Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2025 – 12:38 PM EDT

PDB ID	:	3EXF / pdb_00003exf
Title	:	Crystal structure of the pyruvate dehydrogenase (E1p) component of human pyruvate dehydrogenase complex
Authors	:	Kato, M.; Wynn, R.M.; Chuang, J.L.; Tso, S.-C.; Machius, M.; Li, J.; Chuang, D.T.
Deposited on	:	2008-10-16
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

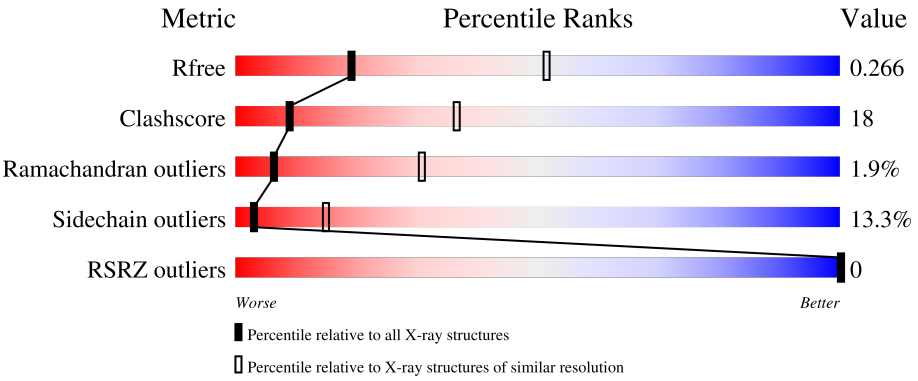
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	382	49% 40% 6% 5%
1	C	382	53% 31% 9% • 5%
1	E	382	57% 31% 8% 5%
1	G	382	61% 27% 6% • 5%

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Mol	Chain	Length	Quality of chain
2	B	329	57% 35% 9%
2	D	329	57% 35% 7%
2	F	329	60% 33% 7%
2	H	329	60% 33% 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 21507 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 E1 component subunit alpha, somatic form, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2821	1772	496	529	24			
1	C	363	Total	C	N	O	S	0	0	0
			2834	1780	499	530	25			
1	E	363	Total	C	N	O	S	0	0	0
			2834	1780	499	530	25			
1	G	362	Total	C	N	O	S	0	0	0
			2821	1772	496	529	24			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P08559
A	-19	GLY	-	expression tag	UNP P08559
A	-18	SER	-	expression tag	UNP P08559
A	-17	SER	-	expression tag	UNP P08559
A	-16	HIS	-	expression tag	UNP P08559
A	-15	HIS	-	expression tag	UNP P08559
A	-14	HIS	-	expression tag	UNP P08559
A	-13	HIS	-	expression tag	UNP P08559
A	-12	HIS	-	expression tag	UNP P08559
A	-11	HIS	-	expression tag	UNP P08559
A	-10	SER	-	expression tag	UNP P08559
A	-9	SER	-	expression tag	UNP P08559
A	-8	GLY	-	expression tag	UNP P08559
A	-7	LEU	-	expression tag	UNP P08559
A	-6	VAL	-	expression tag	UNP P08559
A	-5	PRO	-	expression tag	UNP P08559
A	-4	ARG	-	expression tag	UNP P08559
A	-3	GLY	-	expression tag	UNP P08559
A	-2	SER	-	expression tag	UNP P08559
A	-1	HIS	-	expression tag	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP P08559
A	203	ALA	SER	engineered mutation	UNP P08559
A	271	ALA	SER	engineered mutation	UNP P08559
C	-20	MET	-	expression tag	UNP P08559
C	-19	GLY	-	expression tag	UNP P08559
C	-18	SER	-	expression tag	UNP P08559
C	-17	SER	-	expression tag	UNP P08559
C	-16	HIS	-	expression tag	UNP P08559
C	-15	HIS	-	expression tag	UNP P08559
C	-14	HIS	-	expression tag	UNP P08559
C	-13	HIS	-	expression tag	UNP P08559
C	-12	HIS	-	expression tag	UNP P08559
C	-11	HIS	-	expression tag	UNP P08559
C	-10	SER	-	expression tag	UNP P08559
C	-9	SER	-	expression tag	UNP P08559
C	-8	GLY	-	expression tag	UNP P08559
C	-7	LEU	-	expression tag	UNP P08559
C	-6	VAL	-	expression tag	UNP P08559
C	-5	PRO	-	expression tag	UNP P08559
C	-4	ARG	-	expression tag	UNP P08559
C	-3	GLY	-	expression tag	UNP P08559
C	-2	SER	-	expression tag	UNP P08559
C	-1	HIS	-	expression tag	UNP P08559
C	0	MET	-	expression tag	UNP P08559
C	203	ALA	SER	engineered mutation	UNP P08559
C	271	ALA	SER	engineered mutation	UNP P08559
E	-20	MET	-	expression tag	UNP P08559
E	-19	GLY	-	expression tag	UNP P08559
E	-18	SER	-	expression tag	UNP P08559
E	-17	SER	-	expression tag	UNP P08559
E	-16	HIS	-	expression tag	UNP P08559
E	-15	HIS	-	expression tag	UNP P08559
E	-14	HIS	-	expression tag	UNP P08559
E	-13	HIS	-	expression tag	UNP P08559
E	-12	HIS	-	expression tag	UNP P08559
E	-11	HIS	-	expression tag	UNP P08559
E	-10	SER	-	expression tag	UNP P08559
E	-9	SER	-	expression tag	UNP P08559
E	-8	GLY	-	expression tag	UNP P08559
E	-7	LEU	-	expression tag	UNP P08559
E	-6	VAL	-	expression tag	UNP P08559
E	-5	PRO	-	expression tag	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	ARG	-	expression tag	UNP P08559
E	-3	GLY	-	expression tag	UNP P08559
E	-2	SER	-	expression tag	UNP P08559
E	-1	HIS	-	expression tag	UNP P08559
E	0	MET	-	expression tag	UNP P08559
E	203	ALA	SER	engineered mutation	UNP P08559
E	271	ALA	SER	engineered mutation	UNP P08559
G	-20	MET	-	expression tag	UNP P08559
G	-19	GLY	-	expression tag	UNP P08559
G	-18	SER	-	expression tag	UNP P08559
G	-17	SER	-	expression tag	UNP P08559
G	-16	HIS	-	expression tag	UNP P08559
G	-15	HIS	-	expression tag	UNP P08559
G	-14	HIS	-	expression tag	UNP P08559
G	-13	HIS	-	expression tag	UNP P08559
G	-12	HIS	-	expression tag	UNP P08559
G	-11	HIS	-	expression tag	UNP P08559
G	-10	SER	-	expression tag	UNP P08559
G	-9	SER	-	expression tag	UNP P08559
G	-8	GLY	-	expression tag	UNP P08559
G	-7	LEU	-	expression tag	UNP P08559
G	-6	VAL	-	expression tag	UNP P08559
G	-5	PRO	-	expression tag	UNP P08559
G	-4	ARG	-	expression tag	UNP P08559
G	-3	GLY	-	expression tag	UNP P08559
G	-2	SER	-	expression tag	UNP P08559
G	-1	HIS	-	expression tag	UNP P08559
G	0	MET	-	expression tag	UNP P08559
G	203	ALA	SER	engineered mutation	UNP P08559
G	271	ALA	SER	engineered mutation	UNP P08559

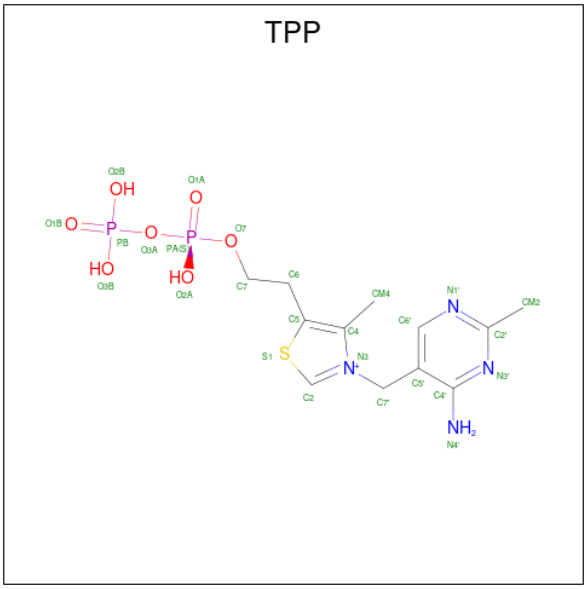
- Molecule 2 is a protein called Pyruvate dehydrogenase E1 component subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	D	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	F	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	H	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0

- Molecule 4 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 26 12 4 7 2 1	0	0
4	C	1	Total C N O P S 26 12 4 7 2 1	0	0
4	E	1	Total C N O P S 26 12 4 7 2 1	0	0
4	G	1	Total C N O P S 26 12 4 7 2 1	0	0

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total K 1 1	0	0
5	F	1	Total K 1 1	0	0
5	H	1	Total K 1 1	0	0

- Molecule 6 is water.

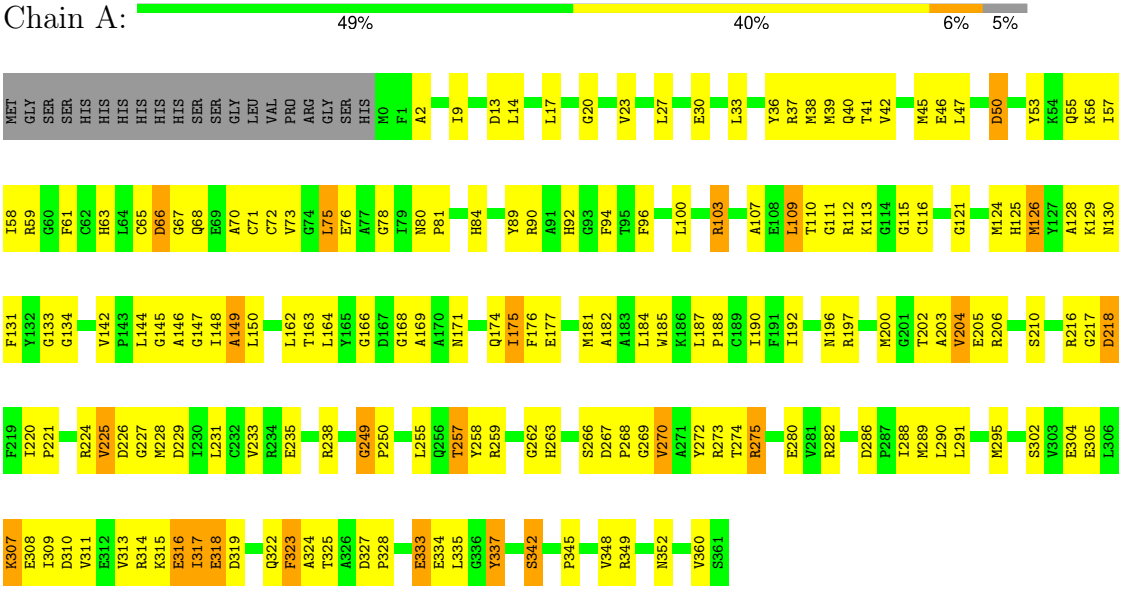
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O 1 1	0	0
6	C	3	Total O 3 3	0	0
6	D	1	Total O 1 1	0	0
6	E	1	Total O 1 1	0	0
6	F	2	Total O 2 2	0	0
6	H	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

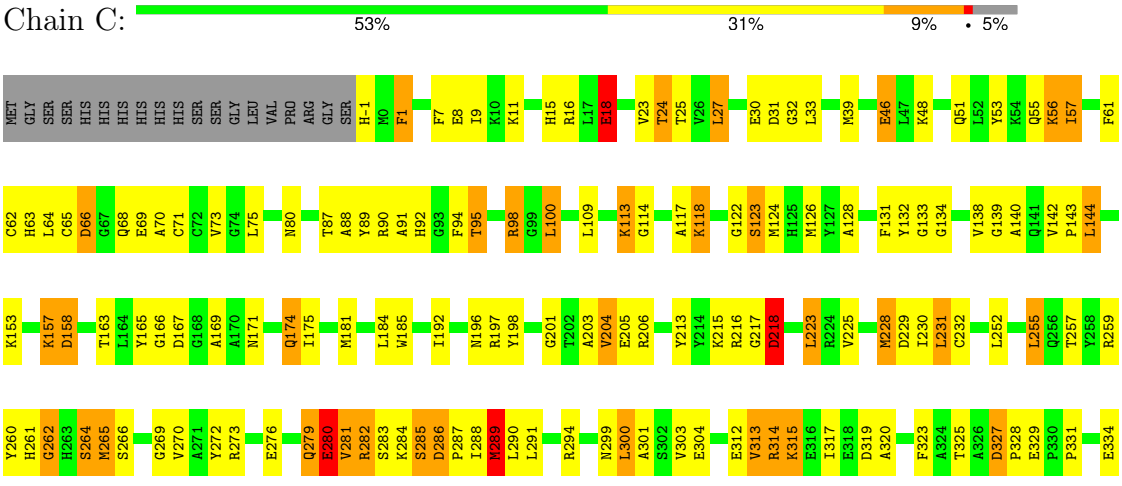
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

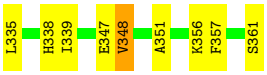
Chain A:



• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

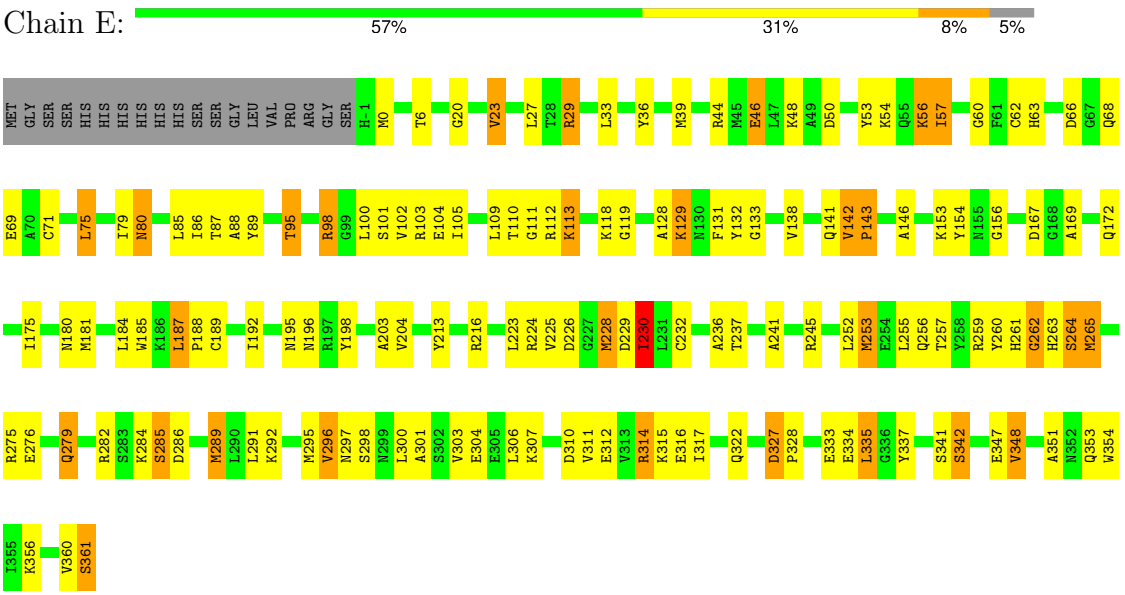
Chain C:





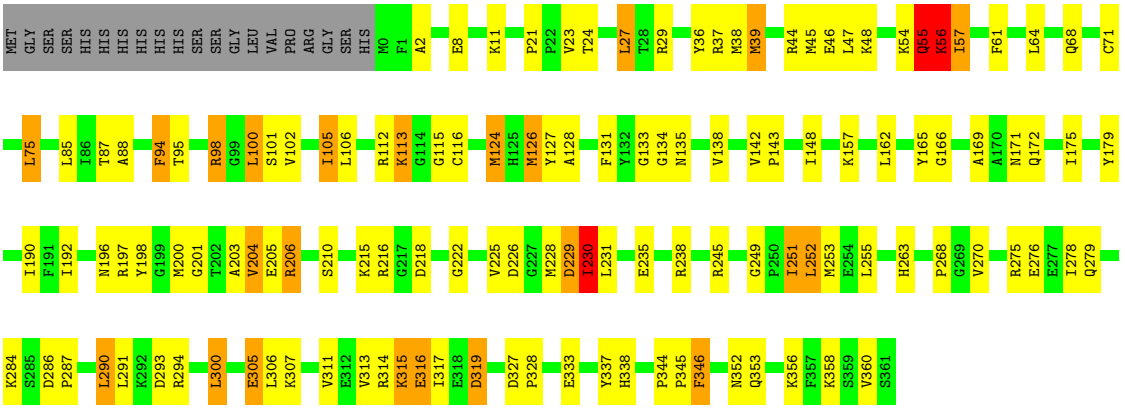
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain E:



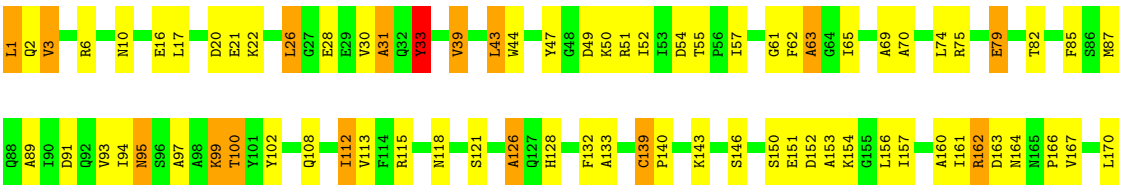
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

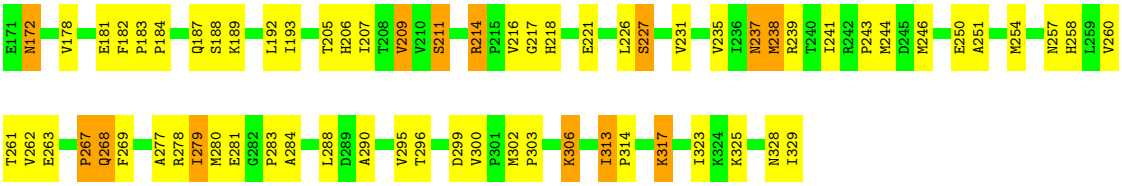
Chain G:



• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

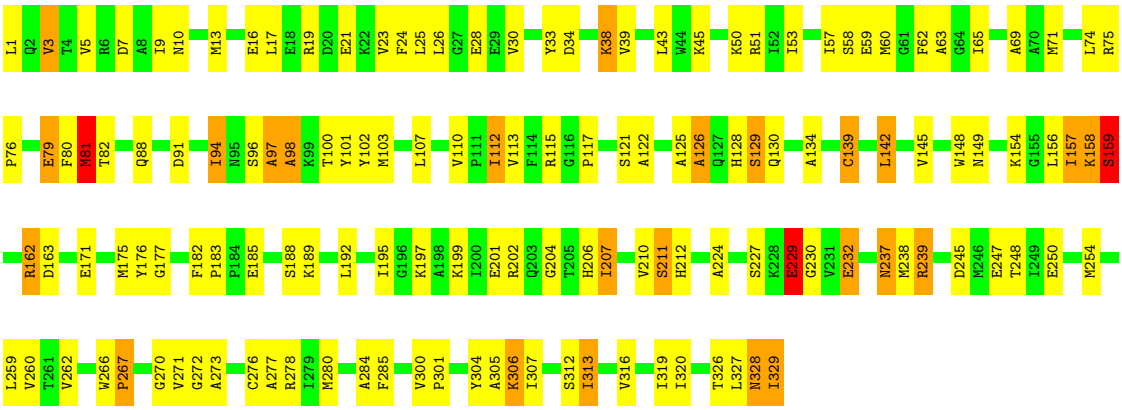
Chain B:





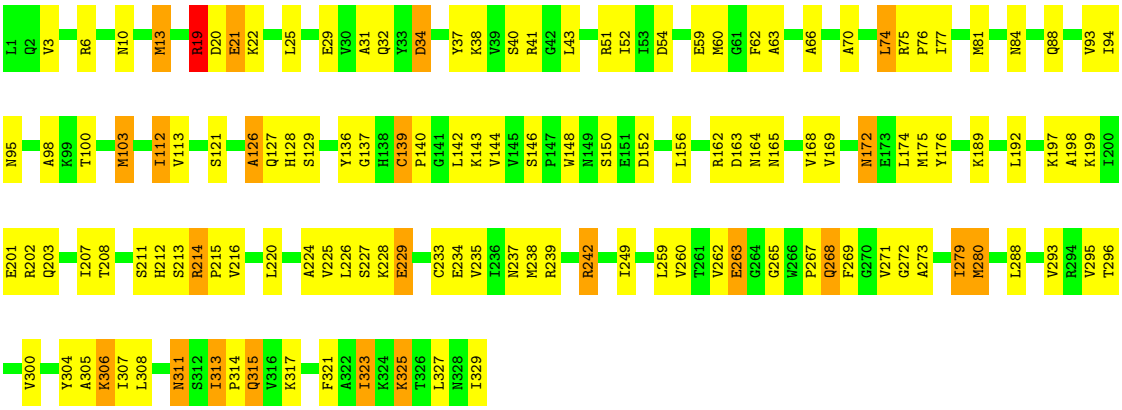
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain D:



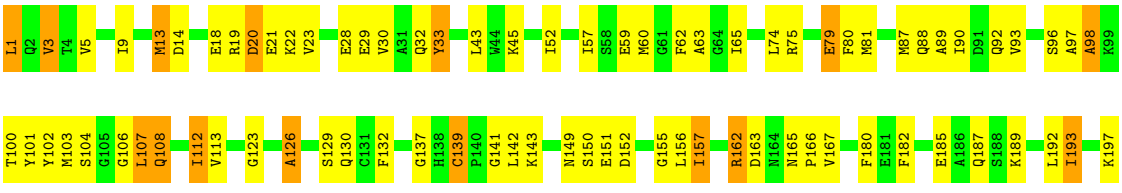
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

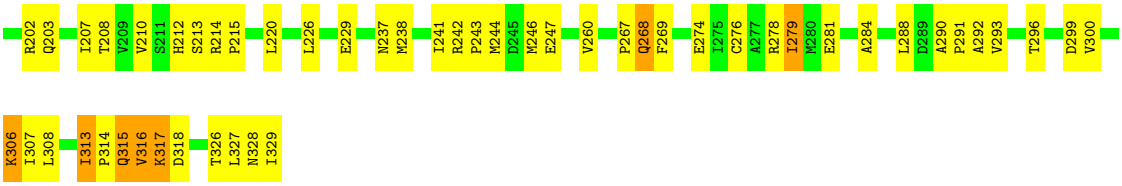
Chain F:



• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain H:




R202
Q203
I207
T208
V209
V210
S211
H212
S213
R214
P215
L220
L226
E229
N237
M238
I241
R242
P243
M244
D245
M246
E247
V260
P267
Q268
F269
E274
I275
C276
A277
R278
I279
M280
E281
A284
L288
D289
A290
P291
A292
V293
T296
D299
V300
K306
I307
L308
I313
P314
Q315
V316
K317
D318
T326
L327
N328
I329

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.39Å 129.67Å 144.95Å 90.00° 109.15° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-3.00) 99.4 (50.00-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.58 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.185 , 0.263 0.190 , 0.266	Depositor DCC
R_{free} test set	3624 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 5.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.117 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21507	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TPP, K, MG

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	1.14	4/2877 (0.1%)	1.30	15/3875 (0.4%)
1	C	1.17	3/2891 (0.1%)	1.34	20/3893 (0.5%)
1	E	1.13	2/2891 (0.1%)	1.29	19/3893 (0.5%)
1	G	1.15	1/2877 (0.0%)	1.29	16/3875 (0.4%)
2	B	1.20	3/2574 (0.1%)	1.37	23/3488 (0.7%)
2	D	1.17	3/2574 (0.1%)	1.33	19/3488 (0.5%)
2	F	1.21	6/2574 (0.2%)	1.32	15/3488 (0.4%)
2	H	1.19	1/2574 (0.0%)	1.37	15/3488 (0.4%)
All	All	1.17	23/21832 (0.1%)	1.32	142/29488 (0.5%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	313	ILE	CA-CB	-8.12	1.46	1.55
2	F	77	ILE	CA-CB	-6.55	1.46	1.54
1	A	149	ALA	CA-CB	-5.64	1.44	1.53
2	B	153	ALA	CA-CB	-5.60	1.44	1.53
2	F	6	ARG	CA-C	5.58	1.60	1.52
2	F	242	ARG	C-O	-5.53	1.20	1.25
2	F	70	ALA	CA-CB	-5.44	1.44	1.53
2	B	166	PRO	CA-C	-5.41	1.47	1.52
1	C	192	ILE	CA-CB	-5.34	1.48	1.54
2	F	249	ILE	CA-CB	-5.32	1.48	1.54
1	E	296	VAL	CA-C	5.28	1.59	1.52
1	C	281	VAL	CA-CB	-5.26	1.47	1.54
2	B	33	TYR	CA-C	5.24	1.60	1.52
2	D	129	SER	N-CA	-5.22	1.40	1.46
2	F	203	GLN	CA-C	-5.18	1.46	1.52
1	E	314	ARG	CA-C	5.17	1.59	1.52
1	G	204	VAL	CA-CB	5.17	1.61	1.54
1	A	175	ILE	CA-C	5.17	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	139	CYS	N-CA	5.15	1.53	1.46
1	C	257	THR	CA-CB	5.15	1.61	1.54
2	H	18	GLU	C-O	-5.13	1.18	1.24
1	A	257	THR	CA-CB	5.03	1.61	1.53
1	A	78	GLY	C-O	-5.01	1.20	1.24

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	249	GLY	CA-C-N	10.65	130.57	120.03
1	A	249	GLY	C-N-CA	10.65	130.57	120.03
1	A	67	GLY	N-CA-C	-9.04	103.90	113.58
1	G	344	PRO	CA-C-N	-8.61	111.02	120.14
1	G	344	PRO	C-N-CA	-8.61	111.02	120.14
2	F	139	CYS	N-CA-C	8.33	125.01	109.10
2	H	20	ASP	N-CA-C	7.84	120.25	107.32
2	D	300	VAL	CA-C-N	-7.80	112.30	120.03
2	D	300	VAL	C-N-CA	-7.80	112.30	120.03
1	E	347	GLU	N-CA-C	7.71	122.03	109.85
2	D	224	ALA	N-CA-C	-7.66	102.87	111.14
2	H	139	CYS	N-CA-C	7.64	119.28	109.72
2	H	23	VAL	CB-CA-C	-7.64	101.08	111.63
2	H	281	GLU	N-CA-C	-7.52	104.08	113.18
2	D	126	ALA	N-CA-C	7.32	119.05	111.14
2	D	204	GLY	N-CA-C	-7.15	102.45	110.96
1	A	2	ALA	N-CA-C	-6.97	101.14	110.55
1	C	280	GLU	N-CA-C	6.90	118.80	111.28
1	C	339	ILE	N-CA-C	-6.85	104.51	110.74
2	H	79	GLU	N-CA-C	6.79	120.00	107.99
2	D	139	CYS	CB-CA-C	-6.75	101.08	110.13
2	D	81	MET	N-CA-C	-6.75	103.93	111.28
1	E	142	VAL	CA-C-N	-6.73	111.65	119.32
1	E	142	VAL	C-N-CA	-6.73	111.65	119.32
2	B	126	ALA	N-CA-C	6.69	118.22	111.07
2	F	139	CYS	CB-CA-C	-6.67	102.77	110.17
2	D	98	ALA	N-CA-C	6.65	119.08	111.11
1	E	298	SER	N-CA-C	-6.64	105.15	112.72
2	H	32	GLN	N-CA-C	6.59	118.47	111.28
2	H	126	ALA	N-CA-C	6.51	118.04	111.07
1	E	297	ASN	N-CA-C	6.44	119.29	111.82
2	D	53	ILE	N-CA-C	6.32	116.97	107.75
1	A	168	GLY	N-CA-C	-6.24	107.14	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	231	LEU	N-CA-C	6.24	118.16	111.36
1	C	228	MET	N-CA-C	-6.23	105.46	114.12
1	E	20	GLY	CA-C-N	6.20	126.77	120.38
1	E	20	GLY	C-N-CA	6.20	126.77	120.38
2	D	139	CYS	N-CA-C	6.17	120.46	108.85
1	C	171	ASN	N-CA-C	6.11	119.77	112.93
2	H	316	VAL	CB-CA-C	-6.07	104.11	111.88
2	F	300	VAL	CA-C-N	-5.98	113.62	119.78
2	F	300	VAL	C-N-CA	-5.98	113.62	119.78
1	C	73	VAL	N-CA-C	-5.90	105.32	111.58
1	C	114	GLY	N-CA-C	5.88	121.28	114.16
2	B	6	ARG	N-CA-C	-5.88	104.95	111.36
2	F	34	ASP	N-CA-C	5.86	119.64	111.90
1	G	313	VAL	CB-CA-C	-5.84	104.49	111.97
1	E	119	GLY	N-CA-C	-5.84	107.04	115.27
1	G	124	MET	N-CA-C	5.83	119.65	112.54
1	C	281	VAL	CB-CA-C	-5.82	102.84	112.26
2	B	238	MET	N-CA-C	5.80	117.60	111.28
2	B	133	ALA	CA-C-N	5.79	128.36	120.54
2	B	133	ALA	C-N-CA	5.79	128.36	120.54
2	B	94	ILE	N-CA-C	5.79	115.97	110.42
1	G	225	VAL	N-CA-C	5.78	117.07	108.46
1	G	293	ASP	CB-CA-C	-5.76	102.02	110.95
2	B	300	VAL	CA-C-N	-5.76	113.85	119.90
2	B	300	VAL	C-N-CA	-5.76	113.85	119.90
2	F	189	LYS	N-CA-C	-5.76	106.23	113.20
1	E	154	TYR	CA-CB-CG	5.76	124.26	113.90
2	B	193	ILE	CA-C-N	-5.73	113.33	119.98
2	B	193	ILE	C-N-CA	-5.73	113.33	119.98
2	B	178	VAL	CA-C-N	5.72	126.99	119.84
2	B	178	VAL	C-N-CA	5.72	126.99	119.84
2	H	33	TYR	N-CA-C	-5.70	106.19	113.02
1	E	29	ARG	N-CA-C	-5.61	105.06	111.07
2	F	197	LYS	N-CA-C	5.60	117.82	108.02
2	B	100	THR	N-CA-C	5.59	117.82	111.11
1	E	310	ASP	N-CA-C	5.59	118.09	111.33
2	F	93	VAL	CB-CA-C	-5.59	104.60	112.14
2	H	98	ALA	N-CA-C	5.58	119.95	113.20
2	D	88	GLN	N-CA-C	-5.57	105.98	112.89
2	D	232	GLU	N-CA-C	5.57	117.38	108.41
1	E	187	LEU	CA-C-N	5.57	126.80	119.84
1	E	187	LEU	C-N-CA	5.57	126.80	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	316	GLU	N-CA-CB	5.55	118.39	110.06
1	G	204	VAL	N-CA-C	5.55	120.88	109.34
2	H	193	ILE	N-CA-C	-5.54	101.02	107.61
1	C	117	ALA	N-CA-C	-5.54	106.31	112.57
2	D	229	GLU	N-CA-CB	5.54	118.51	110.65
2	B	262	VAL	N-CA-C	5.54	115.86	108.11
2	F	224	ALA	N-CA-C	-5.50	105.18	111.07
2	D	69	ALA	N-CA-C	-5.50	105.18	111.07
1	G	21	PRO	CA-C-N	5.49	125.50	119.90
1	G	21	PRO	C-N-CA	5.49	125.50	119.90
2	F	19	ARG	N-CA-C	5.46	118.00	111.71
2	B	235	VAL	CB-CA-C	-5.45	104.70	111.08
1	A	175	ILE	N-CA-C	5.44	115.65	110.42
1	A	225	VAL	N-CA-C	5.44	117.47	108.99
2	B	108	GLN	CA-C-N	-5.43	115.15	120.52
2	B	108	GLN	C-N-CA	-5.43	115.15	120.52
2	B	26	LEU	N-CA-C	5.42	117.50	108.99
1	C	286	ASP	N-CA-C	5.41	116.23	109.57
1	G	39	MET	N-CA-C	-5.41	104.79	111.33
1	G	2	ALA	N-CA-C	-5.41	103.25	110.55
2	B	95	ASN	N-CA-C	5.40	117.99	111.40
1	G	38	MET	N-CA-C	5.40	116.85	110.97
1	C	1	PHE	N-CA-C	-5.38	102.08	110.42
2	B	217	GLY	N-CA-C	-5.38	105.79	113.86
1	C	122	GLY	N-CA-C	-5.36	104.37	112.84
1	C	327	ASP	N-CA-C	5.36	116.16	109.57
1	A	228	MET	N-CA-C	-5.35	107.12	113.97
1	C	312	GLU	N-CA-C	5.35	117.11	111.28
1	G	249	GLY	CA-C-N	5.33	125.79	120.14
1	G	249	GLY	C-N-CA	5.33	125.79	120.14
2	F	77	ILE	CB-CA-C	-5.33	103.18	110.96
1	C	289	MET	N-CA-C	-5.31	105.57	111.36
1	C	232	CYS	CB-CA-C	-5.31	99.86	110.42
1	E	342	SER	N-CA-C	5.30	119.70	113.23
2	D	17	LEU	N-CA-C	-5.25	105.46	111.07
1	C	282	ARG	N-CA-C	-5.25	106.83	113.18
1	A	205	GLU	N-CA-C	5.23	119.28	113.01
1	E	23	VAL	CB-CA-C	-5.21	104.75	111.88
1	G	138	VAL	N-CA-C	5.21	115.81	109.30
2	D	177	GLY	N-CA-C	5.20	120.34	113.37
2	F	225	VAL	CB-CA-C	-5.18	104.12	112.16
2	D	128	HIS	CB-CA-C	-5.18	101.13	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	304	GLU	N-CA-C	5.18	116.92	111.28
2	B	63	ALA	N-CA-C	-5.16	104.92	111.11
2	F	126	ALA	N-CA-C	5.16	117.69	111.40
1	A	270	VAL	CB-CA-C	-5.16	105.30	112.36
2	B	139	CYS	N-CA-C	5.15	116.14	109.65
2	F	37	TYR	N-CA-C	-5.15	104.61	111.87
1	E	327	ASP	N-CA-C	5.13	116.87	109.48
1	G	94	PHE	N-CA-C	5.13	117.27	111.11
1	A	337	TYR	N-CA-C	5.12	117.65	110.23
2	H	33	TYR	CB-CA-C	5.11	119.46	110.37
2	D	80	PHE	N-CA-C	-5.10	101.84	109.95
2	H	45	LYS	N-CA-C	-5.10	105.85	111.71
1	A	268	PRO	N-CA-C	-5.09	107.22	113.84
1	A	311	VAL	N-CA-C	5.08	115.22	110.30
1	C	87	THR	N-CA-C	5.07	115.74	108.74
2	F	150	SER	N-CA-C	5.06	116.61	111.14
1	A	349	ARG	N-CA-C	5.03	117.76	109.76
2	H	75	ARG	CA-C-N	5.03	124.96	119.78
2	H	75	ARG	C-N-CA	5.03	124.96	119.78
2	B	47	TYR	N-CA-C	5.03	119.56	113.38
2	D	247	GLU	CB-CA-C	-5.03	102.99	110.88
1	E	146	ALA	N-CA-C	-5.02	105.81	111.28
1	E	228	MET	N-CA-C	-5.01	107.55	113.97
1	C	80	ASN	CA-C-N	-5.00	114.51	119.56
1	C	80	ASN	C-N-CA	-5.00	114.51	119.56

