



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:55 PM GMT

PDB ID : 1MJG  
Title : CRYSTAL STRUCTURE OF BIFUNCTIONAL CARBON MONOXIDE  
DEHYDROGENASE / ACETYL-COA SYNTHASE(CODH/ACS)  
FROM MOORELLA THERMOACETICA (F. CLOSTRIDIUM THER-  
MOACETICUM)  
Authors : Doukov, T.I.; Iverson, T.M.; Seravalli, J.; Ragsdale, S.W.; Drennan, C.L.  
Deposited on : 2002-08-27  
Resolution : 2.20 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

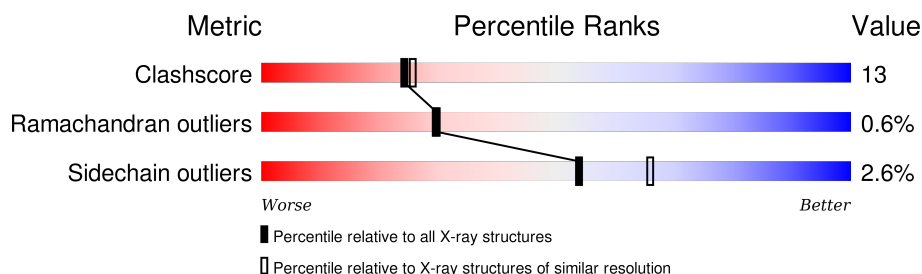
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)


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	674	 78% 20% •
1	B	674	 78% 20% •
1	C	674	 78% 20% •
1	D	674	 78% 21% •
2	M	729	 77% 21% •
2	N	729	 77% 21% •
2	O	729	 72% 26% •

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	P	729	 <div>75% 24%</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
5	ACT	M	950	-	-	X	-
5	ACT	N	950	-	-	X	-
7	XCC	A	800	-	-	X	-
7	XCC	C	800	-	-	X	-
7	XCC	D	800	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 44653 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 CARBON MONOXIDE DEHYDROGENASE BETA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	S	0	0	0
			5087	3197	890	958	42			
1	B	672	Total	C	N	O	S	0	0	0
			5087	3197	890	958	42			
1	C	672	Total	C	N	O	S	0	0	0
			5087	3197	890	958	42			
1	D	672	Total	C	N	O	S	0	0	0
			5087	3197	890	958	42			

- Molecule 2 is a protein called Carbon monoxide dehydrogenase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	728	Total	C	N	O	S	0	0	0
			5735	3678	953	1069	35			
2	N	728	Total	C	N	O	S	0	0	0
			5735	3678	953	1069	35			
2	O	728	Total	C	N	O	S	0	0	0
			5735	3678	953	1069	35			
2	P	728	Total	C	N	O	S	0	0	0
			5735	3678	953	1069	35			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	685	SER	ARG	SEE REMARK 999	UNP P27988
N	685	SER	ARG	SEE REMARK 999	UNP P27988
O	685	SER	ARG	SEE REMARK 999	UNP P27988
P	685	SER	ARG	SEE REMARK 999	UNP P27988

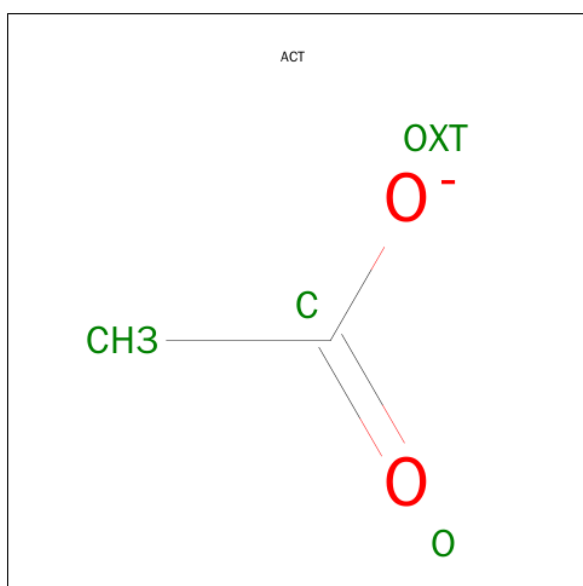
- Molecule 3 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total Cu 1 1	0	0
3	O	1	Total Cu 1 1	0	0
3	N	1	Total Cu 1 1	0	0
3	M	1	Total Cu 1 1	0	0

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total Ni 1 1	0	0
4	O	1	Total Ni 1 1	0	0
4	N	1	Total Ni 1 1	0	0
4	M	1	Total Ni 1 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



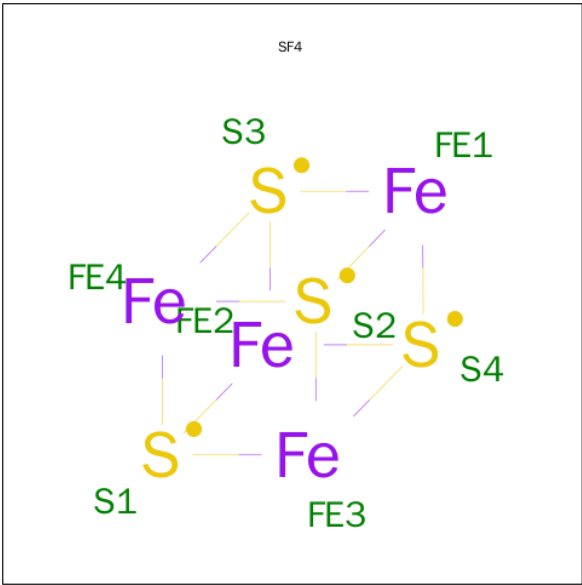
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total C O 3 2 1	0	0
5	N	1	Total C O 3 2 1	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	O	1	Total	C	O	0	0
			3	2	1		
5	P	1	Total	C	O	0	0
			3	2	1		

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



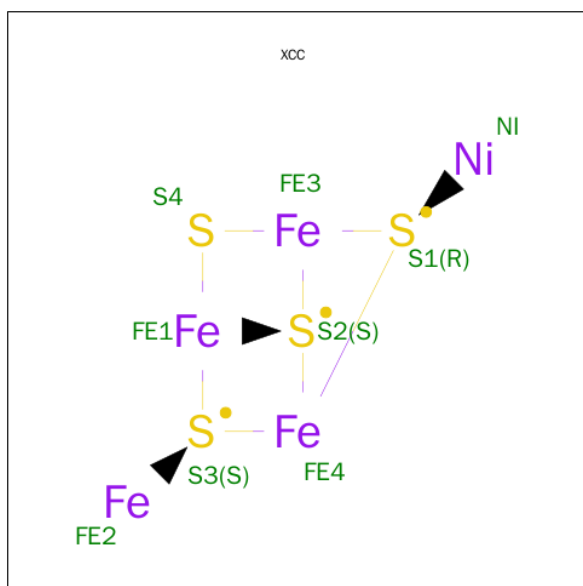
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	C	1	Total	Fe	S	0	0
			8	4	4		
6	C	1	Total	Fe	S	0	0
			8	4	4		
6	D	1	Total	Fe	S	0	0
			8	4	4		
6	M	1	Total	Fe	S	0	0
			8	4	4		
6	N	1	Total	Fe	S	0	0
			8	4	4		
6	O	1	Total	Fe	S	0	0
			8	4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	P	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 7 is FE(4)-NI(1)-S(4) CLUSTER (three-letter code: XCC) (formula:  $\text{Fe}_4\text{NiS}_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
7	B	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
7	C	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
7	D	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	179	Total	O	0	0
			179	179		
8	B	217	Total	O	0	0
			217	217		
8	C	148	Total	O	0	0
			148	148		
8	D	131	Total	O	0	0
			131	131		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	206	Total 206	O 206	0	0
8	N	221	Total 221	O 221	0	0
8	O	26	Total 26	O 26	0	0
8	P	101	Total 101	O 101	0	0

