



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:53 am GMT

PDB ID : 1DI0  
Title : CRYSTAL STRUCTURE OF LUMAZINE SYNTHASE FROM BRUCELLA ABORTUS  
Authors : Braden, B.C.; Velikovsky, C.A.; Cauwerhff, A.A.; Polikarpov, I.; Goldbaum, F.A.  
Deposited on : 1999-11-28  
Resolution : 2.70 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.

---

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

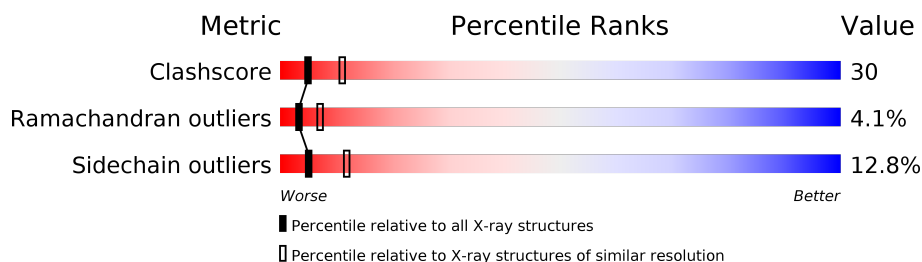
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	158	
1	B	158	
1	C	158	
1	D	158	
1	E	158	

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
2	PO4	A	190	-	-	X	-
2	PO4	A	192	-	-	X	-
2	PO4	B	195	-	-	X	-
2	PO4	C	196	-	-	X	-
2	PO4	C	197	-	-	X	-
2	PO4	D	198	-	-	X	-
2	PO4	D	199	-	-	X	-
2	PO4	E	202	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5818 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 LUMAZINE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1147	738	201	206	2			
1	B	148	Total	C	N	O	S	0	0	0
			1147	738	201	206	2			
1	C	146	Total	C	N	O	S	0	0	0
			1135	731	199	203	2			
1	D	147	Total	C	N	O	S	0	0	0
			1142	735	200	205	2			
1	E	146	Total	C	N	O	S	0	0	0
			1135	731	199	203	2			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	ASP	ARG	CONFLICT	UNP P61711
B	88	ASP	ARG	CONFLICT	UNP P61711
C	88	ASP	ARG	CONFLICT	UNP P61711
D	88	ASP	ARG	CONFLICT	UNP P61711
E	88	ASP	ARG	CONFLICT	UNP P61711

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total 10	O 10	0	0
3	B	8	Total 8	O 8	0	0
3	C	12	Total 12	O 12	0	0
3	D	7	Total 7	O 7	0	0
3	E	10	Total 10	O 10	0	0

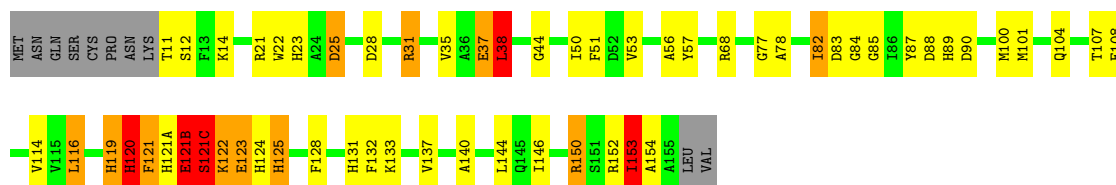
### 3 Residue-property plots

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

Note EDS was not executed.

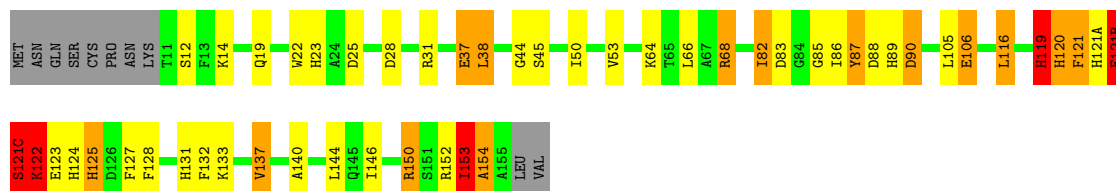
#### • Molecule 1: LUMAZINE SYNTHASE

Chain A: 



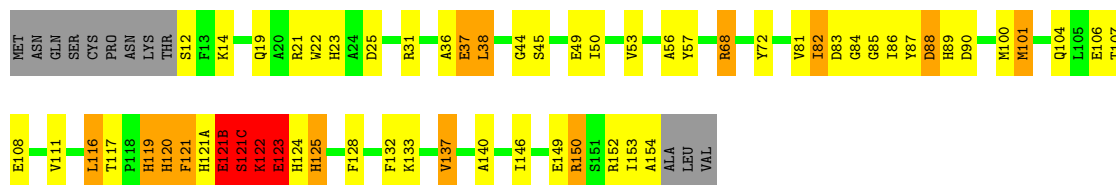
#### • Molecule 1: LUMAZINE SYNTHASE

Chain B: 



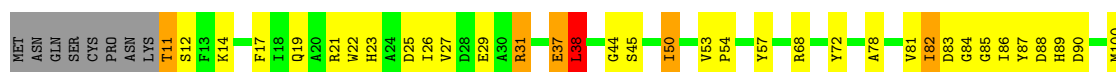
#### • Molecule 1: LUMAZINE SYNTHASE

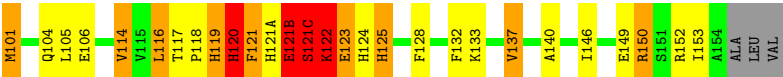
Chain C: 



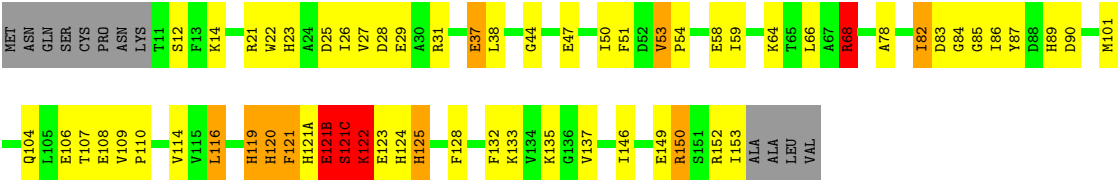
#### • Molecule 1: LUMAZINE SYNTHASE

Chain D: 





