Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:31 AM GMT

PDB ID	:	3EXF
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
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:

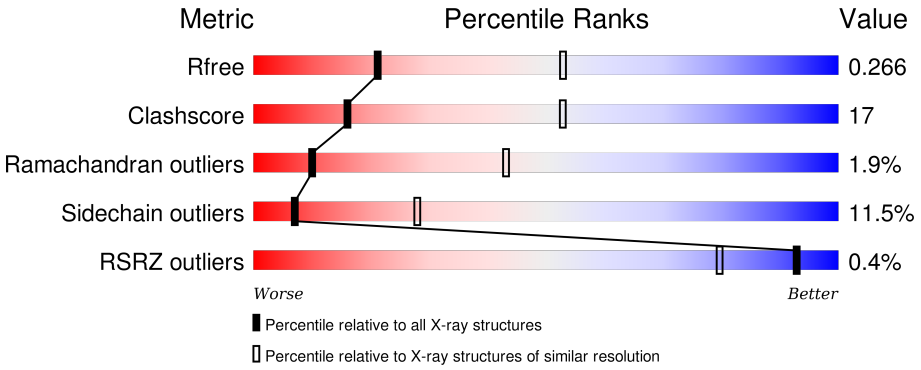
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 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	382	52% 38% • 5%
1	C	382	58% 29% 8% • 5%
1	E	382	60% 30% 5% 5%
1	G	382	% 65% 25% • • 5%
2	B	329	61% 33% 6%

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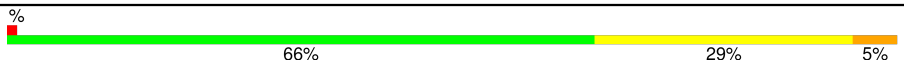
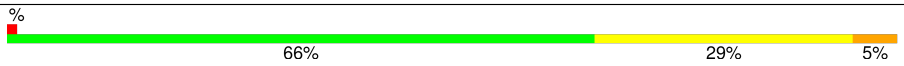
Mol	Chain	Length	Quality of chain
2	D	329	
2	F	329	
2	H	329	

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	UNP P08559
A	271	ALA	SER	ENGINEERED	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	UNP P08559
C	271	ALA	SER	ENGINEERED	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	UNP P08559
E	271	ALA	SER	ENGINEERED	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	UNP P08559
G	271	ALA	SER	ENGINEERED	UNP P08559

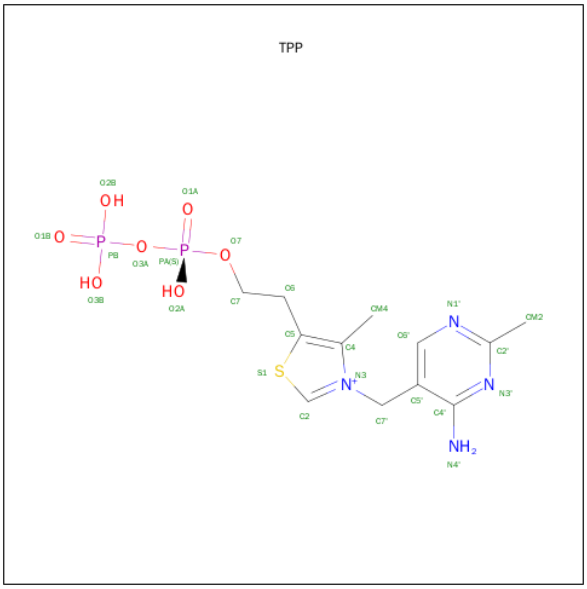
- Molecule 2 is a protein called Pyruvate dehydrogenase E1 component subunit beta, mitochondrial.

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is THIAMINE DIPHOSPHATE (three-letter code: 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 (three-letter code: K) (formula: K).

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

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

- Molecule 6 is water.

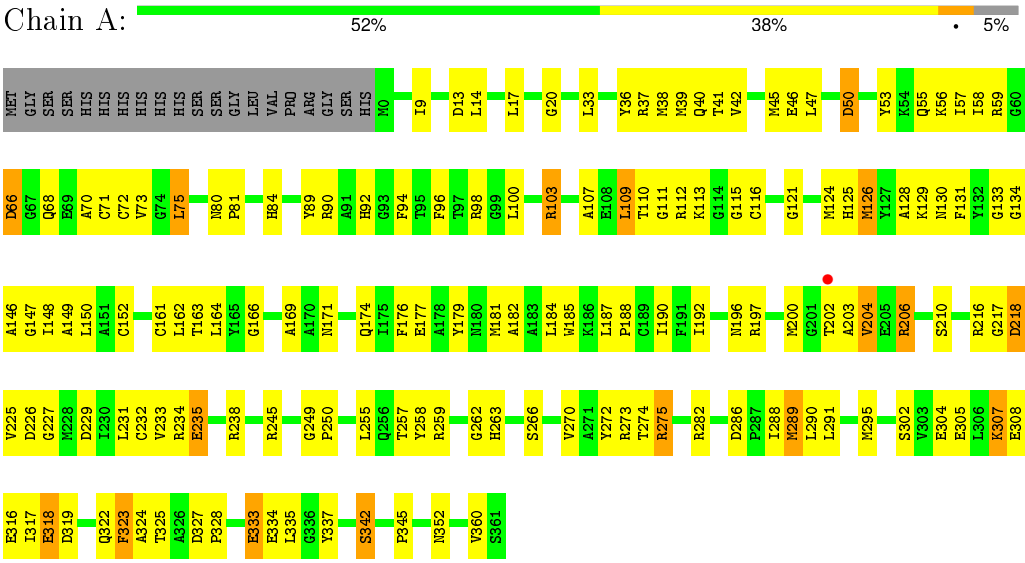
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O 1 1	0	0
6	C	3	Total O 3 3	0	0
6	D	1	Total O 1 1	0	0
6	E	1	Total O 1 1	0	0
6	F	2	Total O 2 2	0	0
6	H	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

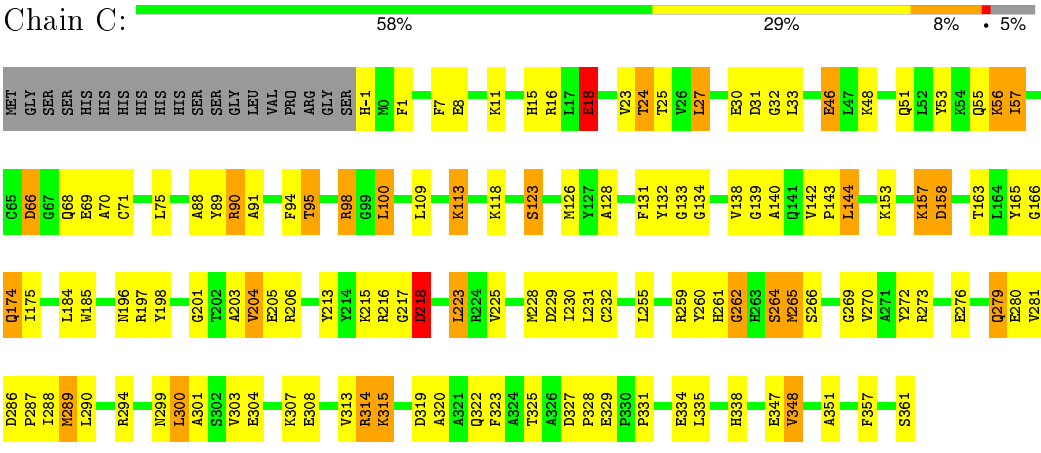
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain A:



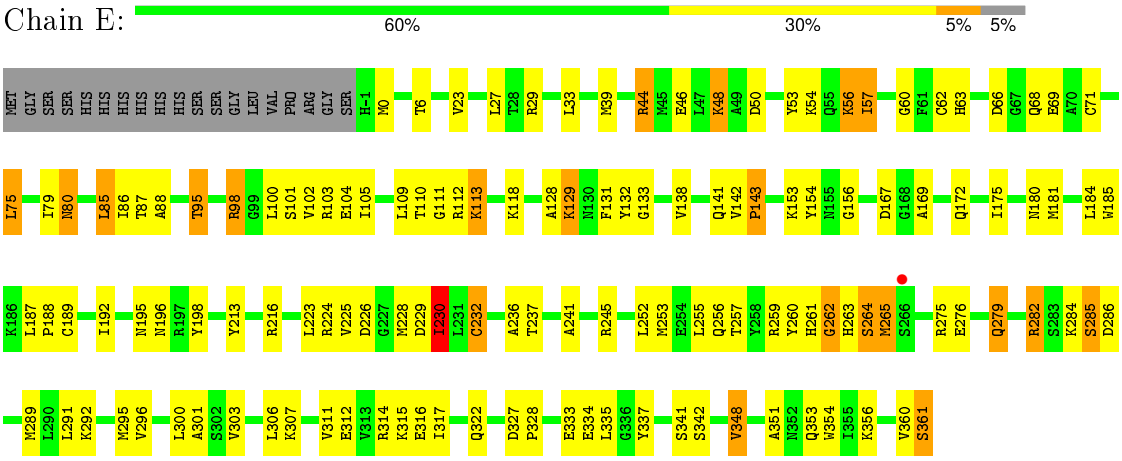
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain C:



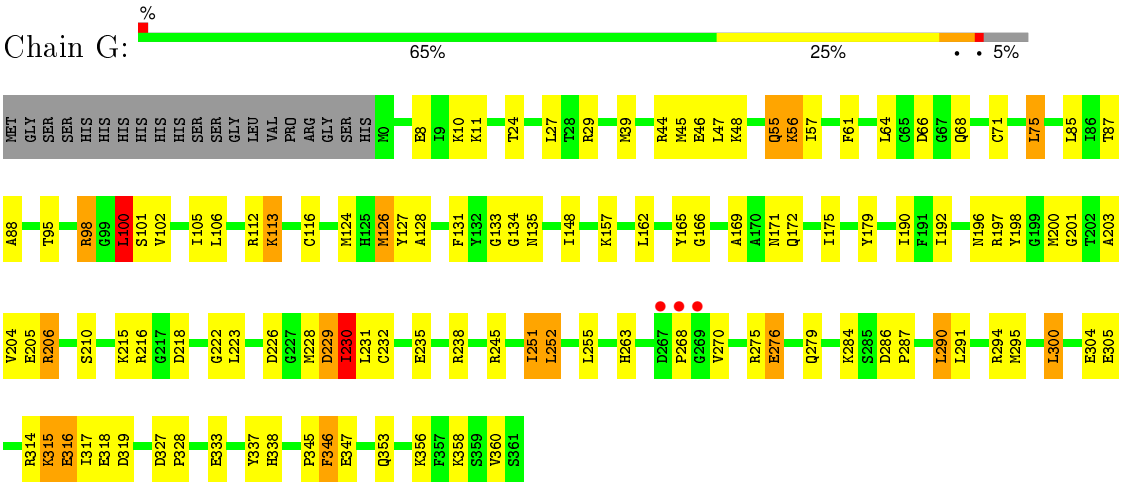
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain E:



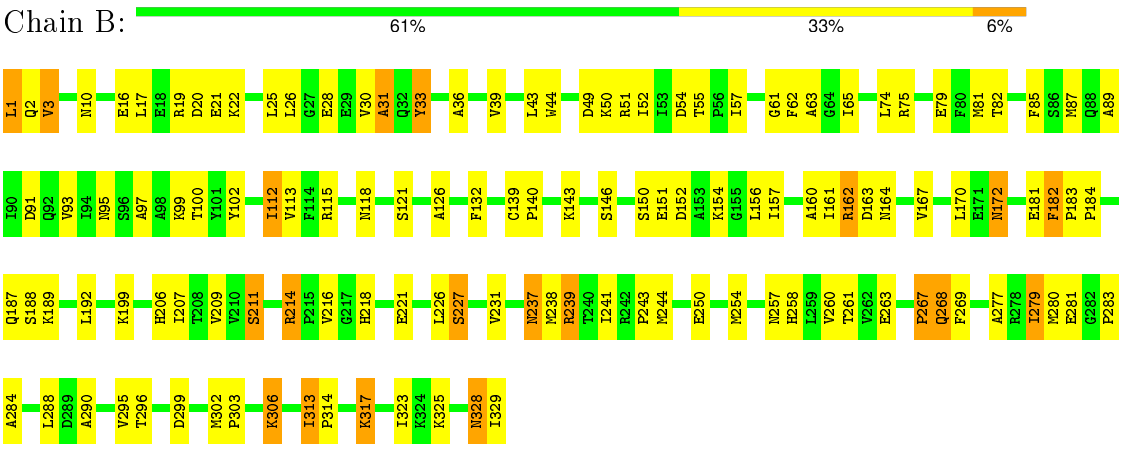
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain G:



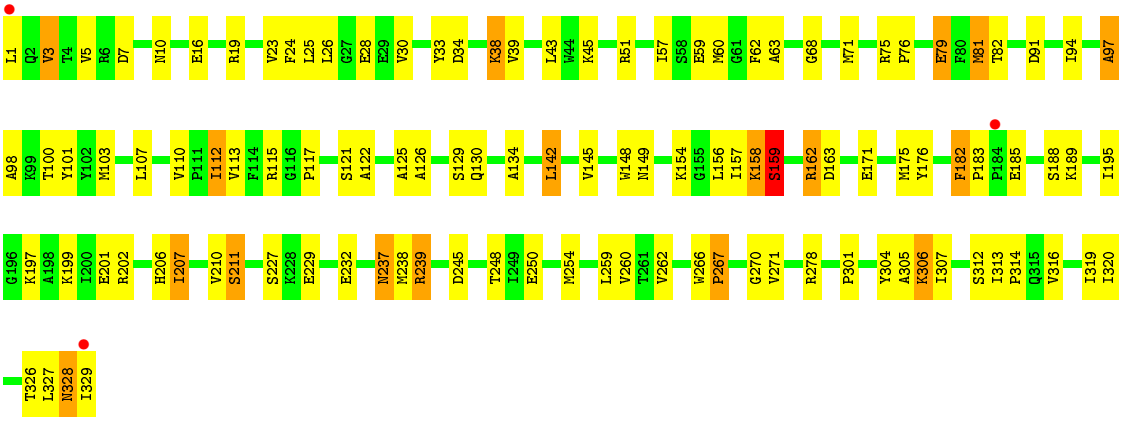
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain B:

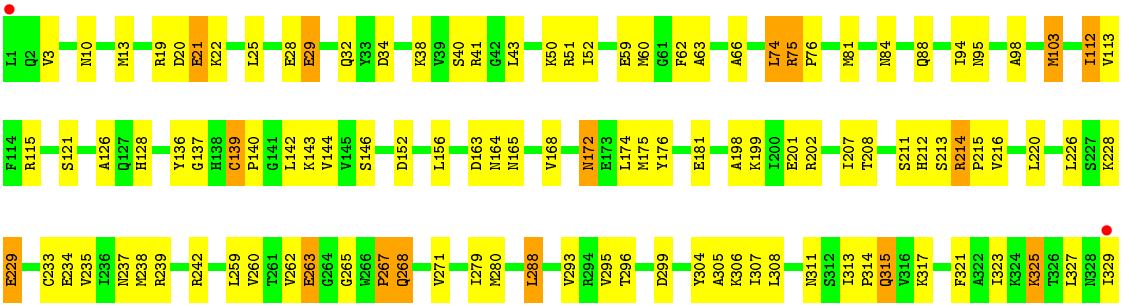


• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

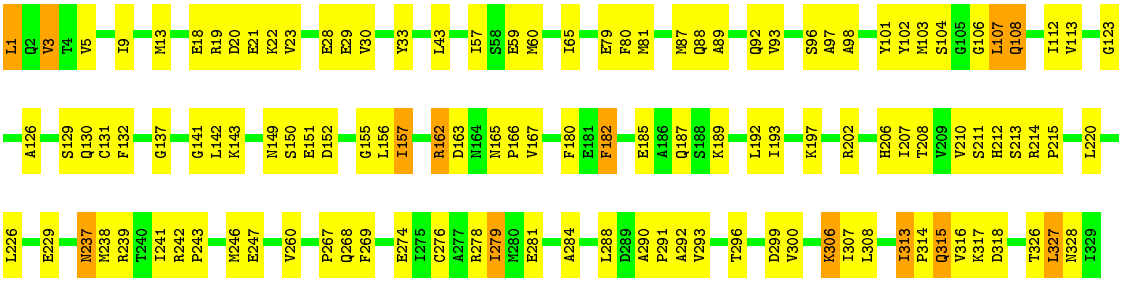
Chain D:



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



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



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 48.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-3.00) 99.4 (48.00-3.00)	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	Depositor
R, R_{free}	0.185 , 0.263 0.190 , 0.266	Depositor DCC
R_{free} test set	3624 reflections (5.29%)	DCC
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 , 1.1	EDS
Estimated twinning fraction	0.117 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 72119 reflections	Xtriage
F_o,F_c correlation	0.91	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, 0.375 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: K, MG, TPP

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	0.96	6/2877 (0.2%)	0.96	3/3875 (0.1%)
1	C	0.97	4/2891 (0.1%)	1.00	4/3893 (0.1%)
1	E	0.95	1/2891 (0.0%)	0.99	3/3893 (0.1%)
1	G	0.98	5/2877 (0.2%)	0.97	3/3875 (0.1%)
2	B	0.94	0/2574	0.97	2/3488 (0.1%)
2	D	0.90	0/2574	0.95	0/3488
2	F	0.96	1/2574 (0.0%)	0.98	4/3488 (0.1%)
2	H	0.95	2/2574 (0.1%)	0.98	3/3488 (0.1%)
All	All	0.95	19/21832 (0.1%)	0.98	22/29488 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	232	CYS	CB-SG	-10.18	1.65	1.82
2	H	131	CYS	CB-SG	-7.86	1.68	1.82
1	A	318	GLU	CG-CD	7.59	1.63	1.51
1	A	152	CYS	CB-SG	-6.76	1.70	1.82
1	C	308	GLU	CG-CD	6.63	1.61	1.51
1	G	232	CYS	CB-SG	-6.62	1.71	1.82
1	A	161	CYS	CB-SG	-6.27	1.71	1.82
1	A	232	CYS	CB-SG	-6.26	1.71	1.82
1	E	232	CYS	CB-SG	-5.75	1.72	1.81
1	G	318	GLU	CG-CD	5.61	1.60	1.51
1	G	276	GLU	CG-CD	5.58	1.60	1.51
2	F	29	GLU	CG-CD	5.54	1.60	1.51
1	C	8	GLU	CG-CD	5.44	1.60	1.51
2	H	281	GLU	CG-CD	5.34	1.59	1.51
1	A	235	GLU	CG-CD	5.33	1.59	1.51
1	A	179	TYR	CD2-CE2	-5.26	1.31	1.39
1	C	62	CYS	CB-SG	-5.18	1.73	1.81
1	G	347	GLU	CG-CD	5.16	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	304	GLU	CG-CD	5.03	1.59	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	282	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	C	90	ARG	NE-CZ-NH1	-7.05	116.78	120.30
1	C	282	ARG	NE-CZ-NH1	-6.99	116.80	120.30
2	F	75	ARG	NE-CZ-NH1	6.37	123.49	120.30
2	B	239	ARG	NE-CZ-NH2	-6.19	117.20	120.30
2	F	75	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	G	223	LEU	CA-CB-CG	5.86	128.78	115.30
1	E	44	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	E	154	TYR	CA-CB-CG	5.72	124.26	113.40
2	H	239	ARG	NE-CZ-NH2	-5.45	117.57	120.30
2	H	23	VAL	CB-CA-C	-5.43	101.08	111.40
2	F	288	LEU	CB-CG-CD2	-5.38	101.85	111.00
1	A	234	ARG	NE-CZ-NH1	-5.35	117.63	120.30
2	B	25	LEU	CA-CB-CG	5.34	127.59	115.30
1	C	232	CYS	CB-CA-C	-5.27	99.86	110.40
1	C	144	LEU	CA-CB-CG	5.25	127.39	115.30
1	A	206	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	F	139	CYS	N-CA-C	5.19	125.01	111.00
2	H	327	LEU	CA-CB-CG	-5.11	103.54	115.30
1	G	238	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	G	100	LEU	CA-CB-CG	5.04	126.88	115.30
1	A	289	MET	CG-SD-CE	5.02	108.24	100.20

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	108	0
1	C	2834	0	2791	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2834	0	2791	104	0
1	G	2821	0	2777	72	0
2	B	2519	0	2517	93	0
2	D	2519	0	2517	84	0
2	F	2519	0	2517	100	0
2	H	2519	0	2517	102	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	1	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	722	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 17.

