Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2023 – 11:46 PM EDT

PDB ID	:	2PNR
Title	:	Crystal Structure of the asymmetric Pdk3-l2 Complex
Authors	:	Vassylyev, D.G.; Steussy, C.N.; Devedjiev, Y.
Deposited on	:	2007-04-25
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

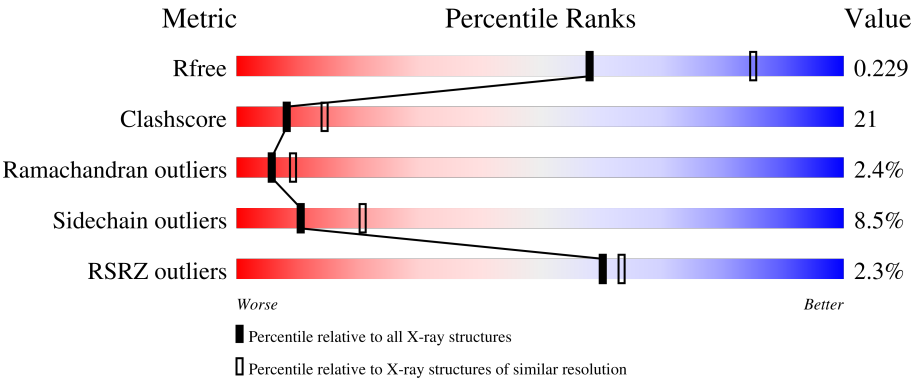
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	419	3% 52% 32% 5% 11%
1	B	419	2% 46% 30% 5% 19%
1	E	419	2% 53% 33% • 11%
1	F	419	% 47% 30% • 19%
2	C	128	2% 30% 26% 5% 38%

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Mol	Chain	Length	Quality of chain
2	G	128	35% 22% 5% 38%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13603 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 [lipoamide]] kinase isozyme 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			3038	1956	508	562	12			
1	B	341	Total	C	N	O	S	0	0	0
			2789	1796	467	513	13			
1	E	374	Total	C	N	O	S	0	0	0
			3038	1956	508	562	12			
1	F	341	Total	C	N	O	S	0	0	0
			2789	1796	467	513	13			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	GLY	-	cloning artifact	UNP Q15120
A	-11	GLY	-	cloning artifact	UNP Q15120
A	-10	SER	-	cloning artifact	UNP Q15120
A	-9	HIS	-	cloning artifact	UNP Q15120
A	-8	HIS	-	cloning artifact	UNP Q15120
A	-7	HIS	-	cloning artifact	UNP Q15120
A	-6	HIS	-	cloning artifact	UNP Q15120
A	-5	HIS	-	cloning artifact	UNP Q15120
A	-4	HIS	-	cloning artifact	UNP Q15120
A	-3	GLY	-	cloning artifact	UNP Q15120
A	-2	MET	-	cloning artifact	UNP Q15120
A	-1	ALA	-	cloning artifact	UNP Q15120
A	0	ARG	-	cloning artifact	UNP Q15120
A	1	LEU	-	cloning artifact	UNP Q15120
A	2	GLU	-	cloning artifact	UNP Q15120
A	3	ASN	-	cloning artifact	UNP Q15120
A	4	LEU	-	cloning artifact	UNP Q15120
A	5	TYR	-	cloning artifact	UNP Q15120
A	6	PHE	-	cloning artifact	UNP Q15120
A	7	GLN	-	cloning artifact	UNP Q15120
A	8	GLY	-	cloning artifact	UNP Q15120

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	GLY	-	cloning artifact	UNP Q15120
B	-11	GLY	-	cloning artifact	UNP Q15120
B	-10	SER	-	cloning artifact	UNP Q15120
B	-9	HIS	-	cloning artifact	UNP Q15120
B	-8	HIS	-	cloning artifact	UNP Q15120
B	-7	HIS	-	cloning artifact	UNP Q15120
B	-6	HIS	-	cloning artifact	UNP Q15120
B	-5	HIS	-	cloning artifact	UNP Q15120
B	-4	HIS	-	cloning artifact	UNP Q15120
B	-3	GLY	-	cloning artifact	UNP Q15120
B	-2	MET	-	cloning artifact	UNP Q15120
B	-1	ALA	-	cloning artifact	UNP Q15120
B	0	ARG	-	cloning artifact	UNP Q15120
B	1	LEU	-	cloning artifact	UNP Q15120
B	2	GLU	-	cloning artifact	UNP Q15120
B	3	ASN	-	cloning artifact	UNP Q15120
B	4	LEU	-	cloning artifact	UNP Q15120
B	5	TYR	-	cloning artifact	UNP Q15120
B	6	PHE	-	cloning artifact	UNP Q15120
B	7	GLN	-	cloning artifact	UNP Q15120
B	8	GLY	-	cloning artifact	UNP Q15120
E	-12	GLY	-	cloning artifact	UNP Q15120
E	-11	GLY	-	cloning artifact	UNP Q15120
E	-10	SER	-	cloning artifact	UNP Q15120
E	-9	HIS	-	cloning artifact	UNP Q15120
E	-8	HIS	-	cloning artifact	UNP Q15120
E	-7	HIS	-	cloning artifact	UNP Q15120
E	-6	HIS	-	cloning artifact	UNP Q15120
E	-5	HIS	-	cloning artifact	UNP Q15120
E	-4	HIS	-	cloning artifact	UNP Q15120
E	-3	GLY	-	cloning artifact	UNP Q15120
E	-2	MET	-	cloning artifact	UNP Q15120
E	-1	ALA	-	cloning artifact	UNP Q15120
E	0	ARG	-	cloning artifact	UNP Q15120
E	1	LEU	-	cloning artifact	UNP Q15120
E	2	GLU	-	cloning artifact	UNP Q15120
E	3	ASN	-	cloning artifact	UNP Q15120
E	4	LEU	-	cloning artifact	UNP Q15120
E	5	TYR	-	cloning artifact	UNP Q15120
E	6	PHE	-	cloning artifact	UNP Q15120
E	7	GLN	-	cloning artifact	UNP Q15120
E	8	GLY	-	cloning artifact	UNP Q15120

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-12	GLY	-	cloning artifact	UNP Q15120
F	-11	GLY	-	cloning artifact	UNP Q15120
F	-10	SER	-	cloning artifact	UNP Q15120
F	-9	HIS	-	cloning artifact	UNP Q15120
F	-8	HIS	-	cloning artifact	UNP Q15120
F	-7	HIS	-	cloning artifact	UNP Q15120
F	-6	HIS	-	cloning artifact	UNP Q15120
F	-5	HIS	-	cloning artifact	UNP Q15120
F	-4	HIS	-	cloning artifact	UNP Q15120
F	-3	GLY	-	cloning artifact	UNP Q15120
F	-2	MET	-	cloning artifact	UNP Q15120
F	-1	ALA	-	cloning artifact	UNP Q15120
F	0	ARG	-	cloning artifact	UNP Q15120
F	1	LEU	-	cloning artifact	UNP Q15120
F	2	GLU	-	cloning artifact	UNP Q15120
F	3	ASN	-	cloning artifact	UNP Q15120
F	4	LEU	-	cloning artifact	UNP Q15120
F	5	TYR	-	cloning artifact	UNP Q15120
F	6	PHE	-	cloning artifact	UNP Q15120
F	7	GLN	-	cloning artifact	UNP Q15120
F	8	GLY	-	cloning artifact	UNP Q15120

- Molecule 2 is a protein called Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	79	Total	C	N	O	S	0	0	0
			602	384	94	121	3			
2	G	79	Total	C	N	O	S	0	0	0
			602	384	94	121	3			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	106	GLY	-	cloning artifact	UNP P10515
C	107	GLY	-	cloning artifact	UNP P10515
C	108	SER	-	cloning artifact	UNP P10515
C	109	HIS	-	cloning artifact	UNP P10515
C	110	HIS	-	cloning artifact	UNP P10515
C	111	HIS	-	cloning artifact	UNP P10515
C	112	HIS	-	cloning artifact	UNP P10515
C	113	HIS	-	cloning artifact	UNP P10515

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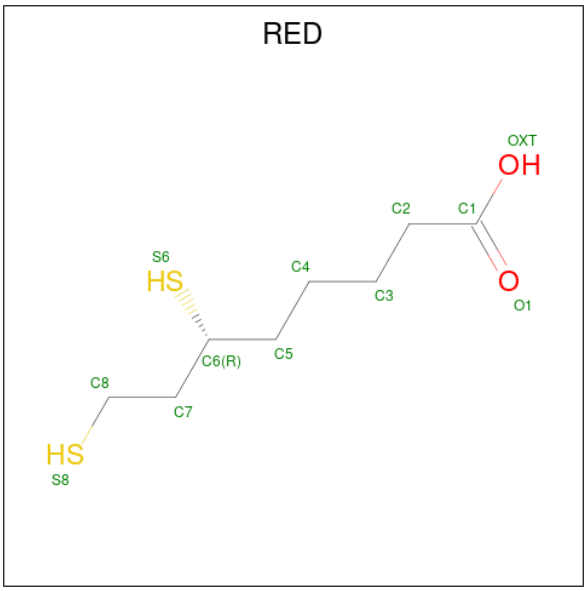
Chain	Residue	Modelled	Actual	Comment	Reference
C	114	HIS	-	cloning artifact	UNP P10515
C	115	GLY	-	cloning artifact	UNP P10515
C	116	MET	-	cloning artifact	UNP P10515
C	117	ALA	-	cloning artifact	UNP P10515
C	118	ARG	-	cloning artifact	UNP P10515
C	119	LEU	-	cloning artifact	UNP P10515
C	120	GLU	-	cloning artifact	UNP P10515
C	121	ASN	-	cloning artifact	UNP P10515
C	122	LEU	-	cloning artifact	UNP P10515
C	123	TYR	-	cloning artifact	UNP P10515
C	124	PHE	-	cloning artifact	UNP P10515
C	125	GLN	-	cloning artifact	UNP P10515
G	106	GLY	-	cloning artifact	UNP P10515
G	107	GLY	-	cloning artifact	UNP P10515
G	108	SER	-	cloning artifact	UNP P10515
G	109	HIS	-	cloning artifact	UNP P10515
G	110	HIS	-	cloning artifact	UNP P10515
G	111	HIS	-	cloning artifact	UNP P10515
G	112	HIS	-	cloning artifact	UNP P10515
G	113	HIS	-	cloning artifact	UNP P10515
G	114	HIS	-	cloning artifact	UNP P10515
G	115	GLY	-	cloning artifact	UNP P10515
G	116	MET	-	cloning artifact	UNP P10515
G	117	ALA	-	cloning artifact	UNP P10515
G	118	ARG	-	cloning artifact	UNP P10515
G	119	LEU	-	cloning artifact	UNP P10515
G	120	GLU	-	cloning artifact	UNP P10515
G	121	ASN	-	cloning artifact	UNP P10515
G	122	LEU	-	cloning artifact	UNP P10515
G	123	TYR	-	cloning artifact	UNP P10515
G	124	PHE	-	cloning artifact	UNP P10515
G	125	GLN	-	cloning artifact	UNP P10515

- Molecule 3 is DIHYDROLIPOIC ACID (three-letter code: RED) (formula: $C_8H_{16}O_2S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O S 11 8 1 2	0	0
3	G	1	Total C O S 11 8 1 2	0	0

- Molecule 4 is water.

