Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:33 PM GMT

PDB ID	:	1PKN
Title	:	STRUCTURE OF RABBIT MUSCLE PYRUVATE KINASE COMPLEXED WITH MN2+, K+, AND PYRUVATE
Authors	:	Larsen, T.M.; Laughlin, L.T.; Holden, H.M.; Rayment, I.; Reed, G.H.
Deposited on	:	1994-03-25
Resolution	:	2.90 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 (i)) were used in the production of this report:

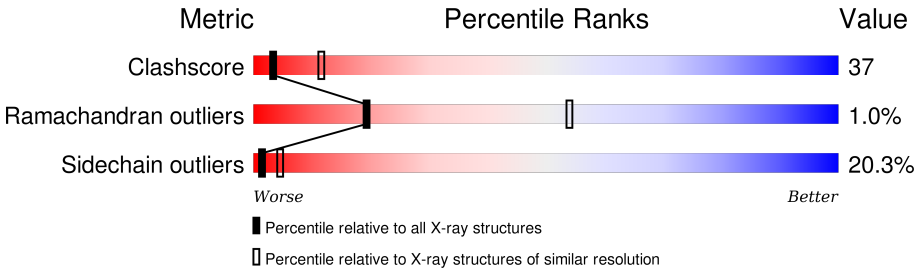
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	530	32% 44% 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3937 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 KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			3929	2469	698	734	28			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	149	ALA	GLU	CONFLICT	UNP P11974
A	150	ALA	LYS	CONFLICT	UNP P11974
A	168	GLU	ASP	CONFLICT	UNP P11974
A	233	ASP	GLU	CONFLICT	UNP P11974
A	234	GLU	GLN	CONFLICT	UNP P11974
A	499	ALA	ARG	CONFLICT	UNP P11974

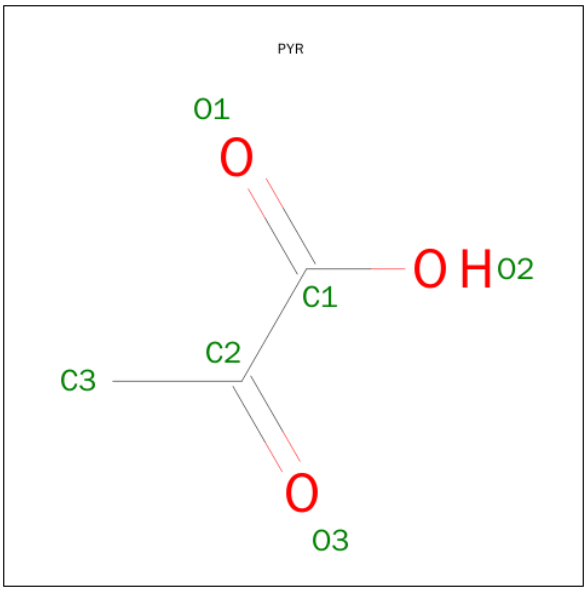
- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0

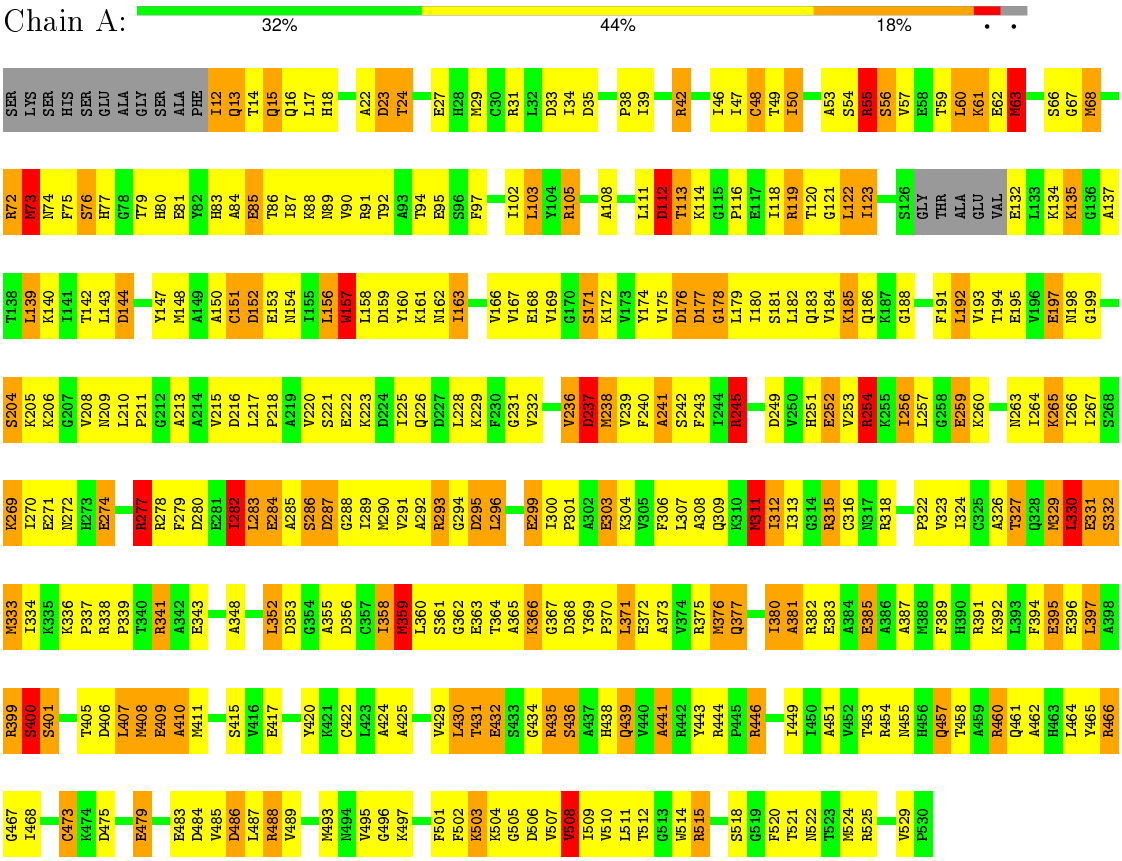
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: PYRUVATE KINASE