All (722) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LEU:HD13	2:D:71:MET:HE1	1.18	1.14
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:314:ARG:HG3	1:C:314:ARG:HH21	0.93	1.09
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:HA	1:C:18:GLU:OE2	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:NH1	2:F:214:ARG:HG2	1.81	0.92
2:F:214:ARG:CG	2:F:214:ARG:HH11	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:CG	1:C:314:ARG:HH21	1.83	0.87
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
1:E:103:ARG:HH11	1:E:103:ARG:HG3	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: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
1:E:71:CYS:O	1:E:75:LEU:HD22	1.84	0.76
2:D:266:TRP:HB3	2:D:267:PRO:HD2	1.66	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:F:280:MET:CE	2:H:292:ALA:HB3	2.16	0.76
2:B:1:LEU:HD12	2:B:3:VAL:HG12	1.68	0.75
1:A:103:ARG:CG	1:A:103:ARG:HH11	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
2:B:33:TYR:HD1	1:C:201:GLY:HA3	1.53	0.74
1:C:289:MET:CG	1:C:290:LEU:N	2.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:198:TYR:CD1	1:G:203:ALA:HB2	2.23	0.73
2:B:184:PRO:HA	2:B:187:GLN:NE2	2.03	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
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
2:H:3:VAL:CG1	2:H:182:PHE:CG	2.73	0.71
1:G:112:ARG:HD2	1:G:327:ASP:O	1.89	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:C:314:ARG:NH2	1:C:314:ARG:CG	2.49	0.70
2:B:214:ARG:HG2	2:B:214:ARG:HH11	1.57	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
2:F:172:ASN:HD22	2:F:172:ASN:C	1.96	0.69
1:A:40:GLN:HE21	1:A:288:ILE:HD13	1.56	0.69
2:H:237:ASN:HD22	2:H:238:MET:N	1.90	0.69
1:C:338:HIS:ND1	1:C:361:SER:O	2.25	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: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:CA	1:C:46:GLU:OE1	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
2:F:19:ARG:HG2	2:F:19:ARG:HH11	1.58	0.68
1:A:229:ASP:OD1	1:A:229:ASP:C	2.33	0.68
1:C:144:LEU:CD1	2:D:71:MET:HE1	2.11	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
2:F:280:MET:HE2	2:H:292:ALA:HB3	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LEU:CD1	2:D:71:MET:CE	2.66	0.67
2:H:3:VAL:HG11	2:H:182:PHE:CG	2.29	0.66
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: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
2:H:229:GLU:O	2:H:229:GLU:HG2	1.96	0.66
1:A:61:PHE:HD2	1:A:124:MET:HE1	1.60	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:118:ASN:HD21	2:B:132:PHE:N	1.92	0.64
2:B:102:TYR:CD2	2:D:301:PRO:HG2	2.32	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:B:99:LYS:NZ	2:D:130:GLN:OE1	2.30	0.64
2:H:3:VAL:CG1	2:H:182:PHE:HB2	2.27	0.64
2:H:108:GLN:C	2:H:108:GLN:HE21	2.01	0.64
2:D:207:ILE:O	2:D:207:ILE:HG23	1.98	0.64
1:C:113:LYS:HD3	1:C:328:PRO:HG2	1.80	0.64
2:B:33:TYR:CD1	1:C:201:GLY:HA3	2.32	0.64
2:D:199:LYS:HE3	2:D:201:GLU:CD	2.18	0.64
2:D:237:ASN:HD22	2:D:237:ASN:C	2.01	0.64
2:F:103:MET:SD	2:H:126:ALA:HB3	2.36	0.64
2:H:108:GLN:HA	2:H:108:GLN:NE2	2.12	0.64
2:B:207:ILE:HG13	2:B:258:HIS:HB2	1.79	0.64
1:A:103:ARG:HG2	1:A:103:ARG:HH11	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
1:C:-1:HIS:HE1	1:C:299:ASN:OD1	1.82	0.63
1:C:204:VAL:HG12	1:C:213:TYR:OH	1.99	0.63
2:B:63:ALA:CB	2:B:89:ALA:HB1	2.29	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:OXT	2:B:329:ILE:HD12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:GLU:O	1:C:284:LYS:HG3	2.00	0.62
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
1:G:333:GLU:CD	1:G:333:GLU:H	2.04	0.61
1:C:228:MET:HE3	1:C:285:SER:O	2.01	0.61
2:F:20:ASP:C	2:F:20:ASP:OD1	2.39	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
2:B:87:MET:HE3	2:D:91:ASP:OD1	2.00	0.61
2:B:75:ARG:HH22	2:B:164:ASN:ND2	1.98	0.61
1:A:229:ASP:OD1	1:A:231:LEU:N	2.33	0.61
1:G:222:GLY:HA2	1:G:252:LEU:O	2.00	0.61
1:C:157:LYS:O	1:C:158:ASP:HB2	1.99	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
2:F:172:ASN:ND2	2:F:172:ASN:C	2.55	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: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
1:A:144:LEU:O	1:A:148:ILE:HG13	2.01	0.59
2:B:267:PRO:HD2	2:B:299:ASP:OD1	2.03	0.59
1:E:172:GLN:HE21	2:H:57:ILE:HG22	1.67	0.59
1:E:225:VAL:HG12	1:E:226:ASP:N	2.18	0.59
1:A:225:VAL:HG12	1:A:226:ASP:N	2.17	0.59
1:G:162:LEU:HG	1:G:192:ILE:HD11	1.84	0.58
2:F:228:LYS:O	2:F:229:GLU:HG3	2.02	0.58
1:A:334:GLU:HG2	1:A:337:TYR:CE2	2.38	0.58
2:B:172:ASN:C	2:B:172:ASN:HD22	2.06	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:E:46:GLU:HA	1:E:46:GLU:OE1	2.03	0.58
1:C:335:LEU:C	1:C:335:LEU:HD23	2.23	0.58
1:C:100:LEU:HD22	1:C:128:ALA:HB2	1.84	0.58
1:A:235:GLU:OE2	1:A:238:ARG:NH1	2.36	0.58
1:E:348:VAL:HG12	2:H:299:ASP:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:ILE:HG21	1:C:138:VAL:HG11	1.84	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:B:313:ILE:HG22	2:B:314:PRO:HD2	1.87	0.57
2:D:33:TYR:O	2:D:33:TYR:CD2	2.57	0.57
1:E:261:HIS:O	1:E:262:GLY:O	2.21	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:H:212:HIS:HB3	2:H:238:MET:CE	2.34	0.57
2:B:237:ASN:ND2	2:B:237:ASN:C	2.58	0.57
2:D:23:VAL:HG22	2:D:75:ARG:HB2	1.86	0.57
2:F:293:VAL:HG12	1:G:353:GLN:HE22	1.69	0.57
1:E:172:GLN:HB2	1:E:175:ILE:HD12	1.87	0.57
2:D:57:ILE:HG22	2:D:57:ILE:O	2.05	0.57
1:G:55:GLN:O	1:G:57:ILE:N	2.38	0.56
1:C:231:LEU:HB2	1:C:294:ARG:HH12	1.70	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:CE	2:B:317:LYS:HA	2.35	0.56
1:C:313:VAL:HG12	1:C:314:ARG:N	2.19	0.56
2:B:51:ARG:NH1	2:B:51:ARG:HG3	2.15	0.56
2:D:100:THR:O	2:D:101:TYR:C	2.41	0.56
2:D:25:LEU:HD12	2:D:26:LEU:H	1.71	0.56
1:A:147:GLY:HA2	2:B:65:ILE:HG23	1.88	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
1:A:111:GLY:O	1:A:112:ARG:HD3	2.06	0.56
2:H:3:VAL:HG11	2:H:182:PHE:CD2	2.41	0.56
2:F:28:GLU:HB2	2:F:81:MET:HE3	1.88	0.56
1:A:177:GLU:OE1	2:B:61:GLY:N	2.34	0.56
1:C:68:GLN:HE21	1:C:259:ARG:HB3	1.71	0.56
1:C:261:HIS:O	1:C:262:GLY:O	2.25	0.55
1:C:24:THR:HG22	1:C:24:THR:O	2.07	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:28:GLU:OE2	2:D:59:GLU:OE2	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:ASN:HD22	2:B:237:ASN:C	2.09	0.55
2:D:16:GLU:OE2	2:D:162:ARG:NH1	2.39	0.55
1:E:241:ALA:O	1:E:245:ARG:HB2	2.07	0.55
2:H:89:ALA:O	2:H:92:GLN:N	2.40	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
1:C:217:GLY:O	1:C:218:ASP:HB3	2.06	0.55
2:F:172:ASN:ND2	2:F:174:LEU:H	2.04	0.55
1:E:53:TYR:CE1	1:E:265:MET:HB3	2.42	0.55
1:A:121:GLY:O	1:A:125:HIS:HD2	1.90	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:E:295:MET:HE2	1:E:300:LEU:HB3	1.90	0.54
1:E:53:TYR:C	1:E:53:TYR:CD1	2.81	0.54
2:H:112:ILE:CG1	2:H:113:VAL:N	2.70	0.54
2:B:328:ASN:ND2	2:B:328:ASN:O	2.40	0.54
1:E:335:LEU:C	1:E:335:LEU:HD23	2.27	0.54
1:E:213:TYR:HA	1:E:216:ARG:HG2	1.90	0.54
2:B:288:LEU:HG	2:B:290:ALA:O	2.08	0.54
2:H:165:ASN:HB3	2:H:166:PRO:CD	2.38	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
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
1:G:196:ASN:O	1:G:197:ARG:HB2	2.07	0.54
1:C:144:LEU:CD1	2:D:71:MET:HE3	2.38	0.54
2:B:16:GLU:CD	2:B:162:ARG:HH11	2.11	0.54
2:B:214:ARG:HG2	2:B:214:ARG:NH1	2.22	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
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:A:70:ALA:HB3	1:A:227:GLY:O	2.09	0.53
1:E:63:HIS:HA	1:E:264:SER:HB2	1.91	0.53
1:A:38:MET:O	1:A:39:MET:C	2.44	0.53
2:D:145:VAL:HG11	2:D:195:ILE:HG12	1.90	0.53
1:C:61:PHE:HB3	1:C:63:HIS:CE1	2.43	0.53
1:C:286:ASP:O	1:C:290:LEU:HB2	2.08	0.53
1:E:282:ARG:CG	1:E:282:ARG:HH11	2.13	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:CYS:SG	1:E:255:LEU:HD23	2.48	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:A:286:ASP:O	1:A:290:LEU:HG	2.08	0.53
2:D:59:GLU:O	2:D:60:MET:C	2.42	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:F:20:ASP:OD1	2:F:21:GLU:N	2.42	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:75:ARG:NH2	2:F:163:ASP:O	2.42	0.53
1:A:309:ILE:O	1:A:310:ASP:C	2.45	0.53
2:H:80:PHE:O	2:H:81:MET:C	2.44	0.53
2:H:3:VAL:CG1	2:H:182:PHE:CB	2.88	0.52
2:D:206:HIS:O	2:D:207:ILE:HB	2.08	0.52
2:B:2:GLN:HA	2:B:181:GLU:HA	1.92	0.52
2:B:51:ARG:O	2:B:52:ILE:HD13	2.09	0.52
2:F:19:ARG:HG2	2:F:19:ARG:NH1	2.24	0.52
2:D:75:ARG:NH2	2:D:163:ASP:O	2.42	0.52
1:G:116:CYS:SG	1:G:126:MET:HG2	2.50	0.52
2:F:136:TYR:HB3	2:F:144:VAL:HG21	1.91	0.52
2:H:57:ILE:HG22	2:H:57:ILE:O	2.10	0.52
1:G:61:PHE:HD2	1:G:124:MET:CE	2.22	0.52
1:G:263:HIS:CE1	4:G:1012:TPP:S1	3.03	0.52
1:E:341:SER:H	2:F:165:ASN:ND2	2.06	0.52
2:B:279:ILE:HG22	2:B:280:MET:N	2.24	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
2:F:280:MET:HE3	2:H:292:ALA:HB3	1.92	0.52
1:G:228:MET:HE3	1:G:287:PRO:HD3	1.91	0.52
1:E:100:LEU:HD13	1:E:128:ALA:CB	2.35	0.52
2:F:263:GLU:OE2	2:F:296:THR:HG22	2.09	0.52
1:C:62:CYS:HB3	1:C:265:MET:HG2	1.91	0.52