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	2821	0	2777	111	0
1	C	2834	0	2791	119	0
1	E	2834	0	2791	112	0
1	G	2821	0	2777	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2519	0	2517	97	0
2	D	2519	0	2517	95	0
2	F	2519	0	2517	105	0
2	H	2519	0	2517	110	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	26	0	16	2	0
4	C	26	0	16	1	0
4	E	26	0	16	2	0
4	G	26	0	16	2	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
6	B	1	0	0	0	0
6	C	3	0	0	1	0
6	D	1	0	0	1	0
6	E	1	0	0	0	0
6	F	2	0	0	0	0
6	H	1	0	0	1	0
All	All	21507	0	21268	780	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (780) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:280:MET:HE3	2:H:292:ALA:HB3	1.21	1.13
2:F:214:ARG:HG2	2:F:214:ARG:HH11	0.99	1.10
1:C:144:LEU:HD13	2:D:71:MET:CE	1.81	1.10
1:C:144:LEU:HD13	2:D:71:MET:HE1	1.20	1.09
1:C:314:ARG:HH21	1:C:314:ARG:HG3	0.93	1.09
1:C:144:LEU:CD1	2:D:71:MET:HE1	1.82	1.08
2:F:329:ILE:HD12	2:F:329:ILE:OXT	1.53	1.06
1:C:314:ARG:HG3	1:C:314:ARG:NH2	1.64	0.99
1:C:331:PRO:HD2	1:C:334:GLU:OE1	1.62	0.99
2:H:143:LYS:HB2	2:H:167:VAL:HG22	1.45	0.98
1:C:18:GLU:OE2	1:C:18:GLU:HA	1.67	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:271:VAL:HA	2:H:269:PHE:HE1	1.32	0.95
2:F:214:ARG:HG2	2:F:214:ARG:NH1	1.81	0.92
2:F:214:ARG:HH11	2:F:214:ARG:CG	1.81	0.92
2:B:118:ASN:HD21	2:B:132:PHE:H	1.16	0.90
1:G:95:THR:HG22	1:G:131:PHE:CE2	2.08	0.89
2:B:277:ALA:O	2:B:281:GLU:HG3	1.72	0.88
2:D:211:SER:HB2	2:D:262:VAL:O	1.74	0.87
2:B:51:ARG:HG3	2:B:51:ARG:HH11	1.40	0.87
1:C:314:ARG:HH21	1:C:314:ARG:CG	1.83	0.87
2:H:212:HIS:HB3	2:H:238:MET:HE3	1.57	0.86
2:D:76:PRO:HG2	2:D:112:ILE:HD12	1.58	0.86
2:H:162:ARG:HH21	2:H:192:LEU:HD11	1.38	0.85
1:E:224:ARG:HD2	1:E:256:GLN:NE2	1.92	0.84
1:C:289:MET:HG2	1:C:290:LEU:N	1.93	0.84
1:G:98:ARG:HG2	1:G:131:PHE:HB2	1.60	0.83
1:E:279:GLN:NE2	1:E:279:GLN:HA	1.93	0.82
1:C:46:GLU:OE1	1:C:46:GLU:HA	1.77	0.82
1:C:91:ALA:O	1:C:95:THR:HG23	1.79	0.82
2:H:98:ALA:HB2	2:H:142:LEU:HD13	1.60	0.82
1:A:116:CYS:SG	1:A:126:MET:HG2	2.20	0.81
2:F:280:MET:HE3	2:H:292:ALA:CB	2.09	0.81
1:E:103:ARG:HG3	1:E:103:ARG:HH11	1.45	0.81
2:F:88:GLN:HE22	1:G:172:GLN:HE22	1.29	0.80
1:C:98:ARG:HG2	1:C:131:PHE:HB2	1.61	0.80
1:E:282:ARG:HG3	1:E:282:ARG:HH11	1.46	0.79
1:E:100:LEU:HD13	1:E:128:ALA:HB2	1.63	0.79
1:C:113:LYS:O	1:C:118:LYS:HD3	1.83	0.78
2:H:155:GLY:HA3	2:H:193:ILE:HG13	1.64	0.78
1:C:91:ALA:O	1:C:95:THR:CG2	2.32	0.77
2:F:34:ASP:HB3	2:F:41:ARG:HA	1.67	0.77
2:D:212:HIS:HB3	2:D:238:MET:HE3	1.65	0.77
2:F:271:VAL:HA	2:H:269:PHE:CE1	2.19	0.77
2:B:226:LEU:HD11	2:B:323:ILE:HG21	1.66	0.76
2:D:266:TRP:HB3	2:D:267:PRO:HD2	1.66	0.76
1:E:71:CYS:O	1:E:75:LEU:HD22	1.84	0.76
1:E:44:ARG:HB2	1:E:317:ILE:HG13	1.67	0.76
2:H:207:ILE:HD11	2:H:260:VAL:HG23	1.68	0.76
2:B:1:LEU:HD12	2:B:3:VAL:HG12	1.68	0.75
1:A:103:ARG:HH11	1:A:103:ARG:CG	1.99	0.75
1:E:341:SER:H	2:F:165:ASN:HD21	1.34	0.75
1:A:327:ASP:OD1	1:A:328:PRO:HD2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:TYR:HD1	1:C:201:GLY:HA3	1.53	0.74
2:F:172:ASN:C	2:F:172:ASN:HD22	1.96	0.74
1:C:289:MET:CG	1:C:290:LEU:N	2.51	0.74
2:B:184:PRO:HA	2:B:187:GLN:NE2	2.03	0.73
1:G:198:TYR:CD1	1:G:203:ALA:HB2	2.23	0.73
1:G:198:TYR:HD1	1:G:203:ALA:HB2	1.53	0.73
1:E:282:ARG:HG3	1:E:282:ARG:NH1	2.03	0.72
2:F:21:GLU:O	2:F:21:GLU:HG2	1.88	0.72
1:A:45:MET:HE3	1:A:92:HIS:HB3	1.71	0.72
1:A:229:ASP:OD1	1:A:229:ASP:C	2.33	0.72
2:H:313:ILE:HG12	2:H:314:PRO:HD2	1.71	0.72
1:C:55:GLN:O	1:C:56:LYS:HB2	1.89	0.72
1:G:112:ARG:HD2	1:G:327:ASP:O	1.89	0.71
2:H:3:VAL:CG1	2:H:182:PHE:CG	2.73	0.71
1:G:29:ARG:NH2	1:G:305:GLU:OE1	2.23	0.71
1:E:68:GLN:HG2	1:E:257:THR:OG1	1.91	0.71
1:G:71:CYS:O	1:G:75:LEU:HD22	1.89	0.71
2:H:19:ARG:NH1	2:H:162:ARG:HD2	2.06	0.71
1:G:171:ASN:OD1	1:G:216:ARG:NH2	2.22	0.71
2:B:143:LYS:HB2	2:B:167:VAL:HG22	1.71	0.70
2:B:16:GLU:OE2	2:B:162:ARG:NH1	2.24	0.70
1:G:228:MET:HE3	1:G:287:PRO:HD3	1.73	0.70
2:B:214:ARG:HG2	2:B:214:ARG:HH11	1.57	0.70
1:C:314:ARG:NH2	1:C:314:ARG:CG	2.49	0.70
2:D:9:ILE:HG22	2:D:13:MET:HE2	1.73	0.70
2:B:226:LEU:CD1	2:B:323:ILE:HG21	2.22	0.70
2:F:126:ALA:HB3	2:H:103:MET:SD	2.30	0.70
2:B:75:ARG:HH12	2:B:164:ASN:ND2	1.89	0.69
1:A:40:GLN:HE21	1:A:288:ILE:HD13	1.56	0.69
1:C:338:HIS:ND1	1:C:361:SER:O	2.25	0.69
2:H:237:ASN:HD22	2:H:238:MET:N	1.90	0.69
1:C:15:HIS:ND1	1:C:215:LYS:HG2	2.07	0.69
2:F:199:LYS:HE2	2:F:201:GLU:OE1	1.93	0.69
2:H:108:GLN:C	2:H:108:GLN:HE21	2.01	0.69
2:D:199:LYS:HE3	2:D:201:GLU:CD	2.18	0.69
2:D:237:ASN:C	2:D:237:ASN:HD22	2.01	0.69
2:H:268:GLN:NE2	2:H:299:ASP:OD2	2.26	0.68
2:F:88:GLN:HE22	1:G:172:GLN:NE2	1.91	0.68
1:C:46:GLU:OE1	1:C:46:GLU:CA	2.42	0.68
1:C:139:GLY:HA3	1:C:174:GLN:HE22	1.59	0.68
1:E:311:VAL:HG12	1:E:315:LYS:HE3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:19:ARG:HG2	2:F:19:ARG:HH11	1.58	0.68
1:A:146:ALA:O	1:A:149:ALA:HB3	1.94	0.68
1:C:94:PHE:O	1:C:98:ARG:HB2	1.94	0.67
1:E:286:ASP:HB3	1:E:289:MET:HB3	1.77	0.67
2:H:98:ALA:CB	2:H:142:LEU:HD13	2.24	0.67
2:H:98:ALA:HB2	2:H:142:LEU:CD1	2.24	0.67
2:D:199:LYS:HE3	2:D:201:GLU:OE1	1.95	0.66
2:F:142:LEU:HD21	2:F:168:VAL:CG2	2.25	0.66
2:H:3:VAL:HG11	2:H:182:PHE:CG	2.29	0.66
2:F:268:GLN:HG3	6:H:2003:HOH:O	1.94	0.66
1:A:270:VAL:CG1	1:A:275:ARG:HG3	2.26	0.66
1:G:333:GLU:CD	1:G:333:GLU:H	2.04	0.66
2:F:20:ASP:OD1	2:F:20:ASP:C	2.39	0.66
2:H:229:GLU:O	2:H:229:GLU:HG2	1.96	0.66
1:A:272:TYR:CE1	1:A:273:ARG:HD3	2.32	0.65
1:E:66:ASP:HA	1:E:69:GLU:OE2	1.96	0.65
1:A:291:LEU:O	1:A:295:MET:HG3	1.96	0.65
2:D:259:LEU:HD12	2:D:260:VAL:N	2.12	0.65
2:H:112:ILE:HG13	2:H:113:VAL:N	2.12	0.65
1:A:270:VAL:HG11	1:A:275:ARG:HG3	1.79	0.65
2:B:102:TYR:CD2	2:D:301:PRO:HG2	2.32	0.64
2:B:118:ASN:HD21	2:B:132:PHE:N	1.92	0.64
2:B:99:LYS:NZ	2:D:130:GLN:OE1	2.30	0.64
1:E:295:MET:HE2	1:E:300:LEU:CB	2.27	0.64
2:F:329:ILE:OXT	2:F:329:ILE:CD1	2.37	0.64
1:G:95:THR:HG22	1:G:131:PHE:HE2	1.60	0.64
2:H:3:VAL:CG1	2:H:182:PHE:HB2	2.27	0.64
2:F:172:ASN:C	2:F:172:ASN:ND2	2.55	0.64
1:G:113:LYS:HB2	1:G:113:LYS:HZ2	1.63	0.64
2:D:207:ILE:HG23	2:D:207:ILE:O	1.98	0.64
2:B:33:TYR:CD1	1:C:201:GLY:HA3	2.32	0.64
1:C:113:LYS:HD3	1:C:328:PRO:HG2	1.80	0.64
2:F:103:MET:SD	2:H:126:ALA:HB3	2.36	0.64
2:B:207:ILE:HG13	2:B:258:HIS:HB2	1.79	0.64
2:H:108:GLN:NE2	2:H:108:GLN:HA	2.12	0.64
1:A:103:ARG:HH11	1:A:103:ARG:HG2	1.62	0.63
2:D:79:GLU:HG3	2:D:115:ARG:NH1	2.13	0.63
2:H:59:GLU:HB2	2:H:88:GLN:HE21	1.63	0.63
2:D:112:ILE:HG13	2:D:113:VAL:N	2.13	0.63
1:G:345:PRO:HB3	1:G:360:VAL:HG12	1.80	0.63
2:B:172:ASN:C	2:B:172:ASN:HD22	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-1:HIS:HE1	1:C:299:ASN:OD1	1.82	0.63
1:C:335:LEU:C	1:C:335:LEU:HD23	2.23	0.63
1:C:144:LEU:HD13	2:D:71:MET:HE2	1.79	0.63
1:C:204:VAL:HG12	1:C:213:TYR:OH	1.99	0.63
2:F:127:GLN:HE21	2:H:103:MET:HE1	1.64	0.63
2:B:63:ALA:CB	2:B:89:ALA:HB1	2.29	0.62
1:C:228:MET:HE3	1:C:287:PRO:HD3	1.81	0.62
2:F:262:VAL:HG22	2:F:295:VAL:HB	1.81	0.62
2:H:214:ARG:N	2:H:215:PRO:HD2	2.14	0.62
1:G:101:SER:O	1:G:105:ILE:HG13	2.00	0.62
2:B:329:ILE:HD12	2:B:329:ILE:OXT	1.99	0.62
1:C:280:GLU:O	1:C:284:LYS:HG3	2.00	0.62
2:B:237:ASN:C	2:B:237:ASN:ND2	2.58	0.61
1:E:113:LYS:HG2	1:E:328:PRO:HG2	1.81	0.61
2:H:112:ILE:HG13	2:H:113:VAL:H	1.64	0.61
2:B:20:ASP:OD1	2:B:21:GLU:N	2.32	0.61
2:D:100:THR:O	2:D:101:TYR:C	2.41	0.61
2:F:313:ILE:HG22	2:F:314:PRO:HD2	1.83	0.61
1:A:129:LYS:O	1:A:130:ASN:HB2	2.01	0.61
1:A:229:ASP:OD1	1:A:231:LEU:N	2.33	0.61
2:B:75:ARG:HH22	2:B:164:ASN:ND2	1.98	0.61
1:C:157:LYS:O	1:C:158:ASP:HB2	1.99	0.61
1:G:222:GLY:HA2	1:G:252:LEU:O	2.00	0.61
2:D:237:ASN:HD22	2:D:238:MET:N	1.99	0.60
2:F:220:LEU:HD23	2:F:235:VAL:HG21	1.82	0.60
1:E:138:VAL:HG13	1:E:169:ALA:HB2	1.82	0.60
1:G:230:ILE:HG13	1:G:230:ILE:O	2.01	0.60
1:C:300:LEU:O	1:C:301:ALA:HB2	2.02	0.60
2:F:76:PRO:HG2	2:F:112:ILE:HD12	1.82	0.60
1:A:171:ASN:OD1	1:A:216:ARG:NH2	2.34	0.60
1:E:263:HIS:O	1:E:264:SER:HB3	2.01	0.60
1:C:144:LEU:HD12	2:D:71:MET:HE1	1.82	0.60
1:G:39:MET:CE	1:G:291:LEU:HD23	2.32	0.60
1:C:279:GLN:HA	1:C:279:GLN:OE1	2.02	0.60
2:H:60:MET:HE2	2:H:88:GLN:O	2.02	0.60
1:A:144:LEU:O	1:A:148:ILE:HG13	2.01	0.59
2:B:87:MET:HE3	2:D:91:ASP:OD1	2.01	0.59
2:B:267:PRO:HD2	2:B:299:ASP:OD1	2.03	0.59
2:D:238:MET:HE1	2:D:271:VAL:HG11	1.85	0.59
2:B:237:ASN:C	2:B:237:ASN:HD22	2.09	0.59
1:E:53:TYR:CD1	1:E:53:TYR:C	2.81	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:GLN:HE21	2:H:57:ILE:HG22	1.67	0.59
1:A:225:VAL:HG12	1:A:226:ASP:N	2.17	0.59
1:E:225:VAL:HG12	1:E:226:ASP:N	2.18	0.59
1:E:335:LEU:C	1:E:335:LEU:HD23	2.27	0.59
2:F:228:LYS:O	2:F:229:GLU:HG3	2.02	0.58
1:G:162:LEU:HG	1:G:192:ILE:HD11	1.84	0.58
1:A:334:GLU:HG2	1:A:337:TYR:CE2	2.38	0.58
2:B:16:GLU:CD	2:B:162:ARG:HH11	2.11	0.58
2:D:157:ILE:HG13	2:D:158:LYS:N	2.18	0.58
2:F:213:SER:O	2:F:216:VAL:HG23	2.03	0.58
1:A:235:GLU:OE2	1:A:238:ARG:NH1	2.36	0.58
1:C:100:LEU:HD22	1:C:128:ALA:HB2	1.84	0.58
1:A:38:MET:O	1:A:39:MET:C	2.44	0.58
2:B:57:ILE:HG21	1:C:138:VAL:HG11	1.84	0.58
1:E:348:VAL:HG12	2:H:299:ASP:HB3	1.86	0.58
2:H:108:GLN:NE2	2:H:108:GLN:CA	2.66	0.57
1:A:57:ILE:HG22	1:A:110:THR:HG22	1.85	0.57
2:D:59:GLU:O	2:D:60:MET:C	2.42	0.57
1:A:309:ILE:O	1:A:310:ASP:C	2.45	0.57
2:H:80:PHE:O	2:H:81:MET:C	2.44	0.57
2:B:313:ILE:HG22	2:B:314:PRO:HD2	1.87	0.57
2:D:33:TYR:CD2	2:D:33:TYR:O	2.57	0.57
1:E:261:HIS:O	1:E:262:GLY:O	2.21	0.57
2:F:127:GLN:NE2	2:H:103:MET:HE1	2.19	0.57
1:A:55:GLN:O	1:A:56:LYS:HB2	2.05	0.57
2:F:315:GLN:HB2	2:F:317:LYS:HB2	1.86	0.57
1:E:167:ASP:HB3	1:E:195:ASN:HA	1.87	0.57
2:F:95:ASN:ND2	2:H:87:MET:CE	2.68	0.57
2:D:23:VAL:HG22	2:D:75:ARG:HB2	1.86	0.57
1:E:46:GLU:OE1	1:E:46:GLU:HA	2.03	0.57
2:F:293:VAL:HG12	1:G:353:GLN:HE22	1.69	0.57
2:D:57:ILE:HG22	2:D:57:ILE:O	2.05	0.57
1:E:172:GLN:HB2	1:E:175:ILE:HD12	1.87	0.57
1:C:231:LEU:HB2	1:C:294:ARG:HH12	1.70	0.56
1:E:295:MET:HE2	1:E:300:LEU:HB3	1.85	0.56
1:G:55:GLN:O	1:G:57:ILE:N	2.38	0.56
1:A:103:ARG:HH22	1:A:319:ASP:HB3	1.70	0.56
2:B:250:GLU:O	2:B:254:MET:HG3	2.03	0.56
2:B:317:LYS:HA	2:B:317:LYS:CE	2.35	0.56
1:A:147:GLY:HA2	2:B:65:ILE:HG23	1.88	0.56
2:B:51:ARG:HG3	2:B:51:ARG:NH1	2.15	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:25:LEU:HD12	2:D:26:LEU:H	1.71	0.56
1:G:95:THR:HG21	1:G:126:MET:HE3	1.86	0.56
2:B:126:ALA:HB3	2:D:103:MET:SD	2.46	0.56
1:C:231:LEU:HB2	1:C:294:ARG:NH1	2.20	0.56
2:H:237:ASN:HD22	2:H:237:ASN:C	2.11	0.56
1:A:111:GLY:O	1:A:112:ARG:HD3	2.06	0.56
1:A:177:GLU:OE1	2:B:61:GLY:N	2.34	0.56
2:F:148:TRP:CD1	2:F:175:MET:HE2	2.41	0.56
2:H:3:VAL:HG11	2:H:182:PHE:CD2	2.41	0.56
1:C:68:GLN:HE21	1:C:259:ARG:HB3	1.71	0.56
1:C:24:THR:HG22	1:C:24:THR:O	2.07	0.55
1:C:261:HIS:O	1:C:262:GLY:O	2.25	0.55
2:B:157:ILE:O	2:B:160:ALA:HB3	2.07	0.55
4:C:1006:TPP:HN42	4:C:1006:TPP:H2	1.72	0.55
2:B:279:ILE:HD13	2:B:284:ALA:HB3	1.87	0.55
1:C:139:GLY:HA3	1:C:174:GLN:NE2	2.22	0.55
2:F:307:ILE:HG23	2:F:308:LEU:N	2.21	0.55
2:D:16:GLU:OE2	2:D:162:ARG:NH1	2.39	0.55
2:D:28:GLU:OE2	2:D:59:GLU:OE2	2.25	0.55
2:H:328:ASN:CG	2:H:328:ASN:O	2.49	0.55
1:E:241:ALA:O	1:E:245:ARG:HB2	2.07	0.55
1:A:65:CYS:HB3	1:A:90:ARG:HG2	1.89	0.55
1:A:72:CYS:HA	1:A:94:PHE:CE1	2.42	0.55
2:B:172:ASN:C	2:B:172:ASN:ND2	2.63	0.55
2:H:89:ALA:O	2:H:92:GLN:N	2.40	0.55
1:C:217:GLY:O	1:C:218:ASP:HB3	2.06	0.55
1:E:53:TYR:CE1	1:E:265:MET:HB3	2.42	0.55
2:F:172:ASN:ND2	2:F:174:LEU:H	2.04	0.55
1:A:121:GLY:O	1:A:125:HIS:HD2	1.90	0.54
2:F:327:LEU:C	2:F:329:ILE:H	2.15	0.54
1:G:55:GLN:C	1:G:57:ILE:H	2.14	0.54
1:G:165:TYR:HH	1:G:179:TYR:HH	1.51	0.54
1:A:345:PRO:HB3	1:A:360:VAL:HG12	1.88	0.54
1:E:351:ALA:HA	2:H:296:THR:O	2.08	0.54
1:C:313:VAL:HG12	1:C:314:ARG:N	2.19	0.54