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	83.60Å 109.90Å 146.80Å 94.90° 93.60° 112.30°	Depositor
Resolution (Å)	30.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3937	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.02	19/3991 (0.5%)	1.92	147/5384 (2.7%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	432	GLU	CD-OE1	8.72	1.35	1.25
1	A	259	GLU	CD-OE1	8.47	1.34	1.25
1	A	331	GLU	CD-OE1	8.29	1.34	1.25
1	A	95	GLU	CD-OE1	7.50	1.33	1.25
1	A	479	GLU	CD-OE1	7.38	1.33	1.25
1	A	85	GLU	CD-OE1	7.17	1.33	1.25
1	A	372	GLU	CD-OE1	6.96	1.33	1.25
1	A	222	GLU	CD-OE1	6.23	1.32	1.25
1	A	81	GLU	CD-OE2	6.04	1.32	1.25
1	A	284	GLU	CD-OE1	6.01	1.32	1.25
1	A	385	GLU	CD-OE1	5.98	1.32	1.25
1	A	303	GLU	CD-OE2	5.79	1.32	1.25
1	A	195	GLU	CD-OE1	5.64	1.31	1.25
1	A	417	GLU	CD-OE1	5.47	1.31	1.25
1	A	483	GLU	CD-OE1	5.46	1.31	1.25
1	A	396	GLU	CD-OE1	5.23	1.31	1.25
1	A	395	GLU	CD-OE1	5.20	1.31	1.25
1	A	409	GLU	CD-OE1	5.18	1.31	1.25
1	A	252	GLU	CD-OE1	5.16	1.31	1.25

