



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:52 PM UTC

PDB ID : 3BG5 / pdb_00003bg5
Title : Crystal Structure of Staphylococcus Aureus Pyruvate Carboxylase
Authors : Xiang, S.; Tong, L.
Deposited on : 2007-11-26
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

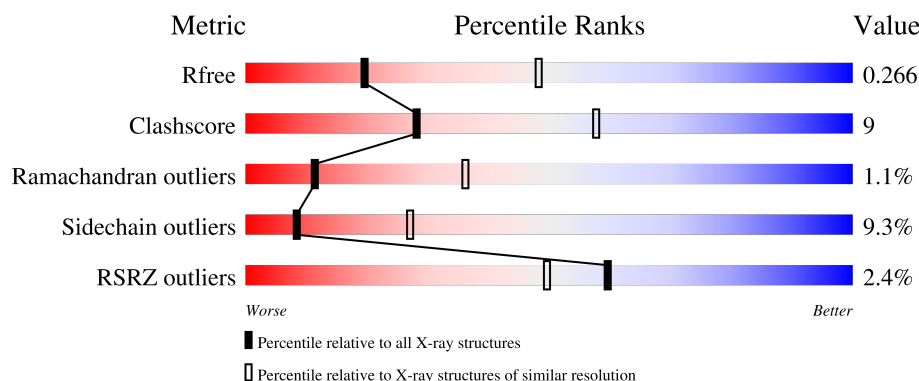
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	1173	 2% 73% 21% • •
1	B	1173	 3% 70% 19% • 8%
1	C	1173	 2% 68% 21% • 9%
1	D	1173	 2% 68% 19% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PYR	A	2001	-	X	-	-
4	PYR	B	2001	-	X	-	-
4	PYR	C	2001	-	X	-	-
4	PYR	D	2001	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 34438 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 carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1137	Total	C	N	O	S	0	0	0
			8969	5682	1510	1747	30			
1	B	1074	Total	C	N	O	S	0	0	0
			8465	5365	1427	1644	29			
1	C	1067	Total	C	N	O	S	0	0	0
			8441	5350	1421	1640	30			
1	D	1067	Total	C	N	O	S	0	0	0
			8413	5334	1416	1634	29			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	expression tag	UNP Q99UY8
A	12	GLY	-	expression tag	UNP Q99UY8
A	13	SER	-	expression tag	UNP Q99UY8
A	14	SER	-	expression tag	UNP Q99UY8
A	15	HIS	-	expression tag	UNP Q99UY8
A	16	HIS	-	expression tag	UNP Q99UY8
A	17	HIS	-	expression tag	UNP Q99UY8
A	18	HIS	-	expression tag	UNP Q99UY8
A	19	HIS	-	expression tag	UNP Q99UY8
A	20	HIS	-	expression tag	UNP Q99UY8
A	21	SER	-	expression tag	UNP Q99UY8
A	22	SER	-	expression tag	UNP Q99UY8
A	23	GLY	-	expression tag	UNP Q99UY8
A	24	LEU	-	expression tag	UNP Q99UY8
A	25	VAL	-	expression tag	UNP Q99UY8
A	26	PRO	-	expression tag	UNP Q99UY8
A	27	ARG	-	expression tag	UNP Q99UY8
A	28	GLY	-	expression tag	UNP Q99UY8
A	29	SER	-	expression tag	UNP Q99UY8
A	30	HIS	-	expression tag	UNP Q99UY8
A	31	MET	-	expression tag	UNP Q99UY8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	-	expression tag	UNP Q99UY8
A	33	SER	-	expression tag	UNP Q99UY8
B	11	MET	-	expression tag	UNP Q99UY8
B	12	GLY	-	expression tag	UNP Q99UY8
B	13	SER	-	expression tag	UNP Q99UY8
B	14	SER	-	expression tag	UNP Q99UY8
B	15	HIS	-	expression tag	UNP Q99UY8
B	16	HIS	-	expression tag	UNP Q99UY8
B	17	HIS	-	expression tag	UNP Q99UY8
B	18	HIS	-	expression tag	UNP Q99UY8
B	19	HIS	-	expression tag	UNP Q99UY8
B	20	HIS	-	expression tag	UNP Q99UY8
B	21	SER	-	expression tag	UNP Q99UY8
B	22	SER	-	expression tag	UNP Q99UY8
B	23	GLY	-	expression tag	UNP Q99UY8
B	24	LEU	-	expression tag	UNP Q99UY8
B	25	VAL	-	expression tag	UNP Q99UY8
B	26	PRO	-	expression tag	UNP Q99UY8
B	27	ARG	-	expression tag	UNP Q99UY8
B	28	GLY	-	expression tag	UNP Q99UY8
B	29	SER	-	expression tag	UNP Q99UY8
B	30	HIS	-	expression tag	UNP Q99UY8
B	31	MET	-	expression tag	UNP Q99UY8
B	32	ALA	-	expression tag	UNP Q99UY8
B	33	SER	-	expression tag	UNP Q99UY8
C	11	MET	-	expression tag	UNP Q99UY8
C	12	GLY	-	expression tag	UNP Q99UY8
C	13	SER	-	expression tag	UNP Q99UY8
C	14	SER	-	expression tag	UNP Q99UY8
C	15	HIS	-	expression tag	UNP Q99UY8
C	16	HIS	-	expression tag	UNP Q99UY8
C	17	HIS	-	expression tag	UNP Q99UY8
C	18	HIS	-	expression tag	UNP Q99UY8
C	19	HIS	-	expression tag	UNP Q99UY8
C	20	HIS	-	expression tag	UNP Q99UY8
C	21	SER	-	expression tag	UNP Q99UY8
C	22	SER	-	expression tag	UNP Q99UY8
C	23	GLY	-	expression tag	UNP Q99UY8
C	24	LEU	-	expression tag	UNP Q99UY8
C	25	VAL	-	expression tag	UNP Q99UY8
C	26	PRO	-	expression tag	UNP Q99UY8
C	27	ARG	-	expression tag	UNP Q99UY8

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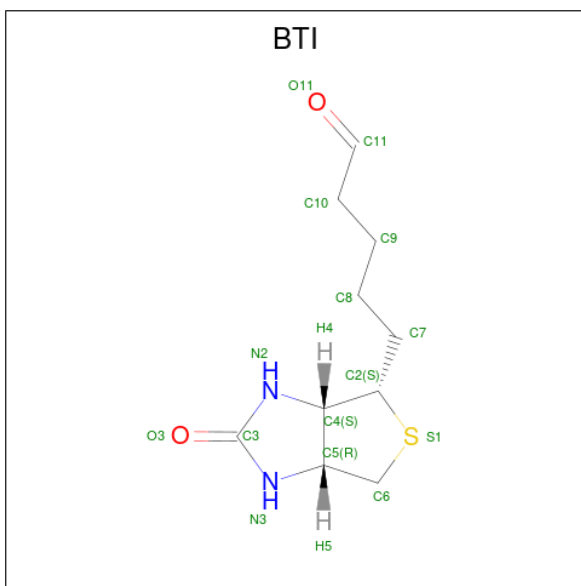
Chain	Residue	Modelled	Actual	Comment	Reference
C	28	GLY	-	expression tag	UNP Q99UY8
C	29	SER	-	expression tag	UNP Q99UY8
C	30	HIS	-	expression tag	UNP Q99UY8
C	31	MET	-	expression tag	UNP Q99UY8
C	32	ALA	-	expression tag	UNP Q99UY8
C	33	SER	-	expression tag	UNP Q99UY8
D	11	MET	-	expression tag	UNP Q99UY8
D	12	GLY	-	expression tag	UNP Q99UY8
D	13	SER	-	expression tag	UNP Q99UY8
D	14	SER	-	expression tag	UNP Q99UY8
D	15	HIS	-	expression tag	UNP Q99UY8
D	16	HIS	-	expression tag	UNP Q99UY8
D	17	HIS	-	expression tag	UNP Q99UY8
D	18	HIS	-	expression tag	UNP Q99UY8
D	19	HIS	-	expression tag	UNP Q99UY8
D	20	HIS	-	expression tag	UNP Q99UY8
D	21	SER	-	expression tag	UNP Q99UY8
D	22	SER	-	expression tag	UNP Q99UY8
D	23	GLY	-	expression tag	UNP Q99UY8
D	24	LEU	-	expression tag	UNP Q99UY8
D	25	VAL	-	expression tag	UNP Q99UY8
D	26	PRO	-	expression tag	UNP Q99UY8
D	27	ARG	-	expression tag	UNP Q99UY8
D	28	GLY	-	expression tag	UNP Q99UY8
D	29	SER	-	expression tag	UNP Q99UY8
D	30	HIS	-	expression tag	UNP Q99UY8
D	31	MET	-	expression tag	UNP Q99UY8
D	32	ALA	-	expression tag	UNP Q99UY8
D	33	SER	-	expression tag	UNP Q99UY8

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0

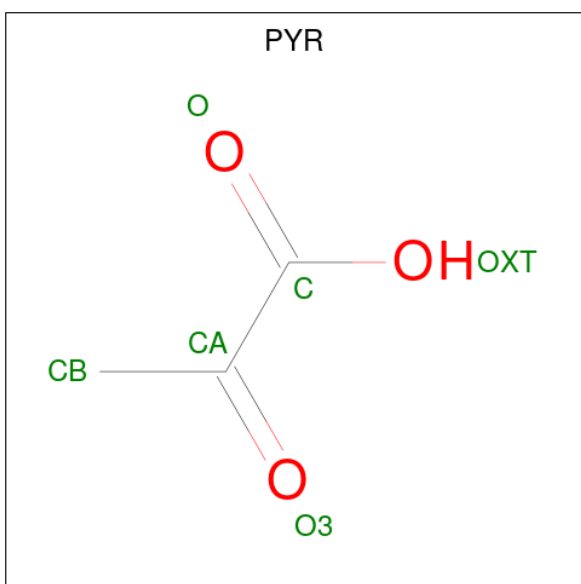
- Molecule 3 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL

(CCD ID: BTI) (formula: $C_{10}H_{16}N_2O_2S$).



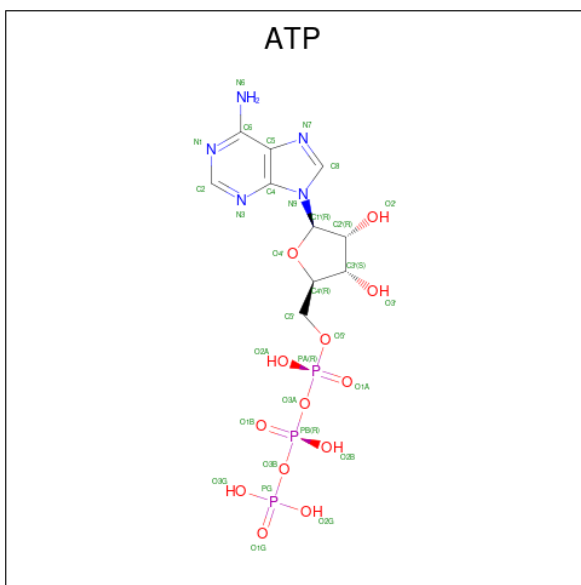
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	B	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	C	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	D	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