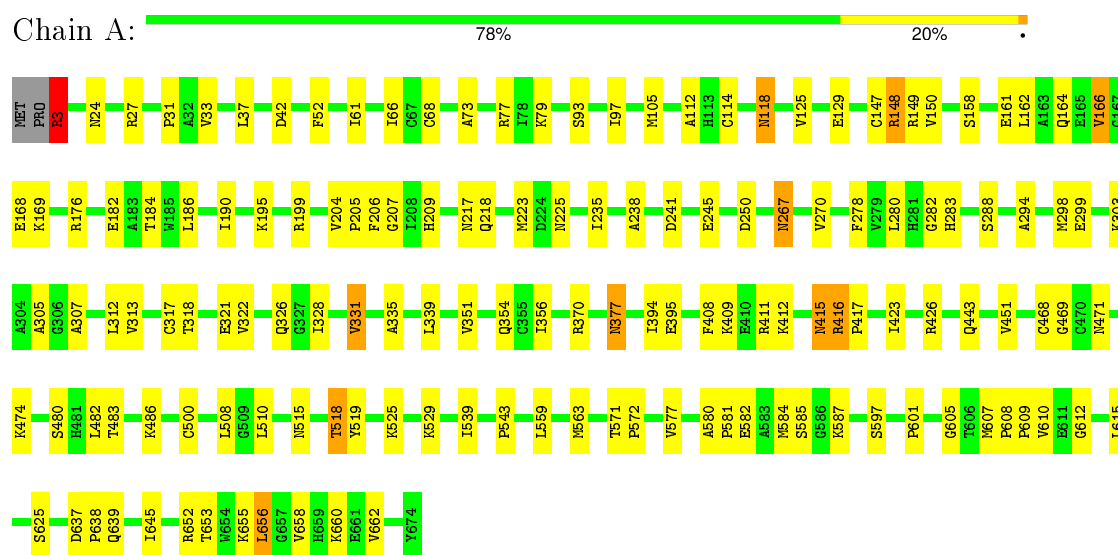


### 3 Residue-property plots

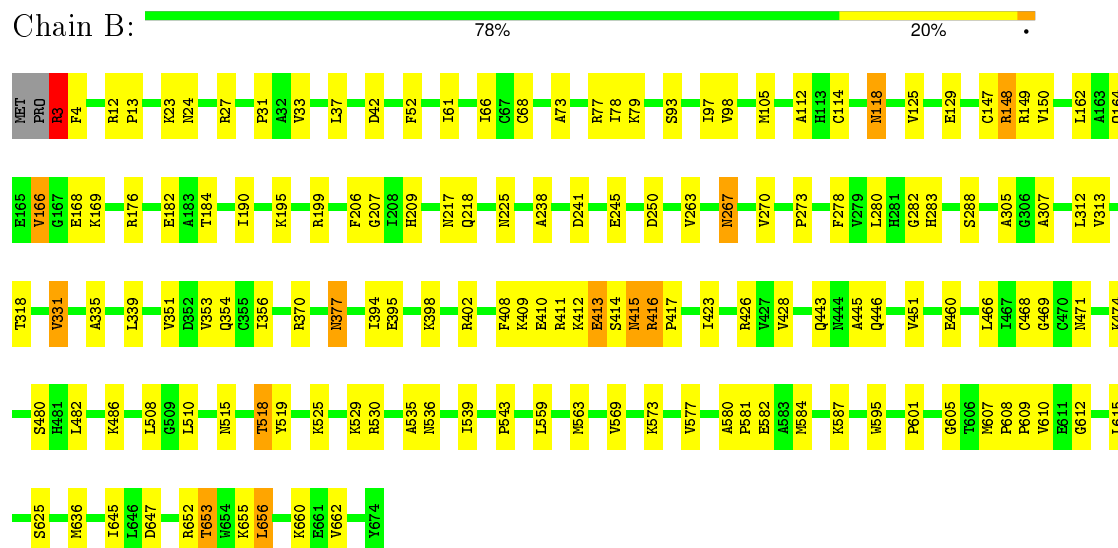
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

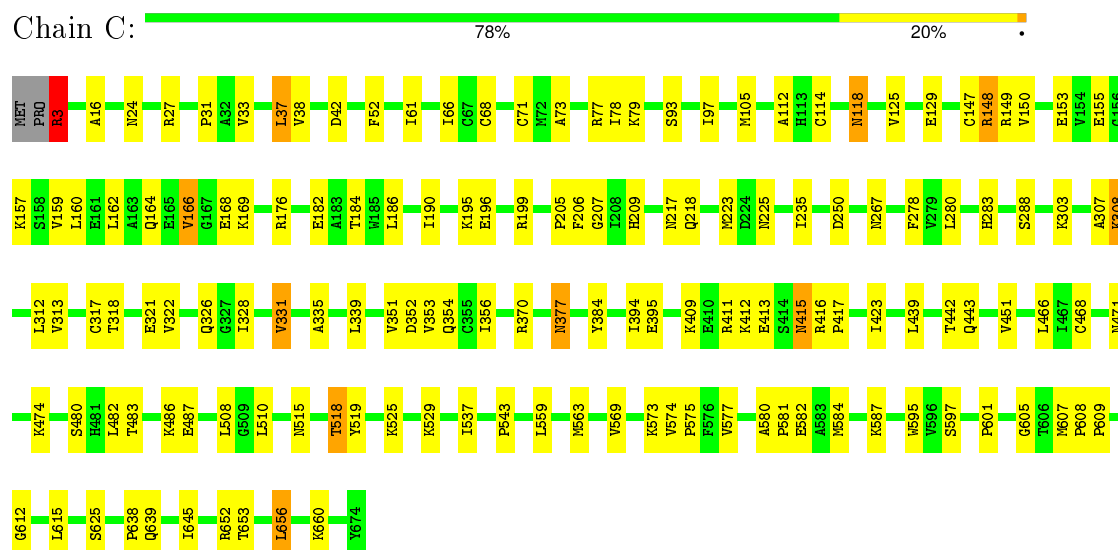
#### • Molecule 1: CARBON MONOXIDE DEHYDROGENASE BETA SUBUNIT



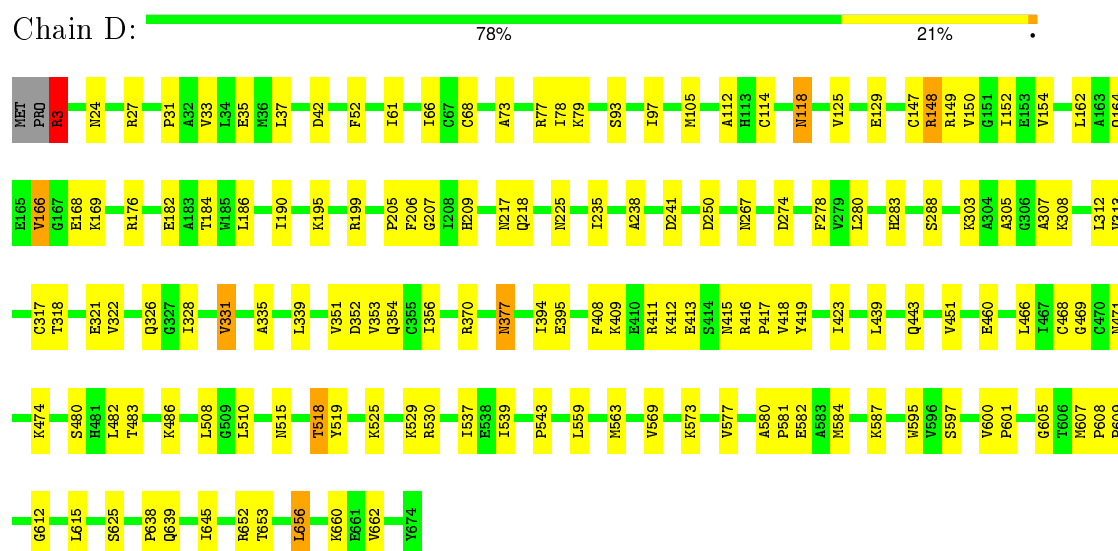
#### • Molecule 1: CARBON MONOXIDE DEHYDROGENASE BETA SUBUNIT



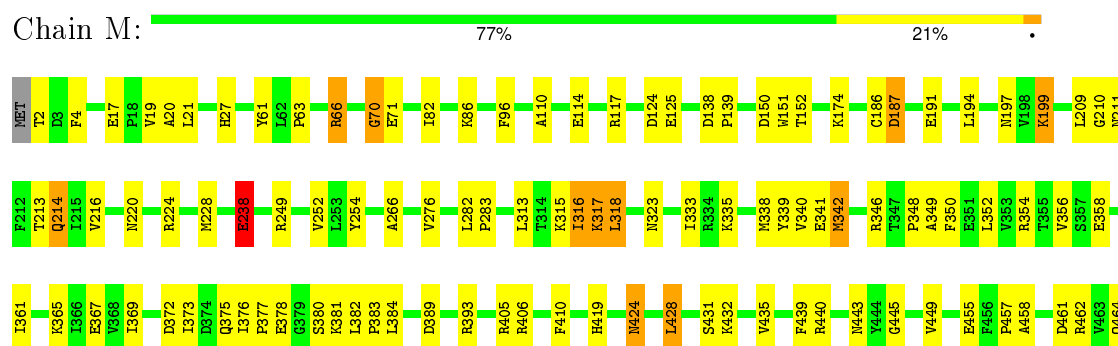
• Molecule 1: CARBON MONOXIDE DEHYDROGENASE BETA SUBUNIT