● Molecule 1: LUMAZINE SYNTHASE





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.25Å 142.25Å 242.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	150.00 – 2.70	Depositor
% Data completeness (in resolution range)	90.0 (150.00-2.70)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.180 , 0.230	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5818	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.34	3/1176 (0.3%)	1.30	8/1596 (0.5%)
1	B	1.36	3/1176 (0.3%)	1.20	5/1596 (0.3%)
1	C	1.45	8/1164 (0.7%)	1.27	6/1579 (0.4%)
1	D	1.44	10/1171 (0.9%)	1.26	5/1589 (0.3%)
1	E	1.34	6/1164 (0.5%)	1.22	7/1579 (0.4%)
All	All	1.39	30/5851 (0.5%)	1.25	31/7939 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	101	MET	CG-SD	-6.55	1.64	1.81
1	D	106	GLU	CG-CD	6.54	1.61	1.51
1	B	106	GLU	CD-OE2	6.45	1.32	1.25
1	E	121(B)	GLU	CD-OE2	6.37	1.32	1.25
1	C	36	ALA	CA-CB	-6.24	1.39	1.52
1	D	137	VAL	CB-CG2	-6.15	1.40	1.52
1	D	114	VAL	CB-CG2	-6.10	1.40	1.52
1	A	35	VAL	CB-CG2	-5.92	1.40	1.52
1	E	121(B)	GLU	CG-CD	5.89	1.60	1.51
1	C	88	ASP	CB-CG	5.87	1.64	1.51
1	D	17	PHE	CE2-CZ	5.79	1.48	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	111	VAL	CB-CG2	-5.78	1.40	1.52
1	B	121(B)	GLU	CD-OE2	5.75	1.31	1.25
1	E	121(B)	GLU	CD-OE1	5.57	1.31	1.25
1	D	17	PHE	CG-CD2	5.56	1.47	1.38
1	E	108	GLU	CB-CG	-5.54	1.41	1.52
1	A	100	MET	SD-CE	-5.43	1.47	1.77
1	C	106	GLU	CD-OE2	5.41	1.31	1.25
1	C	137	VAL	CB-CG2	-5.40	1.41	1.52
1	D	100	MET	SD-CE	-5.39	1.47	1.77
1	A	11	THR	CA-CB	5.35	1.67	1.53
1	C	100	MET	SD-CE	-5.30	1.48	1.77
1	D	72	TYR	CD1-CE1	-5.29	1.31	1.39
1	B	137	VAL	CB-CG2	-5.25	1.41	1.52
1	D	11	THR	CA-CB	5.22	1.67	1.53
1	D	101	MET	CG-SD	-5.18	1.67	1.81
1	C	123	GLU	CD-OE2	5.17	1.31	1.25
1	E	107	THR	CB-CG2	-5.17	1.35	1.52
1	E	59	ILE	C-O	-5.12	1.13	1.23
1	D	50	ILE	C-O	-5.01	1.13	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ARG	NE-CZ-NH1	-13.78	113.41	120.30
1	C	68	ARG	NE-CZ-NH2	-12.80	113.90	120.30
1	E	150	ARG	NE-CZ-NH1	-11.64	114.48	120.30
1	D	150	ARG	NE-CZ-NH1	-10.19	115.20	120.30
1	A	68	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	C	150	ARG	NE-CZ-NH1	-7.65	116.47	120.30
1	A	38	LEU	CB-CG-CD1	-6.92	99.23	111.00
1	C	150	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	B	150	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	E	90	ASP	CB-CG-OD1	6.70	124.33	118.30
1	E	68	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	D	50	ILE	CG1-CB-CG2	-6.43	97.26	111.40
1	E	153	ILE	CB-CA-C	-6.42	98.76	111.60
1	B	88	ASP	CB-CG-OD1	6.41	124.07	118.30
1	D	31	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	C	68	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	31	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	D	88	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	150	ARG	NE-CZ-NH2	5.82	123.21	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	ASP	CB-CG-OD1	5.77	123.49	118.30
1	D	38	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	B	90	ASP	CB-CG-OD1	5.73	123.45	118.30
1	A	50	ILE	CG1-CB-CG2	-5.67	98.93	111.40
1	A	77	GLY	N-CA-C	-5.54	99.25	113.10
1	A	25	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	119	HIS	N-CA-C	5.38	125.52	111.00
1	E	150	ARG	NH1-CZ-NH2	5.28	125.20	119.40
1	E	109	VAL	N-CA-C	-5.22	96.91	111.00
1	B	153	ILE	CB-CA-C	-5.07	101.46	111.60
1	C	106	GLU	CA-CB-CG	5.02	124.44	113.40
1	E	50	ILE	CG1-CB-CG2	-5.00	100.39	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	87	TYR	Sidechain
1	C	72	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1147	0	1127	72	0
1	B	1147	0	1127	69	0
1	C	1135	0	1115	78	0
1	D	1142	0	1122	76	0
1	E	1135	0	1112	71	0
2	A	15	0	0	5	0
2	B	15	0	0	3	0
2	C	10	0	0	8	0
2	D	10	0	0	5	0
2	E	15	0	0	3	0
3	A	10	0	0	1	0
3	B	8	0	0	0	0
3	C	12	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	7	0	0	0	0
3	E	10	0	0	3	0
All	All	5818	0	5603	342	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 30.

