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

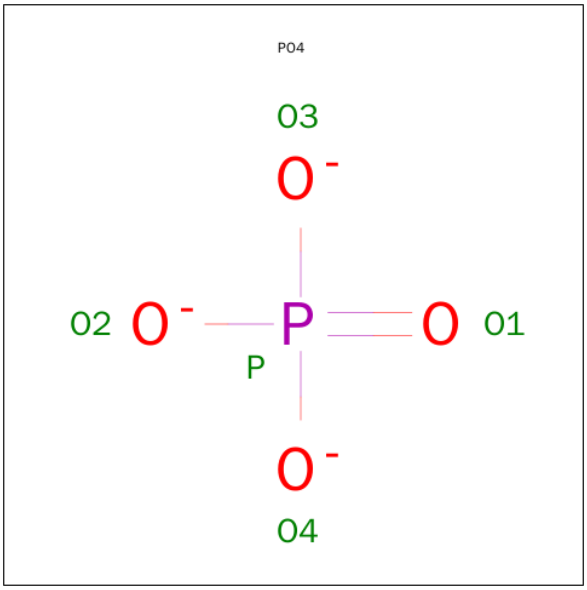


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	I	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	J	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	L	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	K	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	I	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	L	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	C	1	Total O P 5 4 1	0	0
5	C	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	E	1	Total O P 5 4 1	0	0
5	E	1	Total O P 5 4 1	0	0
5	F	1	Total O P 5 4 1	0	0
5	F	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total O P 5 4 1	0	0
5	G	1	Total O P 5 4 1	0	0
5	G	1	Total O P 5 4 1	0	0
5	H	1	Total O P 5 4 1	0	0
5	H	1	Total O P 5 4 1	0	0
5	I	1	Total O P 5 4 1	0	0
5	I	1	Total O P 5 4 1	0	0
5	J	1	Total O P 5 4 1	0	0
5	K	1	Total O P 5 4 1	0	0
5	L	1	Total O P 5 4 1	0	0
5	L	1	Total O P 5 4 1	0	0
5	L	1	Total O P 5 4 1	0	0
5	L	1	Total O P 5 4 1	0	0
5	L	1	Total O P 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	280	Total O 280 280	0	0
6	B	60	Total O 60 60	0	0
6	C	73	Total O 73 73	0	0
6	D	88	Total O 88 88	0	0
6	E	43	Total O 43 43	0	0

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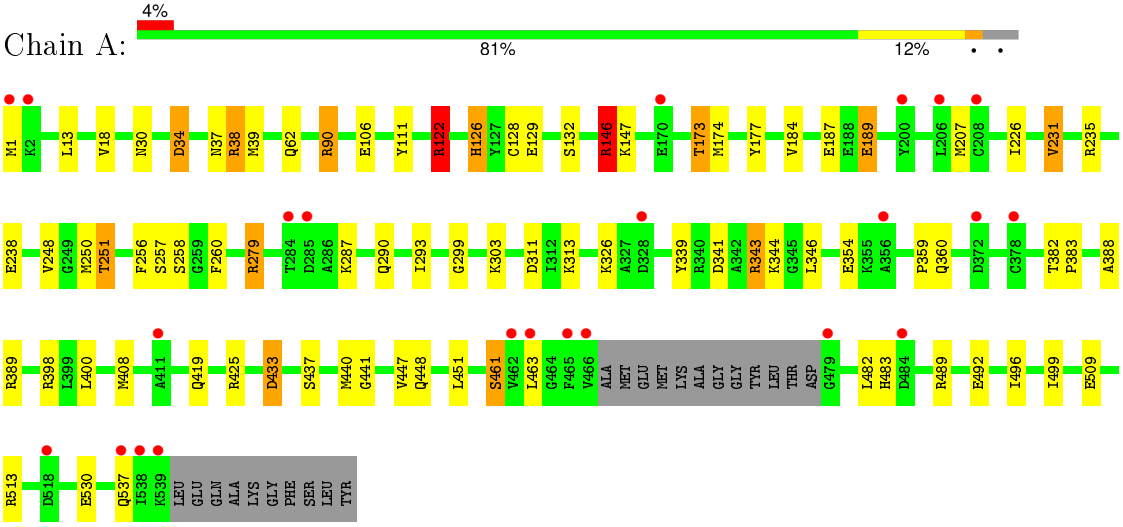
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	41	Total O 41 41	0	0
6	G	40	Total O 40 40	0	0
6	H	64	Total O 64 64	0	0
6	I	62	Total O 62 62	0	0
6	J	50	Total O 50 50	0	0
6	K	77	Total O 77 77	0	0
6	L	451	Total O 451 451	0	0

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.

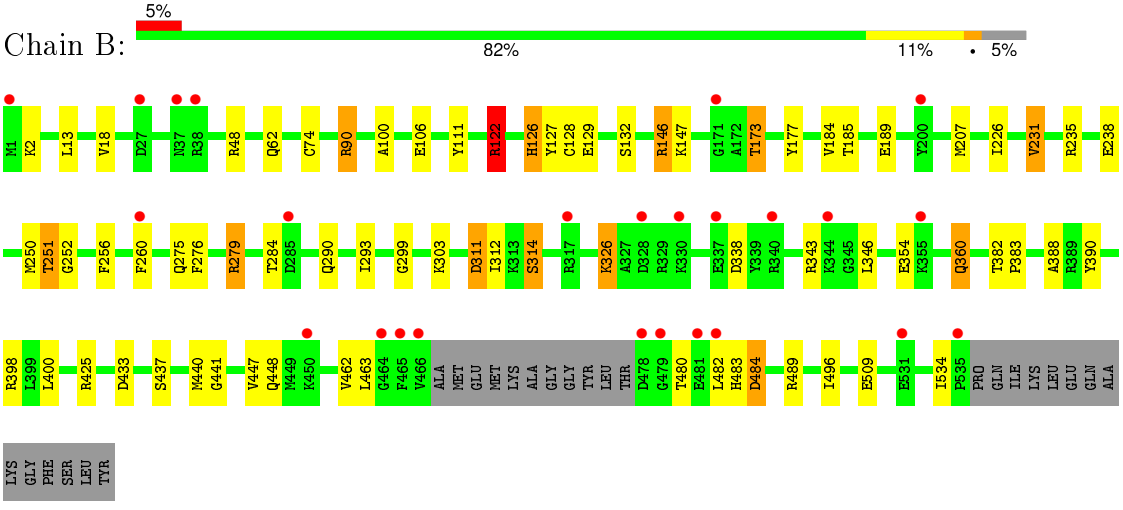
- Molecule 1: Pyruvate dehydrogenase [cytochrome]

Chain A:



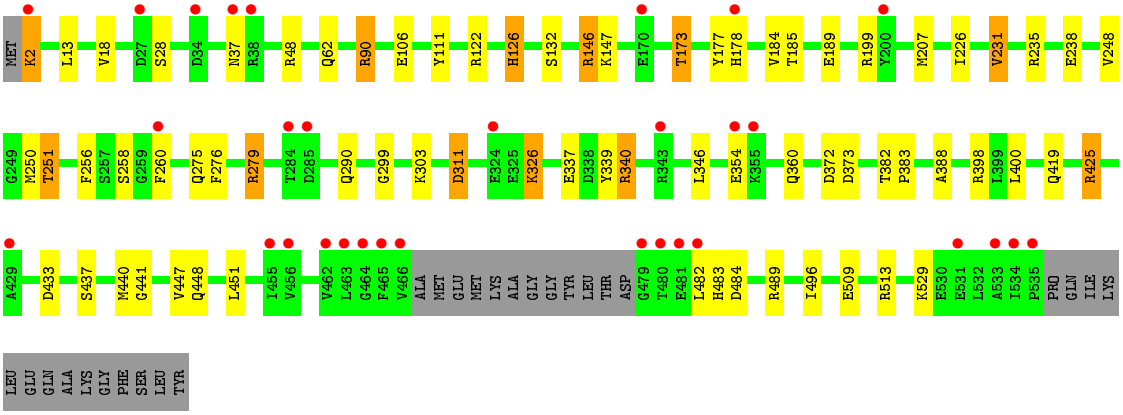
- Molecule 1: Pyruvate dehydrogenase [cytochrome]

Chain B:



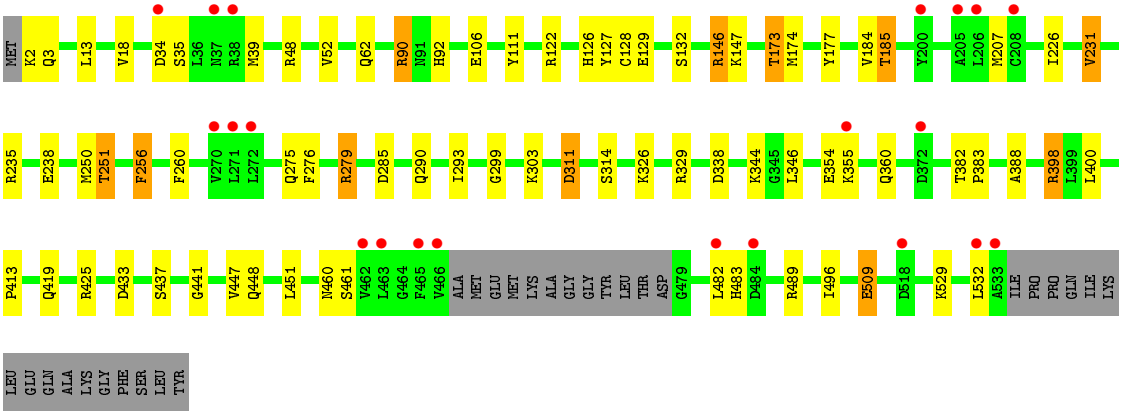
- Molecule 1: Pyruvate dehydrogenase [cytochrome]

Chain C:



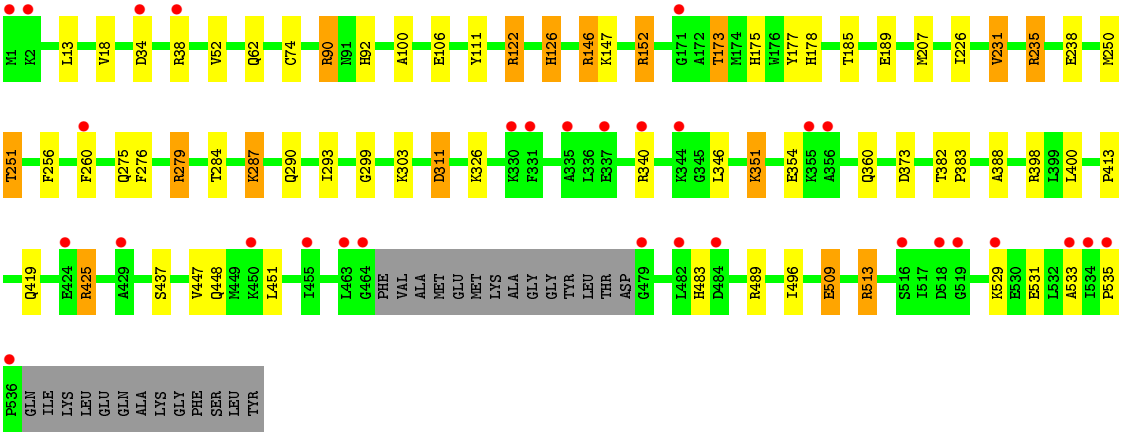
• Molecule 1: Pyruvate dehydrogenase [cytochrome]

Chain D:



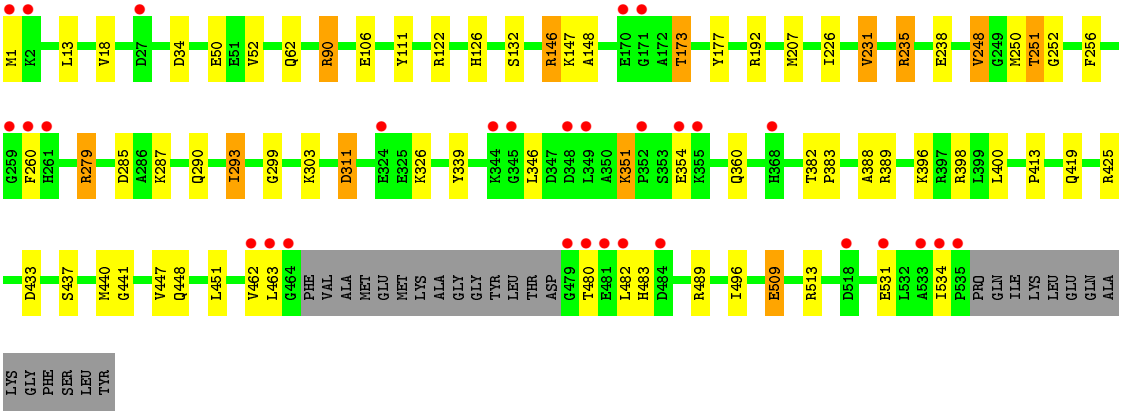
• Molecule 1: Pyruvate dehydrogenase [cytochrome]

Chain E:

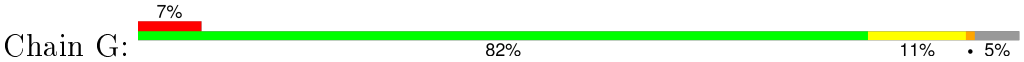


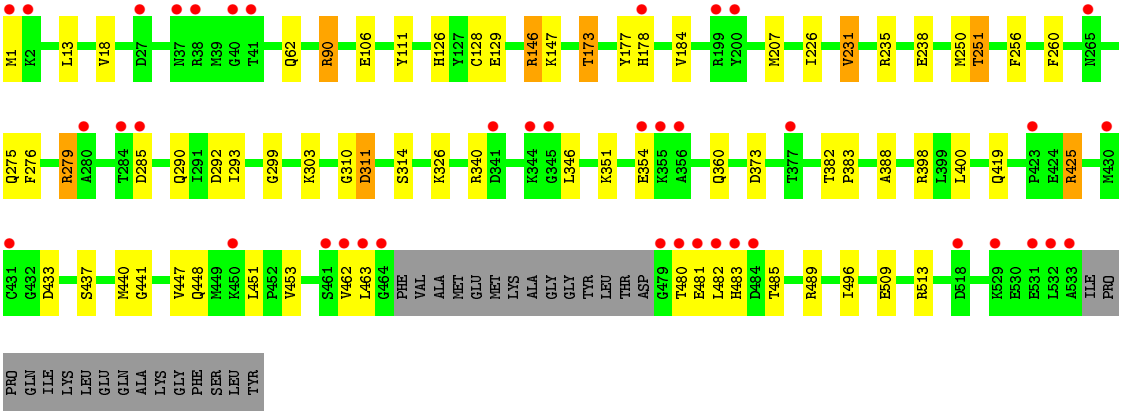
• Molecule 1: Pyruvate dehydrogenase [cytochrome]

Chain F:

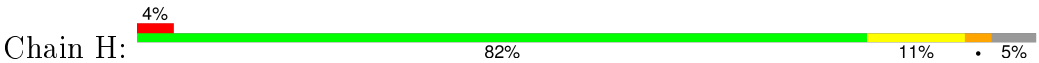


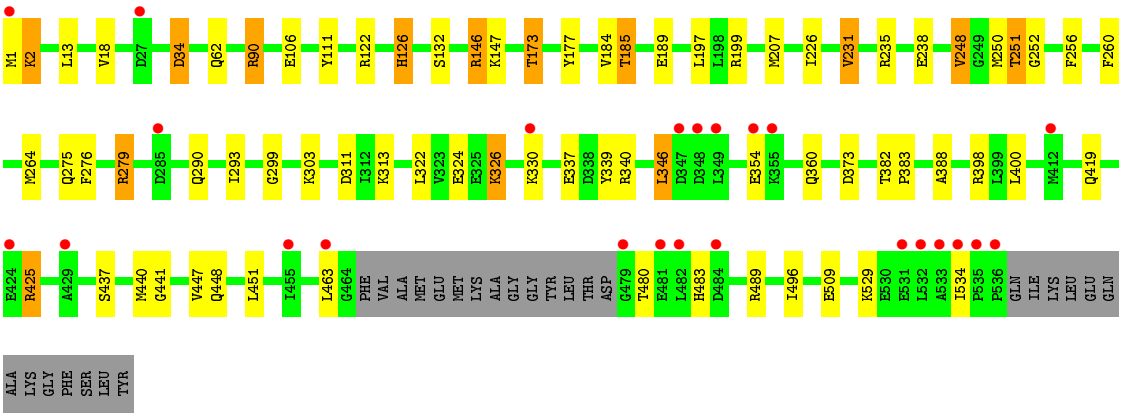
• Molecule 1: Pyruvate dehydrogenase [cytochrome]



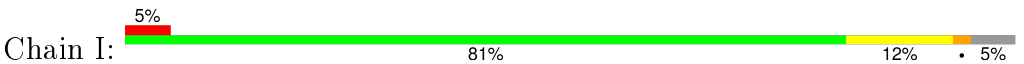


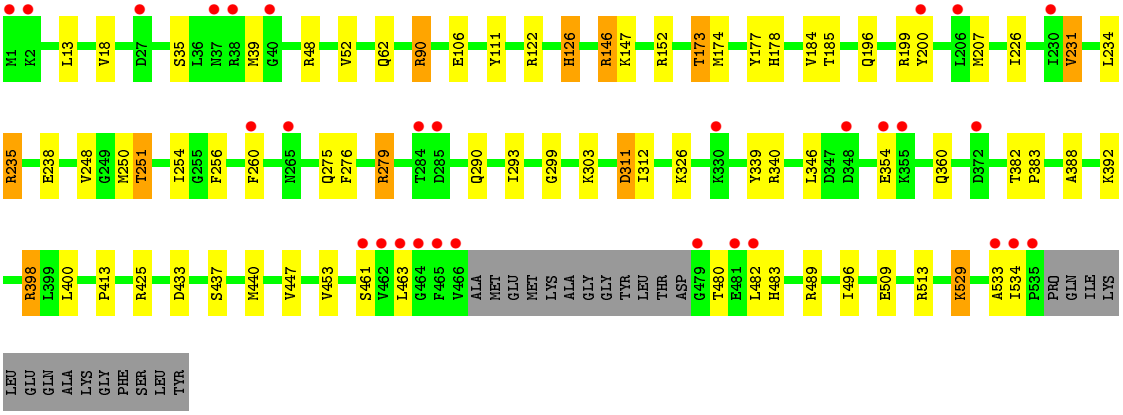
• Molecule 1: Pyruvate dehydrogenase [cytochrome]





