



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:37 AM GMT

PDB ID : 3BG5  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

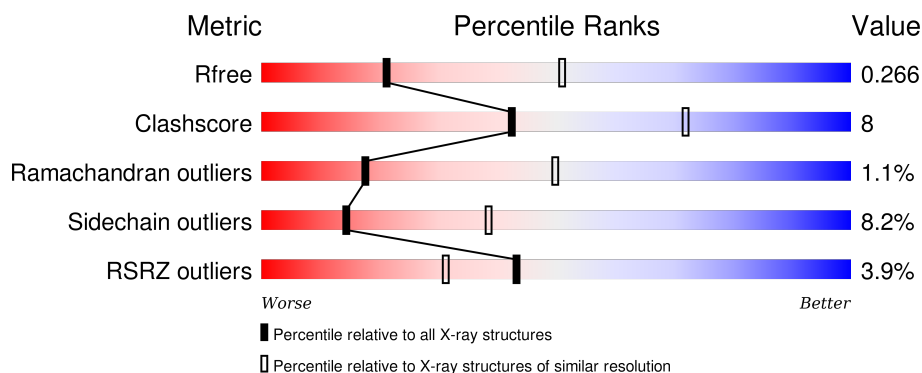
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>4%</div> <div>72% 21% . .</div> </div>
1	B	1173	<div> <div>4%</div> <div>70% 18% . 8%</div> </div>
1	C	1173	<div> <div>2%</div> <div>66% 22% . 9%</div> </div>
1	D	1173	<div> <div>4%</div> <div>68% 20% . 9%</div> </div>

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	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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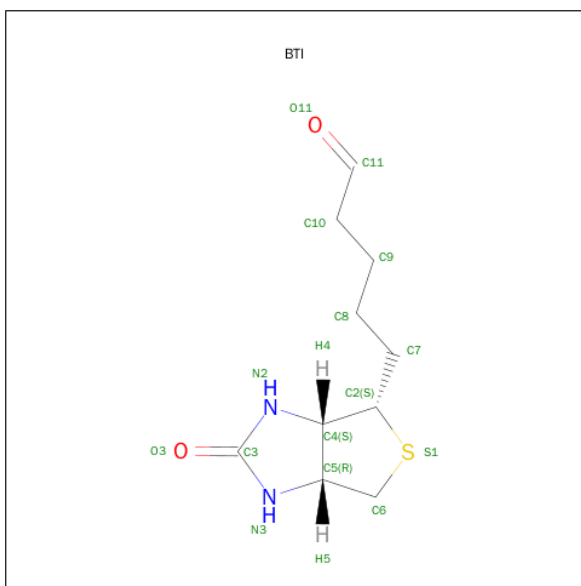
Chain	Residue	Modelled	Actual	Comment	Reference
C	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	29	SER	-	EXPRESSION TAG	UNP Q99UY8
C	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	31	MET	-	EXPRESSION TAG	UNP Q99UY8
C	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
C	33	SER	-	EXPRESSION TAG	UNP Q99UY8
D	11	MET	-	EXPRESSION TAG	UNP Q99UY8
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 (three-letter code: MN) (formula: Mn).

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

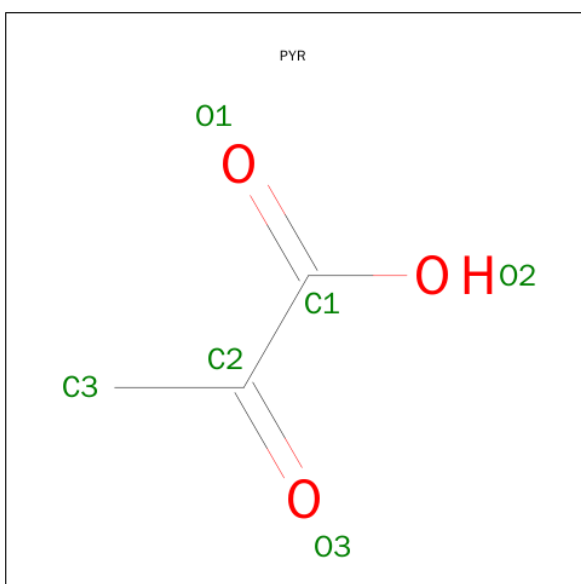
- Molecule 3 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL

(three-letter code: BTI) (formula:  $C_{10}H_{16}N_2O_2S$ ).



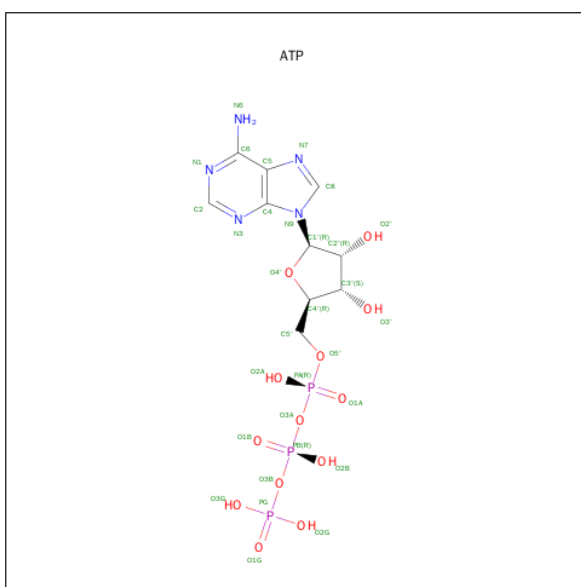
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	B	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	C	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	D	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

- Molecule 4 is PYRUVIC ACID (three-letter code: 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 (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



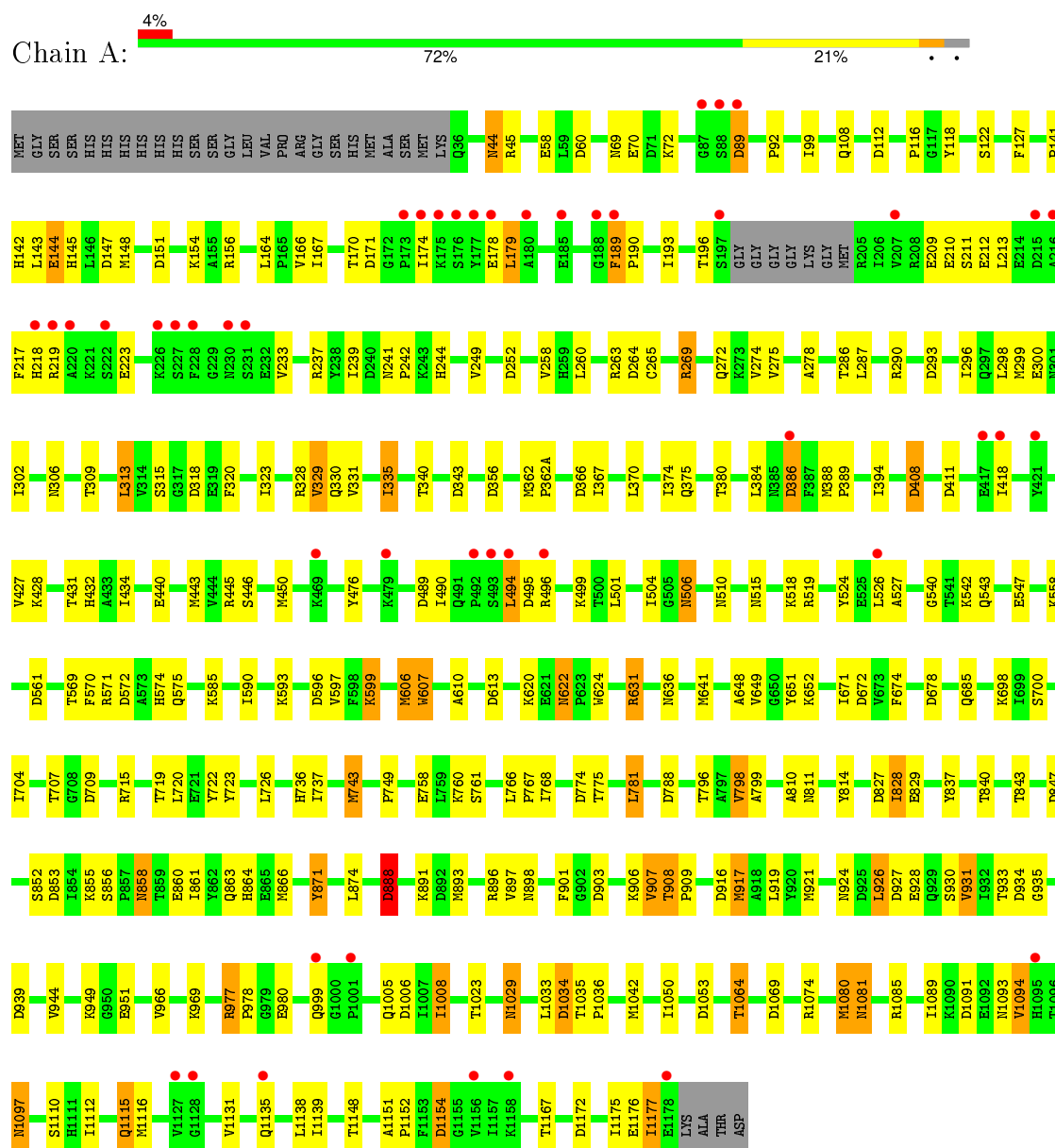
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		