All (342) 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:D:152:ARG:NH2	1:D:153:ILE:HD13	1.61	1.14
1:D:152:ARG:HH21	1:D:153:ILE:CD1	1.64	1.11
1:D:153:ILE:HG12	1:E:51:PHE:HE2	1.09	1.05
1:B:121(B):GLU:O	1:B:121(C):SER:HB3	1.56	1.03
1:D:152:ARG:HH21	1:D:153:ILE:HD13	0.88	1.02
1:C:83:ASP:HB3	3:C:2027:HOH:O	1.59	1.02
1:B:85:GLY:HA3	2:B:195:PO4:O4	1.58	1.00
1:E:121(B):GLU:O	1:E:121(C):SER:HB3	1.57	1.00
1:D:121(B):GLU:O	1:D:121(C):SER:HB3	1.62	0.99
1:C:121(B):GLU:O	1:C:121(C):SER:HB3	1.60	0.98
1:D:121(C):SER:OG	1:D:123:GLU:HB2	1.63	0.98
1:A:85:GLY:HA3	2:A:192:PO4:O3	1.65	0.97
1:A:121(B):GLU:O	1:A:121(C):SER:HB3	1.59	0.96
1:D:153:ILE:HG12	1:E:51:PHE:CE2	2.02	0.94
1:A:37:GLU:HG3	1:A:137:VAL:HG13	1.53	0.90
1:C:121:PHE:HD2	1:C:128:PHE:HE1	1.21	0.89
1:C:121(C):SER:OG	1:C:123:GLU:HB2	1.71	0.88
1:D:153:ILE:O	1:D:153:ILE:HG22	1.70	0.88
1:D:153:ILE:CG2	1:D:153:ILE:O	2.21	0.87
1:C:121:PHE:CD2	1:C:128:PHE:CE1	2.64	0.86
1:B:121(C):SER:OG	1:B:123:GLU:HB2	1.76	0.85
1:A:153:ILE:O	1:A:153:ILE:HD13	1.78	0.83
1:D:22:TRP:CE3	1:D:23:HIS:HD2	1.97	0.83
1:D:12:SER:HA	1:D:45:SER:O	1.80	0.81
1:C:121:PHE:HD2	1:C:128:PHE:CE1	1.97	0.81
1:E:121:PHE:CD2	1:E:128:PHE:CE1	2.69	0.80
1:E:121:PHE:HD2	1:E:128:PHE:HE1	1.28	0.80
1:A:121(C):SER:OG	1:A:123:GLU:HB2	1.79	0.80
1:C:56:ALA:N	2:C:196:PO4:O2	2.15	0.79
1:B:37:GLU:HG3	1:B:137:VAL:HG13	1.65	0.79
1:D:37:GLU:HG3	1:D:137:VAL:HG13	1.64	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:GLU:HG3	1:E:137:VAL:HG13	1.65	0.78
1:E:121(C):SER:OG	1:E:123:GLU:HB2	1.83	0.78
1:A:56:ALA:HB3	2:A:190:PO4:O1	1.83	0.78
1:A:153:ILE:HD11	1:B:66:LEU:HD23	1.66	0.78
1:E:22:TRP:CE3	1:E:23:HIS:HD2	2.00	0.78
1:A:22:TRP:CE3	1:A:23:HIS:HD2	2.01	0.78
1:A:121:PHE:HD2	1:A:128:PHE:HE1	1.32	0.77
1:C:121:PHE:CD2	1:C:128:PHE:HE1	1.99	0.77
1:E:121:PHE:HD2	1:E:128:PHE:CE1	2.04	0.76
1:E:146:ILE:O	1:E:150:ARG:HG3	1.86	0.75
1:B:22:TRP:CE3	1:B:23:HIS:HD2	2.04	0.74
1:A:121:PHE:CD2	1:A:128:PHE:CE1	2.75	0.74
1:E:121:PHE:CD2	1:E:128:PHE:HE1	2.06	0.74
1:C:37:GLU:HG3	1:C:137:VAL:HG13	1.70	0.74
1:C:82:ILE:HG23	1:C:82:ILE:O	1.87	0.73
1:D:121:PHE:HD2	1:D:128:PHE:HE1	1.36	0.73
1:D:85:GLY:HA3	2:D:199:PO4:P	2.28	0.73
1:D:82:ILE:HG23	1:D:82:ILE:O	1.89	0.72
1:E:119:HIS:O	1:E:120:HIS:HB2	1.86	0.72
1:B:121:PHE:CD2	1:B:128:PHE:CE1	2.78	0.72
1:D:119:HIS:O	1:D:120:HIS:HB2	1.89	0.72
1:A:82:ILE:O	1:A:82:ILE:HG23	1.88	0.72
1:B:22:TRP:HH2	1:B:82:ILE:CG2	2.02	0.72
1:D:85:GLY:HA3	2:D:199:PO4:O1	1.89	0.72
1:C:119:HIS:O	1:C:120:HIS:HB2	1.89	0.71
1:A:121:PHE:CD2	1:A:128:PHE:HE1	2.10	0.70
1:E:116:LEU:HD23	1:E:132:PHE:CZ	2.27	0.70
1:C:22:TRP:CE3	1:C:23:HIS:HD2	2.10	0.70
1:C:12:SER:HA	1:C:45:SER:O	1.91	0.70
1:D:121:PHE:CD2	1:D:128:PHE:CE1	2.79	0.70
1:C:121(C):SER:O	1:C:123:GLU:N	2.25	0.70
1:A:146:ILE:O	1:A:150:ARG:HG3	1.92	0.69
1:D:25:ASP:OD1	1:D:125:HIS:HE1	1.75	0.69
1:B:119:HIS:O	1:B:120:HIS:HB2	1.92	0.69
1:B:82:ILE:C	1:B:82:ILE:HD13	2.13	0.69
1:A:121:PHE:HD2	1:A:128:PHE:CE1	2.09	0.69
1:A:22:TRP:HH2	1:A:82:ILE:CG2	2.06	0.69
1:B:121:PHE:HD2	1:B:128:PHE:HE1	1.41	0.69
1:B:22:TRP:CH2	1:B:82:ILE:HG22	2.28	0.69
1:D:57:TYR:N	2:D:198:PO4:O2	2.19	0.68
1:C:128:PHE:HD2	1:D:87:TYR:HH	1.40	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:HD23	1:A:140:ALA:HB1	1.76	0.68
1:A:153:ILE:HD11	1:B:66:LEU:CD2	2.24	0.68
1:C:22:TRP:HH2	1:C:82:ILE:CG2	2.06	0.67
1:B:82:ILE:HG23	1:B:82:ILE:O	1.95	0.67
1:E:83:ASP:OD1	3:E:2045:HOH:O	2.13	0.67
1:D:153:ILE:HG21	1:E:66:LEU:HD21	1.77	0.67
1:D:121:PHE:CD2	1:D:128:PHE:HE1	2.14	0.67
1:D:121:PHE:HD2	1:D:128:PHE:CE1	2.13	0.67
1:D:57:TYR:HB2	2:D:198:PO4:O2	1.95	0.67
1:C:85:GLY:HA3	2:C:197:PO4:P	2.35	0.66
1:A:85:GLY:HA3	2:A:192:PO4:P	2.34	0.66
1:C:25:ASP:OD1	1:C:125:HIS:HE1	1.77	0.66
1:B:89:HIS:HD2	2:B:194:PO4:O1	1.78	0.66