- Molecule 4 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



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

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

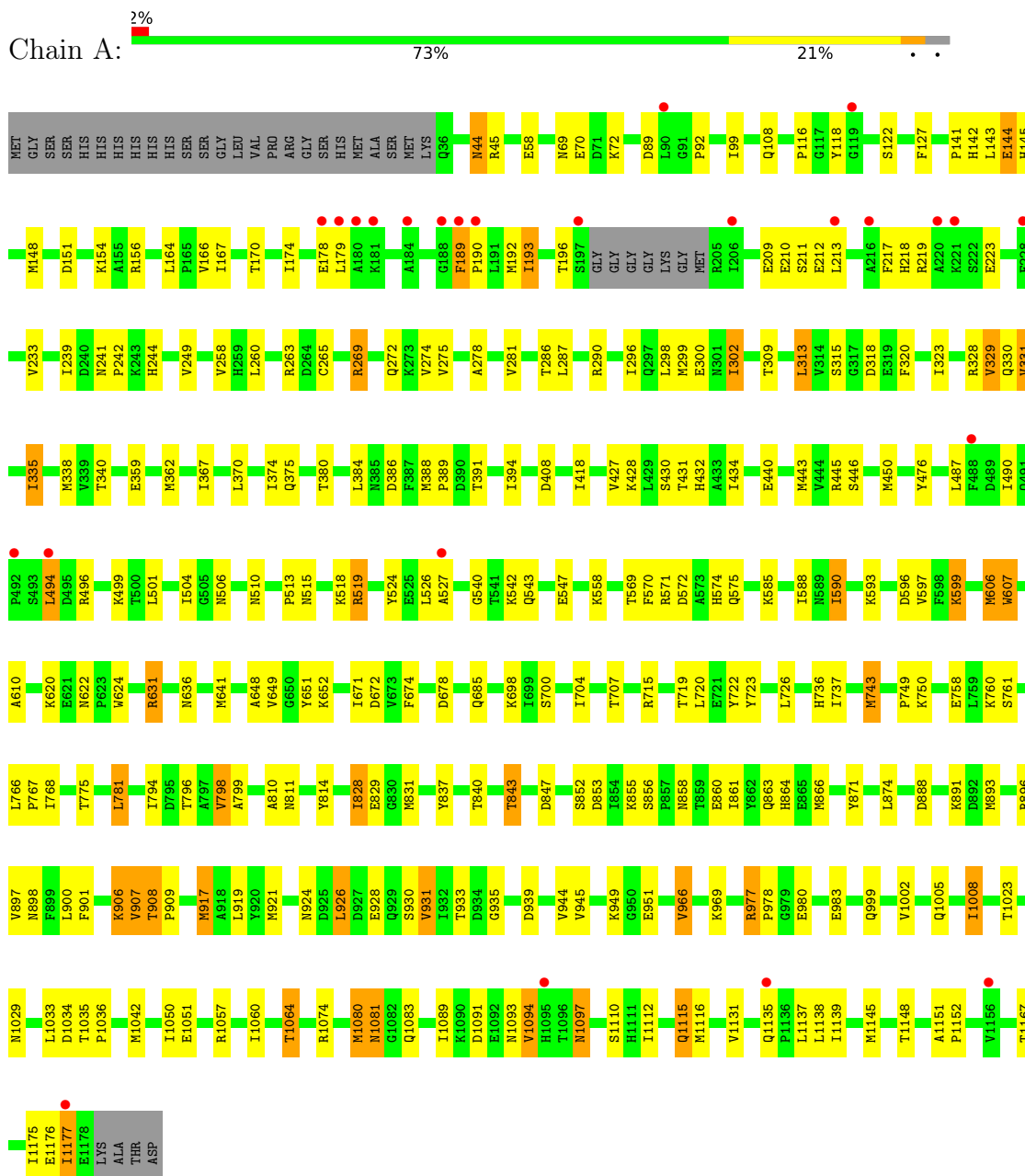


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

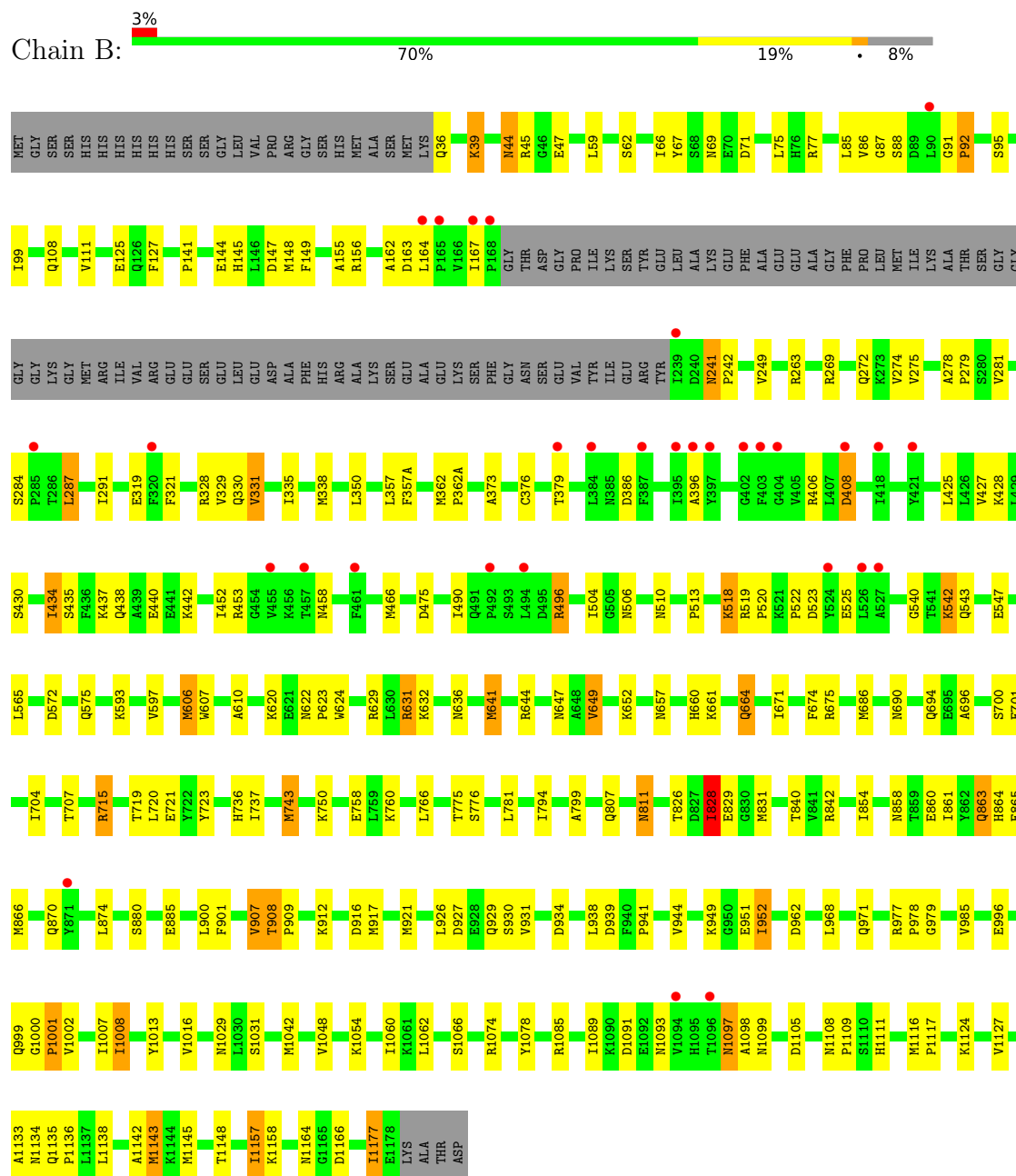
3 Residue-property plots [i](#)

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.

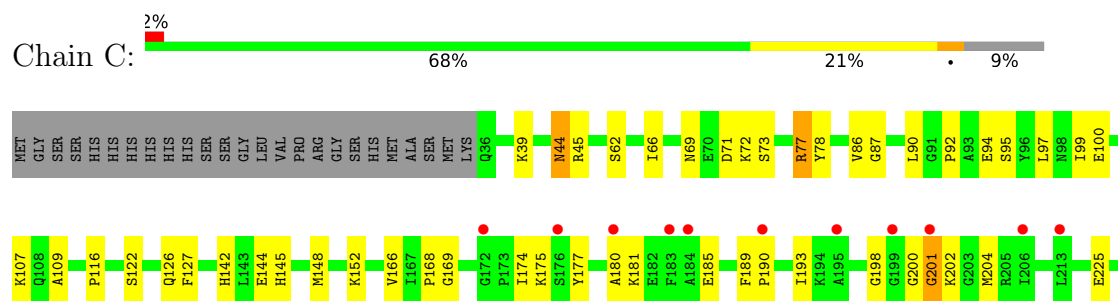
• Molecule 1: Pyruvate carboxylase

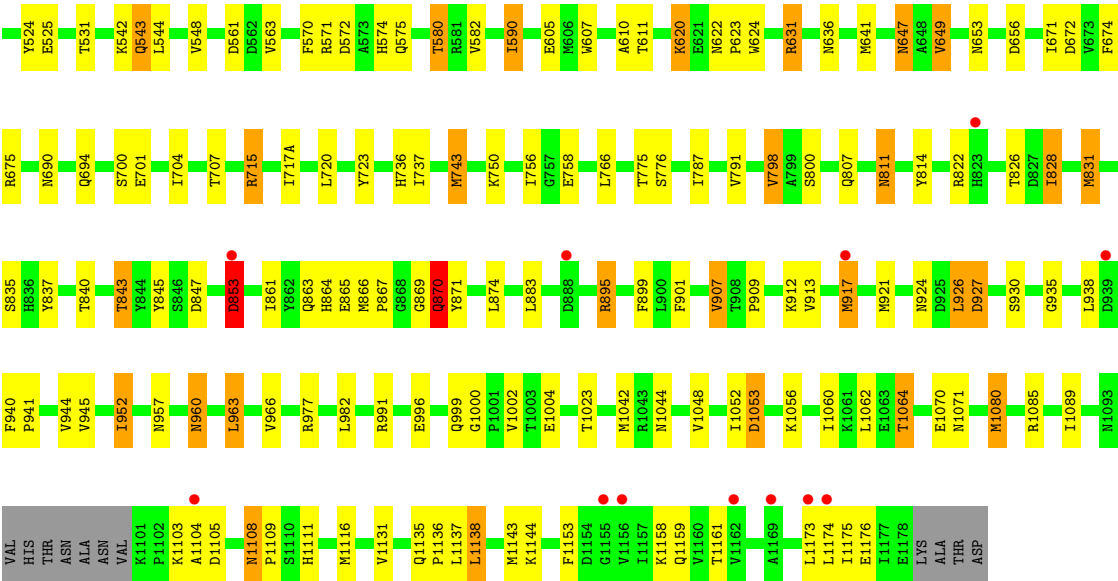


● Molecule 1: Pyruvate carboxylase



● Molecule 1: Pyruvate carboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.43Å 256.08Å 126.01Å 90.00° 109.47° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-2.80) 98.4 (30.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.59 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.215 , 0.268 0.215 , 0.266	Depositor DCC
R_{free} test set	7343 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	34438	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.51	0/9139	0.88	0/12364
1	B	0.49	0/8625	0.89	4/11675 (0.0%)
1	C	0.50	1/8603 (0.0%)	0.88	2/11627 (0.0%)
1	D	0.52	0/8571	0.88	2/11598 (0.0%)
All	All	0.50	1/34938 (0.0%)	0.88	8/47264 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	315	SER	CB-OG	7.26	1.56	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	972	GLU	N-CA-C	7.25	117.54	108.19
1	B	163	ASP	N-CA-C	6.05	119.52	111.30
1	D	938	LEU	N-CA-C	5.86	117.75	111.36
1	C	69	ASN	N-CA-C	5.85	117.46	111.14
1	B	95	SER	N-CA-C	5.61	117.84	111.11
1	D	649	VAL	N-CA-C	-5.60	107.27	112.43
1	B	1007	ILE	N-CA-C	5.54	115.74	110.53
1	B	828	ILE	N-CA-C	5.03	115.47	110.23

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	8969	0	8894	176	0
1	B	8465	0	8412	141	0
1	C	8441	0	8350	150	0
1	D	8413	0	8361	153	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	15	0	15	1	0
3	B	15	0	15	0	0
3	C	15	0	15	1	0
3	D	15	0	15	1	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	C	6	0	0	0	0
4	D	6	0	0	0	0
5	A	31	0	12	0	0
5	C	31	0	12	1	0
All	All	34438	0	34101	609	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 9.

