



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:09 AM GMT

PDB ID : 3HB9  
Title : Crystal Structure of S. aureus Pyruvate Carboxylase A610T Mutant  
Authors : Tong, L.; Yu, L.P.C.  
Deposited on : 2009-05-04  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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

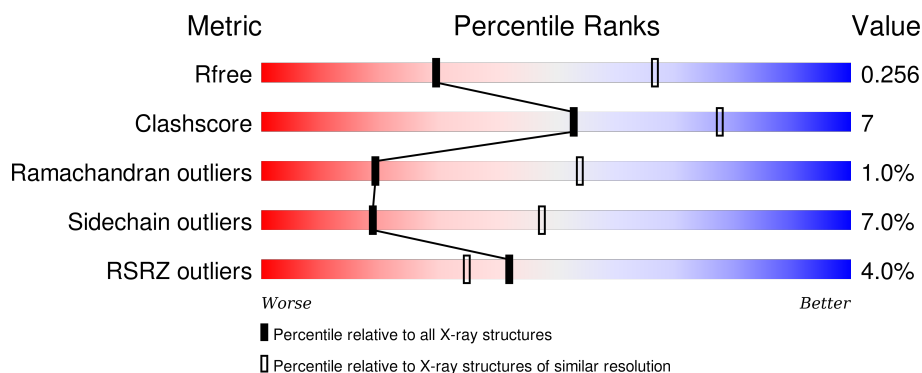
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1150	<div> <div>5%</div> <div>79% 17% ..</div> </div>
1	B	1150	<div> <div>4%</div> <div>75% 16% • 7%</div> </div>
1	C	1150	<div> <div>3%</div> <div>74% 16% • 7%</div> </div>
1	D	1150	<div> <div>3%</div> <div>70% 14% • 14%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33840 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.

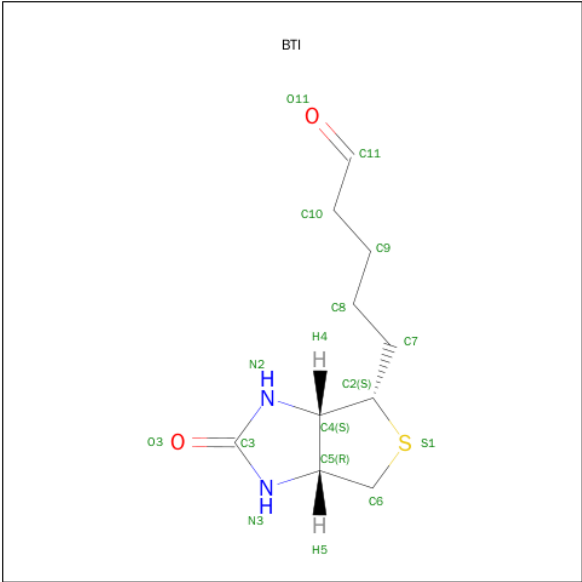
- Molecule 1 is a protein called Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1133	Total	C	N	O	S	0	0	0
			8942	5665	1505	1742	30			
1	B	1074	Total	C	N	O	S	0	0	0
			8467	5366	1427	1645	29			
1	C	1067	Total	C	N	O	S	0	0	0
			8443	5351	1421	1641	30			
1	D	993	Total	C	N	O	S	0	0	0
			7870	4995	1326	1521	28			

There are 4 discrepancies between the modelled and reference sequences:

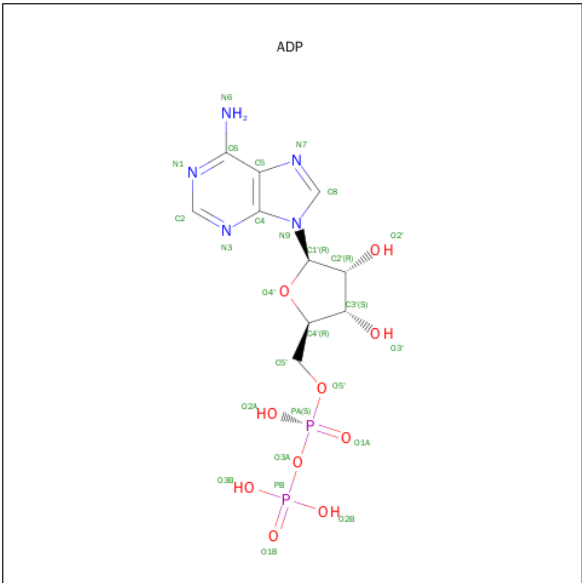
Chain	Residue	Modelled	Actual	Comment	Reference
A	610	THR	ALA	ENGINEERED	UNP Q99UY8
B	610	THR	ALA	ENGINEERED	UNP Q99UY8
C	610	THR	ALA	ENGINEERED	UNP Q99UY8
D	610	THR	ALA	ENGINEERED	UNP Q99UY8

- Molecule 2 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>S).



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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