1:B:121(C):SER:O	1:B:123:GLU:N	2.29	0.65
1:A:82:ILE:C	1:A:82:ILE:HD13	2.16	0.65
1:E:116:LEU:HD23	1:E:132:PHE:CE1	2.32	0.65
1:C:82:ILE:C	1:C:82:ILE:HD13	2.17	0.65
1:D:22:TRP:HH2	1:D:82:ILE:CG2	2.10	0.65
1:C:22:TRP:CH2	1:C:82:ILE:HG22	2.32	0.65
1:E:22:TRP:HH2	1:E:82:ILE:CG2	2.09	0.65
1:D:146:ILE:O	1:D:150:ARG:HG3	1.97	0.64
1:B:121:PHE:HD2	1:B:128:PHE:CE1	2.14	0.64
1:B:85:GLY:HA3	2:B:195:PO4:P	2.38	0.64
1:A:25:ASP:OD1	1:A:125:HIS:HE1	1.80	0.64
1:A:22:TRP:CH2	1:A:82:ILE:HG22	2.33	0.64
1:E:121(C):SER:O	1:E:123:GLU:N	2.31	0.63
1:A:87:TYR:HH	1:E:128:PHE:HD2	1.46	0.63
1:C:116:LEU:HD23	1:C:132:PHE:CE1	2.34	0.63
1:E:22:TRP:CH2	1:E:82:ILE:HG22	2.33	0.63
1:D:121(C):SER:O	1:D:123:GLU:N	2.32	0.62
1:E:82:ILE:O	1:E:82:ILE:HG23	1.98	0.62
1:E:85:GLY:HA3	2:E:202:PO4:P	2.40	0.62
1:C:128:PHE:HD2	1:D:87:TYR:OH	1.83	0.62
1:B:152:ARG:O	1:B:153:ILE:C	2.37	0.61
1:B:38:LEU:HD23	1:B:140:ALA:HB1	1.82	0.61
1:E:22:TRP:CZ3	1:E:23:HIS:HD2	2.18	0.61
1:C:119:HIS:HB2	1:D:86:ILE:O	2.00	0.61
1:D:121(A):HIS:O	1:D:121(B):GLU:O	2.18	0.61
1:B:116:LEU:HD23	1:B:132:PHE:CZ	2.35	0.61
1:B:121(B):GLU:O	1:B:121(C):SER:CB	2.41	0.60
1:D:19:GLN:HE22	1:D:31:ARG:HE	1.48	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ILE:HD13	1:D:82:ILE:C	2.22	0.60
1:B:12:SER:HA	1:B:45:SER:O	2.00	0.60
1:D:22:TRP:CZ3	1:D:23:HIS:HD2	2.18	0.60
1:D:22:TRP:CH2	1:D:82:ILE:HG22	2.37	0.60
1:E:82:ILE:HD13	1:E:82:ILE:C	2.22	0.60
1:B:121(A):HIS:O	1:B:121(B):GLU:O	2.20	0.60
1:A:121(C):SER:O	1:A:123:GLU:N	2.35	0.59
1:C:19:GLN:HE22	1:C:31:ARG:HE	1.50	0.59
1:C:22:TRP:HH2	1:C:82:ILE:HG21	1.67	0.59
1:C:85:GLY:HA3	2:C:197:PO4:O3	2.02	0.59
1:D:22:TRP:CZ3	1:D:23:HIS:CD2	2.91	0.59
1:E:25:ASP:OD1	1:E:125:HIS:HE1	1.85	0.59
1:C:107:THR:O	1:C:108:GLU:HB2	2.02	0.59
1:C:82:ILE:CG2	1:C:82:ILE:O	2.51	0.58
1:A:22:TRP:HH2	1:A:82:ILE:HG21	1.67	0.58
1:E:22:TRP:CZ3	1:E:23:HIS:CD2	2.91	0.58
1:C:86:ILE:N	2:C:197:PO4:O4	2.37	0.57
1:A:119:HIS:O	1:A:120:HIS:HB2	2.05	0.57
1:A:82:ILE:CG2	1:A:82:ILE:O	2.53	0.57
1:B:22:TRP:HH2	1:B:82:ILE:HG21	1.68	0.57
1:E:64:LYS:NZ	1:E:106:GLU:OE1	2.34	0.57
1:C:128:PHE:CD2	1:D:87:TYR:OH	2.55	0.56
1:C:50:ILE:HD12	1:C:50:ILE:N	2.20	0.56
1:E:121(A):HIS:O	1:E:121(B):GLU:O	2.23	0.56
1:B:122:LYS:N	1:B:122:LYS:HD2	2.20	0.55
1:B:116:LEU:HD23	1:B:132:PHE:CE1	2.42	0.55
1:D:22:TRP:HH2	1:D:82:ILE:HG21	1.72	0.55
1:A:87:TYR:OH	1:E:128:PHE:HD2	1.89	0.55
1:B:121:PHE:CD2	1:B:128:PHE:HE1	2.19	0.55
1:D:116:LEU:HD23	1:D:132:PHE:CZ	2.41	0.54
1:B:146:ILE:O	1:B:150:ARG:HG3	2.06	0.54
1:B:22:TRP:CZ3	1:B:23:HIS:HD2	2.25	0.54
1:C:122:LYS:HD2	1:C:122:LYS:N	2.22	0.54
1:B:25:ASP:OD1	1:B:125:HIS:HE1	1.89	0.54
1:E:83:ASP:CG	3:E:2045:HOH:O	2.45	0.54
1:B:152:ARG:O	1:B:153:ILE:O	2.26	0.54
1:D:82:ILE:CG2	1:D:82:ILE:O	2.54	0.54
1:A:22:TRP:CZ3	1:A:23:HIS:HD2	2.26	0.54
1:C:121(A):HIS:O	1:C:121(B):GLU:O	2.26	0.53
1:E:22:TRP:HH2	1:E:82:ILE:HG21	1.72	0.53
1:A:116:LEU:HD23	1:A:132:PHE:CZ	2.42	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:PHE:HB2	1:C:128:PHE:CZ	2.43	0.53
1:A:150:ARG:HA	1:A:153:ILE:HG22	1.91	0.53
1:D:152:ARG:CZ	1:D:153:ILE:HD13	2.37	0.53
1:A:21:ARG:NE	1:A:21:ARG:HA	2.23	0.53
1:C:121(C):SER:C	1:C:123:GLU:N	2.62	0.53
1:D:26:ILE:O	1:D:27:VAL:C	2.47	0.53
1:B:50:ILE:N	1:B:50:ILE:HD12	2.23	0.53
1:A:121(B):GLU:O	1:A:121(C):SER:CB	2.43	0.52
1:A:22:TRP:CZ3	1:A:23:HIS:CD2	2.97	0.52
1:D:121(C):SER:O	1:D:124:HIS:N	2.42	0.52
1:A:89:HIS:HD2	2:A:191:PO4:O2	1.92	0.52
1:E:121:PHE:HB2	1:E:128:PHE:CZ	2.44	0.52
1:C:22:TRP:CH2	1:C:82:ILE:CG2	2.88	0.52
1:D:81:VAL:O	1:D:117:THR:HG23	2.10	0.52
1:B:22:TRP:CH2	1:B:82:ILE:CG2	2.86	0.51
1:D:84:GLY:HA3	1:D:120:HIS:CE1	2.45	0.51
1:D:25:ASP:OD1	1:D:125:HIS:CE1	2.61	0.51
1:D:22:TRP:CH2	1:D:82:ILE:CG2	2.93	0.51
1:B:121:PHE:HB2	1:B:128:PHE:CZ	2.46	0.51
1:D:121(C):SER:C	1:D:123:GLU:N	2.64	0.51