2:B:328:ASN:O	2:B:328:ASN:ND2	2.40	0.54
2:H:112:ILE:CG1	2:H:113:VAL:N	2.70	0.54
2:B:288:LEU:HG	2:B:290:ALA:O	2.08	0.54
1:E:213:TYR:HA	1:E:216:ARG:HG2	1.90	0.54
2:B:295:VAL:HG13	1:C:351:ALA:O	2.08	0.54
1:G:229:ASP:OD1	1:G:294:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:165:ASN:HB3	2:H:166:PRO:CD	2.38	0.54
2:B:227:SER:HA	2:B:231:VAL:O	2.08	0.54
1:E:196:ASN:ND2	1:E:259:ARG:HG2	2.22	0.54
2:B:214:ARG:HG2	2:B:214:ARG:NH1	2.22	0.54
1:E:261:HIS:C	1:E:262:GLY:O	2.51	0.54
1:E:295:MET:HE2	1:E:300:LEU:HB2	1.89	0.54
1:G:190:ILE:HG22	1:G:192:ILE:HG13	1.90	0.53
2:H:20:ASP:O	2:H:22:LYS:N	2.40	0.53
1:C:270:VAL:HG22	1:C:270:VAL:O	2.07	0.53
2:H:165:ASN:HB3	2:H:166:PRO:HD2	1.89	0.53
1:A:70:ALA:HB3	1:A:227:GLY:O	2.09	0.53
1:G:196:ASN:O	1:G:197:ARG:HB2	2.07	0.53
2:H:3:VAL:HG12	2:H:182:PHE:HB2	1.90	0.53
2:H:28:GLU:O	2:H:29:GLU:HB2	2.07	0.53
1:C:61:PHE:HB3	1:C:63:HIS:CE1	2.43	0.53
2:D:145:VAL:HG11	2:D:195:ILE:HG12	1.90	0.53
1:E:63:HIS:HA	1:E:264:SER:HB2	1.91	0.53
2:B:99:LYS:HE2	2:D:126:ALA:O	2.08	0.53
1:C:169:ALA:O	1:C:175:ILE:HD12	2.08	0.53
1:C:286:ASP:O	1:C:290:LEU:HB2	2.08	0.53
1:E:71:CYS:SG	1:E:255:LEU:HD23	2.48	0.53
1:E:282:ARG:HH11	1:E:282:ARG:CG	2.13	0.53
2:F:280:MET:HE2	2:H:276:CYS:HB3	1.90	0.53
1:A:286:ASP:O	1:A:290:LEU:HG	2.08	0.53
2:F:142:LEU:HD21	2:F:168:VAL:HG21	1.91	0.53
2:B:184:PRO:HA	2:B:187:GLN:HE21	1.72	0.53
1:E:225:VAL:HG21	1:E:236:ALA:CB	2.39	0.53
2:F:211:SER:OG	2:F:212:HIS:N	2.41	0.53
2:D:125:ALA:O	2:D:129:SER:HB2	2.09	0.53
1:E:312:GLU:O	1:E:316:GLU:HG2	2.08	0.53
2:F:20:ASP:OD1	2:F:21:GLU:N	2.42	0.53
2:F:75:ARG:NH2	2:F:163:ASP:O	2.42	0.53
2:B:2:GLN:HA	2:B:181:GLU:HA	1.92	0.52
2:H:3:VAL:CG1	2:H:182:PHE:CB	2.88	0.52
2:B:51:ARG:O	2:B:52:ILE:HD13	2.09	0.52
2:D:75:ARG:NH2	2:D:163:ASP:O	2.42	0.52
2:F:19:ARG:HG2	2:F:19:ARG:NH1	2.24	0.52
2:F:136:TYR:HB3	2:F:144:VAL:HG21	1.91	0.52
1:G:61:PHE:HD2	1:G:124:MET:CE	2.22	0.52
1:G:116:CYS:SG	1:G:126:MET:HG2	2.50	0.52
1:A:50:ASP:OD2	1:A:50:ASP:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:263:HIS:CE1	4:G:1012:TPP:S1	3.03	0.52
2:B:279:ILE:HG22	2:B:280:MET:N	2.24	0.52
1:E:341:SER:H	2:F:165:ASN:ND2	2.06	0.52
2:F:207:ILE:HD11	2:F:260:VAL:HG23	1.91	0.52
1:G:172:GLN:HB2	1:G:175:ILE:HD12	1.91	0.52
1:C:62:CYS:HB3	1:C:265:MET:HG2	1.91	0.52
1:E:100:LEU:HD13	1:E:128:ALA:CB	2.35	0.52
2:F:228:LYS:C	2:F:229:GLU:HG3	2.35	0.52
2:F:263:GLU:OE2	2:F:296:THR:HG22	2.09	0.52
2:H:202:ARG:HH11	2:H:202:ARG:HG2	1.74	0.52
1:A:182:ALA:HA	1:A:187:LEU:HD12	1.91	0.52
2:F:202:ARG:HD3	2:F:233:CYS:O	2.10	0.52
1:A:113:LYS:HG2	1:A:328:PRO:O	2.10	0.52
1:A:190:ILE:HG22	1:A:192:ILE:HG13	1.91	0.52
2:B:237:ASN:HD22	2:B:238:MET:N	2.07	0.52
2:F:112:ILE:HG13	2:F:113:VAL:N	2.24	0.52
2:F:175:MET:O	2:F:176:TYR:C	2.53	0.52
2:F:327:LEU:C	2:F:329:ILE:N	2.66	0.52
2:H:212:HIS:HB3	2:H:238:MET:CE	2.34	0.52
2:H:246:MET:O	2:H:247:GLU:C	2.53	0.52
2:B:31:ALA:HB3	2:B:54:ASP:CG	2.35	0.51
2:B:246:MET:HE2	2:B:278:ARG:CB	2.40	0.51
2:B:251:ALA:HA	2:B:254:MET:HE2	1.90	0.51
2:D:206:HIS:O	2:D:207:ILE:HB	2.08	0.51
1:C:1:PHE:CE1	1:C:301:ALA:HA	2.45	0.51
1:C:196:ASN:O	1:C:197:ARG:HB2	2.10	0.51
1:E:153:LYS:NZ	1:E:185:TRP:O	2.34	0.51
1:G:286:ASP:OD1	1:G:287:PRO:HD2	2.09	0.51
2:B:246:MET:HE2	2:B:278:ARG:HB3	1.92	0.51
1:G:206:ARG:HB3	1:G:206:ARG:CZ	2.40	0.51
1:A:45:MET:CE	1:A:92:HIS:HB3	2.40	0.51
2:B:93:VAL:O	2:B:97:ALA:HB3	2.10	0.51
1:A:275:ARG:HH11	1:A:275:ARG:CG	2.24	0.51
1:E:62:CYS:HB3	1:E:265:MET:HG2	1.91	0.51
2:F:142:LEU:HD21	2:F:168:VAL:HG23	1.92	0.51
2:F:311:ASN:N	2:F:311:ASN:HD22	2.09	0.51
1:G:68:GLN:HE22	1:G:196:ASN:HD22	1.58	0.51
2:F:59:GLU:O	2:F:60:MET:C	2.51	0.51
2:B:20:ASP:OD1	2:B:22:LYS:N	2.39	0.51
2:D:121:SER:OG	2:D:122:ALA:N	2.41	0.51
2:D:171:GLU:OE1	2:D:176:TYR:OH	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3:VAL:HG13	2:H:182:PHE:CD1	2.46	0.51
2:H:57:ILE:HG22	2:H:57:ILE:O	2.10	0.51
2:D:158:LYS:O	2:D:159:SER:C	2.53	0.51
1:E:327:ASP:OD1	1:E:328:PRO:HD2	2.09	0.51
2:F:208:THR:O	2:F:259:LEU:HA	2.11	0.51
1:G:316:GLU:O	1:G:316:GLU:HG2	2.08	0.50
2:H:155:GLY:HA3	2:H:193:ILE:CG1	2.36	0.50
2:H:290:ALA:HB1	2:H:291:PRO:HD2	1.92	0.50
1:G:39:MET:HE2	1:G:291:LEU:HD23	1.92	0.50
1:C:174:GLN:HB3	2:D:60:MET:HG2	1.93	0.50
2:D:98:ALA:HB2	2:D:142:LEU:HD13	1.94	0.50
2:D:328:ASN:O	2:D:328:ASN:CG	2.53	0.50
1:E:279:GLN:HA	1:E:279:GLN:HE21	1.75	0.50
1:G:268:PRO:HB2	1:G:270:VAL:HG12	1.92	0.50
2:H:316:VAL:O	2:H:317:LYS:C	2.53	0.50
1:A:103:ARG:NH2	1:A:319:ASP:HB3	2.26	0.50
1:G:346:PHE:CD1	1:G:346:PHE:N	2.78	0.50
1:A:66:ASP:N	1:A:66:ASP:OD2	2.45	0.50
2:B:99:LYS:HG2	2:D:301:PRO:HB3	1.93	0.50
2:D:237:ASN:C	2:D:237:ASN:ND2	2.66	0.50
1:E:296:VAL:HA	1:E:301:ALA:O	2.12	0.50
2:H:98:ALA:O	2:H:141:GLY:HA3	2.12	0.50
2:B:143:LYS:NZ	2:B:163:ASP:OD2	2.45	0.50
2:B:206:HIS:ND1	2:B:231:VAL:HA	2.27	0.50
1:C:269:GLY:HA2	1:C:272:TYR:CE1	2.47	0.50
1:C:282:ARG:HG2	1:C:282:ARG:O	2.11	0.50
1:E:327:ASP:CG	1:E:328:PRO:HD2	2.37	0.50
1:G:27:LEU:HD13	1:G:300:LEU:HD21	1.93	0.50
1:A:61:PHE:HD2	1:A:124:MET:CE	2.25	0.50
2:B:268:GLN:NE2	2:B:299:ASP:OD2	2.45	0.50
1:G:127:TYR:CD1	2:H:104:SER:HB3	2.47	0.50
1:A:128:ALA:HB3	1:A:131:PHE:HB3	1.94	0.49
2:B:150:SER:O	2:B:151:GLU:C	2.54	0.49
1:C:71:CYS:SG	1:C:255:LEU:HD23	2.52	0.49
1:C:228:MET:HE2	1:C:285:SER:HB2	1.93	0.49
2:D:19:ARG:HD2	2:D:162:ARG:NH1	2.26	0.49
1:E:225:VAL:HG12	1:E:226:ASP:H	1.77	0.49
2:F:13:MET:HE3	2:F:43:LEU:HD21	1.94	0.49
2:H:9:ILE:HA	2:H:157:ILE:CD1	2.42	0.49
2:H:149:ASN:HB2	2:H:180:PHE:CE2	2.47	0.49
2:H:279:ILE:HD12	2:H:284:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:279:ILE:CD1	2:H:284:ALA:HB3	2.41	0.49
1:A:107:ALA:HA	1:A:324:ALA:HB1	1.95	0.49
1:A:302:SER:C	1:A:304:GLU:N	2.67	0.49
1:A:352:ASN:C	1:A:352:ASN:OD1	2.54	0.49
1:C:92:HIS:HD2	1:C:126:MET:HE1	1.77	0.49
2:D:23:VAL:HG22	2:D:75:ARG:CB	2.42	0.49
2:D:326:THR:C	2:D:328:ASN:H	2.20	0.49
1:E:63:HIS:CD2	1:E:264:SER:HB3	2.47	0.49
2:H:214:ARG:HB3	2:H:215:PRO:CD	2.42	0.49
2:H:316:VAL:C	2:H:318:ASP:N	2.69	0.49
1:A:202:THR:HG23	1:A:206:ARG:CZ	2.42	0.49
2:B:16:GLU:OE1	2:B:162:ARG:HD2	2.11	0.49
1:C:132:TYR:CD1	1:C:132:TYR:N	2.80	0.49
1:E:286:ASP:HB3	1:E:289:MET:CB	2.42	0.49
2:D:206:HIS:O	2:D:327:LEU:HD21	2.12	0.49
1:G:128:ALA:HB3	1:G:131:PHE:HB3	1.93	0.49
2:B:91:ASP:OD1	2:B:95:ASN:ND2	2.41	0.49
2:B:218:HIS:O	2:B:221:GLU:HB2	2.12	0.49
1:C:229:ASP:O	1:C:230:ILE:C	2.55	0.49
1:E:335:LEU:C	1:E:335:LEU:CD2	2.84	0.49
1:G:44:ARG:HB2	1:G:317:ILE:HG13	1.94	0.49
1:A:36:TYR:O	1:A:37:ARG:C	2.54	0.49
2:B:112:ILE:HG13	2:B:113:VAL:N	2.28	0.49
1:E:128:ALA:O	1:E:129:LYS:C	2.55	0.49
2:B:269:PHE:HE1	2:D:271:VAL:HA	1.77	0.49
2:D:24:PHE:HB2	2:D:51:ARG:O	2.12	0.49
2:F:76:PRO:CG	2:F:112:ILE:HD12	2.41	0.49
1:A:164:LEU:N	1:A:164:LEU:HD12	2.27	0.49
2:B:44:TRP:NE1	2:B:49:ASP:OD1	2.40	0.49
1:E:142:VAL:O	1:E:143:PRO:C	2.54	0.49
1:G:39:MET:CE	1:G:291:LEU:CD2	2.91	0.49
1:C:109:LEU:HD21	1:C:123:SER:HB2	1.94	0.49
1:G:166:GLY:O	1:G:169:ALA:HB3	2.11	0.49
1:C:198:TYR:CE1	1:C:203:ALA:HB2	2.47	0.49
1:C:281:VAL:O	1:C:281:VAL:CG1	2.59	0.48
2:D:266:TRP:HB3	2:D:267:PRO:CD	2.39	0.48
1:A:46:GLU:O	1:A:47:LEU:C	2.56	0.48
1:E:56:LYS:HA	1:E:56:LYS:HD3	1.59	0.48
1:G:68:GLN:NE2	1:G:196:ASN:HD22	2.11	0.48
1:E:86:ILE:HD12	1:E:132:TYR:HB2	1.94	0.48
1:E:342:SER:N	1:E:361:SER:OG	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:ASP:OD1	1:E:260:TYR:HB2	2.14	0.48
2:F:84:ASN:ND2	2:F:128:HIS:HA	2.27	0.48
2:B:62:PHE:O	2:B:63:ALA:C	2.56	0.48
2:B:91:ASP:O	2:B:95:ASN:HB2	2.13	0.48
1:C:95:THR:HG21	1:C:126:MET:HE3	1.95	0.48
2:D:306:LYS:O	2:D:307:ILE:C	2.53	0.48
1:E:142:VAL:HG21	1:E:175:ILE:HG12	1.95	0.48
1:E:279:GLN:NE2	1:E:279:GLN:CA	2.72	0.48
2:H:3:VAL:HG13	2:H:182:PHE:CG	2.47	0.48
2:H:152:ASP:HA	2:H:193:ILE:CD1	2.43	0.48
1:A:107:ALA:HB3	1:A:115:GLY:HA2	1.95	0.48
1:E:101:SER:O	1:E:105:ILE:HG13	2.13	0.48
1:G:39:MET:HE2	1:G:291:LEU:CD2	2.43	0.48
1:G:327:ASP:OD1	1:G:328:PRO:HD2	2.13	0.48
2:B:154:LYS:O	2:B:157:ILE:HG22	2.14	0.48
2:F:202:ARG:O	2:F:234:GLU:HA	2.13	0.48
2:H:93:VAL:O	2:H:97:ALA:HB3	2.14	0.48
1:A:150:LEU:HA	1:A:187:LEU:HD22	1.94	0.48
1:A:162:LEU:N	1:A:162:LEU:HD12	2.29	0.48
2:D:82:THR:HG22	2:D:117:PRO:HG2	1.95	0.48
2:H:104:SER:O	2:H:107:LEU:HD22	2.14	0.48
2:B:79:GLU:HG3	2:B:115:ARG:NH1	2.28	0.47
2:B:296:THR:O	1:C:351:ALA:HA	2.14	0.47
2:F:62:PHE:O	2:F:63:ALA:C	2.57	0.47
1:A:217:GLY:O	1:A:218:ASP:HB3	2.14	0.47
1:A:275:ARG:HH11	1:A:275:ARG:CB	2.27	0.47
2:B:241:ILE:O	2:B:241:ILE:CG2	2.61	0.47
2:B:39:VAL:HG11	2:B:115:ARG:NH2	2.29	0.47
2:B:207:ILE:HG13	2:B:258:HIS:CB	2.43	0.47
1:C:223:LEU:HD12	1:C:225:VAL:CG2	2.44	0.47
1:G:231:LEU:HD23	1:G:231:LEU:HA	1.68	0.47
1:A:323:PHE:CD2	1:A:323:PHE:C	2.91	0.47
2:H:143:LYS:NZ	2:H:163:ASP:OD2	2.46	0.47
2:F:152:ASP:O	2:F:156:LEU:HB2	2.15	0.47
2:F:269:PHE:CZ	2:H:244:MET:HE1	2.49	0.47
1:A:112:ARG:NH1	1:A:327:ASP:O	2.47	0.47
1:C:71:CYS:O	1:C:75:LEU:HD13	2.15	0.47
2:H:229:GLU:O	2:H:229:GLU:CG	2.63	0.47
1:A:58:ILE:HG12	1:A:109:LEU:O	2.15	0.47
2:B:152:ASP:O	2:B:156:LEU:HB2	2.14	0.47
2:B:302:MET:SD	2:B:303:PRO:HD2	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:VAL:HB	1:C:255:LEU:HD12	1.96	0.47
2:D:156:LEU:HD11	2:D:239:ARG:HB3	1.97	0.47
1:E:196:ASN:C	1:E:198:TYR:H	2.21	0.47
1:E:279:GLN:OE1	1:E:282:ARG:HD2	2.15	0.47
1:E:353:GLN:OE1	2:H:293:VAL:HG12	2.15	0.47
2:F:304:TYR:O	2:F:305:ALA:C	2.58	0.47
1:A:103:ARG:HH11	1:A:103:ARG:HG3	1.78	0.47
1:A:196:ASN:O	1:A:197:ARG:HB2	2.14	0.47
1:C:166:GLY:HA3	6:C:2002:HOH:O	2.15	0.47
1:C:167:ASP:OD1	1:C:198:TYR:C	2.58	0.47
1:C:281:VAL:O	1:C:281:VAL:HG12	2.11	0.47
2:D:5:VAL:HB	2:D:175:MET:O	2.15	0.47
2:D:25:LEU:HD12	2:D:26:LEU:N	2.29	0.47
2:F:311:ASN:N	2:F:311:ASN:ND2	2.63	0.47
1:G:55:GLN:C	1:G:57:ILE:N	2.69	0.47
2:H:237:ASN:C	2:H:237:ASN:ND2	2.73	0.47
2:B:82:THR:HG23	2:B:85:PHE:CE2	2.50	0.47
2:D:270:GLY:HA3	6:D:2001:HOH:O	2.15	0.47
1:G:338:HIS:O	2:H:102:TYR:HA	2.15	0.47
1:A:103:ARG:HG2	1:A:103:ARG:NH1	2.25	0.46
1:C:264:SER:O	1:C:266:SER:N	2.48	0.46
2:B:182:PHE:HA	2:B:183:PRO:HD2	1.74	0.46
1:C:53:TYR:C	1:C:53:TYR:CD1	2.93	0.46
1:C:139:GLY:CA	1:C:174:GLN:HE22	2.28	0.46
1:E:62:CYS:O	1:E:264:SER:HB2	2.14	0.46
1:G:263:HIS:CE1	4:G:1012:TPP:H62	2.51	0.46
2:H:59:GLU:O	2:H:60:MET:C	2.59	0.46
1:A:257:THR:OG1	1:A:258:TYR:N	2.45	0.46
2:D:10:ASN:ND2	2:D:39:VAL:O	2.41	0.46
2:F:40:SER:O	2:F:41:ARG:C	2.58	0.46
1:A:203:ALA:O	1:A:204:VAL:C	2.59	0.46
1:C:282:ARG:NH1	1:C:282:ARG:HG3	2.31	0.46
2:H:307:ILE:HG23	2:H:308:LEU:HG	1.96	0.46
2:F:94:ILE:O	2:F:98:ALA:HB3	2.15	0.46
1:G:200:MET:HG2	1:G:201:GLY:H	1.81	0.46
1:G:251:ILE:HG12	1:G:252:LEU:H	1.81	0.46
1:A:307:LYS:HD2	1:A:307:LYS:HA	1.51	0.46
1:A:334:GLU:HG2	1:A:337:TYR:CD2	2.51	0.46
2:D:254:MET:HE2	2:D:284:ALA:HA	1.96	0.46
2:H:101:TYR:CE1	2:H:106:GLY:HA2	2.51	0.46
1:A:42:VAL:O	1:A:46:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:ILE:O	2:B:241:ILE:HG22	2.15	0.46
1:C:15:HIS:CD2	1:C:16:ARG:HG3	2.51	0.46
2:D:62:PHE:O	2:D:63:ALA:C	2.56	0.46
1:G:216:ARG:NH1	1:G:216:ARG:HG3	2.30	0.46
2:H:150:SER:O	2:H:151:GLU:C	2.59	0.46
2:B:118:ASN:ND2	2:B:132:PHE:H	1.97	0.46
1:C:7:PHE:HE1	1:C:27:LEU:HB3	1.81	0.46
1:C:89:TYR:CD1	1:C:89:TYR:C	2.94	0.46
1:C:140:ALA:O	1:C:143:PRO:HD2	2.16	0.46
1:E:50:ASP:O	1:E:54:LYS:HG3	2.16	0.46
1:E:87:THR:HG22	1:E:133:GLY:O	2.16	0.46
1:C:39:MET:HE1	1:C:291:LEU:HD22	1.98	0.45
1:E:60:GLY:HA3	2:H:123:GLY:O	2.16	0.45
1:E:229:ASP:O	1:E:230:ILE:C	2.57	0.45
2:F:136:TYR:CB	2:F:144:VAL:HG21	2.47	0.45
2:H:279:ILE:HD13	2:H:279:ILE:HA	1.72	0.45
1:A:176:PHE:HZ	1:A:216:ARG:HE	1.64	0.45
1:E:68:GLN:HE21	1:E:259:ARG:HB3	1.82	0.45