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	369	TYR	CB-CG-CD1	-17.72	110.37	121.00
1	A	55	ARG	NE-CZ-NH2	-16.21	112.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	369	TYR	CB-CG-CD2	16.16	130.69	121.00
1	A	119	ARG	NE-CZ-NH1	15.81	128.21	120.30
1	A	55	ARG	NE-CZ-NH1	12.89	126.75	120.30
1	A	42	ARG	NE-CZ-NH1	12.34	126.47	120.30
1	A	356	ASP	CB-CG-OD2	-11.27	108.16	118.30
1	A	341	ARG	NE-CZ-NH2	-11.10	114.75	120.30
1	A	408	MET	CA-CB-CG	-10.92	94.74	113.30
1	A	318	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	A	249	ASP	CB-CG-OD2	-9.90	109.39	118.30
1	A	356	ASP	CB-CG-OD1	9.84	127.15	118.30
1	A	236	VAL	CA-CB-CG1	-9.40	96.80	110.90
1	A	119	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	A	466	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	287	ASP	CB-CG-OD2	-8.97	110.23	118.30
1	A	12	ILE	O-C-N	8.81	136.80	122.70
1	A	435	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	A	176	ASP	CB-CG-OD1	-8.44	110.70	118.30
1	A	286	SER	N-CA-CB	8.44	123.15	110.50
1	A	387	ALA	CB-CA-C	8.31	122.57	110.10
1	A	81	GLU	N-CA-CB	8.20	125.35	110.60
1	A	80	HIS	N-CA-CB	7.99	124.99	110.60
1	A	119	ARG	CD-NE-CZ	7.89	134.64	123.60
1	A	451	ALA	N-CA-CB	7.87	121.11	110.10
1	A	239	VAL	CA-CB-CG2	-7.86	99.11	110.90
1	A	77	HIS	CB-CA-C	-7.84	94.72	110.40
1	A	83	HIS	CA-CB-CG	-7.72	100.47	113.60
1	A	410	ALA	CB-CA-C	-7.69	98.57	110.10
1	A	399	ARG	NE-CZ-NH2	7.65	124.12	120.30
1	A	105	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	A	330	LEU	N-CA-CB	-7.55	95.31	110.40
1	A	399	ARG	N-CA-CB	7.52	124.14	110.60
1	A	375	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	A	280	ASP	CB-CG-OD1	-7.51	111.54	118.30
1	A	446	ARG	NE-CZ-NH2	7.49	124.05	120.30
1	A	33	ASP	CB-CG-OD2	7.48	125.03	118.30
1	A	72	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	A	466	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	488	ARG	NE-CZ-NH2	7.41	124.01	120.30
1	A	515	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	A	254	ARG	NE-CZ-NH2	7.39	123.99	120.30
1	A	444	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	A	277	ARG	NE-CZ-NH1	7.36	123.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	338	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	A	35	ASP	CB-CG-OD2	7.30	124.87	118.30
1	A	241	ALA	N-CA-CB	-7.28	99.91	110.10
1	A	510	VAL	CA-CB-CG2	7.27	121.80	110.90
1	A	441	ALA	CB-CA-C	7.15	120.83	110.10
1	A	238	MET	N-CA-CB	-7.14	97.74	110.60
1	A	506	ASP	CB-CG-OD1	-7.08	111.93	118.30
1	A	66	SER	CB-CA-C	7.04	123.49	110.10
1	A	287	ASP	CB-CG-OD1	7.03	124.63	118.30
1	A	293	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	A	397	LEU	CB-CG-CD2	-6.90	99.27	111.00
1	A	249	ASP	CB-CG-OD1	6.87	124.48	118.30
1	A	399	ARG	CD-NE-CZ	-6.82	114.05	123.60
1	A	495	VAL	CA-CB-CG2	-6.78	100.73	110.90
1	A	12	ILE	CA-C-N	-6.77	102.30	117.20
1	A	157	TRP	CE2-CD2-CG	6.71	112.66	107.30
1	A	371	LEU	CB-CG-CD1	-6.67	99.66	111.00
1	A	12	ILE	N-CA-CB	6.59	125.95	110.80
1	A	373	ALA	N-CA-CB	6.58	119.31	110.10
1	A	303	GLU	N-CA-CB	-6.52	98.87	110.60
1	A	443	TYR	CB-CG-CD1	6.49	124.89	121.00
1	A	376	MET	CG-SD-CE	6.48	110.57	100.20
1	A	312	ILE	CA-CB-CG2	-6.47	97.96	110.90
1	A	316	CYS	CB-CA-C	-6.43	97.53	110.40
1	A	35	ASP	CB-CG-OD1	-6.43	112.51	118.30
1	A	394	PHE	CB-CG-CD2	6.40	125.28	120.80
1	A	23	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	296	LEU	N-CA-CB	-6.40	97.61	110.40
1	A	381	ALA	N-CA-CB	6.39	119.05	110.10
1	A	497	LYS	CB-CA-C	-6.33	97.74	110.40
1	A	157	TRP	CA-CB-CG	6.31	125.69	113.70
1	A	397	LEU	CB-CA-C	-6.30	98.23	110.20
1	A	460	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	A	285	ALA	CB-CA-C	6.27	119.50	110.10
1	A	333	MET	CA-CB-CG	-6.27	102.64	113.30
1	A	113	THR	N-CA-CB	-6.25	98.43	110.30
1	A	359	MET	CG-SD-CE	6.24	110.19	100.20
1	A	176	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	358	ILE	CB-CA-C	6.21	124.02	111.60
1	A	73	MET	CG-SD-CE	6.19	110.10	100.20
1	A	259	GLU	CB-CA-C	-6.18	98.03	110.40
1	A	443	TYR	CB-CG-CD2	-6.18	117.29	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	148	MET	CG-SD-CE	6.16	110.06	100.20
1	A	97	PHE	CB-CG-CD1	-6.14	116.50	120.80
1	A	359	MET	O-C-N	6.14	132.53	122.70
1	A	237	ASP	CB-CG-OD2	6.14	123.82	118.30
1	A	240	PHE	CB-CG-CD2	-6.08	116.54	120.80
1	A	318	ARG	N-CA-CB	-6.05	99.70	110.60
1	A	24	THR	N-CA-CB	-6.04	98.83	110.30
1	A	429	VAL	CA-CB-CG1	6.01	119.92	110.90
1	A	329	MET	CG-SD-CE	6.00	109.80	100.20
1	A	84	ALA	N-CA-CB	5.96	118.45	110.10
1	A	400	SER	CB-CA-C	-5.96	98.78	110.10
1	A	63	MET	CG-SD-CE	5.96	109.73	100.20
1	A	92	THR	CA-CB-CG2	-5.96	104.06	112.40
1	A	382	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	48	CYS	CB-CA-C	-5.93	98.53	110.40
1	A	462	ALA	CB-CA-C	5.92	118.99	110.10
1	A	29	MET	CB-CA-C	-5.88	98.64	110.40
1	A	265	LYS	CB-CA-C	5.88	122.15	110.40
1	A	356	ASP	CB-CA-C	-5.87	98.65	110.40
1	A	524	MET	CG-SD-CE	5.87	109.59	100.20
1	A	177	ASP	CB-CG-OD2	5.86	123.58	118.30
1	A	226	GLN	CB-CA-C	-5.80	98.80	110.40
1	A	237	ASP	CB-CG-OD1	-5.69	113.17	118.30
1	A	370	PRO	N-CA-CB	5.69	110.12	103.30
1	A	185	LYS	CB-CA-C	5.67	121.74	110.40
1	A	112	ASP	CB-CG-OD1	-5.67	113.20	118.30
1	A	380	ILE	CA-CB-CG2	-5.66	99.58	110.90
1	A	222	GLU	N-CA-CB	5.66	120.78	110.60
1	A	33	ASP	CB-CA-C	-5.65	99.09	110.40
1	A	353	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	A	94	THR	N-CA-CB	5.59	120.92	110.30
1	A	341	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	97	PHE	CB-CG-CD2	5.53	124.67	120.80
1	A	430	LEU	CB-CA-C	-5.51	99.74	110.20
1	A	501	PHE	N-CA-CB	-5.50	100.71	110.60
1	A	61	LYS	CB-CA-C	-5.48	99.44	110.40
1	A	525	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	177	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	A	245	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	420	TYR	CB-CG-CD1	5.37	124.22	121.00
1	A	435	ARG	CG-CD-NE	5.37	123.08	111.80
1	A	420	TYR	CB-CG-CD2	-5.35	117.79	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	218	PRO	N-CA-CB	5.33	109.69	103.30
1	A	508	VAL	N-CA-CB	-5.32	99.79	111.50
1	A	366	LYS	CD-CE-NZ	5.27	123.83	111.70
1	A	216	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	A	506	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	432	GLU	CA-CB-CG	-5.20	101.97	113.40
1	A	226	GLN	N-CA-CB	5.18	119.93	110.60
1	A	291	VAL	CA-CB-CG2	-5.17	103.15	110.90
1	A	108	ALA	N-CA-CB	5.16	117.33	110.10
1	A	220	VAL	CG1-CB-CG2	-5.16	102.65	110.90
1	A	466	ARG	CB-CG-CD	-5.15	98.20	111.60
1	A	311	MET	CA-CB-CG	-5.14	104.56	113.30
1	A	443	TYR	N-CA-CB	5.10	119.78	110.60
1	A	132	GLU	O-C-N	5.08	130.82	122.70
1	A	486	ASP	N-CA-CB	-5.07	101.47	110.60
1	A	42	ARG	NH1-CZ-NH2	-5.06	113.83	119.40
1	A	282	ILE	N-CA-CB	5.05	122.42	110.80
1	A	411	MET	CB-CA-C	-5.04	100.32	110.40
1	A	368	ASP	CB-CG-OD1	-5.02	113.78	118.30

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	3929	0	4001	294	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	6	0	3	3	0
All	All	3937	0	4004	294	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 37.