1:A:128:PHE:CD2	1:B:87:TYR:OH	2.64	0.51
1:B:82:ILE:C	1:B:82:ILE:CD1	2.78	0.50
1:D:22:TRP:HH2	1:D:82:ILE:HG22	1.76	0.50
1:C:81:VAL:O	1:C:117:THR:HG23	2.10	0.50
1:B:28:ASP:OD2	1:B:31:ARG:NH2	2.38	0.50
1:A:116:LEU:HD23	1:A:132:PHE:CE1	2.47	0.50
1:D:122:LYS:N	1:D:122:LYS:HD2	2.26	0.50
1:D:128:PHE:HD2	1:E:87:TYR:OH	1.93	0.50
1:A:121(A):HIS:O	1:A:121(B):GLU:O	2.29	0.50
1:A:150:ARG:O	1:A:153:ILE:HG22	2.11	0.49
1:D:101:MET:HA	1:D:104:GLN:HE21	1.77	0.49
1:D:116:LEU:HD23	1:D:132:PHE:CE1	2.47	0.49
1:E:28:ASP:OD2	1:E:31:ARG:NH2	2.44	0.49
1:B:82:ILE:CG2	1:B:82:ILE:O	2.60	0.49
1:D:128:PHE:CD2	1:E:87:TYR:OH	2.63	0.49
1:A:51:PHE:HB3	3:A:2036:HOH:O	2.12	0.49
1:A:128:PHE:HD2	1:B:87:TYR:OH	1.95	0.49
1:A:25:ASP:OD1	1:A:125:HIS:CE1	2.64	0.49
1:A:82:ILE:CD1	1:A:82:ILE:C	2.81	0.49
1:B:22:TRP:CZ3	1:B:23:HIS:CD2	3.00	0.49
1:C:82:ILE:CD1	1:C:82:ILE:C	2.80	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:GLU:OE2	1:D:152:ARG:NH1	2.45	0.49
1:E:82:ILE:O	1:E:82:ILE:CG2	2.61	0.49
1:C:119:HIS:N	1:D:86:ILE:O	2.27	0.49
1:B:64:LYS:NZ	1:B:106:GLU:OE1	2.39	0.49
1:D:57:TYR:CB	2:D:198:PO4:O2	2.61	0.48
1:D:19:GLN:NE2	1:D:31:ARG:HE	2.11	0.48
1:E:68:ARG:HH11	1:E:68:ARG:HG2	1.78	0.48
1:C:19:GLN:NE2	1:C:31:ARG:HE	2.10	0.48
1:C:88:ASP:OD1	1:C:90:ASP:OD2	2.32	0.48
1:A:22:TRP:CH2	1:A:82:ILE:CG2	2.89	0.48
1:C:121:PHE:HB2	1:C:128:PHE:CE1	2.48	0.48
1:C:152:ARG:O	1:C:154:ALA:N	2.46	0.48
1:A:28:ASP:OD2	1:A:31:ARG:NH2	2.38	0.48
1:E:68:ARG:HH11	1:E:68:ARG:CG	2.25	0.48
1:B:90:ASP:OD2	1:B:90:ASP:N	2.46	0.48
1:E:21:ARG:HA	1:E:21:ARG:NE	2.28	0.48
1:A:57:TYR:N	2:A:190:PO4:O1	2.43	0.48
1:B:121(C):SER:C	1:B:123:GLU:N	2.65	0.48
1:C:116:LEU:HD23	1:C:132:PHE:CZ	2.49	0.48
1:A:121(C):SER:C	1:A:123:GLU:N	2.67	0.48
1:A:150:ARG:HA	1:A:153:ILE:CG2	2.44	0.48
1:B:121:PHE:HB2	1:B:128:PHE:CE1	2.48	0.48
1:E:85:GLY:HA3	2:E:202:PO4:O3	2.14	0.48
1:A:152:ARG:O	1:A:154:ALA:N	2.47	0.47
1:D:21:ARG:HA	1:D:21:ARG:NE	2.29	0.47
1:E:121(C):SER:C	1:E:123:GLU:N	2.68	0.47
1:B:87:TYR:CD1	1:B:87:TYR:N	2.83	0.47
1:E:101:MET:HA	1:E:104:GLN:HE21	1.79	0.47
1:D:152:ARG:HB3	1:D:152:ARG:HE	1.41	0.47
1:B:68:ARG:HG2	1:B:68:ARG:HH11	1.80	0.47
1:C:146:ILE:O	1:C:150:ARG:HG3	2.15	0.47
1:C:57:TYR:N	2:C:196:PO4:O2	2.43	0.46
1:C:22:TRP:CD2	1:C:23:HIS:HD2	2.33	0.46
1:D:29:GLU:HG3	1:D:133:LYS:HE3	1.97	0.46
1:A:84:GLY:HA3	1:A:120:HIS:CE1	2.51	0.46
1:A:121:PHE:HB2	1:A:128:PHE:CZ	2.50	0.46
1:C:121(C):SER:O	1:C:124:HIS:N	2.49	0.46
1:A:133:LYS:HE3	1:A:133:LYS:HB2	1.74	0.46
1:E:121:PHE:CD1	1:E:121:PHE:C	2.88	0.46
1:A:131:HIS:ND1	1:B:87:TYR:CZ	2.84	0.46
1:B:119:HIS:HB2	1:C:86:ILE:O	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:TRP:CD2	1:E:23:HIS:HD2	2.34	0.46
1:B:19:GLN:HE22	1:B:31:ARG:HE	1.64	0.45
1:B:83:ASP:HA	1:B:89:HIS:HB2	1.98	0.45
1:E:83:ASP:HA	1:E:89:HIS:HB2	1.98	0.45
1:C:85:GLY:HA3	2:C:197:PO4:O1	2.17	0.45
1:E:53:VAL:HG13	1:E:58:GLU:HB2	1.98	0.45
1:A:101:MET:HA	1:A:104:GLN:HE21	1.81	0.45
1:B:124:HIS:O	1:B:127:PHE:N	2.49	0.45
1:E:116:LEU:CD2	1:E:132:PHE:CZ	2.98	0.45
1:C:25:ASP:OD1	1:C:125:HIS:CE1	2.64	0.45
1:D:50:ILE:HD12	1:D:50:ILE:N	2.30	0.45
1:E:135:LYS:NZ	3:E:2032:HOH:O	2.47	0.45
1:E:82:ILE:HD13	1:E:83:ASP:C	2.37	0.45
1:A:150:ARG:HH11	1:A:150:ARG:HD3	1.38	0.45
1:E:22:TRP:CH2	1:E:82:ILE:CG2	2.91	0.45
1:C:101:MET:HA	1:C:104:GLN:HE21	1.82	0.45
1:A:83:ASP:HA	1:A:89:HIS:HB2	1.98	0.45
1:C:38:LEU:HD23	1:C:140:ALA:HB1	1.99	0.45
1:E:122:LYS:HD2	1:E:122:LYS:N	2.32	0.45
1:E:82:ILE:C	1:E:82:ILE:CD1	2.86	0.45
1:D:153:ILE:CG2	1:E:66:LEU:HD21	2.45	0.44
1:A:87:TYR:OH	1:E:128:PHE:CD2	2.63	0.44
1:C:50:ILE:N	1:C:50:ILE:CD1	2.80	0.44
1:E:86:ILE:N	2:E:202:PO4:O3	2.47	0.44
1:B:133:LYS:HB2	1:B:133:LYS:HE3	1.81	0.44
1:A:153:ILE:C	1:A:153:ILE:HD13	2.38	0.44
1:B:128:PHE:CD2	1:C:87:TYR:OH	2.70	0.44