### 3 Residue-property plots

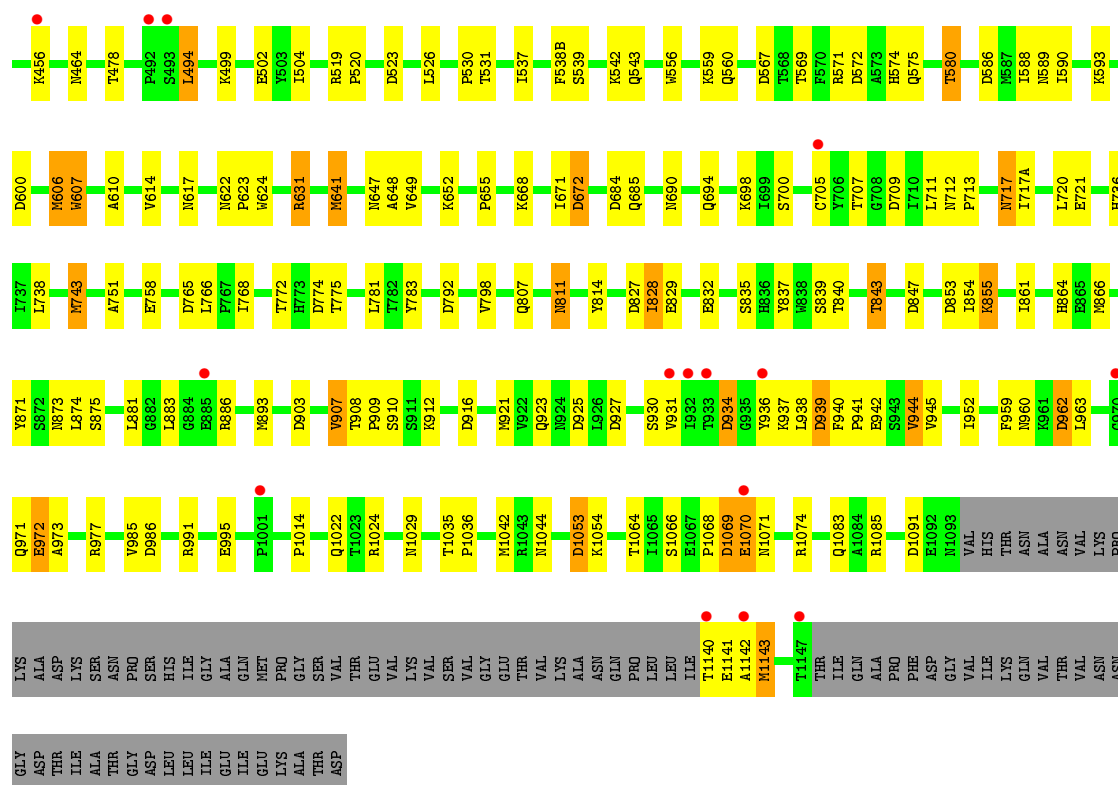
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Pyruvate carboxylase

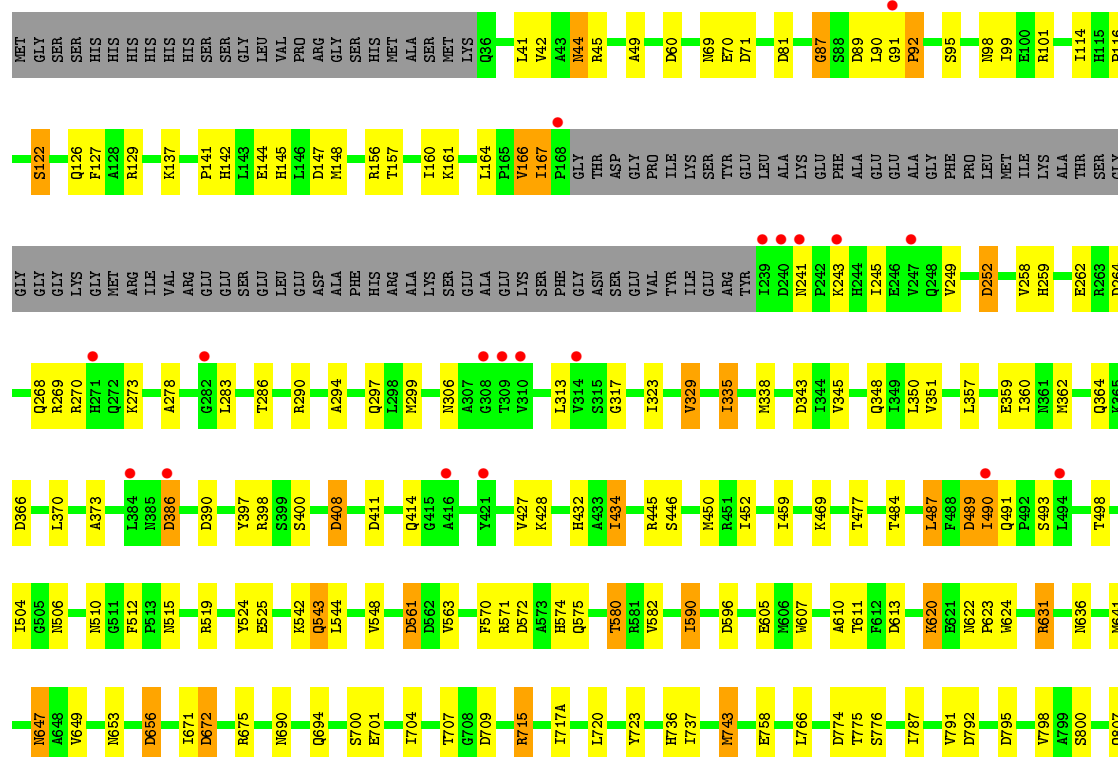


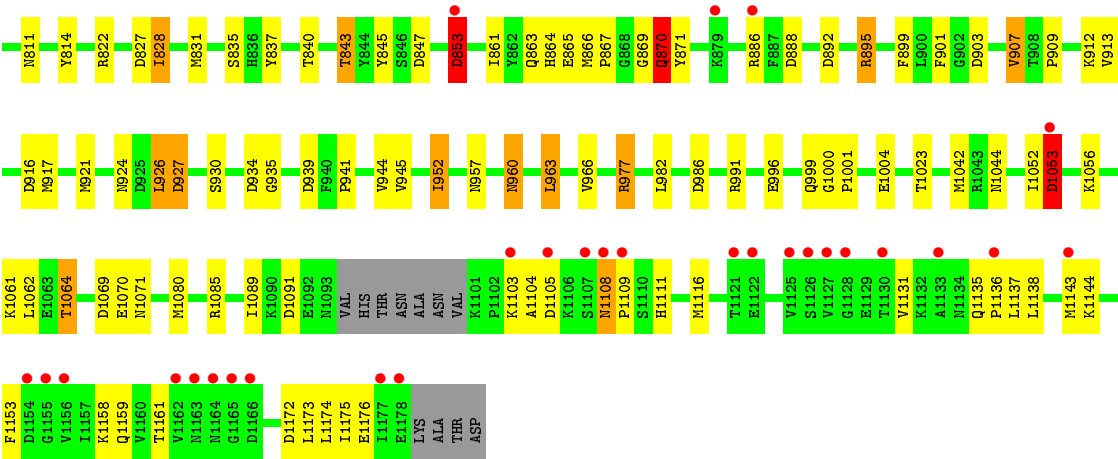
#### • Molecule 1: Pyruvate carboxylase





• Molecule 1: Pyruvate carboxylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.43 Å   256.08 Å   126.01 Å 90.00°   109.47°   90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.63 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-2.80) 91.9 (29.63-2.69)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.59 (at 2.68 Å)	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	6977 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.7	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.7	EDS
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 145662 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	34438	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.40	0/9139	0.73	33/12364 (0.3%)
1	B	0.38	0/8625	0.74	47/11675 (0.4%)
1	C	0.40	1/8603 (0.0%)	0.73	39/11627 (0.3%)
1	D	0.40	0/8571	0.75	35/11598 (0.3%)
All	All	0.40	1/34938 (0.0%)	0.74	154/47264 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	315	SER	CB-OG	11.09	1.56	1.42