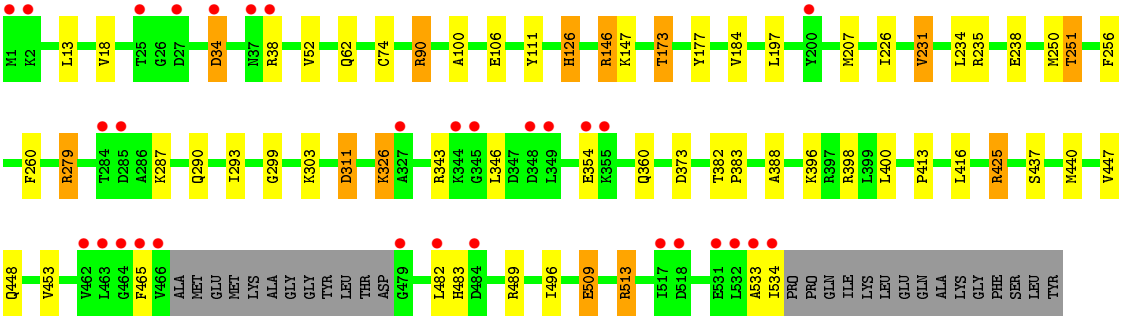
• Molecule 1: Pyruvate dehydrogenase [cytochrome]





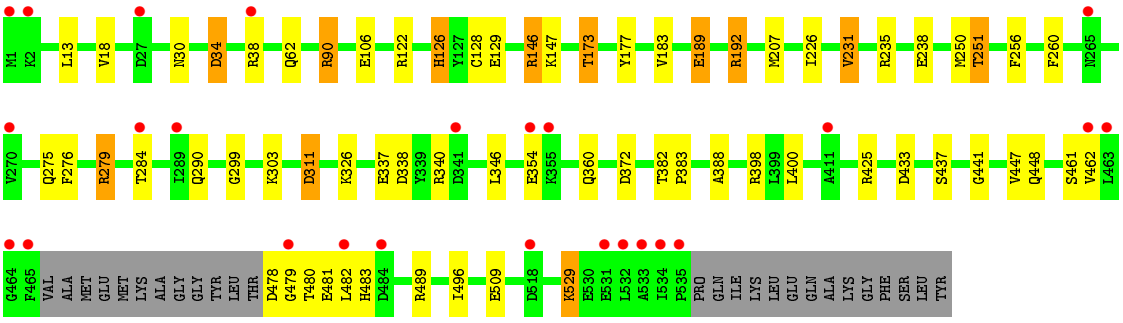
• Molecule 1: Pyruvate dehydrogenase [cytochrome]

Chain J:



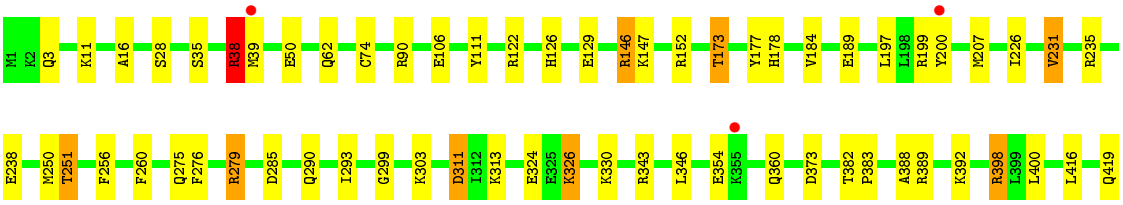
• Molecule 1: Pyruvate dehydrogenase [cytochrome]

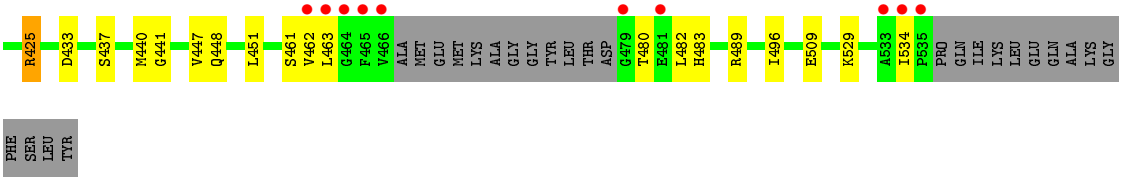
Chain K:



• Molecule 1: Pyruvate dehydrogenase [cytochrome]

Chain L:




R425
D433
S437
M440
G441
V447
Q448
L451
S461
V462
L463
G464
F465
V466
ALA
MET
GLU
MET
LYS
ALA
GLY
GLY
TYR
LEU
THR
ASP
G479
T480
E481
L482
H483
R489
I496
E509
K529
A533
I534
P535
PRO
GLN
ILE
LYS
LEU
GLU
GLN
ALA
LYS
GLY
PHE
SER
LEU
TYR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	203.24Å 207.05Å 214.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.50) 99.6 (29.99-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.4.0062	Depositor
R, R_{free}	0.183 , 0.198 0.186 , 0.186	Depositor DCC
R_{free} test set	15607 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 38.6	EDS
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 309367 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	50360	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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: PO4, TDP, MG, FAD

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	0.68	1/4186 (0.0%)	0.76	12/5670 (0.2%)
1	B	0.61	0/4096	0.73	10/5550 (0.2%)
1	C	0.66	3/4088 (0.1%)	0.77	12/5540 (0.2%)
1	D	0.65	0/4076	0.74	8/5522 (0.1%)
1	E	0.63	4/4063 (0.1%)	0.70	8/5508 (0.1%)
1	F	0.57	1/4060 (0.0%)	0.69	9/5502 (0.2%)
1	G	0.55	1/4024 (0.0%)	0.67	6/5453 (0.1%)
1	H	0.62	1/4066 (0.0%)	0.72	9/5513 (0.2%)
1	I	0.66	8/4065 (0.2%)	0.81	16/5507 (0.3%)
1	J	0.64	6/4092 (0.1%)	0.82	11/5543 (0.2%)
1	K	0.64	0/4102	0.75	9/5556 (0.2%)
1	L	0.68	2/4123 (0.0%)	0.75	10/5584 (0.2%)
All	All	0.63	27/49041 (0.1%)	0.74	120/66448 (0.2%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	351	LYS	CG-CD	12.22	1.94	1.52
1	E	351	LYS	CE-NZ	12.20	1.79	1.49
1	E	513[A]	ARG	CD-NE	11.85	1.66	1.46
1	E	513[B]	ARG	CD-NE	11.85	1.66	1.46
1	I	513[A]	ARG	NE-CZ	9.84	1.45	1.33
1	I	513[B]	ARG	NE-CZ	9.84	1.45	1.33
1	C	340	ARG	CZ-NH1	8.49	1.44	1.33
1	J	513[A]	ARG	CZ-NH1	8.40	1.44	1.33
1	J	513[B]	ARG	CZ-NH1	8.40	1.44	1.33
1	I	513[A]	ARG	CG-CD	-6.77	1.35	1.51
1	I	513[B]	ARG	CG-CD	-6.77	1.35	1.51
1	J	513[A]	ARG	CG-CD	6.28	1.67	1.51
1	J	513[B]	ARG	CG-CD	6.28	1.67	1.51
1	C	340	ARG	CD-NE	6.06	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	340	ARG	CZ-NH2	6.00	1.40	1.33
1	J	513[A]	ARG	CD-NE	-5.93	1.36	1.46
1	J	513[B]	ARG	CD-NE	-5.93	1.36	1.46
1	I	513[A]	ARG	CZ-NH1	-5.91	1.25	1.33
1	I	513[B]	ARG	CZ-NH1	-5.91	1.25	1.33
1	E	351	LYS	CG-CD	5.73	1.72	1.52
1	L	189	GLU	CG-CD	5.72	1.60	1.51
1	H	122	ARG	CG-CD	5.45	1.65	1.51
1	I	513[A]	ARG	CB-CG	-5.40	1.38	1.52
1	I	513[B]	ARG	CB-CG	-5.40	1.38	1.52
1	L	129	GLU	CD-OE1	5.15	1.31	1.25
1	G	351	LYS	CE-NZ	5.08	1.61	1.49
1	A	187	GLU	CD-OE2	5.03	1.31	1.25

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	513[A]	ARG	NE-CZ-NH1	18.57	129.59	120.30
1	J	513[B]	ARG	NE-CZ-NH1	18.57	129.59	120.30
1	C	340	ARG	NE-CZ-NH1	-14.26	113.17	120.30
1	I	513[A]	ARG	NE-CZ-NH1	14.22	127.41	120.30
1	I	513[B]	ARG	NE-CZ-NH1	14.22	127.41	120.30
1	J	513[A]	ARG	NE-CZ-NH2	-12.43	114.08	120.30
1	J	513[B]	ARG	NE-CZ-NH2	-12.43	114.08	120.30
1	L	90	ARG	NE-CZ-NH2	-11.92	114.34	120.30
1	B	90	ARG	NE-CZ-NH2	-11.35	114.63	120.30
1	K	90	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	A	90	ARG	NE-CZ-NH2	-10.91	114.85	120.30
1	D	90	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	I	90	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	J	90	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	H	90	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	I	513[A]	ARG	NH1-CZ-NH2	-10.49	107.86	119.40
1	I	513[B]	ARG	NH1-CZ-NH2	-10.49	107.86	119.40
1	C	90	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	G	90	ARG	NE-CZ-NH2	-10.05	115.27	120.30
1	E	90	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	F	90	ARG	NE-CZ-NH2	-9.67	115.47	120.30
1	A	235	ARG	NE-CZ-NH2	-8.95	115.82	120.30
1	I	513[A]	ARG	NE-CZ-NH2	8.82	124.71	120.30
1	I	513[B]	ARG	NE-CZ-NH2	8.82	124.71	120.30
1	I	279	ARG	NE-CZ-NH2	-8.82	115.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	279	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	D	279	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	L	279	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	K	279	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	K	192[A]	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	K	192[B]	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	L	235	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	H	279	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	A	279	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	B	279	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	B	235	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	D	235	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	E	122	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	H	235	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	G	279	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	C	90	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	E	279	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	E	235	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	J	279	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	D	235	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	D	90	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	G	235	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	C	235	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	C	279	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	I	235	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	F	279	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	K	235	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	F	235	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	B	235	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	C	122	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	J	90	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	L	279	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	B	90	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	K	90	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	F	351	LYS	CB-CG-CD	-6.65	94.31	111.60
1	A	235	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	L	235	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	K	279	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	I	90	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	122	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	B	122	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	F	235	ARG	NE-CZ-NH1	6.29	123.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	484	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	L	90	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	C	513[A]	ARG	NE-CZ-NH1	-6.09	117.26	120.30
1	C	513[B]	ARG	NE-CZ-NH1	-6.09	117.26	120.30
1	C	513[A]	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	C	513[B]	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	B	279	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	I	279	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	E	90	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	H	90	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	90	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	90	ARG	CG-CD-NE	-5.95	99.31	111.80
1	F	90	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	K	235	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	D	90	ARG	CG-CD-NE	-5.85	99.51	111.80
1	L	398	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	I	90	ARG	CG-CD-NE	-5.80	99.61	111.80
1	L	122	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	279	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	90	ARG	CG-CD-NE	-5.74	99.74	111.80
1	J	235	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	E	90	ARG	CG-CD-NE	-5.67	99.90	111.80
1	I	122[A]	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	I	122[B]	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	H	279	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	279	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	H	122	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	K	90	ARG	CG-CD-NE	-5.58	100.08	111.80
1	L	90	ARG	CG-CD-NE	-5.57	100.10	111.80
1	F	279	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	G	90	ARG	CG-CD-NE	-5.55	100.14	111.80
1	J	235	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	H	90	ARG	CG-CD-NE	-5.49	100.27	111.80
1	G	279	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	122	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	E	152	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	G	90	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	L	38	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	H	235	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	I	235	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	I	398	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	90	ARG	CG-CD-NE	-5.34	100.59	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	398	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	146	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	J	90	ARG	CG-CD-NE	-5.29	100.70	111.80
1	F	90	ARG	CG-CD-NE	-5.23	100.83	111.80
1	J	279	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	433	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	38	ARG	CB-CA-C	5.10	120.61	110.40
1	F	293	ILE	CB-CA-C	-5.07	101.46	111.60
1	A	122	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	H	34	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	E	351	LYS	CD-CE-NZ	-5.01	100.19	111.70

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	4066	0	4095	79	2
1	B	3999	0	3991	51	0
1	C	4001	0	3990	63	0
1	D	3977	0	3975	71	0
1	E	3975	0	3967	57	0
1	F	3969	0	3969	53	0
1	G	3939	0	3938	56	0
1	H	3973	0	3982	65	0
1	I	3978	0	3978	47	0
1	J	3993	0	3999	43	0
1	K	4005	0	4014	69	0
1	L	4016	0	4027	61	2
2	A	26	0	16	4	0
2	B	26	0	16	2	0
2	C	26	0	16	3	0
2	D	26	0	16	2	0
2	E	26	0	16	3	0
2	F	26	0	16	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	26	0	16	3	0
2	H	26	0	16	3	0
2	I	26	0	16	3	0
2	J	26	0	16	3	0
2	K	26	0	16	6	0
2	L	26	0	16	5	0
3	A	53	0	31	1	0
3	B	53	0	31	3	0
3	C	53	0	31	1	0
3	D	53	0	31	3	0
3	E	53	0	31	5	0
3	F	53	0	31	4	0
3	G	53	0	31	4	0
3	H	53	0	31	2	0
3	I	53	0	31	6	0
3	J	53	0	31	4	0
3	K	53	0	31	2	0
3	L	53	0	31	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	30	0	0	8	0
5	B	15	0	0	1	0
5	C	10	0	0	0	0
5	D	35	0	0	3	0
5	E	10	0	0	1	0
5	F	10	0	0	1	0
5	G	15	0	0	0	0
5	H	10	0	0	1	0
5	I	10	0	0	1	0
5	J	5	0	0	0	0
5	K	5	0	0	1	0
5	L	25	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	280	0	0	15	0
6	B	60	0	0	0	0
6	C	73	0	0	4	0
6	D	88	0	0	6	0
6	E	43	0	0	8	0
6	F	41	0	0	2	0
6	G	40	0	0	1	0
6	H	64	0	0	4	0
6	I	62	0	0	1	0
6	J	50	0	0	3	0
6	K	77	0	0	4	0
6	L	451	0	0	28	0
All	All	50360	0	48489	659	2