All (294) 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:279:PHE:CE2	1:A:283:LEU:HD12	1.65	1.29
1:A:122:LEU:O	1:A:151:CYS:HB2	1.29	1.26
1:A:134:LYS:NZ	1:A:139:LEU:HD13	1.56	1.20
1:A:139:LEU:HD12	1:A:153:GLU:O	1.44	1.16
1:A:72:ARG:HD2	1:A:359:MET:HE3	1.32	1.07
1:A:134:LYS:CE	1:A:139:LEU:HD13	1.84	1.07
1:A:134:LYS:NZ	1:A:139:LEU:CD1	2.17	1.06
1:A:72:ARG:HD2	1:A:359:MET:CE	1.87	1.05
1:A:511:LEU:HB3	1:A:521:THR:HG21	1.09	1.04
1:A:431:THR:HG21	1:A:434:GLY:HA2	1.40	1.03
1:A:511:LEU:HB3	1:A:521:THR:CG2	1.89	1.03
1:A:49:THR:OG1	1:A:72:ARG:HD3	1.63	0.98
1:A:134:LYS:HZ3	1:A:139:LEU:HD13	1.16	0.96
1:A:294:GLY:CA	1:A:327:THR:HG21	1.96	0.95
1:A:279:PHE:CE2	1:A:283:LEU:CD1	2.53	0.91
1:A:15:GLN:HG3	1:A:39:ILE:HG23	1.50	0.90
1:A:122:LEU:O	1:A:151:CYS:CB	2.21	0.89
1:A:454:ARG:HG2	1:A:473:CYS:HB3	1.54	0.89
1:A:49:THR:HA	1:A:72:ARG:HB3	1.54	0.87
1:A:294:GLY:HA3	1:A:327:THR:HG21	1.54	0.87
1:A:139:LEU:HG	1:A:140:LYS:H	1.39	0.87
1:A:24:THR:CG2	1:A:27:GLU:HB2	2.05	0.87
1:A:24:THR:HG23	1:A:27:GLU:HB2	1.57	0.86
1:A:425:ALA:HB1	1:A:502:PHE:HB3	1.58	0.86
1:A:139:LEU:CD1	1:A:153:GLU:O	2.24	0.85
1:A:406:ASP:HB3	1:A:409:GLU:HB2	1.58	0.85
1:A:186:GLN:HB3	1:A:193:VAL:HB	1.56	0.85
1:A:134:LYS:HZ3	1:A:139:LEU:CD1	1.82	0.84
1:A:431:THR:CG2	1:A:434:GLY:HA2	2.08	0.82
1:A:511:LEU:CB	1:A:521:THR:HG21	2.03	0.81
1:A:162:ASN:O	1:A:166:VAL:HG23	1.79	0.81
1:A:134:LYS:HE2	1:A:139:LEU:HD13	1.62	0.81
1:A:225:ILE:HG22	1:A:229:LYS:HE2	1.64	0.80
1:A:54:SER:HA	1:A:59:THR:HG21	1.63	0.80
1:A:293:ARG:HD3	1:A:326:ALA:O	1.82	0.80
1:A:504:LYS:O	1:A:529:VAL:O	1.98	0.80
1:A:405:THR:HG22	1:A:405:THR:O	1.82	0.80
1:A:181:SER:OG	1:A:197:GLU:OE1	1.98	0.79
1:A:75:PHE:HB2	1:A:112:ASP:O	1.84	0.78
1:A:279:PHE:HE2	1:A:283:LEU:HD12	1.45	0.78
1:A:134:LYS:CE	1:A:139:LEU:CD1	2.60	0.77
1:A:15:GLN:HG3	1:A:39:ILE:CG2	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LEU:HB3	1:A:194:THR:HG21	1.66	0.77
1:A:485:VAL:O	1:A:489:VAL:HG23	1.84	0.77
1:A:237:ASP:OD1	1:A:460:ARG:NH1	2.18	0.76
1:A:57:VAL:O	1:A:61:LYS:HG3	1.86	0.75
1:A:139:LEU:HG	1:A:140:LYS:N	2.00	0.74
1:A:333:MET:HE3	1:A:339:PRO:HD3	1.69	0.74
1:A:322:PRO:HB3	1:A:464:LEU:O	1.88	0.74
1:A:332:SER:HB3	1:A:343:GLU:OE2	1.87	0.74
1:A:333:MET:HE3	1:A:337:PRO:O	1.87	0.74
1:A:331:GLU:HG2	1:A:334:ILE:HD12	1.68	0.74
1:A:15:GLN:CG	1:A:39:ILE:HG23	2.17	0.73
1:A:512:THR:N	1:A:521:THR:HG23	2.03	0.73
1:A:134:LYS:HE2	1:A:139:LEU:CD1	2.17	0.73
1:A:215:VAL:HG12	1:A:217:LEU:H	1.52	0.73
1:A:308:ALA:O	1:A:312:ILE:HG13	1.88	0.72
1:A:176:ASP:O	1:A:179:LEU:HB2	1.89	0.72
1:A:139:LEU:HD21	1:A:156:LEU:HD12	1.72	0.72
1:A:116:PRO:HB3	1:A:217:LEU:HB2	1.71	0.71
1:A:122:LEU:C	1:A:151:CYS:HB2	2.10	0.71
1:A:167:VAL:CG1	1:A:171:SER:HB3	2.21	0.71
1:A:134:LYS:HZ1	1:A:139:LEU:CD1	2.04	0.71
1:A:134:LYS:HE2	1:A:153:GLU:O	1.90	0.71
1:A:134:LYS:HZ1	1:A:139:LEU:HD11	1.53	0.70
1:A:225:ILE:O	1:A:229:LYS:HG3	1.90	0.70
1:A:333:MET:HA	1:A:336:LYS:O	1.91	0.70
1:A:47:ILE:HD13	1:A:324:ILE:HD13	1.73	0.70
1:A:279:PHE:CZ	1:A:283:LEU:HD12	2.26	0.70
1:A:333:MET:CE	1:A:339:PRO:HD3	2.22	0.70
1:A:120:THR:HG23	1:A:156:LEU:HD23	1.73	0.70
1:A:174:TYR:HB3	1:A:178:GLY:HA2	1.74	0.69
1:A:72:ARG:CD	1:A:359:MET:CE	2.70	0.68
1:A:371:LEU:N	1:A:371:LEU:HD12	2.09	0.68