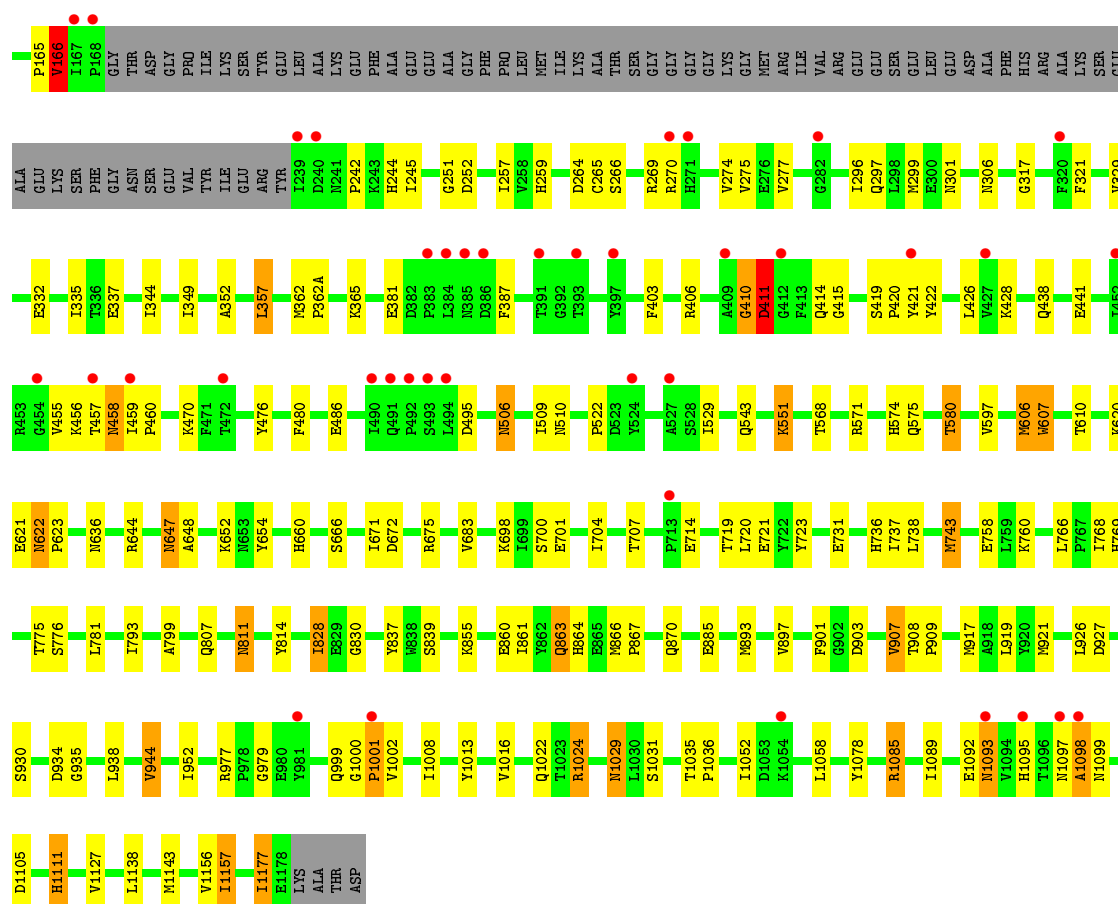


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

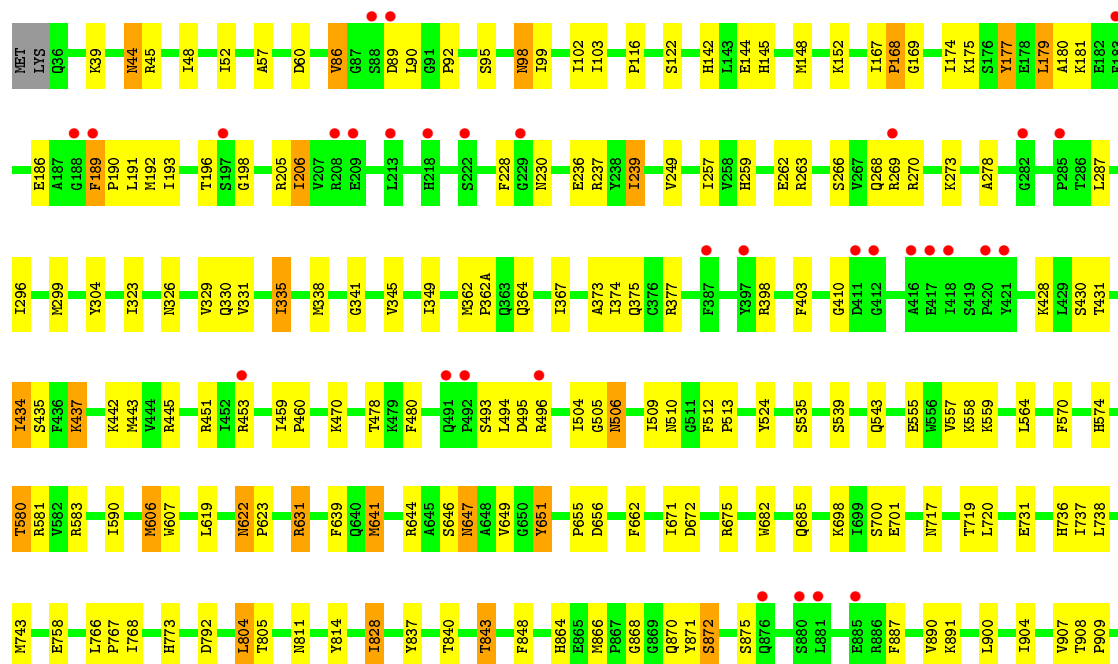
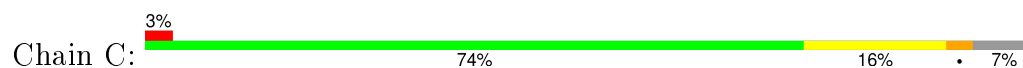
- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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





• Molecule 1: Pyruvate carboxylase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.57Å 256.76Å 126.48Å 90.00° 109.65° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.58 – 2.82	Depositor EDS
% Data completeness (in resolution range)	92.8 (30.00-2.90) 90.1 (29.58-2.82)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.220 , 0.266 0.213 , 0.256	Depositor DCC
$R_{free}$ test set	5983 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 30.3	EDS
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 124490 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	33840	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.34	0/9110	0.50	0/12324
1	B	0.33	0/8627	0.49	0/11678
1	C	0.33	0/8605	0.49	0/11630
1	D	0.33	0/8021	0.50	0/10848
All	All	0.33	0/34363	0.49	0/46480

There are no bond length outliers.

There are no bond angle outliers.

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	8942	0	8872	118	0
1	B	8467	0	8413	115	0
1	C	8443	0	8352	118	0
1	D	7870	0	7808	102	0
2	A	15	0	15	1	0
2	B	15	0	15	1	0
2	C	30	0	31	1	0
3	A	27	0	12	0	0
3	C	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	33840	0	33530	444	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 7.