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 (659) 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:G:611:TDP:C2	2:G:611:TDP:H2	0.97	1.50
2:L:611:TDP:C2	2:L:611:TDP:H2	0.97	1.50
2:F:611:TDP:H2	2:F:611:TDP:C2	0.97	1.50
2:A:611:TDP:C2	2:A:611:TDP:H2	0.97	1.49
2:K:611:TDP:C2	2:K:611:TDP:H2	0.97	1.49
1:K:337:GLU:CG	1:K:340:ARG:HH22	1.26	1.49
2:I:611:TDP:H2	2:I:611:TDP:C2	0.97	1.48
2:H:611:TDP:C2	2:H:611:TDP:H2	0.97	1.48
2:E:611:TDP:H2	2:E:611:TDP:C2	0.97	1.48
2:C:611:TDP:H2	2:C:611:TDP:C2	0.97	1.48
2:B:611:TDP:H2	2:B:611:TDP:C2	0.97	1.47
2:J:611:TDP:C2	2:J:611:TDP:H2	0.97	1.47
2:D:611:TDP:H2	2:D:611:TDP:C2	0.97	1.47
1:C:337:GLU:CG	1:C:340:ARG:HH21	1.25	1.46
1:F:351:LYS:CG	1:F:351:LYS:CD	1.94	1.42
1:E:351:LYS:NZ	1:E:351:LYS:CE	1.79	1.41
1:C:337:GLU:CG	1:C:340:ARG:NH2	1.80	1.40
1:K:337:GLU:CG	1:K:340:ARG:NH2	1.97	1.27
1:D:355:LYS:CE	1:H:322:LEU:HA	1.64	1.25
1:C:337:GLU:HG3	1:C:340:ARG:NH2	0.93	1.24
1:K:337:GLU:HG3	1:K:340:ARG:NH2	1.52	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:509:GLU:OE2	1:J:513[A]:ARG:NH1	1.78	1.16
1:F:396:LYS:NZ	6:F:625:HOH:O	1.80	1.14
6:A:682:HOH:O	1:J:251:THR:HG21	1.48	1.12
1:K:337:GLU:HG3	1:K:340:ARG:HH22	0.98	1.11
6:A:699:HOH:O	1:L:251:THR:HG21	1.50	1.10
1:D:355:LYS:HE2	1:H:322:LEU:HA	1.27	1.09
1:D:355:LYS:HE3	1:H:322:LEU:HD23	1.34	1.09
1:C:251:THR:HG21	6:L:721:HOH:O	1.50	1.09
6:D:672:HOH:O	1:H:330:LYS:HE2	1.49	1.08
1:C:248:VAL:HG23	1:C:339:TYR:HB2	1.32	1.07
6:A:684:HOH:O	1:G:251:THR:HG21	1.53	1.07
6:A:760:HOH:O	1:D:251:THR:HG21	1.54	1.06
1:K:478:ASP:OD2	1:K:480:THR:HB	1.57	1.05
1:A:251:THR:HG21	6:A:696:HOH:O	1.56	1.04
1:E:178[B]:HIS:HD2	6:E:770:HOH:O	1.39	1.03
1:H:2:LYS:N	1:H:2:LYS:HE2	1.79	0.98
1:K:337:GLU:HG3	1:K:340:ARG:CZ	1.92	0.97
1:A:39:MET:O	1:L:11:LYS:HE3	1.63	0.97
1:A:122:ARG:HH11	1:A:122:ARG:HG3	1.27	0.96
1:H:2:LYS:H	1:H:2:LYS:HE2	1.29	0.95
1:K:251:THR:HG21	6:L:634:HOH:O	1.64	0.95
1:I:251:THR:HG23	1:I:260:PHE:HA	1.49	0.95
1:K:337:GLU:HG2	1:K:340:ARG:NH2	1.82	0.94
1:H:251:THR:HG21	6:L:949:HOH:O	1.65	0.94
1:C:248:VAL:CG2	1:C:339:TYR:HB2	2.00	0.91
1:D:251:THR:HG23	1:D:260:PHE:HA	1.52	0.91
1:I:251:THR:CG2	1:I:260:PHE:HA	2.00	0.90
1:H:251:THR:HG23	1:H:260:PHE:HA	1.52	0.90
1:L:324:GLU:HG2	5:L:617:PO4:O4	1.72	0.89
1:K:337:GLU:HG3	1:K:340:ARG:NH1	1.86	0.89
1:A:39:MET:O	1:L:11:LYS:CE	2.21	0.88
1:C:448:GLN:HE21	1:D:483:HIS:H	1.20	0.88
1:L:250:MET:HE2	6:L:1043:HOH:O	1.74	0.88
1:A:251:THR:HG23	1:A:260[A]:PHE:HA	1.56	0.88
2:G:611:TDP:H352	5:H:615:PO4:O3	1.74	0.88
1:J:251:THR:HG23	1:J:260:PHE:HA	1.57	0.87
1:J:251:THR:CG2	1:J:260:PHE:HA	2.04	0.87
1:K:251:THR:HG23	1:K:260:PHE:HA	1.57	0.86
1:C:251:THR:HG23	1:C:260:PHE:HA	1.58	0.86
1:K:251:THR:CG2	1:K:260:PHE:HA	2.05	0.86
1:H:251:THR:CG2	1:H:260:PHE:HA	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:THR:CG2	1:E:260:PHE:HA	2.06	0.86
1:A:248[B]:VAL:HG13	1:A:339:TYR:HB2	1.56	0.86
1:C:251:THR:CG2	1:C:260:PHE:HA	2.07	0.85
1:E:251:THR:HG23	1:E:260:PHE:HA	1.58	0.85
1:G:251:THR:HG23	1:G:260:PHE:HA	1.59	0.84
1:H:324:GLU:OE2	6:H:663:HOH:O	1.94	0.84
1:E:311:ASP:HB3	6:E:1065:HOH:O	1.77	0.84
1:D:251:THR:CG2	1:D:260:PHE:HA	2.07	0.84
1:A:313:LYS:NZ	5:A:619:PO4:O1	2.09	0.84
1:K:337:GLU:CD	1:K:340:ARG:HH22	1.81	0.84
1:L:251:THR:CG2	1:L:260:PHE:HA	2.08	0.84
1:G:251:THR:CG2	1:G:260:PHE:HA	2.07	0.83
1:C:337:GLU:HG3	1:C:340:ARG:HH22	1.40	0.83
1:L:251:THR:HG23	1:L:260:PHE:HA	1.59	0.83
1:K:483:HIS:H	1:L:448:GLN:HE21	1.24	0.83
1:B:251:THR:HG23	1:B:260:PHE:HA	1.61	0.83
1:C:337:GLU:HA	1:C:340:ARG:HE	1.43	0.82
1:A:251:THR:CG2	1:A:260[A]:PHE:HA	2.08	0.82
1:B:251:THR:CG2	1:B:260:PHE:HA	2.09	0.81
1:K:462:VAL:CG2	1:K:480:THR:HG22	2.11	0.81
1:C:433:ASP:OD2	1:C:482:LEU:HD12	1.78	0.81
1:G:483:HIS:H	1:H:448:GLN:HE21	1.29	0.81
1:K:478:ASP:OD2	1:K:480:THR:CB	2.28	0.81
1:E:311:ASP:OD2	6:E:1065:HOH:O	2.00	0.80
1:F:251:THR:HG23	1:F:260:PHE:HA	1.62	0.80
1:G:433:ASP:OD2	1:G:482:LEU:HD12	1.81	0.80
1:F:251:THR:CG2	1:F:260:PHE:HA	2.11	0.80
1:E:483:HIS:H	1:F:448:GLN:HE21	1.29	0.80
1:I:174:MET:N	5:I:614:PO4:O1	2.11	0.79
1:D:250:MET:HE2	6:L:629:HOH:O	1.83	0.79
1:A:174:MET:N	5:A:618:PO4:O1	2.13	0.79
1:A:344:LYS:HD3	1:A:537:GLN:NE2	1.98	0.78
1:I:483:HIS:H	1:J:448:GLN:HE21	1.31	0.78
1:K:337:GLU:HG3	1:K:340:ARG:HH12	1.45	0.78
2:K:611:TDP:H4'2	2:K:611:TDP:H2	1.49	0.77
1:C:184[A]:VAL:HG23	1:C:311:ASP:HB3	1.65	0.77
1:A:448:GLN:HE21	1:B:483:HIS:H	1.32	0.77
1:D:355:LYS:HE3	1:H:322:LEU:HA	1.64	0.77
1:F:462:VAL:HG23	1:F:480:THR:O	1.84	0.76
1:H:2:LYS:CE	1:H:2:LYS:H	1.98	0.76
1:F:351:LYS:CB	1:F:351:LYS:CD	2.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:465:PHE:CD2	1:J:465:PHE:O	2.38	0.76
1:G:448:GLN:HE21	1:H:483:HIS:H	1.34	0.76
1:K:448:GLN:HE21	1:L:483:HIS:H	1.34	0.75
6:A:685:HOH:O	1:C:250:MET:HE2	1.87	0.74
1:C:448:GLN:NE2	1:D:483:HIS:H	1.84	0.74
1:K:337:GLU:HA	1:K:340:ARG:NH1	2.02	0.74
5:E:614:PO4:O2	2:F:611:TDP:H352	1.88	0.74
1:G:279:ARG:HD3	1:H:106:GLU:OE1	1.88	0.74
1:B:433:ASP:OD2	1:B:482:LEU:HD12	1.88	0.74
6:A:825:HOH:O	1:D:146:ARG:HD2	1.88	0.73
1:K:279:ARG:HD3	1:L:106:GLU:OE1	1.88	0.73
1:H:185:THR:HG21	6:H:670:HOH:O	1.89	0.73
6:E:1066:HOH:O	1:H:146:ARG:HD2	1.89	0.73
1:L:433:ASP:OD2	1:L:482:LEU:HD12	1.89	0.73
1:A:448:GLN:NE2	1:B:483:HIS:H	1.86	0.73
1:A:106:GLU:OE1	1:B:279:ARG:HD3	1.89	0.72
1:A:251:THR:CG2	1:A:260[B]:PHE:HA	2.20	0.72
1:K:483:HIS:H	1:L:448:GLN:NE2	1.87	0.72
1:E:483:HIS:H	1:F:448:GLN:NE2	1.87	0.71
1:D:355:LYS:HE3	1:H:322:LEU:CD2	2.16	0.71
1:C:173:THR:CG2	6:C:619:HOH:O	2.39	0.71
1:E:279:ARG:HD3	1:F:106:GLU:OE1	1.90	0.70
1:G:178:HIS:HB3	6:G:630:HOH:O	1.91	0.70
1:C:279:ARG:HD3	1:D:106:GLU:OE1	1.92	0.70
1:I:483:HIS:H	1:J:448:GLN:NE2	1.89	0.70
1:I:199:ARG:HD3	1:I:200:TYR:CE2	2.26	0.70
1:D:355:LYS:HE2	1:H:322:LEU:CA	2.15	0.70
1:I:392:LYS:HE3	6:L:931:HOH:O	1.91	0.70
1:D:355:LYS:CE	1:H:322:LEU:HD23	2.18	0.69
1:L:28[B]:SER:HG	1:L:74:CYS:HG	1.37	0.69
1:E:351:LYS:NZ	1:E:351:LYS:CG	2.56	0.69
6:A:756:HOH:O	1:K:250:MET:HE2	1.91	0.69
1:A:447:VAL:HG23	1:A:496:ILE:HD11	1.75	0.69
1:G:447:VAL:HG23	1:G:496:ILE:HD11	1.75	0.69
1:C:447:VAL:HG23	1:C:496:ILE:HD11	1.75	0.68
1:A:339:TYR:OH	1:A:343[B]:ARG:HD3	1.93	0.68
1:B:311:ASP:OD2	1:B:314:SER:HB3	1.92	0.68
1:E:351:LYS:CD	1:E:351:LYS:NZ	2.57	0.68
1:I:447:VAL:HG23	1:I:496:ILE:HD11	1.76	0.68
1:J:447:VAL:HG23	1:J:496:ILE:HD11	1.75	0.68
1:H:313:LYS:NZ	6:H:650:HOH:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:279:ARG:HD3	1:J:106:GLU:OE1	1.93	0.68
1:F:248:VAL:HG22	1:F:339:TYR:HB2	1.76	0.68
1:L:447:VAL:HG23	1:L:496:ILE:HD11	1.74	0.68
1:D:344:LYS:HD3	6:D:672:HOH:O	1.94	0.67
1:H:447:VAL:HG23	1:H:496:ILE:HD11	1.76	0.67
1:C:337:GLU:HA	1:C:340:ARG:NE	2.09	0.67
1:A:250:MET:HE2	6:A:632:HOH:O	1.94	0.67
1:B:447:VAL:HG23	1:B:496:ILE:HD11	1.76	0.67
1:A:251:THR:HG23	1:A:260[B]:PHE:HA	1.76	0.67
1:A:343[A]:ARG:NH1	1:A:389:ARG:O	2.25	0.67
1:K:448:GLN:NE2	1:L:483:HIS:H	1.93	0.67
1:A:146:ARG:HD2	6:A:625:HOH:O	1.95	0.67
1:D:509:GLU:HG2	6:D:637:HOH:O	1.94	0.67
1:D:173:THR:HG23	6:D:641:HOH:O	1.95	0.67
1:D:447:VAL:HG23	1:D:496:ILE:HD11	1.77	0.66
1:C:337:GLU:HG2	1:C:340:ARG:NH2	2.04	0.66
1:E:311:ASP:CB	6:E:1065:HOH:O	2.38	0.66
1:E:447:VAL:HG23	1:E:496:ILE:HD11	1.76	0.66
1:F:447:VAL:HG23	1:F:496:ILE:HD11	1.77	0.66
1:H:337:GLU:HG3	1:H:340:ARG:HH22	1.61	0.66
1:D:173:THR:CG2	6:D:641:HOH:O	2.44	0.65
1:K:447:VAL:HG23	1:K:496:ILE:HD11	1.76	0.65
1:E:146:ARG:HD2	6:L:877:HOH:O	1.97	0.65
1:H:146:ARG:NH2	1:H:177:TYR:O	2.28	0.65
1:E:351:LYS:NZ	1:E:351:LYS:HG2	2.12	0.64
1:L:313:LYS:NZ	6:L:1062:HOH:O	2.30	0.64
1:F:462:VAL:CG2	1:F:480:THR:O	2.44	0.64
1:G:448:GLN:NE2	1:H:483:HIS:H	1.94	0.64
1:H:463:LEU:HB3	2:H:611:TDP:H5A1	1.80	0.64
2:C:611:TDP:H352	5:D:615:PO4:O2	1.97	0.64
2:J:611:TDP:H4'2	2:J:611:TDP:H2	1.63	0.63
6:A:751:HOH:O	1:B:146:ARG:HD2	1.98	0.63
1:A:483:HIS:H	1:B:448:GLN:HE21	1.46	0.63
1:A:251:THR:HG22	1:A:260[B]:PHE:HD1	1.64	0.62
1:I:303:LYS:HD3	1:L:173:THR:HG21	1.81	0.62
1:H:248:VAL:HG22	1:H:339:TYR:HB2	1.80	0.62
1:C:106:GLU:OE1	1:D:279:ARG:HD3	1.98	0.62
1:D:355:LYS:CE	1:H:322:LEU:CA	2.60	0.62
1:J:303:LYS:HD3	1:K:173:THR:HG21	1.80	0.62
1:B:462:VAL:HG23	1:B:480:THR:O	1.99	0.62
1:A:38:ARG:HB2	1:L:38:ARG:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:HB2	6:L:800:HOH:O	1.99	0.61
1:A:38:ARG:HA	1:L:38:ARG:O	2.01	0.61
1:C:337:GLU:CG	1:C:340:ARG:HH22	2.02	0.61
1:A:257:SER:HA	1:A:260[B]:PHE:CD2	2.36	0.61
1:F:303:LYS:HD3	1:G:173:THR:HG21	1.81	0.61
1:F:146:ARG:NH2	1:F:177:TYR:O	2.31	0.61
1:J:173:THR:HG21	1:K:303:LYS:HD3	1.82	0.61
1:E:173:THR:HG21	1:H:303:LYS:HD3	1.83	0.61
1:H:337:GLU:HG3	1:H:340:ARG:NH2	2.16	0.60
1:E:250:MET:HE2	6:L:688:HOH:O	2.01	0.60
1:J:396:LYS:NZ	6:J:1235:HOH:O	2.35	0.60
1:F:433:ASP:OD2	1:F:482:LEU:HD12	1.99	0.60
1:A:122:ARG:NH1	1:A:122:ARG:HG3	2.05	0.60
1:G:482:LEU:O	1:G:483:HIS:C	2.39	0.60
1:A:492:GLU:OE2	5:A:617:PO4:O4	2.19	0.60
1:B:303:LYS:HD3	1:C:173:THR:HG21	1.83	0.59
1:K:189:GLU:HA	1:K:192[B]:ARG:NH1	2.17	0.59
1:B:173:THR:HG21	1:C:303:LYS:HD3	1.84	0.59
1:K:122[B]:ARG:CG	1:K:122[B]:ARG:HH11	2.15	0.59
1:D:146:ARG:NH2	1:D:177:TYR:O	2.33	0.59
1:L:250:MET:CE	6:L:1043:HOH:O	2.43	0.59
1:L:392:LYS:HE3	6:L:713:HOH:O	2.02	0.59
1:I:173:THR:HG21	1:L:303:LYS:HD3	1.83	0.59
1:E:106:GLU:OE1	1:F:279:ARG:HD3	2.02	0.59
1:A:483:HIS:H	1:B:448:GLN:NE2	2.01	0.59
1:D:355:LYS:NZ	1:H:322:LEU:HA	2.16	0.59
1:C:173:THR:HG23	6:C:619:HOH:O	1.99	0.59
1:G:483:HIS:O	1:G:485:THR:OG1	2.21	0.58
1:K:433:ASP:OD2	1:K:482:LEU:HD12	2.03	0.58
1:K:461:SER:HB2	6:K:622:HOH:O	2.02	0.58
1:G:483:HIS:H	1:H:448:GLN:NE2	2.01	0.58
1:A:339:TYR:CZ	1:A:343[B]:ARG:HD3	2.38	0.58
1:J:146:ARG:NH2	1:J:177:TYR:O	2.31	0.58
2:I:611:TDP:H4'2	2:I:611:TDP:H2	1.69	0.57
1:C:248:VAL:HG23	1:C:339:TYR:CB	2.19	0.57
1:I:248:VAL:HG22	1:I:339:TYR:HB2	1.86	0.57
1:D:532:LEU:O	1:D:532:LEU:CG	2.50	0.57
1:L:152[A]:ARG:HD2	6:L:1046:HOH:O	2.04	0.57
1:L:146:ARG:NH2	1:L:177:TYR:O	2.31	0.57
1:K:337:GLU:HA	1:K:340:ARG:HH12	1.69	0.57
1:I:106:GLU:OE1	1:J:279:ARG:HD3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:462:VAL:HG22	1:K:480:THR:HG22	1.85	0.57
1:C:178:HIS:HB3	6:C:646:HOH:O	2.05	0.56
1:H:251:THR:HG23	1:H:260:PHE:CA	2.32	0.56
1:F:463:LEU:HB3	2:F:611:TDP:H5A1	1.86	0.56
2:K:611:TDP:H352	5:L:616:PO4:O4	2.05	0.56
1:F:351:LYS:CE	1:F:351:LYS:CG	2.81	0.56
1:B:462:VAL:CG2	1:B:480:THR:O	2.52	0.56
1:K:106:GLU:OE1	1:L:279:ARG:HD3	2.05	0.56
1:E:303:LYS:HD3	1:H:173:THR:HG21	1.86	0.56
1:L:285:ASP:N	1:L:285:ASP:OD1	2.37	0.56
1:I:90:ARG:NH2	1:J:111:TYR:O	2.38	0.56
1:H:199:ARG:NH1	1:H:324:GLU:OE1	2.38	0.56
1:G:106:GLU:OE1	1:H:279:ARG:HD3	2.06	0.56
1:E:92:HIS:HE1	3:E:612:FAD:O2A	1.89	0.56
1:B:146:ARG:NH2	1:B:177:TYR:O	2.34	0.56
1:J:173:THR:CG2	6:J:1258:HOH:O	2.53	0.56
1:A:146:ARG:NH2	1:A:177:TYR:O	2.35	0.55
1:I:146:ARG:NH2	1:I:177:TYR:O	2.32	0.55
1:K:529:LYS:HD3	1:K:529:LYS:N	2.21	0.55
1:G:90:ARG:NH2	1:H:111:TYR:O	2.39	0.55
1:A:238:GLU:OE1	1:A:398:ARG:HD2	2.06	0.55
1:D:532:LEU:O	1:D:532:LEU:HG	2.05	0.55
1:D:532:LEU:O	1:D:532:LEU:HD12	2.07	0.55
1:D:185[B]:THR:OG1	1:D:314:SER:OG	2.24	0.55
1:E:311:ASP:CG	6:E:1065:HOH:O	2.41	0.55
1:J:173:THR:HG23	6:J:1258:HOH:O	2.07	0.55
1:A:30:ASN:O	1:A:34:ASP:HB2	2.06	0.55
1:C:483:HIS:H	1:D:448:GLN:HE21	1.55	0.55
1:J:238:GLU:OE1	1:J:398:ARG:HD2	2.07	0.55
1:K:90:ARG:NH2	1:L:111:TYR:O	2.40	0.55
1:A:279:ARG:HD3	1:B:106:GLU:OE1	2.06	0.55
1:K:238:GLU:OE1	1:K:398:ARG:HD2	2.07	0.55
1:K:146:ARG:NH2	1:K:177:TYR:O	2.32	0.55
1:E:146:ARG:NH2	1:E:177:TYR:O	2.33	0.54
1:G:146:ARG:NH2	1:G:177:TYR:O	2.33	0.54
6:F:627:HOH:O	1:G:146:ARG:HD2	2.05	0.54
1:D:238:GLU:OE1	1:D:398:ARG:HD2	2.08	0.54
1:A:313:LYS:HZ1	5:A:619:PO4:P	2.25	0.54
1:G:437:SER:O	1:H:441:GLY:HA3	2.08	0.54
1:C:146:ARG:NH2	1:C:177:TYR:O	2.32	0.54
1:G:462:VAL:CG2	1:G:480:THR:O	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:290:GLN:HE22	1:F:299:GLY:H	1.56	0.54
1:K:462:VAL:HG22	1:K:480:THR:CG2	2.37	0.53
1:G:173:THR:CG2	6:L:806:HOH:O	2.55	0.53
1:C:238:GLU:OE1	1:C:398:ARG:HD2	2.08	0.53
1:A:313:LYS:NZ	5:A:619:PO4:P	2.81	0.53
1:I:126:HIS:O	1:I:147:LYS:HE3	2.08	0.53
1:C:126:HIS:O	1:C:147:LYS:HE3	2.08	0.53
1:E:448:GLN:HE21	1:F:483:HIS:HB2	1.74	0.53
1:F:238:GLU:OE1	1:F:398:ARG:HD2	2.08	0.53
1:A:111:TYR:O	1:B:90:ARG:NH2	2.41	0.53
1:L:238:GLU:OE1	1:L:398:ARG:HD2	2.09	0.53
1:D:251:THR:HG23	1:D:260:PHE:CA	2.32	0.53
1:L:251:THR:HG23	1:L:260:PHE:CA	2.36	0.53
1:D:126:HIS:O	1:D:147:LYS:HE3	2.09	0.53
1:H:238:GLU:OE1	1:H:398:ARG:HD2	2.09	0.53
1:I:238:GLU:OE1	1:I:398:ARG:HD2	2.09	0.53
1:G:462:VAL:HG23	1:G:480:THR:O	2.09	0.52
1:L:207:MET:SD	1:L:231:VAL:HG22	2.50	0.52
1:B:238:GLU:OE1	1:B:398:ARG:HD2	2.08	0.52
1:L:461:SER:HB3	6:L:752:HOH:O	2.10	0.52
1:E:126:HIS:O	1:E:147:LYS:HE3	2.09	0.52
1:I:251:THR:HG23	1:I:260:PHE:CA	2.31	0.52
1:J:465:PHE:HD2	1:J:465:PHE:O	1.91	0.52
1:A:248[B]:VAL:CG1	1:A:258:SER:HB2	2.39	0.52
1:D:293:ILE:HG12	3:D:612:FAD:C4A	2.39	0.52
1:F:248:VAL:O	1:F:248:VAL:HG13	2.10	0.52
1:H:90:ARG:HD2	6:L:892:HOH:O	2.09	0.52
1:E:238:GLU:OE1	1:E:398:ARG:HD2	2.10	0.52
1:I:290:GLN:HE22	1:I:299:GLY:H	1.58	0.52
2:K:611:TDP:N4'	2:K:611:TDP:C2	2.77	0.52
1:K:437:SER:O	1:L:441:GLY:HA3	2.10	0.52
1:J:34:ASP:O	1:J:38[B]:ARG:HG3	2.10	0.52
1:G:238:GLU:OE1	1:G:398:ARG:HD2	2.09	0.51
1:D:185[A]:THR:HG23	6:L:731:HOH:O	2.10	0.51
1:K:337:GLU:CG	1:K:340:ARG:CZ	2.66	0.51
1:E:251:THR:HG23	1:E:260:PHE:CA	2.37	0.51
1:E:90:ARG:NH2	1:F:111:TYR:O	2.43	0.51
1:A:303:LYS:HD3	1:D:173:THR:HG21	1.93	0.51
1:K:337:GLU:CG	1:K:340:ARG:HH12	2.21	0.51
1:K:478:ASP:C	1:K:480:THR:H	2.14	0.51
1:D:174:MET:N	5:D:614:PO4:O1	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ILE:HD11	1:A:513[B]:ARG:HD3	1.92	0.50
2:E:611:TDP:H352	5:F:614:PO4:O3	2.11	0.50
1:C:207:MET:SD	1:C:231:VAL:HG22	2.51	0.50
1:L:3:GLN:NE2	6:L:743:HOH:O	2.44	0.50
1:C:337:GLU:CB	1:C:340:ARG:HH21	2.13	0.50
1:A:122:ARG:HH11	1:A:122:ARG:CG	2.11	0.50
1:H:290:GLN:HE22	1:H:299:GLY:H	1.60	0.50
1:F:126[B]:HIS:CE1	1:F:148:ALA:HA	2.47	0.50
5:K:614:PO4:O1	2:L:611:TDP:H352	2.12	0.50
1:B:132:SER:HB3	1:D:132:SER:HB3	1.94	0.50
1:I:463:LEU:HB3	2:I:611:TDP:H5A1	1.94	0.50
1:L:392:LYS:CE	6:L:713:HOH:O	2.60	0.50
1:G:126:HIS:O	1:G:147:LYS:HE3	2.12	0.50
1:F:226:ILE:HA	1:F:326:LYS:HG3	1.94	0.50
1:J:146:ARG:HD2	6:K:624:HOH:O	2.10	0.49
1:K:441:GLY:HA3	1:L:437:SER:O	2.12	0.49
1:J:251:THR:HG23	1:J:260:PHE:CA	2.36	0.49
1:K:483:HIS:HD2	6:K:687:HOH:O	1.94	0.49