2:H:202:ARG:HG2	2:H:202:ARG:HH11	1.74	0.52
2:F:202:ARG:HD3	2:F:233:CYS:O	2.10	0.52
1:A:182:ALA:HA	1:A:187:LEU:HD12	1.91	0.52
2:H:237:ASN:HD22	2:H:237:ASN:C	2.11	0.52
1:A:113:LYS:HG2	1:A:328:PRO:O	2.10	0.52
2:F:112:ILE:HG13	2:F:113:VAL:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:ASN:HD22	2:B:238:MET:N	2.07	0.52
1:A:190:ILE:HG22	1:A:192:ILE:HG13	1.91	0.52
1:C:1:PHE:CE1	1:C:301:ALA:HA	2.45	0.51
1:G:286:ASP:OD1	1:G:287:PRO:HD2	2.09	0.51
1:C:196:ASN:O	1:C:197:ARG:HB2	2.10	0.51
2:D:121:SER:OG	2:D:122:ALA:N	2.41	0.51
1:E:153:LYS:NZ	1:E:185:TRP:O	2.34	0.51
1:G:95:THR:HG21	1:G:126:MET:HE3	1.91	0.51
1:G:206:ARG:HB3	1:G:206:ARG:CZ	2.40	0.51
2:B:93:VAL:O	2:B:97:ALA:HB3	2.10	0.51
1:A:45:MET:CE	1:A:92:HIS:HB3	2.40	0.51
2:D:68:GLY:HA2	2:D:71:MET:HE2	1.93	0.51
2:F:142:LEU:HD21	2:F:168:VAL:HG23	1.92	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
1:G:68:GLN:HE22	1:G:196:ASN:HD22	1.58	0.51
2:F:311:ASN:HD22	2:F:311:ASN:N	2.09	0.51
2:B:20:ASP:OD1	2:B:22:LYS:N	2.39	0.51
2:B:172:ASN:ND2	2:B:172:ASN:C	2.63	0.51
2:H:3:VAL:HG13	2:H:182:PHE:CD1	2.46	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
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:316:GLU:O	1:G:316:GLU:HG2	2.08	0.50
1:C:144:LEU:HD13	2:D:71:MET:HE3	1.81	0.50
1:E:279:GLN:HE21	1:E:279:GLN:HA	1.75	0.50
1:C:174:GLN:HB3	2:D:60:MET:HG2	1.93	0.50
1:G:268:PRO:HB2	1:G:270:VAL:HG12	1.92	0.50
2:D:98:ALA:HB2	2:D:142:LEU:HD13	1.94	0.50
2:H:328:ASN:O	2:H:328:ASN:CG	2.49	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:OD2	1:A:66:ASP:N	2.45	0.50
2:B:99:LYS:HG2	2:D:301:PRO:HB3	1.93	0.50
2:H:98:ALA:O	2:H:141:GLY:HA3	2.12	0.50
1:E:296:VAL:HA	1:E:301:ALA:O	2.12	0.50
1:G:55:GLN:C	1:G:57:ILE:H	2.14	0.50
2:B:206:HIS:ND1	2:B:231:VAL:HA	2.27	0.50
1:G:27:LEU:HD13	1:G:300:LEU:HD21	1.93	0.50
1:C:269:GLY:HA2	1:C:272:TYR:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ARG:HG2	1:C:282:ARG:O	2.11	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:E:225:VAL:HG12	1:E:226:ASP:H	1.77	0.49
1:C:71:CYS:SG	1:C:255:LEU:HD23	2.52	0.49
2:D:19:ARG:HD2	2:D:162:ARG:NH1	2.26	0.49
2:H:149:ASN:HB2	2:H:180:PHE:CE2	2.47	0.49
2:F:13:MET:HE3	2:F:43:LEU:HD21	1.94	0.49
2:H:279:ILE:CD1	2:H:284:ALA:HB3	2.41	0.49
2:H:279:ILE:HD12	2:H:284:ALA:HB3	1.93	0.49
2:H:9:ILE:HA	2:H:157:ILE:CD1	2.42	0.49
1:A:128:ALA:HB3	1:A:131:PHE:HB3	1.94	0.49
2:H:214:ARG:HB3	2:H:215:PRO:CD	2.42	0.49
1:E:63:HIS:CD2	1:E:264:SER:HB3	2.47	0.49
2:D:23:VAL:HG22	2:D:75:ARG:CB	2.42	0.49
1:A:107:ALA:HA	1:A:324:ALA:HB1	1.95	0.49
2:F:327:LEU:C	2:F:329:ILE:H	2.15	0.49
2:B:16:GLU:OE1	2:B:162:ARG:HD2	2.11	0.49
1:E:286:ASP:HB3	1:E:289:MET:CB	2.42	0.49
1:A:202:THR:HG23	1:A:206:ARG:CZ	2.42	0.49
1:C:132:TYR:CD1	1:C:132:TYR:N	2.80	0.49
1:G:128:ALA:HB3	1:G:131:PHE:HB3	1.93	0.49
2:D:206:HIS:O	2:D:327:LEU:HD21	2.12	0.49
1:G:113:LYS:HZ2	1:G:113:LYS:HB2	1.77	0.49
2:B:218:HIS:O	2:B:221:GLU:HB2	2.12	0.49
2:B:91:ASP:OD1	2:B:95:ASN:ND2	2.41	0.49
1:G:44:ARG:HB2	1:G:317:ILE:HG13	1.94	0.49
2:B:112:ILE:HG13	2:B:113:VAL:N	2.28	0.49
2:D:24:PHE:HB2	2:D:51:ARG:O	2.12	0.49
2:D:237:ASN:ND2	2:D:237:ASN:C	2.66	0.49
2:F:76:PRO:CG	2:F:112:ILE:HD12	2.41	0.49
2:B:269:PHE:HE1	2:D:271:VAL:HA	1.77	0.49
1:G:39:MET:CE	1:G:291:LEU:CD2	2.91	0.49
1:E:261:HIS:C	1:E:262:GLY:O	2.51	0.49
2:B:44:TRP:NE1	2:B:49:ASP:OD1	2.40	0.49
1:A:164:LEU:HD12	1:A:164:LEU:N	2.27	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
2:D:266:TRP:HB3	2:D:267:PRO:CD	2.39	0.48
1:C:281:VAL:CG1	1:C:281:VAL:O	2.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:68:GLN:NE2	1:G:196:ASN:HD22	2.11	0.48
1:E:56:LYS:HA	1:E:56:LYS:HD3	1.59	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
2:F:327:LEU:C	2:F:329:ILE:N	2.66	0.48
1:A:61:PHE:HD2	1:A:124:MET:CE	2.25	0.48
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
1:E:279:GLN:CA	1:E:279:GLN:NE2	2.72	0.48
2:H:152:ASP:HA	2:H:193:ILE:CD1	2.43	0.48
2:H:3:VAL:HG13	2:H:182:PHE:CG	2.47	0.48
2:H:108:GLN:HE21	2:H:108:GLN:CA	2.27	0.48
1:E:142:VAL:HG21	1:E:175:ILE:HG12	1.95	0.48
2:B:91:ASP:O	2:B:95:ASN:HB2	2.13	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: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
2:H:104:SER:O	2:H:107:LEU:HD22	2.14	0.48
2:D:82:THR:HG22	2:D:117:PRO:HG2	1.95	0.48
1:A:162:LEU:HD12	1:A:162:LEU:N	2.29	0.48
2:B:296:THR:O	1:C:351:ALA:HA	2.14	0.47
2:B:79:GLU:HG3	2:B:115:ARG:NH1	2.28	0.47
1:A:275:ARG:CB	1:A:275:ARG:HH11	2.27	0.47
1:A:217:GLY:O	1:A:218:ASP:HB3	2.14	0.47
2:B:241:ILE:CG2	2:B:241:ILE:O	2.61	0.47
1:A:50:ASP:C	1:A:50:ASP:OD2	2.52	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:C:281:VAL:HG12	1:C:281:VAL:O	2.11	0.47
2:B:39:VAL:HG11	2:B:115:ARG:NH2	2.29	0.47
1:A:196:ASN:O	1:A:197:ARG:HB2	2.14	0.47
1:G:231:LEU:HA	1:G:231:LEU:HD23	1.68	0.47
2:H:143:LYS:NZ	2:H:163:ASP:OD2	2.46	0.47
2:F:228:LYS:C	2:F:229:GLU:HG3	2.35	0.47
2:F:152:ASP:O	2:F:156:LEU:HB2	2.15	0.47
1:A:112:ARG:NH1	1:A:327:ASP:O	2.47	0.47
2:H:229:GLU:CG	2:H:229:GLU:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:CYS:O	1:C:75:LEU:HD13	2.15	0.47
2:F:175:MET:O	2:F:176:TYR:C	2.53	0.47
1:E:279:GLN:OE1	1:E:282:ARG:HD2	2.15	0.47
1:C:225:VAL:HB	1:C:255:LEU:HD12	1.96	0.47
2:B:152:ASP:O	2:B:156:LEU:HB2	2.14	0.47
2:D:156:LEU:HD11	2:D:239:ARG:HB3	1.97	0.47
2:H:246:MET:O	2:H:247:GLU:C	2.53	0.47
1:A:58:ILE:HG12	1:A:109:LEU:O	2.15	0.47
1:E:353:GLN:OE1	2:H:293:VAL:HG12	2.15	0.47
2:B:302:MET:SD	2:B:303:PRO:HD2	2.55	0.47
1:A:103:ARG:HG3	1:A:103:ARG:HH11	1.78	0.47
2:D:25:LEU:HD12	2:D:26:LEU:N	2.29	0.47
2:F:311:ASN:ND2	2:F:311:ASN:N	2.63	0.47
1:C:166:GLY:HA3	6:C:2002:HOH:O	2.15	0.47
2:B:31:ALA:HB3	2:B:54:ASP:CG	2.35	0.47
2:D:5:VAL:HB	2:D:175:MET:O	2.15	0.47
1:G:338:HIS:O	2:H:102:TYR:HA	2.15	0.47
2:D:270:GLY:HA3	6:D:2001:HOH:O	2.15	0.47
2:B:82:THR:HG23	2:B:85:PHE:CE2	2.50	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:F:59:GLU:O	2:F:60:MET:C	2.51	0.46
2:D:328:ASN:CG	2:D:328:ASN:O	2.53	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:B:182:PHE:HA	2:B:183:PRO:HD2	1.74	0.46
1:G:228:MET:CE	1:G:287:PRO:HD3	2.46	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
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
1:G:251:ILE:HG12	1:G:252:LEU:H	1.81	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:A:334:GLU:HG2	1:A:337:TYR:CD2	2.51	0.46
2:D:158:LYS:O	2:D:159:SER:C	2.53	0.46
2:H:101:TYR:CE1	2:H:106:GLY:HA2	2.51	0.46
1:A:307:LYS:HD2	1:A:307:LYS:HA	1.51	0.46
1:G:216:ARG:NH1	1:G:216:ARG:HG3	2.30	0.46
1:C:15:HIS:CD2	1:C:16:ARG:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:ILE:HG22	2:B:241:ILE:O	2.15	0.46
1:A:42:VAL:O	1:A:46:GLU:HG2	2.15	0.46
2:B:118:ASN:ND2	2:B:132:PHE:H	1.97	0.46
1:C:140:ALA:O	1:C:143:PRO:HD2	2.16	0.46
1:C:7:PHE:HE1	1:C:27:LEU:HB3	1.81	0.46
1:G:39:MET:HE2	1:G:291:LEU:HD23	1.98	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
2:H:316:VAL:O	2:H:317:LYS:C	2.53	0.46
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:E:60:GLY:HA3	2:H:123:GLY:O	2.16	0.45
2:F:214:ARG:NH1	2:F:214:ARG:CG	2.52	0.45
1:E:68:GLN:HE21	1:E:259:ARG:HB3	1.82	0.45
1:A:176:PHE:HZ	1:A:216:ARG:HE	1.64	0.45
2:D:326:THR:C	2:D:328:ASN:H	2.20	0.45
2:D:81:MET:HB2	2:D:81:MET:HE3	1.87	0.45
1:C:327:ASP:OD1	1:C:328:PRO:HD2	2.16	0.45
2:F:313:ILE:CG2	2:F:314:PRO:HD2	2.44	0.45
1:G:55:GLN:C	1:G:57:ILE:N	2.69	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
2:D:202:ARG:NH1	2:D:232:GLU:OE1	2.38	0.45
2:H:212:HIS:HB3	2:H:238:MET:HE3	1.97	0.45
1:E:142:VAL:HG21	1:E:175:ILE:CG1	2.46	0.45
1:C:30:GLU:N	1:C:30:GLU:OE2	2.47	0.45
1:E:327:ASP:CG	1:E:328:PRO:HD2	2.37	0.45
1:C:300:LEU:HD12	1:C:300:LEU:HA	1.54	0.45
1:A:145:GLY:HA3	1:A:163:THR:OG1	2.17	0.45
1:E:111:GLY:O	1:E:112:ARG:HD3	2.17	0.45
1:E:48:LYS:HD3	1:E:48:LYS:HA	1.77	0.45
1:A:45:MET:HE3	1:A:92:HIS:HB3	1.99	0.45
2:H:316:VAL:C	2:H:318:ASP:N	2.69	0.45
1:E:228:MET:HE3	1:E:285:SER:O	2.17	0.45
1:A:103:ARG:HH22	1:A:319:ASP:CB	2.30	0.45
2:F:199:LYS:HD2	2:F:239:ARG:NH2	2.31	0.45
1:A:270:VAL:HG12	1:A:275:ARG:HG3	1.97	0.45
2:B:150:SER:O	2:B:151:GLU:C	2.54	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:B:263:GLU:HG2	2:B:296:THR:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:SER:C	1:A:304:GLU:N	2.67	0.45
1:G:165:TYR:HH	1:G:179:TYR:HH	1.54	0.45
1:A:352:ASN:OD1	1:A:352:ASN:C	2.54	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
1:E:335:LEU:C	1:E:335:LEU:CD2	2.84	0.45
2:H:208:THR:HG22	2:H:210:VAL:HG23	1.99	0.45
1:E:57:ILE:HG22	1:E:110:THR:HG22	1.98	0.45
1:G:112:ARG:HG3	1:G:327:ASP:HB3	1.98	0.44
1:C:229:ASP:O	1:C:230:ILE:C	2.55	0.44
1:E:80:ASN:O	1:E:98:ARG:NH2	2.50	0.44
2:D:94:ILE:HD13	2:D:94:ILE:HA	1.75	0.44
1:E:128:ALA:O	1:E:129:LYS:C	2.55	0.44
2:F:280:MET:HE3	2:H:292:ALA:CB	2.47	0.44
1:C:-1:HIS:CE1	1:C:299:ASN:OD1	2.67	0.44
2:H:213:SER:OG	2:H:214:ARG:N	2.50	0.44
1:E:335:LEU:HD21	2:H:300:VAL:HG21	1.98	0.44