1:A:120:THR:HG22	1:A:121:GLY:H	1.57	0.68
1:A:188:GLY:HA3	1:A:191:PHE:CE1	2.28	0.68
1:A:167:VAL:HG13	1:A:171:SER:HB3	1.75	0.67
1:A:102:ILE:HG22	1:A:103:LEU:HD12	1.75	0.67
1:A:511:LEU:C	1:A:521:THR:CG2	2.63	0.67
1:A:182:LEU:HB3	1:A:194:THR:CG2	2.24	0.67
1:A:391:ARG:HH11	1:A:391:ARG:HG2	1.61	0.66
1:A:22:ALA:O	1:A:391:ARG:NH2	2.29	0.66
1:A:120:THR:HG23	1:A:156:LEU:CD2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ASN:OD1	1:A:76:SER:OG	2.14	0.66
1:A:270:ILE:HD13	1:A:312:ILE:HD13	1.79	0.65
1:A:265:LYS:HA	1:A:287:ASP:OD2	1.97	0.64
1:A:355:ALA:O	1:A:466:ARG:NH1	2.30	0.64
1:A:279:PHE:HE2	1:A:283:LEU:CD1	2.05	0.64
1:A:160:TYR:CE1	1:A:162:ASN:HB2	2.32	0.63
1:A:120:THR:HG22	1:A:121:GLY:N	2.14	0.63
1:A:466:ARG:HG3	1:A:467:GLY:N	2.14	0.62
1:A:228:LEU:CD1	1:A:256:ILE:HG21	2.28	0.62
1:A:408:MET:SD	1:A:436:SER:HA	2.39	0.62
1:A:143:LEU:N	1:A:143:LEU:HD12	2.14	0.62
1:A:435:ARG:O	1:A:438:HIS:HB2	1.99	0.62
1:A:457:GLN:O	1:A:461:GLN:HG3	2.00	0.62
1:A:334:ILE:HD11	1:A:362:GLY:HA3	1.80	0.62
1:A:119:ARG:H	1:A:159:ASP:HB2	1.64	0.61
1:A:358:ILE:HG13	1:A:377:GLN:NE2	2.16	0.61
1:A:511:LEU:CB	1:A:521:THR:CG2	2.74	0.60
1:A:504:LYS:HG3	1:A:505:GLY:N	2.16	0.60
1:A:134:LYS:HE3	1:A:153:GLU:HA	1.83	0.60
1:A:360:LEU:HB3	1:A:364:THR:HG23	1.83	0.60
1:A:188:GLY:HA3	1:A:191:PHE:CD1	2.36	0.60
1:A:225:ILE:CG2	1:A:229:LYS:HE2	2.31	0.60
1:A:24:THR:HG23	1:A:27:GLU:H	1.67	0.59
1:A:50:ILE:HD11	1:A:68:MET:CE	2.31	0.59
1:A:177:ASP:O	1:A:179:LEU:N	2.35	0.59
1:A:134:LYS:CE	1:A:153:GLU:HA	2.31	0.59
1:A:181:SER:HB3	1:A:198:ASN:HB2	1.83	0.59
1:A:446:ARG:HG3	1:A:446:ARG:O	2.02	0.59
1:A:135:LYS:C	1:A:137:ALA:H	2.05	0.59
1:A:118:ILE:HG12	1:A:160:TYR:HB2	1.84	0.59
1:A:47:ILE:CD1	1:A:324:ILE:HD13	2.33	0.59
1:A:511:LEU:C	1:A:521:THR:HG23	2.21	0.59
1:A:503:LYS:O	1:A:529:VAL:HG11	2.03	0.58
1:A:18:HIS:CE1	1:A:31:ARG:NH1	2.71	0.58
1:A:264:ILE:HG22	1:A:265:LYS:N	2.17	0.58
1:A:182:LEU:CB	1:A:194:THR:HG21	2.32	0.58
1:A:270:ILE:HD13	1:A:312:ILE:CD1	2.33	0.58
1:A:484:ASP:O	1:A:487:LEU:HB3	2.04	0.58
1:A:333:MET:CE	1:A:337:PRO:O	2.52	0.58
1:A:73:MET:HE2	1:A:86:THR:HG21	1.86	0.58
1:A:430:LEU:N	1:A:430:LEU:HD12	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:O	1:A:359:MET:HB2	2.03	0.57
1:A:228:LEU:HD12	1:A:256:ILE:HG21	1.87	0.57
1:A:14:THR:O	1:A:17:LEU:HG	2.04	0.57
1:A:15:GLN:CG	1:A:39:ILE:CG2	2.80	0.57
1:A:277:ARG:O	1:A:277:ARG:HG2	2.03	0.56
1:A:271:GLU:HG3	1:A:292:ALA:HB3	1.87	0.56
1:A:73:MET:CE	1:A:86:THR:HG21	2.35	0.56
1:A:142:THR:HG22	1:A:144:ASP:N	2.20	0.56
1:A:381:ALA:O	1:A:385:GLU:HG3	2.05	0.56
1:A:182:LEU:CG	1:A:194:THR:HG21	2.34	0.56
1:A:431:THR:O	1:A:432:GLU:HG2	2.05	0.56
1:A:12:ILE:HG22	1:A:13:GLN:O	2.05	0.56
1:A:186:GLN:HB3	1:A:193:VAL:CB	2.31	0.56
1:A:512:THR:CA	1:A:521:THR:HG23	2.36	0.56
1:A:209:ASN:C	1:A:211:PRO:HD3	2.26	0.56
1:A:142:THR:HG22	1:A:144:ASP:H	1.72	0.55
1:A:293:ARG:CD	1:A:326:ALA:O	2.54	0.55
1:A:48:CYS:SG	1:A:68:MET:HG3	2.46	0.55
1:A:142:THR:O	1:A:157:TRP:HA	2.07	0.54
1:A:241:ALA:O	1:A:269:LYS:HG3	2.07	0.54
1:A:38:PRO:HG3	1:A:383:GLU:OE1	2.08	0.54
1:A:408:MET:SD	1:A:436:SER:HB3	2.47	0.54
1:A:143:LEU:HD23	1:A:161:LYS:HA	1.89	0.54
1:A:177:ASP:C	1:A:179:LEU:H	2.11	0.54