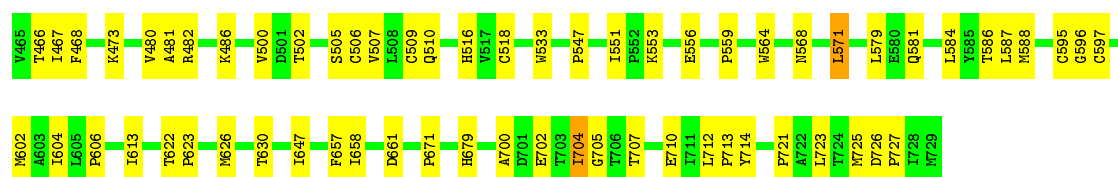


• Molecule 1: CARBON MONOXIDE DEHYDROGENASE BETA SUBUNIT



• Molecule 2: Carbon monoxide dehydrogenase alpha subunit





Q705	WET	L209	E358	A458	W568	W609	W626	W630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
I706	T2	G210	T361	D461	L571	T613	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
I707	D3	M211	T362	R462	W572	W613	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
E710	F4	F212	D363	Q463	W579	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
I711	P13	T213	Q364	Q464	W579	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
I712	Q214	Q214	Q364	Q464	W579	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
P713	D115	D115	Q365	Q465	W579	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
Y714	V216	V216	Q366	Q466	W579	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	N220	N220	Q367	Q467	W579	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	L21	L21	Q368	Q468	W579	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	E27	E27	Q369	Q469	W579	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	W61	W61	D372	E471	W585	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	L62	L62	L373	A472	W586	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	P63	P63	D374	K473	W587	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	R66	R66	Q375	Q474	W588	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	G70	G70	E376	E476	W595	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	E71	E71	E377	E477	W596	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	I82	I82	E378	E478	W602	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	K86	K86	S379	V480	W603	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	R87	R87	A481	A481	W604	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	A88	A88	R482	R482	W605	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	F96	F96	K381	K381	W606	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	A110	A110	L382	L382	W607	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	E114	E114	P383	P383	W608	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	R117	R117	L384	L384	W609	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	D124	D124	D389	D389	W610	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	E125	E125	R393	R393	W611	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	D138	D138	F399	F399	W612	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	P139	P139	L403	L403	W613	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	D150	D150	R406	R406	W614	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	H153	H153	F410	F410	W615	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	T152	T152	H419	H419	W616	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	R162	R162	N424	N424	W617	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	K167	K167	L428	L428	W618	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	K174	K174	S431	S431	W619	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	C186	C186	K432	K432	W620	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	D187	D187	V435	V435	W621	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	E188	E188	F439	F439	W622	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	L194	L194	R440	R440	W623	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
	K199	K199	G445	G445	W624	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
			V449	V449	W625	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
			E455	E455	W626	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
			F456	F456	W627	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
			P457	P457	W628	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704
					W629	W622	A603	T630	Q640	T647	F657	S658	A660	W666	P671	W679	W684	A700	W701	W702	W703	I704

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.75Å 136.97Å 141.53Å 101.45° 109.05° 103.94°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	90.6 (20.00-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.215 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	44653	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	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: XCC, SF4, ACT, CU1, NI

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	0.38	0/5179	0.61	1/7017 (0.0%)
1	B	0.39	0/5179	0.62	1/7017 (0.0%)
1	C	0.36	0/5179	0.61	2/7017 (0.0%)
1	D	0.34	0/5179	0.60	1/7017 (0.0%)
2	M	0.36	0/5869	0.61	3/7948 (0.0%)
2	N	0.37	0/5869	0.61	0/7948
2	O	0.30	0/5869	0.58	1/7948 (0.0%)
2	P	0.32	0/5869	0.59	0/7948
All	All	0.35	0/44192	0.60	9/59860 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	A	3	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	D	3	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	3	ARG	NE-CZ-NH2	6.54	123.57	120.30
2	M	238	GLU	CA-CB-CG	6.13	126.88	113.40
2	M	595	CYS	C-N-CA	-5.21	111.37	122.30
2	O	70	GLY	N-CA-C	5.19	126.08	113.10
2	M	70	GLY	N-CA-C	5.08	125.79	113.10
1	C	196	GLU	CA-CB-CG	5.01	124.42	113.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5087	0	5089	126	0
1	B	5087	0	5089	139	0
1	C	5087	0	5089	128	0
1	D	5087	0	5089	118	0
2	M	5735	0	5693	155	0
2	N	5735	0	5693	148	0
2	O	5735	0	5693	190	0
2	P	5735	0	5693	166	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
5	M	3	0	3	2	0
5	N	3	0	3	2	0
5	O	3	0	3	1	0
5	P	3	0	3	1	0
6	A	16	0	0	0	0
6	B	8	0	0	0	0
6	C	16	0	0	0	0
6	D	8	0	0	0	0
6	M	8	0	0	0	0
6	N	8	0	0	0	0
6	O	8	0	0	0	0
6	P	8	0	0	0	0
7	A	9	0	0	3	0
7	B	9	0	0	1	0
7	C	9	0	0	2	0
7	D	9	0	0	2	0
8	A	179	0	0	3	0
8	B	217	0	0	6	0
8	C	148	0	0	3	0
8	D	131	0	0	0	0
8	M	206	0	0	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	N	221	0	0	7	0
8	O	26	0	0	0	0
8	P	101	0	0	1	0
All	All	44653	0	43140	1127	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 13.

All (1127) 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)
2:O:335:LYS:HD2	2:O:335:LYS:H	1.21	1.06
2:M:335:LYS:H	2:M:335:LYS:HD2	1.20	1.03
2:P:335:LYS:HD2	2:P:335:LYS:H	1.21	1.03
1:B:446:GLN:HE22	1:C:38:VAL:HG11	1.22	1.02
2:N:335:LYS:HD2	2:N:335:LYS:H	1.20	1.02
1:A:426:ARG:NH2	1:A:539:ILE:HG13	1.81	0.93
1:B:3:ARG:HH12	1:B:625:SER:CB	1.83	0.92
1:B:3:ARG:HG2	1:B:3:ARG:HH21	1.35	0.91
2:M:318:LEU:HD23	2:M:318:LEU:H	1.35	0.89
1:B:446:GLN:HE22	1:C:38:VAL:CG1	1.86	0.88
2:M:213:THR:O	2:M:216:VAL:HG23	1.73	0.88
2:P:318:LEU:H	2:P:318:LEU:HD23	1.38	0.88
1:A:3:ARG:NH2	1:A:625:SER:OG	2.06	0.88
1:B:263:VAL:HG22	1:B:539:ILE:HD12	1.57	0.87
1:B:428:VAL:HG22	1:B:539:ILE:HD11	1.55	0.86
2:N:71:GLU:HG3	2:N:82:ILE:HD11	1.56	0.86
2:N:213:THR:O	2:N:216:VAL:HG23	1.75	0.85
2:P:213:THR:O	2:P:216:VAL:HG23	1.76	0.85
1:D:274:ASP:HB2	1:D:308:LYS:HE2	1.54	0.85
2:M:602:MET:HE2	2:M:647:ILE:HD13	1.58	0.85
2:N:478:MET:O	2:N:482:ARG:HG2	1.77	0.84
1:B:446:GLN:NE2	1:C:38:VAL:HG11	1.92	0.84
2:P:602:MET:HE2	2:P:647:ILE:HD13	1.59	0.84
1:B:313:VAL:HB	1:B:331:VAL:HG22	1.60	0.83
2:M:71:GLU:HG3	2:M:82:ILE:HD11	1.61	0.82
1:D:313:VAL:HB	1:D:331:VAL:HG22	1.59	0.82
1:B:412:LYS:HD3	1:B:416:ARG:HD3	1.61	0.82
2:O:213:THR:O	2:O:216:VAL:HG23	1.79	0.82
1:A:313:VAL:HB	1:A:331:VAL:HG22	1.61	0.82
1:B:482:LEU:HD12	1:B:486:LYS:HE3	1.62	0.81