1:B:184:VAL:HG22	1:C:184[A]:VAL:HG12	1.94	0.49
1:C:290:GLN:HE22	1:C:299:GLY:H	1.60	0.49
1:L:290:GLN:HE22	1:L:299:GLY:H	1.60	0.49
1:D:460:ASN:O	1:D:461:SER:HB3	2.11	0.49
2:H:611:TDP:H2	2:H:611:TDP:H4'2	1.77	0.49
1:E:178[B]:HIS:CD2	6:E:770:HOH:O	2.28	0.49
1:J:290:GLN:HE22	1:J:299:GLY:H	1.60	0.49
1:K:126:HIS:O	1:K:147:LYS:HE3	2.11	0.49
1:G:226:ILE:HA	1:G:326:LYS:HG3	1.95	0.49
1:E:351:LYS:HZ3	1:E:351:LYS:CG	2.26	0.49
1:D:290:GLN:HE22	1:D:299:GLY:H	1.61	0.49
1:K:290:GLN:HE22	1:K:299:GLY:H	1.58	0.49
1:J:126:HIS:O	1:J:147:LYS:HE3	2.11	0.49
1:G:207:MET:SD	1:G:231:VAL:HG22	2.53	0.49
1:G:441:GLY:HA3	1:H:437:SER:O	2.12	0.49
1:G:481:GLU:O	1:G:482:LEU:HD23	2.12	0.49
1:D:461:SER:HB2	6:L:679:HOH:O	2.13	0.49
1:C:90:ARG:NH2	1:D:111:TYR:O	2.45	0.49
1:E:290:GLN:HE22	1:E:299:GLY:H	1.60	0.49
1:F:207:MET:SD	1:F:231:VAL:HG22	2.53	0.49
1:F:173:THR:HG21	1:G:303:LYS:HD3	1.93	0.49
1:A:461[A]:SER:HB3	6:L:785:HOH:O	2.11	0.48
1:K:462:VAL:CG2	1:K:480:THR:CG2	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:178:HIS:HB3	6:I:636:HOH:O	2.13	0.48
1:A:37:ASN:O	1:L:38:ARG:HD2	2.13	0.48
1:H:226:ILE:HA	1:H:326:LYS:HG3	1.95	0.48
1:C:251:THR:HG23	1:C:260:PHE:CA	2.37	0.48
1:A:290:GLN:HE22	1:A:299:GLY:H	1.61	0.48
1:B:290:GLN:HE22	1:B:299:GLY:H	1.59	0.48
1:D:250:MET:CE	6:L:629:HOH:O	2.52	0.48
6:A:756:HOH:O	1:K:250:MET:CE	2.56	0.48
1:F:290:GLN:NE2	1:F:299:GLY:H	2.11	0.48
1:A:207:MET:SD	1:A:231:VAL:HG22	2.53	0.48
3:E:612:FAD:H2'	3:E:612:FAD:N1	2.29	0.48
1:G:251:THR:HG23	1:G:260:PHE:CA	2.37	0.48
1:I:290:GLN:NE2	1:I:299:GLY:H	2.12	0.48
1:A:126:HIS:O	1:A:147:LYS:HE3	2.12	0.48
1:K:34:ASP:O	1:K:38:ARG:HG2	2.14	0.48
1:E:290:GLN:NE2	1:E:299:GLY:H	2.12	0.48
1:K:337:GLU:CG	1:K:340:ARG:NH1	2.68	0.48
1:D:344:LYS:CD	6:D:672:HOH:O	2.59	0.48
1:L:199:ARG:HG2	1:L:200:TYR:CD2	2.49	0.48
1:K:311:ASP:HA	3:K:612:FAD:N1A	2.29	0.48
1:G:290:GLN:HE22	1:G:299:GLY:H	1.60	0.48
1:B:207:MET:SD	1:B:231:VAL:HG22	2.54	0.48
1:B:127:TYR:CZ	1:B:129[A]:GLU:HG3	2.49	0.48
1:I:207:MET:SD	1:I:231:VAL:HG22	2.54	0.48
1:B:311:ASP:HA	3:B:612:FAD:N1A	2.28	0.47
1:K:290:GLN:NE2	1:K:299:GLY:H	2.11	0.47
1:L:126:HIS:O	1:L:147:LYS:HE3	2.13	0.47
1:C:248:VAL:HG22	1:C:258:SER:HB2	1.96	0.47
1:C:290:GLN:NE2	1:C:299:GLY:H	2.12	0.47
1:B:290:GLN:NE2	1:B:299:GLY:H	2.12	0.47
1:H:126:HIS:O	1:H:147:LYS:HE3	2.13	0.47
1:A:132:SER:HB3	1:C:132:SER:HB3	1.97	0.47
1:B:126:HIS:O	1:B:147:LYS:HE3	2.13	0.47
1:B:251:THR:HG23	1:B:260:PHE:CA	2.38	0.47
1:G:290:GLN:NE2	1:G:299:GLY:H	2.13	0.47
1:A:226:ILE:HA	1:A:326:LYS:HG3	1.96	0.47
1:A:250:MET:CE	1:A:388:ALA:HB1	2.45	0.47
1:B:312:ILE:HG12	3:B:612:FAD:C2A	2.45	0.47
1:K:251:THR:HG23	1:K:260:PHE:CA	2.37	0.47
1:G:463:LEU:HB3	2:G:611:TDP:H5A1	1.96	0.47
1:J:290:GLN:NE2	1:J:299:GLY:H	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:226:ILE:HA	1:I:326:LYS:HG3	1.97	0.47
1:G:250:MET:CE	1:G:388:ALA:HB1	2.45	0.47
1:C:189[B]:GLU:H	1:C:189[B]:GLU:CD	2.17	0.47
1:L:226:ILE:HA	1:L:326:LYS:HG3	1.97	0.47
1:L:250:MET:CE	1:L:388:ALA:HB1	2.45	0.47
1:A:359:PRO:HD2	1:A:530:GLU:OE2	2.15	0.47
1:E:207:MET:SD	1:E:231:VAL:HG22	2.55	0.47
1:K:226:ILE:HA	1:K:326:LYS:HG3	1.96	0.47
1:A:447:VAL:CG2	1:A:496:ILE:HD11	2.45	0.47
1:H:290:GLN:NE2	1:H:299:GLY:H	2.13	0.47
1:D:226:ILE:HA	1:D:326:LYS:HG3	1.96	0.47
1:I:146:ARG:HD2	6:L:741:HOH:O	2.15	0.47
1:B:226:ILE:HA	1:B:326:LYS:HG3	1.96	0.47
1:D:92:HIS:HE1	3:D:612:FAD:O2A	1.98	0.46
1:J:226:ILE:HA	1:J:326:LYS:HG3	1.96	0.46
6:A:739:HOH:O	1:C:90:ARG:HD2	2.15	0.46
1:F:389:ARG:NH1	1:F:534:ILE:HD11	2.30	0.46
1:K:207:MET:SD	1:K:231:VAL:HG22	2.55	0.46
1:K:250:MET:CE	1:K:388:ALA:HB1	2.45	0.46
1:D:128:CYS:C	1:D:129:GLU:HG2	2.35	0.46
2:L:611:TDP:H2	2:L:611:TDP:H4'2	1.81	0.46
1:I:311:ASP:HA	3:I:612:FAD:N1A	2.30	0.46
1:H:207:MET:SD	1:H:231:VAL:HG22	2.55	0.46
1:L:463:LEU:HB3	2:L:611:TDP:H5A1	1.98	0.46
1:G:482:LEU:HA	1:H:448:GLN:NE2	2.31	0.46
1:C:111:TYR:O	1:D:90:ARG:NH2	2.48	0.46
1:E:351:LYS:HZ2	1:E:351:LYS:HG2	1.81	0.46
1:D:433:ASP:OD2	1:D:482:LEU:HD12	2.16	0.46
1:F:132:SER:HB3	1:H:132:SER:HB3	1.98	0.46
1:D:285:ASP:N	1:D:285:ASP:OD1	2.47	0.46
1:D:311:ASP:HA	3:D:612:FAD:N1A	2.31	0.46
1:A:290:GLN:NE2	1:A:299:GLY:H	2.14	0.46
1:I:62:GLN:HG2	1:I:400:LEU:HD22	1.98	0.46
1:A:257:SER:HA	1:A:260[B]:PHE:HD2	1.78	0.46
1:G:482:LEU:HA	1:H:448:GLN:HE22	1.81	0.46
1:A:173:THR:HB	5:A:618:PO4:O2	2.16	0.46
1:E:250:MET:CE	1:E:388:ALA:HB1	2.46	0.46
1:D:207:MET:SD	1:D:231:VAL:HG22	2.56	0.45
1:J:207:MET:SD	1:J:231:VAL:HG22	2.56	0.45
1:C:437:SER:O	1:D:441:GLY:HA3	2.17	0.45
1:C:184[A]:VAL:HG23	1:C:311:ASP:CB	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:250:MET:CE	1:I:388:ALA:HB1	2.46	0.45
1:F:146:ARG:HD2	6:L:923:HOH:O	2.15	0.45
1:J:482:LEU:O	1:J:483:HIS:C	2.53	0.45
1:C:226:ILE:HA	1:C:326:LYS:HG3	1.97	0.45
1:E:226:ILE:HA	1:E:326:LYS:HG3	1.97	0.45
1:D:256:PHE:HA	5:D:618:PO4:O2	2.16	0.45
1:A:90:ARG:NH2	1:B:111:TYR:O	2.50	0.45
1:L:383:PRO:HD3	2:L:611:TDP:O22	2.17	0.45
1:B:463:LEU:HB3	2:B:611:TDP:H5A1	1.98	0.45
1:C:2:LYS:HG3	1:C:2:LYS:O	2.16	0.45
1:J:62:GLN:HG2	1:J:400:LEU:HD22	1.99	0.45
1:A:441:GLY:HA3	1:B:437:SER:O	2.16	0.45
1:I:111:TYR:O	1:J:90:ARG:NH2	2.49	0.45
1:F:351:LYS:CD	1:F:351:LYS:HB2	2.45	0.45
1:K:447:VAL:CG2	1:K:496:ILE:HD11	2.46	0.45
1:C:483:HIS:H	1:D:448:GLN:NE2	2.13	0.45
1:D:382:THR:N	1:D:383:PRO:CD	2.79	0.45
1:F:62:GLN:HG2	1:F:400:LEU:HD22	1.99	0.45
1:D:250:MET:CE	1:D:388:ALA:HB1	2.47	0.45
1:D:62:GLN:HG2	1:D:400:LEU:HD22	1.99	0.45
1:A:408:MET:SD	2:A:611:TDP:H4A2	2.57	0.45
1:A:448:GLN:HE21	1:B:483:HIS:N	2.07	0.45
1:J:533:ALA:C	1:J:534:ILE:HG13	2.37	0.45
1:L:293:ILE:HG12	3:L:612:FAD:C4A	2.47	0.45
1:G:448:GLN:HE21	1:H:483:HIS:N	2.09	0.45
1:F:90:ARG:HD2	6:L:737:HOH:O	2.16	0.45
1:C:184[A]:VAL:CG2	1:C:311:ASP:HB3	2.42	0.45
1:B:447:VAL:CG2	1:B:496:ILE:HD11	2.46	0.45
1:L:290:GLN:NE2	1:L:299:GLY:H	2.14	0.45
1:G:293:ILE:HG12	3:G:612:FAD:C4A	2.47	0.45
1:K:462:VAL:HG23	1:K:480:THR:HG22	1.96	0.44
1:E:92:HIS:CE1	3:E:612:FAD:O2A	2.68	0.44
3:I:612:FAD:H1'1	3:I:612:FAD:H9	1.79	0.44
1:L:462:VAL:HG23	1:L:480:THR:O	2.17	0.44
1:I:13:LEU:O	1:I:18:VAL:HG13	2.17	0.44
1:J:250:MET:CE	1:J:388:ALA:HB1	2.47	0.44
1:K:13:LEU:O	1:K:18:VAL:HG13	2.17	0.44
3:H:612:FAD:H1'1	3:H:612:FAD:H9	1.84	0.44
1:B:250:MET:CE	1:B:388:ALA:HB1	2.47	0.44
1:L:447:VAL:CG2	1:L:496:ILE:HD11	2.45	0.44
1:H:293:ILE:HG12	3:H:612:FAD:C4A	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:509:GLU:OE2	1:F:513:ARG:CD	2.65	0.44
1:B:122:ARG:HH12	1:D:122[A]:ARG:HH22	1.64	0.44
1:L:389:ARG:NH1	1:L:534:ILE:HD11	2.33	0.44
1:D:13:LEU:O	1:D:18:VAL:HG13	2.17	0.44
2:K:611:TDP:N4'	2:K:611:TDP:H2	2.26	0.44
1:E:447:VAL:CG2	1:E:496:ILE:HD11	2.46	0.44
1:D:290:GLN:NE2	1:D:299:GLY:H	2.15	0.44
1:L:311:ASP:HA	3:L:612:FAD:N1A	2.32	0.44
1:B:251:THR:HB	1:B:252:GLY:H	1.56	0.44
1:C:37:ASN:HA	1:C:37:ASN:HD22	1.69	0.44
1:A:343[A]:ARG:NH2	5:A:616:PO4:P	2.91	0.44
1:K:483:HIS:CD2	6:K:687:HOH:O	2.69	0.44
1:F:251:THR:HB	1:F:252:GLY:H	1.54	0.44
1:C:447:VAL:CG2	1:C:496:ILE:HD11	2.46	0.44
1:K:30:ASN:O	1:K:34:ASP:HB2	2.17	0.44
1:F:293:ILE:HG12	3:F:612:FAD:C4A	2.48	0.44
1:E:62:GLN:HG2	1:E:400:LEU:HD22	1.98	0.44
1:F:13:LEU:O	1:F:18:VAL:HG13	2.18	0.44
1:C:250:MET:CE	1:C:388:ALA:HB1	2.48	0.44
1:H:447:VAL:CG2	1:H:496:ILE:HD11	2.46	0.44
1:F:447:VAL:CG2	1:F:496:ILE:HD11	2.47	0.44
1:K:382:THR:N	1:K:383:PRO:CD	2.81	0.44
1:G:382:THR:N	1:G:383:PRO:CD	2.81	0.44
1:G:62:GLN:HG2	1:G:400:LEU:HD22	1.99	0.44
2:A:611:TDP:H352	5:B:614:PO4:O4	2.18	0.44
2:J:611:TDP:C2	2:J:611:TDP:N4'	2.86	0.44
1:F:251:THR:HG23	1:F:260:PHE:CA	2.41	0.44
1:A:341:ASP:HB3	1:A:537:GLN:HB2	1.99	0.44
1:C:311:ASP:HA	3:C:612:FAD:N1A	2.32	0.44
1:E:437:SER:O	1:F:441:GLY:HA3	2.18	0.44
1:A:433:ASP:OD2	1:A:482:LEU:HD12	2.17	0.44
1:C:441:GLY:HA3	1:D:437:SER:O	2.18	0.44
1:J:234:LEU:HB3	3:J:612:FAD:H1'2	2.00	0.44
2:E:611:TDP:N1'	1:F:50:GLU:OE2	2.51	0.44
1:G:311:ASP:OD2	1:G:314[A]:SER:HB3	2.17	0.44
1:C:62:GLN:HG2	1:C:400:LEU:HD22	2.00	0.44
1:H:250:MET:CE	1:H:388:ALA:HB1	2.48	0.44
1:E:509:GLU:OE2	1:E:513[A]:ARG:NE	2.49	0.44
3:K:612:FAD:H1'1	3:K:612:FAD:H9	1.77	0.43
1:E:382:THR:N	1:E:383:PRO:CD	2.81	0.43
1:E:152:ARG:HB2	1:E:152:ARG:HE	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:279:ARG:NH1	1:L:106:GLU:OE2	2.51	0.43
1:F:248:VAL:O	1:F:248:VAL:CG1	2.66	0.43
1:J:437:SER:HA	1:J:440:MET:HB2	2.01	0.43
1:J:373:ASP:O	1:J:425:ARG:NH1	2.45	0.43
1:J:382:THR:N	1:J:383:PRO:CD	2.80	0.43
1:I:196:GLN:O	1:I:199:ARG:HB3	2.18	0.43
1:D:532:LEU:O	1:D:532:LEU:CD1	2.65	0.43
1:G:184[A]:VAL:HG23	1:G:310:GLY:HA2	2.00	0.43
1:L:382:THR:N	1:L:383:PRO:CD	2.82	0.43
1:G:279:ARG:NH1	1:H:106:GLU:OE2	2.51	0.43
1:G:437:SER:HA	1:G:440:MET:HB2	2.01	0.43
1:L:275:GLN:O	1:L:276:PHE:C	2.57	0.43
1:G:128:CYS:C	1:G:129:GLU:HG2	2.39	0.43
1:B:2:LYS:HB2	1:B:2:LYS:HE3	1.65	0.43
1:I:382:THR:N	1:I:383:PRO:CD	2.82	0.43
1:B:62:GLN:HG2	1:B:400:LEU:HD22	1.99	0.43
6:A:644:HOH:O	1:D:329:ARG:HA	2.18	0.43
1:H:62:GLN:HG2	1:H:400:LEU:HD22	2.00	0.43
1:G:447:VAL:CG2	1:G:496:ILE:HD11	2.45	0.43
1:E:34:ASP:O	1:E:38:ARG:HG3	2.19	0.43
1:K:128:CYS:C	1:K:129:GLU:HG2	2.39	0.43
1:I:437:SER:HA	1:I:440:MET:HB2	2.00	0.43
1:A:128:CYS:C	1:A:129:GLU:HG2	2.39	0.43
1:F:250:MET:CE	1:F:388:ALA:HB1	2.49	0.43
1:H:251:THR:HB	1:H:252:GLY:H	1.55	0.43
1:A:106:GLU:OE2	1:B:279:ARG:NH1	2.52	0.43
1:B:293:ILE:HG12	3:B:612:FAD:C4A	2.49	0.43
1:F:311:ASP:HA	3:F:612:FAD:N1A	2.34	0.43
1:J:13:LEU:O	1:J:18:VAL:HG13	2.19	0.43
1:K:62:GLN:HG2	1:K:400:LEU:HD22	1.99	0.43
1:A:173:THR:HG21	1:D:303:LYS:HD3	2.01	0.42
1:F:235:ARG:HB2	3:F:612:FAD:O1P	2.19	0.42
1:A:382:THR:N	1:A:383:PRO:CD	2.82	0.42
1:A:62:GLN:HG2	1:A:400:LEU:HD22	2.01	0.42
1:C:373:ASP:O	1:C:425:ARG:NH1	2.46	0.42
1:H:382:THR:N	1:H:383:PRO:CD	2.82	0.42
1:I:529:LYS:HG2	1:I:529:LYS:H	1.54	0.42
1:K:183:VAL:HA	6:L:856:HOH:O	2.19	0.42
2:D:611:TDP:H2	2:D:611:TDP:H4'2	1.84	0.42
1:L:62:GLN:HG2	1:L:400:LEU:HD22	2.01	0.42
1:B:382:THR:N	1:B:383:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:TYR:O	1:F:90:ARG:NH2	2.52	0.42
1:A:339:TYR:OH	1:A:343[B]:ARG:NH2	2.47	0.42
1:H:437:SER:HA	1:H:440:MET:HB2	2.00	0.42
1:G:275:GLN:O	1:G:276:PHE:C	2.57	0.42
1:E:52:VAL:HG13	1:E:413:PRO:HB3	2.01	0.42
1:G:285:ASP:OD1	1:G:285:ASP:N	2.42	0.42
1:E:311:ASP:HA	3:E:612:FAD:N1A	2.35	0.42
1:J:311:ASP:HA	3:J:612:FAD:N1A	2.34	0.42
1:B:275:GLN:O	1:B:276:PHE:C	2.58	0.42
1:E:293:ILE:HG12	3:E:612:FAD:C4A	2.48	0.42
1:L:437:SER:HA	1:L:440:MET:HB2	2.02	0.42
3:J:612:FAD:H1'1	3:J:612:FAD:H9	1.78	0.42
1:H:13:LEU:O	1:H:18:VAL:HG13	2.19	0.42
1:A:437:SER:HA	1:A:440:MET:HB2	2.02	0.42
1:D:52:VAL:HG13	1:D:413:PRO:HB3	2.01	0.42
1:H:275:GLN:O	1:H:276:PHE:C	2.57	0.42
1:I:433:ASP:OD2	1:I:482:LEU:HD12	2.19	0.42
1:K:189:GLU:HA	1:K:192[B]:ARG:CZ	2.49	0.42
6:A:735:HOH:O	1:I:235:ARG:HD2	2.20	0.42
1:B:13:LEU:O	1:B:18:VAL:HG13	2.19	0.42
1:E:419:GLN:HG2	1:E:451:LEU:HB3	2.02	0.42
1:I:392:LYS:CE	6:L:931:HOH:O	2.59	0.42
1:G:111:TYR:O	1:H:90:ARG:NH2	2.53	0.42
3:F:612:FAD:H9	3:F:612:FAD:H1'1	1.63	0.42
1:I:48:ARG:HD3	1:I:48:ARG:HA	1.85	0.42
1:A:499:ILE:CD1	1:A:513[B]:ARG:HD3	2.50	0.42
1:F:382:THR:N	1:F:383:PRO:CD	2.83	0.42
1:J:52:VAL:HG13	1:J:413:PRO:HB3	2.01	0.42
1:J:416:LEU:HA	1:J:416:LEU:HD12	1.88	0.42
1:A:419:GLN:HG2	1:A:451:LEU:HB3	2.02	0.42
1:A:257:SER:O	1:A:260[B]:PHE:HB2	2.19	0.41
1:G:311:ASP:HA	3:G:612:FAD:N1A	2.35	0.41
1:J:293:ILE:HG12	3:J:612:FAD:C4A	2.50	0.41
1:E:373:ASP:O	1:E:425:ARG:NH1	2.47	0.41
1:G:373:ASP:O	1:G:425:ARG:NH1	2.48	0.41
1:A:463:LEU:HB3	2:A:611:TDP:H5A1	2.01	0.41
1:I:234:LEU:HB3	3:I:612:FAD:H1'2	2.02	0.41
1:E:13:LEU:O	1:E:18:VAL:HG13	2.20	0.41
1:I:52:VAL:HG13	1:I:413:PRO:HB3	2.02	0.41
1:E:275:GLN:O	1:E:276:PHE:C	2.59	0.41
1:D:447:VAL:CG2	1:D:496:ILE:HD11	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:437:SER:HA	1:F:440:MET:HB2	2.02	0.41
1:L:16:ALA:O	1:L:178[B]:HIS:HE1	2.02	0.41
1:B:360:GLN:HB2	1:B:390:TYR:CZ	2.56	0.41
1:A:343[A]:ARG:HH22	5:A:616:PO4:P	2.43	0.41
1:A:293:ILE:HG12	3:A:612:FAD:C4A	2.50	0.41
1:L:373:ASP:O	1:L:425:ARG:NH1	2.47	0.41
1:H:346:LEU:CD1	1:H:534:ILE:HD13	2.51	0.41
1:D:419:GLN:HG2	1:D:451:LEU:HB3	2.02	0.41
1:K:275:GLN:O	1:K:276:PHE:C	2.59	0.41
1:J:447:VAL:CG2	1:J:496:ILE:HD11	2.45	0.41
1:I:312:ILE:HG12	3:I:612:FAD:C2A	2.50	0.41
1:A:13:LEU:O	1:A:18:VAL:HG13	2.21	0.41
1:I:447:VAL:CG2	1:I:496:ILE:HD11	2.46	0.41
1:A:437:SER:O	1:B:441:GLY:HA3	2.20	0.41
1:H:419:GLN:HG2	1:H:451:LEU:HB3	2.03	0.41
1:I:533:ALA:C	1:I:534:ILE:HG13	2.41	0.41
1:C:382:THR:N	1:C:383:PRO:CD	2.83	0.41
1:G:13:LEU:O	1:G:18:VAL:HG13	2.20	0.41
1:L:35:SER:O	1:L:39:MET:HB2	2.21	0.41
1:G:419:GLN:HG2	1:G:451:LEU:HB3	2.02	0.41
2:K:611:TDP:N1'	1:L:50:GLU:OE2	2.54	0.41
1:B:437:SER:HA	1:B:440:MET:HB2	2.02	0.41
1:C:13:LEU:O	1:C:18:VAL:HG13	2.21	0.41
1:I:275:GLN:O	1:I:276:PHE:C	2.59	0.41
1:E:175:HIS:CD2	6:H:657:HOH:O	2.73	0.41
1:F:52:VAL:HG13	1:F:413:PRO:HB3	2.03	0.41
1:E:279:ARG:NH1	1:F:106:GLU:OE2	2.53	0.41
1:J:74:CYS:HA	1:J:100:ALA:O	2.21	0.41
1:E:235:ARG:NH2	6:E:1269:HOH:O	2.44	0.41
1:I:35:SER:O	1:I:39:MET:HB2	2.20	0.41
1:C:275:GLN:O	1:C:276:PHE:C	2.58	0.41
1:G:292:ASP:OD1	3:G:612:FAD:O2B	2.39	0.40
1:L:419:GLN:HG2	1:L:451:LEU:HB3	2.03	0.40
1:C:48:ARG:HA	1:C:48:ARG:HD3	1.85	0.40
1:D:48:ARG:HA	1:D:48:ARG:HD3	1.87	0.40
1:E:287:LYS:HE3	1:E:287:LYS:HB2	1.71	0.40
2:C:611:TDP:H4'2	2:C:611:TDP:H2	1.87	0.40
1:L:28[B]:SER:OG	1:L:74:CYS:SG	2.59	0.40
1:B:128:CYS:C	1:B:129[A]:GLU:HG2	2.41	0.40
1:D:127:TYR:CZ	1:D:129:GLU:HG3	2.55	0.40
1:I:254:ILE:HG12	3:I:612:FAD:C4	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:SER:HA	1:C:440:MET:HB2	2.04	0.40
1:H:373:ASP:O	1:H:425:ARG:NH1	2.46	0.40
1:D:275:GLN:O	1:D:276:PHE:C	2.59	0.40
1:K:337:GLU:OE1	1:K:340:ARG:NH2	2.52	0.40
1:C:173:THR:HG22	6:C:619:HOH:O	2.15	0.40
1:B:48:ARG:HA	1:B:48:ARG:HD3	1.85	0.40
1:F:419:GLN:HG2	1:F:451:LEU:HB3	2.03	0.40
1:H:264:MET:HE3	6:L:647:HOH:O	2.21	0.40
1:L:416:LEU:HD12	1:L:416:LEU:HA	1.88	0.40
1:D:35:SER:O	1:D:39:MET:HB2	2.22	0.40
1:B:74:CYS:HA	1:B:100:ALA:O	2.22	0.40
1:K:122[B]:ARG:NH1	1:K:122[B]:ARG:HG3	2.37	0.40
1:I:293:ILE:HG12	3:I:612:FAD:C4A	2.52	0.40
3:G:612:FAD:H9	3:G:612:FAD:H1'1	1.76	0.40
1:E:74:CYS:HA	1:E:100:ALA:O	2.22	0.40
1:C:419:GLN:HG2	1:C:451:LEU:HB3	2.03	0.40
1:E:533:ALA:O	1:E:535:PRO:HD3	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:GLU:OE1	1:L:200:TYR:OH[4_545]	1.76	0.44
1:A:344:LYS:NZ	1:L:330:LYS:CE[4_545]	1.92	0.28