All (609) 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:189:PHE:HB3	1:A:190:PRO:HD3	1.35	1.06
1:C:504:ILE:HG21	1:C:1042:MET:HE2	1.38	1.03
1:C:893:MET:HE1	1:C:921:MET:HB2	1.39	1.03
1:C:504:ILE:HG21	1:C:1042:MET:CE	1.95	0.96
1:B:1000:GLY:H	1:B:1001:PRO:HD3	1.30	0.96
1:A:44:ASN:HD22	1:A:45:ARG:H	0.92	0.91
1:D:1042:MET:HE3	1:D:1062:LEU:HB2	1.52	0.89
1:D:44:ASN:HD22	1:D:45:ARG:H	1.18	0.88
1:C:700:SER:H	1:C:736:HIS:HD2	1.24	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:700:SER:H	1:D:736:HIS:HD2	1.23	0.86
1:A:44:ASN:ND2	1:A:45:ARG:H	1.75	0.84
1:D:720:LEU:HD21	1:D:758:GLU:HG3	1.60	0.84
1:C:44:ASN:HD22	1:C:45:ARG:H	1.26	0.83
1:D:258:VAL:HG21	1:D:362:MET:HE2	1.58	0.83
1:A:840:THR:O	1:A:843:THR:HB	1.79	0.83
1:B:858:ASN:HD21	1:B:860:GLU:HG2	1.42	0.82
1:D:647:ASN:HD22	1:D:647:ASN:C	1.88	0.82
1:A:501:LEU:HD11	1:A:1080:MET:HG3	1.61	0.81
1:D:357:LEU:O	1:D:362:MET:HB2	1.80	0.80
1:A:864:HIS:CD2	1:A:866:MET:HG3	2.17	0.80
1:A:44:ASN:HD22	1:A:45:ARG:N	1.76	0.80
1:A:620:LYS:HG2	1:A:1023:THR:HG21	1.62	0.80
1:B:331:VAL:HG12	1:B:428:LYS:HD3	1.63	0.79
1:B:519:ARG:HB2	1:B:520:PRO:HD2	1.65	0.79
1:B:1105:ASP:H	1:B:1111:HIS:HD2	1.28	0.79
1:A:743:MET:HG3	1:A:907:VAL:HG13	1.66	0.78
1:A:504:ILE:HG21	1:A:1042:MET:HE2	1.66	0.77
1:A:543:GLN:O	1:A:547:GLU:HG2	1.85	0.77
1:C:590:ILE:HG12	1:C:837:TYR:CE2	2.19	0.76
1:C:814:TYR:CE2	1:C:828:ILE:HG12	2.21	0.76
1:D:641:MET:HE3	1:D:674:PHE:CE1	2.21	0.75
1:D:329:VAL:HG22	1:D:348:GLN:HE22	1.52	0.75
1:B:811:ASN:H	1:B:811:ASN:HD22	1.35	0.74
1:B:864:HIS:HD2	1:B:866:MET:H	1.36	0.74
1:B:700:SER:H	1:B:736:HIS:HD2	1.34	0.73
1:B:144:GLU:O	1:B:148:MET:HB2	1.89	0.72
1:A:898:ASN:ND2	1:A:906:LYS:HE3	2.04	0.72
1:B:44:ASN:HD22	1:B:45:ARG:H	1.36	0.72
1:D:864:HIS:CD2	1:D:866:MET:HG3	2.24	0.72
1:D:543:GLN:HE22	1:D:636:ASN:HA	1.54	0.71
1:D:840:THR:O	1:D:843:THR:HB	1.91	0.71
1:A:864:HIS:HD2	1:A:866:MET:HG3	1.54	0.71
1:C:338:MET:HE3	1:C:373:ALA:HB1	1.73	0.71
1:A:810:ALA:HB1	1:A:831:MET:HE1	1.71	0.71
1:B:1042:MET:HE3	1:B:1062:LEU:HB2	1.73	0.70
1:A:1081:ASN:HB2	1:C:78:TYR:CE2	2.26	0.70
1:D:259:HIS:H	1:D:364:GLN:HE22	1.39	0.70
1:A:313:LEU:HB2	1:A:323:ILE:HD11	1.73	0.70
1:D:1159:GLN:HG2	1:D:1176:GLU:HG2	1.73	0.69
1:D:864:HIS:HD2	1:D:866:MET:H	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:GLN:HA	1:B:664:GLN:HE21	1.57	0.68
1:C:116:PRO:HB2	1:C:122:SER:HA	1.76	0.67
1:A:700:SER:H	1:A:736:HIS:HD2	1.39	0.67
1:C:960:ASN:HB2	1:C:963:LEU:CB	2.24	0.67
1:D:921:MET:HG3	1:D:926:LEU:HB2	1.76	0.67
1:C:606:MET:HE1	1:C:671:ILE:CD1	2.25	0.67
1:A:189:PHE:HB3	1:A:190:PRO:CD	2.19	0.67
1:B:1177:ILE:HD13	1:B:1177:ILE:N	2.09	0.67
1:C:866:MET:HE1	1:C:871:TYR:HA	1.77	0.66
1:A:362:MET:CE	1:A:367:ILE:HD11	2.26	0.66
1:D:543:GLN:NE2	1:D:636:ASN:HA	2.11	0.66
1:A:606:MET:HE1	1:A:671:ILE:CD1	2.25	0.66
1:D:574:HIS:HD2	1:D:580:THR:HA	1.61	0.66
1:B:977:ARG:HG2	1:B:979:GLY:H	1.61	0.65
1:C:201:GLY:HA2	1:C:204:MET:HE3	1.77	0.65
1:C:622:ASN:HD21	1:C:624:TRP:HD1	1.45	0.65
1:C:811:ASN:HD22	1:C:811:ASN:H	1.44	0.65
1:A:263:ARG:HH21	1:A:330:GLN:NE2	1.94	0.65
1:B:506:ASN:HD22	1:B:510:ASN:HD22	1.43	0.65
1:C:260:LEU:HD21	1:C:362:MET:HE1	1.78	0.65
1:D:142:HIS:H	1:D:145:HIS:HD2	1.43	0.65
1:D:690:ASN:O	1:D:694:GLN:HG2	1.97	0.65
1:B:543:GLN:HE22	1:B:636:ASN:HA	1.61	0.65
1:B:1029:ASN:C	1:B:1029:ASN:HD22	2.05	0.65
1:D:570:PHE:O	1:D:574:HIS:HE1	1.80	0.65
1:D:575:GLN:NE2	1:D:610:ALA:H	1.95	0.65
1:A:164:LEU:HD11	1:A:298:LEU:HB2	1.80	0.64
1:A:527:ALA:HB2	1:A:840:THR:HG21	1.77	0.64
1:A:278:ALA:HB3	1:A:335:ILE:HG23	1.80	0.64
1:C:306:ASN:OD1	1:C:348:GLN:HG2	1.98	0.64
1:A:1042:MET:HE1	1:A:1060:ILE:CG2	2.28	0.64
1:C:700:SER:H	1:C:736:HIS:CD2	2.12	0.64
1:A:901:PHE:CZ	1:A:917:MET:HG3	2.33	0.63
1:C:260:LEU:HD21	1:C:362:MET:CE	2.28	0.63
1:A:142:HIS:H	1:A:145:HIS:HD2	1.45	0.63
1:D:241:ASN:HD21	1:D:477:THR:HG21	1.63	0.63
1:B:504:ILE:HG21	1:B:1042:MET:HE2	1.80	0.63
1:C:539:SER:HA	1:C:543:GLN:HG3	1.80	0.63
1:C:960:ASN:HB2	1:C:963:LEU:HB2	1.79	0.63
1:A:145:HIS:HE1	1:A:302:ILE:O	1.82	0.63
1:C:152:LYS:HE2	1:C:198:GLY:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:ASN:HD21	1:B:624:TRP:HD1	1.46	0.63
1:D:498:THR:OG1	1:D:1085:ARG:NH2	2.32	0.63
1:C:77:ARG:HD3	1:C:78:TYR:CE2	2.34	0.62
1:C:840:THR:O	1:C:843:THR:HB	1.99	0.62
1:D:1137:LEU:HD13	1:D:1175:ILE:HG13	1.79	0.62
1:D:575:GLN:HE22	1:D:610:ALA:H	1.45	0.62
1:A:338:MET:HE1	1:A:430:SER:HB3	1.80	0.62
1:C:269:ARG:HG3	1:C:270:ARG:H	1.64	0.62
1:A:1097:ASN:HD22	1:A:1097:ASN:H	1.47	0.62
1:A:1112:ILE:HD11	1:A:1177:ILE:HD11	1.82	0.62
1:B:85:LEU:HD21	1:B:88:SER:HB3	1.82	0.62
1:A:540:GLY:H	1:A:543:GLN:HE21	1.48	0.62
1:A:590:ILE:HG12	1:A:837:TYR:CE2	2.35	0.62
1:A:700:SER:H	1:A:736:HIS:CD2	2.18	0.62
1:B:901:PHE:HZ	1:B:917:MET:HG3	1.63	0.61
1:B:927:ASP:H	1:B:930:SER:HB2	1.65	0.61
1:A:720:LEU:HD11	1:A:758:GLU:HG3	1.83	0.61
1:A:1115:GLN:CD	1:A:1115:GLN:H	2.08	0.61
1:B:700:SER:H	1:B:736:HIS:CD2	2.18	0.61
1:C:991:ARG:O	1:C:995:GLU:HG2	2.01	0.61
1:A:269:ARG:HD3	1:A:272:GLN:NE2	2.16	0.60
1:B:435:SER:HB3	1:B:438:GLN:HB2	1.83	0.60
1:D:701:GLU:HG2	1:D:737:ILE:HB	1.84	0.60
1:A:1042:MET:HE1	1:A:1060:ILE:HG22	1.81	0.60
1:B:1074:ARG:NH1	1:B:1091:ASP:OD1	2.35	0.60
1:C:419:SER:HB2	1:C:421:TYR:CD1	2.37	0.60
1:C:370:LEU:O	1:C:432:HIS:HE1	1.84	0.60
1:C:556:TRP:O	1:C:560:GLN:HG2	2.02	0.60
1:A:814:TYR:CE2	1:A:828:ILE:HG12	2.36	0.60
1:B:519:ARG:HB2	1:B:520:PRO:CD	2.32	0.60
1:A:167:ILE:HD11	1:A:323:ILE:HD13	1.84	0.60
1:D:901:PHE:CZ	1:D:917:MET:HG3	2.36	0.60
1:A:858:ASN:ND2	1:A:860:GLU:H	2.00	0.60
1:B:99:ILE:HG23	1:B:127:PHE:HD1	1.67	0.60
1:A:1139:ILE:HG12	1:A:1148:THR:HG22	1.84	0.59
1:C:200:GLY:C	1:C:202:LYS:H	2.10	0.59
1:C:775:THR:HG22	1:C:861:ILE:HG13	1.84	0.59
1:D:87:GLY:HA3	1:D:90:LEU:HD12	1.85	0.59
1:D:278:ALA:HB3	1:D:335:ILE:HG23	1.85	0.59
1:B:44:ASN:ND2	1:B:45:ARG:H	2.00	0.59
1:C:275:VAL:HG11	1:C:466:MET:HE1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:571:ARG:HH11	1:C:575:GLN:NE2	1.99	0.59
1:C:145:HIS:HE1	1:C:302:ILE:O	1.86	0.59
1:C:814:TYR:CZ	1:C:828:ILE:HG12	2.38	0.58
1:A:370:LEU:O	1:A:432:HIS:HE1	1.86	0.58
1:C:398:ARG:NE	1:C:1083:GLN:HG2	2.18	0.58
1:A:58:GLU:HG3	1:C:445:ARG:HD3	1.85	0.58
1:C:437:LYS:H	1:C:437:LYS:HD3	1.68	0.58
1:D:717(A):ILE:HG13	1:D:957:ASN:HD21	1.68	0.58
1:B:540:GLY:H	1:B:543:GLN:HE21	1.52	0.58
1:B:664:GLN:HA	1:B:664:GLN:NE2	2.18	0.58
1:D:400:SER:HB2	1:D:445:ARG:HH21	1.68	0.58
1:A:569:THR:OG1	1:A:798:VAL:HG23	2.03	0.58
1:D:909:PRO:HG2	1:D:952:ILE:HG12	1.85	0.58
1:A:524:TYR:CD2	1:A:843:THR:HG22	2.39	0.57
1:A:571:ARG:HH11	1:A:575:GLN:NE2	2.01	0.57
1:A:296:ILE:O	1:A:300:GLU:HB2	2.04	0.57
1:C:230:ASN:HD22	1:C:232:GLU:H	1.52	0.57
1:A:864:HIS:HD2	1:A:866:MET:H	1.52	0.57
1:B:269:ARG:HG3	1:B:272:GLN:HB3	1.86	0.57
1:B:1177:ILE:HD13	1:B:1177:ILE:H	1.70	0.57
1:D:935:GLY:HA3	1:D:966:VAL:CG1	2.35	0.57
1:A:494:LEU:HD12	1:A:494:LEU:H	1.70	0.57
1:B:641:MET:HE2	1:B:671:ILE:HG13	1.86	0.57
1:D:590:ILE:HG12	1:D:837:TYR:CE2	2.40	0.57
1:B:715:ARG:HH12	1:B:865:GLU:CD	2.11	0.57
1:B:263:ARG:HH21	1:B:330:GLN:NE2	2.03	0.56
1:B:1116:MET:HB3	1:B:1117:PRO:HD2	1.86	0.56
1:A:901:PHE:HZ	1:A:917:MET:HG3	1.69	0.56
1:A:167:ILE:HD11	1:A:323:ILE:CD1	2.36	0.56
1:C:396:ALA:HB3	1:C:453:ARG:NH1	2.20	0.56
1:A:1131:VAL:HB	1:A:1135:GLN:CD	2.31	0.56
1:A:69:ASN:O	1:A:72:LYS:HG2	2.05	0.56
1:B:860:GLU:O	1:B:863:GLN:HG2	2.04	0.56
1:D:519:ARG:NH2	1:D:847:ASP:OD2	2.35	0.56
1:D:675:ARG:HA	1:D:701:GLU:HB2	1.86	0.56
1:A:69:ASN:HD22	1:A:72:LYS:HE2	1.71	0.56
1:A:575:GLN:NE2	1:A:610:ALA:H	2.04	0.56
1:A:1081:ASN:HB2	1:C:78:TYR:CD2	2.41	0.56
1:A:380:THR:HG21	1:A:418:ILE:HD13	1.88	0.55
1:C:655:PRO:HG2	1:C:985:VAL:HG23	1.87	0.55
1:D:90:LEU:HD21	1:D:98:ASN:HD22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:ARG:NH1	1:C:408:ASP:OD1	2.37	0.55
1:D:867:PRO:O	1:D:870:GLN:HB2	2.05	0.55
1:A:210:GLU:C	1:A:212:GLU:H	2.14	0.55
1:D:631:ARG:NH2	1:D:672:ASP:OD1	2.40	0.55
1:A:641:MET:HE3	1:A:674:PHE:CE1	2.41	0.55
1:A:858:ASN:HD21	1:A:860:GLU:HB2	1.70	0.55
1:A:258:VAL:HG21	1:A:362:MET:HE2	1.89	0.55
1:A:596:ASP:O	1:A:599:LYS:HG2	2.06	0.55
1:C:622:ASN:HD22	1:C:623:PRO:HD2	1.72	0.55
1:D:269:ARG:HG3	1:D:270:ARG:H	1.72	0.55
1:C:174:ILE:HG21	1:C:180:ALA:HB2	1.90	0.55
1:C:622:ASN:HD21	1:C:624:TRP:CD1	2.25	0.55
1:C:641:MET:HG2	1:C:671:ILE:HG21	1.87	0.55
1:C:144:GLU:O	1:C:148:MET:HB2	2.07	0.54
1:C:71:ASP:C	1:C:73:SER:H	2.15	0.54
1:A:504:ILE:HG21	1:A:1042:MET:CE	2.34	0.54
1:C:263:ARG:HH21	1:C:330:GLN:NE2	2.04	0.54
1:C:775:THR:CG2	1:C:861:ILE:HG13	2.36	0.54
1:C:960:ASN:HB2	1:C:963:LEU:HB3	1.89	0.54
1:D:574:HIS:CD2	1:D:580:THR:HA	2.41	0.54
1:B:917:MET:HE2	1:B:944:VAL:HG21	1.89	0.54
1:D:826:THR:HG21	1:D:831:MET:HE1	1.88	0.54
1:C:504:ILE:HG21	1:C:1042:MET:HE3	1.82	0.54
1:A:606:MET:HE1	1:A:671:ILE:HD12	1.90	0.54
1:C:569:THR:OG1	1:C:798:VAL:HG23	2.07	0.54
1:B:1000:GLY:N	1:B:1001:PRO:HD3	2.09	0.54
1:A:1064:THR:HG21	1:C:1066:SER:HA	1.89	0.53
1:D:1052:ILE:HG22	1:D:1053:ASP:H	1.73	0.53
1:A:1145:MET:HE3	1:B:513:PRO:HB3	1.89	0.53
1:B:45:ARG:HD2	1:B:71:ASP:OD2	2.08	0.53
1:C:44:ASN:ND2	1:C:45:ARG:H	2.02	0.53
1:C:909:PRO:O	1:C:912:LYS:HB3	2.09	0.53
1:D:1052:ILE:O	1:D:1053:ASP:C	2.50	0.53
1:C:607:TRP:HE3	1:C:641:MET:HE2	1.73	0.53
1:A:622:ASN:HD22	1:A:622:ASN:C	2.17	0.53
1:C:607:TRP:CE3	1:C:641:MET:HE2	2.44	0.53
1:B:1105:ASP:H	1:B:1111:HIS:CD2	2.18	0.53
1:D:90:LEU:HD13	1:D:95:SER:HA	1.90	0.53
1:B:543:GLN:O	1:B:547:GLU:HG2	2.08	0.53
1:C:263:ARG:HH21	1:C:330:GLN:HE21	1.55	0.53
1:D:164:LEU:HD21	1:D:294:ALA:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:ASN:HD22	1:A:811:ASN:H	1.57	0.53
1:B:641:MET:HE3	1:B:674:PHE:CE1	2.43	0.53
1:B:720:LEU:HD21	1:B:758:GLU:HG3	1.91	0.53
1:D:814:TYR:CE2	1:D:828:ILE:HG12	2.44	0.53
1:D:935:GLY:HA3	1:D:966:VAL:HG13	1.91	0.53
1:B:506:ASN:ND2	1:B:510:ASN:HD22	2.06	0.53
1:D:408:ASP:HB2	1:D:428:LYS:HB3	1.91	0.53
1:B:575:GLN:HE22	1:B:610:ALA:H	1.56	0.52
1:A:210:GLU:O	1:A:212:GLU:N	2.38	0.52
1:B:408:ASP:CB	1:B:428:LYS:HE3	2.39	0.52
1:B:1029:ASN:ND2	1:B:1031:SER:OG	2.40	0.52
1:A:1033:LEU:HD23	1:A:1050:ILE:HG12	1.91	0.52
1:A:1074:ARG:NH1	1:A:1091:ASP:OD2	2.41	0.52
1:C:296:ILE:O	1:C:300:GLU:HB2	2.09	0.52
1:B:900:LEU:HD23	1:B:921:MET:HE1	1.90	0.52
1:C:398:ARG:HE	1:C:1083:GLN:HG2	1.75	0.52
1:A:394:ILE:HD11	1:A:418:ILE:HD11	1.91	0.52
1:A:519:ARG:NH2	1:A:847:ASP:OD2	2.42	0.52
1:A:144:GLU:O	1:A:148:MET:HB2	2.09	0.52
1:A:362:MET:HE1	1:A:367:ILE:CD1	2.40	0.52
1:B:811:ASN:H	1:B:811:ASN:ND2	2.06	0.52
1:D:249:VAL:HG21	1:D:299:MET:HG3	1.90	0.52
1:D:563:VAL:HG21	1:D:787:ILE:HG12	1.91	0.52
1:A:515:ASN:HA	1:B:1143:MET:HG3	1.91	0.52
1:A:672:ASP:HA	1:A:698:LYS:HD2	1.92	0.52
1:A:239:ILE:HD11	1:A:315:SER:HB2	1.91	0.52
1:C:334:THR:O	1:C:338:MET:HG3	2.10	0.52
1:D:811:ASN:H	1:D:811:ASN:HD22	1.57	0.52
1:A:575:GLN:HE22	1:A:610:ALA:H	1.56	0.51
1:C:435:SER:HB2	1:C:437:LYS:HE3	1.91	0.51
1:C:772:THR:HG22	1:C:783:TYR:CE2	2.46	0.51
1:D:622:ASN:HD22	1:D:623:PRO:HD2	1.74	0.51
1:C:142:HIS:H	1:C:145:HIS:HD2	1.58	0.51
1:C:810:ALA:HB1	1:C:831:MET:HE1	1.91	0.51
1:D:44:ASN:ND2	1:D:45:ARG:H	1.99	0.51
1:A:328:ARG:HD2	1:A:329:VAL:O	2.10	0.51
1:B:776:SER:HB3	1:B:861:ILE:HD11	1.92	0.51
1:B:274:VAL:HG12	1:B:275:VAL:HG23	1.92	0.51
1:C:606:MET:HE2	1:C:639:PHE:HB3	1.93	0.51
1:B:1042:MET:HE1	1:B:1060:ILE:HG22	1.93	0.51
1:A:504:ILE:HD13	1:A:1042:MET:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:864:HIS:CD2	1:B:866:MET:H	2.23	0.51
1:D:743:MET:HG3	1:D:907:VAL:HG13	1.92	0.51
1:A:737:ILE:HG12	1:A:767:PRO:HG2	1.92	0.50
1:B:675:ARG:HA	1:B:701:GLU:HB2	1.93	0.50
1:A:1005:GLN:HA	1:A:1008:ILE:HD11	1.92	0.50
1:B:622:ASN:HD22	1:B:623:PRO:HD2	1.76	0.50
1:A:543:GLN:HE22	1:A:636:ASN:HA	1.77	0.50
1:C:1145:MET:HE2	1:C:1145:MET:HA	1.93	0.50
1:B:858:ASN:ND2	1:B:860:GLU:HG2	2.17	0.50
1:C:1035:THR:HB	1:C:1036:PRO:HD3	1.94	0.50
1:C:419:SER:HB2	1:C:421:TYR:HD1	1.76	0.50
1:B:664:GLN:HE22	1:B:696:ALA:HB2	1.77	0.50
1:B:799:ALA:H	1:B:811:ASN:ND2	2.10	0.50
1:C:504:ILE:HD13	1:C:1042:MET:HE2	1.93	0.50
1:A:871:TYR:CD1	1:A:871:TYR:O	2.65	0.49
1:B:338:MET:HE3	1:B:373:ALA:HB1	1.92	0.49
1:C:66:ILE:HB	1:C:86:VAL:CG2	2.41	0.49
1:C:278:ALA:HB3	1:C:335:ILE:HG23	1.94	0.49
1:D:504:ILE:CG2	1:D:1042:MET:HG3	2.42	0.49
1:D:776:SER:HB3	1:D:861:ILE:HD11	1.93	0.49
1:D:1158:LYS:HG3	1:D:1176:GLU:HG3	1.94	0.49
1:A:309:THR:HG21	1:A:330:GLN:HE22	1.78	0.49
1:D:370:LEU:O	1:D:432:HIS:HE1	1.96	0.49
1:B:406:ARG:NH1	1:B:408:ASP:OD1	2.46	0.49
1:D:1104:ALA:HB2	1:D:1173:LEU:HA	1.95	0.49
1:A:70:GLU:HG3	1:A:92:PRO:HG3	1.94	0.49
1:D:501:LEU:HD11	1:D:1080:MET:HE2	1.95	0.49
1:D:620:LYS:HG2	1:D:1023:THR:HG21	1.94	0.49
1:D:1137:LEU:CD1	1:D:1175:ILE:HG13	2.42	0.49
1:A:760:LYS:HG2	1:A:768:ILE:HD12	1.95	0.49
1:A:935:GLY:HA3	1:A:966:VAL:HG13	1.95	0.49
1:B:496:ARG:H	1:B:496:ARG:HD2	1.78	0.49
1:B:719:THR:HG22	1:B:721:GLU:H	1.78	0.49
1:B:1066:SER:HB2	1:D:1064:THR:HG21	1.95	0.49
1:C:641:MET:CG	1:C:671:ILE:HG21	2.43	0.49
1:A:335:ILE:HD11	1:A:375:GLN:N	2.28	0.48
1:B:408:ASP:HB2	1:B:428:LYS:HE3	1.94	0.48
1:D:506:ASN:ND2	1:D:510:ASN:HD22	2.11	0.48
1:A:720:LEU:HD21	1:A:758:GLU:HG3	1.95	0.48
1:B:934:ASP:O	1:B:938:LEU:HG	2.13	0.48
1:B:67:TYR:CD1	1:B:77:ARG:HG3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:LYS:HD3	1:C:62:SER:HB3	1.95	0.48
1:D:863:GLN:O	1:D:895:ARG:HD2	2.12	0.48
1:D:1137:LEU:HD12	1:D:1138:LEU:HB2	1.95	0.48
1:A:949:LYS:HB3	1:A:951:GLU:HG3	1.95	0.48
1:B:141:PRO:HB2	1:B:145:HIS:HB2	1.95	0.48
1:B:1097:ASN:C	1:B:1099:ASN:H	2.21	0.48
1:C:169:GLY:HA2	1:C:236:GLU:HA	1.96	0.48
1:C:940:PHE:HB3	1:C:944:VAL:CG1	2.43	0.48
1:D:452:ILE:HD12	1:D:459:ILE:HD11	1.95	0.48
1:D:853:ASP:OD2	1:D:853:ASP:N	2.47	0.48