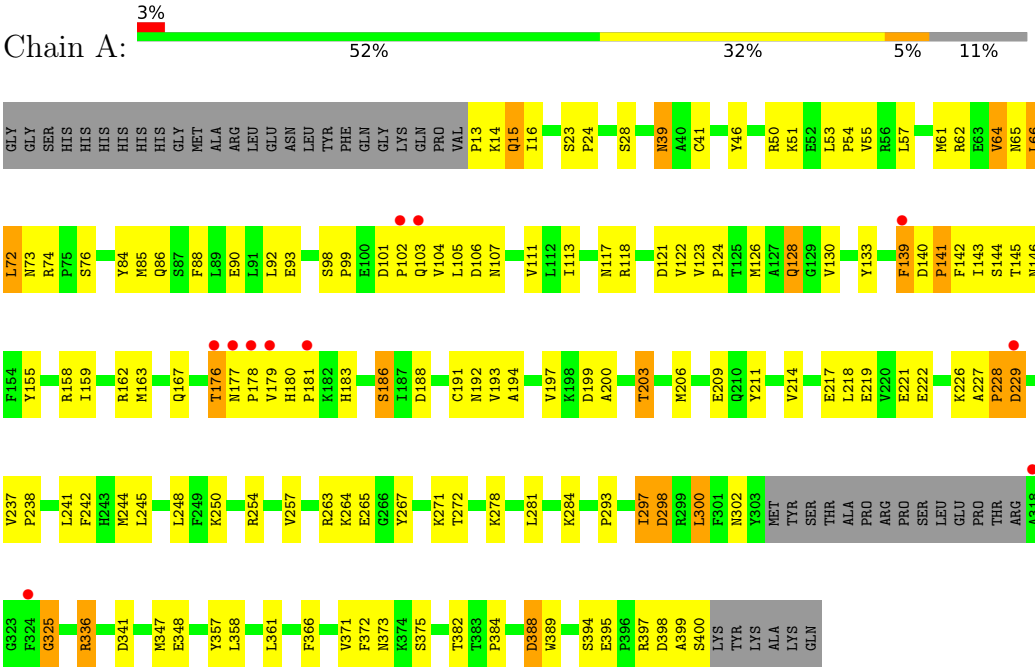
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	172	Total O 172 172	0	0
4	B	165	Total O 165 165	0	0
4	C	26	Total O 26 26	0	0
4	E	172	Total O 172 172	0	0
4	F	155	Total O 155 155	0	0
4	G	33	Total O 33 33	0	0

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.

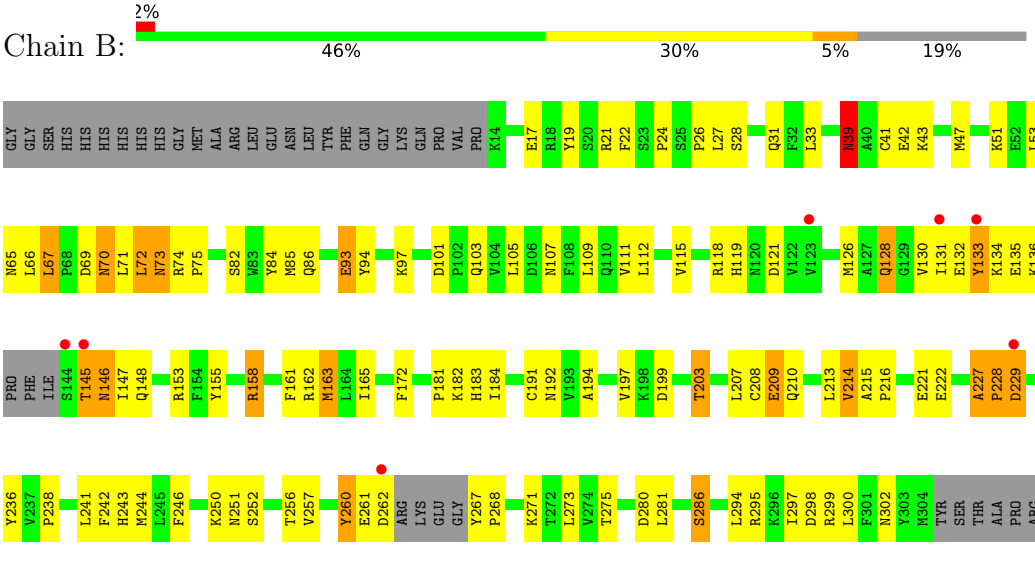
• Molecule 1: [Pyruvate dehydrogenase [lipoamide]] kinase isozyme 3

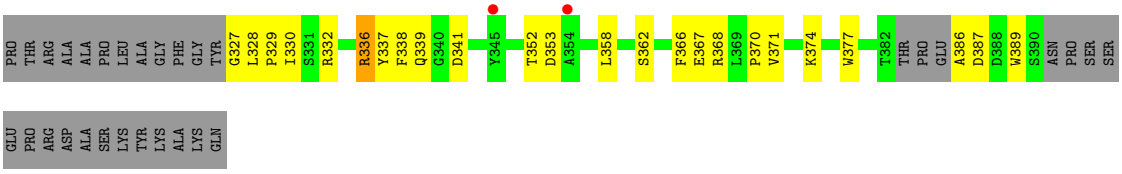
Chain A:



• Molecule 1: [Pyruvate dehydrogenase [lipoamide]] kinase isozyme 3

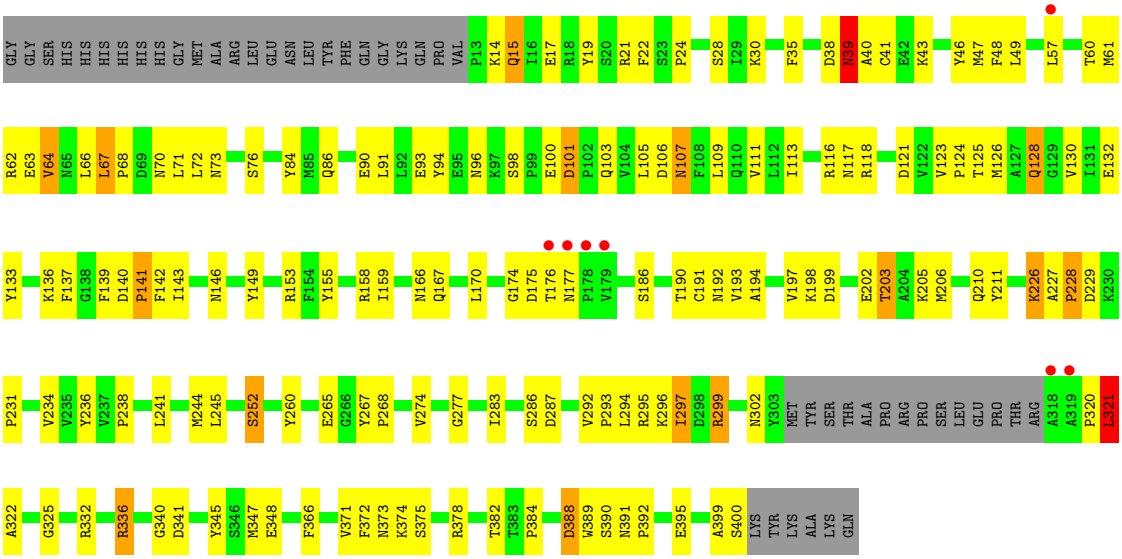
Chain B:





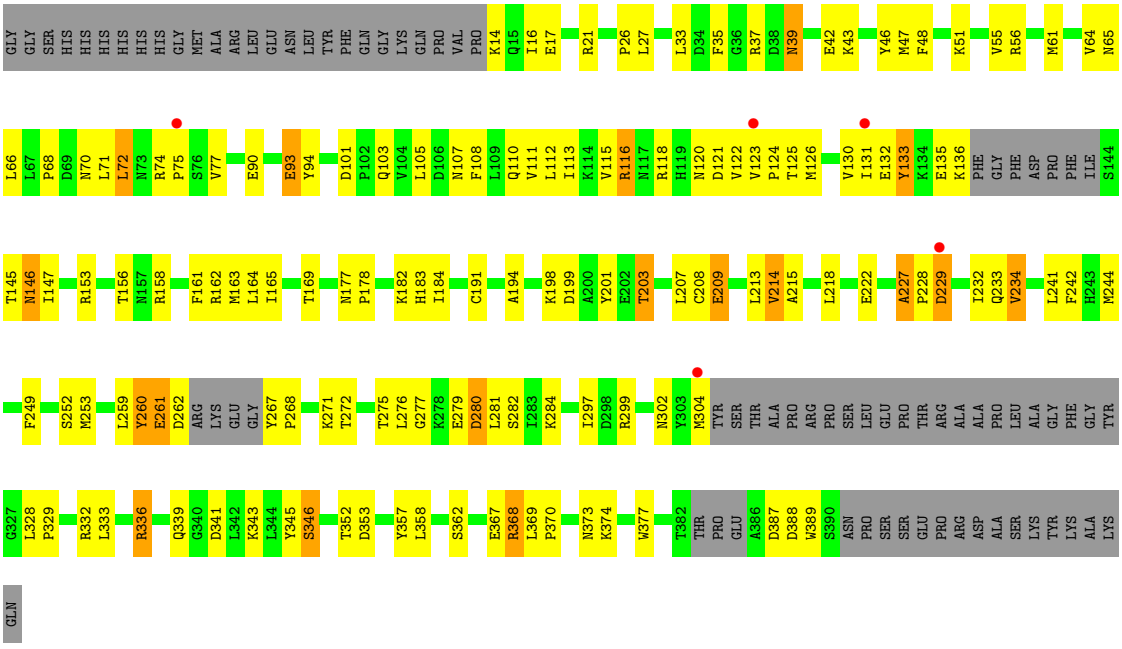
• Molecule 1: [Pyruvate dehydrogenase [lipoamide]] kinase isozyme 3

Chain E:



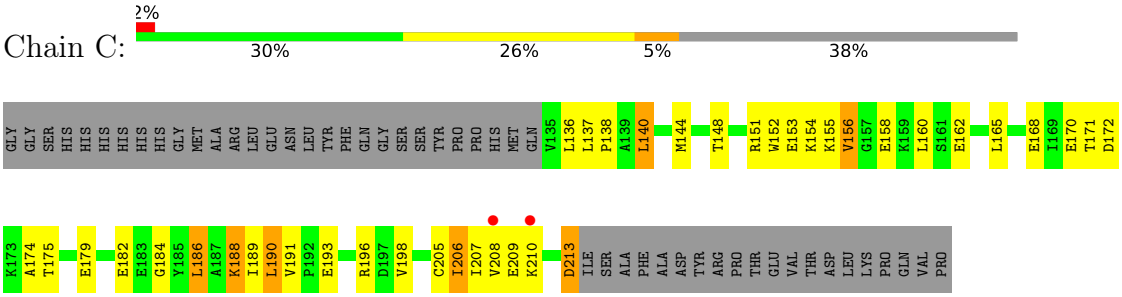
• Molecule 1: [Pyruvate dehydrogenase [lipoamide]] kinase isozyme 3

Chain F:



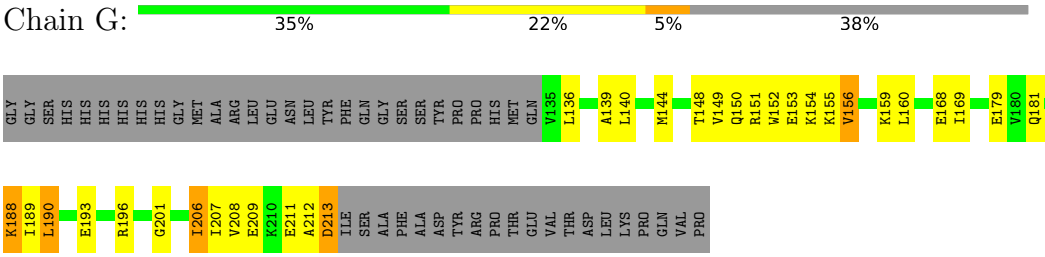
• Molecule 2: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex

Chain C:



• Molecule 2: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	96.16Å 96.16Å 222.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.43 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.9 (30.00-2.50) 93.0 (29.43-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.176 , 0.229 0.176 , 0.229	Depositor DCC
R_{free} test set	3746 reflections (5.79%)	wwPDB-VP
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 83.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.190 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13603	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RED

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	0.69	0/3116	0.77	1/4222 (0.0%)
1	B	0.68	0/2853	0.75	0/3858
1	E	0.69	0/3116	0.78	1/4222 (0.0%)
1	F	0.68	0/2853	0.76	0/3858
2	C	0.57	0/610	0.77	0/827
2	G	0.59	0/610	0.78	0/827
All	All	0.68	0/13158	0.77	2/17814 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	321	LEU	N-CA-C	7.43	131.07	111.00
1	E	321	LEU	N-CA-C	7.10	130.18	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3038	0	3003	113	0
1	B	2789	0	2774	139	0
1	E	3038	0	3003	129	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2789	0	2774	125	0
2	C	602	0	618	35	0
2	G	602	0	618	33	0
3	C	11	0	15	0	0
3	G	11	0	15	2	0
4	A	172	0	0	31	0
4	B	165	0	0	22	0
4	C	26	0	0	7	0
4	E	172	0	0	25	0
4	F	155	0	0	23	0
4	G	33	0	0	6	0
All	All	13603	0	12820	541	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 21.