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	535/549 (97%)	513 (96%)	22 (4%)	0	100	100
1	B	525/549 (96%)	505 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	524/549 (95%)	509 (97%)	14 (3%)	1 (0%)	52 75
1	D	522/549 (95%)	503 (96%)	19 (4%)	0	100 100
1	E	521/549 (95%)	504 (97%)	17 (3%)	0	100 100
1	F	520/549 (95%)	502 (96%)	18 (4%)	0	100 100
1	G	517/549 (94%)	502 (97%)	15 (3%)	0	100 100
1	H	522/549 (95%)	507 (97%)	15 (3%)	0	100 100
1	I	521/549 (95%)	506 (97%)	15 (3%)	0	100 100
1	J	524/549 (95%)	507 (97%)	17 (3%)	0	100 100
1	K	524/549 (95%)	504 (96%)	19 (4%)	1 (0%)	52 75
1	L	527/549 (96%)	509 (97%)	18 (3%)	0	100 100
All	All	6282/6588 (95%)	6071 (97%)	209 (3%)	2 (0%)	100 100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	484	ASP
1	K	479	GLY

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	434/439 (99%)	411 (95%)	23 (5%)	28 50
1	B	424/439 (97%)	401 (95%)	23 (5%)	27 49
1	C	423/439 (96%)	402 (95%)	21 (5%)	30 53
1	D	421/439 (96%)	401 (95%)	20 (5%)	31 55
1	E	420/439 (96%)	399 (95%)	21 (5%)	30 53
1	F	420/439 (96%)	400 (95%)	20 (5%)	31 55
1	G	417/439 (95%)	401 (96%)	16 (4%)	40 67
1	H	422/439 (96%)	397 (94%)	25 (6%)	24 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	420/439 (96%)	399 (95%)	21 (5%)	30 53
1	J	423/439 (96%)	402 (95%)	21 (5%)	30 53
1	K	424/439 (97%)	404 (95%)	20 (5%)	32 56
1	L	426/439 (97%)	407 (96%)	19 (4%)	34 59
All	All	5074/5268 (96%)	4824 (95%)	250 (5%)	31 55

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	34	ASP
1	A	122	ARG
1	A	126	HIS
1	A	146	ARG
1	A	173	THR
1	A	184	VAL
1	A	189	GLU
1	A	231	VAL
1	A	251	THR
1	A	256	PHE
1	A	287	LYS
1	A	311	ASP
1	A	343[A]	ARG
1	A	343[B]	ARG
1	A	346	LEU
1	A	354	GLU
1	A	360	GLN
1	A	425	ARG
1	A	461[A]	SER
1	A	461[B]	SER
1	A	489	ARG
1	A	509	GLU
1	B	122	ARG
1	B	126	HIS
1	B	146	ARG
1	B	173	THR
1	B	185	THR
1	B	189	GLU
1	B	231	VAL
1	B	251	THR
1	B	256	PHE

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Mol	Chain	Res	Type
1	B	284	THR
1	B	311	ASP
1	B	314	SER
1	B	326	LYS
1	B	338	ASP
1	B	343	ARG
1	B	346	LEU
1	B	354	GLU
1	B	360	GLN
1	B	425	ARG
1	B	484	ASP
1	B	489	ARG
1	B	509	GLU
1	B	534	ILE
1	C	2	LYS
1	C	28	SER
1	C	126	HIS
1	C	146	ARG
1	C	173	THR
1	C	185	THR
1	C	199	ARG
1	C	231	VAL
1	C	251	THR
1	C	256	PHE
1	C	311	ASP
1	C	326	LYS
1	C	346	LEU
1	C	354	GLU
1	C	360	GLN
1	C	372[A]	ASP
1	C	372[B]	ASP
1	C	425	ARG
1	C	489	ARG
1	C	509	GLU
1	C	529	LYS
1	D	2	LYS
1	D	3	GLN
1	D	34	ASP
1	D	146	ARG
1	D	173	THR
1	D	184	VAL
1	D	185[A]	THR

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Mol	Chain	Res	Type
1	D	185[B]	THR
1	D	231	VAL
1	D	251	THR
1	D	256	PHE
1	D	311	ASP
1	D	338	ASP
1	D	346	LEU
1	D	354	GLU
1	D	360	GLN
1	D	425	ARG
1	D	489	ARG
1	D	509	GLU
1	D	529	LYS
1	E	122	ARG
1	E	126	HIS
1	E	146	ARG
1	E	173	THR
1	E	185	THR
1	E	189	GLU
1	E	231	VAL
1	E	251	THR
1	E	256	PHE
1	E	284	THR
1	E	287	LYS
1	E	311	ASP
1	E	340	ARG
1	E	346	LEU
1	E	354	GLU
1	E	360	GLN
1	E	425	ARG
1	E	489	ARG
1	E	509	GLU
1	E	529	LYS
1	E	531	GLU
1	F	1	MET
1	F	34	ASP
1	F	122	ARG
1	F	146	ARG
1	F	173	THR
1	F	192	ARG
1	F	231	VAL
1	F	248	VAL

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Mol	Chain	Res	Type
1	F	251	THR
1	F	256	PHE
1	F	285	ASP
1	F	287	LYS
1	F	311	ASP
1	F	346	LEU
1	F	354	GLU
1	F	360	GLN
1	F	425	ARG
1	F	489	ARG
1	F	509	GLU
1	F	531	GLU
1	G	1	MET
1	G	146	ARG
1	G	173	THR
1	G	231	VAL
1	G	251	THR
1	G	256	PHE
1	G	311	ASP
1	G	340	ARG
1	G	346	LEU
1	G	354	GLU
1	G	360	GLN
1	G	425	ARG
1	G	453	VAL
1	G	489	ARG
1	G	509	GLU
1	G	513	ARG
1	H	1	MET
1	H	2	LYS
1	H	34	ASP
1	H	126	HIS
1	H	146	ARG
1	H	173	THR
1	H	184[A]	VAL
1	H	184[B]	VAL
1	H	185	THR
1	H	189	GLU
1	H	197	LEU
1	H	231	VAL
1	H	248	VAL
1	H	251	THR

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Mol	Chain	Res	Type
1	H	256	PHE
1	H	311	ASP
1	H	326	LYS
1	H	346	LEU
1	H	354	GLU
1	H	360	GLN
1	H	425	ARG
1	H	480	THR
1	H	489	ARG
1	H	509	GLU
1	H	529	LYS
1	I	126	HIS
1	I	146	ARG
1	I	152	ARG
1	I	173	THR
1	I	184	VAL
1	I	185	THR
1	I	231	VAL
1	I	251	THR
1	I	256	PHE
1	I	311	ASP
1	I	340	ARG
1	I	346	LEU
1	I	354	GLU
1	I	360	GLN
1	I	425	ARG
1	I	453	VAL
1	I	461	SER
1	I	480	THR
1	I	489	ARG
1	I	509	GLU
1	I	529	LYS
1	J	34	ASP
1	J	126	HIS
1	J	146	ARG
1	J	173	THR
1	J	184[A]	VAL
1	J	184[B]	VAL
1	J	197	LEU
1	J	231	VAL
1	J	251	THR
1	J	256	PHE

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Mol	Chain	Res	Type
1	J	287	LYS
1	J	311	ASP
1	J	326	LYS
1	J	343	ARG
1	J	346	LEU
1	J	354	GLU
1	J	360	GLN
1	J	425	ARG
1	J	453	VAL
1	J	489	ARG
1	J	509	GLU
1	K	34	ASP
1	K	126	HIS
1	K	146	ARG
1	K	173	THR
1	K	189	GLU
1	K	231	VAL
1	K	251	THR
1	K	256	PHE
1	K	284	THR
1	K	311	ASP
1	K	338	ASP
1	K	346	LEU
1	K	354	GLU
1	K	360	GLN
1	K	372	ASP
1	K	425	ARG
1	K	481	GLU
1	K	489	ARG
1	K	509	GLU
1	K	529	LYS
1	L	38	ARG
1	L	146	ARG
1	L	173	THR
1	L	184	VAL
1	L	197	LEU
1	L	231	VAL
1	L	251	THR
1	L	256	PHE
1	L	311	ASP
1	L	326	LYS
1	L	343[A]	ARG