1:D:895:ARG:HE	1:D:899:PHE:HE1	1.61	0.48
1:A:362:MET:HE1	1:A:367:ILE:HD11	1.95	0.48
1:A:921:MET:HE2	1:A:931:VAL:HG21	1.95	0.48
1:D:126:GLN:HG2	1:D:129:ARG:HH12	1.79	0.48
1:D:864:HIS:HD2	1:D:866:MET:HG3	1.77	0.48
1:D:941:PRO:O	1:D:944:VAL:HG12	2.14	0.48
1:A:446:SER:O	1:A:450:MET:HG2	2.13	0.48
1:A:799:ALA:H	1:A:811:ASN:ND2	2.12	0.48
1:C:174:ILE:HG22	1:C:175:LYS:N	2.29	0.48
1:C:861:ILE:HD13	1:C:864:HIS:NE2	2.29	0.48
1:C:1143:MET:HG3	1:D:515:ASN:HA	1.94	0.48
1:C:590:ILE:CG1	1:C:837:TYR:CE2	2.95	0.48
1:C:705:CYS:HB3	1:C:743:MET:SD	2.54	0.47
1:C:828:ILE:O	1:C:832:GLU:HG2	2.14	0.47
1:C:1069:ASP:C	1:C:1071:ASN:H	2.20	0.47
1:A:704:ILE:HG21	1:A:723:TYR:HD2	1.79	0.47
1:B:149:PHE:HA	1:B:155:ALA:HB2	1.96	0.47
1:B:328:ARG:HD3	1:B:329:VAL:O	2.14	0.47
1:D:268:GLN:HB3	1:D:273:LYS:HA	1.95	0.47
1:D:641:MET:HE2	1:D:671:ILE:HG13	1.96	0.47
1:A:930:SER:HA	1:A:933:THR:HB	1.95	0.47
1:C:266:SER:O	1:C:478:THR:HA	2.15	0.47
1:C:811:ASN:H	1:C:811:ASN:ND2	2.07	0.47
1:C:940:PHE:HB3	1:C:944:VAL:HG12	1.97	0.47
1:A:856:SER:OG	1:D:800:SER:HA	2.14	0.47
1:B:287:LEU:HD22	1:B:291:ILE:HD11	1.97	0.47
1:C:273:LYS:HB3	1:C:276:GLU:OE2	2.14	0.47
1:C:991:ARG:O	1:C:995:GLU:CG	2.62	0.47
1:C:99:ILE:HG23	1:C:127:PHE:HD1	1.80	0.47
1:D:917:MET:HE1	1:D:940:PHE:HD2	1.78	0.47
1:A:494:LEU:HD23	1:A:499:LYS:HZ2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:LEU:HB3	1:D:114:ILE:HG12	1.97	0.47
1:D:631:ARG:HA	1:D:631:ARG:HD3	1.59	0.47
1:D:656:ASP:OD2	1:D:977:ARG:NH2	2.48	0.47
1:D:1108:ASN:HB2	1:D:1109:PRO:CD	2.45	0.47
1:B:44:ASN:HD22	1:B:45:ARG:N	2.07	0.47
1:B:572:ASP:HB3	1:B:807:GLN:NE2	2.29	0.47
1:B:949:LYS:HG2	1:B:968:LEU:HD22	1.96	0.47
1:A:888:ASP:HA	1:A:891:LYS:HE3	1.96	0.47
1:B:622:ASN:HD21	1:B:624:TRP:CD1	2.32	0.47
1:A:1029:ASN:C	1:A:1029:ASN:HD22	2.22	0.47
1:A:179:LEU:HD23	1:A:179:LEU:H	1.80	0.46
1:A:335:ILE:HD11	1:A:374:ILE:HA	1.97	0.46
1:A:513:PRO:HB2	1:B:1145:MET:HE2	1.96	0.46
1:B:999:GLN:H	1:B:999:GLN:CD	2.23	0.46
1:D:243:LYS:HD2	1:D:245:ILE:HD11	1.96	0.46
1:B:743:MET:HG3	1:B:907:VAL:HG13	1.98	0.46
1:B:941:PRO:O	1:B:944:VAL:HG12	2.14	0.46
1:B:376:CYS:SG	1:B:466:MET:HE3	2.55	0.46
1:C:403:PHE:O	1:C:442:LYS:HE3	2.15	0.46
1:C:941:PRO:HG2	1:C:944:VAL:HB	1.97	0.46
1:D:434:ILE:H	1:D:434:ILE:HG13	1.48	0.46
1:D:647:ASN:C	1:D:647:ASN:ND2	2.60	0.46
1:D:1143:MET:HG2	1:D:1144:LYS:HE3	1.98	0.46
1:A:209:GLU:HA	1:A:213:LEU:HG	1.96	0.46
1:B:406:ARG:HB3	1:B:430:SER:HB2	1.97	0.46
1:C:200:GLY:C	1:C:202:LYS:N	2.73	0.46
1:D:960:ASN:HB3	1:D:963:LEU:HB2	1.97	0.46
1:B:525:GLU:HB3	1:B:840:THR:HG23	1.97	0.46
1:B:664:GLN:NE2	1:B:696:ALA:HB2	2.30	0.46
1:C:274:VAL:HG12	1:C:275:VAL:HG23	1.98	0.46
1:D:1042:MET:HE1	1:D:1060:ILE:HG22	1.97	0.46
1:A:1097:ASN:H	1:A:1097:ASN:ND2	2.13	0.46
1:D:157:THR:HG22	1:D:161:LYS:HE2	1.98	0.46
1:B:241:ASN:N	1:B:242:PRO:HD3	2.31	0.46
1:B:379:THR:HG22	1:B:425:LEU:HA	1.98	0.46
1:D:286:THR:O	1:D:290:ARG:HG3	2.15	0.46
1:D:1044:ASN:HD22	1:D:1062:LEU:HD22	1.80	0.46
1:A:524:TYR:HD2	1:A:843:THR:CG2	2.29	0.46
1:A:864:HIS:CD2	1:A:866:MET:CG	2.96	0.46
1:B:66:ILE:HB	1:B:86:VAL:HG23	1.98	0.46
1:D:313:LEU:HB2	1:D:323:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1105:ASP:HB3	1:D:1109:PRO:HG2	1.98	0.46
1:A:290:ARG:HB3	1:A:320:PHE:CE1	2.51	0.46
1:A:814:TYR:CZ	1:A:828:ILE:HG12	2.50	0.46
1:A:1042:MET:HE1	1:A:1060:ILE:HG21	1.98	0.46
1:C:278:ALA:CB	1:C:335:ILE:HG23	2.45	0.46
1:D:338:MET:HE3	1:D:373:ALA:HB1	1.98	0.46
1:A:641:MET:HE2	1:A:671:ILE:HG13	1.98	0.46
1:A:719:THR:H	1:A:722:TYR:HB3	1.81	0.45
1:B:704:ILE:HG21	1:B:723:TYR:HD2	1.81	0.45
1:B:921:MET:HE2	1:B:931:VAL:HG11	1.97	0.45
1:C:152:LYS:NZ	5:C:2100:ATP:O2A	2.49	0.45
1:D:350:LEU:HD22	1:D:359:GLU:HB3	1.97	0.45
1:A:408:ASP:HB2	1:A:428:LYS:HB3	1.97	0.45
1:D:99:ILE:HG23	1:D:127:PHE:HD1	1.81	0.45
1:D:278:ALA:CB	1:D:335:ILE:HG23	2.46	0.45
1:D:927:ASP:H	1:D:930:SER:HB2	1.81	0.45
1:A:1112:ILE:HD12	1:A:1175:ILE:HB	1.98	0.45
1:B:949:LYS:HE2	1:B:951:GLU:OE1	2.17	0.45
1:D:269:ARG:HG3	1:D:270:ARG:N	2.31	0.45
1:A:570:PHE:O	1:A:574:HIS:HE1	2.00	0.45
1:A:749:PRO:HG3	1:A:781:LEU:HB3	1.98	0.45
1:C:331:VAL:HG12	1:C:428:LYS:HE2	1.99	0.45
1:D:446:SER:O	1:D:450:MET:HG2	2.16	0.45
1:A:249:VAL:HG11	1:A:299:MET:HG3	1.98	0.45
1:A:1138:LEU:HD13	1:A:1175:ILE:HD11	1.99	0.45
1:D:941:PRO:HD2	1:D:944:VAL:HG11	1.98	0.45
1:A:893:MET:O	1:A:897:VAL:HG23	2.17	0.45
1:B:901:PHE:CZ	1:B:917:MET:HG3	2.49	0.45
1:D:917:MET:HA	1:D:917:MET:HE2	1.98	0.45
1:B:162:ALA:O	1:B:164:LEU:HG	2.17	0.45
1:B:593:LYS:O	1:B:597:VAL:HG23	2.17	0.45
1:B:715:ARG:NH1	1:B:865:GLU:OE2	2.50	0.45
1:B:1042:MET:CE	1:B:1078:TYR:HE2	2.29	0.45
1:C:606:MET:HE1	1:C:671:ILE:HD12	1.97	0.45
1:C:181:LYS:O	1:C:185:GLU:HG2	2.17	0.45
1:C:685:GLN:HA	1:C:685:GLN:HE21	1.82	0.45
1:D:798:VAL:CG1	1:D:835:SER:HA	2.47	0.45
1:A:263:ARG:NH2	1:A:330:GLN:NE2	2.62	0.45
1:C:909:PRO:HG2	1:C:952:ILE:HG12	1.99	0.45
1:D:544:LEU:O	1:D:548:VAL:HG22	2.16	0.45
1:A:490:ILE:H	1:A:490:ILE:HG13	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:GLU:HA	1:B:147:ASP:HB3	1.99	0.44
1:B:575:GLN:NE2	1:B:610:ALA:H	2.14	0.44
1:B:1097:ASN:HB2	1:B:1166:ASP:HA	1.98	0.44
1:D:1131:VAL:HG13	1:D:1135:GLN:HB3	1.98	0.44
1:C:256:ASN:C	1:C:257:ILE:HG13	2.41	0.44
1:D:524:TYR:CD2	1:D:843:THR:HG22	2.53	0.44
1:B:811:ASN:HD22	1:B:811:ASN:N	2.11	0.44
1:C:1068:PRO:HD3	1:C:1074:ARG:CZ	2.47	0.44
1:D:397:TYR:N	1:D:414:GLN:HG3	2.32	0.44
1:D:704:ILE:HG21	1:D:723:TYR:HD2	1.82	0.44
1:D:798:VAL:HG13	1:D:835:SER:HA	1.98	0.44
1:A:585:LYS:HG2	1:A:1034:ASP:HA	1.99	0.44
1:B:908:THR:HA	1:B:909:PRO:HA	1.67	0.44
1:C:580:THR:HB	1:C:614:VAL:HG21	1.98	0.44
1:A:192:MET:HE2	1:A:192:MET:HB3	1.86	0.44
1:B:278:ALA:HA	1:B:279:PRO:HA	1.83	0.44
1:A:99:ILE:HG23	1:A:127:PHE:HD1	1.83	0.44
1:A:828:ILE:H	1:A:828:ILE:HG13	1.58	0.44
1:A:900:LEU:HD22	1:A:921:MET:HE1	1.99	0.44
1:A:1051:GLU:CD	1:A:1057:ARG:HH21	2.26	0.44
1:B:496:ARG:H	1:B:496:ARG:CD	2.31	0.44
1:C:908:THR:HA	1:C:909:PRO:HA	1.72	0.44
1:D:901:PHE:HZ	1:D:917:MET:HG3	1.81	0.44
1:A:260:LEU:HB3	1:A:340:THR:HG21	1.99	0.44
1:C:883:LEU:HG	1:C:923:GLN:HE21	1.83	0.44
1:A:116:PRO:HB2	1:A:122:SER:HA	2.00	0.44
1:A:156:ARG:HH11	1:A:166:VAL:HG11	1.83	0.44
1:A:651:TYR:CE1	1:A:652:LYS:HG3	2.53	0.44
1:A:796:THR:HB	1:A:810:ALA:HB2	1.99	0.44
1:B:1127:VAL:HA	1:B:1157:ILE:HG22	1.99	0.44
1:D:345:VAL:O	1:D:348:GLN:HB2	2.18	0.44
1:B:319:GLU:HG3	1:B:321:PHE:HE1	1.83	0.43
1:D:580:THR:HG22	1:D:611:THR:HG22	2.00	0.43
1:A:241:ASN:N	1:A:242:PRO:HD3	2.33	0.43
1:A:1151:ALA:HA	1:A:1152:PRO:HD3	1.85	0.43
1:B:912:LYS:NZ	1:B:916:ASP:OD1	2.44	0.43
1:D:571:ARG:HH11	1:D:575:GLN:NE2	2.15	0.43
1:A:431:THR:HG21	1:A:443:MET:HA	2.00	0.43
1:A:506:ASN:HD22	1:A:510:ASN:HD22	1.65	0.43
1:A:829:GLU:OE1	1:A:829:GLU:HA	2.18	0.43
1:B:690:ASN:O	1:B:694:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1013:TYR:HB3	1:B:1016:VAL:HB	2.00	0.43
1:A:1110:SER:O	1:A:1176:GLU:HA	2.18	0.43
3:A:2000:BTI:H63	1:B:620:LYS:CG	2.49	0.43
1:C:107:LYS:C	1:C:109:ALA:H	2.26	0.43
1:C:396:ALA:HB3	1:C:453:ARG:HH11	1.83	0.43
1:C:873:ASN:HB3	3:D:2000:BTI:H83	2.00	0.43
1:D:156:ARG:HD2	1:D:166:VAL:HG11	1.99	0.43
1:D:388:MET:HE2	1:D:388:MET:HA	2.01	0.43
1:A:949:LYS:HB2	1:A:949:LYS:HE3	1.80	0.43
1:C:375:GLN:NE2	1:C:428:LYS:HD3	2.32	0.43
1:D:144:GLU:O	1:D:148:MET:HB2	2.18	0.43
1:D:252:ASP:C	1:D:254:HIS:H	2.26	0.43
1:D:524:TYR:HD2	1:D:843:THR:CG2	2.32	0.43
1:D:1108:ASN:HB2	1:D:1109:PRO:HD3	1.99	0.43
1:A:593:LYS:O	1:A:597:VAL:HG23	2.19	0.43
1:A:1035:THR:HB	1:A:1036:PRO:HD3	2.00	0.43
1:C:66:ILE:HB	1:C:86:VAL:HG21	2.01	0.43
1:A:1093:ASN:O	1:A:1094:VAL:HB	2.19	0.43
1:C:712:ASN:HA	1:C:713:PRO:HD2	1.91	0.43
1:C:927:ASP:OD2	1:C:930:SER:HB2	2.18	0.43
1:D:252:ASP:HA	1:D:351:VAL:HG13	2.01	0.43
1:D:622:ASN:HD21	1:D:624:TRP:HD1	1.67	0.43
1:D:653:ASN:HB3	1:D:982:LEU:HD11	2.01	0.43
1:A:141:PRO:HB2	1:A:145:HIS:HB2	1.99	0.43
1:C:672:ASP:HA	1:C:698:LYS:HD2	2.01	0.43
1:C:711:LEU:HG	1:C:751:ALA:HB2	2.00	0.43
1:A:977:ARG:HA	1:A:978:PRO:HD3	1.90	0.43
1:B:661:LYS:HG2	1:B:1008:ILE:HG12	2.00	0.43
1:C:166:VAL:HG22	1:C:322:PHE:HB3	2.01	0.43
1:C:738:LEU:HD23	1:C:768:ILE:HG12	1.99	0.43
1:C:309:THR:HG21	1:C:330:GLN:NE2	2.34	0.43
1:D:42:VAL:HG11	1:D:49:ALA:HA	2.00	0.43
1:A:166:VAL:HG12	1:A:167:ILE:N	2.34	0.42
1:C:225:GLU:HB2	1:C:231:SER:HB3	2.01	0.42
1:C:519:ARG:HG3	1:C:520:PRO:O	2.19	0.42
1:D:360:ILE:HG22	1:D:362:MET:HG2	2.01	0.42
1:A:219:ARG:HG2	1:A:223:GLU:HG3	2.01	0.42
1:A:622:ASN:ND2	1:A:624:TRP:H	2.17	0.42
1:A:908:THR:HA	1:A:909:PRO:HA	1.83	0.42
1:A:274:VAL:HG12	1:A:275:VAL:HG23	2.01	0.42
1:B:59:LEU:HD22	1:B:350:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ILE:HB	1:B:86:VAL:CG2	2.49	0.42
1:B:125:GLU:CD	1:B:147:ASP:HA	2.44	0.42
1:D:924:ASN:HB2	1:D:926:LEU:HD22	2.02	0.42
1:D:999:GLN:HG2	1:D:1000:GLY:N	2.34	0.42
1:A:151:ASP:HB3	1:A:154:LYS:CG	2.49	0.42
1:A:244:HIS:CD2	1:A:265:CYS:HB2	2.54	0.42
1:C:499:LYS:HA	1:C:502:GLU:HG3	2.01	0.42
1:D:811:ASN:H	1:D:811:ASN:ND2	2.16	0.42
1:B:39:LYS:HG3	1:B:111:VAL:HA	2.00	0.42
1:B:657:ASN:HD21	1:B:985:VAL:H	1.68	0.42
1:D:116:PRO:HB2	1:D:122:SER:HA	2.01	0.42
1:D:490:ILE:H	1:D:490:ILE:HG13	1.65	0.42
1:A:193:ILE:HD11	1:A:233:VAL:HB	2.02	0.42
1:A:1115:GLN:CD	1:A:1115:GLN:N	2.77	0.42
1:B:284:SER:OG	1:B:287:LEU:HB2	2.19	0.42
1:B:826:THR:OG1	1:B:831:MET:HE2	2.19	0.42
1:C:952:ILE:O	1:C:952:ILE:CG2	2.68	0.42
1:D:141:PRO:HB2	1:D:145:HIS:HB2	2.01	0.42
1:A:631:ARG:HA	1:A:631:ARG:HD3	1.75	0.42
1:A:828:ILE:O	1:A:829:GLU:C	2.60	0.42
1:B:977:ARG:HA	1:B:978:PRO:HD3	1.95	0.42
1:C:309:THR:HG21	1:C:330:GLN:HE22	1.85	0.42
1:D:484:THR:HG21	1:D:487:LEU:HD13	2.01	0.42
1:D:582:VAL:HA	1:D:845:TYR:CZ	2.54	0.42
1:B:542:LYS:HE2	1:B:631:ARG:CZ	2.49	0.42
1:D:484:THR:HB	1:D:487:LEU:HD22	2.01	0.42
1:D:952:ILE:HG23	1:D:952:ILE:O	2.19	0.42
1:B:842:ARG:CZ	1:C:855:LYS:HE2	2.50	0.42
1:D:572:ASP:HB2	1:D:605:GLU:OE1	2.19	0.42
1:D:869:GLY:O	1:D:871:TYR:N	2.52	0.42
1:B:701:GLU:HG2	1:B:737:ILE:HB	2.02	0.42
1:C:575:GLN:NE2	1:C:610:ALA:H	2.18	0.42
1:A:263:ARG:NH2	1:A:330:GLN:HE21	2.17	0.41
1:A:384:LEU:HD11	1:A:490:ILE:HG12	2.02	0.41
1:A:924:ASN:HB2	1:A:926:LEU:HD22	2.01	0.41
1:B:362:MET:HA	1:B:362(A):PRO:HD3	1.92	0.41
1:B:1000:GLY:H	1:B:1001:PRO:CD	2.15	0.41
1:C:907:VAL:O	1:C:910:SER:N	2.53	0.41
1:C:1069:ASP:O	1:C:1071:ASN:N	2.48	0.41
1:D:91:GLY:HA3	1:D:92:PRO:HD3	1.80	0.41
1:D:504:ILE:HG21	1:D:1042:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1109:PRO:HB2	1:D:1111:HIS:CE1	2.55	0.41
1:A:263:ARG:HH21	1:A:330:GLN:HE22	1.66	0.41
1:C:589:ASN:HD22	1:C:589:ASN:HA	1.69	0.41
3:C:2000:BTI:H5	1:D:512:PHE:CZ	2.55	0.41
1:B:91:GLY:HA2	1:B:92:PRO:HD2	1.89	0.41
1:B:811:ASN:ND2	1:B:811:ASN:N	2.68	0.41
1:B:828:ILE:HD12	1:B:829:GLU:H	1.85	0.41
1:B:1133:ALA:O	1:B:1134:ASN:HB2	2.21	0.41
1:C:338:MET:CE	1:C:430:SER:HB3	2.50	0.41
1:C:530:PRO:HB2	1:C:593:LYS:HD3	2.02	0.41
1:D:294:ALA:HA	1:D:297:GLN:HG3	2.01	0.41
1:C:631:ARG:C	1:C:631:ARG:HD3	2.43	0.41
1:C:1024:ARG:HH11	1:C:1024:ARG:HG2	1.85	0.41
1:A:678:ASP:OD2	1:A:685:GLN:NE2	2.54	0.41
1:C:571:ARG:HH11	1:C:575:GLN:HE22	1.66	0.41
1:A:606:MET:CE	1:A:607:TRP:HB2	2.51	0.41
1:A:864:HIS:CD2	1:A:866:MET:H	2.35	0.41
1:B:1135:GLN:HA	1:B:1136:PRO:HD2	1.93	0.41
1:C:866:MET:CE	1:C:871:TYR:HA	2.48	0.41
1:D:506:ASN:HD21	1:D:510:ASN:HD22	1.68	0.41
1:B:606:MET:HE1	1:B:671:ILE:CD1	2.51	0.41
1:C:854:ILE:H	1:C:854:ILE:HG13	1.71	0.41
1:D:941:PRO:O	1:D:944:VAL:CG1	2.68	0.41
1:A:313:LEU:HD13	1:A:323:ILE:HG13	2.02	0.41
1:B:396:ALA:HB3	1:B:453:ARG:HH11	1.86	0.41
1:C:174:ILE:CG2	1:C:175:LYS:N	2.83	0.41
1:A:704:ILE:HG23	1:A:726:LEU:HD23	2.01	0.41
1:A:921:MET:CE	1:A:931:VAL:HG21	2.51	0.41
1:A:1008:ILE:H	1:A:1008:ILE:HG13	1.70	0.41
1:B:828:ILE:H	1:B:828:ILE:HG13	1.54	0.41
1:B:949:LYS:HG2	1:B:968:LEU:CD2	2.51	0.41
1:C:142:HIS:N	1:C:145:HIS:HD2	2.19	0.41
1:C:258:VAL:HG21	1:C:362:MET:HE2	2.03	0.41
1:C:631:ARG:NH2	1:C:672:ASP:OD1	2.54	0.41
1:D:167:ILE:H	1:D:167:ILE:HG13	1.69	0.41
1:D:715:ARG:NH1	1:D:865:GLU:OE2	2.54	0.41
1:B:542:LYS:HE2	1:B:631:ARG:NH2	2.36	0.41
1:C:835:SER:O	1:C:839:SER:HB2	2.21	0.41
1:D:561:ASP:O	1:D:822:ARG:HD2	2.20	0.41
1:D:866:MET:HE2	1:D:871:TYR:HA	2.03	0.41
1:A:298:LEU:O	1:A:302:ILE:HG13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:MET:HA	1:A:389:PRO:HD3	1.90	0.40
1:C:717:ASN:HD22	1:C:717(A):ILE:HD12	1.86	0.40
1:A:156:ARG:NH2	1:A:170:THR:O	2.53	0.40
1:A:896:ARG:HD2	1:A:928:GLU:OE2	2.22	0.40
1:A:118:TYR:OH	1:A:331:VAL:HG13	2.21	0.40
1:A:571:ARG:HB3	1:A:572:ASP:H	1.80	0.40
1:A:1033:LEU:CD2	1:A:1050:ILE:HG12	2.51	0.40
1:B:506:ASN:ND2	1:B:510:ASN:ND2	2.69	0.40
1:B:909:PRO:HG2	1:B:952:ILE:HG12	2.04	0.40
1:B:1108:ASN:HA	1:B:1109:PRO:HD2	1.94	0.40
1:B:1164:ASN:ND2	1:B:1164:ASN:H	2.18	0.40
1:C:419:SER:C	1:C:421:TYR:H	2.29	0.40
1:C:537:ILE:HA	1:C:538(B):PHE:CD1	2.56	0.40
1:C:720:LEU:HD21	1:C:758:GLU:HG3	2.03	0.40
1:C:893:MET:HE2	1:C:893:MET:HB3	1.87	0.40
1:D:622:ASN:ND2	1:D:624:TRP:H	2.20	0.40
1:B:39:LYS:HB3	1:B:62:SER:HB3	2.03	0.40
1:B:434:ILE:H	1:B:434:ILE:HG13	1.68	0.40
1:B:622:ASN:HA	1:B:623:PRO:HD2	1.86	0.40
1:C:574:HIS:CD2	1:C:580:THR:HA	2.56	0.40
1:C:972:GLU:HB2	1:C:973:ALA:H	1.70	0.40
1:D:329:VAL:HG22	1:D:348:GLN:NE2	2.29	0.40
1:D:913:VAL:HG13	1:D:944:VAL:HA	2.03	0.40
1:D:991:ARG:NH2	1:D:1004:GLU:OE1	2.54	0.40
1:D:1135:GLN:HA	1:D:1136:PRO:HD2	1.93	0.40
1:C:690:ASN:O	1:C:694:GLN:HG2	2.21	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	1133/1173 (97%)	1049 (93%)	77 (7%)	7 (1%)	21	51
1	B	1070/1173 (91%)	999 (93%)	58 (5%)	13 (1%)	10	34
1	C	1063/1173 (91%)	980 (92%)	65 (6%)	18 (2%)	7	25
1	D	1061/1173 (90%)	980 (92%)	73 (7%)	8 (1%)	16	44
All	All	4327/4692 (92%)	4008 (93%)	273 (6%)	46 (1%)	11	36