2:F:214:ARG:NH1	2:F:214:ARG:CG	2.52	0.45
2:H:212:HIS:CB	2:H:238:MET:HE3	2.39	0.45
1:A:166:GLY:O	1:A:169:ALA:HB3	2.17	0.45
1:A:259:ARG:HH12	1:A:262:GLY:HA2	1.81	0.45
1:C:327:ASP:OD1	1:C:328:PRO:HD2	2.16	0.45
2:D:202:ARG:NH1	2:D:232:GLU:OE1	2.38	0.45
2:F:313:ILE:CG2	2:F:314:PRO:HD2	2.44	0.45
1:C:30:GLU:OE2	1:C:30:GLU:N	2.47	0.45
1:C:261:HIS:C	1:C:262:GLY:O	2.59	0.45
2:D:319:ILE:O	2:D:320:ILE:C	2.60	0.45
1:E:142:VAL:HG21	1:E:175:ILE:CG1	2.46	0.45
1:A:145:GLY:HA3	1:A:163:THR:OG1	2.17	0.45
1:C:31:ASP:O	1:C:32:GLY:C	2.58	0.45
1:C:300:LEU:HD12	1:C:300:LEU:HA	1.54	0.45
2:D:304:TYR:O	2:D:305:ALA:C	2.58	0.45
1:E:48:LYS:HA	1:E:48:LYS:HD3	1.77	0.45
1:E:111:GLY:O	1:E:112:ARG:HD3	2.17	0.45
1:A:103:ARG:HH22	1:A:319:ASP:CB	2.30	0.45
1:A:270:VAL:HG12	1:A:275:ARG:HG3	1.97	0.45
1:C:264:SER:O	1:C:265:MET:C	2.60	0.45
2:D:316:VAL:HG12	2:D:320:ILE:HD12	1.99	0.45
2:F:137:GLY:O	2:F:242:ARG:NH1	2.42	0.45
2:F:199:LYS:HD2	2:F:239:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:227:SER:C	2:F:229:GLU:H	2.25	0.45
2:H:108:GLN:HE21	2:H:108:GLN:CA	2.27	0.45
2:B:263:GLU:HG2	2:B:296:THR:HG22	1.97	0.45
1:E:187:LEU:O	1:E:189:CYS:N	2.47	0.45
2:B:250:GLU:OE2	2:B:283:PRO:HD2	2.16	0.45
2:H:208:THR:HG22	2:H:210:VAL:HG23	1.99	0.45
1:C:65:CYS:O	1:C:66:ASP:C	2.60	0.45
1:E:57:ILE:HG22	1:E:110:THR:HG22	1.98	0.45
2:D:94:ILE:HD13	2:D:94:ILE:HA	1.75	0.44
1:E:80:ASN:O	1:E:98:ARG:NH2	2.50	0.44
1:G:36:TYR:C	1:G:36:TYR:CD2	2.95	0.44
1:G:112:ARG:HG3	1:G:327:ASP:HB3	1.98	0.44
1:A:109:LEU:HD12	1:A:109:LEU:HA	1.80	0.44
1:C:-1:HIS:CE1	1:C:299:ASN:OD1	2.67	0.44
1:C:228:MET:HE3	1:C:285:SER:O	2.17	0.44
2:D:182:PHE:HA	2:D:183:PRO:HD2	1.83	0.44
1:E:335:LEU:HD21	2:H:300:VAL:HG21	1.98	0.44
2:F:51:ARG:O	2:F:52:ILE:HD13	2.17	0.44
1:G:94:PHE:O	1:G:95:THR:C	2.58	0.44
2:H:213:SER:OG	2:H:214:ARG:N	2.50	0.44
1:A:61:PHE:HB3	1:A:63:HIS:CE1	2.53	0.44
1:A:112:ARG:HD2	1:A:327:ASP:O	2.17	0.44
2:D:33:TYR:O	2:D:33:TYR:HD2	1.98	0.44
2:F:307:ILE:CG2	2:F:308:LEU:N	2.80	0.44
1:C:48:LYS:HD3	1:C:51:GLN:HE21	1.83	0.44
2:D:250:GLU:O	2:D:254:MET:HG3	2.17	0.44
1:E:282:ARG:O	1:E:282:ARG:HG2	2.17	0.44
2:F:306:LYS:O	2:F:307:ILE:C	2.58	0.44
1:G:36:TYR:O	1:G:37:ARG:C	2.59	0.44
1:A:13:ASP:HB2	1:A:224:ARG:HB3	2.00	0.44
1:C:24:THR:O	1:C:24:THR:CG2	2.65	0.44
1:C:68:GLN:NE2	1:C:259:ARG:HB3	2.32	0.44
1:E:103:ARG:HH11	1:E:103:ARG:CG	2.22	0.44
2:F:25:LEU:HD23	2:F:52:ILE:HG23	1.99	0.44
2:F:144:VAL:HG22	2:F:168:VAL:HB	1.98	0.44
1:G:54:LYS:C	1:G:56:LYS:H	2.26	0.44
1:G:142:VAL:O	1:G:143:PRO:C	2.59	0.44
1:A:272:TYR:HE1	1:A:273:ARG:HD3	1.80	0.44
1:E:102:VAL:HG11	1:E:317:ILE:HD13	1.98	0.44
1:G:228:MET:CE	1:G:287:PRO:HD3	2.46	0.44
2:H:182:PHE:HD2	2:H:187:GLN:HG3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:VAL:HA	1:A:163:THR:HG21	1.99	0.44
1:E:228:MET:HE3	1:E:285:SER:O	2.18	0.44
2:H:149:ASN:HB2	2:H:180:PHE:CD2	2.53	0.44
1:A:39:MET:HG2	1:A:73:VAL:HG21	2.00	0.44
2:B:299:ASP:HB3	1:C:348:VAL:HG12	1.99	0.44
2:D:259:LEU:HD12	2:D:260:VAL:H	1.82	0.44
1:E:172:GLN:HB2	1:E:175:ILE:CD1	2.47	0.44
1:A:65:CYS:O	1:A:65:CYS:SG	2.76	0.44
1:A:267:ASP:C	1:A:269:GLY:N	2.76	0.44
1:E:50:ASP:OD1	1:E:265:MET:HE1	2.17	0.44
2:F:259:LEU:CD2	2:F:279:ILE:HG13	2.47	0.44
2:H:313:ILE:HG12	2:H:314:PRO:CD	2.43	0.44
2:H:327:LEU:HD23	2:H:327:LEU:HA	1.76	0.44
1:A:80:ASN:HB3	1:A:81:PRO:HD2	1.99	0.43
2:H:59:GLU:OE1	2:H:59:GLU:N	2.51	0.43
2:H:156:LEU:HD23	2:H:156:LEU:HA	1.58	0.43
2:D:148:TRP:CE3	2:D:149:ASN:ND2	2.85	0.43
1:E:44:ARG:CB	1:E:317:ILE:HG13	2.41	0.43
1:E:138:VAL:HG13	1:E:169:ALA:CB	2.48	0.43
1:E:203:ALA:O	1:E:204:VAL:C	2.61	0.43
4:E:1009:TPP:N1'	2:H:59:GLU:OE2	2.51	0.43
2:H:19:ARG:CZ	2:H:162:ARG:HD2	2.48	0.43
1:A:335:LEU:HD23	1:A:335:LEU:C	2.43	0.43
2:H:329:ILE:HD12	2:H:329:ILE:C	2.43	0.43
1:A:305:GLU:O	1:A:309:ILE:HG13	2.18	0.43
2:D:24:PHE:CE1	2:D:76:PRO:HB3	2.52	0.43
1:E:103:ARG:HG3	1:E:103:ARG:NH1	2.21	0.43
1:E:141:GLN:N	1:E:141:GLN:OE1	2.51	0.43
2:F:81:MET:HE3	2:F:81:MET:HB2	1.80	0.43
2:F:327:LEU:O	2:F:329:ILE:N	2.52	0.43
1:C:320:ALA:O	1:C:323:PHE:HB3	2.18	0.43
2:D:96:SER:O	2:D:100:THR:OG1	2.27	0.43
1:E:225:VAL:CG1	1:E:226:ASP:N	2.82	0.43
1:A:202:THR:HG23	1:A:206:ARG:NH2	2.34	0.43
1:C:69:GLU:OE1	1:C:69:GLU:N	2.48	0.43
2:F:10:ASN:HD21	2:F:43:LEU:HD13	1.82	0.43
2:H:62:PHE:O	2:H:63:ALA:C	2.61	0.43
1:A:220:ILE:HG23	1:A:221:PRO:HD2	2.00	0.43
1:E:95:THR:O	1:E:100:LEU:HB2	2.19	0.43
1:A:58:ILE:CG2	1:A:59:ARG:N	2.81	0.43
2:B:211:SER:HB3	2:B:216:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:207:ILE:O	2:D:207:ILE:CG2	2.66	0.43
1:E:53:TYR:CG	1:E:265:MET:HG3	2.53	0.43
1:E:335:LEU:HD23	1:E:335:LEU:O	2.18	0.43
2:F:66:ALA:O	2:F:76:PRO:HG3	2.19	0.43
1:G:113:LYS:C	1:G:115:GLY:H	2.27	0.43
2:H:274:GLU:OE2	2:H:278:ARG:HG2	2.18	0.43
1:A:75:LEU:O	1:A:76:GLU:C	2.61	0.43
1:A:181:MET:HG2	1:A:185:TRP:CH2	2.54	0.43
2:D:272:GLY:O	2:D:273:ALA:C	2.61	0.43
2:F:75:ARG:HH12	2:F:164:ASN:ND2	2.16	0.43
1:A:270:VAL:HG11	1:A:275:ARG:CG	2.48	0.43
1:A:314:ARG:HD2	1:A:314:ARG:HA	1.84	0.43
2:F:142:LEU:HD23	2:F:143:LYS:N	2.34	0.43
2:F:293:VAL:HG12	1:G:353:GLN:NE2	2.33	0.43
1:G:87:THR:O	1:G:135:ASN:ND2	2.49	0.43
2:H:5:VAL:O	2:H:9:ILE:HG13	2.19	0.43
1:C:68:GLN:O	1:C:71:CYS:HB2	2.19	0.42
1:C:153:LYS:NZ	1:C:185:TRP:O	2.44	0.42
2:F:146:SER:OG	2:F:213:SER:HB2	2.19	0.42
2:F:214:ARG:N	2:F:215:PRO:HD2	2.34	0.42
1:G:337:TYR:N	1:G:337:TYR:CD1	2.88	0.42
2:B:306:LYS:HB2	1:C:329:GLU:OE2	2.19	0.42
1:C:90:ARG:NH1	1:C:90:ARG:HG3	2.34	0.42
1:C:174:GLN:H	1:C:174:GLN:HG3	1.38	0.42
2:D:100:THR:C	2:D:102:TYR:N	2.75	0.42
2:D:156:LEU:HD23	2:D:156:LEU:HA	1.79	0.42
1:E:180:ASN:O	1:E:184:LEU:HB2	2.19	0.42
2:B:156:LEU:HD23	2:B:156:LEU:HA	1.89	0.42
1:C:300:LEU:O	1:C:301:ALA:CB	2.67	0.42
1:E:79:ILE:HG23	1:E:237:THR:CG2	2.50	0.42
1:E:279:GLN:CD	1:E:282:ARG:HD2	2.44	0.42
2:F:272:GLY:O	2:F:273:ALA:C	2.61	0.42
1:G:290:LEU:HD12	1:G:290:LEU:HA	1.96	0.42
1:A:317:ILE:O	1:A:318:GLU:C	2.60	0.42
2:B:325:LYS:HD2	2:B:325:LYS:HA	1.94	0.42
1:E:334:GLU:HG2	1:E:337:TYR:CD2	2.54	0.42
2:F:198:ALA:HA	2:F:238:MET:O	2.19	0.42
2:F:288:LEU:HD12	2:F:288:LEU:HA	1.77	0.42
2:B:10:ASN:HD21	2:B:43:LEU:HD13	1.85	0.42
2:B:112:ILE:HG13	2:B:113:VAL:H	1.84	0.42
1:C:143:PRO:O	1:C:144:LEU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ASP:OD2	1:C:167:ASP:N	2.52	0.42
1:G:133:GLY:HA2	1:G:134:GLY:HA3	1.72	0.42
1:G:352:ASN:OD1	1:G:352:ASN:C	2.62	0.42
4:A:1003:TPP:HN42	4:A:1003:TPP:H2	1.84	0.42
2:D:245:ASP:OD2	2:D:248:THR:OG1	2.32	0.42
2:F:22:LYS:HB3	2:F:75:ARG:HG3	2.01	0.42
2:H:212:HIS:CG	2:H:241:ILE:HD11	2.54	0.42
1:A:333:GLU:H	1:A:333:GLU:HG3	1.61	0.42
1:C:109:LEU:HD23	1:C:109:LEU:HA	1.81	0.42
2:D:112:ILE:HG13	2:D:113:VAL:H	1.81	0.42
2:D:327:LEU:C	2:D:329:ILE:H	2.27	0.42
1:E:29:ARG:NH1	1:E:300:LEU:O	2.53	0.42
2:F:34:ASP:O	2:F:38:LYS:HA	2.20	0.42
1:A:53:TYR:O	1:A:56:LYS:N	2.43	0.42
2:B:139:CYS:HA	2:B:140:PRO:HD2	1.85	0.42
1:C:181:MET:HE1	2:D:58:SER:HB2	2.00	0.42
2:D:3:VAL:HG13	2:D:182:PHE:HB2	2.01	0.42
2:D:81:MET:HB2	2:D:81:MET:HE3	1.71	0.42
1:E:132:TYR:CD1	1:E:132:TYR:N	2.87	0.42
2:F:60:MET:O	2:F:60:MET:HG3	2.19	0.42
2:F:88:GLN:NE2	1:G:172:GLN:HE22	2.07	0.42
1:G:315:LYS:O	1:G:319:ASP:OD2	2.38	0.42
2:B:69:ALA:O	2:B:70:ALA:C	2.63	0.42
1:E:353:GLN:HG2	1:E:354:TRP:CE3	2.55	0.42
2:H:13:MET:O	2:H:14:ASP:C	2.62	0.42
2:D:34:ASP:O	2:D:38:LYS:HA	2.20	0.42
1:G:106:LEU:HD23	1:G:106:LEU:HA	1.71	0.42
2:H:100:THR:O	2:H:101:TYR:C	2.62	0.42
1:A:41:THR:HG21	1:A:96:PHE:CZ	2.55	0.41
2:B:75:ARG:HH12	2:B:164:ASN:HD21	1.62	0.41
2:D:3:VAL:HG13	2:D:182:PHE:CG	2.56	0.41
2:D:24:PHE:CZ	2:D:76:PRO:HB3	2.55	0.41
2:D:97:ALA:HA	2:D:110:VAL:HG11	2.01	0.41
1:G:216:ARG:HD2	1:G:216:ARG:HA	1.90	0.41
1:C:184:LEU:HD12	1:C:184:LEU:HA	1.88	0.41
1:C:334:GLU:O	1:C:335:LEU:C	2.63	0.41
1:E:39:MET:HE2	1:E:291:LEU:HD22	2.03	0.41
1:E:89:TYR:OH	4:E:1009:TPP:O3B	2.35	0.41
1:E:229:ASP:HB3	1:E:232:CYS:HB3	2.03	0.41
1:A:14:LEU:HD21	1:A:20:GLY:HA3	2.02	0.41
1:A:58:ILE:HD11	1:A:109:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:189:LYS:NZ	2:D:189:LYS:HB2	2.34	0.41
1:E:44:ARG:HA	1:E:44:ARG:NE	2.35	0.41
1:E:192:ILE:HA	1:E:253:MET:O	2.20	0.41
1:G:200:MET:CG	1:G:201:GLY:H	2.32	0.41
1:A:184:LEU:HD21	1:C:206:ARG:O	2.21	0.41
1:A:302:SER:C	1:A:304:GLU:H	2.28	0.41
1:A:335:LEU:HD11	2:D:312:SER:OG	2.20	0.41
1:E:292:LYS:HG3	1:E:306:LEU:HD13	2.02	0.41
2:F:31:ALA:HB3	2:F:54:ASP:CG	2.46	0.41
2:F:327:LEU:HD23	2:F:327:LEU:HA	1.86	0.41
1:G:306:LEU:O	1:G:307:LYS:C	2.64	0.41
1:A:58:ILE:CD1	1:A:109:LEU:HB3	2.51	0.41
1:C:142:VAL:HA	1:C:163:THR:CG2	2.51	0.41
1:E:36:TYR:CD2	1:E:36:TYR:C	2.98	0.41
1:E:181:MET:HB3	1:E:185:TRP:CZ3	2.56	0.41
1:G:251:ILE:HG12	1:G:252:LEU:N	2.35	0.41
2:H:1:LEU:H3	2:H:1:LEU:HG	1.72	0.41
1:A:133:GLY:HA2	1:A:134:GLY:HA3	1.77	0.41
1:A:142:VAL:HA	1:A:163:THR:CG2	2.50	0.41
2:B:209:VAL:HA	2:B:260:VAL:O	2.21	0.41
2:B:269:PHE:CE1	2:D:271:VAL:HA	2.55	0.41
2:D:229:GLU:O	2:D:230:GLY:C	2.62	0.41
1:E:39:MET:CE	1:E:291:LEU:HD22	2.50	0.41
1:E:279:GLN:NE2	1:E:282:ARG:HD2	2.36	0.41
2:F:175:MET:SD	2:F:214:ARG:HD2	2.61	0.41
2:F:279:ILE:HD13	2:F:279:ILE:HA	1.76	0.41
1:G:126:MET:HE3	1:G:126:MET:HB2	1.59	0.41
2:H:130:GLN:HB3	2:H:132:PHE:CE1	2.56	0.41
2:H:315:GLN:O	2:H:318:ASP:HB2	2.21	0.41
4:A:1003:TPP:H6'	2:D:28:GLU:OE1	2.20	0.41
1:C:66:ASP:OD2	1:C:260:TYR:HB2	2.20	0.41
2:F:139:CYS:HA	2:F:140:PRO:HD3	1.98	0.41
1:G:46:GLU:HA	1:G:46:GLU:OE1	2.21	0.41
1:G:200:MET:CG	1:G:201:GLY:N	2.83	0.41
2:H:143:LYS:HZ2	2:H:163:ASP:CG	2.28	0.41
1:A:282:ARG:HG3	1:A:282:ARG:HH11	1.85	0.41
2:D:276:CYS:O	2:D:277:ALA:C	2.63	0.41
2:F:226:LEU:HD13	2:F:323:ILE:HG21	2.03	0.41
1:G:45:MET:HG3	1:G:102:VAL:HG13	2.03	0.41
1:G:192:ILE:HG12	1:G:253:MET:HE2	2.01	0.41
1:A:68:GLN:HE22	1:A:196:ASN:HD22	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:ASP:OD1	2:B:20:ASP:C	2.63	0.41
2:B:128:HIS:ND1	1:C:124:MET:HE1	2.36	0.41
1:E:225:VAL:HG21	1:E:236:ALA:HB1	2.03	0.41
1:E:341:SER:N	2:F:165:ASN:HD21	2.09	0.41
2:H:137:GLY:O	2:H:242:ARG:HD2	2.20	0.41
1:C:70:ALA:HB2	1:C:287:PRO:HB3	2.03	0.41
2:F:321:PHE:CE2	2:F:325:LYS:HE3	2.56	0.41
2:H:226:LEU:HD23	2:H:226:LEU:HA	1.84	0.41
1:A:313:VAL:O	1:A:314:ARG:C	2.62	0.40
1:C:57:ILE:HG21	1:C:325:THR:HG22	2.02	0.40
1:C:348:VAL:HG23	1:C:357:PHE:O	2.21	0.40
1:E:224:ARG:HD2	1:E:256:GLN:CD	2.44	0.40
2:H:316:VAL:C	2:H:318:ASP:H	2.28	0.40
1:A:249:GLY:HA3	1:A:250:PRO:HD2	1.69	0.40
2:B:65:ILE:HG21	2:B:65:ILE:HD13	1.81	0.40
1:C:133:GLY:HA3	1:C:134:GLY:HA3	1.87	0.40
1:C:315:LYS:HZ3	1:C:315:LYS:HG3	1.58	0.40
2:D:280:MET:HE2	2:D:285:PHE:CE1	2.56	0.40
1:G:95:THR:HB	1:G:100:LEU:HD22	2.04	0.40
1:A:84:HIS:CE1	1:A:130:ASN:ND2	2.90	0.40
1:A:89:TYR:HB2	1:A:124:MET:HG2	2.02	0.40
1:C:203:ALA:O	1:C:204:VAL:C	2.65	0.40
2:D:254:MET:HE2	2:D:284:ALA:CA	2.51	0.40
1:A:58:ILE:HG22	1:A:59:ARG:N	2.35	0.40
1:E:85:LEU:HD23	1:E:131:PHE:CE1	2.56	0.40
2:H:313:ILE:HD13	2:H:313:ILE:C	2.47	0.40
1:A:75:LEU:HD13	1:A:233:VAL:CG1	2.52	0.40
1:C:165:TYR:CD1	1:C:165:TYR:N	2.88	0.40
2:F:29:GLU:OE1	2:F:29:GLU:HA	2.19	0.40
1:G:55:GLN:O	1:G:56:LYS:C	2.64	0.40
2:H:315:GLN:H	2:H:315:GLN:HG2	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	360/382 (94%)	321 (89%)	32 (9%)	7 (2%)	6 31
1	C	361/382 (94%)	322 (89%)	31 (9%)	8 (2%)	5 27
1	E	361/382 (94%)	333 (92%)	19 (5%)	9 (2%)	4 24
1	G	360/382 (94%)	318 (88%)	35 (10%)	7 (2%)	6 31
2	B	327/329 (99%)	297 (91%)	26 (8%)	4 (1%)	11 41
2	D	327/329 (99%)	277 (85%)	41 (12%)	9 (3%)	4 21
2	F	327/329 (99%)	287 (88%)	37 (11%)	3 (1%)	14 49
2	H	327/329 (99%)	295 (90%)	28 (9%)	4 (1%)	11 41
All	All	2750/2844 (97%)	2450 (89%)	249 (9%)	51 (2%)	6 31