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	343	ASP	CB-CG-OD2	8.58	126.02	118.30
1	B	613	ASP	CB-CG-OD2	8.02	125.52	118.30
1	D	561	ASP	CB-CG-OD2	7.92	125.43	118.30
1	A	927	ASP	CB-CG-OD2	7.86	125.38	118.30
1	A	827	ASP	CB-CG-OD2	7.72	125.25	118.30
1	D	1053	ASP	CB-CG-OD2	7.50	125.05	118.30
1	A	1069	ASP	CB-CG-OD2	7.22	124.80	118.30
1	C	1069	ASP	CB-CG-OD2	7.14	124.73	118.30
1	C	774	ASP	CB-CG-OD2	6.94	124.55	118.30
1	A	252	ASP	CB-CG-OD2	6.92	124.53	118.30
1	C	827	ASP	CB-CG-OD2	6.81	124.42	118.30
1	D	252	ASP	CB-CG-OD2	6.80	124.42	118.30
1	C	252	ASP	CB-CG-OD2	6.76	124.38	118.30
1	B	1069	ASP	CB-CG-OD2	6.75	124.37	118.30
1	A	264	ASP	CB-CG-OD2	6.64	124.28	118.30
1	D	390	ASP	CB-CG-OD2	6.61	124.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	1172	ASP	CB-CG-OD2	6.55	124.20	118.30
1	A	489	ASP	CB-CG-OD2	6.53	124.17	118.30
1	B	163	ASP	CB-CG-OD2	6.40	124.06	118.30
1	C	1091	ASP	CB-CG-OD2	6.36	124.02	118.30
1	B	252	ASP	CB-CG-OD2	6.35	124.01	118.30
1	B	939	ASP	CB-CG-OD2	6.33	124.00	118.30
1	C	386	ASP	CB-CG-OD2	6.30	123.97	118.30
1	D	81	ASP	CB-CG-OD2	6.29	123.96	118.30
1	B	1172	ASP	CB-CG-OD2	6.28	123.95	118.30
1	B	489	ASP	CB-CG-OD2	6.26	123.93	118.30
1	B	853	ASP	CB-CG-OD2	6.21	123.89	118.30
1	D	934	ASP	CB-CG-OD2	6.20	123.88	118.30
1	D	147	ASP	CB-CG-OD2	6.19	123.87	118.30
1	D	343	ASP	CB-CG-OD2	6.19	123.87	118.30
1	D	853	ASP	CB-CG-OD2	6.19	123.87	118.30
1	C	356	ASP	CB-CG-OD2	6.19	123.87	118.30
1	D	774	ASP	CB-CG-OD2	6.17	123.86	118.30
1	D	613	ASP	CB-CG-OD2	6.17	123.85	118.30
1	B	151	ASP	CB-CG-OD2	6.14	123.83	118.30
1	B	986	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	888	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	788	ASP	CB-CG-OD2	6.09	123.79	118.30
1	C	60	ASP	CB-CG-OD2	6.08	123.78	118.30
1	C	390	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	1053	ASP	CB-CG-OD2	6.05	123.75	118.30
1	B	847	ASP	CB-CG-OD2	6.05	123.75	118.30
1	D	827	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	1091	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	903	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	1154	ASP	CB-CG-OD2	5.99	123.69	118.30
1	D	1172	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	774	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	934	ASP	CB-CG-OD2	5.92	123.63	118.30
1	D	1069	ASP	CB-CG-OD2	5.85	123.56	118.30
1	B	1034	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	1154	ASP	CB-CG-OD2	5.84	123.56	118.30
1	C	709	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	147	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	916	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	903	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	827	ASP	CB-CG-OD2	5.78	123.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	709	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	561	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	1053	ASP	CB-CG-OD2	5.73	123.45	118.30
1	B	962	ASP	CB-CG-OD2	5.73	123.45	118.30
1	C	104	ASP	CB-CG-OD2	5.72	123.44	118.30
1	A	774	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	81	ASP	CB-CG-OD2	5.66	123.39	118.30
1	D	709	ASP	CB-CG-OD2	5.65	123.39	118.30
1	D	903	ASP	CB-CG-OD2	5.64	123.38	118.30
1	D	71	ASP	CB-CG-OD2	5.64	123.37	118.30
1	C	1053	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	1091	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	264	ASP	CB-CG-OD2	5.59	123.33	118.30
1	D	986	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	523	ASP	CB-CG-OD2	5.58	123.32	118.30
1	C	264	ASP	CB-CG-OD2	5.58	123.32	118.30
1	C	939	ASP	CB-CG-OD2	5.57	123.31	118.30
1	C	847	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	916	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	684	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	596	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	709	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	600	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	600	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	147	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	112	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	343	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	962	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	408	ASP	CB-CG-OD2	5.46	123.21	118.30
1	D	264	ASP	CB-CG-OD2	5.45	123.20	118.30
1	C	684	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	572	ASP	CB-CG-OD2	5.43	123.19	118.30
1	D	89	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	523	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	765	ASP	CB-CG-OD2	5.40	123.16	118.30
1	D	411	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	60	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	934	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	765	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	1034	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	408	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	934	ASP	CB-CG-OD2	5.32	123.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1006	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	390	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	318	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	356	ASP	CB-CG-OD2	5.26	123.04	118.30
1	D	795	ASP	CB-CG-OD2	5.26	123.04	118.30
1	D	596	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	171	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	411	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	903	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	888	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	104	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	672	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	489	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	475	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	386	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	89	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	572	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	986	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	112	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	112	ASP	CB-CG-OD2	5.16	122.94	118.30
1	D	792	ASP	CB-CG-OD2	5.15	122.94	118.30
1	C	163	ASP	CB-CG-OD2	5.15	122.94	118.30
1	C	586	ASP	CB-CG-OD2	5.14	122.93	118.30
1	C	925	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	916	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	60	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	892	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	586	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	494	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	293	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	792	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	495	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	408	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	888	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	939	ASP	CB-CG-OD2	5.07	122.87	118.30
1	A	386	ASP	CB-CG-OD2	5.06	122.86	118.30
1	C	567	ASP	CB-CG-OD2	5.06	122.86	118.30
1	B	546	ASP	CB-CG-OD2	5.06	122.85	118.30
1	C	81	ASP	CB-CG-OD2	5.05	122.85	118.30
1	D	366	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	366	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	411	ASP	CB-CG-OD2	5.04	122.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	318	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	613	ASP	CB-CG-OD2	5.04	122.83	118.30
1	B	356	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	495	ASP	CB-CG-OD2	5.04	122.83	118.30
1	C	853	ASP	CB-CG-OD2	5.04	122.83	118.30
1	B	386	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	89	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	411	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	408	ASP	CB-CG-OD2	5.03	122.82	118.30
1	D	656	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	672	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	916	ASP	CB-CG-OD2	5.01	122.81	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	8969	0	8894	163	0
1	B	8465	0	8412	127	0
1	C	8441	0	8350	141	0
1	D	8413	0	8361	148	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	3	0	0
4	B	6	0	3	0	0
4	C	6	0	3	0	0
4	D	6	0	3	0	0
5	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	31	0	12	1	0
All	All	34438	0	34113	570	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 8.