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	SER
1	B	386	ASP
1	B	522	PRO
1	B	1001	PRO
1	C	92	PRO
1	D	92	PRO
1	D	870	GLN
1	A	648	ALA
1	A	1081	ASN
1	B	87	GLY
1	C	87	GLY
1	C	168	PRO
1	C	177	TYR
1	C	201	GLY
1	C	931	VAL
1	C	1070	GLU
1	D	853	ASP
1	D	1053	ASP
1	A	476	TYR
1	B	408	ASP
1	B	1093	ASN
1	B	1142	ALA
1	C	72	LYS
1	C	936	TYR
1	C	938	LEU
1	C	939	ASP
1	B	1002	VAL
1	B	1098	ALA
1	C	648	ALA
1	D	493	SER
1	D	1108	ASN
1	A	89	ASP
1	A	1094	VAL

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Mol	Chain	Res	Type
1	B	939	ASP
1	C	189	PHE
1	C	1142	ALA
1	D	87	GLY
1	D	317	GLY
1	A	189	PHE
1	B	518	LYS
1	C	190	PRO
1	C	886	ARG
1	C	1014	PRO
1	B	649	VAL
1	B	92	PRO
1	C	229	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	980/1006 (97%)	892 (91%)	88 (9%)	9	28
1	B	928/1006 (92%)	846 (91%)	82 (9%)	9	29
1	C	917/1006 (91%)	825 (90%)	92 (10%)	7	24
1	D	922/1006 (92%)	837 (91%)	85 (9%)	8	27
All	All	3747/4024 (93%)	3400 (91%)	347 (9%)	8	27