1:A:109:LEU:HA	1:A:109:LEU:HD12	1.80	0.44
2:D:182:PHE:HA	2:D:183:PRO:HD2	1.83	0.44
2:F:51:ARG:O	2:F:52:ILE:HD13	2.17	0.44
1:A:112:ARG:HD2	1:A:327:ASP:O	2.17	0.44
1:A:61:PHE:HB3	1:A:63:HIS:CE1	2.53	0.44
2:D:33:TYR:HD2	2:D:33:TYR:O	1.98	0.44
2:F:307:ILE:CG2	2:F:308:LEU:N	2.80	0.44
1:A:36:TYR:O	1:A:37:ARG:C	2.54	0.44
1:E:282:ARG:HG2	1:E:282:ARG:O	2.17	0.44
2:F:280:MET:HE1	2:H:276:CYS:HB3	2.00	0.44
1:G:39:MET:HE1	1:G:291:LEU:CD2	2.48	0.44
1:E:142:VAL:O	1:E:143:PRO:C	2.54	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:103:ARG:HH11	1:E:103:ARG:CG	2.22	0.44
2:F:144:VAL:HG22	2:F:168:VAL:HB	1.98	0.44
1:C:68:GLN:NE2	1:C:259:ARG:HB3	2.32	0.44
1:C:24:THR:CG2	1:C:24:THR:O	2.65	0.44
2:F:25:LEU:HD23	2:F:52:ILE:HG23	1.99	0.44
1:A:13:ASP:HB2	1:A:224:ARG:HB3	2.00	0.44
1:E:102:VAL:HG11	1:E:317:ILE:HD13	1.98	0.44
2:H:182:PHE:HD2	2:H:187:GLN:HG3	1.81	0.44
1:A:272:TYR:HE1	1:A:273:ARG:HD3	1.80	0.44
2:H:149:ASN:HB2	2:H:180:PHE:CD2	2.53	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
2:D:259:LEU:HD12	2:D:260:VAL:H	1.82	0.44
2:B:299:ASP:HB3	1:C:348:VAL:HG12	1.99	0.44
1:E:172:GLN:HB2	1:E:175:ILE:CD1	2.47	0.44
1:A:39:MET:HG2	1:A:73:VAL:HG21	2.00	0.44
2:H:313:ILE:HG12	2:H:314:PRO:CD	2.43	0.44
1:A:65:CYS:O	1:A:65:CYS:SG	2.76	0.44
2:F:259:LEU:CD2	2:F:279:ILE:HG13	2.47	0.44
1:A:46:GLU:O	1:A:47:LEU:C	2.56	0.44
2:H:327:LEU:HA	2:H:327:LEU:HD23	1.76	0.44
2:H:59:GLU:N	2:H:59:GLU:OE1	2.51	0.43
2:F:95:ASN:ND2	2:H:87:MET:HE2	2.32	0.43
2:H:156:LEU:HA	2:H:156:LEU:HD23	1.58	0.43
1:A:80:ASN:HB3	1:A:81:PRO:HD2	1.99	0.43
2:H:19:ARG:CZ	2:H:162:ARG:HD2	2.48	0.43
1:E:44:ARG:CB	1:E:317:ILE:HG13	2.41	0.43
4:E:1009:TPP:N1'	2:H:59:GLU:OE2	2.51	0.43
1:E:138:VAL:HG13	1:E:169:ALA:CB	2.48	0.43
2:D:306:LYS:O	2:D:307:ILE:C	2.53	0.43
2:D:148:TRP:CE3	2:D:149:ASN:ND2	2.85	0.43
2:F:327:LEU:O	2:F:329:ILE:N	2.52	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
2:B:62:PHE:O	2:B:63:ALA:C	2.56	0.43
1:A:305:GLU:O	1:A:309:ILE:HG13	2.18	0.43
1:E:141:GLN:OE1	1:E:141:GLN:N	2.51	0.43
1:E:225:VAL:CG1	1:E:226:ASP:N	2.82	0.43
1:C:320:ALA:O	1:C:323:PHE:HB3	2.18	0.43
2:B:19:ARG:O	2:B:19:ARG:HG2	2.19	0.43
2:F:10:ASN:HD21	2:F:43:LEU:HD13	1.82	0.43
1:A:202:THR:HG23	1:A:206:ARG:NH2	2.34	0.43
1:C:69:GLU:N	1:C:69:GLU:OE1	2.48	0.43
1:E:95:THR:O	1:E:100:LEU:HB2	2.19	0.43
1:A:220:ILE:HG23	1:A:221:PRO:HD2	2.00	0.43
2:D:207:ILE:CG2	2:D:207:ILE:O	2.66	0.43
2:F:66:ALA:O	2:F:76:PRO:HG3	2.19	0.43
1:E:53:TYR:CG	1:E:265:MET:HG3	2.53	0.43
1:E:335:LEU:O	1:E:335:LEU:HD23	2.18	0.43
1:A:58:ILE:CG2	1:A:59:ARG:N	2.81	0.43
2:H:274:GLU:OE2	2:H:278:ARG:HG2	2.18	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:F:75:ARG:HH12	2:F:164:ASN:ND2	2.16	0.43
1:A:181:MET:HG2	1:A:185:TRP:CH2	2.54	0.43
2:F:62:PHE:O	2:F:63:ALA:C	2.57	0.43
2:F:142:LEU:HD23	2:F:143:LYS:N	2.34	0.43
1:A:270:VAL:HG11	1:A:275:ARG:CG	2.48	0.43
2:F:293:VAL:HG12	1:G:353:GLN:NE2	2.33	0.43
2:H:5:VAL:O	2:H:9:ILE:HG13	2.19	0.43
1:G:87:THR:O	1:G:135:ASN:ND2	2.49	0.43
1:A:314:ARG:HD2	1:A:314:ARG:HA	1.84	0.43
2:F:214:ARG:N	2:F:215:PRO:HD2	2.34	0.42
2:F:146:SER:OG	2:F:213:SER:HB2	2.19	0.42
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
1:A:323:PHE:CD2	1:A:323:PHE:C	2.91	0.42
1:G:337:TYR:CD1	1:G:337:TYR:N	2.88	0.42
2:F:29:GLU:OE1	2:F:29:GLU:HA	2.19	0.42
1:C:174:GLN:HG3	1:C:174:GLN:H	1.38	0.42
2:D:156:LEU:HD23	2:D:156:LEU:HA	1.79	0.42
1:C:126:MET:HE2	1:C:126:MET:HB2	1.82	0.42
1:C:90:ARG:HG3	1:C:90:ARG:NH1	2.34	0.42
2:B:306:LYS:HB2	1:C:329:GLU:OE2	2.19	0.42
1:E:180:ASN:O	1:E:184:LEU:HB2	2.19	0.42
1:C:300:LEU:O	1:C:301:ALA:CB	2.67	0.42
2:B:156:LEU:HD23	2:B:156:LEU:HA	1.89	0.42
1:E:79:ILE:HG23	1:E:237:THR:CG2	2.50	0.42
1:G:290:LEU:HD12	1:G:290:LEU:HA	1.96	0.42
2:F:198:ALA:HA	2:F:238:MET:O	2.19	0.42
1:E:334:GLU:HG2	1:E:337:TYR:CD2	2.54	0.42
2:B:325:LYS:HA	2:B:325:LYS:HD2	1.94	0.42
2:F:288:LEU:HA	2:F:288:LEU:HD12	1.77	0.42
1:E:196:ASN:C	1:E:198:TYR:H	2.21	0.42
2:B:112:ILE:HG13	2:B:113:VAL:H	1.84	0.42
1:C:167:ASP:OD2	1:C:167:ASP:N	2.52	0.42
2:D:304:TYR:O	2:D:305:ALA:C	2.58	0.42
2:F:304:TYR:O	2:F:305:ALA:C	2.58	0.42
2:B:10:ASN:HD21	2:B:43:LEU:HD13	1.85	0.42
1:G:133:GLY:HA2	1:G:134:GLY:HA3	1.72	0.42
2:H:212:HIS:CG	2:H:241:ILE:HD11	2.54	0.42
2:H:211:SER:C	2:H:238:MET:HE3	2.40	0.42
4:A:1003:TPP:HN42	4:A:1003:TPP:H2	1.84	0.42
2:F:22:LYS:HB3	2:F:75:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ASP:OD1	1:C:198:TYR:C	2.58	0.42
2:D:245:ASP:OD2	2:D:248:THR:OG1	2.32	0.42
2:D:112:ILE:HG13	2:D:113:VAL:H	1.81	0.42
2:F:34:ASP:O	2:F:38:LYS:HA	2.20	0.42
1:E:29:ARG:NH1	1:E:300:LEU:O	2.53	0.42
1:C:109:LEU:HA	1:C:109:LEU:HD23	1.81	0.42
1:A:333:GLU:HG3	1:A:333:GLU:H	1.61	0.42
2:F:88:GLN:NE2	1:G:172:GLN:HE22	2.07	0.42
1:A:53:TYR:O	1:A:56:LYS:N	2.43	0.42
1:E:132:TYR:N	1:E:132:TYR:CD1	2.87	0.42
2:F:60:MET:HG3	2:F:60:MET:O	2.19	0.42
2:D:3:VAL:HG13	2:D:182:PHE:HB2	2.01	0.42
2:B:139:CYS:HA	2:B:140:PRO:HD2	1.85	0.42
1:G:315:LYS:O	1:G:319:ASP:OD2	2.38	0.42
1:E:353:GLN:HG2	1:E:354:TRP:CE3	2.55	0.42
1:G:106:LEU:HD23	1:G:106:LEU:HA	1.71	0.42
2:D:34:ASP:O	2:D:38:LYS:HA	2.20	0.42
2:D:171:GLU:OE1	2:D:176:TYR:OH	2.29	0.42
2:D:24:PHE:CZ	2:D:76:PRO:HB3	2.55	0.41
1:G:216:ARG:HA	1:G:216:ARG:HD2	1.90	0.41
2:B:143:LYS:NZ	2:B:163:ASP:OD2	2.45	0.41
2:B:75:ARG:HH12	2:B:164:ASN:HD21	1.62	0.41
2:H:237:ASN:C	2:H:237:ASN:ND2	2.73	0.41
1:A:124:MET:HB2	1:A:124:MET:HE3	1.97	0.41
2:H:59:GLU:O	2:H:60:MET:C	2.59	0.41
1:A:45:MET:HE1	1:A:92:HIS:HB3	2.02	0.41
2:D:3:VAL:HG13	2:D:182:PHE:CG	2.56	0.41
2:D:97:ALA:HA	2:D:110:VAL:HG11	2.01	0.41
1:A:41:THR:HG21	1:A:96:PHE:CZ	2.55	0.41
1:C:53:TYR:C	1:C:53:TYR:CD1	2.93	0.41
2:F:40:SER:O	2:F:41:ARG:C	2.58	0.41
1:E:229:ASP:HB3	1:E:232:CYS:HB3	2.03	0.41
1:C:184:LEU:HA	1:C:184:LEU:HD12	1.88	0.41
1:E:44:ARG:HA	1:E:44:ARG:NE	2.35	0.41
1:A:58:ILE:HD11	1:A:109:LEU:HB3	2.02	0.41
1:G:200:MET:CG	1:G:201:GLY:H	2.32	0.41
1:A:14:LEU:HD21	1:A:20:GLY:HA3	2.02	0.41
1:E:192:ILE:HA	1:E:253:MET:O	2.20	0.41
1:A:203:ALA:O	1:A:204:VAL:C	2.59	0.41
2:D:189:LYS:NZ	2:D:189:LYS:HB2	2.34	0.41
2:F:327:LEU:HA	2:F:327:LEU:HD23	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LEU:HD11	2:D:312:SER:OG	2.20	0.41
1:A:184:LEU:HD21	1:C:206:ARG:O	2.21	0.41
1:E:292:LYS:HG3	1:E:306:LEU:HD13	2.02	0.41
1:G:251:ILE:HG12	1:G:252:LEU:N	2.35	0.41
1:E:181:MET:HB3	1:E:185:TRP:CZ3	2.56	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
2:H:1:LEU:H3	2:H:1:LEU:HG	1.72	0.41
2:F:175:MET:SD	2:F:214:ARG:HD2	2.61	0.41
1:E:279:GLN:NE2	1:E:282:ARG:HD2	2.36	0.41
2:F:279:ILE:HD13	2:F:279:ILE:HA	1.76	0.41
2:B:269:PHE:CE1	2:D:271:VAL:HA	2.55	0.41
1:G:200:MET:CG	1:G:201:GLY:N	2.83	0.41
2:H:315:GLN:O	2:H:318:ASP:HB2	2.21	0.41
1:A:142:VAL:HA	1:A:163:THR:CG2	2.50	0.41
2:D:62:PHE:O	2:D:63:ALA:C	2.56	0.41
1:E:39:MET:CE	1:E:291:LEU:HD22	2.50	0.41
2:H:150:SER:O	2:H:151:GLU:C	2.59	0.41
2:B:209:VAL:HA	2:B:260:VAL:O	2.21	0.41
1:A:133:GLY:HA2	1:A:134:GLY:HA3	1.77	0.41
2:B:36:ALA:HB2	2:B:81:MET:HE2	2.03	0.41
2:H:130:GLN:HB3	2:H:132:PHE:CE1	2.56	0.41
4:A:1003:TPP:H6'	2:D:28:GLU:OE1	2.20	0.41
2:F:139:CYS:HA	2:F:140:PRO:HD3	1.98	0.41
1:C:66:ASP:OD2	1:C:260:TYR:HB2	2.20	0.41
1:C:89:TYR:CD1	1:C:89:TYR:C	2.94	0.41
1:G:46:GLU:OE1	1:G:46:GLU:HA	2.21	0.41
1:G:45:MET:HG3	1:G:102:VAL:HG13	2.03	0.41
2:F:226:LEU:HD13	2:F:323:ILE:HG21	2.03	0.41
1:A:282:ARG:HH11	1:A:282:ARG:HG3	1.85	0.41
1:E:341:SER:N	2:F:165:ASN:HD21	2.09	0.41
1:E:225:VAL:HG21	1:E:236:ALA:HB1	2.03	0.41
1:A:68:GLN:HE22	1:A:196:ASN:HD22	1.69	0.41
1:E:229:ASP:O	1:E:230:ILE:C	2.57	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:C:348:VAL:HG23	1:C:357:PHE:O	2.21	0.40
1:C:261:HIS:C	1:C:262:GLY:O	2.59	0.40
2:D:319:ILE:O	2:D:320:ILE:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ILE:HG21	1:C:325:THR:HG22	2.02	0.40
1:G:95:THR:HB	1:G:100:LEU:HD22	2.04	0.40
2:B:65:ILE:HG21	2:B:65:ILE:HD13	1.81	0.40
1:A:249:GLY:HA3	1:A:250:PRO:HD2	1.69	0.40
1:C:133:GLY:HA3	1:C:134:GLY:HA3	1.87	0.40
1:C:31:ASP:O	1:C:32:GLY:C	2.58	0.40
1:C:315:LYS:HZ3	1:C:315:LYS:HG3	1.58	0.40
1:A:89:TYR:HB2	1:A:124:MET:HG2	2.02	0.40
1:A:84:HIS:CE1	1:A:130:ASN:ND2	2.90	0.40
1:E:295:MET:HE2	1:E:300:LEU:CB	2.50	0.40
1:C:264:SER:O	1:C:265:MET:C	2.60	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:315:GLN:H	2:H:315:GLN:HG2	1.70	0.40
1:C:165:TYR:CD1	1:C:165:TYR:N	2.88	0.40
1:A:75:LEU:HD13	1:A:233:VAL:CG1	2.52	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%)	10 43
1	C	361/382 (94%)	322 (89%)	31 (9%)	8 (2%)	8 38
1	E	361/382 (94%)	333 (92%)	19 (5%)	9 (2%)	7 34
1	G	360/382 (94%)	318 (88%)	35 (10%)	7 (2%)	10 43
2	B	327/329 (99%)	297 (91%)	26 (8%)	4 (1%)	16 56
2	D	327/329 (99%)	277 (85%)	41 (12%)	9 (3%)	6 30
2	F	327/329 (99%)	287 (88%)	37 (11%)	3 (1%)	21 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	327/329 (99%)	295 (90%)	28 (9%)	4 (1%)	16 56
All	All	2750/2844 (97%)	2450 (89%)	249 (9%)	51 (2%)	10 43