All (541) 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:A:211:TYR:HB3	1:A:321:LEU:HD21	1.47	0.94
2:C:182:GLU:HG3	4:C:924:HOH:O	1.72	0.90
1:A:278:LYS:HD3	4:B:541:HOH:O	1.72	0.89
1:E:14:LYS:HB2	4:E:492:HOH:O	1.74	0.88
1:B:241:LEU:HA	1:B:244:MET:HE3	1.54	0.86
1:F:343:LYS:HA	4:F:475:HOH:O	1.75	0.85
1:A:149:TYR:HA	4:A:488:HOH:O	1.76	0.83
1:A:395:GLU:HG2	4:A:531:HOH:O	1.77	0.83
1:F:70:ASN:HB3	1:F:136:LYS:HE2	1.60	0.83
1:F:131:ILE:HG12	4:F:545:HOH:O	1.80	0.81
1:E:399:ALA:HB1	1:F:35:PHE:HB2	1.62	0.80
1:F:125:THR:HB	4:F:506:HOH:O	1.79	0.80
1:F:68:PRO:HB2	4:F:496:HOH:O	1.81	0.80
1:F:199:ASP:O	1:F:203:THR:HG23	1.81	0.80
1:E:395:GLU:HG2	4:E:453:HOH:O	1.80	0.80
1:B:24:PRO:HD2	1:B:371:VAL:HG22	1.64	0.79
1:A:167:GLN:HE22	1:A:186:SER:H	1.31	0.78
1:B:70:ASN:HB3	1:B:136:LYS:HE2	1.65	0.78
1:E:211:TYR:HB3	1:E:321:LEU:HD21	1.66	0.78
1:A:15:GLN:HA	1:A:15:GLN:HE21	1.49	0.78
1:B:203:THR:HG21	1:B:242:PHE:HZ	1.49	0.77
1:A:70:ASN:HB2	1:A:133:TYR:HE2	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:ASN:HD21	1:F:388:ASP:HA	1.51	0.76
1:A:14:LYS:HB2	4:A:462:HOH:O	1.85	0.75
1:E:96:ASN:HB2	4:E:519:HOH:O	1.86	0.75
2:G:190:LEU:HD11	2:G:206:ILE:HD11	1.68	0.75
1:F:120:ASN:HA	4:F:503:HOH:O	1.87	0.75
1:F:68:PRO:HB3	4:F:550:HOH:O	1.86	0.74
1:A:254:ARG:HD2	4:A:432:HOH:O	1.86	0.74
1:F:74:ARG:HD3	1:F:132:GLU:HB2	1.68	0.73
1:A:221:GLU:HG3	4:A:481:HOH:O	1.87	0.73
2:G:208:VAL:HG21	2:G:213:ASP:HB2	1.68	0.73
1:F:368:ARG:O	1:F:368:ARG:HG3	1.88	0.72
1:A:13:PRO:HB3	4:A:456:HOH:O	1.88	0.72
2:C:190:LEU:HD11	2:C:206:ILE:HD11	1.71	0.72
1:B:134:LYS:HG3	4:B:515:HOH:O	1.89	0.71
1:E:293:PRO:HA	1:F:280:ASP:OD2	1.91	0.71
2:C:148:THR:HG23	2:C:196:ARG:HA	1.70	0.71
1:E:126:MET:HE2	1:E:130:VAL:HG13	1.71	0.71
1:E:98:SER:OG	1:E:100:GLU:HG2	1.91	0.71
1:B:330:ILE:HG12	4:B:434:HOH:O	1.90	0.70
1:B:74:ARG:HD3	1:B:132:GLU:HB2	1.71	0.70
1:E:167:GLN:HE22	1:E:186:SER:H	1.38	0.70
1:F:110:GLN:HG3	4:F:554:HOH:O	1.92	0.69
1:F:336:ARG:HD3	1:F:341:ASP:OD1	1.92	0.69
1:B:298:ASP:HB2	4:B:436:HOH:O	1.91	0.69
1:A:74:ARG:HB3	4:A:425:HOH:O	1.92	0.69
1:E:62:ARG:O	1:E:66:LEU:HD13	1.93	0.69
1:B:368:ARG:HG3	1:B:368:ARG:O	1.92	0.69
1:A:72:LEU:HD12	4:A:577:HOH:O	1.94	0.68
1:B:199:ASP:O	1:B:203:THR:HG23	1.94	0.68
1:E:192:ASN:HB2	4:E:411:HOH:O	1.94	0.68
2:G:151:ARG:HB3	2:G:168:GLU:HG3	1.74	0.68
1:A:39:ASN:ND2	1:A:41:CYS:HB2	2.09	0.68
1:F:68:PRO:HG3	4:F:435:HOH:O	1.94	0.68
2:G:212:ALA:HA	4:G:914:HOH:O	1.93	0.68
1:E:211:TYR:HB3	1:E:321:LEU:CD2	2.22	0.68
1:B:332:ARG:O	1:B:336:ARG:HG2	1.94	0.67
1:E:390:SER:HB2	1:F:26:PRO:HG3	1.75	0.67
1:F:281:LEU:HD23	1:F:358:LEU:HD12	1.75	0.67
1:A:397:ARG:NE	2:C:172:ASP:OD2	2.27	0.67
1:B:28:SER:OG	1:B:31:GLN:HG3	1.94	0.67
1:A:57:LEU:O	1:A:61:MET:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:156:VAL:HA	2:C:186:LEU:HB3	1.76	0.67
1:A:102:PRO:O	1:A:106:ASP:HB2	1.95	0.67
1:F:101:ASP:OD2	1:F:103:GLN:HB3	1.95	0.67
4:A:420:HOH:O	1:B:386:ALA:HB3	1.95	0.66
1:B:42:GLU:HG2	1:B:105:LEU:HD23	1.77	0.66
1:A:167:GLN:NE2	1:A:186:SER:H	1.93	0.66
1:A:336:ARG:HD3	1:A:341:ASP:OD1	1.96	0.66
1:B:332:ARG:HD3	1:B:336:ARG:CZ	2.26	0.66
1:B:158:ARG:HB2	4:B:499:HOH:O	1.96	0.65
1:E:15:GLN:HE21	1:E:15:GLN:HA	1.62	0.65
1:F:232:ILE:HG23	1:F:276:LEU:HD22	1.79	0.64
1:A:197:VAL:HA	1:A:245:LEU:HD13	1.79	0.64
1:A:199:ASP:O	1:A:203:THR:HG23	1.96	0.64
1:B:101:ASP:OD2	1:B:103:GLN:HB3	1.98	0.64
1:E:155:TYR:O	1:E:159:ILE:HG13	1.98	0.64
1:F:21:ARG:HH11	1:F:21:ARG:HB2	1.62	0.64
2:C:208:VAL:HG21	2:C:213:ASP:HB2	1.80	0.63
1:E:321:LEU:HD11	4:E:484:HOH:O	1.97	0.63
1:A:28:SER:HB3	1:A:366:PHE:CE1	2.33	0.63
1:E:226:LYS:HE2	1:E:277:GLY:O	1.98	0.63
1:A:140:ASP:HB2	1:A:141:PRO:HD2	1.81	0.63
1:A:236:TYR:O	1:A:238:PRO:HD3	1.98	0.63
1:A:62:ARG:O	1:A:66:LEU:HD13	1.99	0.62
1:A:62:ARG:HG2	1:A:372:PHE:CE2	2.34	0.62
1:B:208:CYS:SG	1:B:215:ALA:HB2	2.40	0.62
1:B:51:LYS:HE3	4:B:533:HOH:O	1.98	0.62
1:E:64:VAL:O	1:E:67:LEU:HD22	1.99	0.62
1:A:99:PRO:HD3	4:A:417:HOH:O	1.99	0.62
1:F:234:VAL:HG23	4:F:479:HOH:O	1.98	0.62
1:F:74:ARG:CZ	1:F:74:ARG:HA	2.29	0.62
1:A:382:THR:HB	4:A:501:HOH:O	2.00	0.62
1:E:60:THR:O	1:E:64:VAL:HG12	1.99	0.62
1:F:271:LYS:HE2	4:F:446:HOH:O	2.00	0.62
1:E:336:ARG:HD3	1:E:341:ASP:OD1	2.00	0.61
1:E:336:ARG:HA	1:E:340:GLY:O	2.01	0.61
1:E:35:PHE:HD1	4:E:469:HOH:O	1.84	0.61
1:B:61:MET:HA	1:B:64:VAL:HG12	1.82	0.61
2:G:181:GLN:NE2	2:G:181:GLN:HA	2.14	0.61
1:E:206:MET:O	1:E:210:GLN:HG2	2.00	0.61
1:A:126:MET:HE2	1:A:130:VAL:HG13	1.82	0.60
1:F:61:MET:HA	1:F:64:VAL:HG12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:384:PRO:HA	4:E:483:HOH:O	2.00	0.60
1:F:74:ARG:HD3	1:F:132:GLU:CB	2.32	0.60
1:F:162:ARG:HD3	4:F:503:HOH:O	2.01	0.60
1:B:192:ASN:HD21	1:B:233:GLN:HE21	1.49	0.60
1:A:145:THR:HG21	4:A:530:HOH:O	2.01	0.60
1:E:48:PHE:HD2	1:E:49:LEU:HD23	1.67	0.60
1:B:146:ASN:H	1:B:147:ILE:HD12	1.67	0.59
1:E:62:ARG:HG2	1:E:372:PHE:CE2	2.37	0.59
1:A:180:HIS:HB2	4:A:447:HOH:O	2.02	0.59
1:A:158:ARG:HH22	1:A:162:ARG:HH21	1.50	0.59
1:A:302:ASN:HB3	4:A:450:HOH:O	2.00	0.59
2:C:154:LYS:HA	4:C:903:HOH:O	2.02	0.59
2:G:151:ARG:H	2:G:168:GLU:HB2	1.67	0.59
1:E:143:ILE:O	1:E:146:ASN:HB2	2.01	0.59
1:F:74:ARG:HB3	1:F:132:GLU:OE1	2.02	0.59
1:A:14:LYS:HG2	4:A:438:HOH:O	2.03	0.59
1:F:213:LEU:O	1:F:214:VAL:HG23	2.02	0.59
1:F:203:THR:HG21	1:F:242:PHE:HZ	1.68	0.58
1:E:30:LYS:HE3	4:E:553:HOH:O	2.02	0.58
1:A:86:GLN:O	1:A:90:GLU:HG3	2.04	0.58
1:A:24:PRO:HD2	1:A:371:VAL:HG22	1.85	0.58
1:B:147:ILE:HD12	1:B:147:ILE:H	1.69	0.58
1:A:293:PRO:HD3	1:A:348:GLU:OE2	2.03	0.58
1:F:70:ASN:CB	1:F:136:LYS:HE2	2.31	0.58
1:E:227:ALA:O	1:E:229:ASP:N	2.34	0.57
1:B:241:LEU:HA	1:B:244:MET:CE	2.30	0.57
1:E:35:PHE:HB2	4:E:469:HOH:O	2.04	0.57
2:G:151:ARG:N	2:G:168:GLU:HB2	2.20	0.57
1:B:213:LEU:HB2	4:B:428:HOH:O	2.04	0.57
1:E:123:VAL:HB	1:E:124:PRO:HD3	1.87	0.57
1:E:24:PRO:HD2	1:E:371:VAL:HG22	1.87	0.56
1:E:136:LYS:HE2	4:E:568:HOH:O	2.05	0.56
1:A:176:THR:O	1:A:178:PRO:HD3	2.04	0.56
1:E:17:GLU:O	1:E:21:ARG:HG3	2.05	0.56
1:A:227:ALA:O	1:A:229:ASP:N	2.38	0.56
1:B:374:LYS:HB2	2:C:179:GLU:OE2	2.05	0.56
1:E:137:PHE:HB3	4:E:516:HOH:O	2.05	0.56
1:F:121:ASP:HB2	4:F:542:HOH:O	2.06	0.56
1:F:332:ARG:HD3	1:F:336:ARG:CZ	2.36	0.56
2:C:138:PRO:HG2	2:C:140:LEU:CD1	2.35	0.56
1:A:144:SER:HB2	4:A:496:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ASP:O	1:B:73:ASN:HB2	2.05	0.56
1:E:109:LEU:O	1:E:113:ILE:HD13	2.06	0.56
1:A:123:VAL:HB	1:A:124:PRO:HD3	1.87	0.56
1:A:142:PHE:CD2	1:A:384:PRO:HG3	2.40	0.56
1:F:51:LYS:HE3	4:F:427:HOH:O	2.06	0.56
2:G:188:LYS:O	2:G:206:ILE:HD12	2.06	0.56
1:E:106:ASP:HB2	4:E:548:HOH:O	2.06	0.56
1:A:62:ARG:HG2	1:A:372:PHE:CD2	2.41	0.56
1:E:231:PRO:HB3	4:E:558:HOH:O	2.05	0.56
1:B:107:ASN:O	1:B:111:VAL:HG23	2.07	0.56
1:F:27:LEU:HD21	3:G:901:RED:H32	1.87	0.55
1:A:244:MET:O	1:A:248:LEU:HG	2.06	0.55
1:A:139:PHE:HD1	4:A:483:HOH:O	1.89	0.55
1:A:217:GLU:HG2	4:A:439:HOH:O	2.06	0.55
1:B:118:ARG:HB3	1:B:119:HIS:ND1	2.22	0.55
1:F:124:PRO:HG3	4:F:438:HOH:O	2.05	0.55
1:B:260:TYR:CE2	1:B:268:PRO:HG2	2.41	0.55
1:E:241:LEU:HA	1:E:244:MET:CE	2.36	0.55
1:B:75:PRO:HD2	1:B:132:GLU:OE1	2.06	0.55
1:E:197:VAL:HA	1:E:245:LEU:HD13	1.87	0.55
2:G:151:ARG:HG2	2:G:153:GLU:OE2	2.07	0.55
1:B:74:ARG:HD3	1:B:132:GLU:CB	2.37	0.55
1:B:228:PRO:HA	4:B:447:HOH:O	2.07	0.55
1:B:236:TYR:O	1:B:238:PRO:HD3	2.06	0.55
1:E:389:TRP:CZ3	1:F:370:PRO:HG3	2.42	0.55
1:E:28:SER:HA	1:E:366:PHE:HA	1.88	0.55
1:F:90:GLU:O	1:F:93:GLU:HG3	2.07	0.55
1:F:21:ARG:HB2	1:F:21:ARG:NH1	2.21	0.55
1:A:62:ARG:O	1:A:65:ASN:HB3	2.07	0.54
1:B:93:GLU:O	1:B:97:LYS:HE3	2.08	0.54
1:F:116:ARG:HG3	1:F:116:ARG:HH11	1.72	0.54
1:B:181:PRO:HD2	4:B:410:HOH:O	2.07	0.54
1:B:281:LEU:HD23	1:B:358:LEU:HD12	1.89	0.54
1:B:257:VAL:HA	1:B:267:TYR:CE1	2.41	0.54
1:E:63:GLU:HG2	1:E:372:PHE:HD1	1.71	0.54
1:F:16:ILE:HD12	4:F:415:HOH:O	2.06	0.54
2:G:156:VAL:HA	2:G:186:LEU:HB3	1.89	0.54
1:B:19:TYR:HA	1:B:22:PHE:HD1	1.71	0.54