All (570) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:ILE:HG21	1:C:1042:MET:HE2	1.34	1.07
1:A:189:PHE:HB3	1:A:190:PRO:HD3	1.35	1.06
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: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
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: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: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:504:ILE:HG21	1:A:1042:MET:HE3	1.64	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:D:647:ASN:HD22	1:D:647:ASN:C	1.88	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.72	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
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:C:960:ASN:HB2	1:C:963:LEU:CB	2.24	0.67
1:A:700:SER:H	1:A:736:HIS:HD2	1.39	0.67
1:D:921:MET:HG3	1:D:926:LEU:HB2	1.76	0.67
1:A:189:PHE:HB3	1:A:190:PRO:CD	2.19	0.67
1:B:1177:ILE:N	1:B:1177:ILE:HD13	2.09	0.67
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:HE3	1:A:607:TRP:HB2	1.78	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:622:ASN:HD21	1:C:624:TRP:HD1	1.45	0.65
1:C:811:ASN:H	1:C:811:ASN:HD22	1.44	0.65
1:B:506:ASN:HD22	1:B:510:ASN:HD22	1.43	0.65
1:A:263:ARG:HH21	1:A:330:GLN:NE2	1.94	0.65
1:D:690:ASN:O	1:D:694:GLN:HG2	1.97	0.65
1:D:142:HIS:H	1:D:145:HIS:HD2	1.43	0.65
1:D:570:PHE:O	1:D:574:HIS:HE1	1.80	0.65
1:B:543:GLN:HE22	1:B:636:ASN:HA	1.61	0.65
1:D:575:GLN:NE2	1:D:610:ALA:H	1.95	0.65
1:A:921:MET:HE2	1:A:931:VAL:HG21	1.79	0.65
1:A:527:ALA:HB2	1:A:840:THR:HG21	1.77	0.64
1:A:164:LEU:HD11	1:A:298:LEU:HB2	1.80	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:HIS:H	1:A:145:HIS:HD2	1.45	0.63
1:C:893:MET:CE	1:C:921:MET:HB2	2.29	0.63
1:D:241:ASN:HD21	1:D:477:THR:HG21	1.63	0.63
1:C:960:ASN:HB2	1:C:963:LEU:HB2	1.79	0.63
1:C:539:SER:HA	1:C:543:GLN:HG3	1.80	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
1:D:498:THR:OG1	1:D:1085:ARG:NH2	2.32	0.63
1:B:622:ASN:HD21	1:B:624:TRP:HD1	1.46	0.63
1:C:77:ARG:HD3	1:C:78:TYR:CE2	2.34	0.62
1:D:1137:LEU:HD13	1:D:1175:ILE:HG13	1.79	0.62
1:C:840:THR:O	1:C:843:THR:HB	1.99	0.62
1:D:575:GLN:HE22	1:D:610:ALA:H	1.45	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: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:720:LEU:HD11	1:A:758:GLU:HG3	1.83	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: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:B:519:ARG:HB2	1:B:520:PRO:CD	2.32	0.60
1:A:814:TYR:CE2	1:A:828:ILE:HG12	2.36	0.60
1:B:1029:ASN:HD22	1:B:1029:ASN:C	2.05	0.60
1:D:641:MET:HE3	1:D:671:ILE:HG21	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:571:ARG:HH11	1:C:575:GLN:NE2	1.99	0.59
1:A:606:MET:HE1	1:A:671:ILE:CD1	2.32	0.59
1:C:145:HIS:HE1	1:C:302:ILE:O	1.86	0.59
1:C:260:LEU:HD21	1:C:362:MET:HE1	1.85	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:C:437:LYS:HD3	1:C:437:LYS:H	1.68	0.58
1:A:58:GLU:HG3	1:C:445:ARG:HD3	1.85	0.58
1:D:717(A):ILE:HG13	1:D:957:ASN:HD21	1.68	0.58
1:B:664:GLN:HA	1:B:664:GLN:NE2	2.18	0.58
1:B:540:GLY:H	1:B:543:GLN:HE21	1.52	0.58
1:D:400:SER:HB2	1:D:445:ARG:HH21	1.68	0.58
1:D:909:PRO:HG2	1:D:952:ILE:HG12	1.85	0.58
1:A:569:THR:OG1	1:A:798:VAL:HG23	2.03	0.58
1:A:1115:GLN:H	1:A:1115:GLN:CD	2.08	0.58
1:A:524:TYR:CD2	1:A:843:THR:HG22	2.39	0.57
1:A:504:ILE:HG21	1:A:1042:MET:CE	2.34	0.57
1:A:571:ARG:HH11	1:A:575:GLN:NE2	2.01	0.57
1:C:230:ASN:HD22	1:C:232:GLU:H	1.52	0.57
1:A:296:ILE:O	1:A:300:GLU:HB2	2.04	0.57
1:A:864:HIS:HD2	1:A:866:MET:H	1.52	0.57
1:B:1177:ILE:H	1:B:1177:ILE:HD13	1.70	0.57
1:D:935:GLY:HA3	1:D:966:VAL:CG1	2.35	0.57
1:B:269:ARG:HG3	1:B:272:GLN:HB3	1.86	0.57
1:A:494:LEU:H	1:A:494:LEU:HD12	1.70	0.57
1:D:590:ILE:HG12	1:D:837:TYR:CE2	2.40	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:B:860:GLU:O	1:B:863:GLN:HG2	2.04	0.56
1:D:675:ARG:HA	1:D:701:GLU:HB2	1.86	0.56
1:D:519:ARG:NH2	1:D:847:ASP:OD2	2.35	0.56
1:A:69:ASN:O	1:A:72:LYS:HG2	2.05	0.56
1:A:575:GLN:NE2	1:A:610:ALA:H	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASN:HD22	1:A:72:LYS:HE2	1.71	0.56
1:A:1081:ASN:HB2	1:C:78:TYR:CD2	2.41	0.56
1:D:90:LEU:HD21	1:D:98:ASN:HD22	1.71	0.55
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: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:D:631:ARG:NH2	1:D:672:ASP:OD1	2.40	0.55
1:A:858:ASN:HD21	1:A:860:GLU:HB2	1.70	0.55
1:C:622:ASN:HD22	1:C:623:PRO:HD2	1.72	0.55
1:A:596:ASP:O	1:A:599:LYS:HG2	2.06	0.55
1:D:269:ARG:HG3	1:D:270:ARG:H	1.72	0.55
1:C:200:GLY:C	1:C:202:LYS:H	2.10	0.55
1:C:641:MET:HG2	1:C:671:ILE:HG21	1.87	0.55
1:C:174:ILE:HG21	1:C:180:ALA:HB2	1.90	0.55
1:C:144:GLU:O	1:C:148:MET:HB2	2.07	0.54
1:A:641:MET:HE3	1:A:674:PHE:CE1	2.42	0.54
1:C:960:ASN:HB2	1:C:963:LEU:HB3	1.89	0.54
1:C:775:THR:CG2	1:C:861:ILE:HG13	2.36	0.54
1:C:263:ARG:HH21	1:C:330:GLN:NE2	2.04	0.54
1:D:574:HIS:CD2	1:D:580:THR:HA	2.41	0.54
1:A:362:MET:HE1	1:A:367:ILE:CD1	2.38	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:C:893:MET:HE1	1:C:921:MET:HB2	1.90	0.53
1:D:1052:ILE:HG22	1:D:1053:ASP:H	1.73	0.53
1:C:44:ASN:ND2	1:C:45:ARG:H	2.02	0.53
1:B:45:ARG:HD2	1:B:71:ASP:OD2	2.08	0.53
1:C:909:PRO:O	1:C:912:LYS:HB3	2.09	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
1:D:935:GLY:HA3	1:D:966:VAL:HG13	1.91	0.53
1:B:720:LEU:HD21	1:B:758:GLU:HG3	1.91	0.53
1:A:811:ASN:HD22	1:A:811:ASN:H	1.57	0.53
1:D:814:TYR:CE2	1:D:828:ILE:HG12	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:GLN:HE22	1:B:610:ALA:H	1.56	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:210:GLU:O	1:A:212:GLU:N	2.38	0.52
1:A:1074:ARG:NH1	1:A:1091:ASP:OD2	2.41	0.52
1:A:1033:LEU:HD23	1:A:1050:ILE:HG12	1.91	0.52
1:C:296:ILE:O	1:C:300:GLU:HB2	2.09	0.52
1:C:398:ARG:HE	1:C:1083:GLN:HG2	1.75	0.52
1:B:715:ARG:HH12	1:B:865:GLU:CD	2.11	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:B:811:ASN:ND2	1:B:811:ASN:H	2.06	0.52
1:B:606:MET:HE3	1:B:607:TRP:HB2	1.91	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:672:ASP:HA	1:A:698:LYS:HD2	1.92	0.52
1:A:515:ASN:HA	1:B:1143:MET:HG3	1.91	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:HD22	1:D:811:ASN:H	1.57	0.52
1:C:435:SER:HB2	1:C:437:LYS:HE3	1.91	0.51
1:A:575:GLN:HE22	1:A:610:ALA:H	1.56	0.51
1:C:772:THR:HG22	1:C:783:TYR:CE2	2.46	0.51
1:D:1042:MET:CE	1:D:1062:LEU:HB2	2.41	0.51
1:D:622:ASN:HD22	1:D:623:PRO:HD2	1.74	0.51
1:A:1131:VAL:HB	1:A:1135:GLN:CD	2.31	0.51
1:A:362:MET:HE1	1:A:367:ILE:HD11	1.93	0.51
1:C:142:HIS:H	1:C:145:HIS:HD2	1.58	0.51
1:D:44:ASN:ND2	1:D:45:ARG:H	1.99	0.51
1:B:776:SER:HB3	1:B:861:ILE:HD11	1.92	0.51
1:A:328:ARG:HD2	1:A:329:VAL:O	2.10	0.51
1:D:1042:MET:HE3	1:D:1062:LEU:HB2	1.92	0.51
1:B:274:VAL:HG12	1:B:275:VAL:HG23	1.92	0.51
1:B:864:HIS:CD2	1:B:866:MET:H	2.23	0.51
1:A:210:GLU:C	1:A:212:GLU:H	2.14	0.51
1:D:743:MET:HG3	1:D:907:VAL:HG13	1.92	0.51
1:B:675:ARG:HA	1:B:701:GLU:HB2	1.93	0.50
1:A:737:ILE:HG12	1:A:767:PRO:HG2	1.92	0.50
1:B:622:ASN:HD22	1:B:623:PRO:HD2	1.76	0.50
1:A:1005:GLN:HA	1:A:1008:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:866:MET:HE2	1:C:871:TYR:HA	1.94	0.50
1:A:543:GLN:HE22	1:A:636:ASN:HA	1.77	0.50
1:B:858:ASN:ND2	1:B:860:GLU:HG2	2.17	0.50
1:C:606:MET:HE3	1:C:607:TRP:HB2	1.94	0.50
1:C:1035:THR:HB	1:C:1036:PRO:HD3	1.94	0.50
1:C:504:ILE:HG21	1:C:1042:MET:HE3	1.86	0.50
1:C:811:ASN:ND2	1:C:811:ASN:H	2.07	0.50
1:C:419:SER:HB2	1:C:421:TYR:HD1	1.76	0.50
1:B:799:ALA:H	1:B:811:ASN:ND2	2.10	0.50
1:B:664:GLN:HE22	1:B:696:ALA:HB2	1.77	0.50
1:C:606:MET:HE1	1:C:671:ILE:CD1	2.42	0.50
1:C:71:ASP:C	1:C:73:SER:H	2.15	0.50
1:A:871:TYR:O	1:A:871:TYR:CD1	2.65	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:1158:LYS:HG3	1:D:1176:GLU:HG3	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: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:D:1137:LEU:CD1	1:D:1175:ILE:HG13	2.42	0.49
1:D:620:LYS:HG2	1:D:1023:THR:HG21	1.94	0.49
1:A:70:GLU:HG3	1:A:92:PRO:HG3	1.94	0.49
1:C:641:MET:CG	1:C:671:ILE:HG21	2.43	0.49
1:B:1066:SER:HB2	1:D:1064:THR:HG21	1.95	0.49
1:B:719:THR:HG22	1:B:721:GLU:H	1.78	0.49
1:A:760:LYS:HG2	1:A:768:ILE:HD12	1.95	0.49
1:B:496:ARG:H	1:B:496:ARG:HD2	1.78	0.49
1:A:935:GLY:HA3	1:A:966:VAL:HG13	1.95	0.49
1:B:408:ASP:HB2	1:B:428:LYS:HE3	1.94	0.48
1:A:335:ILE:HD11	1:A:375:GLN:N	2.28	0.48
1:D:1052:ILE:O	1:D:1053:ASP:C	2.50	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:A:622:ASN:C	1:A:622:ASN:HD22	2.17	0.48
1:D:1137:LEU:HD12	1:D:1138:LEU:HB2	1.95	0.48
1:D:863:GLN:O	1:D:895:ARG:HD2	2.12	0.48
1:C:39:LYS:HD3	1:C:62:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:TYR:CD1	1:B:77:ARG:HG3	2.49	0.48
1:D:895:ARG:HE	1:D:899:PHE:HE1	1.61	0.48
1:B:141:PRO:HB2	1:B:145:HIS:HB2	1.95	0.48
1:C:169:GLY:HA2	1:C:236:GLU:HA	1.96	0.48
1:A:949:LYS:HB3	1:A:951:GLU:HG3	1.95	0.48
1:D:853:ASP:N	1:D:853:ASP:OD2	2.47	0.48
1:D:452:ILE:HD12	1:D:459:ILE:HD11	1.95	0.48
1:C:940:PHE:HB3	1:C:944:VAL:CG1	2.43	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:D:126:GLN:HG2	1:D:129:ARG:HH12	1.79	0.48
1:C:861:ILE:HD13	1:C:864:HIS:NE2	2.29	0.48
1:C:174:ILE:HG22	1:C:175:LYS:N	2.29	0.48
1:A:799:ALA:H	1:A:811:ASN:ND2	2.12	0.48
1:A:446:SER:O	1:A:450:MET:HG2	2.13	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:828:ILE:O	1:C:832:GLU:HG2	2.14	0.47
1:C:705:CYS:HB3	1:C:743:MET:SD	2.54	0.47
1:B:328:ARG:HD3	1:B:329:VAL:O	2.14	0.47
1:B:149:PHE:HA	1:B:155:ALA:HB2	1.96	0.47
1:A:704:ILE:HG21	1:A:723:TYR:HD2	1.79	0.47
1:D:268:GLN:HB3	1:D:273:LYS:HA	1.95	0.47
1:C:266:SER:O	1:C:478:THR:HA	2.15	0.47
1:A:930:SER:HA	1:A:933:THR:HB	1.95	0.47
1:C:940:PHE:HB3	1:C:944:VAL:HG12	1.97	0.47
1:A:362:MET:HE3	1:A:362(A):PRO:HD2	1.96	0.47
1:C:991:ARG:O	1:C:995:GLU:CG	2.62	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:A:856:SER:OG	1:D:800:SER:HA	2.14	0.47
1:C:99:ILE:HG23	1:C:127:PHE:HD1	1.80	0.47
1:C:504:ILE:HD13	1:C:1042:MET:HE2	1.96	0.47
1:D:917:MET:SD	1:D:921:MET:HE3	2.54	0.47