All (347) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	108	GLN
1	A	143	LEU
1	A	144	GLU
1	A	174	ILE
1	A	178	GLU
1	A	193	ILE
1	A	196	THR

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Mol	Chain	Res	Type
1	A	217	PHE
1	A	218	HIS
1	A	269	ARG
1	A	281	VAL
1	A	286	THR
1	A	287	LEU
1	A	302	ILE
1	A	313	LEU
1	A	318	ASP
1	A	329	VAL
1	A	331	VAL
1	A	335	ILE
1	A	359	GLU
1	A	386	ASP
1	A	391	THR
1	A	427	VAL
1	A	434	ILE
1	A	440	GLU
1	A	445	ARG
1	A	487	LEU
1	A	494	LEU
1	A	496	ARG
1	A	518	LYS
1	A	519	ARG
1	A	526	LEU
1	A	542	LYS
1	A	558	LYS
1	A	588	ILE
1	A	590	ILE
1	A	599	LYS
1	A	606	MET
1	A	607	TRP
1	A	631	ARG
1	A	649	VAL
1	A	707	THR
1	A	715	ARG
1	A	743	MET
1	A	750	LYS
1	A	761	SER
1	A	766	LEU
1	A	775	THR
1	A	781	LEU

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Mol	Chain	Res	Type
1	A	794	ILE
1	A	798	VAL
1	A	828	ILE
1	A	843	THR
1	A	852	SER
1	A	853	ASP
1	A	855	LYS
1	A	861	ILE
1	A	863	GLN
1	A	874	LEU
1	A	906	LYS
1	A	907	VAL
1	A	908	THR
1	A	917	MET
1	A	919	LEU
1	A	926	LEU
1	A	931	VAL
1	A	939	ASP
1	A	944	VAL
1	A	945	VAL
1	A	966	VAL
1	A	969	LYS
1	A	977	ARG
1	A	980	GLU
1	A	983	GLU
1	A	999	GLN
1	A	1002	VAL
1	A	1008	ILE
1	A	1064	THR
1	A	1080	MET
1	A	1083	GLN
1	A	1089	ILE
1	A	1097	ASN
1	A	1115	GLN
1	A	1116	MET
1	A	1137	LEU
1	A	1167	THR
1	A	1177	ILE
1	B	36	GLN
1	B	39	LYS
1	B	44	ASN
1	B	47	GLU

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Mol	Chain	Res	Type
1	B	69	ASN
1	B	75	LEU
1	B	108	GLN
1	B	156	ARG
1	B	167	ILE
1	B	241	ASN
1	B	249	VAL
1	B	281	VAL
1	B	287	LEU
1	B	331	VAL
1	B	335	ILE
1	B	357	LEU
1	B	357(A)	PHE
1	B	427	VAL
1	B	434	ILE
1	B	437	LYS
1	B	440	GLU
1	B	442	LYS
1	B	452	ILE
1	B	458	ASN
1	B	475	ASP
1	B	490	ILE
1	B	496	ARG
1	B	518	LYS
1	B	523	ASP
1	B	542	LYS
1	B	565	LEU
1	B	606	MET
1	B	607	TRP
1	B	629	ARG
1	B	631	ARG
1	B	632	LYS
1	B	641	MET
1	B	644	ARG
1	B	647	ASN
1	B	649	VAL
1	B	652	LYS
1	B	660	HIS
1	B	664	GLN
1	B	686	MET
1	B	707	THR
1	B	715	ARG

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Mol	Chain	Res	Type
1	B	743	MET
1	B	750	LYS
1	B	760	LYS
1	B	766	LEU
1	B	775	THR
1	B	781	LEU
1	B	794	ILE
1	B	811	ASN
1	B	828	ILE
1	B	854	ILE
1	B	863	GLN
1	B	870	GLN
1	B	874	LEU
1	B	880	SER
1	B	885	GLU
1	B	907	VAL
1	B	908	THR
1	B	926	LEU
1	B	929	GLN
1	B	952	ILE
1	B	962	ASP
1	B	971	GLN
1	B	996	GLU
1	B	1008	ILE
1	B	1048	VAL
1	B	1054	LYS
1	B	1085	ARG
1	B	1089	ILE
1	B	1097	ASN
1	B	1124	LYS
1	B	1138	LEU
1	B	1143	MET
1	B	1148	THR
1	B	1157	ILE
1	B	1158	LYS
1	B	1177	ILE
1	C	44	ASN
1	C	77	ARG
1	C	90	LEU
1	C	94	GLU
1	C	95	SER
1	C	97	LEU

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Mol	Chain	Res	Type
1	C	100	GLU
1	C	126	GLN
1	C	193	ILE
1	C	237	ARG
1	C	249	VAL
1	C	250	ILE
1	C	262	GLU
1	C	268	GLN
1	C	287	LEU
1	C	313	LEU
1	C	323	ILE
1	C	329	VAL
1	C	331	VAL
1	C	335	ILE
1	C	342	ILE
1	C	398	ARG
1	C	406	ARG
1	C	417	GLU
1	C	427	VAL
1	C	434	ILE
1	C	437	LYS
1	C	456	LYS
1	C	472	THR
1	C	494	LEU
1	C	519	ARG
1	C	526	LEU
1	C	531	THR
1	C	542	LYS
1	C	559	LYS
1	C	580	THR
1	C	588	ILE
1	C	590	ILE
1	C	606	MET
1	C	607	TRP
1	C	631	ARG
1	C	641	MET
1	C	647	ASN
1	C	649	VAL
1	C	652	LYS
1	C	660	HIS
1	C	707	THR
1	C	717	ASN

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Mol	Chain	Res	Type
1	C	717(A)	ILE
1	C	721	GLU
1	C	743	MET
1	C	748	LYS
1	C	750	LYS
1	C	756	ILE
1	C	766	LEU
1	C	781	LEU
1	C	793	ILE
1	C	794	ILE
1	C	807	GLN
1	C	811	ASN
1	C	828	ILE
1	C	829	GLU
1	C	843	THR
1	C	854	ILE
1	C	855	LYS
1	C	866	MET
1	C	875	SER
1	C	876	GLN
1	C	881	LEU
1	C	907	VAL
1	C	931	VAL
1	C	934	ASP
1	C	937	LYS
1	C	942	GLU
1	C	944	VAL
1	C	945	VAL
1	C	952	ILE
1	C	959	PHE
1	C	962	ASP
1	C	971	GLN
1	C	972	GLU
1	C	977	ARG
1	C	1008	ILE
1	C	1022	GLN
1	C	1053	ASP
1	C	1054	LYS
1	C	1064	THR
1	C	1070	GLU
1	C	1085	ARG
1	C	1140	THR

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Mol	Chain	Res	Type
1	C	1141	GLU
1	C	1143	MET
1	D	44	ASN
1	D	60	ASP
1	D	69	ASN
1	D	70	GLU
1	D	122	SER
1	D	136	ILE
1	D	137	LYS
1	D	160	ILE
1	D	166	VAL
1	D	167	ILE
1	D	250	ILE
1	D	262	GLU
1	D	267	VAL
1	D	283	LEU
1	D	296	ILE
1	D	306	ASN
1	D	329	VAL
1	D	331	VAL
1	D	335	ILE
1	D	386	ASP
1	D	398	ARG
1	D	427	VAL
1	D	434	ILE
1	D	437	LYS
1	D	456	LYS
1	D	469	LYS
1	D	487	LEU
1	D	489	ASP
1	D	490	ILE
1	D	491	GLN
1	D	519	ARG
1	D	525	GLU
1	D	531	THR
1	D	542	LYS
1	D	543	GLN
1	D	580	THR
1	D	590	ILE
1	D	607	TRP
1	D	620	LYS
1	D	631	ARG

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Mol	Chain	Res	Type
1	D	647	ASN
1	D	649	VAL
1	D	707	THR
1	D	715	ARG
1	D	743	MET
1	D	750	LYS
1	D	756	ILE
1	D	766	LEU
1	D	775	THR
1	D	791	VAL
1	D	798	VAL
1	D	807	GLN
1	D	811	ASN
1	D	828	ILE
1	D	831	MET
1	D	843	THR
1	D	853	ASP
1	D	870	GLN
1	D	874	LEU
1	D	883	LEU
1	D	895	ARG
1	D	907	VAL
1	D	912	LYS
1	D	917	MET
1	D	926	LEU
1	D	927	ASP
1	D	945	VAL
1	D	952	ILE
1	D	960	ASN
1	D	963	LEU
1	D	996	GLU
1	D	1002	VAL
1	D	1048	VAL
1	D	1056	LYS
1	D	1064	THR
1	D	1070	GLU
1	D	1071	ASN
1	D	1080	MET
1	D	1089	ILE
1	D	1103	LYS
1	D	1116	MET
1	D	1138	LEU