1:F:103:GLN:HA	1:F:103:GLN:OE1	2.07	0.54
1:A:13:PRO:HA	1:A:16:ILE:HB	1.90	0.54
1:B:158:ARG:CB	4:B:499:HOH:O	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:LEU:HA	1:F:244:MET:CE	2.38	0.54
2:G:148:THR:HG23	2:G:196:ARG:HA	1.88	0.54
1:A:46:TYR:HD2	1:A:99:PRO:HB3	1.72	0.53
1:E:67:LEU:HG	1:E:71:LEU:HD23	1.90	0.53
1:E:123:VAL:HG13	1:E:155:TYR:CE1	2.43	0.53
1:B:82:SER:O	1:B:85:MET:HB3	2.08	0.53
1:B:192:ASN:HD21	1:B:233:GLN:NE2	2.05	0.53
1:A:84:TYR:HE1	1:A:122:VAL:HG21	1.73	0.53
1:B:27:LEU:O	1:B:367:GLU:HG3	2.09	0.53
1:E:274:VAL:HG22	1:E:283:ILE:HG23	1.89	0.53
1:F:27:LEU:O	1:F:367:GLU:HG3	2.08	0.53
1:F:108:PHE:CE2	1:F:112:LEU:HD11	2.44	0.53
1:E:86:GLN:O	1:E:90:GLU:HG3	2.07	0.53
1:F:14:LYS:N	4:F:415:HOH:O	2.41	0.53
2:G:185:TYR:CE1	2:G:211:GLU:HB3	2.43	0.53
1:B:192:ASN:ND2	1:B:233:GLN:HE21	2.07	0.53
1:E:389:TRP:CZ2	1:F:153:ARG:HG2	2.44	0.53
1:F:147:ILE:HD12	1:F:147:ILE:H	1.74	0.53
1:E:48:PHE:CD2	1:E:49:LEU:HD23	2.43	0.53
1:B:158:ARG:HA	1:B:161:PHE:CD1	2.44	0.53
1:F:135:GLU:O	1:F:136:LYS:HB2	2.08	0.53
1:E:60:THR:HG21	1:E:84:TYR:HE2	1.74	0.53
1:E:126:MET:CE	1:E:130:VAL:HG13	2.38	0.53
1:F:208:CYS:SG	1:F:215:ALA:HB2	2.49	0.53
2:C:210:LYS:HA	4:C:916:HOH:O	2.09	0.52
1:F:272:THR:HA	1:F:284:LYS:O	2.09	0.52
1:E:193:VAL:O	1:E:197:VAL:HG23	2.08	0.52
1:E:295:ARG:HD3	4:F:504:HOH:O	2.09	0.52
1:F:123:VAL:HG11	4:F:473:HOH:O	2.08	0.52
1:F:299:ARG:HD2	1:F:304:MET:CE	2.40	0.52
2:C:155:LYS:HB2	2:C:158:GLU:HG3	1.91	0.52
1:B:339:GLN:NE2	1:B:368:ARG:HB3	2.24	0.52
1:E:389:TRP:HZ3	1:F:156:THR:HG21	1.75	0.52
1:E:15:GLN:HE21	1:E:15:GLN:CA	2.21	0.52
1:E:17:GLU:OE2	1:E:21:ARG:HD2	2.10	0.52
1:A:361:LEU:HD13	4:A:470:HOH:O	2.10	0.52
1:F:297:ILE:HD11	1:F:346:SER:HB2	1.90	0.52
1:E:194:ALA:O	1:E:198:LYS:HG3	2.09	0.52
1:F:61:MET:O	1:F:64:VAL:HG12	2.10	0.52
2:G:155:LYS:HB3	4:G:927:HOH:O	2.08	0.52
1:E:117:ASN:ND2	4:E:507:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:LYS:O	1:F:47:MET:HG2	2.10	0.51
1:F:72:LEU:HA	1:F:77:VAL:HG11	1.92	0.51
2:G:207:ILE:HG22	2:G:208:VAL:N	2.25	0.51
1:A:271:LYS:HE3	4:A:431:HOH:O	2.11	0.51
1:B:260:TYR:CZ	1:B:268:PRO:HG2	2.45	0.51
1:F:56:ARG:NH1	1:F:164:LEU:HD11	2.26	0.51
1:F:75:PRO:HD2	1:F:132:GLU:OE1	2.10	0.51
1:B:163:MET:CE	1:B:163:MET:HA	2.41	0.51
1:E:39:ASN:HD21	1:E:41:CYS:HB3	1.75	0.51
1:E:68:PRO:CB	4:E:563:HOH:O	2.59	0.51
1:B:107:ASN:ND2	4:B:570:HOH:O	2.42	0.51
1:B:336:ARG:HD3	1:B:341:ASP:OD1	2.11	0.51
2:C:170:GLU:HG3	2:C:175:THR:OG1	2.10	0.51
1:B:21:ARG:NH1	1:B:21:ARG:HB2	2.26	0.51
1:B:112:LEU:HB3	1:B:165:ILE:HG23	1.93	0.51
1:B:153:ARG:HB3	1:B:370:PRO:HB3	1.93	0.51
1:E:140:ASP:HB2	1:E:141:PRO:HD2	1.93	0.51
1:E:153:ARG:HG2	1:F:389:TRP:CZ2	2.46	0.51
1:E:15:GLN:HA	1:E:15:GLN:NE2	2.25	0.51
1:F:165:ILE:O	1:F:169:THR:HG23	2.11	0.51
1:B:213:LEU:O	1:B:214:VAL:HG23	2.10	0.50
1:E:202:GLU:O	1:E:205:LYS:HB3	2.11	0.50
1:F:373:ASN:HB2	2:G:179:GLU:OE1	2.11	0.50
1:A:64:VAL:O	1:A:67:LEU:HD22	2.10	0.50
1:B:199:ASP:O	1:B:203:THR:CG2	2.59	0.50
2:C:154:LYS:HG2	2:C:160:LEU:CD2	2.41	0.50
1:A:140:ASP:OD2	1:A:143:ILE:HB	2.11	0.50
1:A:398:ASP:HA	4:A:548:HOH:O	2.11	0.50
2:G:139:ALA:HA	2:G:144:MET:SD	2.51	0.50
1:A:85:MET:O	1:A:88:PHE:HB3	2.12	0.50
1:B:33:LEU:HD12	1:B:184:ILE:HG13	1.94	0.50
2:G:159:LYS:HE3	4:G:904:HOH:O	2.12	0.50
1:B:222:GLU:HB3	1:B:232:ILE:HD12	1.94	0.49
2:C:153:GLU:HG3	2:C:165:LEU:HD21	1.93	0.49
1:E:140:ASP:OD2	1:E:143:ILE:HB	2.12	0.49
1:E:345:TYR:CZ	1:F:345:TYR:HB3	2.47	0.49
1:B:115:VAL:HG12	1:B:118:ARG:NH2	2.27	0.49
1:B:221:GLU:OE2	1:B:221:GLU:HA	2.12	0.49
1:F:374:LYS:O	1:F:377:TRP:HB3	2.12	0.49
1:B:286:SER:HB3	1:B:353:ASP:OD1	2.12	0.49
1:B:338:PHE:HB2	4:B:409:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:ILE:HD12	1:F:147:ILE:N	2.28	0.49
1:E:70:ASN:HB2	4:E:563:HOH:O	2.11	0.49
1:E:107:ASN:O	1:E:111:VAL:HG23	2.13	0.49
1:E:322:ALA:CB	4:E:525:HOH:O	2.60	0.49
1:F:51:LYS:O	1:F:55:VAL:HG23	2.13	0.49
1:A:67:LEU:HG	1:A:71:LEU:HD23	1.93	0.49
1:A:163:MET:HE1	1:A:237:VAL:HG21	1.94	0.49
1:B:162:ARG:NH2	4:B:499:HOH:O	2.42	0.49
1:B:132:GLU:C	1:B:134:LYS:H	2.16	0.49
1:B:135:GLU:O	1:B:136:LYS:HB2	2.13	0.49
1:B:271:LYS:HG3	4:B:424:HOH:O	2.12	0.49
1:A:121:ASP:C	1:A:124:PRO:HD2	2.33	0.49
1:B:208:CYS:O	1:B:210:GLN:N	2.46	0.49
1:B:28:SER:H	1:B:31:GLN:HE21	1.60	0.48
1:F:227:ALA:O	1:F:229:ASP:N	2.45	0.48
1:E:137:PHE:HD2	4:E:516:HOH:O	1.95	0.48
1:F:339:GLN:NE2	1:F:368:ARG:HB3	2.29	0.48
1:B:221:GLU:O	1:B:273:LEU:HD12	2.13	0.48
1:E:39:ASN:C	1:E:39:ASN:HD22	2.17	0.48
1:E:142:PHE:CD2	1:E:384:PRO:HG3	2.49	0.48
1:A:347:MET:HE1	1:B:275:THR:HG23	1.96	0.48
1:B:28:SER:HA	1:B:366:PHE:HA	1.95	0.48
1:B:121:ASP:OD1	1:B:162:ARG:NH2	2.47	0.48
1:B:257:VAL:HG22	1:B:267:TYR:CZ	2.49	0.48
1:B:297:ILE:O	1:B:300:LEU:HB2	2.13	0.48
1:F:42:GLU:HG2	1:F:105:LEU:HD23	1.96	0.48
1:B:250:LYS:HE2	1:B:251:ASN:ND2	2.28	0.48
1:F:46:TYR:OH	1:F:94:TYR:HB3	2.14	0.48
1:F:135:GLU:O	1:F:136:LYS:CB	2.61	0.48
1:A:90:GLU:CD	1:A:118:ARG:HH12	2.16	0.48
1:B:74:ARG:HB3	1:B:132:GLU:OE1	2.14	0.48
1:B:135:GLU:O	1:B:136:LYS:CB	2.62	0.48
1:B:136:LYS:NZ	1:B:136:LYS:HB3	2.28	0.48
2:C:137:LEU:HD12	2:C:138:PRO:HD2	1.95	0.48
4:A:519:HOH:O	1:B:295:ARG:HG3	2.14	0.48
1:B:43:LYS:O	1:B:47:MET:HG2	2.14	0.48
1:F:94:TYR:CD1	1:F:94:TYR:N	2.82	0.47
1:E:241:LEU:HA	1:E:244:MET:HE3	1.96	0.47
1:E:373:ASN:OD1	1:E:375:SER:HB3	2.14	0.47
2:C:138:PRO:O	2:C:144:MET:HE1	2.14	0.47
1:E:375:SER:HB3	1:F:388:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:LEU:HA	1:F:244:MET:HE3	1.96	0.47
1:A:107:ASN:O	1:A:111:VAL:HG23	2.13	0.47
1:A:399:ALA:O	1:A:400:SER:CB	2.61	0.47
1:E:299:ARG:HA	1:E:302:ASN:ND2	2.28	0.47
1:F:37:ARG:HB2	1:F:184:ILE:HD12	1.96	0.47
1:F:146:ASN:ND2	4:F:435:HOH:O	2.46	0.47
1:A:15:GLN:HG3	1:A:92:LEU:HD21	1.97	0.47
1:A:193:VAL:O	1:A:197:VAL:HG23	2.15	0.47
1:E:132:GLU:O	1:E:132:GLU:HG2	2.14	0.47
2:G:136:LEU:HD22	2:G:201:GLY:O	2.14	0.47
1:A:191:CYS:O	1:A:233:GLN:HA	2.14	0.47
2:C:190:LEU:HD22	2:C:205:CYS:HA	1.97	0.47
1:F:27:LEU:HD11	1:F:48:PHE:CZ	2.50	0.47
1:F:177:ASN:N	1:F:178:PRO:HD3	2.29	0.47
1:A:297:ILE:HG22	1:A:298:ASP:OD1	2.15	0.47
1:B:128:GLN:HA	1:B:131:ILE:HD12	1.97	0.47
1:E:391:ASN:HA	1:E:392:PRO:HD3	1.63	0.47
1:E:388:ASP:HB3	1:E:389:TRP:CD1	2.49	0.47
1:F:107:ASN:O	1:F:111:VAL:HG23	2.15	0.47
1:A:121:ASP:HB3	4:A:553:HOH:O	2.15	0.47
1:A:153:ARG:HG2	1:B:389:TRP:CZ2	2.50	0.46
1:A:241:LEU:HD13	1:A:358:LEU:HD11	1.97	0.46
1:A:264:LYS:CD	4:A:514:HOH:O	2.63	0.46
1:A:264:LYS:HD2	4:A:514:HOH:O	2.14	0.46
1:A:28:SER:HA	1:A:366:PHE:HA	1.98	0.46
1:A:146:ASN:O	1:A:149:TYR:HB3	2.15	0.46
1:F:146:ASN:H	1:F:147:ILE:HD12	1.79	0.46
1:B:328:LEU:N	1:B:329:PRO:CD	2.79	0.46
2:C:151:ARG:HA	2:C:193:GLU:HG2	1.96	0.46
1:E:40:ALA:HB3	4:E:530:HOH:O	2.15	0.46
1:E:57:LEU:O	1:E:61:MET:HG3	2.15	0.46
2:G:181:GLN:CA	2:G:181:GLN:HE21	2.27	0.46
1:A:88:PHE:CE2	1:A:92:LEU:HD22	2.50	0.46
1:B:86:GLN:NE2	1:B:118:ARG:HD3	2.30	0.46
1:E:43:LYS:HB2	4:E:512:HOH:O	2.14	0.46
1:F:260:TYR:CE2	1:F:268:PRO:HG2	2.50	0.46
1:F:332:ARG:HD3	1:F:336:ARG:NH1	2.30	0.46
1:A:373:ASN:OD1	1:A:375:SER:HB3	2.16	0.46
1:F:262:ASP:HA	4:F:425:HOH:O	2.14	0.46
2:G:207:ILE:HG22	2:G:208:VAL:H	1.80	0.46
1:B:109:LEU:O	1:B:109:LEU:HG	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:921:HOH:O	1:E:205:LYS:NZ	2.48	0.46
1:E:62:ARG:HG2	1:E:372:PHE:CD2	2.50	0.46
1:E:146:ASN:O	1:E:149:TYR:HB3	2.16	0.46
1:E:348:GLU:HG2	1:F:277:GLY:HA3	1.96	0.46
1:F:194:ALA:O	1:F:198:LYS:HG3	2.15	0.46
1:B:33:LEU:CD1	1:B:184:ILE:HG13	2.45	0.46
1:E:241:LEU:HA	1:E:244:MET:HE2	1.97	0.46
1:A:257:VAL:HA	1:A:267:TYR:CE1	2.51	0.46
1:B:216:PRO:HA	4:B:422:HOH:O	2.16	0.46
1:E:294:LEU:HD22	1:F:357:TYR:CG	2.51	0.46
1:E:390:SER:HB3	1:F:369:LEU:HB2	1.98	0.46
1:F:122:VAL:O	1:F:124:PRO:HD3	2.15	0.46
2:G:168:GLU:O	2:G:169:ILE:HD13	2.16	0.46
1:A:200:ALA:HA	1:A:242:PHE:CE1	2.51	0.45
1:A:234:VAL:HG22	1:A:235:VAL:H	1.80	0.45
1:E:142:PHE:CG	1:E:384:PRO:HG3	2.52	0.45