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Mol	Chain	Res	Type
1	L	343[B]	ARG
1	L	346	LEU
1	L	354	GLU
1	L	360	GLN
1	L	425	ARG
1	L	489	ARG
1	L	509	GLU
1	L	529	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	37	ASN
1	A	275	GLN
1	A	290	GLN
1	A	364	GLN
1	A	365	GLN
1	A	448	GLN
1	A	537	GLN
1	B	151	ASN
1	B	275	GLN
1	B	290	GLN
1	B	364	GLN
1	B	365	GLN
1	B	448	GLN
1	C	3	GLN
1	C	37	ASN
1	C	151	ASN
1	C	178	HIS
1	C	275	GLN
1	C	290	GLN
1	C	364	GLN
1	C	365	GLN
1	C	448	GLN
1	D	3	GLN
1	D	37	ASN
1	D	92	HIS
1	D	151	ASN
1	D	290	GLN
1	D	364	GLN
1	D	365	GLN

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Mol	Chain	Res	Type
1	D	448	GLN
1	E	3	GLN
1	E	37	ASN
1	E	92	HIS
1	E	151	ASN
1	E	290	GLN
1	E	364	GLN
1	E	365	GLN
1	E	448	GLN
1	F	3	GLN
1	F	151	ASN
1	F	275	GLN
1	F	290	GLN
1	F	364	GLN
1	F	365	GLN
1	F	448	GLN
1	G	3	GLN
1	G	37	ASN
1	G	151	ASN
1	G	178	HIS
1	G	275	GLN
1	G	290	GLN
1	G	364	GLN
1	G	365	GLN
1	G	448	GLN
1	H	3	GLN
1	H	113	GLN
1	H	151	ASN
1	H	275	GLN
1	H	290	GLN
1	H	364	GLN
1	H	365	GLN
1	H	448	GLN
1	I	3	GLN
1	I	37	ASN
1	I	151	ASN
1	I	178	HIS
1	I	275	GLN
1	I	290	GLN
1	I	364	GLN
1	I	365	GLN
1	I	448	GLN

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Mol	Chain	Res	Type
1	J	151	ASN
1	J	275	GLN
1	J	290	GLN
1	J	364	GLN
1	J	365	GLN
1	J	448	GLN
1	K	3	GLN
1	K	37	ASN
1	K	92	HIS
1	K	151	ASN
1	K	290	GLN
1	K	364	GLN
1	K	365	GLN
1	K	448	GLN
1	L	3	GLN
1	L	151	ASN
1	L	275	GLN
1	L	290	GLN
1	L	364	GLN
1	L	365	GLN
1	L	448	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 72 ligands modelled in this entry, 12 are monoatomic - leaving 60 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	$\#\|Z\| > 2$
2	TDP	A	611	4	21,27,27	0.96	1 (4%)	31,40,40	3.17	9 (29%)
3	FAD	A	612	-	48,58,58	0.95	2 (4%)	54,89,89	2.18	12 (22%)
5	PO4	A	614	-	4,4,4	0.40	0	6,6,6	0.30	0
5	PO4	A	615	-	4,4,4	0.23	0	6,6,6	0.27	0
5	PO4	A	616	-	4,4,4	0.41	0	6,6,6	0.28	0
5	PO4	A	617	-	4,4,4	0.46	0	6,6,6	0.32	0
5	PO4	A	618	-	4,4,4	0.38	0	6,6,6	0.27	0
5	PO4	A	619	-	4,4,4	0.33	0	6,6,6	0.28	0
2	TDP	B	611	4	21,27,27	1.10	2 (9%)	31,40,40	2.17	11 (35%)
3	FAD	B	612	-	48,58,58	1.11	3 (6%)	54,89,89	2.17	14 (25%)
5	PO4	B	614	-	4,4,4	0.24	0	6,6,6	0.29	0
5	PO4	B	615	-	4,4,4	0.37	0	6,6,6	0.28	0
5	PO4	B	616	-	4,4,4	0.18	0	6,6,6	0.29	0
2	TDP	C	611	4	21,27,27	0.72	0	31,40,40	2.04	9 (29%)
3	FAD	C	612	-	48,58,58	1.05	3 (6%)	54,89,89	2.49	14 (25%)
5	PO4	C	614	-	4,4,4	0.25	0	6,6,6	0.35	0
5	PO4	C	615	-	4,4,4	0.25	0	6,6,6	0.26	0
2	TDP	D	611	4	21,27,27	1.59	2 (9%)	31,40,40	1.98	10 (32%)
3	FAD	D	612	-	48,58,58	1.08	4 (8%)	54,89,89	2.24	12 (22%)
5	PO4	D	614	-	4,4,4	0.47	0	6,6,6	0.29	0
5	PO4	D	615	-	4,4,4	0.19	0	6,6,6	0.36	0
5	PO4	D	616	-	4,4,4	0.41	0	6,6,6	0.27	0
5	PO4	D	617	-	4,4,4	0.47	0	6,6,6	0.29	0
5	PO4	D	618	-	4,4,4	0.44	0	6,6,6	0.26	0
5	PO4	D	619	-	4,4,4	0.42	0	6,6,6	0.27	0
5	PO4	D	620	-	4,4,4	0.44	0	6,6,6	0.25	0
2	TDP	E	611	4	21,27,27	0.86	1 (4%)	31,40,40	2.28	10 (32%)
3	FAD	E	612	-	48,58,58	0.91	2 (4%)	54,89,89	2.34	13 (24%)
5	PO4	E	614	-	4,4,4	0.33	0	6,6,6	0.32	0
5	PO4	E	615	-	4,4,4	0.30	0	6,6,6	0.29	0
2	TDP	F	611	4	21,27,27	0.97	0	31,40,40	2.30	9 (29%)
3	FAD	F	612	-	48,58,58	0.98	3 (6%)	54,89,89	2.17	10 (18%)
5	PO4	F	614	-	4,4,4	0.25	0	6,6,6	0.32	0
5	PO4	F	615	-	4,4,4	0.19	0	6,6,6	0.29	0
2	TDP	G	611	4	21,27,27	1.04	1 (4%)	31,40,40	2.37	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FAD	G	612	-	48,58,58	0.91	1 (2%)	54,89,89	2.10	12 (22%)
5	PO4	G	614	-	4,4,4	0.47	0	6,6,6	0.29	0
5	PO4	G	615	-	4,4,4	0.31	0	6,6,6	0.32	0
5	PO4	G	616	-	4,4,4	0.37	0	6,6,6	0.27	0
2	TDP	H	611	4	21,27,27	0.82	1 (4%)	31,40,40	2.16	11 (35%)
3	FAD	H	612	-	48,58,58	1.09	4 (8%)	54,89,89	2.34	10 (18%)
5	PO4	H	614	-	4,4,4	0.24	0	6,6,6	0.29	0
5	PO4	H	615	-	4,4,4	0.28	0	6,6,6	0.27	0
2	TDP	I	611	4	21,27,27	0.99	2 (9%)	31,40,40	1.84	9 (29%)
3	FAD	I	612	-	48,58,58	1.12	5 (10%)	54,89,89	2.07	7 (12%)
5	PO4	I	614	-	4,4,4	0.32	0	6,6,6	0.31	0
5	PO4	I	615	-	4,4,4	0.22	0	6,6,6	0.28	0
2	TDP	J	611	4	21,27,27	0.97	1 (4%)	31,40,40	2.38	11 (35%)
3	FAD	J	612	-	48,58,58	1.08	3 (6%)	54,89,89	2.03	12 (22%)
5	PO4	J	614	-	4,4,4	0.21	0	6,6,6	0.28	0
2	TDP	K	611	4	21,27,27	1.10	1 (4%)	31,40,40	2.38	10 (32%)
3	FAD	K	612	-	48,58,58	0.91	2 (4%)	54,89,89	1.76	12 (22%)
5	PO4	K	614	-	4,4,4	0.23	0	6,6,6	0.34	0
2	TDP	L	611	4	21,27,27	0.93	1 (4%)	31,40,40	2.33	10 (32%)
3	FAD	L	612	-	48,58,58	0.88	2 (4%)	54,89,89	2.44	13 (24%)
5	PO4	L	614	-	4,4,4	0.20	0	6,6,6	0.28	0
5	PO4	L	615	-	4,4,4	0.17	0	6,6,6	0.27	0
5	PO4	L	616	-	4,4,4	0.44	0	6,6,6	0.28	0
5	PO4	L	617	-	4,4,4	0.41	0	6,6,6	0.27	0
5	PO4	L	618	-	4,4,4	0.27	0	6,6,6	0.28	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
2	TDP	A	611	4	-	0/16/17/17	0/2/2/2
3	FAD	A	612	-	-	0/30/50/50	0/6/6/6
5	PO4	A	614	-	-	0/0/0/0	0/0/0/0
5	PO4	A	615	-	-	0/0/0/0	0/0/0/0
5	PO4	A	616	-	-	0/0/0/0	0/0/0/0
5	PO4	A	617	-	-	0/0/0/0	0/0/0/0
5	PO4	A	618	-	-	0/0/0/0	0/0/0/0
5	PO4	A	619	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TDP	B	611	4	-	0/16/17/17	0/2/2/2
3	FAD	B	612	-	-	0/30/50/50	0/6/6/6
5	PO4	B	614	-	-	0/0/0/0	0/0/0/0
5	PO4	B	615	-	-	0/0/0/0	0/0/0/0
5	PO4	B	616	-	-	0/0/0/0	0/0/0/0
2	TDP	C	611	4	-	0/16/17/17	0/2/2/2
3	FAD	C	612	-	-	0/30/50/50	0/6/6/6
5	PO4	C	614	-	-	0/0/0/0	0/0/0/0
5	PO4	C	615	-	-	0/0/0/0	0/0/0/0
2	TDP	D	611	4	-	0/16/17/17	0/2/2/2
3	FAD	D	612	-	-	0/30/50/50	0/6/6/6
5	PO4	D	614	-	-	0/0/0/0	0/0/0/0
5	PO4	D	615	-	-	0/0/0/0	0/0/0/0
5	PO4	D	616	-	-	0/0/0/0	0/0/0/0
5	PO4	D	617	-	-	0/0/0/0	0/0/0/0
5	PO4	D	618	-	-	0/0/0/0	0/0/0/0
5	PO4	D	619	-	-	0/0/0/0	0/0/0/0
5	PO4	D	620	-	-	0/0/0/0	0/0/0/0
2	TDP	E	611	4	-	0/16/17/17	0/2/2/2
3	FAD	E	612	-	-	0/30/50/50	0/6/6/6
5	PO4	E	614	-	-	0/0/0/0	0/0/0/0
5	PO4	E	615	-	-	0/0/0/0	0/0/0/0
2	TDP	F	611	4	-	0/16/17/17	0/2/2/2
3	FAD	F	612	-	-	0/30/50/50	0/6/6/6
5	PO4	F	614	-	-	0/0/0/0	0/0/0/0
5	PO4	F	615	-	-	0/0/0/0	0/0/0/0
2	TDP	G	611	4	-	0/16/17/17	0/2/2/2
3	FAD	G	612	-	-	0/30/50/50	0/6/6/6
5	PO4	G	614	-	-	0/0/0/0	0/0/0/0
5	PO4	G	615	-	-	0/0/0/0	0/0/0/0
5	PO4	G	616	-	-	0/0/0/0	0/0/0/0
2	TDP	H	611	4	-	0/16/17/17	0/2/2/2
3	FAD	H	612	-	-	0/30/50/50	0/6/6/6
5	PO4	H	614	-	-	0/0/0/0	0/0/0/0
5	PO4	H	615	-	-	0/0/0/0	0/0/0/0
2	TDP	I	611	4	-	0/16/17/17	0/2/2/2
3	FAD	I	612	-	-	0/30/50/50	0/6/6/6
5	PO4	I	614	-	-	0/0/0/0	0/0/0/0
5	PO4	I	615	-	-	0/0/0/0	0/0/0/0
2	TDP	J	611	4	-	0/16/17/17	0/2/2/2
3	FAD	J	612	-	-	0/30/50/50	0/6/6/6
5	PO4	J	614	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TDP	K	611	4	-	0/16/17/17	0/2/2/2
3	FAD	K	612	-	-	0/30/50/50	0/6/6/6
5	PO4	K	614	-	-	0/0/0/0	0/0/0/0
2	TDP	L	611	4	-	0/16/17/17	0/2/2/2
3	FAD	L	612	-	-	0/30/50/50	0/6/6/6
5	PO4	L	614	-	-	0/0/0/0	0/0/0/0
5	PO4	L	615	-	-	0/0/0/0	0/0/0/0
5	PO4	L	616	-	-	0/0/0/0	0/0/0/0
5	PO4	L	617	-	-	0/0/0/0	0/0/0/0
5	PO4	L	618	-	-	0/0/0/0	0/0/0/0

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	611	TDP	C4-N3	-5.94	1.34	1.39
3	J	612	FAD	C10-N10	-4.17	1.34	1.39
3	B	612	FAD	C10-N10	-3.76	1.34	1.39
2	G	611	TDP	C4-N3	-3.47	1.36	1.39
3	H	612	FAD	C10-N10	-3.24	1.35	1.39
3	F	612	FAD	C10-N10	-3.20	1.35	1.39
3	C	612	FAD	C6-C5X	-3.19	1.36	1.41
2	J	611	TDP	C4-N3	-3.17	1.37	1.39
3	K	612	FAD	C10-N10	-3.06	1.35	1.39
2	E	611	TDP	C4-N3	-3.05	1.37	1.39
2	I	611	TDP	C4-N3	-2.94	1.37	1.39
2	K	611	TDP	C4-N3	-2.90	1.37	1.39
2	B	611	TDP	C4-N3	-2.85	1.37	1.39
3	J	612	FAD	C9A-N10	-2.83	1.34	1.38
3	I	612	FAD	C6-C5X	-2.67	1.37	1.41
3	I	612	FAD	C10-N10	-2.55	1.36	1.39
3	A	612	FAD	C6-C5X	-2.52	1.37	1.41
3	B	612	FAD	C9A-N10	-2.50	1.35	1.38
3	D	612	FAD	C10-N10	-2.50	1.36	1.39
3	K	612	FAD	C9A-N10	-2.39	1.35	1.38
2	H	611	TDP	C4-N3	-2.35	1.37	1.39
3	C	612	FAD	C10-N10	-2.31	1.36	1.39
3	J	612	FAD	C9A-C5X	-2.24	1.38	1.42
3	H	612	FAD	C9A-N10	-2.17	1.35	1.38
3	F	612	FAD	C9A-N10	-2.02	1.36	1.38
3	C	612	FAD	C9A-N10	-2.01	1.36	1.38
2	L	611	TDP	P2-O11	2.06	1.65	1.61
3	D	612	FAD	C2A-N3A	2.08	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	612	FAD	C4X-N5	2.10	1.36	1.33
3	A	612	FAD	O4B-C1B	2.13	1.43	1.41
2	D	611	TDP	C4'-N3'	2.14	1.38	1.35
2	A	611	TDP	C2'-N3'	2.20	1.38	1.34
2	I	611	TDP	C2'-N1'	2.23	1.38	1.34
3	L	612	FAD	C2A-N3A	2.24	1.36	1.32
3	B	612	FAD	C2A-N3A	2.27	1.36	1.32
2	B	611	TDP	C2'-N1'	2.31	1.38	1.34
3	I	612	FAD	C2A-N3A	2.39	1.36	1.32
3	G	612	FAD	C2A-N3A	2.46	1.36	1.32
3	E	612	FAD	C4X-N5	2.47	1.37	1.33
3	I	612	FAD	C4X-N5	2.50	1.37	1.33
3	E	612	FAD	O4B-C1B	2.52	1.44	1.41
3	D	612	FAD	O4B-C1B	2.67	1.44	1.41
3	H	612	FAD	C4X-N5	2.74	1.37	1.33
3	H	612	FAD	O4B-C1B	2.80	1.44	1.41
3	F	612	FAD	C4X-N5	3.20	1.38	1.33
3	D	612	FAD	C4X-N5	3.29	1.38	1.33
3	I	612	FAD	O4B-C1B	3.33	1.45	1.41