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	18	GLU
1	C	88	ALA
1	C	204	VAL
2	D	207	ILE
2	D	328	ASN
1	E	156	GLY
2	H	21	GLU
1	A	204	VAL
1	A	263	HIS
1	C	66	ASP
1	C	262	GLY
1	C	265	MET
2	D	239	ARG
1	E	88	ALA
1	E	262	GLY
1	E	264	SER
1	E	265	MET
1	G	56	LYS
1	G	204	VAL
1	G	226	ASP
1	A	218	ASP
1	A	342	SER
1	C	218	ASP
2	D	38	LYS

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Mol	Chain	Res	Type
2	D	159	SER
1	G	218	ASP
2	H	267	PRO
1	A	71	CYS
1	A	200	MET
2	B	31	ALA
2	B	239	ARG
2	B	243	PRO
2	D	97	ALA
2	D	158	LYS
1	E	129	LYS
1	E	188	PRO
1	E	285	SER
2	F	74	LEU
1	G	55	GLN
2	H	306	LYS
1	C	205	GLU
2	D	134	ALA
1	A	188	PRO
1	G	88	ALA
1	G	230	ILE
2	B	267	PRO
2	F	267	PRO
2	H	243	PRO
1	E	230	ILE
2	D	267	PRO
2	F	265	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	292/310 (94%)	258 (88%)	34 (12%)	4 20
1	C	294/310 (95%)	246 (84%)	48 (16%)	2 9
1	E	294/310 (95%)	258 (88%)	36 (12%)	4 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	292/310 (94%)	244 (84%)	48 (16%)	2 9
2	B	268/268 (100%)	229 (85%)	39 (15%)	2 12
2	D	268/268 (100%)	234 (87%)	34 (13%)	3 17
2	F	268/268 (100%)	240 (90%)	28 (10%)	5 23
2	H	268/268 (100%)	236 (88%)	32 (12%)	4 19
All	All	2244/2312 (97%)	1945 (87%)	299 (13%)	3 15