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:602:MET:HE2	2:N:647:ILE:HD13	1.62	0.81
1:A:3:ARG:HH22	1:A:625:SER:CB	1.93	0.80
1:B:93:SER:H	1:B:225:ASN:HD21	1.29	0.80
2:M:187:ASP:HA	2:M:211:ASN:HD22	1.46	0.80
1:B:426:ARG:HH21	1:B:539:ILE:HG13	1.47	0.80
2:O:602:MET:HE2	2:O:647:ILE:HD13	1.61	0.80
1:C:93:SER:H	1:C:225:ASN:HD21	1.30	0.79
1:C:313:VAL:HB	1:C:331:VAL:HG22	1.62	0.79
1:C:3:ARG:HH12	1:C:625:SER:CB	1.95	0.79
1:B:263:VAL:CG2	1:B:539:ILE:HD12	2.13	0.78
2:P:71:GLU:HG3	2:P:82:ILE:HD11	1.64	0.77
2:P:700:ALA:HB1	2:P:704:ILE:HD11	1.67	0.77
2:P:604:ILE:O	2:P:604:ILE:HD12	1.84	0.77
1:A:482:LEU:HD12	1:A:486:LYS:HE3	1.67	0.77
1:A:426:ARG:HH22	1:A:539:ILE:HG13	1.50	0.77
1:D:93:SER:H	1:D:225:ASN:HD21	1.31	0.77
1:C:411:ARG:HG2	1:C:416:ARG:HD3	1.68	0.76
2:N:187:ASP:HA	2:N:211:ASN:HD22	1.50	0.76
2:O:187:ASP:HA	2:O:211:ASN:HD22	1.47	0.76
2:P:335:LYS:H	2:P:335:LYS:CD	1.99	0.75
2:O:604:ILE:O	2:O:604:ILE:HD12	1.86	0.75
2:P:187:ASP:HA	2:P:211:ASN:HD22	1.50	0.75
2:O:497:ASP:HA	2:O:500:VAL:HG12	1.67	0.75
1:D:482:LEU:HD12	1:D:486:LYS:HE3	1.67	0.75
1:B:150:VAL:HG11	1:B:169:LYS:HG2	1.68	0.75
2:O:352:LEU:HD22	2:O:481:ALA:HB2	1.69	0.75
2:N:335:LYS:CD	2:N:335:LYS:H	1.98	0.75
2:O:110:ALA:HB1	2:O:216:VAL:HG21	1.68	0.74
2:O:110:ALA:HB1	2:O:216:VAL:CG2	2.17	0.74
2:N:110:ALA:HB1	2:N:216:VAL:CG2	2.18	0.74
2:O:342:MET:HG3	2:O:384:LEU:HD22	1.69	0.74
2:M:604:ILE:HD12	2:M:604:ILE:O	1.87	0.74
1:C:482:LEU:HD12	1:C:486:LYS:HE3	1.69	0.74
1:B:148:ARG:HH11	1:B:148:ARG:HB3	1.52	0.74
1:A:93:SER:H	1:A:225:ASN:HD21	1.34	0.74
2:O:71:GLU:HG3	2:O:82:ILE:HD11	1.69	0.74
1:A:283:HIS:N	1:A:318:THR:HG23	2.03	0.74
1:A:148:ARG:HH11	1:A:148:ARG:HB3	1.52	0.74
1:B:3:ARG:NH1	1:B:625:SER:OG	2.19	0.73
2:P:110:ALA:HB1	2:P:216:VAL:CG2	2.18	0.73
2:M:342:MET:HG3	2:M:384:LEU:HD22	1.69	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:VAL:HG21	1:B:645:ILE:HG23	1.69	0.73
2:N:71:GLU:HG3	2:N:82:ILE:CD1	2.17	0.73
1:C:150:VAL:HG11	1:C:169:LYS:HG2	1.70	0.73
1:A:150:VAL:HG11	1:A:169:LYS:HG2	1.70	0.73
1:D:615:LEU:HD23	2:P:27:HIS:HB3	1.69	0.73
2:O:335:LYS:H	2:O:335:LYS:CD	1.99	0.73
1:D:150:VAL:HG11	1:D:169:LYS:HG2	1.69	0.73
1:D:411:ARG:NH1	1:D:416:ARG:HH21	1.86	0.73
2:N:377:PRO:HG2	2:N:380:SER:HB3	1.71	0.73
1:D:148:ARG:HH11	1:D:148:ARG:HB3	1.54	0.72
1:B:283:HIS:N	1:B:318:THR:HG23	2.04	0.72
2:M:71:GLU:HG3	2:M:82:ILE:CD1	2.19	0.72
1:A:577:VAL:HG21	1:A:645:ILE:HG23	1.72	0.72
1:C:148:ARG:HH11	1:C:148:ARG:HB3	1.55	0.72
2:P:377:PRO:HG2	2:P:380:SER:HB3	1.72	0.72
2:P:71:GLU:HG3	2:P:82:ILE:CD1	2.20	0.71
1:C:577:VAL:HG21	1:C:645:ILE:HG23	1.72	0.71
1:B:469:GLY:HA3	8:B:889:HOH:O	1.90	0.70
1:D:3:ARG:HH22	1:D:625:SER:CB	2.03	0.70
1:C:283:HIS:N	1:C:318:THR:HG23	2.05	0.70
2:N:342:MET:HG3	2:N:384:LEU:HD22	1.72	0.70
1:C:412:LYS:NZ	1:C:416:ARG:HH21	1.88	0.70
2:N:63:PRO:HB2	2:N:220:ASN:HB2	1.73	0.70
1:D:283:HIS:N	1:D:318:THR:HG23	2.07	0.70
2:O:377:PRO:HG2	2:O:380:SER:HB3	1.72	0.70
2:O:63:PRO:HB2	2:O:220:ASN:HB2	1.73	0.70
2:O:342:MET:HG2	2:O:428:LEU:HB2	1.72	0.70
1:B:23:LYS:HD3	8:B:851:HOH:O	1.92	0.70
2:M:110:ALA:HB1	2:M:216:VAL:CG2	2.22	0.70
2:N:586:THR:HG22	2:N:588:MET:H	1.57	0.70
1:B:3:ARG:NH1	1:B:625:SER:CB	2.55	0.70
2:P:342:MET:HG3	2:P:384:LEU:HD22	1.72	0.70
1:D:577:VAL:HG21	1:D:645:ILE:HG23	1.73	0.70
2:M:335:LYS:H	2:M:335:LYS:CD	1.99	0.69
2:O:110:ALA:CB	2:O:216:VAL:HG21	2.22	0.69
1:C:412:LYS:HZ2	1:C:416:ARG:HH21	1.40	0.69
2:O:365:LYS:HB3	2:O:464:GLN:HG3	1.74	0.69
2:P:365:LYS:HB3	2:P:464:GLN:HG3	1.74	0.69
2:O:338:MET:SD	2:O:341:GLU:HB2	2.33	0.69
2:P:318:LEU:H	2:P:318:LEU:CD2	2.03	0.69
1:B:426:ARG:NH2	1:B:539:ILE:HG13	2.07	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLU:OE2	1:B:199:ARG:HD3	1.93	0.69
1:B:263:VAL:HG22	1:B:539:ILE:CD1	2.23	0.69
2:N:335:LYS:HD2	2:N:335:LYS:N	2.02	0.69
2:M:377:PRO:HG2	2:M:380:SER:HB3	1.73	0.69
2:P:342:MET:HG2	2:P:428:LEU:HB2	1.74	0.68
2:N:365:LYS:HB3	2:N:464:GLN:HG3	1.75	0.68
1:B:411:ARG:O	1:B:416:ARG:HB3	1.93	0.68
2:M:586:THR:HG22	2:M:588:MET:H	1.58	0.68
2:P:369:ILE:HG21	2:P:473:LYS:HD2	1.75	0.68
1:B:415:ASN:O	1:B:417:PRO:HD3	1.94	0.68
2:P:335:LYS:HD2	2:P:335:LYS:N	2.04	0.68
1:B:428:VAL:CG2	1:B:539:ILE:HD11	2.24	0.68
2:N:342:MET:HG2	2:N:428:LEU:HB2	1.74	0.68
2:N:500:VAL:HG21	2:N:533:TRP:CZ2	2.28	0.68
1:C:615:LEU:HD23	2:O:27:HIS:HB3	1.74	0.68
1:A:112:ALA:HA	1:B:217:ASN:HD22	1.57	0.68
2:M:342:MET:HG2	2:M:428:LEU:HB2	1.76	0.68
1:A:607:MET:HE3	1:A:608:PRO:HD2	1.74	0.68
1:D:482:LEU:HD21	1:D:508:LEU:HD12	1.75	0.67
1:B:3:ARG:CG	1:B:3:ARG:HH21	2.07	0.67
2:P:63:PRO:HB2	2:P:220:ASN:HB2	1.75	0.67
1:C:607:MET:HE3	1:C:608:PRO:HD2	1.76	0.67
2:O:71:GLU:HG3	2:O:82:ILE:CD1	2.25	0.67
1:D:411:ARG:HH12	1:D:416:ARG:HH21	1.42	0.67