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
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

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Mol	Chain	Res	Type
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%)	262 (90%)	30 (10%)	9 33
1	C	294/310 (95%)	254 (86%)	40 (14%)	5 20
1	E	294/310 (95%)	260 (88%)	34 (12%)	7 27
1	G	292/310 (94%)	251 (86%)	41 (14%)	4 19
2	B	268/268 (100%)	232 (87%)	36 (13%)	5 21
2	D	268/268 (100%)	240 (90%)	28 (10%)	9 32
2	F	268/268 (100%)	247 (92%)	21 (8%)	16 49
2	H	268/268 (100%)	240 (90%)	28 (10%)	9 32
All	All	2244/2312 (97%)	1986 (88%)	258 (12%)	7 28

All (258) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	17	LEU
1	A	33	LEU
1	A	50	ASP
1	A	66	ASP
1	A	75	LEU
1	A	98	ARG
1	A	100	LEU
1	A	103	ARG
1	A	109	LEU
1	A	126	MET
1	A	174	GLN
1	A	210	SER
1	A	245	ARG
1	A	255	LEU
1	A	266	SER
1	A	274	THR
1	A	275	ARG
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
1	A	325	THR
1	A	333	GLU
1	A	342	SER
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	50	LYS
2	B	55	THR
2	B	74	LEU
2	B	100	THR
2	B	112	ILE
2	B	121	SER