All (444) 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:B:1024:ARG:HH11	1:B:1024:ARG:HG3	1.13	1.14
1:D:1085:ARG:HH11	1:D:1085:ARG:HG2	1.21	1.05
1:C:44:ASN:HD22	1:C:45:ARG:H	1.00	0.99
1:B:1000:GLY:H	1:B:1001:PRO:HD3	1.28	0.94
1:C:700:SER:H	1:C:736:HIS:HD2	1.16	0.94
1:A:44:ASN:HD22	1:A:45:ARG:H	1.13	0.93
1:B:1024:ARG:NH1	1:B:1024:ARG:HG3	1.90	0.85
1:D:44:ASN:HD22	1:D:45:ARG:H	1.24	0.84
1:A:700:SER:H	1:A:736:HIS:HD2	1.27	0.82
1:D:644:ARG:HH21	1:D:908:THR:HB	1.44	0.81
1:B:700:SER:H	1:B:736:HIS:HD2	1.25	0.81
1:D:700:SER:H	1:D:736:HIS:HD2	1.28	0.81
1:D:101:ARG:HH21	1:D:101:ARG:HG2	1.46	0.81
1:A:329:VAL:HG22	1:A:348:GLN:HE22	1.47	0.79
1:A:590:ILE:HG12	1:A:837:TYR:CE2	2.18	0.78
1:B:644:ARG:HH11	1:B:647:ASN:HD21	1.32	0.77
1:B:410:GLY:O	1:B:411:ASP:HB2	1.83	0.77
1:C:98:ASN:O	1:C:102:ILE:HG12	1.86	0.76
1:A:811:ASN:HD22	1:A:811:ASN:H	1.31	0.76
1:B:917:MET:HG2	1:B:944:VAL:HG11	1.66	0.76
1:C:700:SER:H	1:C:736:HIS:CD2	2.03	0.76
1:B:1024:ARG:HH11	1:B:1024:ARG:CG	1.94	0.76
1:A:864:HIS:HD2	1:A:866:MET:H	1.34	0.75
1:A:164:LEU:HD11	1:A:298:LEU:HB2	1.68	0.74
1:A:1115:GLN:H	1:A:1115:GLN:CD	1.92	0.73
1:B:48:ILE:O	1:B:52:ILE:HG12	1.89	0.73
1:B:44:ASN:HD22	1:B:45:ARG:H	1.35	0.72
1:C:44:ASN:ND2	1:C:45:ARG:H	1.82	0.72
1:D:743:MET:HG3	1:D:907:VAL:HG13	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:ARG:HD2	1:B:647:ASN:HD21	1.52	0.71
1:B:156:ARG:HE	1:B:166:VAL:HG21	1.53	0.71
1:B:551:LYS:H	1:B:551:LYS:HD3	1.54	0.71
1:D:644:ARG:HH11	1:D:647:ASN:HD21	1.38	0.71
1:D:720:LEU:HD21	1:D:758:GLU:HG3	1.71	0.71
1:A:335:ILE:HD13	1:A:375:GLN:HB2	1.74	0.70
1:C:590:ILE:HG12	1:C:837:TYR:CE2	2.27	0.70
1:A:999:GLN:HG2	1:A:1001:PRO:HD2	1.74	0.69
1:D:864:HIS:HD2	1:D:866:MET:H	1.40	0.69
1:C:672:ASP:HA	1:C:698:LYS:HD2	1.74	0.69
1:D:776:SER:HB3	1:D:861:ILE:HD11	1.73	0.69
1:C:48:ILE:O	1:C:52:ILE:HG12	1.91	0.69
1:D:48:ILE:O	1:D:52:ILE:HG12	1.92	0.69
1:B:811:ASN:H	1:B:811:ASN:HD22	1.40	0.69
1:B:1000:GLY:N	1:B:1001:PRO:HD3	2.06	0.68
1:D:917:MET:HG2	1:D:944:VAL:HG21	1.76	0.68
1:D:44:ASN:HD22	1:D:45:ARG:N	1.91	0.68
1:B:458:ASN:H	1:B:458:ASN:HD22	1.42	0.66
1:D:90:LEU:HD11	1:D:98:ASN:HD22	1.59	0.66
1:C:864:HIS:HD2	1:C:866:MET:H	1.43	0.66
1:D:644:ARG:NH2	1:D:908:THR:HB	2.10	0.66
1:D:1085:ARG:CG	1:D:1085:ARG:HH11	2.05	0.66
1:A:44:ASN:ND2	1:A:45:ARG:H	1.90	0.65
1:A:898:ASN:ND2	1:A:906:LYS:HE3	2.11	0.65
1:A:701:GLU:HG2	1:A:737:ILE:HB	1.78	0.65
1:A:144:GLU:O	1:A:148:MET:HB2	1.98	0.64
1:B:142:HIS:H	1:B:145:HIS:HD2	1.46	0.64
1:A:491:GLN:HE21	1:A:491:GLN:H	1.45	0.64
1:B:864:HIS:HD2	1:B:866:MET:H	1.47	0.63
1:D:1085:ARG:NH1	1:D:1085:ARG:HG2	2.01	0.63
1:C:326:ASN:HD22	1:C:330:GLN:NE2	1.97	0.63
1:C:641:MET:HG2	1:C:671:ILE:HG21	1.81	0.62
1:A:313:LEU:HD13	1:A:323:ILE:HG13	1.81	0.62
1:B:672:ASP:HA	1:B:698:LYS:HD2	1.82	0.62
1:A:901:PHE:HZ	1:A:917:MET:HG3	1.65	0.62
1:A:620:LYS:HG2	1:A:1023:THR:HG21	1.81	0.62
1:D:269:ARG:HD2	1:D:270:ARG:HG3	1.82	0.62
1:C:574:HIS:HD2	1:C:580:THR:HA	1.65	0.61
1:B:901:PHE:HZ	1:B:917:MET:HG3	1.66	0.61
1:B:675:ARG:HA	1:B:701:GLU:HB2	1.82	0.61
1:A:935:GLY:HA3	1:A:966:VAL:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:ILE:HD11	1:D:344:ILE:HG23	1.83	0.61
1:C:434:ILE:HD13	1:C:434:ILE:H	1.66	0.61
1:D:329:VAL:HG22	1:D:348:GLN:HE22	1.66	0.60
1:D:814:TYR:CE2	1:D:828:ILE:HG12	2.36	0.60
1:B:1105:ASP:H	1:B:1111:HIS:HD2	1.49	0.60
1:D:960:ASN:HD22	1:D:963:LEU:H	1.46	0.60
1:C:814:TYR:CE2	1:C:828:ILE:HG12	2.35	0.60
1:D:935:GLY:HA3	1:D:966:VAL:HG13	1.83	0.60
1:C:335:ILE:HD13	1:C:375:GLN:HB2	1.84	0.60
1:B:644:ARG:HD2	1:B:647:ASN:ND2	2.16	0.59
1:D:337:GLU:HG2	1:D:344:ILE:HG12	1.82	0.59
1:A:64:VAL:HG22	1:A:82:GLU:HB2	1.85	0.59
1:B:1105:ASP:H	1:B:1111:HIS:CD2	2.19	0.59
1:B:337:GLU:HG2	1:B:344:ILE:HG12	1.84	0.59
1:C:403:PHE:O	1:C:442:LYS:HE3	2.03	0.59
1:D:901:PHE:HZ	1:D:917:MET:HG3	1.68	0.59
1:B:543:GLN:HE22	1:B:636:ASN:HA	1.68	0.59
1:D:539:SER:HA	1:D:543:GLN:HG3	1.84	0.59
1:A:311:GLU:OE1	1:A:326:ASN:ND2	2.36	0.58
1:A:145:HIS:HE1	1:A:302:ILE:O	1.85	0.58
1:D:1058:LEU:HD23	1:D:1060:ILE:HD11	1.85	0.58
1:C:871:TYR:O	1:C:872:SER:HB2	2.03	0.58
1:B:743:MET:HG3	1:B:907:VAL:HG13	1.85	0.58
1:A:901:PHE:CZ	1:A:917:MET:HG3	2.38	0.58
1:C:647:ASN:N	1:C:647:ASN:OD1	2.37	0.58
1:C:86:VAL:HG11	1:C:102:ILE:HD13	1.85	0.58
1:B:299:MET:HA	1:B:299:MET:HE2	1.85	0.58
1:C:44:ASN:HD22	1:C:45:ARG:N	1.85	0.58
1:B:1000:GLY:H	1:B:1001:PRO:CD	2.11	0.58
1:D:543:GLN:HE21	1:D:636:ASN:HA	1.67	0.58
1:D:949:LYS:HE3	1:D:971:GLN:OE1	2.04	0.58
1:C:1059:ILE:H	1:C:1081:ASN:HD21	1.52	0.57
1:A:142:HIS:H	1:A:145:HIS:HD2	1.51	0.57
1:B:144:GLU:O	1:B:148:MET:HB3	2.04	0.57
1:D:935:GLY:HA3	1:D:966:VAL:CG1	2.35	0.57
1:A:622:ASN:HD22	1:A:623:PRO:HD2	1.70	0.57
1:A:672:ASP:HA	1:A:698:LYS:HD2	1.86	0.57
1:D:901:PHE:CZ	1:D:917:MET:HG3	2.40	0.57
1:C:398:ARG:HB3	1:C:451:ARG:HB2	1.85	0.57
1:C:656:ASP:OD1	1:C:977:ARG:NH2	2.37	0.57
1:D:590:ILE:HG12	1:D:837:TYR:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ASP:HB3	1:B:357:LEU:HD23	1.86	0.56
1:B:1095:HIS:HB3	1:B:1098:ALA:HB3	1.85	0.56
1:D:647:ASN:HD22	1:D:647:ASN:C	2.07	0.56
1:A:675:ARG:HA	1:A:701:GLU:HB2	1.87	0.56
1:C:644:ARG:HD2	1:C:647:ASN:OD1	2.04	0.56
1:B:935:GLY:HA2	1:B:938:LEU:HD12	1.86	0.56
1:D:622:ASN:ND2	1:D:624:TRP:H	2.04	0.56
1:B:622:ASN:HD22	1:B:623:PRO:HD2	1.70	0.56
1:A:575:GLN:NE2	1:A:610:THR:H	2.02	0.56
1:D:357:LEU:HA	1:D:360:ILE:HB	1.88	0.56
1:C:174:ILE:HG21	1:C:180:ALA:HB2	1.87	0.56
1:A:1105:ASP:H	1:A:1111:HIS:HD2	1.53	0.56
1:A:606:MET:HE1	1:A:639:PHE:HB3	1.86	0.56
1:D:506:ASN:ND2	1:D:510:ASN:HD22	2.04	0.56
1:D:287:LEU:HD22	1:D:291:ILE:HD11	1.88	0.56
1:D:44:ASN:ND2	1:D:45:ARG:H	2.00	0.55
1:D:101:ARG:HH21	1:D:101:ARG:CG	2.18	0.55
1:C:871:TYR:O	1:C:872:SER:CB	2.54	0.55
1:A:77:ARG:HH22	1:C:1057:ARG:HD2	1.71	0.55
1:A:446:SER:O	1:A:450:MET:HG2	2.05	0.55
1:C:152:LYS:H	1:C:196:THR:HG23	1.71	0.55
1:C:811:ASN:H	1:C:811:ASN:HD22	1.54	0.55
1:B:149:PHE:HA	1:B:155:ALA:HB2	1.88	0.55
1:D:408:ASP:HB2	1:D:428:LYS:HB3	1.89	0.55
1:C:622:ASN:HD22	1:C:623:PRO:HD2	1.70	0.55
1:C:651:TYR:HD1	1:C:651:TYR:H	1.53	0.55
1:D:701:GLU:HG2	1:D:737:ILE:HB	1.89	0.55
1:D:675:ARG:HA	1:D:701:GLU:HB2	1.89	0.54
1:C:191:LEU:HD23	1:C:237:ARG:HA	1.87	0.54
1:C:169:GLY:HA2	1:C:236:GLU:HA	1.88	0.54
1:B:738:LEU:HD23	1:B:768:ILE:HG12	1.89	0.54
1:B:769:HIS:CD2	1:B:793:ILE:HB	2.42	0.54
1:C:606:MET:HE1	1:C:639:PHE:HB3	1.90	0.54
1:B:41:LEU:HB3	1:B:114:ILE:HG12	1.88	0.54
1:C:375:GLN:NE2	1:C:428:LYS:HD3	2.23	0.54
1:C:453:ARG:HH11	1:C:453:ARG:HB2	1.73	0.54
1:A:791:VAL:O	1:A:822:ARG:NH2	2.36	0.54
1:D:828:ILE:O	1:D:832:GLU:HG2	2.08	0.53
1:C:917:MET:O	1:C:921:MET:HB2	2.07	0.53
1:C:338:MET:HE3	1:C:373:ALA:HB1	1.90	0.53
1:C:700:SER:N	1:C:736:HIS:HD2	1.97	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1013:TYR:HB3	1:D:1016:VAL:HB	1.89	0.53
1:B:40:LEU:HD11	1:B:349:ILE:HD12	1.90	0.53
1:A:811:ASN:H	1:A:811:ASN:ND2	2.02	0.53
1:D:571:ARG:HH11	1:D:575:GLN:NE2	2.06	0.53
1:D:840:THR:O	1:D:843:THR:HB	2.09	0.53
1:D:690:ASN:O	1:D:694:GLN:HG2	2.08	0.53
1:C:655:PRO:HG2	1:C:985:VAL:HG23	1.91	0.52
1:D:561:ASP:O	1:D:822:ARG:HD2	2.10	0.52
1:A:278:ALA:HB3	1:A:335:ILE:HG23	1.91	0.52
1:A:90:LEU:HD12	1:A:98:ASN:HD22	1.74	0.52
1:C:494:LEU:HB3	1:C:496:ARG:NH1	2.24	0.52
1:A:149:PHE:HA	1:A:155:ALA:HB2	1.90	0.52
1:A:345:VAL:O	1:A:348:GLN:HB2	2.10	0.52
1:C:570:PHE:O	1:C:574:HIS:HE1	1.92	0.52
1:C:828:ILE:H	1:C:828:ILE:HD12	1.73	0.52
1:B:1127:VAL:HA	1:B:1157:ILE:HG22	1.91	0.52
1:A:828:ILE:HD12	1:A:829:GLU:H	1.74	0.52
1:B:1052:ILE:HD11	1:B:1058:LEU:HG	1.92	0.52
1:B:1078:TYR:HB2	1:B:1085:ARG:HB3	1.91	0.52
1:A:174:ILE:HD12	1:A:179:LEU:HD11	1.91	0.52
1:C:144:GLU:O	1:C:148:MET:HB2	2.10	0.52
1:A:866:MET:HE2	1:A:870:GLN:HG2	1.91	0.52
1:C:890:VAL:HG22	1:C:922:VAL:HG21	1.92	0.52
1:B:1177:ILE:N	1:B:1177:ILE:HD13	2.25	0.52
1:B:867:PRO:O	1:B:870:GLN:HB2	2.10	0.52
1:C:539:SER:HA	1:C:543:GLN:HG3	1.92	0.51
1:B:860:GLU:O	1:B:863:GLN:HG2	2.11	0.51
1:A:575:GLN:HE22	1:A:610:THR:H	1.58	0.51
1:D:631:ARG:NH2	1:D:672:ASP:OD1	2.43	0.51
1:C:574:HIS:CD2	1:C:580:THR:HA	2.44	0.51
1:C:871:TYR:HE1	1:C:891:LYS:HD3	1.74	0.51
1:B:99:ILE:HG23	1:B:127:PHE:HD1	1.76	0.51
1:B:406:ARG:HD3	1:D:404:GLY:H	1.75	0.51
1:C:335:ILE:HD11	1:C:374:ILE:C	2.30	0.51
1:A:606:MET:HE1	1:A:671:ILE:HD13	1.92	0.51
1:A:274:VAL:HG12	1:A:275:VAL:HG23	1.93	0.51
1:B:1022:GLN:HE21	1:B:1022:GLN:HA	1.75	0.51
1:A:717(A):ILE:HG12	1:A:957:ASN:OD1	2.11	0.51
1:D:334:THR:HB	1:D:375:GLN:NE2	2.25	0.51
1:A:192:MET:HB2	1:A:238:TYR:HB2	1.91	0.51
1:D:64:VAL:HG22	1:D:82:GLU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:977:ARG:HG3	1:D:980:GLU:HG3	1.93	0.51
1:B:814:TYR:CZ	1:B:828:ILE:HG12	2.46	0.51
1:A:207:VAL:HG13	1:A:212:GLU:HB3	1.92	0.51
1:C:505:GLY:O	1:C:509:ILE:HG12	2.10	0.50
1:C:701:GLU:HG2	1:C:737:ILE:HB	1.94	0.50
1:B:909:PRO:HG2	1:B:952:ILE:HD12	1.93	0.50
1:B:411:ASP:HB3	1:B:426:LEU:HD23	1.94	0.50
1:B:266:SER:HB2	1:B:476:TYR:HE2	1.75	0.50
1:C:116:PRO:HB2	1:C:122:SER:HA	1.94	0.50
1:B:244:HIS:HD2	1:B:265:CYS:HB2	1.77	0.50
1:A:329:VAL:HG22	1:A:348:GLN:NE2	2.20	0.50
1:B:381:GLU:HB3	1:B:387:PHE:HA	1.94	0.50
1:B:927:ASP:H	1:B:930:SER:HB2	1.77	0.50
1:D:622:ASN:C	1:D:622:ASN:HD22	2.15	0.49
1:B:406:ARG:HD3	1:D:403:PHE:HA	1.94	0.49
1:D:581:ARG:HG3	1:D:848:PHE:CG	2.47	0.49
1:B:42:VAL:HG12	1:B:44:ASN:H	1.77	0.49
1:A:370:LEU:O	1:A:432:HIS:HE1	1.95	0.49
1:B:720:LEU:HD21	1:B:758:GLU:HG3	1.95	0.49
1:B:1035:THR:HB	1:B:1036:PRO:HD3	1.94	0.49
1:C:1042:MET:HB3	1:C:1062:LEU:HD13	1.94	0.49
1:A:858:ASN:HD21	1:A:860:GLU:HB2	1.77	0.49
1:C:364:GLN:HA	1:C:367:ILE:HD12	1.93	0.49
1:B:652:LYS:HG2	1:B:654:TYR:CZ	2.48	0.49
1:A:313:LEU:HB2	1:A:323:ILE:HD11	1.94	0.49
1:D:622:ASN:HD22	1:D:623:PRO:N	2.11	0.49
1:B:811:ASN:ND2	1:B:811:ASN:H	2.07	0.48
1:C:99:ILE:O	1:C:103:ILE:HG12	2.13	0.48
1:A:1116:MET:HB2	1:A:1117:PRO:CD	2.43	0.48
1:C:583:ARG:HG2	1:C:619:LEU:HD22	1.95	0.48
1:A:335:ILE:HD12	1:A:338:MET:HE2	1.96	0.48
1:A:1013:TYR:HB3	1:A:1016:VAL:HB	1.94	0.48
1:D:99:ILE:HG23	1:D:127:PHE:HD1	1.77	0.48