1:A:50:ILE:HD11	1:A:68:MET:HE1	1.90	0.54
1:A:512:THR:N	1:A:521:THR:CG2	2.71	0.54
1:A:53:ALA:HB3	1:A:365:ALA:O	2.07	0.54
1:A:295:ASP:HB2	4:A:533:PYR:O2	2.08	0.53
1:A:441:ALA:HB1	1:A:466:ARG:O	2.07	0.53
1:A:496:GLY:HA3	1:A:502:PHE:CZ	2.43	0.53
1:A:209:ASN:ND2	1:A:299:GLU:OE1	2.41	0.53
1:A:454:ARG:CG	1:A:473:CYS:HB3	2.34	0.53
1:A:391:ARG:NH1	1:A:391:ARG:HG2	2.23	0.53
1:A:162:ASN:O	1:A:166:VAL:CG2	2.54	0.52
1:A:400:SER:OG	1:A:401:SER:N	2.39	0.52
1:A:24:THR:HG22	1:A:27:GLU:HB2	1.90	0.51
1:A:182:LEU:HD23	1:A:194:THR:HG21	1.92	0.51
1:A:441:ALA:HB2	1:A:449:ILE:HD12	1.92	0.51
1:A:507:VAL:HG12	1:A:508:VAL:N	2.26	0.51
1:A:322:PRO:HD3	1:A:465:TYR:CE1	2.45	0.51
1:A:208:VAL:HG12	1:A:209:ASN:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ARG:HB3	1:A:274:GLU:HB3	1.91	0.51
1:A:301:PRO:O	1:A:304:LYS:HB2	2.10	0.51
1:A:160:TYR:CE2	1:A:166:VAL:HG21	2.46	0.51
1:A:278:ARG:O	1:A:282:ILE:HD12	2.11	0.51
1:A:243:PHE:N	1:A:271:GLU:OE1	2.37	0.50
1:A:166:VAL:HG12	1:A:213:ALA:HB1	1.94	0.50
1:A:294:GLY:N	1:A:327:THR:HG21	2.26	0.50
1:A:274:GLU:O	1:A:278:ARG:HB2	2.12	0.50
1:A:168:GLU:O	1:A:171:SER:HB2	2.11	0.50
1:A:54:SER:HA	1:A:59:THR:CG2	2.38	0.49
1:A:228:LEU:HD22	1:A:257:LEU:HD11	1.95	0.49
1:A:228:LEU:O	1:A:231:GLY:N	2.42	0.49
1:A:120:THR:CG2	1:A:121:GLY:H	2.24	0.49
1:A:221:SER:C	1:A:225:ILE:HD12	2.33	0.49
1:A:140:LYS:HG2	1:A:193:VAL:HG13	1.94	0.49
1:A:76:SER:HA	1:A:114:LYS:HB2	1.93	0.48
1:A:434:GLY:O	1:A:438:HIS:ND1	2.46	0.48
1:A:512:THR:O	1:A:521:THR:HA	2.13	0.48
1:A:139:LEU:HD12	1:A:153:GLU:C	2.25	0.48
1:A:116:PRO:HD2	1:A:243:PHE:HB2	1.95	0.48
1:A:453:THR:HG21	1:A:458:THR:HG22	1.96	0.48
1:A:446:ARG:CG	1:A:446:ARG:O	2.61	0.48
1:A:309:GLN:O	1:A:313:ILE:HG13	2.13	0.48
1:A:330:LEU:O	1:A:363:GLU:HG2	2.13	0.48
1:A:473:CYS:SG	1:A:475:ASP:HB2	2.54	0.47
1:A:38:PRO:HG3	1:A:383:GLU:CD	2.35	0.47
1:A:245:ARG:HD2	1:A:274:GLU:OE1	2.13	0.47
1:A:73:MET:HE1	1:A:86:THR:HG22	1.97	0.47
1:A:329:MET:O	1:A:330:LEU:HD13	2.14	0.47
1:A:55:ARG:NH2	1:A:85:GLU:HB3	2.29	0.47
1:A:266:ILE:O	1:A:287:ASP:HB2	2.15	0.47
1:A:237:ASP:O	1:A:264:ILE:HG23	2.15	0.47
1:A:371:LEU:H	1:A:371:LEU:HD12	1.79	0.47
1:A:311:MET:HG2	1:A:311:MET:O	2.13	0.47
1:A:54:SER:O	1:A:60:LEU:HD13	2.15	0.46
1:A:313:ILE:HG23	1:A:323:VAL:HG11	1.98	0.46
1:A:182:LEU:CB	1:A:194:THR:CG2	2.91	0.46
1:A:142:THR:CG2	1:A:144:ASP:H	2.28	0.46
1:A:348:ALA:O	1:A:352:LEU:HD22	2.15	0.46
1:A:300:ILE:HB	1:A:301:PRO:HD2	1.98	0.46
1:A:23:ASP:OD1	1:A:23:ASP:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ILE:CG2	1:A:102:ILE:O	2.64	0.46
1:A:87:ILE:O	1:A:91:ARG:HG3	2.16	0.46
1:A:186:GLN:O	1:A:192:LEU:HA	2.16	0.46
1:A:143:LEU:CD2	1:A:161:LYS:HA	2.45	0.46
1:A:147:TYR:O	1:A:150:ALA:O	2.34	0.46
1:A:430:LEU:N	1:A:430:LEU:CD1	2.80	0.45
1:A:439:GLN:HE21	1:A:439:GLN:HB2	1.43	0.45
1:A:73:MET:HE1	1:A:86:THR:CG2	2.46	0.45
1:A:294:GLY:HA3	4:A:533:PYR:O1	2.16	0.45
1:A:229:LYS:O	1:A:232:VAL:HB	2.17	0.45
1:A:73:MET:CE	1:A:86:THR:CG2	2.94	0.45
1:A:120:THR:CG2	1:A:121:GLY:N	2.80	0.45
1:A:158:LEU:HD22	1:A:163:ILE:HD12	1.98	0.45
1:A:18:HIS:O	1:A:31:ARG:HD3	2.17	0.45
1:A:252:GLU:O	1:A:256:ILE:CD1	2.65	0.45
1:A:358:ILE:HG13	1:A:377:GLN:HE22	1.81	0.45
1:A:60:LEU:O	1:A:63:MET:HB2	2.16	0.45
1:A:74:ASN:HA	1:A:112:ASP:HB3	1.98	0.45