1:F:249:PHE:O	1:F:253:MET:HG3	2.15	0.45
2:G:156:VAL:N	4:G:927:HOH:O	2.49	0.45
2:G:188:LYS:HG2	2:G:206:ILE:CD1	2.45	0.45
1:B:70:ASN:CB	1:B:136:LYS:HE2	2.41	0.45
1:B:203:THR:HG21	1:B:242:PHE:CZ	2.39	0.45
2:G:181:GLN:NE2	2:G:181:GLN:CA	2.77	0.45
1:A:321:LEU:O	1:A:322:ALA:HB2	2.15	0.45
1:F:71:LEU:HD12	1:F:74:ARG:HG3	1.98	0.45
1:A:347:MET:HE2	1:B:273:LEU:HD23	1.98	0.45
1:A:70:ASN:O	1:A:74:ARG:NH1	2.49	0.45
1:A:397:ARG:HB2	2:C:172:ASP:OD2	2.16	0.45
1:B:327:GLY:N	4:B:434:HOH:O	2.48	0.45
1:E:295:ARG:CZ	1:F:279:GLU:OE1	2.65	0.45
1:E:378:ARG:O	1:E:382:THR:HG23	2.17	0.45
1:B:39:ASN:ND2	1:B:41:CYS:HB2	2.32	0.45
1:B:299:ARG:HG2	4:B:529:HOH:O	2.16	0.45
1:E:41:CYS:SG	1:E:43:LYS:HB2	2.57	0.45
1:E:236:TYR:O	1:E:238:PRO:HD3	2.17	0.45
1:F:215:ALA:HB1	1:F:253:MET:HE2	1.99	0.45
1:F:332:ARG:O	1:F:336:ARG:CG	2.64	0.45
1:B:21:ARG:HB2	1:B:21:ARG:HH11	1.82	0.45
1:B:194:ALA:O	1:B:197:VAL:HB	2.16	0.45
1:E:390:SER:CB	1:F:26:PRO:HG3	2.45	0.45
1:F:111:VAL:O	1:F:115:VAL:HG13	2.17	0.45
1:A:145:THR:CG2	4:A:530:HOH:O	2.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:GLU:HB2	1:B:172:PHE:CD1	2.52	0.45
1:B:64:VAL:O	1:B:67:LEU:HB2	2.17	0.45
1:B:146:ASN:N	1:B:147:ILE:HD12	2.32	0.45
1:E:252:SER:HB3	1:E:287:ASP:HB3	1.99	0.45
1:E:296:LYS:HA	1:E:299:ARG:HD3	1.99	0.45
1:F:153:ARG:HB3	1:F:370:PRO:HB3	1.99	0.45
1:A:74:ARG:HA	1:A:74:ARG:NE	2.32	0.44
1:E:101:ASP:OD2	1:E:101:ASP:N	2.48	0.44
1:E:190:THR:HG23	4:E:437:HOH:O	2.16	0.44
1:E:399:ALA:O	1:E:400:SER:CB	2.65	0.44
1:F:65:ASN:HA	1:F:72:LEU:HD11	1.99	0.44
1:F:328:LEU:N	1:F:329:PRO:CD	2.80	0.44
1:F:357:TYR:O	1:F:358:LEU:HD23	2.17	0.44
1:A:388:ASP:HB3	1:A:389:TRP:CD1	2.52	0.44
1:E:399:ALA:HB1	1:F:35:PHE:CB	2.40	0.44
1:E:399:ALA:CB	1:F:35:PHE:HB2	2.40	0.44
1:A:293:PRO:HA	1:B:280:ASP:OD2	2.17	0.44
1:B:207:LEU:HD12	1:B:246:PHE:HZ	1.82	0.44
1:F:182:LYS:HE3	4:F:459:HOH:O	2.17	0.44
2:G:156:VAL:CG1	4:G:927:HOH:O	2.65	0.44
1:A:46:TYR:CD2	1:A:99:PRO:HB3	2.51	0.44
1:E:19:TYR:O	1:E:22:PHE:HB2	2.17	0.44
1:E:121:ASP:C	1:E:124:PRO:HD2	2.37	0.44
1:F:74:ARG:HA	1:F:74:ARG:NE	2.33	0.44
2:G:151:ARG:HA	2:G:193:GLU:HG2	1.98	0.44
1:F:27:LEU:HD13	3:G:901:RED:S6	2.57	0.44
2:G:206:ILE:HD12	2:G:206:ILE:H	1.82	0.44
2:C:152:TRP:CZ2	2:C:189:ILE:HG23	2.53	0.44
2:C:155:LYS:O	2:C:158:GLU:HG3	2.18	0.44
2:G:152:TRP:CZ2	2:G:189:ILE:HG23	2.53	0.44
2:G:154:LYS:HG2	2:G:160:LEU:CD2	2.48	0.44
1:B:221:GLU:O	1:B:273:LEU:HA	2.17	0.44
1:E:292:VAL:HB	1:E:297:ILE:CD1	2.48	0.44
1:F:329:PRO:O	1:F:333:LEU:HG	2.17	0.44
2:G:185:TYR:CZ	2:G:211:GLU:HB3	2.53	0.44
1:E:43:LYS:O	1:E:47:MET:HG2	2.18	0.44
1:A:15:GLN:HE21	1:A:15:GLN:CA	2.26	0.43
1:A:194:ALA:HB2	1:A:222:GLU:OE2	2.18	0.43
1:A:389:TRP:CZ2	1:B:153:ARG:HG2	2.53	0.43
1:E:46:TYR:OH	1:E:94:TYR:HB3	2.17	0.43
1:E:347:MET:CE	1:F:275:THR:HG23	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:339:GLN:NE2	4:F:511:HOH:O	2.50	0.43
2:G:151:ARG:HB3	2:G:168:GLU:CG	2.46	0.43
2:C:184:GLY:HA3	2:C:207:ILE:CG2	2.48	0.43
1:F:33:LEU:HD12	1:F:184:ILE:HG13	1.99	0.43
1:B:191:CYS:HB3	1:B:234:VAL:O	2.17	0.43
2:C:148:THR:HG21	2:C:196:ARG:HG2	1.99	0.43
2:C:188:LYS:O	2:C:205:CYS:HB2	2.19	0.43
2:C:206:ILE:HG22	4:C:913:HOH:O	2.18	0.43
1:B:155:TYR:HA	1:B:158:ARG:HG3	2.01	0.43
1:B:332:ARG:HD3	1:B:336:ARG:NE	2.33	0.43
1:A:51:LYS:O	1:A:55:VAL:HG23	2.19	0.43
1:A:98:SER:O	1:A:104:VAL:HG21	2.19	0.43
1:A:297:ILE:O	1:A:300:LEU:HB2	2.18	0.43
2:C:136:LEU:HD13	4:C:923:HOH:O	2.19	0.43
2:C:151:ARG:HB3	2:C:168:GLU:HG3	2.01	0.43
1:E:106:ASP:CB	4:E:548:HOH:O	2.66	0.43
1:F:90:GLU:OE1	1:F:118:ARG:NH2	2.52	0.43
1:F:328:LEU:HD12	1:F:328:LEU:HA	1.79	0.43
1:A:234:VAL:HG22	1:A:235:VAL:N	2.34	0.43
1:B:374:LYS:O	1:B:377:TRP:HB3	2.19	0.43
2:G:156:VAL:HG13	4:G:927:HOH:O	2.18	0.43
1:A:250:LYS:HZ3	1:A:325:GLY:H	1.66	0.42
1:B:28:SER:HB3	1:B:366:PHE:CD1	2.53	0.42
1:F:222:GLU:HB3	1:F:232:ILE:HD12	2.01	0.42
1:B:103:GLN:OE1	1:B:103:GLN:HA	2.19	0.42
1:B:256:THR:CG2	1:B:268:PRO:HD2	2.49	0.42
1:E:68:PRO:HB2	4:E:563:HOH:O	2.19	0.42
1:A:192:ASN:HB2	4:A:412:HOH:O	2.18	0.42
1:A:394:SER:C	1:A:395:GLU:HG3	2.39	0.42
1:A:76:SER:OG	1:A:128:GLN:HG3	2.19	0.42
1:A:218:LEU:HG	1:A:219:GLU:N	2.33	0.42
2:C:151:ARG:NE	2:C:153:GLU:OE2	2.46	0.42
1:E:345:TYR:OH	1:F:345:TYR:HB3	2.20	0.42
1:F:131:ILE:C	1:F:133:TYR:N	2.71	0.42
1:F:158:ARG:HA	1:F:161:PHE:CD1	2.54	0.42
1:B:19:TYR:HA	1:B:22:PHE:CD1	2.53	0.42
1:A:113:ILE:O	1:A:117:ASN:ND2	2.52	0.42
1:A:126:MET:CE	1:A:130:VAL:HG13	2.48	0.42
1:E:63:GLU:HG2	1:E:372:PHE:CD1	2.53	0.42
1:E:125:THR:O	1:E:128:GLN:HB3	2.19	0.42
1:E:158:ARG:HD2	4:E:421:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:CYS:HB3	1:E:234:VAL:O	2.19	0.42
1:A:272:THR:HA	1:A:284:LYS:O	2.19	0.42
1:B:267:TYR:HA	1:B:268:PRO:HD3	1.88	0.42
2:C:191:VAL:HG11	2:C:198:VAL:HG21	2.02	0.42
1:F:113:ILE:HG23	4:F:426:HOH:O	2.19	0.42
1:A:188:ASP:HB2	1:A:238:PRO:CG	2.49	0.42
1:B:71:LEU:HD12	1:B:74:ARG:HG3	2.02	0.42
1:B:126:MET:O	1:B:130:VAL:HG23	2.19	0.42
1:B:256:THR:HG23	1:B:268:PRO:HD2	2.02	0.42
1:B:61:MET:SD	1:B:84:TYR:HB3	2.59	0.41
1:B:84:TYR:OH	1:B:158:ARG:HD2	2.19	0.41
1:B:181:PRO:HB2	4:B:555:HOH:O	2.19	0.41
1:E:90:GLU:CD	1:E:118:ARG:HH12	2.23	0.41
1:E:98:SER:HG	1:E:100:GLU:HG2	1.82	0.41
1:A:50:ARG:CZ	4:A:417:HOH:O	2.67	0.41
1:A:155:TYR:O	1:A:159:ILE:HG13	2.20	0.41
1:A:179:VAL:O	1:A:181:PRO:HD3	2.20	0.41
1:B:51:LYS:HB2	4:B:457:HOH:O	2.20	0.41
1:B:262:ASP:C	4:B:470:HOH:O	2.57	0.41
1:B:337:TYR:OH	1:B:367:GLU:OE2	2.36	0.41
1:E:70:ASN:HB2	1:E:133:TYR:HE2	1.84	0.41
1:E:347:MET:HE2	1:F:275:THR:HG23	2.02	0.41
1:B:26:PRO:HD2	2:C:174:ALA:HB2	2.01	0.41
1:F:259:LEU:O	1:F:261:GLU:N	2.49	0.41
1:B:22:PHE:HA	2:C:140:LEU:O	2.20	0.41
1:B:42:GLU:HG2	1:B:105:LEU:CD2	2.46	0.41
1:B:65:ASN:HA	1:B:72:LEU:HD11	2.02	0.41
2:C:206:ILE:HD12	2:C:206:ILE:H	1.85	0.41
1:F:201:TYR:CG	1:F:218:LEU:HD22	2.55	0.41
1:B:243:HIS:CE1	4:B:417:HOH:O	2.73	0.41
1:B:26:PRO:CD	2:C:174:ALA:HB2	2.51	0.41
1:E:76:SER:OG	1:E:128:GLN:HG3	2.20	0.41
1:E:166:ASN:O	1:E:170:LEU:HG	2.21	0.41
1:E:267:TYR:HA	1:E:268:PRO:HD3	1.85	0.41
1:A:357:TYR:CG	1:B:294:LEU:HD22	2.55	0.41
1:B:61:MET:HA	1:B:64:VAL:CG1	2.49	0.41
1:B:227:ALA:O	1:B:229:ASP:N	2.54	0.41
1:B:336:ARG:O	1:B:368:ARG:HG2	2.20	0.41
1:E:14:LYS:CD	4:E:485:HOH:O	2.68	0.41
1:E:260:TYR:CE2	1:E:268:PRO:HG2	2.56	0.41
1:A:13:PRO:CB	4:A:456:HOH:O	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ASN:HD22	1:A:73:ASN:HA	1.73	0.41
1:A:233:GLN:NE2	4:A:412:HOH:O	2.49	0.41
1:B:86:GLN:HE21	1:B:118:ARG:NH1	2.18	0.41
1:B:133:TYR:HB3	4:B:444:HOH:O	2.21	0.41
1:E:39:ASN:ND2	1:E:41:CYS:HB3	2.35	0.41
1:F:191:CYS:O	1:F:233:GLN:HA	2.21	0.41
1:A:53:LEU:N	1:A:54:PRO:HD2	2.36	0.41
1:A:206:MET:HG2	4:A:446:HOH:O	2.20	0.41
1:E:91:LEU:C	1:E:93:GLU:H	2.25	0.41
1:F:233:GLN:O	1:F:234:VAL:HB	2.20	0.41
1:F:352:THR:HG22	1:F:353:ASP:N	2.35	0.41
1:B:115:VAL:HG12	1:B:118:ARG:HH21	1.86	0.40
1:B:145:THR:HA	1:B:147:ILE:HD13	2.03	0.40
1:B:352:THR:HG22	1:B:353:ASP:N	2.36	0.40
1:F:201:TYR:HE1	1:F:253:MET:HE3	1.86	0.40
1:F:267:TYR:HA	1:F:268:PRO:HD3	1.85	0.40
1:B:53:LEU:HD23	1:B:53:LEU:HA	1.81	0.40
1:B:332:ARG:O	1:B:336:ARG:CG	2.67	0.40
2:C:136:LEU:CD1	4:C:923:HOH:O	2.69	0.40
1:F:126:MET:O	1:F:130:VAL:HG23	2.21	0.40
1:B:94:TYR:CD1	1:B:94:TYR:N	2.89	0.40
1:E:199:ASP:O	1:E:203:THR:HG23	2.21	0.40
2:G:150:GLN:HB3	2:G:168:GLU:HB3	2.03	0.40
1:B:147:ILE:HD12	1:B:147:ILE:N	2.36	0.40
2:C:138:PRO:HG2	2:C:140:LEU:HD11	2.04	0.40
1:B:61:MET:O	1:B:64:VAL:HG12	2.21	0.40
1:E:61:MET:SD	1:E:84:TYR:HB3	2.61	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	370/419 (88%)	327 (88%)	36 (10%)	7 (2%)	8 13
1	B	331/419 (79%)	300 (91%)	24 (7%)	7 (2%)	7 11
1	E	370/419 (88%)	329 (89%)	32 (9%)	9 (2%)	6 9
1	F	331/419 (79%)	303 (92%)	20 (6%)	8 (2%)	6 9
2	C	77/128 (60%)	65 (84%)	9 (12%)	3 (4%)	3 4
2	G	77/128 (60%)	64 (83%)	10 (13%)	3 (4%)	3 4
All	All	1556/1932 (80%)	1388 (89%)	131 (8%)	37 (2%)	6 9