1:D:811:ASN:HD22	1:D:811:ASN:H	1.61	0.48
1:A:814:TYR:CE2	1:A:828:ILE:HG12	2.48	0.48
1:A:278:ALA:CB	1:A:335:ILE:HG23	2.44	0.48
1:B:1029:ASN:HD22	1:B:1029:ASN:C	2.17	0.48
1:D:672:ASP:HA	1:D:698:LYS:HD2	1.95	0.48
1:B:1013:TYR:HB3	1:B:1016:VAL:HB	1.94	0.48
1:A:434:ILE:HG12	1:C:341:GLY:O	2.13	0.48
1:A:1033:LEU:HD23	1:A:1050:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:572:ASP:HB3	1:D:807:GLN:NE2	2.27	0.48
1:A:413:PHE:HE1	1:A:416:ALA:HB3	1.77	0.48
1:A:590:ILE:HD11	1:A:838:TRP:CZ2	2.48	0.48
1:D:631:ARG:HG2	1:D:670:GLY:HA3	1.96	0.48
1:B:266:SER:HB2	1:B:476:TYR:CE2	2.49	0.48
1:A:431:THR:HG21	1:A:443:MET:HA	1.96	0.48
1:A:585:LYS:HE2	1:A:589:ASN:HD21	1.78	0.48
1:B:529:ILE:HG12	1:B:837:TYR:HE1	1.79	0.48
1:A:41:LEU:HB3	1:A:114:ILE:HG12	1.95	0.48
1:B:893:MET:O	1:B:897:VAL:HG23	2.14	0.47
1:A:42:VAL:HG11	1:A:49:ALA:HA	1.96	0.47
1:D:274:VAL:HG12	1:D:275:VAL:HG23	1.96	0.47
1:A:394:ILE:HD11	1:A:418:ILE:HD11	1.95	0.47
1:C:174:ILE:HG23	1:C:179:LEU:HB3	1.96	0.47
1:A:219:ARG:HB3	1:A:223:GLU:HB2	1.95	0.47
1:D:787:ILE:HA	1:D:791:VAL:HG12	1.96	0.47
1:C:331:VAL:HG12	1:C:428:LYS:HE2	1.97	0.47
1:A:470:LYS:HB3	1:A:480:PHE:HE1	1.80	0.47
1:C:606:MET:CE	1:C:639:PHE:HB3	2.45	0.47
1:D:563:VAL:HG21	1:D:787:ILE:HG12	1.96	0.47
1:C:1059:ILE:H	1:C:1081:ASN:ND2	2.13	0.47
1:C:142:HIS:HB2	1:C:145:HIS:CD2	2.49	0.47
1:A:743:MET:HG3	1:A:907:VAL:HG13	1.97	0.47
1:A:189:PHE:HB3	1:A:208:ARG:HE	1.79	0.47
1:D:799:ALA:H	1:D:811:ASN:ND2	2.13	0.46
1:C:506:ASN:ND2	1:C:510:ASN:HD22	2.12	0.46
1:A:378:ILE:HB	1:A:427:VAL:HG23	1.97	0.46
1:A:866:MET:CE	1:A:870:GLN:HG2	2.45	0.46
1:A:606:MET:CE	1:A:639:PHE:HB3	2.46	0.46
1:A:1060:ILE:HG12	1:A:1080:MET:HG2	1.96	0.46
1:C:1085:ARG:HH11	1:C:1085:ARG:CG	2.27	0.46
1:B:799:ALA:H	1:B:811:ASN:ND2	2.13	0.46
1:C:875:SER:HA	1:C:887:PHE:CE1	2.50	0.46
1:A:505:GLY:O	1:A:509:ILE:HG12	2.16	0.46
1:A:620:LYS:HB2	2:B:2000:BTI:H63	1.97	0.46
1:B:977:ARG:HG2	1:B:979:GLY:H	1.81	0.46
1:B:506:ASN:ND2	1:B:510:ASN:HD22	2.14	0.46
1:B:606:MET:HE3	1:B:607:TRP:HB2	1.97	0.46
1:C:263:ARG:HG2	1:C:278:ALA:HB2	1.97	0.46
1:B:666:SER:HB3	1:B:671:ILE:HD13	1.98	0.46
1:D:395:ILE:HD12	1:D:1085:ARG:HH22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:917:MET:HG2	1:A:944:VAL:HG11	1.97	0.46
1:D:645:ALA:HB1	1:D:685:GLN:O	2.16	0.46
1:C:675:ARG:HA	1:C:701:GLU:HB2	1.97	0.46
1:A:1127:VAL:HA	1:A:1157:ILE:HG22	1.98	0.46
1:A:787:ILE:HA	1:A:791:VAL:HG12	1.97	0.46
2:A:2000:BTI:H63	1:B:620:LYS:CG	2.46	0.46
1:C:167:ILE:HG12	1:C:239:ILE:HD11	1.98	0.46
1:A:896:ARG:HD2	1:A:928:GLU:OE2	2.16	0.45
1:C:682:TRP:CE3	1:C:685:GLN:HG3	2.51	0.45
1:B:731:GLU:HG3	1:B:766:LEU:HD13	1.98	0.45
1:C:1013:TYR:HB3	1:C:1016:VAL:HB	1.99	0.45
1:B:701:GLU:HG2	1:B:737:ILE:HB	1.98	0.45
1:D:543:GLN:NE2	1:D:636:ASN:HA	2.31	0.45
1:B:406:ARG:CZ	1:B:406:ARG:HA	2.46	0.45
1:C:921:MET:HG3	1:C:926:LEU:HD23	1.98	0.45
1:B:99:ILE:H	1:B:99:ILE:HD12	1.81	0.45
1:D:275:VAL:HG11	1:D:466:MET:HE1	1.97	0.45
1:B:165:PRO:HG2	1:B:321:PHE:HA	1.99	0.45
1:C:662:PHE:HA	1:C:1008:ILE:HD13	1.98	0.45
1:B:700:SER:H	1:B:736:HIS:CD2	2.17	0.45
1:C:504:ILE:HD12	1:C:1037:THR:HG22	1.99	0.45
1:A:543:GLN:HE22	1:A:636:ASN:HA	1.81	0.45
1:D:332:GLU:O	1:D:335:ILE:HG22	2.15	0.45
1:A:362(A):PRO:HG2	1:A:367:ILE:HG12	1.98	0.45
1:C:152:LYS:HE3	1:C:198:GLY:H	1.81	0.45
1:A:1120:VAL:HG21	1:A:1162:VAL:HB	1.99	0.45
1:A:811:ASN:ND2	1:A:811:ASN:N	2.65	0.45
1:D:924:ASN:HB2	1:D:926:LEU:HD22	1.97	0.44
1:B:459:ILE:N	1:B:460:PRO:HD2	2.32	0.44
1:A:840:THR:O	1:A:843:THR:HB	2.17	0.44
1:D:927:ASP:HB3	1:D:930:SER:H	1.82	0.44
1:A:935:GLY:HA3	1:A:966:VAL:CG1	2.46	0.44
1:D:524:TYR:CD2	1:D:843:THR:HG22	2.52	0.44
1:A:521:LYS:HA	1:A:522:PRO:HD3	1.86	0.44
1:B:814:TYR:CE2	1:B:828:ILE:HG12	2.52	0.44
1:D:116:PRO:HB2	1:D:122:SER:HA	1.98	0.44
1:D:717(A):ILE:HG13	1:D:957:ASN:OD1	2.17	0.44
1:C:504:ILE:HG21	1:C:1042:MET:CE	2.48	0.44
1:A:500:THR:O	1:A:504:ILE:HG12	2.17	0.44
1:B:864:HIS:CD2	1:B:866:MET:HG3	2.52	0.44
1:B:704:ILE:HG21	1:B:723:TYR:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:GLY:O	1:B:306:ASN:N	2.46	0.44
1:B:53:PHE:CZ	1:B:65:ALA:HB2	2.53	0.44
1:C:206:ILE:H	1:C:206:ILE:HD13	1.83	0.44
1:C:453:ARG:NH1	1:C:453:ARG:HB2	2.31	0.44
1:B:571:ARG:HH11	1:B:575:GLN:NE2	2.16	0.44
1:D:622:ASN:HD22	1:D:623:PRO:CD	2.30	0.44
1:D:622:ASN:HD22	1:D:623:PRO:HD2	1.83	0.44
1:D:443:MET:HG2	1:D:466:MET:SD	2.58	0.44
1:D:249:VAL:HG21	1:D:299:MET:HG3	2.00	0.44
2:C:2000:BTI:H63	1:D:620:LYS:HB2	2.00	0.44
1:A:828:ILE:O	1:A:832:GLU:HG2	2.18	0.43
1:A:1074:ARG:NH1	1:A:1091:ASP:OD2	2.47	0.43
1:C:459:ILE:HB	1:C:460:PRO:HD3	1.99	0.43
1:D:498:THR:OG1	1:D:1085:ARG:NH2	2.50	0.43
1:C:375:GLN:HG3	1:C:430:SER:OG	2.18	0.43
1:B:760:LYS:HG2	1:B:768:ILE:HD12	2.00	0.43
1:D:257:ILE:HD13	1:D:300:GLU:HA	2.00	0.43
1:C:435:SER:HB2	1:C:437:LYS:HE3	2.00	0.43
1:C:890:VAL:HA	1:C:922:VAL:HG21	2.00	0.43
1:C:964:GLN:O	1:C:968:LEU:HG	2.19	0.43
1:D:494:LEU:H	1:D:494:LEU:HD23	1.83	0.43
1:B:568:THR:OG1	1:B:807:GLN:HG3	2.18	0.43
1:D:334:THR:HB	1:D:375:GLN:HE22	1.84	0.43
1:D:620:LYS:HG2	1:D:1023:THR:HG21	2.00	0.43
1:A:719:THR:HG22	1:A:721:GLU:H	1.83	0.43
1:C:89:ASP:HB2	1:C:90:LEU:HD12	2.01	0.43
1:C:773:HIS:ND1	1:C:805:THR:O	2.47	0.43
1:C:249:VAL:HG11	1:C:299:MET:HG3	2.00	0.43
1:C:437:LYS:HD3	1:C:437:LYS:H	1.83	0.43
1:A:772:THR:HG22	1:A:783:TYR:CZ	2.54	0.43
1:A:406:ARG:HA	1:A:406:ARG:NE	2.34	0.43
1:C:259:HIS:HB3	1:C:296:ILE:HD11	2.00	0.43
1:B:621:GLU:HB2	1:B:1031:SER:HB3	2.01	0.43
1:A:331:VAL:HG12	1:A:428:LYS:HD2	2.00	0.43
1:C:606:MET:HE1	1:C:671:ILE:HD13	2.00	0.43
1:C:335:ILE:HD11	1:C:374:ILE:O	2.19	0.43
1:A:1029:ASN:C	1:A:1029:ASN:HD22	2.22	0.43
1:C:814:TYR:CZ	1:C:828:ILE:HG12	2.54	0.43
1:D:641:MET:HE2	1:D:671:ILE:HG21	2.00	0.43
1:A:769:HIS:NE2	1:A:795:ASP:OD1	2.52	0.43
1:A:811:ASN:HD22	1:A:811:ASN:N	2.08	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:HIS:CD2	1:B:296:ILE:HD11	2.54	0.43
1:B:574:HIS:CD2	1:B:580:THR:HA	2.54	0.43
1:C:840:THR:O	1:C:843:THR:HG22	2.19	0.43
1:C:558:LYS:HG3	1:C:767:PRO:HG3	2.01	0.43
1:B:644:ARG:HH11	1:B:647:ASN:ND2	2.10	0.42
1:A:864:HIS:CD2	1:A:866:MET:HG3	2.54	0.42
1:A:58:GLU:HG3	1:C:445:ARG:HD3	2.01	0.42
1:B:917:MET:O	1:B:921:MET:HB2	2.18	0.42
1:C:512:PHE:HA	1:C:513:PRO:HD2	1.85	0.42
1:C:738:LEU:HD23	1:C:768:ILE:HD12	2.01	0.42
1:D:893:MET:O	1:D:897:VAL:HG23	2.20	0.42
1:A:641:MET:HE2	1:A:671:ILE:HG21	2.01	0.42
1:A:794:ILE:CD1	1:A:813:LEU:HD21	2.49	0.42
1:C:731:GLU:HG3	1:C:766:LEU:HD13	2.01	0.42
1:A:152:LYS:O	1:A:156:ARG:HB2	2.20	0.42
1:C:720:LEU:HD21	1:C:758:GLU:HG3	2.00	0.42
1:C:979:GLY:HA2	1:C:982:LEU:HD12	2.02	0.42
1:B:438:GLN:HA	1:B:441:GLU:HG2	2.00	0.42
1:A:854:ILE:HD11	1:A:872:SER:HB2	2.02	0.42
1:C:470:LYS:HB2	1:C:480:PHE:CE1	2.55	0.42
1:B:776:SER:HB3	1:B:861:ILE:HD11	2.01	0.42
1:A:195:ALA:HA	1:A:233:VAL:HA	2.01	0.42
1:A:252:ASP:HB3	1:A:357:LEU:HG	2.00	0.42
1:A:445:ARG:HD3	1:C:57:ALA:HB1	2.00	0.42
1:C:631:ARG:NH2	1:C:672:ASP:OD1	2.52	0.42
1:C:145:HIS:CE1	1:C:304:TYR:HA	2.55	0.42
1:B:470:LYS:HB2	1:B:480:PHE:HE1	1.84	0.42
1:C:345:VAL:O	1:C:349:ILE:HG12	2.20	0.42
1:D:631:ARG:HD3	1:D:631:ARG:HA	1.71	0.42
1:D:570:PHE:O	1:D:574:HIS:HE1	2.03	0.42
1:B:458:ASN:ND2	1:B:458:ASN:H	2.12	0.42
1:A:408:ASP:HB2	1:A:428:LYS:HB3	2.02	0.42
1:B:103:ILE:HG21	1:B:134:GLU:HG3	2.01	0.42
1:B:597:VAL:HG22	1:B:830:GLY:HA3	2.02	0.42
1:B:297:GLN:O	1:B:301:ASN:HB2	2.20	0.42
1:D:737:ILE:HG12	1:D:767:PRO:HG2	2.02	0.41
1:B:1022:GLN:NE2	1:B:1022:GLN:HA	2.35	0.41
1:B:403:PHE:HB2	1:D:406:ARG:NH1	2.34	0.41
1:D:334:THR:HG23	1:D:406:ARG:NH1	2.35	0.41
1:B:251:GLY:HA3	1:B:257:ILE:HG13	2.02	0.41
1:B:574:HIS:HD2	1:B:580:THR:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:954:GLN:HA	1:C:955:PRO:HD3	1.92	0.41
1:C:555:GLU:HA	1:C:558:LYS:HE3	2.02	0.41
1:B:274:VAL:HG12	1:B:275:VAL:HG23	2.03	0.41
1:B:332:GLU:O	1:B:335:ILE:HG22	2.20	0.41
1:A:1115:GLN:CD	1:A:1115:GLN:N	2.68	0.41
1:A:529:ILE:HG21	1:A:589:ASN:HB3	2.03	0.41
1:C:167:ILE:HA	1:C:168:PRO:HD2	1.83	0.41
1:C:431:THR:HG21	1:C:443:MET:HA	2.01	0.41
1:C:268:GLN:HG2	1:C:273:LYS:HA	2.02	0.41
1:D:853:ASP:N	1:D:853:ASP:OD2	2.53	0.41
1:B:44:ASN:ND2	1:B:45:ARG:H	2.08	0.41
1:C:557:VAL:HG13	1:C:564:LEU:HD12	2.02	0.41
1:A:631:ARG:HD3	1:A:631:ARG:O	2.20	0.41
1:D:101:ARG:CG	1:D:101:ARG:NH2	2.80	0.41
1:C:335:ILE:HA	1:C:335:ILE:HD12	1.78	0.41
1:A:828:ILE:HG13	1:A:828:ILE:H	1.62	0.41
1:A:719:THR:HG22	1:A:720:LEU:N	2.36	0.41
1:C:524:TYR:CD2	1:C:843:THR:HG23	2.56	0.41
1:A:798:VAL:CG1	1:A:835:SER:HA	2.50	0.41
1:C:908:THR:HA	1:C:909:PRO:HA	1.82	0.41
1:A:866:MET:CE	1:A:874:LEU:HD22	2.51	0.41
1:A:58:GLU:OE2	1:C:445:ARG:NH1	2.53	0.41
1:B:82:GLU:HA	1:D:1055:GLY:O	2.21	0.41
1:B:362:MET:HA	1:B:362(A):PRO:HD3	1.94	0.41
1:B:264:ASP:HB3	1:B:277:VAL:HB	2.02	0.41
1:C:266:SER:O	1:C:478:THR:HA	2.21	0.41
1:B:108:GLN:HB3	1:B:108:GLN:HE21	1.72	0.41
1:A:335:ILE:HD12	1:A:335:ILE:HA	1.82	0.40
1:D:828:ILE:HG13	1:D:828:ILE:H	1.59	0.40
1:C:362:MET:CE	1:C:362(A):PRO:HD2	2.52	0.40
1:A:501:LEU:HD21	1:A:1080:MET:HG3	2.03	0.40
1:C:1085:ARG:NH1	1:C:1085:ARG:CG	2.85	0.40
1:B:1092:GLU:O	1:B:1093:ASN:C	2.59	0.40
1:B:509:ILE:HD12	1:B:1089:ILE:HB	2.04	0.40
1:A:1105:ASP:H	1:A:1111:HIS:CD2	2.37	0.40
1:A:174:ILE:HG12	1:A:234:TYR:HA	2.04	0.40
1:D:656:ASP:OD2	1:D:977:ARG:NH2	2.54	0.40
1:B:419:SER:HA	1:B:420:PRO:HD3	1.90	0.40
1:D:142:HIS:H	1:D:145:HIS:HD2	1.69	0.40
1:D:141:PRO:HB2	1:D:145:HIS:HB2	2.02	0.40
1:B:1097:ASN:C	1:B:1099:ASN:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:581:ARG:HG3	1:C:848:PHE:CD2	2.56	0.40
1:D:42:VAL:HG21	1:D:52:ILE:HB	2.03	0.40
1:D:590:ILE:H	1:D:590:ILE:HG13	1.79	0.40
1:B:137:LYS:HG2	1:B:352:ALA:HB1	2.03	0.40
1:C:269:ARG:HG3	1:C:270:ARG:N	2.36	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	1127/1150 (98%)	1044 (93%)	74 (7%)	9 (1%)	24	60
1	B	1070/1150 (93%)	995 (93%)	60 (6%)	15 (1%)	14	44
1	C	1063/1150 (92%)	983 (92%)	69 (6%)	11 (1%)	19	54
1	D	987/1150 (86%)	928 (94%)	52 (5%)	7 (1%)	26	63
All	All	4247/4600 (92%)	3950 (93%)	255 (6%)	42 (1%)	19	54