All (260) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	612	FAD	N3A-C2A-N1A	-12.43	119.37	128.89
3	A	612	FAD	N3A-C2A-N1A	-11.88	119.80	128.89
3	E	612	FAD	N3A-C2A-N1A	-10.92	120.54	128.89
3	L	612	FAD	N3A-C2A-N1A	-10.77	120.65	128.89
3	H	612	FAD	N3A-C2A-N1A	-9.87	121.34	128.89
3	G	612	FAD	N3A-C2A-N1A	-9.68	121.48	128.89
3	I	612	FAD	N3A-C2A-N1A	-9.54	121.59	128.89
3	J	612	FAD	N3A-C2A-N1A	-9.50	121.62	128.89
3	F	612	FAD	N3A-C2A-N1A	-9.45	121.66	128.89
3	D	612	FAD	N3A-C2A-N1A	-9.42	121.69	128.89
3	K	612	FAD	N3A-C2A-N1A	-8.73	122.21	128.89
3	B	612	FAD	N3A-C2A-N1A	-8.40	122.46	128.89
2	A	611	TDP	C5A-C5-S1	-6.40	111.28	120.24
2	L	611	TDP	C4A-C4-C5	-5.44	116.68	128.90
3	H	612	FAD	C1B-N9A-C4A	-5.40	118.80	126.94
2	A	611	TDP	C4A-C4-C5	-5.32	116.94	128.90
2	E	611	TDP	C5'-C35-N3	-5.21	104.62	113.33
2	B	611	TDP	C5'-C35-N3	-5.19	104.65	113.33
3	F	612	FAD	C4-C4X-C10	-4.58	117.01	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	611	TDP	C5'-C35-N3	-4.58	105.67	113.33
2	C	611	TDP	C5'-C35-N3	-4.38	106.01	113.33
2	K	611	TDP	C5'-C35-N3	-4.28	106.17	113.33
3	B	612	FAD	O3P-P-O5'	-4.28	91.58	102.94
2	C	611	TDP	C4A-C4-C5	-4.25	119.35	128.90
2	G	611	TDP	C5A-C5-S1	-4.20	114.36	120.24
2	J	611	TDP	C4A-C4-C5	-4.17	119.53	128.90
3	C	612	FAD	O3P-P-O5'	-4.12	92.00	102.94
3	H	612	FAD	C4-C4X-C10	-4.12	117.31	119.94
2	F	611	TDP	C5'-C35-N3	-4.07	106.53	113.33
3	L	612	FAD	C4X-C4-N3	-4.05	118.05	123.59
2	K	611	TDP	C5A-C5-S1	-4.02	114.61	120.24
3	C	612	FAD	C4X-C4-N3	-4.01	118.11	123.59
2	F	611	TDP	C4A-C4-C5	-3.98	119.96	128.90
2	E	611	TDP	C4A-C4-C5	-3.97	119.99	128.90
3	I	612	FAD	C4X-C4-N3	-3.96	118.17	123.59
3	H	612	FAD	O3P-P-O5'	-3.90	92.60	102.94
2	J	611	TDP	C5A-C5-S1	-3.87	114.82	120.24
2	E	611	TDP	C5A-C5-S1	-3.84	114.87	120.24
3	A	612	FAD	O3P-P-O5'	-3.77	92.94	102.94
2	A	611	TDP	C5'-C35-N3	-3.75	107.05	113.33
3	I	612	FAD	O3P-P-O5'	-3.72	93.06	102.94
3	B	612	FAD	C4X-C4-N3	-3.70	118.53	123.59
3	D	612	FAD	C4X-C4-N3	-3.68	118.55	123.59
3	G	612	FAD	O4'-C4'-C5'	-3.67	102.20	110.19
2	L	611	TDP	C5'-C35-N3	-3.67	107.20	113.33
2	K	611	TDP	C4A-C4-C5	-3.65	120.70	128.90
2	G	611	TDP	C4A-C4-C5	-3.63	120.74	128.90
2	H	611	TDP	C4A-C4-C5	-3.61	120.78	128.90
3	G	612	FAD	O3P-P-O5'	-3.54	93.54	102.94
2	J	611	TDP	C5'-C6'-N1'	-3.54	117.72	123.86
2	B	611	TDP	N1'-C2'-N3'	-3.53	119.06	125.60
2	D	611	TDP	C5'-C35-N3	-3.53	107.42	113.33
2	G	611	TDP	C5'-C35-N3	-3.51	107.46	113.33
2	K	611	TDP	C5'-C6'-N1'	-3.48	117.82	123.86
3	I	612	FAD	C4A-C5A-N7A	-3.41	106.34	109.48
3	E	612	FAD	C4X-C4-N3	-3.38	118.97	123.59
2	B	611	TDP	C4A-C4-C5	-3.38	121.31	128.90
2	G	611	TDP	N1'-C2'-N3'	-3.36	119.38	125.60
2	H	611	TDP	N1'-C2'-N3'	-3.28	119.54	125.60
3	F	612	FAD	C1B-N9A-C4A	-3.27	122.01	126.94
2	J	611	TDP	C5'-C35-N3	-3.24	107.91	113.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	611	TDP	C5'-C6'-N1'	-3.20	118.31	123.86
2	F	611	TDP	C5A-C5-S1	-3.19	115.78	120.24
2	I	611	TDP	C4A-C4-C5	-3.18	121.74	128.90
3	H	612	FAD	C4X-C10-N10	-3.16	118.66	120.52
2	K	611	TDP	N1'-C2'-N3'	-3.10	119.87	125.60
2	L	611	TDP	N1'-C2'-N3'	-3.03	119.99	125.60
3	E	612	FAD	C1B-N9A-C4A	-3.03	122.38	126.94
2	D	611	TDP	C4A-C4-C5	-3.00	122.15	128.90
3	I	612	FAD	C1B-N9A-C4A	-2.98	122.45	126.94
2	H	611	TDP	C5A-C5-S1	-2.95	116.11	120.24
2	L	611	TDP	C5'-C6'-N1'	-2.89	118.84	123.86
2	I	611	TDP	C5A-C5-S1	-2.88	116.20	120.24
3	L	612	FAD	C1B-N9A-C4A	-2.88	122.60	126.94
2	I	611	TDP	C5'-C35-N3	-2.88	108.52	113.33
2	F	611	TDP	N1'-C2'-N3'	-2.85	120.33	125.60
3	L	612	FAD	C9A-C5X-N5	-2.84	118.16	122.36
3	K	612	FAD	C4A-C5A-N7A	-2.82	106.88	109.48
3	G	612	FAD	C1B-N9A-C4A	-2.80	122.72	126.94
3	H	612	FAD	C4A-C5A-N7A	-2.80	106.91	109.48
2	B	611	TDP	C5A-C5-S1	-2.75	116.39	120.24
2	D	611	TDP	N1'-C2'-N3'	-2.75	120.51	125.60
3	J	612	FAD	C4X-C4-N3	-2.74	119.84	123.59
3	J	612	FAD	P-O3P-PA	-2.73	125.06	132.73
2	I	611	TDP	C5'-C6'-N1'	-2.72	119.14	123.86
3	L	612	FAD	O4B-C1B-N9A	-2.67	102.50	108.10
2	E	611	TDP	C5'-C6'-N1'	-2.65	119.27	123.86
2	J	611	TDP	N1'-C2'-N3'	-2.64	120.71	125.60
3	B	612	FAD	O3P-PA-O5B	-2.63	95.96	102.94
3	L	612	FAD	O2'-C2'-C1'	-2.62	103.50	109.94
3	A	612	FAD	O3B-C3B-C4B	-2.62	103.19	111.05
2	H	611	TDP	C5'-C6'-N1'	-2.62	119.32	123.86
2	E	611	TDP	N1'-C2'-N3'	-2.58	120.82	125.60
2	G	611	TDP	O22-P2-O11	-2.58	95.49	106.09
3	A	612	FAD	O4B-C1B-N9A	-2.56	102.75	108.10
2	A	611	TDP	N1'-C2'-N3'	-2.49	121.00	125.60
3	L	612	FAD	O3P-P-O5'	-2.47	96.38	102.94
2	B	611	TDP	C5'-C6'-N1'	-2.47	119.58	123.86
3	C	612	FAD	O5B-C5B-C4B	-2.45	100.09	109.12
3	G	612	FAD	C4X-C10-N10	-2.45	119.08	120.52
3	D	612	FAD	C1B-N9A-C4A	-2.41	123.30	126.94
3	D	612	FAD	O3P-P-O5'	-2.40	96.56	102.94
3	E	612	FAD	C4-C4X-C10	-2.40	118.41	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	612	FAD	C9A-C5X-N5	-2.38	118.84	122.36
2	C	611	TDP	C35-C5'-C6'	-2.37	115.81	120.67
3	C	612	FAD	C4A-C5A-N7A	-2.37	107.30	109.48
3	G	612	FAD	C9A-C5X-N5	-2.36	118.86	122.36
3	E	612	FAD	O3P-P-O5'	-2.36	96.67	102.94
3	A	612	FAD	C4X-C4-N3	-2.36	120.36	123.59
3	H	612	FAD	C4X-C4-N3	-2.35	120.38	123.59
3	J	612	FAD	O3P-PA-O5B	-2.33	96.76	102.94
3	G	612	FAD	C4X-C4-N3	-2.31	120.43	123.59
3	L	612	FAD	C4A-C5A-N7A	-2.31	107.36	109.48
3	E	612	FAD	O3P-PA-O5B	-2.26	96.94	102.94
3	B	612	FAD	O3'-C3'-C2'	-2.26	103.07	108.75
3	D	612	FAD	O4B-C1B-N9A	-2.25	103.38	108.10
2	D	611	TDP	C35-C5'-C6'	-2.25	116.06	120.67
2	J	611	TDP	O22-P2-O11	-2.25	96.87	106.09
3	J	612	FAD	C9A-C5X-N5	-2.24	119.04	122.36
3	D	612	FAD	C9A-C5X-N5	-2.22	119.08	122.36
3	J	612	FAD	C4X-C10-N10	-2.20	119.22	120.52
3	A	612	FAD	C1B-N9A-C4A	-2.19	123.64	126.94
3	K	612	FAD	O3P-PA-O5B	-2.19	97.13	102.94
3	K	612	FAD	C4X-C4-N3	-2.17	120.62	123.59
3	C	612	FAD	C7-C6-C5X	-2.17	117.38	120.92
3	E	612	FAD	P-O3P-PA	-2.14	126.71	132.73
3	K	612	FAD	C1B-N9A-C4A	-2.13	123.73	126.94
2	L	611	TDP	C5A-C5-S1	-2.12	117.26	120.24
3	E	612	FAD	C4X-C10-N10	-2.12	119.27	120.52
3	D	612	FAD	C4-C4X-C10	-2.12	118.58	119.94
3	C	612	FAD	C8M-C8-C7	-2.10	116.11	120.73
2	C	611	TDP	C5'-C6'-N1'	-2.09	120.23	123.86
3	C	612	FAD	C9A-C5X-N5	-2.08	119.27	122.36
2	C	611	TDP	C5A-C5-S1	-2.08	117.33	120.24
3	K	612	FAD	O5B-C5B-C4B	-2.07	101.48	109.12
2	C	611	TDP	N1'-C2'-N3'	-2.07	121.78	125.60
3	F	612	FAD	C4X-C4-N3	-2.06	120.77	123.59
3	A	612	FAD	C4A-C5A-N7A	-2.06	107.59	109.48
3	L	612	FAD	P-O3P-PA	-2.04	127.00	132.73
3	E	612	FAD	C9A-C5X-N5	-2.03	119.35	122.36
2	H	611	TDP	C35-C5'-C6'	-2.01	116.56	120.67
3	B	612	FAD	O3B-C3B-C4B	-2.00	105.04	111.05
2	E	611	TDP	C5-C4-N3	2.00	112.10	107.69
2	B	611	TDP	C2A-C2'-N3'	2.02	120.63	117.20
2	D	611	TDP	N4'-C4'-N3'	2.03	119.89	116.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	612	FAD	C1'-N10-C9A	2.03	121.14	118.86
2	L	611	TDP	C6'-C5'-C4'	2.04	118.64	115.72
2	F	611	TDP	C5-C4-N3	2.08	112.27	107.69
3	K	612	FAD	C1'-C2'-C3'	2.13	115.90	109.82
2	G	611	TDP	C2A-C2'-N3'	2.13	120.83	117.20
3	A	612	FAD	C4B-O4B-C1B	2.15	112.09	109.72
3	J	612	FAD	C5X-C9A-N10	2.16	119.26	117.62
3	F	612	FAD	C4-C4X-N5	2.16	121.34	118.72
3	B	612	FAD	C5X-C9A-N10	2.16	119.26	117.62
2	A	611	TDP	C6'-C5'-C4'	2.20	118.87	115.72
3	K	612	FAD	C1'-N10-C9A	2.27	121.41	118.86
2	E	611	TDP	C2A-C2'-N1'	2.27	119.75	117.03
2	K	611	TDP	C2A-C2'-N3'	2.28	121.08	117.20
2	G	611	TDP	C2A-C2'-N1'	2.30	119.79	117.03
3	G	612	FAD	C1'-C2'-C3'	2.30	116.39	109.82
3	D	612	FAD	C1'-C2'-C3'	2.30	116.40	109.82
2	J	611	TDP	C6'-C5'-C4'	2.33	119.06	115.72
3	F	612	FAD	O2P-P-O1P	2.35	125.24	112.53
3	J	612	FAD	C1'-N10-C9A	2.36	121.51	118.86
3	B	612	FAD	C4X-N5-C5X	2.36	119.48	116.76
2	B	611	TDP	C6'-C5'-C4'	2.37	119.11	115.72
3	J	612	FAD	O2P-P-O1P	2.37	125.36	112.53
2	I	611	TDP	C6'-N1'-C2'	2.37	119.91	115.77
3	K	612	FAD	C5X-C9A-N10	2.39	119.44	117.62
3	J	612	FAD	C1'-C2'-C3'	2.41	116.71	109.82
2	A	611	TDP	O23-P2-O21	2.45	119.83	110.85
3	K	612	FAD	O2P-P-O1P	2.46	125.87	112.53
3	G	612	FAD	C4-C4X-N5	2.48	121.72	118.72
2	F	611	TDP	C2'-N3'-C4'	2.50	123.16	118.19
2	D	611	TDP	C6'-C5'-C4'	2.51	119.32	115.72
3	B	612	FAD	O2P-P-O1P	2.52	126.18	112.53
3	E	612	FAD	C1'-C2'-C3'	2.52	117.03	109.82
3	E	612	FAD	C4-C4X-N5	2.57	121.84	118.72
3	C	612	FAD	C6-C5X-C9A	2.63	122.44	118.98
3	L	612	FAD	C1'-C2'-C3'	2.68	117.49	109.82
3	F	612	FAD	C1'-C2'-C3'	2.70	117.55	109.82
2	B	611	TDP	C2A-C2'-N1'	2.72	120.29	117.03
3	F	612	FAD	C4B-O4B-C1B	2.73	112.72	109.72
3	G	612	FAD	C4B-O4B-C1B	2.73	112.72	109.72
3	A	612	FAD	C1'-N10-C9A	2.74	121.93	118.86
2	A	611	TDP	C6'-N1'-C2'	2.74	120.56	115.77
3	A	612	FAD	C4-C4X-N5	2.76	122.07	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	612	FAD	C4-C4X-N5	2.78	122.09	118.72
2	H	611	TDP	C2A-C2'-N3'	2.78	121.94	117.20
2	C	611	TDP	C6'-N1'-C2'	2.79	120.65	115.77
3	H	612	FAD	C1'-N10-C9A	2.81	122.02	118.86
2	I	611	TDP	C2A-C2'-N1'	2.86	120.47	117.03
3	G	612	FAD	O2P-P-O1P	2.87	128.10	112.53
2	K	611	TDP	C6'-C5'-C4'	2.90	119.88	115.72
2	L	611	TDP	C2A-C2'-N1'	2.91	120.53	117.03
3	A	612	FAD	C1'-C2'-C3'	2.92	118.17	109.82
3	B	612	FAD	C2B-C1B-N9A	2.94	118.78	114.29
2	H	611	TDP	O11-P1-O5G	2.96	110.80	102.94
3	I	612	FAD	C5X-C9A-N10	2.96	119.87	117.62
3	B	612	FAD	C4-C4X-N5	2.99	122.34	118.72
3	K	612	FAD	C4-N3-C2	3.06	117.89	115.25
3	J	612	FAD	C4-C4X-N5	3.07	122.45	118.72
2	C	611	TDP	C5A-C5-C4	3.10	130.34	127.56
3	K	612	FAD	C4-C4X-N5	3.10	122.48	118.72
3	C	612	FAD	C4X-N5-C5X	3.10	120.33	116.76
2	I	611	TDP	C4A-C4-N3	3.10	126.72	122.59
2	L	611	TDP	C5A-C5-C4	3.16	130.40	127.56
3	B	612	FAD	C4B-O4B-C1B	3.21	113.25	109.72
2	G	611	TDP	C6'-N1'-C2'	3.25	121.45	115.77
3	L	612	FAD	C1'-N10-C9A	3.29	122.55	118.86
2	I	611	TDP	C6'-C5'-C4'	3.43	120.65	115.72
2	J	611	TDP	C6'-N1'-C2'	3.47	121.83	115.77
2	F	611	TDP	C2A-C2'-N1'	3.50	121.23	117.03
2	E	611	TDP	C6'-N1'-C2'	3.55	121.98	115.77
3	D	612	FAD	C4-C4X-N5	3.61	123.10	118.72
3	D	612	FAD	C5X-C9A-N10	3.61	120.36	117.62
2	H	611	TDP	C5A-C5-C4	3.65	130.83	127.56
2	D	611	TDP	C2A-C2'-N3'	3.72	123.54	117.20
2	L	611	TDP	C6'-N1'-C2'	3.75	122.33	115.77
2	G	611	TDP	C4A-C4-N3	3.76	127.61	122.59
3	L	612	FAD	C4-C4X-N5	3.77	123.30	118.72
3	E	612	FAD	C5X-C9A-N10	3.84	120.54	117.62
2	F	611	TDP	C4A-C4-N3	3.88	127.77	122.59
2	I	611	TDP	C5A-C5-C4	3.91	131.06	127.56
2	H	611	TDP	C6'-N1'-C2'	3.91	122.60	115.77
2	E	611	TDP	C4A-C4-N3	3.99	127.91	122.59
2	B	611	TDP	C6'-N1'-C2'	4.03	122.81	115.77
2	D	611	TDP	C4A-C4-N3	4.05	127.98	122.59
2	B	611	TDP	C4A-C4-N3	4.05	127.99	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	611	TDP	C4A-C4-N3	4.05	127.99	122.59
3	H	612	FAD	C4-C4X-N5	4.08	123.68	118.72
3	C	612	FAD	C4B-O4B-C1B	4.10	114.22	109.72
2	D	611	TDP	C6'-N1'-C2'	4.15	123.03	115.77
3	A	612	FAD	C4-N3-C2	4.29	118.95	115.25
2	B	611	TDP	C5A-C5-C4	4.37	131.48	127.56
2	K	611	TDP	C6'-N1'-C2'	4.44	123.53	115.77
2	J	611	TDP	C4A-C4-N3	4.48	128.56	122.59
2	J	611	TDP	C2A-C2'-N1'	4.63	122.59	117.03
3	F	612	FAD	C5X-C9A-N10	4.73	121.21	117.62
3	D	612	FAD	C4B-O4B-C1B	4.74	114.92	109.72
2	K	611	TDP	C4A-C4-N3	5.43	129.82	122.59
2	K	611	TDP	C5A-C5-C4	5.45	132.44	127.56
3	J	612	FAD	C4-N3-C2	5.67	120.14	115.25
2	C	611	TDP	C4A-C4-N3	5.72	130.21	122.59
2	J	611	TDP	C5A-C5-C4	5.81	132.77	127.56
3	G	612	FAD	C4-N3-C2	5.91	120.36	115.25
2	E	611	TDP	C5A-C5-C4	6.03	132.97	127.56
3	I	612	FAD	C4-N3-C2	6.04	120.47	115.25
3	C	612	FAD	C4-N3-C2	6.41	120.79	115.25
2	A	611	TDP	C4A-C4-N3	6.61	131.41	122.59
3	B	612	FAD	C4-N3-C2	6.69	121.03	115.25
2	G	611	TDP	C5A-C5-C4	6.78	133.64	127.56
3	F	612	FAD	C4-N3-C2	6.82	121.14	115.25
2	L	611	TDP	C4A-C4-N3	6.83	131.69	122.59
3	H	612	FAD	C4-N3-C2	7.38	121.63	115.25
2	F	611	TDP	C5A-C5-C4	7.39	134.19	127.56
3	D	612	FAD	C4-N3-C2	7.67	121.88	115.25
3	E	612	FAD	C4-N3-C2	8.04	122.20	115.25
3	L	612	FAD	C4-N3-C2	8.61	122.69	115.25
2	A	611	TDP	C5A-C5-C4	11.81	138.15	127.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