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Mol	Chain	Res	Type
2	B	146	SER
2	B	161	ILE
2	B	162	ARG
2	B	170	LEU
2	B	172	ASN
2	B	182	PHE
2	B	188	SER
2	B	189	LYS
2	B	192	LEU
2	B	199	LYS
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
2	B	317	LYS
2	B	328	ASN
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	123	SER
1	C	157	LYS
1	C	158	ASP
1	C	174	GLN

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Mol	Chain	Res	Type
1	C	216	ARG
1	C	218	ASP
1	C	223	LEU
1	C	264	SER
1	C	273	ARG
1	C	276	GLU
1	C	279	GLN
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	307	LYS
1	C	314	ARG
1	C	315	LYS
1	C	319	ASP
1	C	322	GLN
1	C	347	GLU
1	C	348	VAL
2	D	1	LEU
2	D	3	VAL
2	D	7	ASP
2	D	30	VAL
2	D	43	LEU
2	D	45	LYS
2	D	79	GLU
2	D	81	MET
2	D	107	LEU
2	D	112	ILE
2	D	142	LEU
2	D	154	LYS
2	D	159	SER
2	D	162	ARG
2	D	182	PHE
2	D	185	GLU
2	D	188	SER
2	D	197	LYS
2	D	210	VAL
2	D	211	SER
2	D	227	SER

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Mol	Chain	Res	Type
2	D	229	GLU
2	D	237	ASN
2	D	278	ARG
2	D	306	LYS
2	D	313	ILE
2	D	314	PRO
2	D	329	ILE
1	E	0	MET
1	E	6	THR
1	E	23	VAL
1	E	27	LEU
1	E	33	LEU
1	E	48	LYS
1	E	56	LYS
1	E	57	ILE
1	E	75	LEU
1	E	80	ASN
1	E	85	LEU
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	275	ARG
1	E	276	GLU
1	E	279	GLN
1	E	284	LYS
1	E	303	VAL
1	E	307	LYS
1	E	314	ARG
1	E	322	GLN
1	E	333	GLU
1	E	348	VAL
1	E	356	LYS
1	E	360	VAL
1	E	361	SER
2	F	3	VAL

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Mol	Chain	Res	Type
2	F	21	GLU
2	F	32	GLN
2	F	50	LYS
2	F	74	LEU
2	F	103	MET
2	F	112	ILE
2	F	115	ARG
2	F	121	SER
2	F	172	ASN
2	F	181	GLU
2	F	214	ARG
2	F	229	GLU
2	F	237	ASN
2	F	263	GLU
2	F	267	PRO
2	F	268	GLN
2	F	299	ASP
2	F	306	LYS
2	F	315	GLN
2	F	325	LYS
1	G	8	GLU
1	G	10	LYS
1	G	11	LYS
1	G	24	THR
1	G	47	LEU
1	G	48	LYS
1	G	56	LYS
1	G	64	LEU
1	G	66	ASP
1	G	75	LEU
1	G	85	LEU
1	G	98	ARG
1	G	100	LEU
1	G	113	LYS
1	G	126	MET
1	G	148	ILE
1	G	157	LYS
1	G	205	GLU
1	G	206	ARG
1	G	210	SER
1	G	215	LYS
1	G	229	ASP