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	ASP
1	A	1094	VAL
1	B	522	PRO
1	B	1001	PRO
1	B	1093	ASN
1	C	804	LEU
1	C	872	SER
1	D	870	GLN
1	A	397	TYR
1	A	648	ALA

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Mol	Chain	Res	Type
1	B	411	ASP
1	B	415	GLY
1	C	92	PRO
1	C	168	PRO
1	C	868	GLY
1	C	969	LYS
1	D	364	GLN
1	D	868	GLY
1	A	178	GLU
1	A	1093	ASN
1	B	156	ARG
1	B	648	ALA
1	C	177	TYR
1	C	189	PHE
1	C	410	GLY
1	D	648	ALA
1	B	166	VAL
1	B	269	ARG
1	B	1098	ALA
1	C	493	SER
1	D	92	PRO
1	B	903	ASP
1	B	1002	VAL
1	A	210	GLU
1	A	242	PRO
1	B	270	ARG
1	B	410	GLY
1	A	1000	GLY
1	C	190	PRO
1	D	415	GLY
1	B	317	GLY
1	D	91	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	978/988 (99%)	911 (93%)	67 (7%)	19	48
1	B	929/988 (94%)	863 (93%)	66 (7%)	18	47
1	C	918/988 (93%)	855 (93%)	63 (7%)	19	48
1	D	860/988 (87%)	799 (93%)	61 (7%)	18	47
All	All	3685/3952 (93%)	3428 (93%)	257 (7%)	19	47