2:O:439:PHE:O	2:O:440:ARG:HD2	1.95	0.67
1:B:416:ARG:HG3	1:B:416:ARG:O	1.93	0.67
2:P:338:MET:SD	2:P:341:GLU:HB2	2.34	0.67
2:O:500:VAL:HG21	2:O:533:TRP:CZ2	2.30	0.67
2:P:439:PHE:O	2:P:440:ARG:HD2	1.95	0.67
1:D:182:GLU:OE2	1:D:199:ARG:HD3	1.95	0.67
2:M:721:PRO:O	2:M:725:MET:HG3	1.94	0.67
2:N:424:ASN:HD22	2:N:424:ASN:H	1.42	0.67
2:P:211:ASN:H	2:P:214:GLN:NE2	1.92	0.66
1:C:182:GLU:OE2	1:C:199:ARG:HD3	1.95	0.66
1:B:607:MET:HE3	1:B:608:PRO:HD2	1.77	0.66
2:O:348:PRO:HG2	2:O:383:PRO:HB3	1.77	0.66
2:P:586:THR:HG22	2:P:588:MET:H	1.59	0.66
2:O:700:ALA:HB1	2:O:704:ILE:HD11	1.77	0.66
2:M:365:LYS:HB3	2:M:464:GLN:HG3	1.77	0.66
2:P:110:ALA:HB1	2:P:216:VAL:HG21	1.76	0.66
2:M:500:VAL:HG21	2:M:533:TRP:CZ2	2.30	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:439:PHE:O	2:M:440:ARG:HD2	1.96	0.66
2:O:335:LYS:HD2	2:O:335:LYS:N	2.04	0.66
2:P:500:VAL:HG21	2:P:533:TRP:CZ2	2.30	0.66
2:M:424:ASN:H	2:M:424:ASN:HD22	1.43	0.66
1:B:662:VAL:HG21	2:N:194:LEU:HD13	1.77	0.65
2:M:335:LYS:N	2:M:335:LYS:HD2	2.02	0.65
2:N:110:ALA:HB1	2:N:216:VAL:HG21	1.76	0.65
1:B:482:LEU:HD21	1:B:508:LEU:HD12	1.79	0.65
2:M:252:VAL:HB	2:M:276:VAL:HG22	1.79	0.65
2:P:358:GLU:HG3	2:P:462:ARG:NH1	2.12	0.65
2:N:13:PRO:HB2	2:N:16:LYS:HG3	1.79	0.65
2:P:383:PRO:HG2	2:P:471:GLU:HB2	1.78	0.65
2:O:424:ASN:H	2:O:424:ASN:HD22	1.44	0.65
2:N:587:LEU:HD23	2:N:588:MET:HE1	1.78	0.65
1:C:377:ASN:HD22	1:C:377:ASN:H	1.45	0.65
2:M:211:ASN:H	2:M:214:GLN:NE2	1.95	0.65
2:O:358:GLU:HG3	2:O:462:ARG:NH1	2.12	0.65
7:C:800:XCC:FE2	7:C:800:XCC:S3	1.89	0.64
2:N:439:PHE:O	2:N:440:ARG:HD2	1.96	0.64
1:D:607:MET:CE	1:D:608:PRO:HD2	2.27	0.64
2:P:497:ASP:HA	2:P:500:VAL:HG12	1.78	0.64
1:C:377:ASN:ND2	1:C:377:ASN:H	1.96	0.64
1:A:217:ASN:HD22	1:B:112:ALA:HA	1.62	0.64
2:M:63:PRO:HB2	2:M:220:ASN:HB2	1.80	0.64
2:O:586:THR:HG22	2:O:588:MET:H	1.60	0.64
1:C:112:ALA:HA	1:D:217:ASN:HD22	1.62	0.64
2:O:477:TYR:HA	2:O:480:VAL:HG23	1.79	0.64
1:B:607:MET:CE	1:B:608:PRO:HD2	2.27	0.64
2:M:354:ARG:HH21	2:M:480:VAL:HG11	1.62	0.64
2:P:496:THR:H	2:P:499:THR:HG1	1.46	0.64
2:P:110:ALA:CB	2:P:216:VAL:HG21	2.28	0.64
1:C:482:LEU:HD21	1:C:508:LEU:HD12	1.80	0.64
2:N:348:PRO:HG2	2:N:383:PRO:HB3	1.78	0.64
1:A:607:MET:CE	1:A:608:PRO:HD2	2.28	0.64
2:M:151:TRP:CH2	2:M:249:ARG:NH1	2.65	0.64
2:O:252:VAL:HB	2:O:276:VAL:HG22	1.78	0.64
1:D:559:LEU:HG	1:D:563:MET:CE	2.28	0.64
2:P:348:PRO:HG2	2:P:383:PRO:HB3	1.80	0.64
1:A:182:GLU:OE2	1:A:199:ARG:HD3	1.98	0.64
2:P:424:ASN:H	2:P:424:ASN:HD22	1.44	0.64
1:D:607:MET:HE3	1:D:608:PRO:HD2	1.80	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLN:O	1:A:168:GLU:HG3	1.98	0.63
1:A:162:LEU:O	1:A:166:VAL:HG22	1.98	0.63
1:C:195:LYS:O	1:C:199:ARG:HG3	1.98	0.63
1:A:559:LEU:HG	1:A:563:MET:CE	2.28	0.63
2:N:354:ARG:HH21	2:N:480:VAL:HG11	1.61	0.63
1:C:77:ARG:NH1	1:C:79:LYS:HE2	2.13	0.63
2:M:110:ALA:HB1	2:M:216:VAL:HG21	1.81	0.63
2:M:354:ARG:NH2	2:M:480:VAL:HG11	2.14	0.63
2:O:497:ASP:OD1	2:O:522:PRO:HD2	1.99	0.63
1:D:77:ARG:NH1	1:D:79:LYS:HE2	2.13	0.63
2:N:358:GLU:HG3	2:N:462:ARG:NH1	2.14	0.63
2:M:373:ILE:HD11	2:M:435:VAL:HG22	1.80	0.63
1:B:559:LEU:HG	1:B:563:MET:CE	2.29	0.63
2:O:470:ASP:HB3	2:O:473:LYS:HB2	1.79	0.62
2:O:373:ILE:HD11	2:O:435:VAL:HG22	1.80	0.62
2:N:339:TYR:CD2	2:N:435:VAL:HG21	2.34	0.62
1:A:469:GLY:HA3	8:A:921:HOH:O	1.99	0.62
1:A:3:ARG:HH11	1:A:3:ARG:HG2	1.64	0.62
2:N:211:ASN:H	2:N:214:GLN:NE2	1.98	0.62
2:O:475:LYS:HA	2:O:478:MET:HB2	1.80	0.62
1:C:607:MET:CE	1:C:608:PRO:HD2	2.28	0.62
1:B:3:ARG:HD2	8:N:1339:HOH:O	1.99	0.62
2:P:318:LEU:HG	2:P:320:LEU:HG	1.80	0.62
2:N:110:ALA:CB	2:N:216:VAL:HG21	2.29	0.62
1:A:482:LEU:HD21	1:A:508:LEU:HD12	1.82	0.62
2:P:467:ILE:N	2:P:467:ILE:HD12	2.15	0.62
2:O:497:ASP:CA	2:O:500:VAL:HG12	2.30	0.62
2:N:167:LYS:HG2	8:N:1300:HOH:O	1.98	0.62
1:D:164:GLN:O	1:D:168:GLU:HG3	1.99	0.62
2:N:352:LEU:HD22	2:N:481:ALA:HB2	1.80	0.62
2:O:313:LEU:HD12	2:O:313:LEU:O	2.00	0.62
1:D:162:LEU:O	1:D:166:VAL:HG22	2.00	0.62
1:B:114:CYS:SG	1:B:209:HIS:CE1	2.93	0.62
2:O:399:PHE:HZ	2:O:541:GLU:HG3	1.65	0.61
1:B:428:VAL:HG22	1:B:539:ILE:CD1	2.27	0.61
2:P:373:ILE:HD11	2:P:435:VAL:HG22	1.82	0.61
1:D:195:LYS:O	1:D:199:ARG:HG3	2.00	0.61
1:A:468:CYS:O	1:A:580:ALA:HA	2.00	0.61
2:O:482:ARG:NH1	2:O:482:ARG:HA	2.15	0.61
2:N:349:ALA:HA	2:N:384:LEU:O	2.00	0.61
1:C:164:GLN:O	1:C:168:GLU:HG3	1.99	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:373:ILE:HD11	2:N:435:VAL:HG22	1.82	0.61
1:C:217:ASN:HD22	1:D:112:ALA:HA	1.65	0.61
2:N:150:ASP:OD2	2:N:152:THR:HG23	2.01	0.61
2:M:348:PRO:HG2	2:M:383:PRO:HB3	1.81	0.61
1:B:164:GLN:O	1:B:168:GLU:HG3	2.01	0.61
2:O:339:TYR:HD2	2:O:340:VAL:HG23	1.65	0.61
2:M:339:TYR:HD2	2:M:340:VAL:HG23	1.64	0.61
2:P:318:LEU:N	2:P:318:LEU:HD23	2.12	0.61
2:P:722:ALA:HA	2:P:725:MET:CE	2.31	0.61