39 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	611	TDP	4	0
3	A	612	FAD	1	0
5	A	616	PO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	617	PO4	1	0
5	A	618	PO4	2	0
5	A	619	PO4	3	0
2	B	611	TDP	2	0
3	B	612	FAD	3	0
5	B	614	PO4	1	0
2	C	611	TDP	3	0
3	C	612	FAD	1	0
2	D	611	TDP	2	0
3	D	612	FAD	3	0
5	D	614	PO4	1	0
5	D	615	PO4	1	0
5	D	618	PO4	1	0
2	E	611	TDP	3	0
3	E	612	FAD	5	0
5	E	614	PO4	1	0
2	F	611	TDP	3	0
3	F	612	FAD	4	0
5	F	614	PO4	1	0
2	G	611	TDP	3	0
3	G	612	FAD	4	0
2	H	611	TDP	3	0
3	H	612	FAD	2	0
5	H	615	PO4	1	0
2	I	611	TDP	3	0
3	I	612	FAD	6	0
5	I	614	PO4	1	0
2	J	611	TDP	3	0
3	J	612	FAD	4	0
2	K	611	TDP	6	0
3	K	612	FAD	2	0
5	K	614	PO4	1	0
2	L	611	TDP	5	0
3	L	612	FAD	2	0
5	L	616	PO4	1	0
5	L	617	PO4	1	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	527/549 (95%)	-0.07	23 (4%)	38	43	37, 50, 73, 115	10 (1%)
1	B	524/549 (95%)	0.01	25 (4%)	34	39	39, 60, 92, 128	11 (2%)
1	C	522/549 (95%)	-0.03	31 (5%)	26	29	39, 57, 84, 124	10 (1%)
1	D	520/549 (94%)	-0.03	21 (4%)	42	47	39, 54, 78, 94	10 (1%)
1	E	522/549 (95%)	0.13	31 (5%)	26	29	45, 70, 110, 169	8 (1%)
1	F	521/549 (94%)	0.06	30 (5%)	26	30	48, 71, 103, 143	9 (1%)
1	G	519/549 (94%)	0.15	40 (7%)	16	18	46, 71, 104, 137	8 (1%)
1	H	522/549 (95%)	-0.02	24 (4%)	36	41	45, 62, 96, 147	8 (1%)
1	I	523/549 (95%)	0.06	30 (5%)	27	31	44, 64, 98, 137	10 (1%)
1	J	522/549 (95%)	0.12	31 (5%)	26	29	42, 66, 98, 132	10 (1%)
1	K	523/549 (95%)	-0.01	25 (4%)	34	39	39, 55, 81, 118	10 (1%)
1	L	523/549 (95%)	-0.19	13 (2%)	61	65	38, 51, 75, 119	10 (1%)
All	All	6268/6588 (95%)	0.02	324 (5%)	31	35	37, 60, 96, 169	114 (1%)

All (324) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	534	ILE	7.1
1	J	465	PHE	7.0
1	J	466	VAL	6.9
1	F	1	MET	6.5
1	J	1	MET	6.5
1	K	535	PRO	6.4
1	H	535	PRO	6.4
1	K	463	LEU	6.2
1	D	466	VAL	6.0
1	F	463	LEU	6.0
1	E	536	PRO	6.0

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Mol	Chain	Res	Type	RSRZ
1	F	462	VAL	5.9
1	H	479	GLY	5.8
1	J	533	ALA	5.7
1	L	466	VAL	5.5
1	I	1	MET	5.5
1	E	479	GLY	5.5
1	I	535	PRO	5.4
1	D	465	PHE	5.3
1	A	1	MET	5.3
1	J	532	LEU	5.2
1	B	466	VAL	5.2
1	E	534	ILE	5.2
1	K	355	LYS	5.2
1	E	464	GLY	5.2
1	E	535	PRO	5.1
1	K	533	ALA	5.1
1	C	465	PHE	5.1
1	K	465	PHE	5.0
1	L	465	PHE	4.9
1	A	466	VAL	4.9
1	K	482	LEU	4.9
1	H	536	PRO	4.9
1	F	464	GLY	4.9
1	F	481	GLU	4.7
1	C	479	GLY	4.7
1	J	355	LYS	4.7
1	G	479	GLY	4.7
1	F	479	GLY	4.7
1	K	1	MET	4.6
1	L	200	TYR	4.6
1	I	534	ILE	4.5
1	I	465	PHE	4.5
1	E	1	MET	4.5
1	A	2	LYS	4.5
1	B	465	PHE	4.5
1	F	534	ILE	4.4
1	I	482	LEU	4.4
1	B	478	ASP	4.3
1	J	463	LEU	4.3
1	G	532	LEU	4.2
1	J	200	TYR	4.2
1	I	533	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	K	534	ILE	4.1
1	A	539	LYS	4.1
1	I	481	GLU	4.0
1	J	534	ILE	4.0
1	K	462	VAL	4.0
1	I	463	LEU	4.0
1	C	355	LYS	3.9
1	D	533	ALA	3.8
1	L	535	PRO	3.8
1	G	354	GLU	3.8
1	G	462	VAL	3.8
1	F	2	LYS	3.8
1	G	355	LYS	3.8
1	H	463	LEU	3.8
1	H	482	LEU	3.8
1	A	200	TYR	3.8
1	C	480	THR	3.8
1	G	533	ALA	3.7
1	H	533	ALA	3.7
1	K	2	LYS	3.7
1	H	481	GLU	3.7
1	G	341	ASP	3.7
1	C	533	ALA	3.7
1	C	285	ASP	3.7
1	C	38	ARG	3.7
1	A	462	VAL	3.7
1	G	531	GLU	3.7
1	D	38	ARG	3.6
1	G	464	GLY	3.6
1	E	533	ALA	3.6
1	B	27	ASP	3.6
1	J	349	LEU	3.6
1	B	535	PRO	3.5
1	B	481	GLU	3.5
1	F	27	ASP	3.5
1	F	355	LYS	3.5
1	F	533	ALA	3.5
1	G	200	TYR	3.5
1	L	464	GLY	3.5
1	E	2	LYS	3.5
1	F	535	PRO	3.4
1	K	484	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	354	GLU	3.4
1	G	38	ARG	3.4
1	G	27	ASP	3.3
1	L	463	LEU	3.3
1	E	38	ARG	3.3
1	F	484	ASP	3.3
1	C	200	TYR	3.3
1	A	285	ASP	3.3
1	C	27	ASP	3.2
1	L	534	ILE	3.2
1	I	355	LYS	3.2
1	D	206	LEU	3.2
1	F	354	GLU	3.2
1	J	348	ASP	3.2
1	D	463	LEU	3.2
1	C	284	THR	3.2
1	B	340	ARG	3.2
1	D	37	ASN	3.1
1	J	38[A]	ARG	3.1
1	K	270	VAL	3.1
1	G	484	ASP	3.1
1	G	463	LEU	3.1
1	J	482	LEU	3.1
1	E	463	LEU	3.1
1	B	37	ASN	3.1
1	I	285	ASP	3.1
1	I	2	LYS	3.0
1	B	482	LEU	3.0
1	G	280	ALA	3.0
1	G	40	GLY	3.0
1	I	464	GLY	3.0
1	J	464	GLY	3.0
1	H	531	GLU	3.0
1	H	532	LEU	3.0
1	E	450	LYS	3.0
1	C	354	GLU	3.0
1	F	480	THR	3.0
1	B	171	GLY	3.0
1	I	462	VAL	2.9
1	A	465	PHE	2.9
1	G	344	LYS	2.9
1	D	482	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	200	TYR	2.9
1	K	38	ARG	2.9
1	A	463	LEU	2.9
1	E	518	ASP	2.9
1	G	480	THR	2.9
1	J	462	VAL	2.9
1	G	2	LYS	2.9
1	H	354	GLU	2.9
1	L	533	ALA	2.9
1	B	330	LYS	2.9
1	J	354	GLU	2.9
1	I	260	PHE	2.9
1	C	462	VAL	2.8
1	E	356	ALA	2.8
1	H	355	LYS	2.8
1	A	284	THR	2.8
1	I	354	GLU	2.8
1	B	260	PHE	2.8
1	H	429	ALA	2.8
1	L	481	GLU	2.8
1	G	481	GLU	2.8
1	D	518	ASP	2.8
1	C	463	LEU	2.8
1	A	479	GLY	2.8
1	F	482	LEU	2.8
1	G	1	MET	2.8
1	C	466	VAL	2.8
1	C	455	ILE	2.7
1	E	337	GLU	2.7
1	F	352	PRO	2.7
1	E	429	ALA	2.7
1	L	479	GLY	2.7
1	H	1	MET	2.7
1	F	170	GLU	2.7
1	J	479	GLY	2.7
1	G	431	CYS	2.7
1	B	450	LYS	2.7
1	I	40	GLY	2.7
1	A	328	ASP	2.7
1	I	330	LYS	2.7
1	B	344	LYS	2.7
1	H	330	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	284	THR	2.7
1	D	205	ALA	2.7
1	B	355	LYS	2.7
1	K	464	GLY	2.6
1	E	484	ASP	2.6
1	J	518	ASP	2.6
1	I	284	THR	2.6
1	B	531	GLU	2.6
1	C	429	ALA	2.6
1	J	285	ASP	2.6
1	I	38	ARG	2.6
1	J	327	ALA	2.6
1	F	344	LYS	2.6
1	G	199	ARG	2.6
1	I	37	ASN	2.6
1	J	2	LYS	2.6
1	F	260	PHE	2.6
1	J	531	GLU	2.6
1	G	285	ASP	2.6
1	I	479	GLY	2.6
1	J	484	ASP	2.6
1	K	341	ASP	2.6
1	E	331	PHE	2.6
1	K	531	GLU	2.5
1	F	348	ASP	2.5
1	I	230	ILE	2.5
1	J	517	ILE	2.5
1	F	171	GLY	2.5
1	D	271	LEU	2.5
1	F	368	HIS	2.5
1	I	372	ASP	2.5
1	E	529	LYS	2.5
1	F	518	ASP	2.5
1	H	348	ASP	2.5
1	H	412	MET	2.5
1	J	344	LYS	2.4
1	D	270	VAL	2.4
1	H	484	ASP	2.4
1	K	265	ASN	2.4
1	K	479	GLY	2.4
1	L	39	MET	2.4
1	K	27	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	317	ARG	2.4
1	A	411	ALA	2.4
1	C	34	ASP	2.4
1	D	34	ASP	2.4
1	F	531	GLU	2.4
1	H	424	GLU	2.4
1	B	38	ARG	2.4
1	H	347	ASP	2.4
1	I	348	ASP	2.4
1	K	289	ILE	2.4
1	A	208	CYS	2.4
1	A	206	LEU	2.4
1	G	461	SER	2.4
1	E	171	GLY	2.3
1	H	455	ILE	2.3
1	K	411	ALA	2.3
1	C	324	GLU	2.3
1	D	355	LYS	2.3
1	G	482	LEU	2.3
1	D	532	LEU	2.3
1	G	377	THR	2.3
1	G	518	ASP	2.3
1	E	344	LYS	2.3
1	B	200	TYR	2.3
1	C	37	ASN	2.3
1	A	518	ASP	2.3
1	B	1	MET	2.3
1	G	265	ASN	2.3
1	K	518	ASP	2.3
1	G	430	MET	2.2
1	F	349	LEU	2.2
1	J	25	THR	2.2
1	E	340	ARG	2.2
1	C	534	ILE	2.2
1	E	516	SER	2.2
1	C	464	GLY	2.2
1	G	345	GLY	2.2
1	C	535	PRO	2.2
1	G	483	HIS	2.2
1	J	27	ASP	2.2
1	G	450	LYS	2.2
1	C	260	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	272	LEU	2.2
1	E	482	LEU	2.2
1	A	484	ASP	2.2
1	I	265	ASN	2.2
1	A	538	ILE	2.2
1	J	345	GLY	2.2
1	I	206	LEU	2.2
1	D	200	TYR	2.2
1	E	335	ALA	2.2
1	E	455	ILE	2.2
1	C	481	GLU	2.2
1	C	531	GLU	2.2
1	G	41	THR	2.2
1	B	285	ASP	2.2
1	L	462	VAL	2.1
1	E	355	LYS	2.1
1	E	330	LYS	2.1
1	D	484	ASP	2.1
1	J	34	ASP	2.1
1	C	482	LEU	2.1
1	G	37	ASN	2.1
1	E	34	ASP	2.1
1	K	532	LEU	2.1
1	C	178	HIS	2.1
1	G	423	PRO	2.1
1	B	337	GLU	2.1
1	D	372	ASP	2.1
1	H	285[A]	ASP	2.1
1	I	27	ASP	2.1
1	E	260	PHE	2.1
1	B	464	GLY	2.1
1	C	170	GLU	2.1
1	A	372[A]	ASP	2.1
1	L	355	LYS	2.1
1	H	27	ASP	2.1
1	A	356	ALA	2.1
1	G	356	ALA	2.1
1	C	456	VAL	2.1
1	A	378	CYS	2.1
1	F	259	GLY	2.1
1	F	324	GLU	2.1
1	G	284	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	343[A]	ARG	2.0
1	I	466	VAL	2.0
1	E	519	GLY	2.0
1	F	345	GLY	2.0
1	G	529	LYS	2.0
1	I	461	SER	2.0
1	A	537	GLN	2.0
1	A	170	GLU	2.0
1	B	479	GLY	2.0
1	F	261	HIS	2.0
1	B	328	ASP	2.0
1	D	208	CYS	2.0
1	E	424	GLU	2.0
1	C	2	LYS	2.0
1	D	462	VAL	2.0
1	G	178	HIS	2.0
1	H	349	LEU	2.0
1	K	284	THR	2.0
1	J	37[A]	ASN	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
5	PO4	B	616	5/5	0.82	0.41	15.33	71,71,72,73	5
5	PO4	C	615	5/5	0.69	0.33	11.57	72,73,73,74	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	PO4	A	615	5/5	0.77	0.30	11.57	62,62,64,66	5
5	PO4	D	620	5/5	0.86	0.27	7.21	51,53,54,55	5
5	PO4	D	616	5/5	0.62	0.45	6.62	67,67,69,69	5
5	PO4	A	616	5/5	0.86	0.31	4.56	56,57,58,58	5
5	PO4	H	614	5/5	0.79	0.27	4.19	98,99,99,100	0
5	PO4	L	615	5/5	0.88	0.32	3.71	91,92,93,93	0
5	PO4	F	615	5/5	0.91	0.21	2.93	61,61,62,64	5
5	PO4	B	615	5/5	0.84	0.22	2.33	71,71,72,72	5
5	PO4	L	614	5/5	0.89	0.21	1.93	97,97,98,98	0
5	PO4	L	618	5/5	0.91	0.20	0.66	63,63,64,65	5
5	PO4	D	619	5/5	0.89	0.19	0.60	68,69,69,70	5
5	PO4	K	614	5/5	0.95	0.20	0.58	69,72,72,73	0
5	PO4	L	617	5/5	0.85	0.24	0.43	58,58,60,61	5
5	PO4	D	618	5/5	0.89	0.21	0.36	67,68,69,69	5
5	PO4	G	616	5/5	0.89	0.20	0.15	71,71,71,72	5
5	PO4	G	615	5/5	0.94	0.16	0.06	84,85,86,86	0
5	PO4	D	615	5/5	0.96	0.15	-0.03	73,73,74,75	0
5	PO4	A	614	5/5	0.97	0.11	-0.13	70,70,72,73	0
5	PO4	B	614	5/5	0.96	0.16	-0.13	69,70,72,73	0
5	PO4	I	615	5/5	0.94	0.15	-0.18	91,91,92,93	0
5	PO4	J	614	5/5	0.94	0.16	-0.19	89,89,90,91	0
2	TDP	G	611	26/26	0.95	0.14	-0.26	56,59,62,63	0
5	PO4	E	614	5/5	0.95	0.13	-0.26	96,96,97,98	0
5	PO4	F	614	5/5	0.95	0.14	-0.38	91,91,92,93	0
2	TDP	E	611	26/26	0.95	0.13	-0.42	59,65,67,69	0
4	MG	K	613	1/1	0.76	0.19	-0.48	50,50,50,50	0
5	PO4	C	614	5/5	0.94	0.13	-0.50	73,74,75,77	0
3	FAD	G	612	53/53	0.96	0.11	-0.52	52,57,64,64	0
4	MG	D	613	1/1	0.82	0.16	-0.52	57,57,57,57	0
5	PO4	H	615	5/5	0.97	0.12	-0.54	82,83,84,85	0
2	TDP	F	611	26/26	0.97	0.11	-0.55	50,61,63,65	0
2	TDP	C	611	26/26	0.97	0.11	-0.60	43,49,53,54	0
3	FAD	L	612	53/53	0.98	0.10	-0.61	40,45,47,50	0
3	FAD	D	612	53/53	0.97	0.11	-0.62	39,43,48,49	0
3	FAD	C	612	53/53	0.97	0.10	-0.62	38,46,50,53	0
2	TDP	D	611	26/26	0.98	0.11	-0.69	42,48,51,51	0
3	FAD	J	612	53/53	0.97	0.10	-0.69	47,52,57,60	0
2	TDP	L	611	26/26	0.97	0.10	-0.69	43,46,49,50	0
2	TDP	B	611	26/26	0.97	0.10	-0.72	42,50,54,58	0
3	FAD	K	612	53/53	0.97	0.10	-0.73	40,45,52,55	0
2	TDP	H	611	26/26	0.98	0.09	-0.75	55,58,60,63	0
2	TDP	J	611	26/26	0.96	0.11	-0.75	48,61,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	TDP	K	611	26/26	0.98	0.10	-0.77	39,45,48,50	0
2	TDP	I	611	26/26	0.97	0.11	-0.79	44,56,58,60	0
4	MG	L	613	1/1	0.76	0.12	-0.81	47,47,47,47	0
2	TDP	A	611	26/26	0.98	0.10	-0.85	39,46,49,50	0
3	FAD	A	612	53/53	0.98	0.10	-0.87	36,41,44,45	0
3	FAD	B	612	53/53	0.98	0.09	-0.89	43,47,52,52	0
3	FAD	I	612	53/53	0.97	0.10	-0.90	45,49,53,57	0
3	FAD	E	612	53/53	0.97	0.10	-0.97	53,57,63,65	0
3	FAD	F	612	53/53	0.97	0.09	-0.97	50,55,59,63	0
4	MG	C	613	1/1	0.81	0.12	-0.99	63,63,63,63	0
4	MG	J	613	1/1	0.80	0.13	-1.04	72,72,72,72	0
3	FAD	H	612	53/53	0.97	0.09	-1.06	45,49,53,54	0
4	MG	F	613	1/1	0.70	0.08	-1.12	76,76,76,76	0
4	MG	B	613	1/1	0.79	0.12	-1.20	55,55,55,55	0
4	MG	E	613	1/1	0.72	0.07	-1.27	70,70,70,70	0
4	MG	A	613	1/1	0.86	0.11	-1.35	52,52,52,52	0
4	MG	H	613	1/1	0.93	0.07	-1.38	59,59,59,59	0
4	MG	G	613	1/1	0.70	0.10	-1.44	67,67,67,67	0
5	PO4	L	616	5/5	0.99	0.10	-1.44	67,67,68,69	0
4	MG	I	613	1/1	0.92	0.08	-1.52	62,62,62,62	0
5	PO4	G	614	5/5	0.94	0.20	-	65,65,66,66	5
5	PO4	A	619	5/5	0.81	0.32	-	72,73,74,74	5
5	PO4	D	617	5/5	0.91	0.25	-	61,61,62,62	5
5	PO4	A	618	5/5	0.93	0.13	-	56,56,57,57	5
5	PO4	D	614	5/5	0.90	0.20	-	68,68,69,69	5
5	PO4	A	617	5/5	0.84	0.21	-	66,67,68,68	5
5	PO4	E	615	5/5	0.81	0.25	-	73,73,74,74	5
5	PO4	I	614	5/5	0.87	0.15	-	68,68,68,69	5

6.5 Other polymers (i)

There are no such residues in this entry.