1:C:22:TRP:CZ3	1:C:23:HIS:CD2	3.06	0.44
1:E:54:PRO:HD2	1:E:58:GLU:HG2	1.99	0.44
1:E:84:GLY:HA3	1:E:120:HIS:CE1	2.52	0.44
1:B:19:GLN:NE2	1:B:31:ARG:HE	2.16	0.44
1:C:152:ARG:HB3	1:C:152:ARG:HE	1.34	0.44
1:D:29:GLU:HG3	1:D:133:LYS:CE	2.48	0.44
1:C:87:TYR:HD1	2:C:197:PO4:O4	2.00	0.44
1:D:83:ASP:HA	1:D:89:HIS:HB2	2.00	0.44
1:E:133:LYS:HE3	1:E:133:LYS:HB2	1.74	0.43
1:C:146:ILE:HA	1:C:146:ILE:HD12	1.88	0.43
1:C:87:TYR:N	2:C:197:PO4:O4	2.41	0.43
1:D:90:ASP:N	1:D:90:ASP:OD2	2.49	0.43
1:A:121:PHE:HB2	1:A:128:PHE:CE1	2.53	0.43
1:C:87:TYR:N	1:C:87:TYR:CD1	2.86	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121(A):HIS:C	1:E:121(B):GLU:HG3	2.30	0.43
1:E:121:PHE:HB2	1:E:128:PHE:CE1	2.53	0.43
1:E:78:ALA:HA	1:E:114:VAL:O	2.18	0.43
1:A:144:LEU:HA	1:A:144:LEU:HD23	1.85	0.43
1:D:82:ILE:C	1:D:82:ILE:CD1	2.86	0.43
1:A:107:THR:O	1:A:108:GLU:HB2	2.19	0.43
1:E:121(B):GLU:O	1:E:121(C):SER:CB	2.42	0.43
1:A:78:ALA:HA	1:A:114:VAL:O	2.19	0.43
1:D:133:LYS:HE3	1:D:133:LYS:HB2	1.71	0.43
1:A:22:TRP:CE3	1:A:23:HIS:CD2	2.93	0.43
1:D:121(C):SER:C	1:D:123:GLU:H	2.22	0.43
1:D:121:PHE:HB2	1:D:128:PHE:CZ	2.53	0.43
1:E:121(C):SER:O	1:E:124:HIS:N	2.50	0.43
1:B:22:TRP:CD2	1:B:23:HIS:HD2	2.36	0.43
1:B:50:ILE:N	1:B:50:ILE:CD1	2.81	0.43
1:D:121(C):SER:HG	1:D:123:GLU:HB2	1.79	0.42
1:A:121:PHE:CD1	1:A:121:PHE:C	2.90	0.42
1:A:87:TYR:N	1:A:87:TYR:CD1	2.87	0.42
1:C:83:ASP:HA	1:C:89:HIS:HB2	2.01	0.42
1:A:119:HIS:HB2	1:B:86:ILE:O	2.19	0.42
1:C:84:GLY:HA3	1:C:120:HIS:CE1	2.54	0.42
1:C:133:LYS:HE3	1:C:133:LYS:HB2	1.81	0.42
1:B:25:ASP:OD1	1:B:125:HIS:CE1	2.72	0.42
1:C:82:ILE:HD13	1:C:83:ASP:N	2.34	0.42
1:D:22:TRP:CE3	1:D:23:HIS:CD2	2.89	0.42
1:E:29:GLU:HG3	1:E:133:LYS:HE3	2.02	0.42
1:E:47:GLU:H	1:E:47:GLU:HG2	1.70	0.42
1:B:121(C):SER:O	1:B:124:HIS:N	2.52	0.42
1:B:68:ARG:HG2	1:B:68:ARG:NH1	2.35	0.42
1:C:21:ARG:HA	1:C:21:ARG:NE	2.35	0.42
1:D:78:ALA:HA	1:D:114:VAL:O	2.20	0.42
1:E:22:TRP:CE3	1:E:23:HIS:CD2	2.92	0.42
1:C:22:TRP:CZ3	1:C:23:HIS:HD2	2.37	0.42
1:A:88:ASP:OD1	1:A:90:ASP:OD2	2.37	0.42
1:C:19:GLN:O	1:C:19:GLN:HG3	2.20	0.42
1:A:152:ARG:C	1:A:154:ALA:H	2.22	0.42
1:B:153:ILE:HB	1:B:154:ALA:H	1.51	0.42
1:A:121(C):SER:O	1:A:124:HIS:N	2.52	0.41
1:E:110:PRO:HG3	1:E:150:ARG:HD2	2.01	0.41
1:A:90:ASP:N	1:A:90:ASP:OD2	2.53	0.41
1:D:121:PHE:HB2	1:D:128:PHE:CE1	2.55	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LEU:HD23	1:B:144:LEU:HA	1.83	0.41
1:C:121(C):SER:C	1:C:123:GLU:H	2.23	0.41
1:C:121:PHE:CB	1:C:128:PHE:CZ	3.03	0.41
1:B:131:HIS:ND1	1:C:87:TYR:CZ	2.89	0.41
1:C:152:ARG:C	1:C:154:ALA:H	2.24	0.41
1:C:149:GLU:OE2	1:C:152:ARG:NH1	2.54	0.41
1:E:150:ARG:HH11	1:E:150:ARG:HD3	1.51	0.41
1:B:105:LEU:HA	1:B:105:LEU:HD23	1.84	0.41
1:D:38:LEU:HD23	1:D:140:ALA:HB1	2.02	0.41
1:A:152:ARG:HE	1:A:152:ARG:HB3	1.23	0.41
1:E:152:ARG:HB3	1:E:152:ARG:HE	1.33	0.41
1:C:121(B):GLU:O	1:C:121(C):SER:CB	2.44	0.41
1:B:124:HIS:O	1:B:127:PHE:HB3	2.21	0.41
1:B:82:ILE:HD13	1:B:83:ASP:C	2.41	0.41
1:C:121(C):SER:O	1:C:122:LYS:C	2.59	0.41
1:C:82:ILE:HD13	1:C:83:ASP:C	2.41	0.41
1:E:26:ILE:O	1:E:27:VAL:C	2.57	0.41
1:A:21:ARG:HA	1:A:21:ARG:HE	1.86	0.40
1:C:49:GLU:C	1:C:50:ILE:HD12	2.42	0.40
1:B:128:PHE:HD2	1:C:87:TYR:OH	2.04	0.40
1:A:150:ARG:CA	1:A:153:ILE:HG22	2.52	0.40
1:D:105:LEU:HD23	1:D:105:LEU:HA	1.76	0.40
1:B:150:ARG:HD3	1:B:150:ARG:HH11	1.60	0.40
1:E:149:GLU:OE2	1:E:152:ARG:NH1	2.54	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	146/158 (92%)	132 (90%)	8 (6%)	6 (4%)	<b>3</b> <b>7</b>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	146/158 (92%)	135 (92%)	4 (3%)	7 (5%)	2	5
1	C	144/158 (91%)	133 (92%)	5 (4%)	6 (4%)	3	7
1	D	145/158 (92%)	136 (94%)	3 (2%)	6 (4%)	3	7
1	E	144/158 (91%)	134 (93%)	5 (4%)	5 (4%)	4	9
All	All	725/790 (92%)	670 (92%)	25 (3%)	30 (4%)	3	7