2:O:349:ALA:HA	2:O:384:LEU:O	2.00	0.60
2:O:348:PRO:HB3	2:O:475:LYS:NZ	2.16	0.60
2:P:313:LEU:O	2:P:313:LEU:HD12	2.01	0.60
2:P:339:TYR:HD2	2:P:340:VAL:HG23	1.65	0.60
2:P:722:ALA:HA	2:P:725:MET:HE3	1.81	0.60
1:B:468:CYS:O	1:B:580:ALA:HA	2.02	0.60
1:A:662:VAL:HG21	2:M:194:LEU:HD13	1.83	0.60
2:O:110:ALA:CB	2:O:216:VAL:CG2	2.79	0.60
2:M:338:MET:SD	2:M:341:GLU:HB2	2.41	0.60
2:P:252:VAL:HB	2:P:276:VAL:HG22	1.82	0.60
1:B:77:ARG:NH1	1:B:79:LYS:HE2	2.16	0.60
2:M:349:ALA:HA	2:M:384:LEU:O	2.01	0.60
1:A:114:CYS:SG	1:A:209:HIS:CE1	2.95	0.60
2:O:494:GLY:O	2:O:499:THR:HG21	2.02	0.59
2:O:211:ASN:H	2:O:214:GLN:NE2	2.00	0.59
1:A:148:ARG:NH1	1:A:148:ARG:HB3	2.17	0.59
2:O:339:TYR:CD2	2:O:435:VAL:HG21	2.38	0.59
2:N:500:VAL:HG22	2:N:502:THR:H	1.68	0.59
1:A:112:ALA:HA	1:B:217:ASN:ND2	2.18	0.59
2:O:597:CYS:HB3	5:O:950:ACT:H1	1.85	0.59
2:M:313:LEU:HD12	2:M:313:LEU:O	2.02	0.59
2:O:406:ARG:NH1	2:O:406:ARG:HB3	2.17	0.59
2:P:110:ALA:CB	2:P:216:VAL:CG2	2.81	0.59
2:O:467:ILE:N	2:O:467:ILE:HD12	2.17	0.59
1:C:411:ARG:HG2	1:C:416:ARG:CD	2.32	0.59
2:M:339:TYR:CD2	2:M:435:VAL:HG21	2.38	0.59
1:C:3:ARG:NH1	1:C:625:SER:CB	2.65	0.59
1:D:615:LEU:HD23	2:P:27:HIS:CB	2.32	0.59
1:B:195:LYS:O	1:B:199:ARG:HG3	2.02	0.59
2:O:187:ASP:HA	2:O:211:ASN:ND2	2.17	0.59
1:A:195:LYS:O	1:A:199:ARG:HG3	2.02	0.59
1:D:468:CYS:O	1:D:580:ALA:HA	2.02	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:349:ALA:HA	2:P:384:LEU:O	2.01	0.59
1:C:162:LEU:O	1:C:166:VAL:HG22	2.02	0.59
1:C:468:CYS:O	1:C:580:ALA:HA	2.02	0.58
2:P:516:HIS:HE1	2:P:518:CYS:SG	2.26	0.58
2:N:497:ASP:N	2:N:523:GLU:OE2	2.25	0.58
1:C:559:LEU:HG	1:C:563:MET:CE	2.32	0.58
2:N:339:TYR:HD2	2:N:340:VAL:HG23	1.67	0.58
1:C:335:ALA:H	1:C:471:ASN:HD22	1.50	0.58
2:N:338:MET:SD	2:N:341:GLU:HB2	2.44	0.58
2:N:470:ASP:OD2	2:N:473:LYS:HG2	2.03	0.58
2:P:187:ASP:HA	2:P:211:ASN:ND2	2.17	0.58
1:D:482:LEU:CD2	1:D:508:LEU:HD12	2.33	0.58
2:M:339:TYR:CD2	2:M:340:VAL:HG23	2.39	0.58
1:A:77:ARG:NH1	1:A:79:LYS:HE2	2.19	0.58
2:M:500:VAL:HG22	2:M:502:THR:H	1.67	0.58
2:O:477:TYR:HA	2:O:480:VAL:CG2	2.33	0.58
1:A:335:ALA:H	1:A:471:ASN:HD22	1.51	0.58
2:N:313:LEU:HD12	2:N:313:LEU:O	2.03	0.58
2:N:110:ALA:CB	2:N:216:VAL:CG2	2.82	0.58
2:O:339:TYR:CD2	2:O:340:VAL:HG23	2.38	0.58
1:C:615:LEU:CD2	2:O:27:HIS:HB3	2.33	0.57
2:P:339:TYR:CD2	2:P:340:VAL:HG23	2.39	0.57
1:D:114:CYS:SG	1:D:209:HIS:CE1	2.97	0.57
1:B:148:ARG:NH1	1:B:148:ARG:HB3	2.17	0.57
2:N:372:ASP:H	2:N:375:GLN:NE2	2.01	0.57
1:C:515:ASN:HA	1:C:518:THR:HG23	1.86	0.57
1:C:615:LEU:HD23	2:O:27:HIS:CB	2.34	0.57
1:A:3:ARG:NH2	1:A:625:SER:CB	2.65	0.57
1:C:587:LYS:HE3	7:C:800:XCC:S4	2.44	0.57
1:A:105:MET:HE1	1:A:609:PRO:HD2	1.86	0.57
2:M:700:ALA:HB1	2:M:704:ILE:HD11	1.87	0.57
1:B:335:ALA:H	1:B:471:ASN:HD22	1.52	0.57
2:M:318:LEU:H	2:M:318:LEU:CD2	2.14	0.57
1:B:482:LEU:CD2	1:B:508:LEU:HD12	2.35	0.57
1:B:162:LEU:O	1:B:166:VAL:HG22	2.05	0.57
1:D:416:ARG:NH2	1:D:418:VAL:HG21	2.20	0.57
1:A:377:ASN:ND2	1:A:377:ASN:H	2.02	0.57
2:M:110:ALA:CB	2:M:216:VAL:HG21	2.35	0.57
1:D:615:LEU:CD2	2:P:27:HIS:HB3	2.35	0.57
2:M:151:TRP:CZ3	2:M:249:ARG:NH1	2.69	0.57
1:A:33:VAL:HG13	1:A:339:LEU:HD12	1.87	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:728:ILE:HG12	2:O:728:ILE:O	2.05	0.57
2:P:352:LEU:HD22	2:P:481:ALA:HB2	1.86	0.57
2:O:479:GLU:HA	2:O:482:ARG:HB2	1.85	0.56
2:P:339:TYR:HB2	2:P:432:LYS:HA	1.87	0.56
2:M:317:LYS:NZ	2:M:317:LYS:HB2	2.20	0.56
2:O:348:PRO:HG3	2:O:475:LYS:HE2	1.87	0.56
1:C:33:VAL:HG13	1:C:339:LEU:HD12	1.86	0.56
2:M:467:ILE:HD12	2:M:467:ILE:N	2.20	0.56
1:D:148:ARG:NH1	1:D:148:ARG:HB3	2.20	0.56
1:A:559:LEU:HG	1:A:563:MET:HE2	1.87	0.56
2:O:506:CYS:HA	2:O:547:PRO:O	2.05	0.56
2:N:700:ALA:HB1	2:N:704:ILE:HD11	1.88	0.56
2:P:339:TYR:CD2	2:P:435:VAL:HG21	2.41	0.56
2:P:333:ILE:HD12	2:P:431:SER:HB3	1.87	0.56
2:N:595:CYS:HB2	5:N:950:ACT:H1	1.86	0.56
2:P:496:THR:OG1	2:P:499:THR:HG23	2.06	0.56
1:B:351:VAL:HG22	1:B:356:ILE:CD1	2.34	0.56
1:A:426:ARG:HH21	1:A:539:ILE:HG13	1.67	0.56
1:C:482:LEU:CD2	1:C:508:LEU:HD12	2.36	0.56
1:C:114:CYS:SG	1:C:209:HIS:CE1	2.99	0.56
1:A:217:ASN:ND2	1:B:112:ALA:HA	2.21	0.56
2:M:187:ASP:HA	2:M:211:ASN:ND2	2.19	0.56
2:N:467:ILE:N	2:N:467:ILE:HD12	2.21	0.56
2:M:339:TYR:HB2	2:M:432:LYS:HA	1.88	0.56
2:O:516:HIS:HE1	2:O:518:CYS:SG	2.28	0.56
2:P:700:ALA:CB	2:P:704:ILE:HD11	2.35	0.55
2:M:333:ILE:HD12	2:M:431:SER:HB3	1.88	0.55
1:A:307:ALA:HB2	1:A:408:PHE:CE2	2.41	0.55
2:O:571:LEU:HD22	2:O:579:LEU:HB2	1.88	0.55
2:O:61:TYR:O	2:O:63:PRO:HD3	2.06	0.55
2:M:372:ASP:H	2:M:375:GLN:NE2	2.05	0.55
2:M:516:HIS:HE1	2:M:518:CYS:SG	2.29	0.55
1:B:33:VAL:HG13	1:B:339:LEU:HD12	1.89	0.55
2:N:406:ARG:NH1	2:N:406:ARG:HB3	2.22	0.55
2:M:174:LYS:NZ	2:M:174:LYS:HB3	2.21	0.55