1:D:631:ARG:HD3	1:D:631:ARG:HA	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:D:41:LEU:HB3	1:D:114:ILE:HG12	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:888:ASP:HA	1:A:891:LYS:HE3	1.96	0.47
1:A:335:ILE:HD11	1:A:374:ILE:HA	1.97	0.46
1:D:243:LYS:HD2	1:D:245:ILE:HD11	1.96	0.46
1:A:179:LEU:H	1:A:179:LEU:HD23	1.80	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:C:941:PRO:HG2	1:C:944:VAL:HB	1.97	0.46
1:D:1143:MET:HG2	1:D:1144:LYS:HE3	1.98	0.46
1:C:403:PHE:O	1:C:442:LYS:HE3	2.15	0.46
1:D:434:ILE:HG13	1:D:434:ILE:H	1.48	0.46
1:B:406:ARG:HB3	1:B:430:SER:HB2	1.97	0.46
1:D:960:ASN:HB3	1:D:963:LEU:HB2	1.97	0.46
1:A:209:GLU:HA	1:A:213:LEU:HG	1.96	0.46
1:B:664:GLN:NE2	1:B:696:ALA:HB2	2.30	0.46
1:B:525:GLU:HB3	1:B:840:THR:HG23	1.97	0.46
1:C:274:VAL:HG12	1:C:275:VAL:HG23	1.98	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:D:1044:ASN:HD22	1:D:1062:LEU:HD22	1.80	0.46
1:B:379:THR:HG22	1:B:425:LEU:HA	1.98	0.46
1:B:241:ASN:N	1:B:242:PRO:HD3	2.31	0.46
1:D:286:THR:O	1:D:290:ARG:HG3	2.15	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:D:1105:ASP:HB3	1:D:1109:PRO:HG2	1.98	0.46
1:D:313:LEU:HB2	1:D:323:ILE:HD11	1.98	0.46
1:B:66:ILE:HB	1:B:86:VAL:HG23	1.98	0.46
1:C:893:MET:HB3	1:C:893:MET:HE2	1.73	0.46
1:A:814:TYR:CZ	1:A:828:ILE:HG12	2.50	0.46
1:C:278:ALA:CB	1:C:335:ILE:HG23	2.45	0.46
1:A:290:ARG:HB3	1:A:320:PHE:CE1	2.51	0.46
1:C:152:LYS:NZ	5:C:2100:ATP:O2A	2.49	0.45
1:B:704:ILE:HG21	1:B:723:TYR:HD2	1.81	0.45
1:A:719:THR:H	1:A:722:TYR:HB3	1.81	0.45
1:D:350:LEU:HD22	1:D:359:GLU:HB3	1.97	0.45
1:D:278:ALA:CB	1:D:335:ILE:HG23	2.46	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: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:D:269:ARG:HG3	1:D:270:ARG:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:949:LYS:HE2	1:B:951:GLU:OE1	2.17	0.45
1:C:331:VAL:HG12	1:C:428:LYS:HE2	1.99	0.45
1:A:570:PHE:O	1:A:574:HIS:HE1	2.00	0.45
1:D:446:SER:O	1:D:450:MET:HG2	2.16	0.45
1:A:749:PRO:HG3	1:A:781:LEU:HB3	1.98	0.45
1:D:866:MET:HE2	1:D:871:TYR:HA	1.99	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:249:VAL:HG11	1:A:299:MET:HG3	1.98	0.45
1:B:901:PHE:CZ	1:B:917:MET:HG3	2.49	0.45
1:D:1042:MET:HE2	1:D:1062:LEU:HD12	1.99	0.45
1:A:893:MET:O	1:A:897:VAL:HG23	2.17	0.45
1:B:715:ARG:NH1	1:B:865:GLU:OE2	2.50	0.45
1:B:162:ALA:O	1:B:164:LEU:HG	2.17	0.45
1:B:1042:MET:CE	1:B:1078:TYR:HE2	2.29	0.45
1:B:593:LYS:O	1:B:597:VAL:HG23	2.17	0.45
1:A:641:MET:HE2	1:A:671:ILE:HG13	1.99	0.45
1:C:181:LYS:O	1:C:185:GLU:HG2	2.17	0.45
1:C:685:GLN:HE21	1:C:685:GLN:HA	1.82	0.45
1:D:798:VAL:CG1	1:D:835:SER:HA	2.47	0.45
1:D:647:ASN:ND2	1:D:647:ASN:C	2.60	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:B:144:GLU:HA	1:B:147:ASP:HB3	1.99	0.44
1:A:494:LEU:HD23	1:A:499:LYS:HZ2	1.82	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:A:490:ILE:H	1:A:490:ILE:HG13	1.64	0.44
1:D:524:TYR:CD2	1:D:843:THR:HG22	2.53	0.44
1:D:258:VAL:HG21	1:D:362:MET:HE2	1.99	0.44
1:B:811:ASN:HD22	1:B:811:ASN:N	2.11	0.44
1:D:798:VAL:HG13	1:D:835:SER:HA	1.98	0.44
1:D:397:TYR:N	1:D:414:GLN:HG3	2.32	0.44
1:C:1068:PRO:HD3	1:C:1074:ARG:CZ	2.47	0.44
1:D:704:ILE:HG21	1:D:723:TYR:HD2	1.82	0.44
1:C:580:THR:HB	1:C:614:VAL:HG21	1.98	0.44
1:B:908:THR:HA	1:B:909:PRO:HA	1.67	0.44
1:A:585:LYS:HG2	1:A:1034:ASP:HA	1.99	0.44
1:B:278:ALA:HA	1:B:279:PRO:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:MET:HE3	1:D:373:ALA:HB1	2.00	0.44
1:A:828:ILE:H	1:A:828:ILE:HG13	1.58	0.44
1:A:99:ILE:HG23	1:A:127:PHE:HD1	1.83	0.44
1:D:901:PHE:HZ	1:D:917:MET:HG3	1.81	0.44
1:C:908:THR:HA	1:C:909:PRO:HA	1.72	0.44
1:B:496:ARG:CD	1:B:496:ARG:H	2.31	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:D:345:VAL:O	1:D:348:GLN:HB2	2.18	0.44
1:A:156:ARG:HH11	1:A:166:VAL:HG11	1.83	0.44
1:B:1127:VAL:HA	1:B:1157:ILE:HG22	1.99	0.44
1:A:116:PRO:HB2	1:A:122:SER:HA	2.00	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:D:580:THR:HG22	1:D:611:THR:HG22	2.00	0.43
1:B:319:GLU:HG3	1:B:321:PHE:HE1	1.83	0.43
1:D:571:ARG:HH11	1:D:575:GLN:NE2	2.15	0.43
1:C:866:MET:CE	1:C:871:TYR:HA	2.48	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:B:1097:ASN:C	1:B:1099:ASN:H	2.21	0.43
1:B:690:ASN:O	1:B:694:GLN:HG2	2.19	0.43
1:B:1013:TYR:HB3	1:B:1016:VAL:HB	2.00	0.43
1:A:431:THR:HG21	1:A:443:MET:HA	2.00	0.43
1:A:829:GLU:HA	1:A:829:GLU:OE1	2.18	0.43
1:A:506:ASN:HD22	1:A:510:ASN:HD22	1.65	0.43
1:C:201:GLY:HA2	1:C:204:MET:CE	2.49	0.43
1:C:396:ALA:HB3	1:C:453:ARG:HH11	1.83	0.43
3:A:2000:BTI:H63	1:B:620:LYS:CG	2.49	0.43
1:D:156:ARG:HD2	1:D:166:VAL:HG11	1.99	0.43
1:A:1110:SER:O	1:A:1176:GLU:HA	2.18	0.43
1:C:873:ASN:HB3	3:D:2000:BTI:H83	2.00	0.43
1:D:524:TYR:HD2	1:D:843:THR:CG2	2.32	0.43
1:A:949:LYS:HB2	1:A:949:LYS:HE3	1.80	0.43
1:D:1108:ASN:HB2	1:D:1109:PRO:HD3	1.99	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:C:66:ILE:HB	1:C:86:VAL:HG21	2.01	0.43
1:A:1035:THR:HB	1:A:1036:PRO:HD3	2.00	0.43
1:A:593:LYS:O	1:A:597:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:622:ASN:HD21	1:D:624:TRP:HD1	1.67	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:D:653:ASN:HB3	1:D:982:LEU:HD11	2.01	0.43
1:D:252:ASP:HA	1:D:351:VAL:HG13	2.01	0.43
1:C:927:ASP:OD2	1:C:930:SER:HB2	2.18	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:1069:ASP:C	1:C:1071:ASN:H	2.20	0.43
1:C:711:LEU:HG	1:C:751:ALA:HB2	2.00	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:A:977:ARG:HA	1:A:978:PRO:HD3	1.90	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:D:360:ILE:HG22	1:D:362:MET:HG2	2.01	0.42
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: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:219:ARG:HG2	1:A:223:GLU:HG3	2.01	0.42
1:D:924:ASN:HB2	1:D:926:LEU:HD22	2.02	0.42
1:B:66:ILE:HB	1:B:86:VAL:CG2	2.49	0.42
1:B:59:LEU:HD22	1:B:350:LEU:HD21	2.01	0.42
1:A:274:VAL:HG12	1:A:275:VAL:HG23	2.01	0.42
1:D:999:GLN:HG2	1:D:1000:GLY:N	2.34	0.42
1:D:811:ASN:H	1:D:811:ASN:ND2	2.16	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:116:PRO:HB2	1:D:122:SER:HA	2.01	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:490:ILE:HG13	1:D:490:ILE:H	1.65	0.42
1:D:141:PRO:HB2	1:D:145:HIS:HB2	2.01	0.42
1:C:952:ILE:CG2	1:C:952:ILE:O	2.68	0.42
1:B:284:SER:OG	1:B:287:LEU:HB2	2.19	0.42
1:A:193:ILE:HD11	1:A:233:VAL:HB	2.02	0.42
1:B:977:ARG:HA	1:B:978:PRO:HD3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:631:ARG:HA	1:A:631:ARG:HD3	1.75	0.42
1:B:999:GLN:H	1:B:999:GLN:CD	2.23	0.42
1:A:1029:ASN:HD22	1:A:1029:ASN:C	2.22	0.42
1:D:952:ILE:HG23	1:D:952:ILE:O	2.19	0.42
1:C:200:GLY:C	1:C:202:LYS:N	2.73	0.42
1:D:484:THR:HB	1:D:487:LEU:HD22	2.01	0.42
1:B:542:LYS:HE2	1:B:631:ARG:CZ	2.49	0.42
1:D:869:GLY:O	1:D:871:TYR:N	2.52	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:C:575:GLN:NE2	1:C:610:ALA:H	2.18	0.42
1:B:701:GLU:HG2	1:B:737:ILE:HB	2.02	0.42
1:B:1000:GLY:H	1:B:1001:PRO:CD	2.15	0.41
1:A:263:ARG:NH2	1:A:330:GLN:HE21	2.17	0.41
1:D:504:ILE:HG21	1:D:1042:MET:HG3	2.02	0.41
1:D:1109:PRO:HB2	1:D:1111:HIS:CE1	2.55	0.41
1:A:384:LEU:HD11	1:A:490:ILE:HG12	2.02	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: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:C:907:VAL:O	1:C:910:SER:N	2.53	0.41
1:A:263:ARG:HH21	1:A:330:GLN:HE22	1.66	0.41
3:C:2000:BTI:H5	1:D:512:PHE:CZ	2.55	0.41
1:C:589:ASN:HD22	1:C:589:ASN:HA	1.69	0.41
1:B:811:ASN:ND2	1:B:811:ASN:N	2.68	0.41
1:C:338:MET:CE	1:C:430:SER:HB3	2.50	0.41
1:D:294:ALA:HA	1:D:297:GLN:HG3	2.01	0.41
1:B:91:GLY:HA2	1:B:92:PRO:HD2	1.89	0.41
1:C:530:PRO:HB2	1:C:593:LYS:HD3	2.02	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:1024:ARG:HG2	1:C:1024:ARG:HH11	1.85	0.41
1:C:571:ARG:HH11	1:C:575:GLN:HE22	1.66	0.41
1:A:678:ASP:OD2	1:A:685:GLN:NE2	2.54	0.41
1:A:864:HIS:CD2	1:A:866:MET:H	2.35	0.41
1:D:506:ASN:HD21	1:D:510:ASN:HD22	1.68	0.41
1:B:1135:GLN:HA	1:B:1136:PRO:HD2	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:MET:HE1	1:A:671:ILE:HD13	2.01	0.41
1:D:941:PRO:O	1:D:944:VAL:CG1	2.68	0.41
1:C:201:GLY:HA2	1:C:204:MET:HE2	2.01	0.41
1:C:854:ILE:H	1:C:854:ILE:HG13	1.71	0.41
1:A:313:LEU:HD13	1:A:323:ILE:HG13	2.02	0.41
1:C:174:ILE:CG2	1:C:175:LYS:N	2.83	0.41
1:B:396:ALA:HB3	1:B:453:ARG:HH11	1.86	0.41
1:B:641:MET:HE2	1:B:671:ILE:HG21	2.02	0.41
1:C:142:HIS:N	1:C:145:HIS:HD2	2.19	0.41
1:A:1008:ILE:HG13	1:A:1008:ILE:H	1.70	0.41
1:A:704:ILE:HG23	1:A:726:LEU:HD23	2.01	0.41
1:B:949:LYS:HG2	1:B:968:LEU:CD2	2.51	0.41
1:C:631:ARG:NH2	1:C:672:ASP:OD1	2.54	0.41
1:B:828:ILE:HG13	1:B:828:ILE:H	1.54	0.41
1:D:715:ARG:NH1	1:D:865:GLU:OE2	2.54	0.41
1:D:167:ILE:H	1:D:167:ILE:HG13	1.69	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:A:298:LEU:O	1:A:302:ILE:HG13	2.20	0.40
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:258:VAL:HG21	1:A:362:MET:HE2	2.02	0.40
1:B:506:ASN:ND2	1:B:510:ASN:ND2	2.69	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:D:622:ASN:ND2	1:D:624:TRP:H	2.20	0.40
1:B:909:PRO:HG2	1:B:952:ILE:HG12	2.04	0.40
1:A:118:TYR:OH	1:A:331:VAL:HG13	2.21	0.40
1:B:1108:ASN:HA	1:B:1109:PRO:HD2	1.94	0.40
1:C:256:ASN:C	1:C:257:ILE:HG13	2.41	0.40
1:C:537:ILE:HA	1:C:538(B):PHE:CD1	2.56	0.40
1:B:1164:ASN:H	1:B:1164:ASN:ND2	2.18	0.40
1:C:720:LEU:HD21	1:C:758:GLU:HG3	2.03	0.40
1:D:329:VAL:HG22	1:D:348:GLN:NE2	2.29	0.40
1:B:622:ASN:HA	1:B:623:PRO:HD2	1.86	0.40
1:D:913:VAL:HG13	1:D:944:VAL:HA	2.03	0.40
1:D:1135:GLN:HA	1:D:1136:PRO:HD2	1.93	0.40
1:C:574:HIS:CD2	1:C:580:THR:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:LYS:HB3	1:B:62:SER:HB3	2.03	0.40
1:C:972:GLU:HB2	1:C:973:ALA:H	1.70	0.40
1:D:991:ARG:NH2	1:D:1004:GLU:OE1	2.54	0.40
1:B:434:ILE:HG13	1:B:434:ILE:H	1.68	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%)	30	65
1	B	1070/1173 (91%)	999 (93%)	58 (5%)	13 (1%)	16	47
1	C	1063/1173 (91%)	980 (92%)	65 (6%)	18 (2%)	11	36
1	D	1061/1173 (90%)	980 (92%)	73 (7%)	8 (1%)	24	58
All	All	4327/4692 (92%)	4008 (93%)	273 (6%)	46 (1%)	17	50