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Mol	Chain	Res	Type
1	D	1153	PHE
1	D	1161	THR
1	D	1174	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	69	ASN
1	A	98	ASN
1	A	126	GLN
1	A	145	HIS
1	A	241	ASN
1	A	272	GLN
1	A	330	GLN
1	A	361	ASN
1	A	432	HIS
1	A	491	GLN
1	A	506	ASN
1	A	543	GLN
1	A	574	HIS
1	A	575	GLN
1	A	589	ASN
1	A	622	ASN
1	A	736	HIS
1	A	778	ASN
1	A	811	ASN
1	A	818	ASN
1	A	858	ASN
1	A	864	HIS
1	A	877	GLN
1	A	923	GLN
1	A	1005	GLN
1	A	1025	ASN
1	A	1029	ASN
1	A	1044	ASN
1	A	1097	ASN
1	A	1111	HIS
1	B	44	ASN
1	B	69	ASN
1	B	108	GLN
1	B	124	ASN

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Mol	Chain	Res	Type
1	B	145	HIS
1	B	244	HIS
1	B	326	ASN
1	B	330	GLN
1	B	432	HIS
1	B	506	ASN
1	B	543	GLN
1	B	574	HIS
1	B	575	GLN
1	B	589	ASN
1	B	617	ASN
1	B	622	ASN
1	B	660	HIS
1	B	664	GLN
1	B	736	HIS
1	B	811	ASN
1	B	818	ASN
1	B	858	ASN
1	B	864	HIS
1	B	873	ASN
1	B	877	GLN
1	B	924	ASN
1	B	971	GLN
1	B	1005	GLN
1	B	1025	ASN
1	B	1029	ASN
1	B	1071	ASN
1	B	1083	GLN
1	B	1111	HIS
1	B	1115	GLN
1	C	44	ASN
1	C	145	HIS
1	C	230	ASN
1	C	297	GLN
1	C	326	ASN
1	C	330	GLN
1	C	375	GLN
1	C	432	HIS
1	C	464	ASN
1	C	506	ASN
1	C	574	HIS
1	C	575	GLN

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Mol	Chain	Res	Type
1	C	617	ASN
1	C	622	ASN
1	C	717	ASN
1	C	736	HIS
1	C	778	ASN
1	C	785	GLN
1	C	811	ASN
1	C	873	ASN
1	C	877	GLN
1	C	898	ASN
1	C	1005	GLN
1	C	1025	ASN
1	C	1029	ASN
1	C	1083	GLN
1	D	44	ASN
1	D	145	HIS
1	D	241	ASN
1	D	244	HIS
1	D	256	ASN
1	D	289	GLN
1	D	301	ASN
1	D	326	ASN
1	D	330	GLN
1	D	364	GLN
1	D	432	HIS
1	D	468	ASN
1	D	506	ASN
1	D	515	ASN
1	D	543	GLN
1	D	574	HIS
1	D	575	GLN
1	D	589	ASN
1	D	622	ASN
1	D	647	ASN
1	D	685	GLN
1	D	736	HIS
1	D	778	ASN
1	D	811	ASN
1	D	823	HIS
1	D	864	HIS
1	D	898	ASN
1	D	954	GLN

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Mol	Chain	Res	Type
1	D	957	ASN
1	D	1005	GLN
1	D	1019	GLN
1	D	1025	ASN
1	D	1026	GLN
1	D	1044	ASN
1	D	1163	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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
3	BTI	C	2000	1	15,16,16	1.69	3 (20%)	20,21,21	2.03	5 (25%)
3	BTI	A	2000	1	15,16,16	1.72	2 (13%)	20,21,21	2.06	4 (20%)
5	ATP	C	2100	-	32,33,33	1.47	5 (15%)	48,52,52	1.72	8 (16%)
4	PYR	D	2001	-	5,5,5	3.03	3 (60%)	3,6,6	1.81	1 (33%)
5	ATP	A	2100	-	32,33,33	1.46	5 (15%)	48,52,52	1.79	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PYR	C	2001	-	5,5,5	3.02	3 (60%)	3,6,6	1.84	1 (33%)
3	BTI	B	2000	1	15,16,16	1.65	2 (13%)	20,21,21	1.90	4 (20%)
3	BTI	D	2000	1	15,16,16	1.67	2 (13%)	20,21,21	1.89	5 (25%)
4	PYR	A	2001	-	5,5,5	3.09	3 (60%)	3,6,6	1.75	1 (33%)
4	PYR	B	2001	-	5,5,5	3.08	3 (60%)	3,6,6	1.67	1 (33%)

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	BTI	C	2000	1	-	5/6/27/27	0/2/2/2
3	BTI	A	2000	1	-	3/6/27/27	0/2/2/2
5	ATP	C	2100	-	-	5/22/38/38	0/3/3/3
4	PYR	D	2001	-	-	4/4/4/4	-
5	ATP	A	2100	-	-	7/22/38/38	0/3/3/3
4	PYR	C	2001	-	-	3/4/4/4	-
3	BTI	B	2000	1	-	3/6/27/27	0/2/2/2
3	BTI	D	2000	1	-	5/6/27/27	0/2/2/2
4	PYR	A	2001	-	-	3/4/4/4	-
4	PYR	B	2001	-	-	2/4/4/4	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	BTI	O3-C3	4.85	1.33	1.23
5	C	2100	ATP	C5-C4	4.83	1.47	1.39
3	B	2000	BTI	O3-C3	4.81	1.33	1.23
5	A	2100	ATP	C5-C4	4.75	1.47	1.39
3	D	2000	BTI	O3-C3	4.72	1.33	1.23
4	B	2001	PYR	CA-C	-4.44	1.39	1.54
4	C	2001	PYR	CA-C	-4.39	1.39	1.54
3	C	2000	BTI	O3-C3	4.38	1.32	1.23
4	A	2001	PYR	CA-C	-4.38	1.39	1.54
4	D	2001	PYR	CA-C	-4.29	1.40	1.54
4	A	2001	PYR	O-C	3.78	1.31	1.22
4	A	2001	PYR	O3-CA	3.75	1.31	1.23
4	C	2001	PYR	O3-CA	3.71	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2000	BTI	C2-S1	-3.71	1.76	1.82
4	B	2001	PYR	O-C	3.70	1.31	1.22
4	D	2001	PYR	O-C	3.70	1.31	1.22
4	B	2001	PYR	O3-CA	3.69	1.31	1.23
4	D	2001	PYR	O3-CA	3.64	1.31	1.23
4	C	2001	PYR	O-C	3.51	1.31	1.22
3	A	2000	BTI	C2-S1	-3.40	1.77	1.82
3	D	2000	BTI	C2-S1	-3.40	1.77	1.82
5	C	2100	ATP	PB-O3B	3.32	1.63	1.59
3	B	2000	BTI	C2-S1	-3.31	1.77	1.82
5	C	2100	ATP	C5-C6	2.82	1.48	1.41
5	A	2100	ATP	C5-C6	2.76	1.48	1.41
5	A	2100	ATP	PB-O3B	2.62	1.62	1.59
5	A	2100	ATP	C5-N7	-2.41	1.34	1.39
5	C	2100	ATP	C5-N7	-2.38	1.34	1.39
5	A	2100	ATP	C8-N7	2.30	1.36	1.31
5	C	2100	ATP	C8-N7	2.12	1.35	1.31
3	C	2000	BTI	C3-N2	-2.03	1.31	1.35

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	BTI	C2-C4-N2	-6.29	106.68	113.34
5	A	2100	ATP	C5-C4-N3	-6.19	118.20	126.72
3	D	2000	BTI	C6-C5-N3	-6.12	105.30	113.18
5	C	2100	ATP	C5-C4-N3	-5.79	118.74	126.72
3	B	2000	BTI	C6-C5-N3	-5.60	105.96	113.18
3	C	2000	BTI	C6-C5-N3	-5.43	106.19	113.18
3	C	2000	BTI	C2-C4-N2	-5.23	107.80	113.34
3	A	2000	BTI	C6-C5-N3	-4.82	106.97	113.18
5	C	2100	ATP	N3-C4-N9	4.72	135.20	127.17
5	A	2100	ATP	N3-C4-N9	4.71	135.18	127.17
5	A	2100	ATP	C2-N3-C4	3.96	121.51	111.83
3	B	2000	BTI	C2-C4-N2	-3.77	109.35	113.34
5	C	2100	ATP	C2-N3-C4	3.74	120.97	111.83
5	A	2100	ATP	N3-C2-N1	-3.45	123.36	128.58
5	A	2100	ATP	C4-C5-N7	-3.45	106.64	110.58
5	C	2100	ATP	N3-C2-N1	-3.32	123.55	128.58
5	C	2100	ATP	C4-C5-N7	-3.26	106.86	110.58
4	D	2001	PYR	OXT-C-CA	2.68	121.02	113.59
3	D	2000	BTI	C2-C4-N2	-2.65	110.53	113.34
4	C	2001	PYR	OXT-C-CA	2.63	120.88	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2100	ATP	C5-N7-C8	2.50	107.37	103.45
4	A	2001	PYR	OXT-C-CA	2.48	120.47	113.59
3	D	2000	BTI	C4-C2-S1	2.47	107.83	105.03
5	A	2100	ATP	C5-N7-C8	2.44	107.28	103.45
5	C	2100	ATP	C4-N9-C8	2.43	108.29	105.74
3	A	2000	BTI	C4-C2-S1	2.34	107.69	105.03
4	B	2001	PYR	OXT-C-CA	2.31	119.99	113.59
3	C	2000	BTI	C8-C7-C2	-2.30	108.76	114.04
3	C	2000	BTI	C5-C6-S1	2.28	109.21	106.06
3	B	2000	BTI	N2-C3-N3	2.25	111.45	108.85
3	B	2000	BTI	C4-C2-S1	2.19	107.52	105.03
5	A	2100	ATP	C6-C5-N7	2.15	136.24	132.09
3	A	2000	BTI	N2-C3-N3	2.11	111.28	108.85
3	C	2000	BTI	N2-C3-N3	2.08	111.26	108.85
3	D	2000	BTI	C5-C6-S1	2.06	108.90	106.06
5	C	2100	ATP	C6-C5-N7	2.05	136.03	132.09
3	D	2000	BTI	C2-C4-C5	-2.02	106.43	108.89

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2000	BTI	C11-C10-C9-C8
3	B	2000	BTI	S1-C2-C7-C8
3	B	2000	BTI	C4-C2-C7-C8
3	C	2000	BTI	C9-C10-C11-O11
3	C	2000	BTI	C11-C10-C9-C8
3	C	2000	BTI	S1-C2-C7-C8
3	C	2000	BTI	C4-C2-C7-C8
3	D	2000	BTI	C9-C10-C11-O11
3	D	2000	BTI	C11-C10-C9-C8
3	D	2000	BTI	S1-C2-C7-C8
3	D	2000	BTI	C4-C2-C7-C8
4	A	2001	PYR	O-C-CA-CB
4	A	2001	PYR	OXT-C-CA-CB
4	B	2001	PYR	OXT-C-CA-CB
4	C	2001	PYR	O-C-CA-CB
4	C	2001	PYR	OXT-C-CA-CB
4	D	2001	PYR	O-C-CA-CB
4	D	2001	PYR	OXT-C-CA-O3
4	D	2001	PYR	OXT-C-CA-CB
5	A	2100	ATP	O4'-C4'-C5'-O5'

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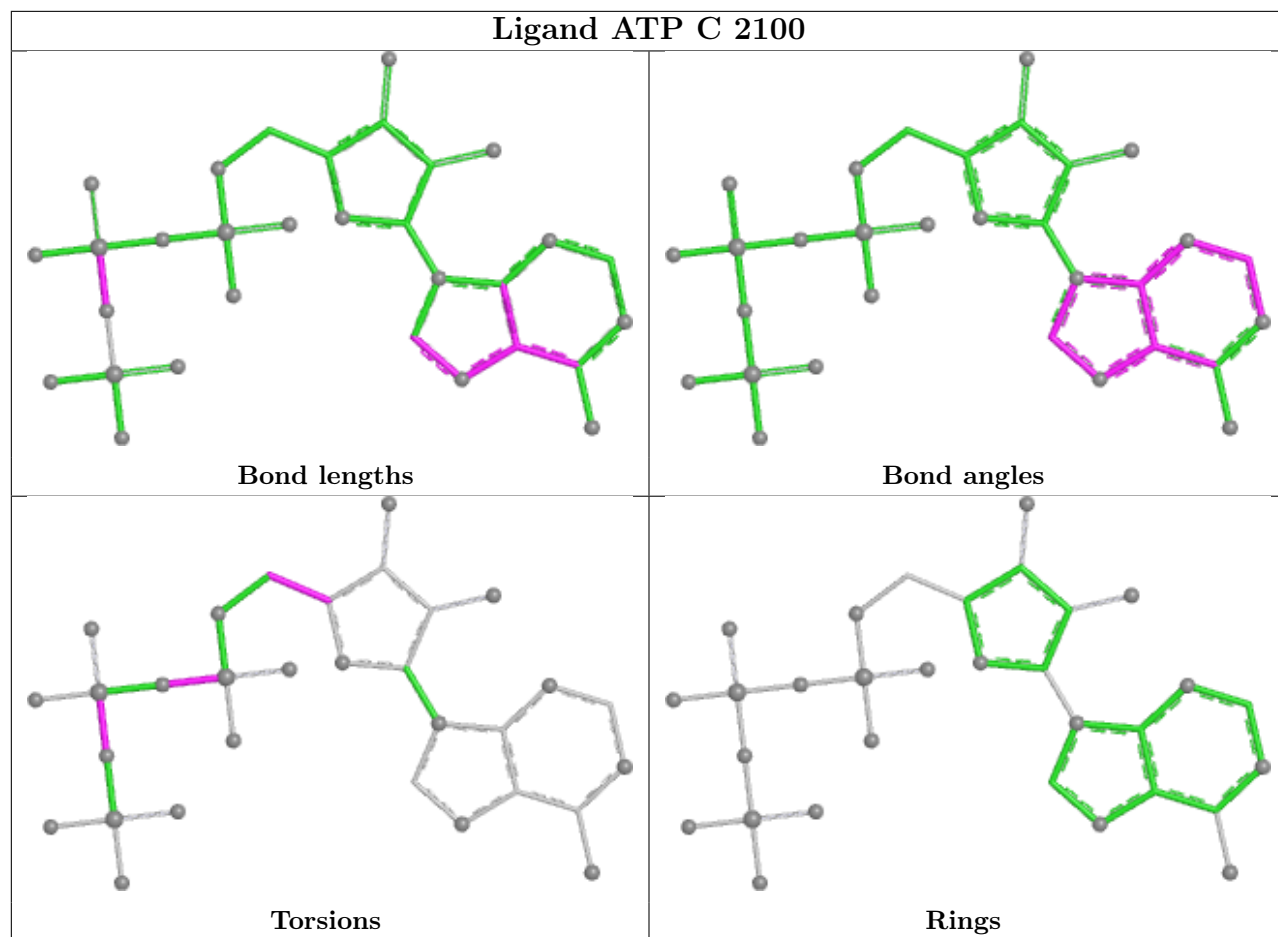
Mol	Chain	Res	Type	Atoms
5	A	2100	ATP	C3'-C4'-C5'-O5'
5	C	2100	ATP	O4'-C4'-C5'-O5'
5	C	2100	ATP	C3'-C4'-C5'-O5'
5	C	2100	ATP	PG-O3B-PB-O1B
5	A	2100	ATP	C4'-C5'-O5'-PA
3	A	2000	BTI	S1-C2-C7-C8
3	A	2000	BTI	C4-C2-C7-C8
4	B	2001	PYR	O-C-CA-CB
5	C	2100	ATP	PB-O3A-PA-O1A
3	C	2000	BTI	C7-C8-C9-C10
5	A	2100	ATP	PA-O3A-PB-O1B
5	A	2100	ATP	PA-O3A-PB-O2B
5	C	2100	ATP	PB-O3A-PA-O2A
5	A	2100	ATP	PB-O3A-PA-O1A
5	A	2100	ATP	PB-O3A-PA-O2A
3	A	2000	BTI	C11-C10-C9-C8
3	D	2000	BTI	C2-C7-C8-C9
4	A	2001	PYR	O-C-CA-O3
4	C	2001	PYR	O-C-CA-O3
4	D	2001	PYR	O-C-CA-O3