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	PRO
1	A	320	PRO
1	B	209	GLU
1	B	214	VAL
2	C	209	GLU
1	E	228	PRO
1	E	320	PRO
1	F	214	VAL
1	F	228	PRO
2	G	209	GLU
1	A	141	PRO
1	B	228	PRO
1	B	261	GLU
2	C	162	GLU
1	E	141	PRO
1	E	176	THR
1	E	325	GLY
1	F	39	ASN
1	F	261	GLU
1	A	300	LEU
1	A	322	ALA
1	B	39	ASN
1	E	39	ASN
1	E	175	ASP
1	F	209	GLU
1	B	260	TYR
1	E	174	GLY
1	A	176	THR
1	A	325	GLY
1	B	227	ALA

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Mol	Chain	Res	Type
2	C	156	VAL
1	E	321	LEU
1	F	234	VAL
1	F	260	TYR
2	G	149	VAL
1	F	227	ALA
2	G	156	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	336/374 (90%)	305 (91%)	31 (9%)	9 18
1	B	311/374 (83%)	285 (92%)	26 (8%)	11 21
1	E	336/374 (90%)	308 (92%)	28 (8%)	11 22
1	F	311/374 (83%)	287 (92%)	24 (8%)	13 25
2	C	67/109 (62%)	60 (90%)	7 (10%)	7 13
2	G	67/109 (62%)	61 (91%)	6 (9%)	9 19
All	All	1428/1714 (83%)	1306 (92%)	122 (8%)	10 21