All (257) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	44	ASN
1	A	60	ASP
1	A	89	ASP
1	A	97	LEU
1	A	101	ARG
1	A	108	GLN
1	A	110	ASN
1	A	147	ASP
1	A	156	ARG
1	A	186	GLU
1	A	221	LYS
1	A	223	GLU
1	A	270	ARG
1	A	287	LEU
1	A	306	ASN
1	A	329	VAL
1	A	334	THR
1	A	335	ILE
1	A	386	ASP
1	A	414	GLN
1	A	427	VAL
1	A	434	ILE
1	A	467	LYS
1	A	469	LYS
1	A	491	GLN
1	A	495	ASP
1	A	496	ARG
1	A	506	ASN
1	A	517	GLU
1	A	519	ARG
1	A	523	ASP
1	A	529	ILE

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Mol	Chain	Res	Type
1	A	580	THR
1	A	590	ILE
1	A	606	MET
1	A	607	TRP
1	A	622	ASN
1	A	649	VAL
1	A	715	ARG
1	A	743	MET
1	A	781	LEU
1	A	784	LYS
1	A	811	ASN
1	A	823	HIS
1	A	828	ILE
1	A	829	GLU
1	A	863	GLN
1	A	871	TYR
1	A	907	VAL
1	A	917	MET
1	A	926	LEU
1	A	931	VAL
1	A	944	VAL
1	A	1008	ILE
1	A	1019	GLN
1	A	1029	ASN
1	A	1048	VAL
1	A	1076	ILE
1	A	1080	MET
1	A	1085	ARG
1	A	1092	GLU
1	A	1097	ASN
1	A	1111	HIS
1	A	1116	MET
1	A	1137	LEU
1	A	1177	ILE
1	B	36	GLN
1	B	44	ASN
1	B	66	ILE
1	B	75	LEU
1	B	98	ASN
1	B	108	GLN
1	B	137	LYS
1	B	148	MET