2:P:406:ARG:HB3	2:P:406:ARG:NH1	2.20	0.55
1:B:147:CYS:SG	1:B:166:VAL:HG13	2.46	0.55
2:N:571:LEU:HD22	2:N:579:LEU:HB2	1.88	0.55
2:O:333:ILE:HD12	2:O:431:SER:HB3	1.87	0.55
2:O:393:ARG:HG2	2:O:461:ASP:OD2	2.06	0.55
2:O:495:LEU:HD21	2:O:533:TRP:CZ3	2.41	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:342:MET:HB3	2:P:382:LEU:O	2.07	0.55
2:O:224:ARG:O	2:O:228:MET:HG3	2.07	0.55
1:D:515:ASN:HA	1:D:518:THR:HG23	1.89	0.55
2:N:602:MET:HE2	2:N:647:ILE:HG21	1.89	0.55
2:M:587:LEU:HD23	2:M:588:MET:HE1	1.88	0.55
1:C:153:GLU:OE2	1:C:155:GLU:HG3	2.07	0.55
1:A:66:ILE:HG23	1:A:612:GLY:HA3	1.88	0.55
2:N:342:MET:HB3	2:N:382:LEU:O	2.07	0.55
2:N:339:TYR:HB2	2:N:432:LYS:HA	1.88	0.55
1:D:31:PRO:HB2	1:D:423:ILE:HD13	1.89	0.55
1:A:33:VAL:HG13	1:A:339:LEU:CD1	2.37	0.55
1:A:415:ASN:O	1:A:417:PRO:HD3	2.06	0.55
2:N:252:VAL:HB	2:N:276:VAL:HG22	1.89	0.55
2:P:587:LEU:HD23	2:P:588:MET:HE1	1.88	0.55
2:O:496:THR:O	2:O:500:VAL:N	2.40	0.54
2:M:342:MET:HB3	2:M:382:LEU:O	2.07	0.54
1:D:559:LEU:HG	1:D:563:MET:HE2	1.89	0.54
2:N:704:ILE:HD13	2:N:714:TYR:CG	2.42	0.54
1:D:335:ALA:H	1:D:471:ASN:HD22	1.53	0.54
2:M:406:ARG:HB3	2:M:406:ARG:NH1	2.22	0.54
2:N:373:ILE:CD1	2:N:435:VAL:HG22	2.37	0.54
2:N:315:LYS:HB3	2:N:315:LYS:NZ	2.22	0.54
2:O:314:THR:O	2:O:316:ILE:N	2.40	0.54
2:P:372:ASP:H	2:P:375:GLN:NE2	2.05	0.54
1:A:77:ARG:HD3	8:A:865:HOH:O	2.07	0.54
2:N:393:ARG:HG2	2:N:461:ASP:OD2	2.07	0.54
2:O:587:LEU:HD23	2:O:588:MET:HE1	1.88	0.54
2:N:315:LYS:HB3	2:N:315:LYS:HZ2	1.72	0.54
1:C:584:MET:HG3	1:D:73:ALA:HB2	1.88	0.54
2:M:393:ARG:HG2	2:M:461:ASP:OD2	2.07	0.54
2:N:339:TYR:CD2	2:N:340:VAL:HG23	2.41	0.54
2:M:369:ILE:HG21	2:M:473:LYS:HG2	1.89	0.54
1:C:442:THR:HG21	1:C:537:ILE:HD11	1.88	0.54
2:P:613:ILE:O	2:P:671:PRO:HD3	2.07	0.54
1:D:377:ASN:ND2	1:D:377:ASN:H	2.05	0.54
2:N:602:MET:CE	2:N:647:ILE:HG21	2.38	0.54
2:O:604:ILE:C	2:O:604:ILE:HD12	2.28	0.54
2:O:266:ALA:HB1	2:O:276:VAL:HG21	1.90	0.54
2:N:174:LYS:HB3	2:N:174:LYS:NZ	2.22	0.54
1:A:377:ASN:H	1:A:377:ASN:HD22	1.55	0.54
1:B:33:VAL:HG13	1:B:339:LEU:CD1	2.38	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:356:VAL:HG21	2:M:361:ILE:HB	1.89	0.54
2:N:6:LYS:O	2:N:9:GLU:HB2	2.07	0.54
2:P:704:ILE:HG13	2:P:705:GLY:N	2.22	0.54
2:N:187:ASP:HA	2:N:211:ASN:ND2	2.20	0.54
1:B:150:VAL:HG12	1:B:150:VAL:O	2.07	0.54
2:O:339:TYR:HB2	2:O:432:LYS:HA	1.88	0.54
2:P:424:ASN:HD22	2:P:424:ASN:N	2.05	0.54
2:M:704:ILE:HD13	2:M:714:TYR:CG	2.43	0.54
2:N:704:ILE:HG13	2:N:705:GLY:N	2.23	0.54
1:D:68:CYS:HB2	1:D:97:ILE:HG23	1.90	0.54
2:M:110:ALA:CB	2:M:216:VAL:CG2	2.86	0.54
1:B:105:MET:HE1	1:B:609:PRO:HD2	1.89	0.54
2:P:356:VAL:HG21	2:P:361:ILE:HB	1.90	0.54
2:O:174:LYS:NZ	2:O:174:LYS:HB3	2.22	0.54
2:M:342:MET:HG3	2:M:384:LEU:CD2	2.38	0.54
1:B:377:ASN:H	1:B:377:ASN:ND2	2.05	0.54
2:M:509:CYS:HB3	5:M:950:ACT:H1	1.89	0.53
2:P:393:ARG:HG2	2:P:461:ASP:OD2	2.08	0.53
2:O:356:VAL:HG21	2:O:361:ILE:HB	1.90	0.53
2:O:346:ARG:HG3	2:O:346:ARG:HH11	1.72	0.53
2:O:373:ILE:CD1	2:O:435:VAL:HG22	2.38	0.53
2:O:469:THR:O	2:O:470:ASP:HB2	2.08	0.53
2:P:150:ASP:OD2	2:P:152:THR:HG23	2.07	0.53
1:D:149:ARG:NH2	1:D:250:ASP:OD2	2.40	0.53
2:O:500:VAL:HG22	2:O:502:THR:H	1.72	0.53
2:O:406:ARG:HB3	2:O:406:ARG:HH11	1.72	0.53
2:N:516:HIS:HE1	2:N:518:CYS:SG	2.32	0.53
1:B:118:ASN:C	1:B:118:ASN:HD22	2.12	0.53
1:B:78:ILE:HD11	1:B:97:ILE:HD12	1.89	0.53
1:D:615:LEU:HD22	2:P:260:MET:SD	2.48	0.53
1:A:147:CYS:SG	1:A:166:VAL:HG13	2.48	0.53
1:B:31:PRO:HB2	1:B:423:ILE:HD13	1.90	0.53
2:O:497:ASP:O	2:O:500:VAL:O	2.26	0.53
2:O:372:ASP:H	2:O:375:GLN:NE2	2.06	0.53
2:N:367:GLU:HG2	8:N:1215:HOH:O	2.08	0.53
2:M:373:ILE:CD1	2:M:435:VAL:HG22	2.37	0.53
1:C:147:CYS:SG	1:C:166:VAL:HG13	2.48	0.53
2:M:151:TRP:CZ2	2:M:249:ARG:NH1	2.76	0.53
2:P:266:ALA:HB1	2:P:276:VAL:HG21	1.90	0.53
1:D:147:CYS:SG	1:D:166:VAL:HG13	2.49	0.53
2:M:4:PHE:HB2	2:M:238:GLU:OE2	2.09	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:604:ILE:C	2:P:604:ILE:HD12	2.28	0.53
2:P:377:PRO:HG2	2:P:380:SER:CB	2.38	0.53
1:C:33:VAL:HG13	1:C:339:LEU:CD1	2.39	0.53
1:D:303:LYS:HA	1:D:307:ALA:O	2.09	0.53
2:P:479:GLU:OE2	2:P:482:ARG:HD3	2.08	0.53
1:C:73:ALA:HB2	1:D:584:MET:HG3	1.90	0.53
1:A:615:LEU:HD23	2:M:27:HIS:HB3	1.90	0.53
1:C:283:HIS:CA	1:C:318:THR:HG23	2.39	0.53
1:C:68:CYS:HB2	1:C:97:ILE:HG23	1.91	0.53
2:P:571:LEU:HD22	2:P:579:LEU:HB2	1.90	0.53
2:N:333:ILE:HD12	2:N:431:SER:HB3	1.90	0.53
2:M:613:ILE:O	2:M:671:PRO:HD3	2.09	0.53
1:D:33:VAL:HG13	1:D:339:LEU:HD12	1.90	0.53
1:B:411:ARG:HG2	1:B:416:ARG:HD2	1.90	0.52
2:P:482:ARG:HG2	2:P:486:LYS:NZ	2.24	0.52
1:C:415:ASN:O	1:C:417:PRO:HD3	2.09	0.52
1:B:66:ILE:HG23	1:B:612:GLY:HA3	1.90	0.52
2:O:725:MET:O	2:O:726:ASP:HB3	2.09	0.52
2:P:500:VAL:HG22	2:P:502:THR:H	1.72	0.52