1:A:406:ASP:HB3	1:A:409:GLU:CB	2.37	0.44
1:A:182:LEU:HG	1:A:194:THR:CG2	2.47	0.44
1:A:264:ILE:CG2	1:A:265:LYS:N	2.80	0.44
1:A:180:ILE:HG23	1:A:199:GLY:HA2	1.99	0.44
1:A:294:GLY:CA	4:A:533:PYR:O1	2.65	0.44
1:A:430:LEU:HD21	1:A:488:ARG:HB2	1.99	0.44
1:A:267:ILE:O	1:A:267:ILE:HG22	2.17	0.44
1:A:228:LEU:HD13	1:A:256:ILE:HG21	1.97	0.44
1:A:424:ALA:HB2	1:A:509:ILE:HD12	1.99	0.44
1:A:134:LYS:HZ3	1:A:139:LEU:CD2	2.30	0.44
1:A:514:TRP:C	1:A:515:ARG:HG2	2.37	0.44
1:A:134:LYS:HZ3	1:A:139:LEU:HD22	1.83	0.44
1:A:431:THR:C	1:A:432:GLU:HG2	2.38	0.44
1:A:238:MET:HA	1:A:264:ILE:CG2	2.47	0.44
1:A:288:GLY:O	1:A:289:ILE:HG13	2.16	0.44
1:A:380:ILE:O	1:A:380:ILE:HG22	2.10	0.44
1:A:50:ILE:HD11	1:A:68:MET:HE2	1.99	0.44
1:A:306:PHE:CE2	1:A:307:LEU:HD23	2.53	0.44
1:A:236:VAL:HG13	1:A:236:VAL:H	1.61	0.44
1:A:464:LEU:HA	1:A:464:LEU:HD12	1.54	0.44
1:A:85:GLU:O	1:A:89:ASN:ND2	2.38	0.44
1:A:407:LEU:O	1:A:410:ALA:HB3	2.18	0.44
1:A:453:THR:HG23	1:A:455:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:NH2	1:A:46:ILE:HD12	2.32	0.43
1:A:56:SER:O	1:A:56:SER:OG	2.33	0.43
1:A:520:PHE:CE2	1:A:522:ASN:HB3	2.53	0.43
1:A:172:LYS:NZ	1:A:197:GLU:OE2	2.49	0.43
1:A:174:TYR:O	1:A:208:VAL:HA	2.17	0.43
1:A:352:LEU:HD12	1:A:352:LEU:HA	1.47	0.43
1:A:123:ILE:HG23	1:A:204:SER:OG	2.18	0.43
1:A:360:LEU:CB	1:A:364:THR:HG23	2.46	0.43
1:A:63:MET:CE	1:A:364:THR:HB	2.48	0.43
1:A:134:LYS:NZ	1:A:156:LEU:HD12	2.32	0.43
1:A:408:MET:O	1:A:408:MET:HG2	2.18	0.43
1:A:134:LYS:HE2	1:A:153:GLU:HA	1.98	0.43
1:A:253:VAL:O	1:A:257:LEU:HD13	2.19	0.43
1:A:49:THR:HB	1:A:361:SER:HA	2.01	0.42
1:A:169:VAL:HG13	1:A:185:LYS:O	2.19	0.42
1:A:289:ILE:CG2	1:A:290:MET:N	2.82	0.42
1:A:251:HIS:O	1:A:254:ARG:N	2.52	0.42
1:A:267:ILE:HD11	1:A:464:LEU:HD21	2.00	0.42
1:A:139:LEU:HD21	1:A:156:LEU:CD1	2.47	0.42
1:A:139:LEU:CD2	1:A:156:LEU:HD12	2.44	0.42
1:A:210:LEU:HB3	1:A:213:ALA:HB3	2.01	0.42
1:A:405:THR:CG2	1:A:405:THR:O	2.54	0.42
1:A:171:SER:O	1:A:184:VAL:HB	2.19	0.42
1:A:143:LEU:N	1:A:143:LEU:CD1	2.83	0.42
1:A:313:ILE:HD13	1:A:313:ILE:HG21	1.54	0.42
1:A:134:LYS:HE2	1:A:153:GLU:C	2.41	0.42
1:A:311:MET:O	1:A:315:ARG:HB2	2.20	0.42
1:A:53:ALA:CB	1:A:365:ALA:O	2.68	0.42
1:A:263:ASN:CB	1:A:457:GLN:HE22	2.33	0.41
1:A:331:GLU:O	1:A:334:ILE:N	2.35	0.41
1:A:119:ARG:HB2	1:A:159:ASP:OD2	2.20	0.41
1:A:507:VAL:CG1	1:A:508:VAL:N	2.82	0.41
1:A:15:GLN:CD	1:A:39:ILE:CG2	2.89	0.41
1:A:391:ARG:O	1:A:395:GLU:HG3	2.20	0.41
1:A:432:GLU:O	1:A:458:THR:HG21	2.20	0.41
1:A:167:VAL:HG13	1:A:171:SER:CB	2.45	0.41
1:A:252:GLU:O	1:A:256:ILE:HD12	2.21	0.41
1:A:175:VAL:HG22	1:A:208:VAL:HG22	2.03	0.41
1:A:228:LEU:HD13	1:A:256:ILE:CG2	2.51	0.41
1:A:139:LEU:CG	1:A:140:LYS:N	2.76	0.41
1:A:152:ASP:C	1:A:154:ASN:H	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ARG:CG	1:A:467:GLY:N	2.82	0.41
1:A:86:THR:O	1:A:90:VAL:HG23	2.21	0.40
1:A:296:LEU:HA	1:A:296:LEU:HD12	1.91	0.40
1:A:72:ARG:CD	1:A:359:MET:HE2	2.51	0.40
1:A:152:ASP:C	1:A:154:ASN:N	2.75	0.40
1:A:204:SER:O	1:A:205:LYS:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	510/530 (96%)	460 (90%)	45 (9%)	5 (1%)	19 54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	GLY
1	A	178	GLY
1	A	259	GLU
1	A	327	THR
1	A	67	GLY