All (299) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	17	LEU
1	A	23	VAL
1	A	27	LEU
1	A	30	GLU
1	A	33	LEU
1	A	50	ASP
1	A	66	ASP
1	A	75	LEU
1	A	100	LEU
1	A	103	ARG
1	A	109	LEU
1	A	126	MET
1	A	174	GLN
1	A	175	ILE
1	A	210	SER
1	A	255	LEU
1	A	266	SER
1	A	274	THR
1	A	275	ARG
1	A	280	GLU
1	A	289	MET
1	A	307	LYS
1	A	308	GLU
1	A	315	LYS
1	A	316	GLU
1	A	317	ILE
1	A	318	GLU
1	A	322	GLN
1	A	323	PHE

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Mol	Chain	Res	Type
1	A	325	THR
1	A	333	GLU
1	A	342	SER
1	A	348	VAL
2	B	1	LEU
2	B	3	VAL
2	B	17	LEU
2	B	26	LEU
2	B	28	GLU
2	B	30	VAL
2	B	33	TYR
2	B	39	VAL
2	B	43	LEU
2	B	50	LYS
2	B	55	THR
2	B	74	LEU
2	B	79	GLU
2	B	99	LYS
2	B	100	THR
2	B	112	ILE
2	B	121	SER
2	B	146	SER
2	B	161	ILE
2	B	162	ARG
2	B	170	LEU
2	B	172	ASN
2	B	188	SER
2	B	189	LYS
2	B	192	LEU
2	B	205	THR
2	B	209	VAL
2	B	211	SER
2	B	214	ARG
2	B	227	SER
2	B	237	ASN
2	B	244	MET
2	B	257	ASN
2	B	261	THR
2	B	268	GLN
2	B	279	ILE
2	B	306	LYS
2	B	313	ILE

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Mol	Chain	Res	Type
2	B	317	LYS
1	C	8	GLU
1	C	9	ILE
1	C	11	LYS
1	C	18	GLU
1	C	23	VAL
1	C	24	THR
1	C	25	THR
1	C	27	LEU
1	C	33	LEU
1	C	46	GLU
1	C	56	LYS
1	C	57	ILE
1	C	64	LEU
1	C	95	THR
1	C	98	ARG
1	C	100	LEU
1	C	113	LYS
1	C	118	LYS
1	C	123	SER
1	C	144	LEU
1	C	157	LYS
1	C	158	ASP
1	C	174	GLN
1	C	216	ARG
1	C	218	ASP
1	C	223	LEU
1	C	252	LEU
1	C	255	LEU
1	C	264	SER
1	C	273	ARG
1	C	276	GLU
1	C	279	GLN
1	C	280	GLU
1	C	283	SER
1	C	285	SER
1	C	288	ILE
1	C	289	MET
1	C	300	LEU
1	C	303	VAL
1	C	304	GLU
1	C	313	VAL

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Mol	Chain	Res	Type
1	C	314	ARG
1	C	315	LYS
1	C	317	ILE
1	C	319	ASP
1	C	347	GLU
1	C	348	VAL
1	C	356	LYS
2	D	1	LEU
2	D	3	VAL
2	D	7	ASP
2	D	21	GLU
2	D	30	VAL
2	D	43	LEU
2	D	45	LYS
2	D	50	LYS
2	D	65	ILE
2	D	74	LEU
2	D	79	GLU
2	D	81	MET
2	D	94	ILE
2	D	107	LEU
2	D	112	ILE
2	D	139	CYS
2	D	142	LEU
2	D	154	LYS
2	D	157	ILE
2	D	159	SER
2	D	162	ARG
2	D	185	GLU
2	D	188	SER
2	D	192	LEU
2	D	197	LYS
2	D	210	VAL
2	D	211	SER
2	D	227	SER
2	D	229	GLU
2	D	237	ASN
2	D	278	ARG
2	D	306	LYS
2	D	313	ILE
2	D	329	ILE
1	E	0	MET

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Mol	Chain	Res	Type
1	E	6	THR
1	E	23	VAL
1	E	27	LEU
1	E	33	LEU
1	E	46	GLU
1	E	56	LYS
1	E	57	ILE
1	E	75	LEU
1	E	80	ASN
1	E	95	THR
1	E	98	ARG
1	E	104	GLU
1	E	109	LEU
1	E	113	LYS
1	E	118	LYS
1	E	143	PRO
1	E	223	LEU
1	E	230	ILE
1	E	252	LEU
1	E	253	MET
1	E	275	ARG
1	E	276	GLU
1	E	279	GLN
1	E	284	LYS
1	E	289	MET
1	E	303	VAL
1	E	307	LYS
1	E	314	ARG
1	E	322	GLN
1	E	333	GLU
1	E	335	LEU
1	E	348	VAL
1	E	356	LYS
1	E	360	VAL
1	E	361	SER
2	F	3	VAL
2	F	13	MET
2	F	19	ARG
2	F	21	GLU
2	F	32	GLN
2	F	74	LEU
2	F	100	THR

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Mol	Chain	Res	Type
2	F	103	MET
2	F	112	ILE
2	F	121	SER
2	F	129	SER
2	F	162	ARG
2	F	169	VAL
2	F	172	ASN
2	F	192	LEU
2	F	214	ARG
2	F	229	GLU
2	F	237	ASN
2	F	263	GLU
2	F	268	GLN
2	F	279	ILE
2	F	280	MET
2	F	306	LYS
2	F	311	ASN
2	F	313	ILE
2	F	315	GLN
2	F	323	ILE
2	F	325	LYS
1	G	8	GLU
1	G	11	LYS
1	G	23	VAL
1	G	24	THR
1	G	27	LEU
1	G	47	LEU
1	G	48	LYS
1	G	55	GLN
1	G	56	LYS
1	G	57	ILE
1	G	64	LEU
1	G	75	LEU
1	G	85	LEU
1	G	98	ARG
1	G	100	LEU
1	G	105	ILE
1	G	113	LYS
1	G	126	MET
1	G	148	ILE
1	G	157	LYS
1	G	205	GLU

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Mol	Chain	Res	Type
1	G	206	ARG
1	G	210	SER
1	G	215	LYS
1	G	229	ASP
1	G	230	ILE
1	G	235	GLU
1	G	238	ARG
1	G	245	ARG
1	G	251	ILE
1	G	252	LEU
1	G	255	LEU
1	G	275	ARG
1	G	276	GLU
1	G	278	ILE
1	G	279	GLN
1	G	284	LYS
1	G	290	LEU
1	G	300	LEU
1	G	305	GLU
1	G	311	VAL
1	G	314	ARG
1	G	315	LYS
1	G	316	GLU
1	G	319	ASP
1	G	346	PHE
1	G	356	LYS
1	G	358	LYS
2	H	1	LEU
2	H	3	VAL
2	H	13	MET
2	H	30	VAL
2	H	33	TYR
2	H	43	LEU
2	H	52	ILE
2	H	65	ILE
2	H	74	LEU
2	H	79	GLU
2	H	90	ILE
2	H	96	SER
2	H	107	LEU
2	H	108	GLN
2	H	112	ILE

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Mol	Chain	Res	Type
2	H	129	SER
2	H	139	CYS
2	H	157	ILE
2	H	162	ARG
2	H	185	GLU
2	H	189	LYS
2	H	197	LYS
2	H	203	GLN
2	H	220	LEU
2	H	268	GLN
2	H	279	ILE
2	H	288	LEU
2	H	306	LYS
2	H	313	ILE
2	H	315	GLN
2	H	317	LYS
2	H	326	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	55	GLN
1	A	68	GLN
1	A	84	HIS
1	A	92	HIS
1	A	125	HIS
1	A	130	ASN
1	A	279	GLN
1	A	353	GLN
2	B	10	ASN
2	B	32	GLN
2	B	88	GLN
2	B	118	ASN
2	B	164	ASN
2	B	172	ASN
2	B	237	ASN
2	B	257	ASN
2	B	328	ASN
1	C	-1	HIS
1	C	3	ASN
1	C	40	GLN

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Mol	Chain	Res	Type
1	C	51	GLN
1	C	55	GLN
1	C	63	HIS
1	C	68	GLN
1	C	84	HIS
1	C	92	HIS
1	C	125	HIS
1	C	155	ASN
1	C	174	GLN
1	C	263	HIS
1	C	353	GLN
2	D	88	GLN
2	D	128	HIS
2	D	172	ASN
2	D	237	ASN
1	E	15	HIS
1	E	55	GLN
1	E	63	HIS
1	E	68	GLN
1	E	80	ASN
1	E	130	ASN
1	E	135	ASN
1	E	172	GLN
1	E	261	HIS
1	E	279	GLN
1	E	297	ASN
2	F	10	ASN
2	F	32	GLN
2	F	92	GLN
2	F	128	HIS
2	F	164	ASN
2	F	165	ASN
2	F	172	ASN
2	F	206	HIS
2	F	237	ASN
2	F	311	ASN
1	G	40	GLN
1	G	51	GLN
1	G	55	GLN
1	G	63	HIS
1	G	68	GLN
1	G	80	ASN

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Mol	Chain	Res	Type
1	G	125	HIS
1	G	172	GLN
1	G	263	HIS
1	G	322	GLN
1	G	353	GLN
2	H	2	GLN
2	H	11	GLN
2	H	88	GLN
2	H	108	GLN
2	H	203	GLN
2	H	237	ASN
2	H	315	GLN
2	H	328	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	TPP	A	1003	3	23,27,27	1.48	5 (21%)	30,40,40	2.08	10 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	TPP	E	1009	3	23,27,27	1.50	5 (21%)	30,40,40	2.08	11 (36%)
4	TPP	G	1012	3	23,27,27	1.70	4 (17%)	30,40,40	2.02	13 (43%)
4	TPP	C	1006	3	23,27,27	1.29	2 (8%)	30,40,40	2.11	11 (36%)

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
4	TPP	A	1003	3	-	1/16/17/17	0/2/2/2
4	TPP	E	1009	3	-	6/16/17/17	0/2/2/2
4	TPP	G	1012	3	-	0/16/17/17	0/2/2/2
4	TPP	C	1006	3	-	4/16/17/17	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1012	TPP	C6-C5	5.67	1.54	1.51
4	A	1003	TPP	C4-N3	-3.86	1.36	1.39
4	C	1006	TPP	C2'-N1'	3.06	1.39	1.34
4	E	1009	TPP	C6-C5	3.02	1.52	1.51
4	E	1009	TPP	C2'-N3'	3.00	1.39	1.34
4	E	1009	TPP	C2'-N1'	2.75	1.38	1.34
4	G	1012	TPP	C2'-N3'	2.62	1.38	1.34
4	A	1003	TPP	C2'-N1'	2.61	1.38	1.34
4	E	1009	TPP	C4'-N3'	2.46	1.38	1.35
4	C	1006	TPP	C4'-N3'	2.41	1.38	1.35
4	G	1012	TPP	C2'-N1'	2.38	1.38	1.34
4	G	1012	TPP	C7'-N3	-2.37	1.44	1.48
4	A	1003	TPP	C4'-N3'	2.27	1.38	1.35
4	A	1003	TPP	C7'-N3	-2.25	1.44	1.48
4	A	1003	TPP	PA-O3A	2.05	1.61	1.59
4	E	1009	TPP	C6'-N1'	2.02	1.38	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1009	TPP	CM4-C4-N3	5.11	129.05	122.53
4	A	1003	TPP	C5'-C7'-N3	-4.99	104.96	113.28
4	A	1003	TPP	C6'-C5'-C4'	4.70	121.33	115.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1006	TPP	C5'-C7'-N3	-4.24	106.22	113.28
4	C	1006	TPP	C6'-N1'-C2'	4.19	122.95	116.07
4	C	1006	TPP	CM4-C4-N3	4.13	127.79	122.53
4	G	1012	TPP	C7'-N3-C2	-3.98	118.16	125.35
4	G	1012	TPP	C6'-C5'-C4'	3.83	120.25	115.55
4	C	1006	TPP	N1'-C2'-N3'	-3.68	119.40	125.53
4	G	1012	TPP	C7'-C5'-C6'	-3.57	113.96	120.69
4	E	1009	TPP	N1'-C2'-N3'	-3.52	119.67	125.53
4	E	1009	TPP	C6'-C5'-C4'	3.50	119.85	115.55
4	G	1012	TPP	O3A-PA-O1A	-3.36	100.59	110.70
4	E	1009	TPP	C5'-C7'-N3	-3.36	107.69	113.28
4	C	1006	TPP	C5'-C6'-N1'	-3.30	118.47	123.83
4	G	1012	TPP	CM4-C4-N3	3.23	126.65	122.53
4	A	1003	TPP	C5'-C6'-N1'	-3.16	118.69	123.83
4	G	1012	TPP	C5'-C7'-N3	-3.15	108.03	113.28
4	E	1009	TPP	CM4-C4-C5	-3.12	120.77	127.60
4	C	1006	TPP	CM2-C2'-N1'	3.10	120.50	117.20
4	E	1009	TPP	C6'-N1'-C2'	3.08	121.13	116.07
4	A	1003	TPP	CM4-C4-N3	3.04	126.41	122.53
4	A	1003	TPP	O2A-PA-O3A	2.91	115.13	107.27
4	C	1006	TPP	C7'-N3-C2	-2.90	120.11	125.35
4	A	1003	TPP	CM2-C2'-N1'	2.82	120.20	117.20
4	E	1009	TPP	C7'-N3-C2	-2.82	120.26	125.35
4	E	1009	TPP	C5'-C6'-N1'	-2.81	119.26	123.83
4	A	1003	TPP	O3A-PA-O1A	-2.81	102.26	110.70
4	E	1009	TPP	CM2-C2'-N1'	2.77	120.14	117.20
4	C	1006	TPP	C7'-C5'-C6'	-2.68	115.64	120.69
4	G	1012	TPP	C5'-C6'-N1'	-2.59	119.62	123.83
4	A	1003	TPP	C6'-N1'-C2'	2.46	120.11	116.07
4	C	1006	TPP	C6'-C5'-C4'	2.31	118.38	115.55
4	G	1012	TPP	C5'-C4'-N4'	2.27	125.20	122.14
4	A	1003	TPP	C7'-C5'-C6'	-2.25	116.46	120.69
4	G	1012	TPP	C6'-N1'-C2'	2.18	119.65	116.07
4	G	1012	TPP	C6-C5-C4	2.17	133.81	127.05
4	G	1012	TPP	CM2-C2'-N3'	2.14	120.34	117.13
4	C	1006	TPP	CM4-C4-C5	-2.12	122.97	127.60
4	A	1003	TPP	O3B-PB-O3A	2.08	111.61	104.64
4	G	1012	TPP	N1'-C2'-N3'	-2.06	122.10	125.53
4	G	1012	TPP	CM4-C4-C5	-2.04	123.14	127.60
4	E	1009	TPP	CM2-C2'-N3'	2.03	120.16	117.13
4	C	1006	TPP	N4'-C4'-N3'	-2.00	114.33	117.03
4	E	1009	TPP	O2B-PB-O3A	2.00	111.35	104.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1009	TPP	C5-C6-C7-O7
4	E	1009	TPP	C7-O7-PA-O1A
4	E	1009	TPP	C7-O7-PA-O3A
4	C	1006	TPP	C4-C5-C6-C7
4	E	1009	TPP	C4-C5-C6-C7
4	C	1006	TPP	C7-O7-PA-O1A
4	E	1009	TPP	C7-O7-PA-O2A
4	C	1006	TPP	PB-O3A-PA-O2A
4	A	1003	TPP	C5-C6-C7-O7
4	E	1009	TPP	PA-O3A-PB-O2B
4	C	1006	TPP	PB-O3A-PA-O1A

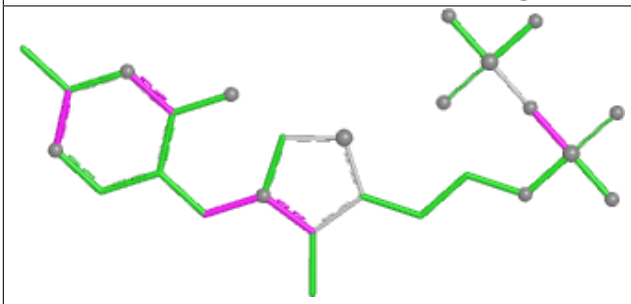
There are no ring outliers.