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

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Mol	Chain	Res	Type
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
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%)	901 (92%)	79 (8%)	15	39
1	B	928/1006 (92%)	857 (92%)	71 (8%)	16	41
1	C	917/1006 (91%)	832 (91%)	85 (9%)	11	32
1	D	922/1006 (92%)	851 (92%)	71 (8%)	16	41
All	All	3747/4024 (93%)	3441 (92%)	306 (8%)	14	38

All (306) 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	179	LEU
1	A	196	THR
1	A	217	PHE
1	A	218	HIS
1	A	237	ARG
1	A	269	ARG
1	A	286	THR
1	A	287	LEU
1	A	306	ASN
1	A	313	LEU
1	A	318	ASP
1	A	329	VAL
1	A	335	ILE
1	A	386	ASP
1	A	427	VAL
1	A	434	ILE
1	A	440	GLU
1	A	445	ARG
1	A	494	LEU
1	A	496	ARG
1	A	506	ASN
1	A	518	LYS
1	A	526	LEU
1	A	542	LYS

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Mol	Chain	Res	Type
1	A	558	LYS
1	A	599	LYS
1	A	606	MET
1	A	607	TRP
1	A	622	ASN
1	A	631	ARG
1	A	649	VAL
1	A	707	THR
1	A	715	ARG
1	A	743	MET
1	A	761	SER
1	A	766	LEU
1	A	775	THR
1	A	781	LEU
1	A	798	VAL
1	A	828	ILE
1	A	852	SER
1	A	853	ASP
1	A	855	LYS
1	A	858	ASN
1	A	861	ILE
1	A	863	GLN
1	A	871	TYR
1	A	874	LEU
1	A	888	ASP
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	969	LYS
1	A	977	ARG
1	A	980	GLU
1	A	999	GLN
1	A	1008	ILE
1	A	1029	ASN
1	A	1064	THR
1	A	1080	MET
1	A	1085	ARG