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	121(B)	GLU
1	A	121(C)	SER
1	A	122	LYS
1	B	120	HIS
1	B	121(B)	GLU
1	B	121(C)	SER
1	B	122	LYS
1	B	153	ILE
1	B	154	ALA
1	C	120	HIS
1	C	121(B)	GLU
1	C	121(C)	SER
1	C	122	LYS
1	D	120	HIS
1	D	121(B)	GLU
1	D	121(C)	SER
1	D	122	LYS
1	E	120	HIS
1	E	121(B)	GLU
1	E	121(C)	SER
1	E	122	LYS
1	A	153	ILE
1	C	153	ILE
1	A	44	GLY
1	C	44	GLY
1	B	44	GLY
1	D	44	GLY
1	E	44	GLY
1	D	54	PRO

### 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	116/126 (92%)	100 (86%)	16 (14%)	4	10
1	B	116/126 (92%)	103 (89%)	13 (11%)	7	16
1	C	115/126 (91%)	101 (88%)	14 (12%)	6	13
1	D	116/126 (92%)	99 (85%)	17 (15%)	3	9
1	E	115/126 (91%)	101 (88%)	14 (12%)	6	13
All	All	578/630 (92%)	504 (87%)	74 (13%)	5	12

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	14	LYS
1	A	37	GLU
1	A	38	LEU
1	A	53	VAL
1	A	82	ILE
1	A	116	LEU
1	A	119	HIS
1	A	120	HIS
1	A	121	PHE
1	A	121(B)	GLU
1	A	121(C)	SER
1	A	122	LYS
1	A	123	GLU
1	A	125	HIS
1	A	153	ILE
1	B	14	LYS
1	B	37	GLU
1	B	38	LEU
1	B	53	VAL
1	B	68	ARG
1	B	82	ILE
1	B	116	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	119	HIS
1	B	121	PHE
1	B	121(B)	GLU
1	B	121(C)	SER
1	B	122	LYS
1	B	125	HIS
1	C	14	LYS
1	C	37	GLU
1	C	38	LEU
1	C	53	VAL
1	C	68	ARG
1	C	82	ILE
1	C	116	LEU
1	C	119	HIS
1	C	121	PHE
1	C	121(B)	GLU
1	C	121(C)	SER
1	C	122	LYS
1	C	123	GLU
1	C	125	HIS
1	D	11	THR
1	D	14	LYS
1	D	37	GLU
1	D	38	LEU
1	D	53	VAL
1	D	68	ARG
1	D	82	ILE
1	D	116	LEU
1	D	118	PRO
1	D	119	HIS
1	D	120	HIS
1	D	121	PHE
1	D	121(B)	GLU
1	D	121(C)	SER
1	D	122	LYS
1	D	123	GLU
1	D	125	HIS
1	E	12	SER
1	E	14	LYS
1	E	37	GLU
1	E	38	LEU
1	E	53	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	68	ARG
1	E	82	ILE
1	E	116	LEU
1	E	119	HIS
1	E	121	PHE
1	E	121(B)	GLU
1	E	121(C)	SER
1	E	122	LYS
1	E	125	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	23	HIS
1	A	89	HIS
1	A	98	ASN
1	A	104	GLN
1	A	125	HIS
1	B	19	GLN
1	B	23	HIS
1	B	89	HIS
1	B	98	ASN
1	B	119	HIS
1	B	121(A)	HIS
1	B	125	HIS
1	C	19	GLN
1	C	23	HIS
1	C	89	HIS
1	C	98	ASN
1	C	104	GLN
1	C	119	HIS
1	C	125	HIS
1	D	19	GLN
1	D	23	HIS
1	D	98	ASN
1	D	104	GLN
1	D	125	HIS
1	E	19	GLN
1	E	23	HIS
1	E	98	ASN
1	E	104	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	119	HIS
1	E	125	HIS