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Mol	Chain	Res	Type
1	B	156	ARG
1	B	166	VAL
1	B	242	PRO
1	B	245	ILE
1	B	329	VAL
1	B	357	LEU
1	B	365	LYS
1	B	411	ASP
1	B	414	GLN
1	B	421	TYR
1	B	422	TYR
1	B	428	LYS
1	B	455	VAL
1	B	456	LYS
1	B	457	THR
1	B	458	ASN
1	B	486	GLU
1	B	495	ASP
1	B	506	ASN
1	B	551	LYS
1	B	580	THR
1	B	606	MET
1	B	607	TRP
1	B	610	THR
1	B	622	ASN
1	B	647	ASN
1	B	660	HIS
1	B	683	VAL
1	B	707	THR
1	B	714	GLU
1	B	719	THR
1	B	721	GLU
1	B	743	MET
1	B	775	THR
1	B	781	LEU
1	B	811	ASN
1	B	828	ILE
1	B	839	SER
1	B	855	LYS
1	B	863	GLN
1	B	885	GLU
1	B	907	VAL

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Mol	Chain	Res	Type
1	B	908	THR
1	B	919	LEU
1	B	926	LEU
1	B	934	ASP
1	B	944	VAL
1	B	999	GLN
1	B	1008	ILE
1	B	1024	ARG
1	B	1029	ASN
1	B	1085	ARG
1	B	1111	HIS
1	B	1138	LEU
1	B	1143	MET
1	B	1156	VAL
1	B	1157	ILE
1	B	1177	ILE
1	C	39	LYS
1	C	44	ASN
1	C	60	ASP
1	C	86	VAL
1	C	95	SER
1	C	98	ASN
1	C	175	LYS
1	C	177	TYR
1	C	179	LEU
1	C	181	LYS
1	C	186	GLU
1	C	189	PHE
1	C	192	MET
1	C	193	ILE
1	C	205	ARG
1	C	206	ILE
1	C	228	PHE
1	C	230	ASN
1	C	239	ILE
1	C	257	ILE
1	C	262	GLU
1	C	287	LEU
1	C	323	ILE
1	C	329	VAL
1	C	335	ILE
1	C	377	ARG

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Mol	Chain	Res	Type
1	C	434	ILE
1	C	437	LYS
1	C	495	ASP
1	C	506	ASN
1	C	535	SER
1	C	559	LYS
1	C	580	THR
1	C	606	MET
1	C	607	TRP
1	C	622	ASN
1	C	631	ARG
1	C	641	MET
1	C	646	SER
1	C	647	ASN
1	C	649	VAL
1	C	651	TYR
1	C	717	ASN
1	C	719	THR
1	C	743	MET
1	C	792	ASP
1	C	804	LEU
1	C	828	ILE
1	C	843	THR
1	C	870	GLN
1	C	900	LEU
1	C	904	ILE
1	C	907	VAL
1	C	923	GLN
1	C	962	ASP
1	C	968	LEU
1	C	969	LYS
1	C	977	ARG
1	C	1008	ILE
1	C	1029	ASN
1	C	1044	ASN
1	C	1085	ARG
1	C	1147	THR
1	D	38	LYS
1	D	44	ASN
1	D	60	ASP
1	D	77	ARG
1	D	101	ARG

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Mol	Chain	Res	Type
1	D	104	ASP
1	D	241	ASN
1	D	262	GLU
1	D	267	VAL
1	D	269	ARG
1	D	272	GLN
1	D	287	LEU
1	D	289	GLN
1	D	303	LYS
1	D	329	VAL
1	D	357	LEU
1	D	365	LYS
1	D	384	LEU
1	D	386	ASP
1	D	411	ASP
1	D	427	VAL
1	D	440	GLU
1	D	475	ASP
1	D	506	ASN
1	D	531	THR
1	D	542	LYS
1	D	580	THR
1	D	607	TRP
1	D	622	ASN
1	D	631	ARG
1	D	647	ASN
1	D	649	VAL
1	D	684	ASP
1	D	707	THR
1	D	714	GLU
1	D	715	ARG
1	D	717	ASN
1	D	725	LYS
1	D	743	MET
1	D	760	LYS
1	D	766	LEU
1	D	775	THR
1	D	798	VAL
1	D	807	GLN
1	D	823	HIS
1	D	828	ILE
1	D	853	ASP

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Mol	Chain	Res	Type
1	D	863	GLN
1	D	873	ASN
1	D	886	ARG
1	D	907	VAL
1	D	908	THR
1	D	917	MET
1	D	919	LEU
1	D	926	LEU
1	D	928	GLU
1	D	931	VAL
1	D	975	THR
1	D	977	ARG
1	D	1064	THR
1	D	1085	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	108	GLN
1	A	145	HIS
1	A	241	ASN
1	A	256	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	617	ASN
1	A	622	ASN
1	A	736	HIS
1	A	778	ASN
1	A	807	GLN
1	A	811	ASN
1	A	818	ASN
1	A	858	ASN
1	A	864	HIS
1	A	898	ASN
1	A	1005	GLN
1	A	1025	ASN

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Mol	Chain	Res	Type
1	A	1029	ASN
1	A	1044	ASN
1	A	1093	ASN
1	A	1099	ASN
1	A	1111	HIS
1	A	1150	GLN
1	B	44	ASN
1	B	69	ASN
1	B	98	ASN
1	B	108	GLN
1	B	126	GLN
1	B	145	HIS
1	B	256	ASN
1	B	364	GLN
1	B	385	ASN
1	B	414	GLN
1	B	432	HIS
1	B	458	ASN
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	647	ASN
1	B	685	GLN
1	B	736	HIS
1	B	773	HIS
1	B	778	ASN
1	B	811	ASN
1	B	818	ASN
1	B	858	ASN
1	B	864	HIS
1	B	876	GLN
1	B	877	GLN
1	B	898	ASN
1	B	923	GLN
1	B	960	ASN
1	B	999	GLN
1	B	1005	GLN
1	B	1022	GLN

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Mol	Chain	Res	Type
1	B	1025	ASN
1	B	1026	GLN
1	B	1029	ASN
1	B	1044	ASN
1	B	1111	HIS
1	C	44	ASN
1	C	98	ASN
1	C	145	HIS
1	C	230	ASN
1	C	330	GLN
1	C	375	GLN
1	C	506	ASN
1	C	515	ASN
1	C	574	HIS
1	C	575	GLN
1	C	589	ASN
1	C	622	ASN
1	C	717	ASN
1	C	736	HIS
1	C	778	ASN
1	C	807	GLN
1	C	811	ASN
1	C	858	ASN
1	C	864	HIS
1	C	870	GLN
1	C	873	ASN
1	C	898	ASN
1	C	923	GLN
1	C	971	GLN
1	C	1005	GLN
1	C	1019	GLN
1	C	1025	ASN
1	C	1029	ASN
1	C	1081	ASN
1	D	44	ASN
1	D	272	GLN
1	D	289	GLN
1	D	326	ASN
1	D	330	GLN
1	D	375	GLN
1	D	432	HIS
1	D	506	ASN

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Mol	Chain	Res	Type
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	717	ASN
1	D	736	HIS
1	D	778	ASN
1	D	807	GLN
1	D	811	ASN
1	D	858	ASN
1	D	864	HIS
1	D	898	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 [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\# Z  > 2$
2	BTI	A	2000	1	14,16,16	1.92	3 (21%)	13,21,21	1.29	1 (7%)
3	ADP	A	2100	-	22,29,29	1.06	2 (9%)	27,45,45	1.93	4 (14%)
2	BTI	B	2000	1	14,16,16	1.91	3 (21%)	13,21,21	1.51	1 (7%)
2	BTI	C	1183	-	14,16,16	1.86	4 (28%)	13,21,21	1.62	1 (7%)
2	BTI	C	2000	1	14,16,16	1.88	4 (28%)	13,21,21	1.31	1 (7%)
3	ADP	C	2100	-	22,29,29	1.07	2 (9%)	27,45,45	2.00	5 (18%)