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Mol	Chain	Res	Type
1	G	230	ILE
1	G	235	GLU
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	279	GLN
1	G	284	LYS
1	G	290	LEU
1	G	295	MET
1	G	300	LEU
1	G	314	ARG
1	G	315	LYS
1	G	316	GLU
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	18	GLU
2	H	30	VAL
2	H	33	TYR
2	H	43	LEU
2	H	65	ILE
2	H	79	GLU
2	H	96	SER
2	H	107	LEU
2	H	108	GLN
2	H	129	SER
2	H	157	ILE
2	H	162	ARG
2	H	182	PHE
2	H	185	GLU
2	H	189	LYS
2	H	197	LYS
2	H	206	HIS
2	H	220	LEU
2	H	237	ASN
2	H	279	ILE

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Mol	Chain	Res	Type
2	H	288	LEU
2	H	306	LYS
2	H	313	ILE
2	H	315	GLN
2	H	326	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	55	GLN
1	A	68	GLN
1	A	92	HIS
1	A	125	HIS
1	A	130	ASN
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	187	GLN
2	B	237	ASN
2	B	257	ASN
2	B	328	ASN
1	C	-1	HIS
1	C	3	ASN
1	C	51	GLN
1	C	55	GLN
1	C	63	HIS
1	C	68	GLN
1	C	125	HIS
1	C	135	ASN
1	C	174	GLN
1	C	263	HIS
1	C	353	GLN
2	D	88	GLN
2	D	237	ASN
1	E	55	GLN
1	E	63	HIS
1	E	68	GLN
1	E	130	ASN

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Mol	Chain	Res	Type
1	E	135	ASN
1	E	172	GLN
1	E	279	GLN
1	E	297	ASN
2	F	10	ASN
2	F	32	GLN
2	F	164	ASN
2	F	165	ASN
2	F	172	ASN
2	F	203	GLN
2	F	206	HIS
2	F	237	ASN
2	F	311	ASN
1	G	40	GLN
1	G	63	HIS
1	G	68	GLN
1	G	172	GLN
1	G	263	HIS
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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	20,27,27	1.37	3 (15%)	31,40,40	2.04	12 (38%)
4	TPP	C	1006	3	20,27,27	1.20	2 (10%)	31,40,40	2.24	11 (35%)
4	TPP	E	1009	3	20,27,27	1.31	3 (15%)	31,40,40	2.28	11 (35%)
4	TPP	G	1012	3	20,27,27	1.24	3 (15%)	31,40,40	2.25	11 (35%)

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	-	0/16/17/17	0/2/2/2
4	TPP	C	1006	3	-	0/16/17/17	0/2/2/2
4	TPP	E	1009	3	-	0/16/17/17	0/2/2/2
4	TPP	G	1012	3	-	0/16/17/17	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	TPP	C4-N3	-3.86	1.36	1.39
4	G	1012	TPP	C7'-N3	-2.40	1.44	1.48
4	A	1003	TPP	C7'-N3	-2.27	1.44	1.48
4	C	1006	TPP	C4'-N3'	2.08	1.38	1.35
4	G	1012	TPP	C2'-N1'	2.10	1.38	1.34
4	E	1009	TPP	C4'-N3'	2.12	1.38	1.35
4	A	1003	TPP	C2'-N1'	2.31	1.38	1.34
4	G	1012	TPP	C2'-N3'	2.39	1.38	1.34
4	E	1009	TPP	C2'-N1'	2.43	1.38	1.34
4	C	1006	TPP	C2'-N1'	2.70	1.39	1.34
4	E	1009	TPP	C2'-N3'	2.73	1.39	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1003	TPP	C5'-C7'-N3	-5.00	104.96	113.33
4	E	1009	TPP	PA-O3A-PB	-4.61	117.20	132.67
4	C	1006	TPP	C5'-C7'-N3	-4.25	106.22	113.33
4	E	1009	TPP	CM4-C4-C5	-3.62	120.77	128.90
4	C	1006	TPP	C6-C5-S1	-3.62	115.18	120.24
4	G	1012	TPP	C6-C5-S1	-3.52	115.31	120.24
4	E	1009	TPP	C5'-C7'-N3	-3.37	107.69	113.33
4	C	1006	TPP	N1'-C2'-N3'	-3.35	119.40	125.60
4	G	1012	TPP	C7'-C5'-C6'	-3.28	113.96	120.67
4	E	1009	TPP	N1'-C2'-N3'	-3.21	119.67	125.60
4	G	1012	TPP	C5'-C7'-N3	-3.17	108.03	113.33
4	C	1006	TPP	PA-O3A-PB	-3.13	122.18	132.67
4	C	1006	TPP	C5'-C6'-N1'	-3.11	118.47	123.86
4	A	1003	TPP	C6-C5-S1	-3.08	115.93	120.24
4	A	1003	TPP	C5'-C6'-N1'	-2.98	118.69	123.86
4	E	1009	TPP	C6-C5-S1	-2.95	116.11	120.24
4	A	1003	TPP	PA-O3A-PB	-2.67	123.72	132.67
4	E	1009	TPP	C5'-C6'-N1'	-2.65	119.26	123.86
4	C	1006	TPP	CM4-C4-C5	-2.64	122.97	128.90
4	G	1012	TPP	CM4-C4-C5	-2.56	123.14	128.90
4	C	1006	TPP	C7'-C5'-C6'	-2.45	115.64	120.67
4	G	1012	TPP	C5'-C6'-N1'	-2.44	119.62	123.86
4	A	1003	TPP	CM4-C4-C5	-2.23	123.88	128.90
4	A	1003	TPP	C7'-C5'-C6'	-2.06	116.46	120.67
4	G	1012	TPP	C5'-C4'-N4'	2.01	125.20	122.25
4	A	1003	TPP	O2A-PA-O3A	2.21	115.13	105.09
4	G	1012	TPP	C6'-N1'-C2'	2.22	119.65	115.77
4	A	1003	TPP	C6'-N1'-C2'	2.48	120.11	115.77
4	E	1009	TPP	CM2-C2'-N1'	2.60	120.14	117.03
4	A	1003	TPP	CM2-C2'-N1'	2.65	120.20	117.03
4	A	1003	TPP	CM4-C4-N3	2.86	126.41	122.59
4	E	1009	TPP	C6'-C5'-C4'	2.88	119.85	115.72
4	C	1006	TPP	CM2-C2'-N1'	2.89	120.50	117.03
4	G	1012	TPP	CM4-C4-N3	3.05	126.65	122.59
4	E	1009	TPP	C6'-N1'-C2'	3.07	121.13	115.77
4	G	1012	TPP	C6'-C5'-C4'	3.16	120.25	115.72
4	A	1003	TPP	C6-C5-C4	3.49	130.69	127.56
4	G	1012	TPP	O3A-PA-O7	3.78	112.97	102.94
4	C	1006	TPP	CM4-C4-N3	3.90	127.79	122.59
4	A	1003	TPP	C6'-C5'-C4'	3.90	121.33	115.72
4	C	1006	TPP	C6'-N1'-C2'	4.11	122.95	115.77
4	C	1006	TPP	C6-C5-C4	4.50	131.60	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1009	TPP	CM4-C4-N3	4.85	129.05	122.59
4	E	1009	TPP	C6-C5-C4	4.92	131.97	127.56
4	G	1012	TPP	C6-C5-C4	6.97	133.81	127.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	362/382 (94%)	-0.07	1 (0%) 94 84	8, 21, 37, 52	0
1	C	363/382 (95%)	-0.12	0 100 100	10, 20, 40, 54	0
1	E	363/382 (95%)	-0.10	1 (0%) 94 84	10, 21, 41, 54	0
1	G	362/382 (94%)	-0.05	3 (0%) 87 67	9, 20, 39, 53	0
2	B	329/329 (100%)	-0.18	0 100 100	8, 19, 29, 38	0
2	D	329/329 (100%)	-0.11	3 (0%) 85 64	12, 20, 30, 41	0
2	F	329/329 (100%)	-0.16	2 (0%) 90 73	10, 20, 29, 40	0
2	H	329/329 (100%)	-0.18	0 100 100	7, 19, 28, 42	0
All	All	2766/2844 (97%)	-0.12	10 (0%) 93 80	7, 20, 33, 54	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	329	ILE	3.0
1	A	202	THR	2.5
2	D	184	PRO	2.4
1	G	268	PRO	2.3
1	G	269	GLY	2.2
1	E	266	SER	2.2
1	G	267	ASP	2.1
2	F	329	ILE	2.1
2	D	1	LEU	2.0
2	F	1	LEU	2.0

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 (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
4	TPP	C	1006	26/26	0.96	0.18	0.24	15,22,34,40	0
4	TPP	A	1003	26/26	0.97	0.18	-0.11	16,21,29,33	0
4	TPP	G	1012	26/26	0.97	0.19	-0.16	17,23,35,41	0
4	TPP	E	1009	26/26	0.97	0.17	-0.45	18,27,37,40	0
3	MG	A	1001	1/1	0.99	0.12	-1.03	6,6,6,6	0
3	MG	E	1007	1/1	0.98	0.08	-1.44	30,30,30,30	0
3	MG	G	1010	1/1	0.98	0.11	-1.59	11,11,11,11	0
5	K	F	1011	1/1	0.97	0.11	-1.91	66,66,66,66	0
3	MG	C	1004	1/1	0.97	0.09	-1.95	22,22,22,22	0
5	K	D	1002	1/1	0.94	0.17	-1.98	50,50,50,50	0
5	K	B	1005	1/1	0.96	0.08	-3.67	37,37,37,37	0
5	K	H	1008	1/1	0.93	0.08	-3.74	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.