4 monomers are involved in 7 short contacts:

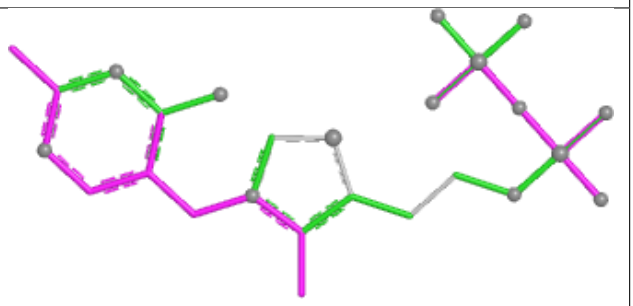
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	TPP	2	0
4	E	1009	TPP	2	0
4	G	1012	TPP	2	0
4	C	1006	TPP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

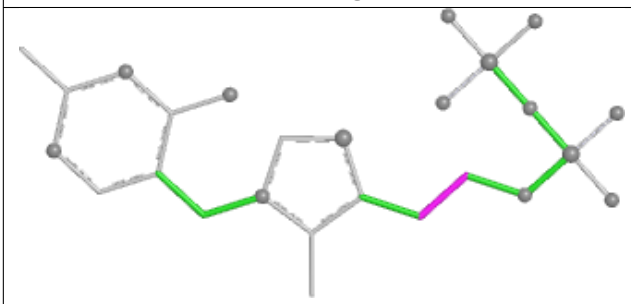
Ligand TPP A 1003



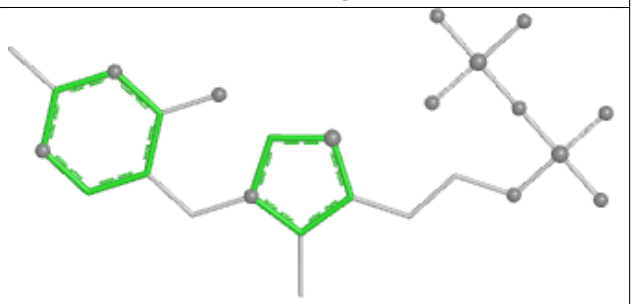
Bond lengths



Bond angles

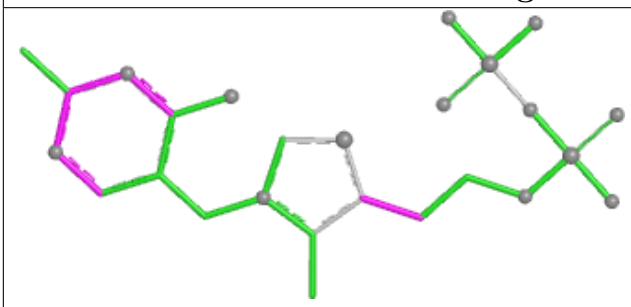


Torsions

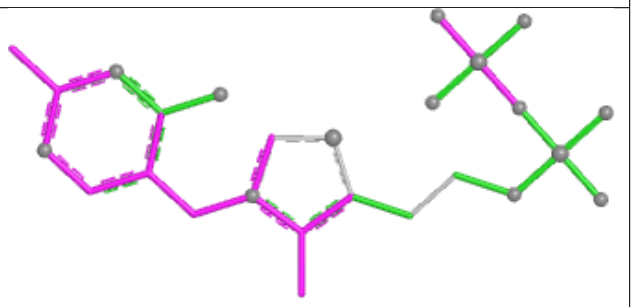


Rings

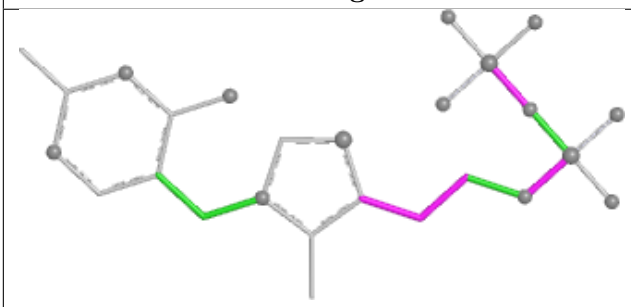
Ligand TPP E 1009



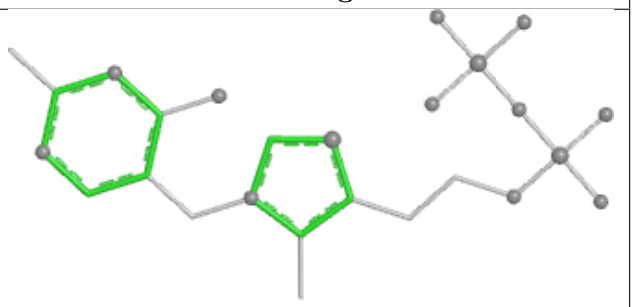
Bond lengths



Bond angles

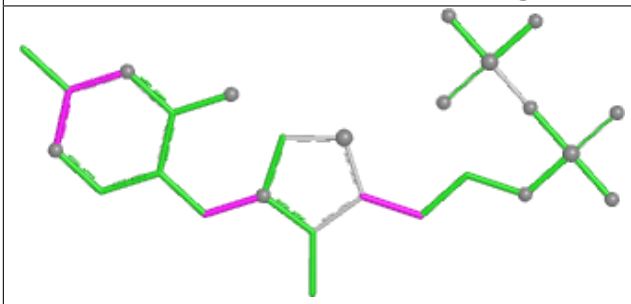


Torsions

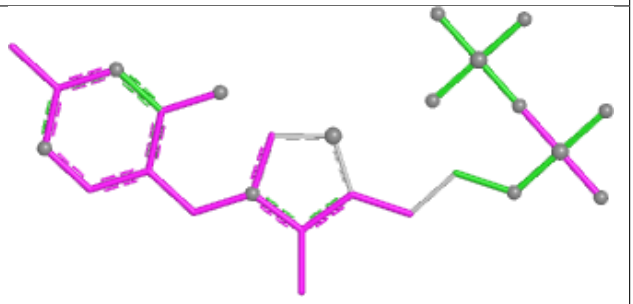


Rings

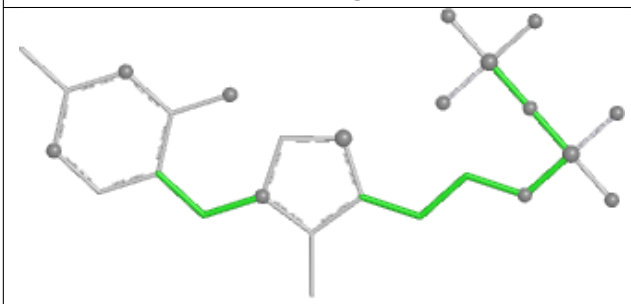
Ligand TPP G 1012



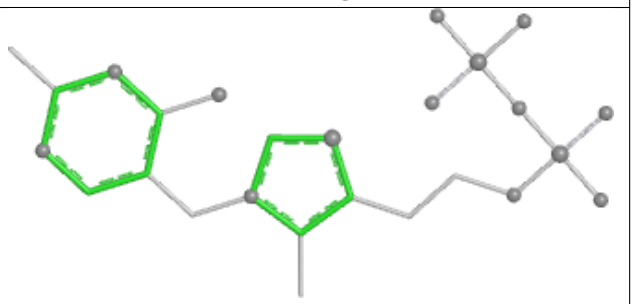
Bond lengths



Bond angles

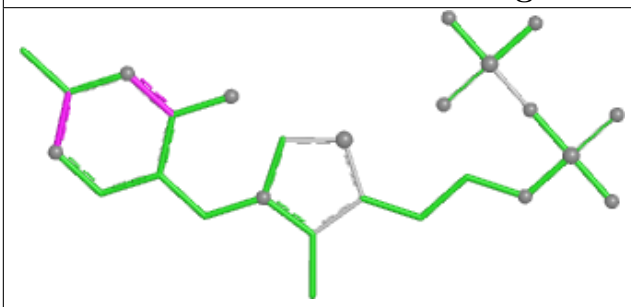


Torsions

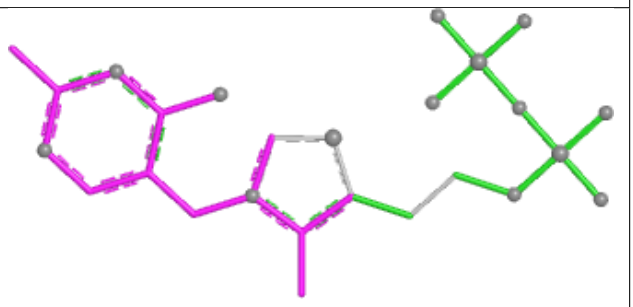


Rings

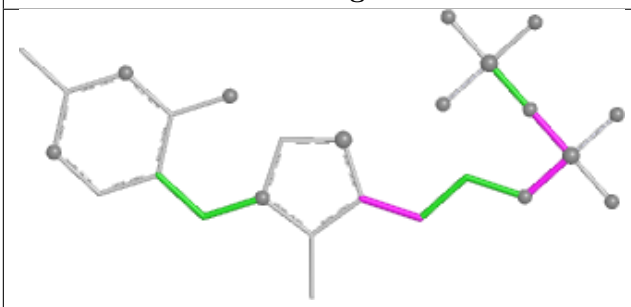
Ligand TPP C 1006



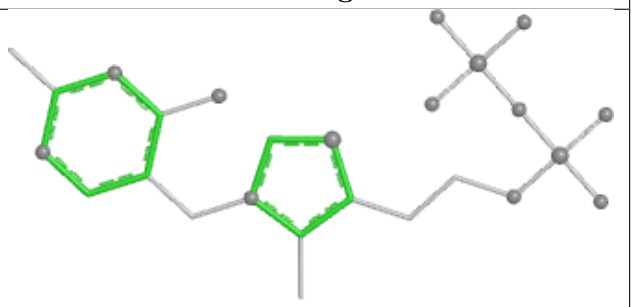
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	362/382 (94%)	-1.96	0	100	100	8, 21, 37, 52	0
1	C	363/382 (95%)	-1.97	0	100	100	10, 20, 40, 54	0
1	E	363/382 (95%)	-1.95	0	100	100	10, 21, 41, 54	0
1	G	362/382 (94%)	-1.96	0	100	100	9, 20, 39, 53	0
2	B	329/329 (100%)	-1.99	0	100	100	8, 19, 29, 38	0
2	D	329/329 (100%)	-2.00	0	100	100	12, 20, 30, 41	0
2	F	329/329 (100%)	-1.98	0	100	100	10, 20, 29, 40	0
2	H	329/329 (100%)	-1.99	0	100	100	7, 19, 28, 42	0
All	All	2766/2844 (97%)	-1.97	0	100	100	7, 20, 33, 54	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

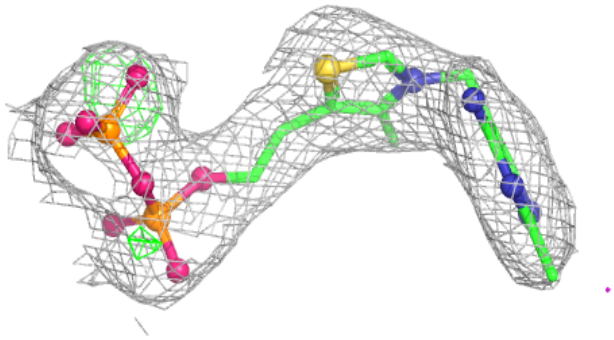
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

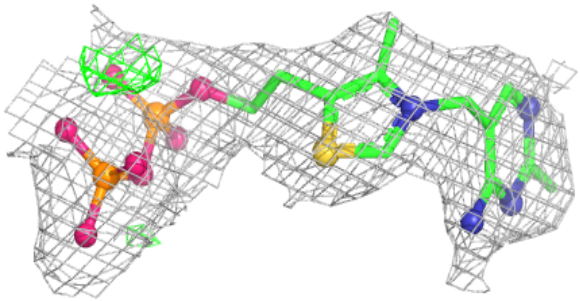
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	K	F	1011	1/1	0.98	0.05	66,66,66,66	0
5	K	D	1002	1/1	0.99	0.03	50,50,50,50	0
5	K	H	1008	1/1	0.99	0.04	36,36,36,36	0
3	MG	G	1010	1/1	1.00	0.02	11,11,11,11	0
4	TPP	A	1003	26/26	1.00	0.02	16,21,29,33	0
4	TPP	C	1006	26/26	1.00	0.02	15,22,34,40	0
4	TPP	E	1009	26/26	1.00	0.02	18,27,37,40	0
4	TPP	G	1012	26/26	1.00	0.02	17,23,35,41	0
5	K	B	1005	1/1	1.00	0.02	37,37,37,37	0
3	MG	A	1001	1/1	1.00	0.03	6,6,6,6	0
3	MG	C	1004	1/1	1.00	0.01	22,22,22,22	0
3	MG	E	1007	1/1	1.00	0.02	30,30,30,30	0

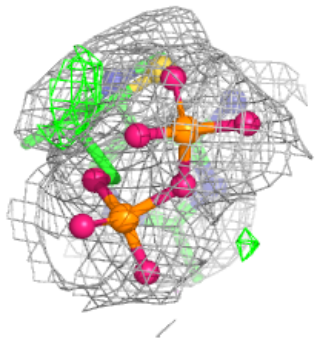
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TPP A 1003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

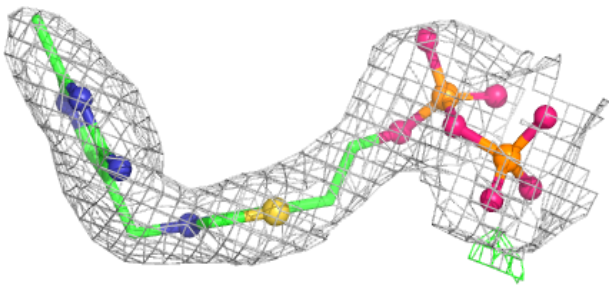


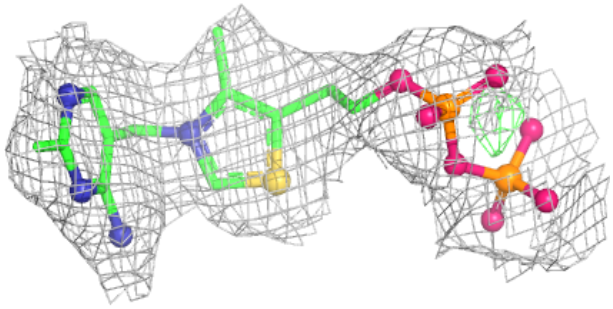


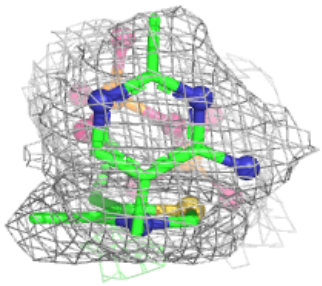


Electron density around TPP C 1006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

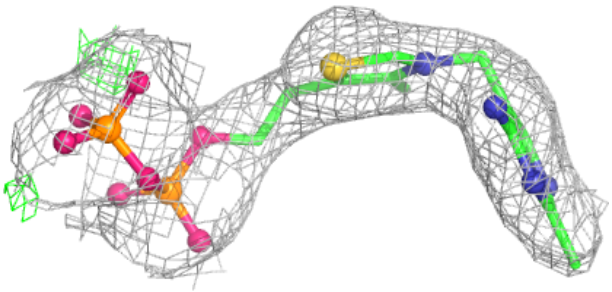


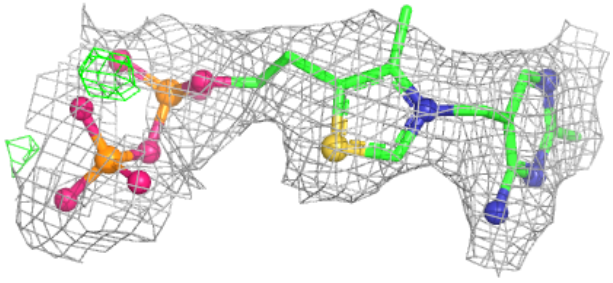


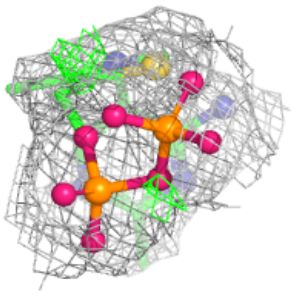


Electron density around TPP E 1009:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

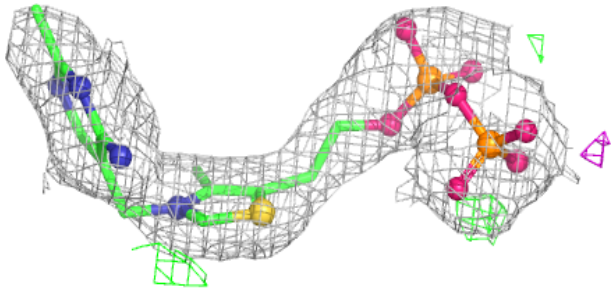


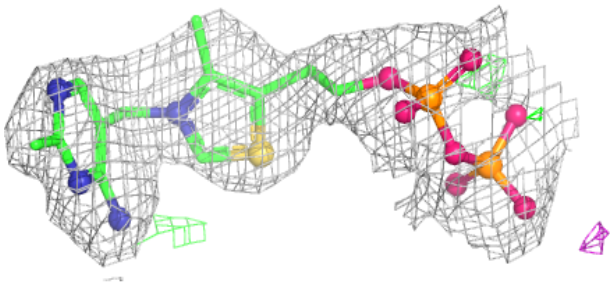


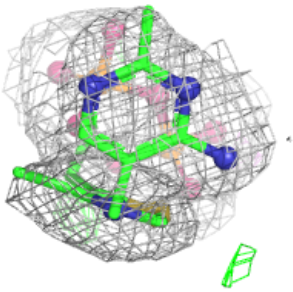


Electron density around TPP G 1012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers

There are no such residues in this entry.