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
2	BTI	A	2000	1	-	0/5/27/27	0/2/2/2
3	ADP	A	2100	-	-	0/12/32/32	0/3/3/3
2	BTI	B	2000	1	-	0/5/27/27	0/2/2/2
2	BTI	C	1183	-	-	0/5/27/27	0/2/2/2
2	BTI	C	2000	1	-	0/5/27/27	0/2/2/2
3	ADP	C	2100	-	-	0/12/32/32	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	BTI	C2-S1	-3.74	1.76	1.82
2	C	2000	BTI	C2-S1	-3.58	1.76	1.82
2	A	2000	BTI	C2-S1	-3.55	1.76	1.82
2	C	1183	BTI	C2-S1	-3.39	1.77	1.82
2	A	2000	BTI	C3-N2	-2.17	1.32	1.35
2	C	2000	BTI	C3-N3	-2.12	1.32	1.35
2	C	2000	BTI	C3-N2	-2.04	1.32	1.35
2	C	1183	BTI	C3-N2	-2.03	1.32	1.35
2	B	2000	BTI	C3-N3	-2.01	1.32	1.35
2	C	1183	BTI	C3-N3	-2.01	1.32	1.35
3	C	2100	ADP	O4'-C1'	2.05	1.43	1.41
3	A	2100	ADP	O4'-C1'	2.09	1.43	1.41
3	C	2100	ADP	C5-C4	3.24	1.47	1.40
3	A	2100	ADP	C5-C4	3.24	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2000	BTI	O3-C3	4.72	1.33	1.23
2	C	1183	BTI	O3-C3	4.87	1.33	1.23
2	B	2000	BTI	O3-C3	4.93	1.33	1.23
2	A	2000	BTI	O3-C3	4.97	1.33	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2100	ADP	N3-C2-N1	-7.07	123.48	128.89
3	C	2100	ADP	N3-C2-N1	-7.04	123.50	128.89
3	C	2100	ADP	C2'-C1'-N9	-4.35	107.64	114.29
3	A	2100	ADP	C2'-C1'-N9	-3.34	109.19	114.29
3	C	2100	ADP	PA-O3A-PB	-3.33	121.51	132.67
3	A	2100	ADP	PA-O3A-PB	-3.28	121.67	132.67
3	A	2100	ADP	C4-C5-N7	-3.20	106.54	109.48
3	C	2100	ADP	C4-C5-N7	-3.16	106.57	109.48
3	C	2100	ADP	O3B-PB-O2B	2.05	115.19	107.38
2	A	2000	BTI	N2-C3-N3	3.10	111.03	108.88
2	C	2000	BTI	N2-C3-N3	3.23	111.11	108.88
2	B	2000	BTI	N2-C3-N3	3.66	111.41	108.88
2	C	1183	BTI	N2-C3-N3	3.75	111.47	108.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2000	BTI	1	0
2	B	2000	BTI	1	0
2	C	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	1133/1150 (98%)	-0.09	52 (4%) 36 30	19, 45, 109, 169	0
1	B	1074/1150 (93%)	0.09	46 (4%) 39 32	29, 60, 127, 178	0
1	C	1067/1150 (92%)	-0.01	39 (3%) 45 38	29, 61, 102, 147	0
1	D	993/1150 (86%)	-0.09	32 (3%) 51 43	17, 44, 138, 192	0
All	All	4267/4600 (92%)	-0.02	169 (3%) 42 35	17, 55, 121, 192	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	492	PRO	9.3
1	B	240	ASP	6.7
1	D	490	ILE	6.5
1	D	494	LEU	5.8
1	C	421	TYR	5.5
1	A	177	TYR	5.3
1	A	185	GLU	5.2
1	B	490	ILE	5.2
1	D	168	PRO	5.2
1	A	181	LYS	5.1
1	D	1142	ALA	5.1
1	B	493	SER	5.1
1	B	491	GLN	5.0
1	A	421	TYR	4.9
1	B	88	SER	4.9
1	D	88	SER	4.8
1	D	239	ILE	4.8
1	B	1095	HIS	4.7
1	A	195	ALA	4.6
1	A	206	ILE	4.5
1	A	233	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	226	LYS	4.4
1	C	491	GLN	4.3
1	A	999	GLN	4.3
1	A	215	ASP	4.2
1	B	89	ASP	4.2
1	A	232	GLU	4.2
1	C	1140	THR	4.0
1	B	421	TYR	3.9
1	A	224	ALA	3.8
1	B	452	ILE	3.8
1	A	1001	PRO	3.8
1	B	494	LEU	3.8
1	A	227	SER	3.8
1	D	417	GLU	3.7
1	A	282	GLY	3.7
1	B	524	TYR	3.6
1	A	196	THR	3.6
1	A	220	ALA	3.6
1	D	282	GLY	3.5
1	D	89	ASP	3.5
1	D	412	GLY	3.5
1	B	271	HIS	3.5
1	C	222	SER	3.5
1	B	38	LYS	3.5
1	B	459	ILE	3.5
1	B	713	PRO	3.4
1	C	218	HIS	3.4
1	C	492	PRO	3.4
1	D	421	TYR	3.4
1	C	229	GLY	3.4
1	B	239	ILE	3.4
1	B	397	TYR	3.4
1	D	87	GLY	3.4
1	B	160	ILE	3.3
1	C	880	SER	3.3
1	C	412	GLY	3.3
1	A	384	LEU	3.3
1	B	527	ALA	3.2
1	B	168	PRO	3.2
1	C	197	SER	3.2
1	A	189	PHE	3.2
1	C	209	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	241	ASN	3.2
1	A	222	SER	3.1
1	D	271	HIS	3.1
1	B	282	GLY	3.1
1	D	386	ASP	3.1
1	A	420	PRO	3.1
1	D	357(A)	PHE	3.1
1	C	420	PRO	3.1
1	C	213	LEU	3.1
1	B	87	GLY	3.1
1	B	1054	LYS	3.1
1	A	180	ALA	3.0
1	A	494	LEU	3.0
1	A	218	HIS	3.0
1	B	412	GLY	3.0
1	A	219	ARG	3.0
1	C	208	ARG	3.0
1	C	416	ALA	3.0
1	C	1093	ASN	3.0
1	C	188	GLY	2.9
1	D	388	MET	2.9
1	A	386	ASP	2.9
1	D	153	VAL	2.9
1	A	234	TYR	2.9
1	A	176	SER	2.9
1	A	1095	HIS	2.9
1	A	526	LEU	2.8
1	A	174	ILE	2.8
1	A	175	LYS	2.8
1	A	493	SER	2.8
1	B	270	ARG	2.8
1	D	358	GLU	2.7
1	A	393	THR	2.7
1	B	1001	PRO	2.7
1	D	156	ARG	2.7
1	A	213	LEU	2.7
1	B	981	TYR	2.7
1	B	384	LEU	2.7
1	C	189	PHE	2.7
1	C	183	PHE	2.6
1	A	418	ILE	2.6
1	D	240	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	885	GLU	2.6
1	A	1128	GLY	2.6
1	C	411	ASP	2.6
1	D	91	GLY	2.6
1	C	496	ARG	2.6
1	C	1001	PRO	2.6
1	C	397	TYR	2.5
1	D	359	GLU	2.5
1	A	207	VAL	2.5
1	B	1093	ASN	2.5
1	A	225	GLU	2.5
1	A	89	ASP	2.5
1	C	936	TYR	2.4
1	D	286	THR	2.4
1	B	320	PHE	2.4
1	B	454	GLY	2.4
1	B	391	THR	2.4
1	A	91	GLY	2.4
1	B	1097	ASN	2.4
1	C	88	SER	2.4
1	A	452	ILE	2.4
1	B	457	THR	2.4
1	D	151	ASP	2.3
1	C	881	LEU	2.3
1	D	999	GLN	2.3
1	C	453	ARG	2.3
1	C	387	PHE	2.3
1	B	386	ASP	2.3
1	B	153	VAL	2.3
1	A	394	ILE	2.3
1	C	418	ILE	2.3
1	A	412	GLY	2.2
1	C	970	GLY	2.2
1	B	1098	ALA	2.2
1	D	93	ALA	2.2
1	C	924	ASN	2.2
1	B	73	SER	2.2
1	C	269	ARG	2.2
1	C	285	PRO	2.2
1	B	409	ALA	2.2
1	A	192	MET	2.2
1	A	1127	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	89	ASP	2.2
1	B	393	THR	2.2
1	A	94	GLU	2.2
1	D	242	PRO	2.2
1	B	427	VAL	2.2
1	C	282	GLY	2.1
1	D	285	PRO	2.1
1	D	1054	LYS	2.1
1	A	223	GLU	2.1
1	A	217	PHE	2.1
1	D	475	ASP	2.1
1	B	167	ILE	2.1
1	A	92	PRO	2.1
1	C	876	GLN	2.1
1	C	417	GLU	2.1
1	A	523	ASP	2.1
1	B	472	THR	2.1
1	B	385	ASN	2.1
1	A	178	GLU	2.1
1	B	383	PRO	2.1
1	C	1147	THR	2.0
1	D	385	ASN	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	MN	D	2002	1/1	0.97	0.19	0.53	57,57,57,57	0
2	BTI	C	2000	15/15	0.95	0.17	0.37	45,45,57,57	0
2	BTI	A	2000	15/15	0.96	0.15	0.15	50,51,53,53	0
2	BTI	C	1183	15/15	0.95	0.16	0.10	48,48,49,49	0
2	BTI	B	2000	15/15	0.95	0.15	-0.06	48,48,51,51	0
3	ADP	A	2100	27/27	0.88	0.20	-0.59	99,100,103,103	0
3	ADP	C	2100	27/27	0.93	0.17	-0.65	78,78,78,79	0
4	MN	B	2002	1/1	0.94	0.14	-0.82	77,77,77,77	0
4	MN	A	2002	1/1	0.91	0.13	-1.27	63,63,63,63	0
4	MN	C	2002	1/1	0.94	0.11	-1.85	75,75,75,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.