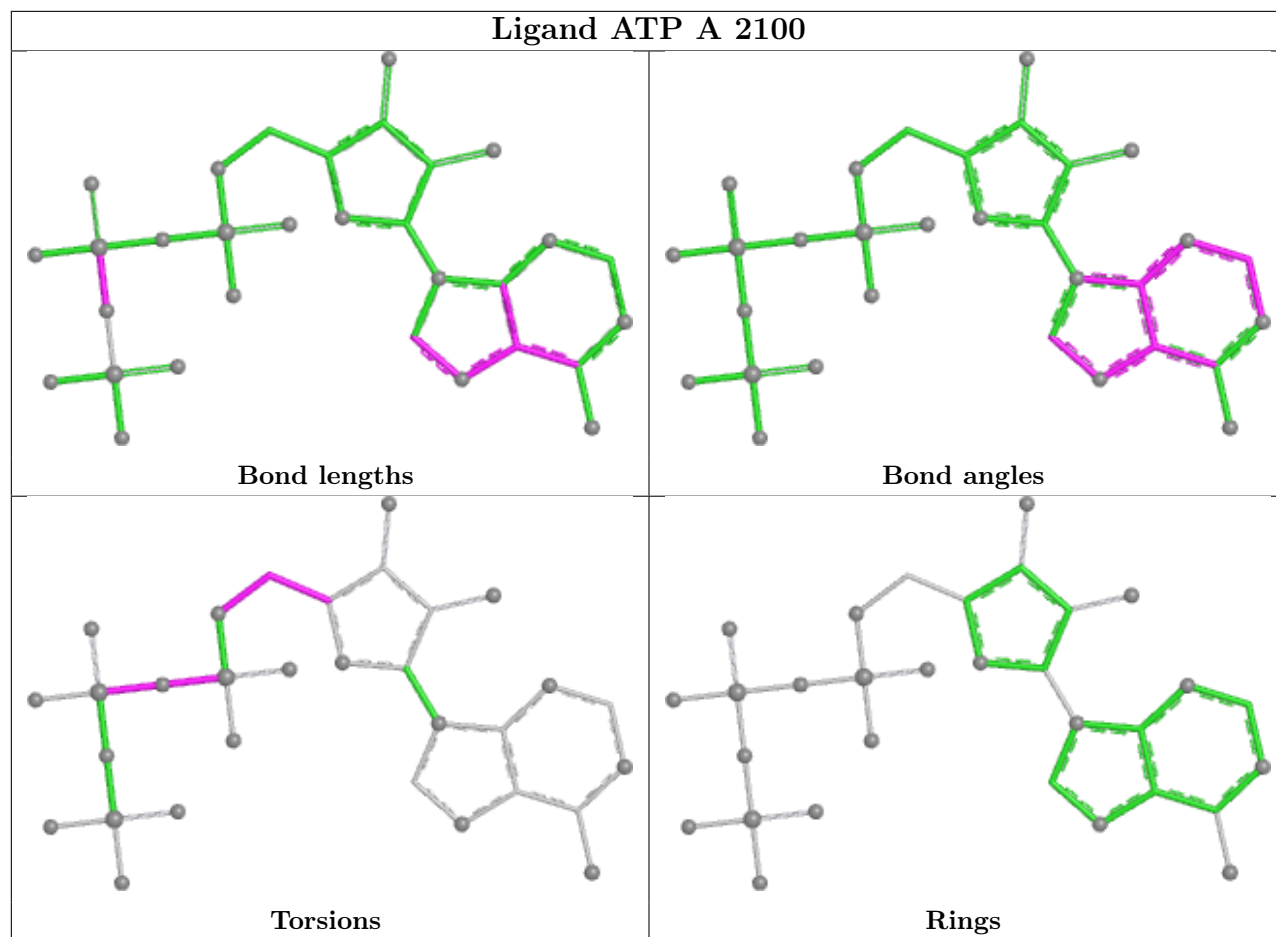
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2000	BTI	1	0
3	A	2000	BTI	1	0
5	C	2100	ATP	1	0
3	D	2000	BTI	1	0

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





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, 95th 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	1137/1173 (96%)	-0.04	25 (2%)	62	52	30, 59, 122, 143	0
1	B	1074/1173 (91%)	0.05	31 (2%)	53	43	39, 69, 119, 152	0
1	C	1067/1173 (90%)	-0.01	26 (2%)	59	49	38, 66, 103, 115	0
1	D	1067/1173 (90%)	-0.11	21 (1%)	65	56	28, 60, 113, 213	0
All	All	4345/4692 (92%)	-0.03	103 (2%)	59	49	28, 64, 114, 213	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	SER	5.1
1	A	180	ALA	4.5
1	A	188	GLY	4.0
1	A	1135	GLN	3.9
1	B	1094	VAL	3.8
1	A	213	LEU	3.6
1	B	396	ALA	3.6
1	B	387	PHE	3.4
1	B	167	ILE	3.3
1	C	931	VAL	3.2
1	B	402	GLY	3.1
1	B	404	GLY	3.1
1	D	1155	GLY	3.1
1	B	494	LEU	3.0
1	B	526	LEU	3.0
1	B	403	PHE	3.0
1	C	176	SER	2.9
1	C	933	THR	2.9
1	A	494	LEU	2.9
1	D	1156	VAL	2.9
1	B	457	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	936	TYR	2.9
1	B	492	PRO	2.9
1	B	1096	THR	2.9
1	B	168	PRO	2.9
1	A	220	ALA	2.8
1	D	1104	ALA	2.8
1	B	455	VAL	2.8
1	C	190	PRO	2.8
1	A	216	ALA	2.8
1	C	282	GLY	2.8
1	B	395	ILE	2.7
1	C	890	VAL	2.7
1	A	90	LEU	2.7
1	B	90	LEU	2.7
1	C	206	ILE	2.6
1	B	164	LEU	2.6
1	C	932	ILE	2.6
1	C	201	GLY	2.6
1	C	415	GLY	2.6
1	D	384	LEU	2.6
1	B	524	TYR	2.6
1	D	92	PRO	2.6
1	B	408	ASP	2.6
1	B	384	LEU	2.5
1	B	527	ALA	2.5
1	B	379	THR	2.5
1	D	434	ILE	2.5
1	B	320	PHE	2.5
1	C	869	GLY	2.5
1	B	285	PRO	2.4
1	D	823	HIS	2.4
1	B	239	ILE	2.4
1	B	418	ILE	2.4
1	D	314	VAL	2.4
1	D	271	HIS	2.4
1	C	183	PHE	2.4
1	A	1095	HIS	2.4
1	A	1177	ILE	2.4
1	D	490	ILE	2.3
1	B	871	TYR	2.3
1	C	935	GLY	2.3
1	C	195	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	119	GLY	2.3
1	C	184	ALA	2.3
1	A	179	LEU	2.3
1	A	492	PRO	2.2
1	B	421	TYR	2.2
1	A	221	LYS	2.2
1	A	1156	VAL	2.2
1	B	397	TYR	2.2
1	A	189	PHE	2.2
1	C	1001	PRO	2.2
1	C	416	ALA	2.2
1	C	199	GLY	2.2
1	D	243	LYS	2.2
1	C	1142	ALA	2.2
1	D	160	ILE	2.1
1	D	917	MET	2.1
1	C	172	GLY	2.1
1	A	228	PHE	2.1
1	D	1173	LEU	2.1
1	A	527	ALA	2.1
1	C	213	LEU	2.1
1	C	180	ALA	2.1
1	D	421	TYR	2.1
1	D	1169	ALA	2.1
1	A	178	GLU	2.1
1	A	190	PRO	2.1
1	A	488	PHE	2.1
1	D	853	ASP	2.1
1	A	184	ALA	2.1
1	C	434	ILE	2.1
1	C	960	ASN	2.1
1	B	461	PHE	2.1
1	C	409	ALA	2.1
1	A	181	LYS	2.0
1	D	1162	VAL	2.0
1	D	1174	LEU	2.0
1	A	206	ILE	2.0
1	D	939	ASP	2.0
1	B	165	PRO	2.0
1	D	888	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

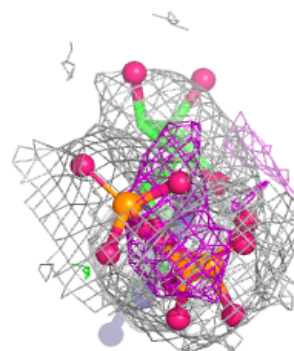
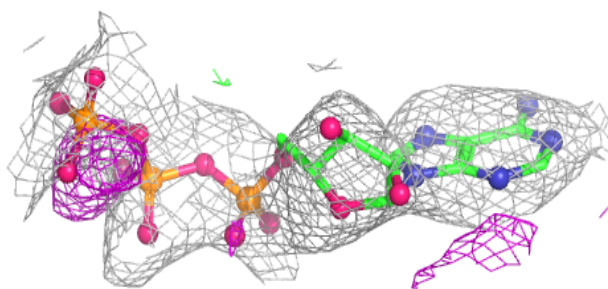
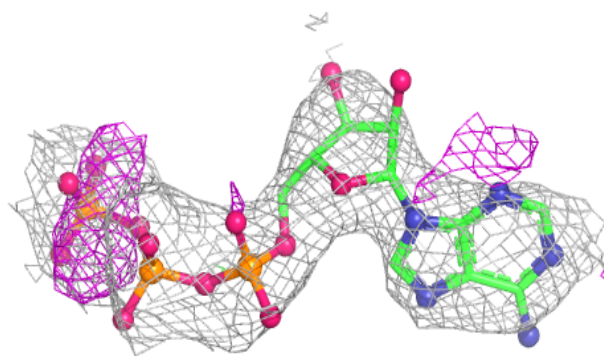
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PYR	D	2001	6/6	0.44	0.25	84,85,85,85	0
4	PYR	B	2001	6/6	0.77	0.18	89,90,91,91	0
5	ATP	A	2100	31/31	0.80	0.15	115,117,126,126	0
4	PYR	C	2001	6/6	0.83	0.20	84,85,85,85	0
4	PYR	A	2001	6/6	0.84	0.20	93,93,93,93	0
2	MN	D	2002	1/1	0.86	0.11	85,85,85,85	0
5	ATP	C	2100	31/31	0.88	0.10	80,82,94,95	0
3	BTI	D	2000	15/15	0.89	0.12	75,75,76,77	0
2	MN	A	2002	1/1	0.92	0.11	123,123,123,123	0
3	BTI	B	2000	15/15	0.94	0.10	51,52,57,58	0
2	MN	B	2002	1/1	0.95	0.08	94,94,94,94	0
2	MN	C	2002	1/1	0.96	0.08	79,79,79,79	0
3	BTI	A	2000	15/15	0.97	0.09	61,63,69,69	0
3	BTI	C	2000	15/15	0.98	0.07	52,52,65,65	0

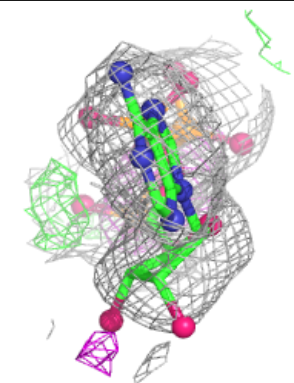
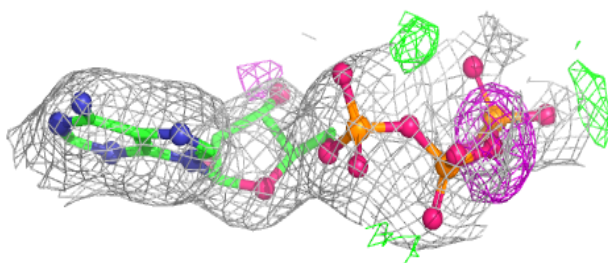
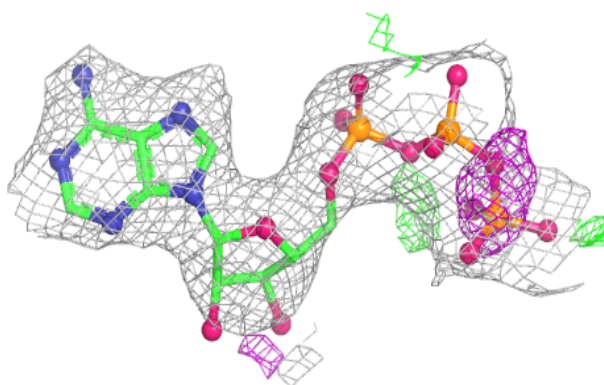
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 2100:

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

**Electron density around ATP C 2100:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.