5.3.2 Protein sidechains

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	419/431 (97%)	334 (80%)	85 (20%)	1 4

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	15	GLN
1	A	16	GLN
1	A	34	ILE
1	A	50	ILE
1	A	55	ARG
1	A	56	SER
1	A	60	LEU
1	A	62	GLU
1	A	63	MET
1	A	68	MET
1	A	73	MET
1	A	76	SER
1	A	79	THR
1	A	88	LYS
1	A	103	LEU
1	A	105	ARG
1	A	111	LEU
1	A	112	ASP
1	A	113	THR
1	A	122	LEU
1	A	123	ILE
1	A	135	LYS
1	A	139	LEU
1	A	144	ASP
1	A	151	CYS
1	A	152	ASP
1	A	156	LEU
1	A	157	TRP
1	A	163	ILE
1	A	171	SER
1	A	183	GLN
1	A	192	LEU
1	A	197	GLU
1	A	204	SER
1	A	206	LYS
1	A	223	LYS
1	A	237	ASP

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Mol	Chain	Res	Type
1	A	242	SER
1	A	245	ARG
1	A	254	ARG
1	A	256	ILE
1	A	260	LYS
1	A	269	LYS
1	A	272	ASN
1	A	274	GLU
1	A	277	ARG
1	A	282	ILE
1	A	283	LEU
1	A	284	GLU
1	A	286	SER
1	A	295	ASP
1	A	299	GLU
1	A	303	GLU
1	A	311	MET
1	A	315	ARG
1	A	330	LEU
1	A	332	SER
1	A	341	ARG
1	A	352	LEU
1	A	359	MET
1	A	366	LYS
1	A	376	MET
1	A	377	GLN
1	A	389	PHE
1	A	392	LYS
1	A	397	LEU
1	A	399	ARG
1	A	400	SER
1	A	401	SER
1	A	407	LEU
1	A	415	SER
1	A	422	CYS
1	A	431	THR
1	A	436	SER
1	A	439	GLN
1	A	457	GLN
1	A	468	ILE
1	A	473	CYS
1	A	479	GLU

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Mol	Chain	Res	Type
1	A	486	ASP
1	A	493	MET
1	A	503	LYS
1	A	508	VAL
1	A	518	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	183	GLN
1	A	209	ASN
1	A	226	GLN
1	A	377	GLN
1	A	439	GLN
1	A	457	GLN
1	A	463	HIS
1	A	478	GLN
1	A	494	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

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	PYR	A	533	3	2,5,5	0.86	0	2,6,6	3.75	1 (50%)

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	PYR	A	533	3	-	0/0/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	533	PYR	O3-C2-C3	5.09	132.33	120.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	533	PYR	3	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.