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Mol	Chain	Res	Type
1	A	1089	ILE
1	A	1097	ASN
1	A	1115	GLN
1	A	1116	MET
1	A	1154	ASP
1	A	1167	THR
1	A	1177	ILE
1	B	36	GLN
1	B	39	LYS
1	B	44	ASN
1	B	47	GLU
1	B	69	ASN
1	B	75	LEU
1	B	108	GLN
1	B	156	ARG
1	B	241	ASN
1	B	269	ARG
1	B	281	VAL
1	B	287	LEU
1	B	328	ARG
1	B	357	LEU
1	B	377	ARG
1	B	417	GLU
1	B	437	LYS
1	B	458	ASN
1	B	475	ASP
1	B	490	ILE
1	B	496	ARG
1	B	506	ASN
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	617	ASN
1	B	631	ARG
1	B	632	LYS
1	B	647	ASN
1	B	649	VAL
1	B	652	LYS
1	B	660	HIS

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Mol	Chain	Res	Type
1	B	664	GLN
1	B	707	THR
1	B	715	ARG
1	B	717	ASN
1	B	743	MET
1	B	750	LYS
1	B	760	LYS
1	B	775	THR
1	B	781	LEU
1	B	784	LYS
1	B	811	ASN
1	B	821	PRO
1	B	828	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	962	ASP
1	B	996	GLU
1	B	1008	ILE
1	B	1029	ASN
1	B	1054	LYS
1	B	1085	ARG
1	B	1097	ASN
1	B	1111	HIS
1	B	1138	LEU
1	B	1143	MET
1	B	1148	THR
1	B	1154	ASP
1	B	1158	LYS
1	B	1177	ILE
1	C	44	ASN
1	C	45	ARG
1	C	77	ARG
1	C	90	LEU
1	C	94	GLU
1	C	95	SER

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Mol	Chain	Res	Type
1	C	97	LEU
1	C	98	ASN
1	C	100	GLU
1	C	126	GLN
1	C	175	LYS
1	C	189	PHE
1	C	193	ILE
1	C	205	ARG
1	C	230	ASN
1	C	237	ARG
1	C	262	GLU
1	C	268	GLN
1	C	269	ARG
1	C	287	LEU
1	C	323	ILE
1	C	329	VAL
1	C	335	ILE
1	C	365	LYS
1	C	377	ARG
1	C	398	ARG
1	C	406	ARG
1	C	434	ILE
1	C	437	LYS
1	C	456	LYS
1	C	464	ASN
1	C	494	LEU
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	606	MET
1	C	607	TRP
1	C	617	ASN
1	C	631	ARG
1	C	641	MET
1	C	647	ASN
1	C	649	VAL
1	C	652	LYS
1	C	668	LYS
1	C	707	THR

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Mol	Chain	Res	Type
1	C	717	ASN
1	C	721	GLU
1	C	743	MET
1	C	766	LEU
1	C	781	LEU
1	C	792	ASP
1	C	807	GLN
1	C	811	ASN
1	C	828	ILE
1	C	829	GLU
1	C	843	THR
1	C	855	LYS
1	C	874	LEU
1	C	875	SER
1	C	881	LEU
1	C	907	VAL
1	C	934	ASP
1	C	937	LYS
1	C	942	GLU
1	C	944	VAL
1	C	945	VAL
1	C	959	PHE
1	C	962	ASP
1	C	971	GLN
1	C	972	GLU
1	C	977	ARG
1	C	1022	GLN
1	C	1029	ASN
1	C	1044	ASN
1	C	1053	ASP
1	C	1054	LYS
1	C	1064	THR
1	C	1070	GLU
1	C	1085	ARG
1	C	1140	THR
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	101	ARG

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Mol	Chain	Res	Type
1	D	122	SER
1	D	137	LYS
1	D	160	ILE
1	D	166	VAL
1	D	167	ILE
1	D	262	GLU
1	D	283	LEU
1	D	306	ASN
1	D	329	VAL
1	D	335	ILE
1	D	386	ASP
1	D	398	ARG
1	D	427	VAL
1	D	434	ILE
1	D	469	LYS
1	D	487	LEU
1	D	489	ASP
1	D	490	ILE
1	D	491	GLN
1	D	525	GLU
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
1	D	647	ASN
1	D	649	VAL
1	D	707	THR
1	D	715	ARG
1	D	743	MET
1	D	766	LEU
1	D	775	THR
1	D	791	VAL
1	D	807	GLN
1	D	828	ILE
1	D	831	MET
1	D	843	THR
1	D	853	ASP
1	D	870	GLN
1	D	886	ARG

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Mol	Chain	Res	Type
1	D	895	ARG
1	D	907	VAL
1	D	912	LYS
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	977	ARG
1	D	996	GLU
1	D	1001	PRO
1	D	1056	LYS
1	D	1061	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	1153	PHE
1	D	1161	THR
1	D	1174	LEU

Some 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	145	HIS
1	A	241	ASN
1	A	254	HIS
1	A	256	ASN
1	A	272	GLN
1	A	297	GLN
1	A	330	GLN
1	A	432	HIS
1	A	506	ASN
1	A	543	GLN
1	A	574	HIS

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Mol	Chain	Res	Type
1	A	575	GLN
1	A	589	ASN
1	A	622	ASN
1	A	694	GLN
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	898	ASN
1	A	999	GLN
1	A	1005	GLN
1	A	1025	ASN
1	A	1026	GLN
1	A	1029	ASN
1	A	1044	ASN
1	A	1097	ASN
1	A	1099	ASN
1	A	1111	HIS
1	B	44	ASN
1	B	69	ASN
1	B	98	ASN
1	B	108	GLN
1	B	145	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	664	GLN
1	B	736	HIS
1	B	778	ASN
1	B	807	GLN
1	B	811	ASN
1	B	818	ASN
1	B	858	ASN

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Mol	Chain	Res	Type
1	B	864	HIS
1	B	873	ASN
1	B	876	GLN
1	B	877	GLN
1	B	898	ASN
1	B	923	GLN
1	B	971	GLN
1	B	1005	GLN
1	B	1025	ASN
1	B	1029	ASN
1	B	1111	HIS
1	C	44	ASN
1	C	145	HIS
1	C	230	ASN
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
1	C	617	ASN
1	C	622	ASN
1	C	653	ASN
1	C	685	GLN
1	C	717	ASN
1	C	736	HIS
1	C	778	ASN
1	C	811	ASN
1	C	863	GLN
1	C	877	GLN
1	C	898	ASN
1	C	1005	GLN
1	C	1025	ASN
1	C	1029	ASN
1	D	44	ASN
1	D	145	HIS
1	D	241	ASN
1	D	272	GLN
1	D	289	GLN
1	D	301	ASN

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Mol	Chain	Res	Type
1	D	326	ASN
1	D	330	GLN
1	D	364	GLN
1	D	432	HIS
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	617	ASN
1	D	622	ASN
1	D	647	ASN
1	D	660	HIS
1	D	685	GLN
1	D	736	HIS
1	D	778	ASN
1	D	811	ASN
1	D	864	HIS
1	D	873	ASN
1	D	898	ASN
1	D	957	ASN
1	D	960	ASN
1	D	1005	GLN
1	D	1019	GLN
1	D	1025	ASN
1	D	1044	ASN
1	D	1083	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates 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	A	2000	1	14,16,16	1.93	3 (21%)	13,21,21	1.41	2 (15%)
4	PYR	A	2001	-	2,5,5	1.86	1 (50%)	2,6,6	0.04	0
5	ATP	A	2100	-	24,33,33	1.00	2 (8%)	31,52,52	1.93	5 (16%)
3	BTI	B	2000	1	14,16,16	1.83	3 (21%)	13,21,21	1.55	2 (15%)
4	PYR	B	2001	-	2,5,5	1.83	1 (50%)	2,6,6	0.13	0
3	BTI	C	2000	1	14,16,16	1.91	3 (21%)	13,21,21	1.47	3 (23%)
4	PYR	C	2001	-	2,5,5	1.85	1 (50%)	2,6,6	0.03	0
5	ATP	C	2100	-	24,33,33	1.00	1 (4%)	31,52,52	1.87	4 (12%)
3	BTI	D	2000	1	14,16,16	1.86	3 (21%)	13,21,21	1.25	2 (15%)
4	PYR	D	2001	-	2,5,5	1.83	1 (50%)	2,6,6	0.44	0