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	23	SER
1	A	39	ASN
1	A	64	VAL
1	A	66	LEU
1	A	67	LEU
1	A	72	LEU
1	A	93	GLU
1	A	101	ASP
1	A	103	GLN
1	A	105	LEU

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Mol	Chain	Res	Type
1	A	128	GLN
1	A	139	PHE
1	A	177	ASN
1	A	183	HIS
1	A	186	SER
1	A	203	THR
1	A	209	GLU
1	A	214	VAL
1	A	226	LYS
1	A	228	PRO
1	A	229	ASP
1	A	263	ARG
1	A	265	GLU
1	A	281	LEU
1	A	297	ILE
1	A	298	ASP
1	A	320	PRO
1	A	321	LEU
1	A	336	ARG
1	A	388	ASP
1	B	17	GLU
1	B	39	ASN
1	B	66	LEU
1	B	67	LEU
1	B	70	ASN
1	B	72	LEU
1	B	73	ASN
1	B	93	GLU
1	B	128	GLN
1	B	133	TYR
1	B	145	THR
1	B	146	ASN
1	B	148	GLN
1	B	158	ARG
1	B	163	MET
1	B	182	LYS
1	B	183	HIS
1	B	203	THR
1	B	209	GLU
1	B	229	ASP
1	B	252	SER
1	B	286	SER

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Mol	Chain	Res	Type
1	B	302	ASN
1	B	336	ARG
1	B	362	SER
1	B	387	ASP
2	C	140	LEU
2	C	171	THR
2	C	186	LEU
2	C	188	LYS
2	C	190	LEU
2	C	206	ILE
2	C	213	ASP
1	E	15	GLN
1	E	38	ASP
1	E	39	ASN
1	E	64	VAL
1	E	67	LEU
1	E	72	LEU
1	E	73	ASN
1	E	101	ASP
1	E	103	GLN
1	E	105	LEU
1	E	107	ASN
1	E	116	ARG
1	E	128	GLN
1	E	139	PHE
1	E	177	ASN
1	E	203	THR
1	E	226	LYS
1	E	228	PRO
1	E	252	SER
1	E	265	GLU
1	E	286	SER
1	E	297	ILE
1	E	299	ARG
1	E	321	LEU
1	E	332	ARG
1	E	336	ARG
1	E	374	LYS
1	E	388	ASP
1	F	17	GLU
1	F	39	ASN
1	F	66	LEU

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Mol	Chain	Res	Type
1	F	72	LEU
1	F	93	GLU
1	F	116	ARG
1	F	133	TYR
1	F	145	THR
1	F	146	ASN
1	F	163	MET
1	F	183	HIS
1	F	203	THR
1	F	207	LEU
1	F	209	GLU
1	F	229	ASP
1	F	252	SER
1	F	280	ASP
1	F	282	SER
1	F	302	ASN
1	F	336	ARG
1	F	346	SER
1	F	362	SER
1	F	368	ARG
1	F	387	ASP
2	G	140	LEU
2	G	186	LEU
2	G	188	LYS
2	G	190	LEU
2	G	206	ILE
2	G	213	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	39	ASN
1	A	70	ASN
1	A	73	ASN
1	A	103	GLN
1	A	107	ASN
1	A	117	ASN
1	A	128	GLN
1	A	157	ASN
1	A	167	GLN
1	A	177	ASN

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Mol	Chain	Res	Type
1	A	192	ASN
1	A	240	HIS
1	B	31	GLN
1	B	39	ASN
1	B	86	GLN
1	B	107	ASN
1	B	128	GLN
1	B	192	ASN
1	B	243	HIS
1	B	251	ASN
1	B	339	GLN
2	C	181	GLN
1	E	15	GLN
1	E	39	ASN
1	E	70	ASN
1	E	73	ASN
1	E	103	GLN
1	E	107	ASN
1	E	128	GLN
1	E	157	ASN
1	E	167	GLN
1	E	177	ASN
1	E	192	ASN
1	E	210	GLN
1	E	233	GLN
1	E	240	HIS
1	E	302	ASN
1	F	39	ASN
1	F	86	GLN
1	F	107	ASN
1	F	119	HIS
1	F	128	GLN
1	F	146	ASN
1	F	157	ASN
1	F	243	HIS
1	F	251	ASN
1	F	302	ASN
1	F	339	GLN
1	F	379	HIS
2	G	181	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
3	RED	G	901	2	9,10,11	1.20	1 (11%)	6,10,12	4.02	1 (16%)
3	RED	C	900	2	9,10,11	1.41	1 (11%)	6,10,12	3.61	1 (16%)

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
3	RED	G	901	2	-	4/7/9/10	-
3	RED	C	900	2	-	4/7/9/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	900	RED	C7-C8	3.26	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	901	RED	C7-C8	2.64	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	901	RED	C7-C8-S8	-9.74	103.59	113.74
3	C	900	RED	C7-C8-S8	-8.70	104.67	113.74

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	900	RED	C1-C2-C3-C4
3	C	900	RED	C5-C6-C7-C8
3	C	900	RED	C6-C7-C8-S8
3	G	901	RED	C1-C2-C3-C4
3	G	901	RED	C5-C6-C7-C8
3	G	901	RED	C6-C7-C8-S8
3	C	900	RED	C2-C3-C4-C5
3	G	901	RED	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	901	RED	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	374/419 (89%)	-0.06	13 (3%) 44 47	23, 51, 83, 96	0
1	B	341/419 (81%)	-0.07	9 (2%) 56 59	27, 49, 70, 94	0
1	E	374/419 (89%)	-0.13	7 (1%) 66 69	24, 49, 77, 99	0
1	F	341/419 (81%)	-0.17	5 (1%) 73 75	23, 46, 74, 85	0
2	C	79/128 (61%)	-0.28	2 (2%) 57 61	42, 55, 79, 89	0
2	G	79/128 (61%)	-0.37	0 100 100	39, 56, 71, 77	0
All	All	1588/1932 (82%)	-0.13	36 (2%) 60 63	23, 51, 76, 99	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	176	THR	4.8
1	A	176	THR	4.6
1	A	318	ALA	4.4
1	B	131	ILE	3.7
1	B	144	SER	3.7
1	A	177	ASN	3.7
1	A	319	ALA	3.5
1	B	123	VAL	3.5
1	F	131	ILE	2.9
1	B	145	THR	2.8
1	F	123	VAL	2.8
1	E	318	ALA	2.8
1	E	179	VAL	2.7
1	B	229	ASP	2.6
1	A	320	PRO	2.5
1	A	178	PRO	2.5
1	E	177	ASN	2.5
1	E	178	PRO	2.4
1	A	102	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	262	ASP	2.4
1	B	345	TYR	2.3
1	E	57	LEU	2.3
1	A	181	PRO	2.2
2	C	210	LYS	2.2
1	A	103	GLN	2.2
1	F	229	ASP	2.2
1	A	229	ASP	2.1
1	F	304	MET	2.1
1	E	319	ALA	2.1
1	A	179	VAL	2.1
1	F	75	PRO	2.1
2	C	208	VAL	2.1
1	A	139	PHE	2.1
1	A	324	PHE	2.1
1	B	133	TYR	2.0
1	B	354	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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
3	RED	C	900	11/12	0.85	0.22	63,64,67,69	0
3	RED	G	901	11/12	0.95	0.14	39,46,54,55	0

6.5 Other polymers (i)

There are no such residues in this entry.