### 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 ⓘ

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PO4	A	190	-	4,4,4	1.17	0	6,6,6	0.45	0
2	PO4	A	191	-	4,4,4	1.21	0	6,6,6	0.51	0
2	PO4	A	192	-	4,4,4	1.90	1 (25%)	6,6,6	0.57	0
2	PO4	B	193	-	4,4,4	1.00	0	6,6,6	0.41	0
2	PO4	B	194	-	4,4,4	1.08	0	6,6,6	0.39	0
2	PO4	B	195	-	4,4,4	1.71	2 (50%)	6,6,6	0.42	0
2	PO4	C	196	-	4,4,4	1.09	0	6,6,6	0.51	0
2	PO4	C	197	-	4,4,4	1.46	0	6,6,6	0.43	0
2	PO4	D	198	-	4,4,4	1.20	1 (25%)	6,6,6	0.41	0
2	PO4	D	199	-	4,4,4	1.79	1 (25%)	6,6,6	0.51	0
2	PO4	E	200	-	4,4,4	1.12	0	6,6,6	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PO4	E	201	-	4,4,4	1.10	0	6,6,6	0.38	0
2	PO4	E	202	-	4,4,4	1.38	0	6,6,6	0.42	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
2	PO4	A	190	-	-	0/0/0/0	0/0/0/0
2	PO4	A	191	-	-	0/0/0/0	0/0/0/0
2	PO4	A	192	-	-	0/0/0/0	0/0/0/0
2	PO4	B	193	-	-	0/0/0/0	0/0/0/0
2	PO4	B	194	-	-	0/0/0/0	0/0/0/0
2	PO4	B	195	-	-	0/0/0/0	0/0/0/0
2	PO4	C	196	-	-	0/0/0/0	0/0/0/0
2	PO4	C	197	-	-	0/0/0/0	0/0/0/0
2	PO4	D	198	-	-	0/0/0/0	0/0/0/0
2	PO4	D	199	-	-	0/0/0/0	0/0/0/0
2	PO4	E	200	-	-	0/0/0/0	0/0/0/0
2	PO4	E	201	-	-	0/0/0/0	0/0/0/0
2	PO4	E	202	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	192	PO4	P-O2	-2.43	1.45	1.54
2	B	195	PO4	P-O2	-2.37	1.46	1.54
2	D	198	PO4	P-O2	-2.25	1.46	1.54
2	D	199	PO4	P-O3	-2.25	1.46	1.54
2	B	195	PO4	P-O4	-2.14	1.46	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	190	PO4	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	191	PO4	1	0
2	A	192	PO4	2	0
2	B	194	PO4	1	0
2	B	195	PO4	2	0
2	C	196	PO4	2	0
2	C	197	PO4	6	0
2	D	198	PO4	3	0
2	D	199	PO4	2	0
2	E	202	PO4	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.