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	A	2000	1	-	0/5/27/27	0/2/2/2
4	PYR	A	2001	-	-	0/0/4/4	0/0/0/0
5	ATP	A	2100	-	-	0/18/38/38	0/3/3/3
3	BTI	B	2000	1	-	0/5/27/27	0/2/2/2
4	PYR	B	2001	-	-	0/0/4/4	0/0/0/0
3	BTI	C	2000	1	-	0/5/27/27	0/2/2/2
4	PYR	C	2001	-	-	0/0/4/4	0/0/0/0
5	ATP	C	2100	-	-	0/18/38/38	0/3/3/3
3	BTI	D	2000	1	-	0/5/27/27	0/2/2/2
4	PYR	D	2001	-	-	0/0/4/4	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2000	BTI	C2-S1	-3.65	1.76	1.82
3	A	2000	BTI	C2-S1	-3.35	1.77	1.82
3	D	2000	BTI	C2-S1	-3.35	1.77	1.82
3	B	2000	BTI	C2-S1	-3.25	1.77	1.82
3	C	2000	BTI	C3-N2	-2.66	1.31	1.35
3	D	2000	BTI	C3-N3	-2.30	1.32	1.35
3	A	2000	BTI	C3-N2	-2.28	1.32	1.35
3	B	2000	BTI	C3-N3	-2.12	1.32	1.35
5	A	2100	ATP	O4'-C1'	2.07	1.43	1.41
4	D	2001	PYR	O3-C2	2.53	1.31	1.22
4	B	2001	PYR	O3-C2	2.56	1.31	1.22
4	C	2001	PYR	O3-C2	2.58	1.31	1.22
4	A	2001	PYR	O3-C2	2.60	1.31	1.22
5	A	2100	ATP	C5-C4	3.13	1.47	1.40
5	C	2100	ATP	C5-C4	3.20	1.47	1.40
3	C	2000	BTI	O3-C3	4.56	1.32	1.23
3	D	2000	BTI	O3-C3	4.92	1.33	1.23
3	B	2000	BTI	O3-C3	5.00	1.33	1.23
3	A	2000	BTI	O3-C3	5.04	1.33	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2100	ATP	N3-C2-N1	-7.23	123.36	128.89
5	C	2100	ATP	N3-C2-N1	-6.98	123.55	128.89
5	C	2100	ATP	PA-O3A-PB	-4.58	119.86	132.73
5	A	2100	ATP	C2'-C1'-N9	-3.44	109.04	114.29
5	A	2100	ATP	PA-O3A-PB	-3.31	123.43	132.73
5	A	2100	ATP	C4-C5-N7	-3.09	106.64	109.48
5	C	2100	ATP	C2'-C1'-N9	-2.91	109.85	114.29
5	C	2100	ATP	C4-C5-N7	-2.85	106.86	109.48
5	A	2100	ATP	PB-O3B-PG	-2.39	124.66	132.67
3	D	2000	BTI	O3-C3-N3	-2.26	123.28	125.90
3	B	2000	BTI	O3-C3-N3	-2.19	123.36	125.90
3	C	2000	BTI	C8-C7-C2	-2.13	108.76	113.70
3	C	2000	BTI	O3-C3-N2	-2.13	123.43	125.90
3	A	2000	BTI	O3-C3-N2	-2.05	123.52	125.90
3	D	2000	BTI	N2-C3-N3	2.65	110.71	108.88
3	C	2000	BTI	N2-C3-N3	3.44	111.26	108.88
3	A	2000	BTI	N2-C3-N3	3.48	111.28	108.88
3	B	2000	BTI	N2-C3-N3	3.72	111.45	108.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1137/1173 (96%)	-0.10	46 (4%)	42	30	30, 59, 122, 143	0
1	B	1074/1173 (91%)	-0.02	52 (4%)	34	23	39, 69, 119, 153	0
1	C	1067/1173 (90%)	-0.10	24 (2%)	65	54	38, 66, 103, 115	0
1	D	1067/1173 (90%)	-0.12	48 (4%)	37	26	28, 60, 113, 213	0
All	All	4345/4692 (92%)	-0.09	170 (3%)	43	31	28, 64, 114, 213	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	936	TYR	6.6
1	A	177	TYR	6.0
1	B	397	TYR	5.9
1	C	933	THR	5.7
1	A	1095	HIS	5.5
1	B	1095	HIS	5.5
1	B	457	THR	5.2
1	B	387	PHE	5.0
1	B	385	ASN	4.8
1	A	218	HIS	4.8
1	D	1128	GLY	4.7
1	D	1155	GLY	4.6
1	A	180	ALA	4.6
1	B	389	PRO	4.5
1	B	492	PRO	4.5
1	A	1156	VAL	4.4
1	B	393	THR	4.4
1	C	1140	THR	4.3
1	B	421	TYR	4.3
1	B	524	TYR	4.3
1	A	231	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	932	ILE	4.2
1	D	1154	ASP	4.2
1	B	270	ARG	4.1
1	A	216	ALA	4.1
1	A	176	SER	4.1
1	A	226	LYS	4.1
1	B	388	MET	4.0
1	B	271	HIS	4.0
1	D	1163	ASN	4.0
1	B	395	ILE	4.0
1	B	386	ASP	3.9
1	A	215	ASP	3.9
1	B	89	ASP	3.9
1	A	494	LEU	3.9
1	D	240	ASP	3.9
1	A	185	GLU	3.8
1	D	282	GLY	3.8
1	A	197	SER	3.8
1	B	384	LEU	3.8
1	B	526	LEU	3.8
1	B	454	GLY	3.7
1	D	1178	GLU	3.7
1	A	219	ARG	3.6
1	B	407	LEU	3.6
1	A	228	PHE	3.6
1	A	227	SER	3.6
1	A	999	GLN	3.6
1	A	189	PHE	3.6
1	B	1096	THR	3.5
1	A	222	SER	3.5
1	B	490	ILE	3.4
1	A	469	LYS	3.3
1	B	383	PRO	3.3
1	C	1001	PRO	3.3
1	D	386	ASP	3.3
1	B	90	LEU	3.2
1	B	402	GLY	3.2
1	C	416	ALA	3.2
1	B	525	GLU	3.2
1	B	240	ASP	3.2
1	C	176	SER	3.2
1	A	493	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	230	ASN	3.1
1	A	386	ASP	3.1
1	B	167	ILE	3.1
1	C	282	GLY	3.1
1	B	88	SER	3.1
1	C	970	GLY	3.1
1	D	1164	ASN	3.0
1	D	1156	VAL	3.0
1	B	91	GLY	3.0
1	A	1135	GLN	3.0
1	D	1130	THR	3.0
1	A	1128	GLY	3.0
1	B	92	PRO	2.9
1	C	89	ASP	2.9
1	C	492	PRO	2.9
1	A	1127	VAL	2.9
1	B	398	ARG	2.9
1	D	1165	GLY	2.8
1	D	271	HIS	2.8
1	A	526	LEU	2.8
1	D	1127	VAL	2.8
1	A	188	GLY	2.8
1	B	527	ALA	2.8
1	A	178	GLU	2.8
1	A	421	TYR	2.8
1	D	1177	ILE	2.8
1	A	417	GLU	2.7
1	D	239	ILE	2.7
1	B	1097	ASN	2.7
1	C	1070	GLU	2.7
1	A	1001	PRO	2.7
1	B	408	ASP	2.7
1	D	1103	LYS	2.7
1	C	493	SER	2.7
1	A	173	PRO	2.6
1	A	89	ASP	2.6
1	D	416	ALA	2.6
1	A	88	SER	2.6
1	B	403	PHE	2.6
1	C	218	HIS	2.6
1	D	1126	SER	2.6
1	B	493	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	1133	ALA	2.5
1	C	885	GLU	2.5
1	D	1105	ASP	2.5
1	C	178	GLU	2.5
1	B	415	GLY	2.5
1	B	394	ILE	2.5
1	B	1094	VAL	2.5
1	D	241	ASN	2.5
1	D	490	ILE	2.5
1	B	391	THR	2.5
1	D	1107	SER	2.5
1	B	409	ALA	2.5
1	B	494	LEU	2.5
1	B	491	GLN	2.5
1	B	157	THR	2.4
1	C	931	VAL	2.4
1	D	309	THR	2.4
1	B	981	TYR	2.4
1	A	496	ARG	2.4
1	A	175	LYS	2.4
1	C	202	LYS	2.3
1	B	418	ILE	2.3
1	D	1125	VAL	2.3
1	C	1147	THR	2.3
1	A	174	ILE	2.3
1	A	220	ALA	2.3
1	D	1166	ASP	2.3
1	D	1162	VAL	2.3
1	B	168	PRO	2.3
1	C	415	GLY	2.3
1	B	399	SER	2.3
1	D	1122	GLU	2.3
1	D	310	VAL	2.3
1	D	879	LYS	2.2
1	A	87	GLY	2.2
1	D	1109	PRO	2.2
1	D	421	TYR	2.2
1	D	1108	ASN	2.2
1	C	1142	ALA	2.2
1	D	247	VAL	2.2
1	D	494	LEU	2.2
1	D	1053	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	314	VAL	2.2
1	D	308	GLY	2.2
1	B	101	ARG	2.1
1	D	243	LYS	2.1
1	D	886	ARG	2.1
1	D	1121	THR	2.1
1	A	1158	LYS	2.1
1	A	492	PRO	2.1
1	C	456	LYS	2.1
1	C	183	PHE	2.1
1	D	1143	MET	2.1
1	D	91	GLY	2.1
1	A	479	LYS	2.1
1	A	1178	GLU	2.1
1	D	384	LEU	2.1
1	A	418	ILE	2.0
1	C	705	CYS	2.0
1	D	853	ASP	2.0
1	D	168	PRO	2.0
1	D	1136	PRO	2.0
1	B	303	LYS	2.0
1	A	207	VAL	2.0
1	B	400	SER	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PYR	D	2001	6/6	0.60	0.50	6.24	84,85,85,85	0
4	PYR	C	2001	6/6	0.92	0.50	5.43	84,85,85,85	0
4	PYR	A	2001	6/6	0.88	0.23	1.88	93,93,93,93	0
4	PYR	B	2001	6/6	0.88	0.24	0.83	89,90,91,91	0
2	MN	C	2002	1/1	0.94	0.29	0.58	79,79,79,79	0
3	BTI	A	2000	15/15	0.95	0.17	0.35	61,63,69,69	0
3	BTI	D	2000	15/15	0.91	0.19	0.21	75,75,76,77	0
5	ATP	A	2100	31/31	0.80	0.25	0.17	115,117,126,126	0
5	ATP	C	2100	31/31	0.87	0.21	-0.16	80,82,94,95	0
3	BTI	C	2000	15/15	0.98	0.14	-0.56	52,52,65,65	0
3	BTI	B	2000	15/15	0.97	0.12	-0.67	51,52,57,58	0
2	MN	B	2002	1/1	0.94	0.11	-1.39	94,94,94,94	0
2	MN	A	2002	1/1	0.92	0.14	-1.63	123,123,123,123	0
2	MN	D	2002	1/1	0.92	0.08	-2.44	85,85,85,85	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.