2:P:506:CYS:HA	2:P:547:PRO:O	2.09	0.52
2:P:167:LYS:HG2	8:P:1026:HOH:O	2.08	0.52
2:O:457:PRO:O	2:O:458:ALA:HB3	2.09	0.52
1:B:414:SER:O	1:B:416:ARG:N	2.43	0.52
1:C:3:ARG:HH12	1:C:625:SER:HB2	1.73	0.52
1:C:148:ARG:HB3	1:C:148:ARG:NH1	2.22	0.52
2:P:373:ILE:CD1	2:P:435:VAL:HG22	2.38	0.52
2:M:317:LYS:O	2:M:317:LYS:HG3	2.08	0.52
2:P:457:PRO:O	2:P:458:ALA:HB3	2.09	0.52
2:M:358:GLU:HG3	2:M:462:ARG:NH1	2.24	0.52
2:P:346:ARG:HG3	2:P:346:ARG:HH11	1.75	0.52
2:M:602:MET:CE	2:M:647:ILE:HG21	2.39	0.52
1:A:482:LEU:CD2	1:A:508:LEU:HD12	2.39	0.52
2:O:342:MET:HG3	2:O:384:LEU:CD2	2.37	0.52
2:N:340:VAL:HG12	2:N:341:GLU:N	2.25	0.52
1:C:66:ILE:HG23	1:C:612:GLY:HA3	1.90	0.52
1:B:615:LEU:HD23	2:N:27:HIS:HB3	1.91	0.52
1:C:31:PRO:HB2	1:C:423:ILE:HD13	1.91	0.52
2:N:727:PRO:HB2	2:N:729:MET:HG3	1.89	0.52
1:A:118:ASN:HD22	1:A:118:ASN:C	2.13	0.52
2:M:704:ILE:HG13	2:M:705:GLY:N	2.24	0.52
2:N:356:VAL:HG21	2:N:361:ILE:HB	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:507:VAL:HB	2:P:510:GLN:HG3	1.92	0.52
2:M:186:CYS:O	2:M:187:ASP:HB2	2.10	0.52
2:M:150:ASP:OD2	2:M:152:THR:HG23	2.10	0.52
1:A:584:MET:HG3	1:B:73:ALA:HB2	1.92	0.52
2:N:377:PRO:HG2	2:N:380:SER:CB	2.39	0.52
1:A:515:ASN:HA	1:A:518:THR:HG23	1.91	0.52
1:D:33:VAL:HG13	1:D:339:LEU:CD1	2.40	0.52
2:P:4:PHE:HB2	2:P:238:GLU:OE2	2.09	0.52
1:B:653:THR:HG22	8:B:907:HOH:O	2.10	0.52
1:D:150:VAL:O	1:D:150:VAL:HG12	2.09	0.52
2:O:613:ILE:O	2:O:671:PRO:HD3	2.09	0.52
1:D:415:ASN:O	1:D:417:PRO:HD3	2.09	0.52
1:D:587:LYS:HE3	7:D:800:XCC:S4	2.49	0.52
2:N:346:ARG:HH11	2:N:346:ARG:HG3	1.74	0.52
2:M:604:ILE:HD12	2:M:604:ILE:C	2.30	0.52
2:P:342:MET:HG3	2:P:384:LEU:CD2	2.38	0.52
1:B:515:ASN:HA	1:B:518:THR:HG23	1.91	0.52
2:O:507:VAL:HB	2:O:510:GLN:HG3	1.92	0.52
2:N:506:CYS:HA	2:N:547:PRO:O	2.10	0.52
2:M:571:LEU:HD22	2:M:579:LEU:HB2	1.91	0.52
1:C:416:ARG:O	1:C:416:ARG:HG3	2.10	0.51
2:O:377:PRO:HG2	2:O:380:SER:CB	2.37	0.51
1:C:351:VAL:HG22	1:C:356:ILE:CD1	2.40	0.51
2:O:456:PHE:HD2	2:O:542:ILE:HD11	1.74	0.51
2:O:342:MET:HB3	2:O:382:LEU:O	2.09	0.51
1:A:150:VAL:HG12	1:A:150:VAL:O	2.10	0.51
1:B:283:HIS:CA	1:B:318:THR:HG23	2.40	0.51
2:P:61:TYR:O	2:P:63:PRO:HD3	2.10	0.51
1:D:377:ASN:HD22	1:D:377:ASN:H	1.59	0.51
2:M:266:ALA:HB1	2:M:276:VAL:HG21	1.91	0.51
1:D:278:PHE:HB3	1:D:312:LEU:HD23	1.92	0.51
2:M:457:PRO:O	2:M:458:ALA:HB3	2.10	0.51
2:O:495:LEU:HD11	2:O:533:TRP:CZ3	2.46	0.51
2:O:350:PHE:HB3	2:O:478:MET:HE1	1.93	0.51
2:P:497:ASP:OD1	2:P:522:PRO:HD2	2.11	0.51
2:P:470:ASP:OD1	2:P:472:ALA:HB3	2.10	0.51
1:A:149:ARG:NH2	1:A:250:ASP:OD2	2.40	0.51
2:O:150:ASP:OD2	2:O:152:THR:HG23	2.10	0.51
1:C:150:VAL:HG12	1:C:150:VAL:O	2.11	0.51
2:P:340:VAL:HG12	2:P:341:GLU:N	2.26	0.51
2:P:626:MET:HB3	2:P:630:THR:HB	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ARG:NH2	1:A:539:ILE:CG1	2.65	0.51
2:O:704:ILE:HD13	2:O:714:TYR:CG	2.45	0.51
2:N:722:ALA:HA	2:N:725:MET:HE3	1.93	0.51
2:N:457:PRO:O	2:N:458:ALA:HB3	2.11	0.51
2:O:609:ASN:OD1	2:O:727:PRO:HA	2.10	0.51
1:B:176:ARG:O	1:B:207:GLY:HA3	2.11	0.51
2:O:495:LEU:HD21	2:O:533:TRP:CE3	2.46	0.51
1:A:283:HIS:CA	1:A:318:THR:HG23	2.41	0.51
2:O:704:ILE:HG13	2:O:705:GLY:N	2.25	0.51
1:C:112:ALA:HA	1:D:217:ASN:ND2	2.25	0.51
2:M:340:VAL:HG12	2:M:341:GLU:N	2.26	0.51
1:C:335:ALA:HB2	1:C:471:ASN:HB3	1.93	0.51
1:A:351:VAL:HG22	1:A:356:ILE:CD1	2.40	0.51
1:A:294:ALA:O	1:A:298:MET:HG2	2.10	0.51
2:P:553:LYS:HZ3	2:P:553:LYS:HB3	1.77	0.50
2:M:346:ARG:HG3	2:M:346:ARG:HH11	1.75	0.50
1:B:412:LYS:HZ3	1:B:416:ARG:CZ	2.24	0.50
1:D:61:ILE:HD13	1:D:77:ARG:HE	1.76	0.50
2:O:482:ARG:CZ	2:O:482:ARG:HA	2.41	0.50
2:N:722:ALA:HA	2:N:725:MET:CE	2.40	0.50
1:A:24:ASN:O	1:A:27:ARG:HG2	2.11	0.50
1:C:24:ASN:O	1:C:27:ARG:HG2	2.12	0.50
2:M:506:CYS:HA	2:M:547:PRO:O	2.10	0.50
2:P:406:ARG:HH11	2:P:406:ARG:HB3	1.76	0.50
2:P:174:LYS:HB3	2:P:174:LYS:NZ	2.27	0.50
2:O:626:MET:HB3	2:O:630:THR:HB	1.93	0.50
2:M:19:VAL:HG23	2:M:20:ALA:N	2.27	0.50
2:P:224:ARG:O	2:P:228:MET:HG3	2.11	0.50
2:N:604:ILE:O	2:N:604:ILE:HD12	2.11	0.50
1:D:66:ILE:HG23	1:D:612:GLY:HA3	1.93	0.50
2:M:602:MET:HE2	2:M:647:ILE:HG21	1.93	0.50
2:O:186:CYS:O	2:O:187:ASP:HB2	2.12	0.50
2:O:471:GLU:O	2:O:475:LYS:HG2	2.11	0.50
2:O:339:TYR:CG	2:O:435:VAL:HG21	2.47	0.50
1:A:278:PHE:HB3	1:A:312:LEU:HD23	1.94	0.50
1:C:118:ASN:HD22	1:C:118:ASN:C	2.15	0.50
1:A:73:ALA:HB2	1:B:584:MET:HG3	1.94	0.50
1:D:283:HIS:CA	1:D:318:THR:HG23	2.42	0.50
2:O:340:VAL:HG12	2:O:341:GLU:N	2.27	0.50
2:N:354:ARG:HD2	2:N:389:ASP:OD2	2.12	0.50
2:N:339:TYR:CG	2:N:435:VAL:HG21	2.47	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:ALA:HB2	1:D:471:ASN:HB3	1.92	0.50
2:O:564:TRP:CZ3	2:O:584:LEU:HD12	2.47	0.50
1:C:280:LEU:HD13	1:C:288:SER:HB2	1.94	0.50
1:B:3:ARG:NH2	1:B:3:ARG:CG	2.70	0.50
2:O:114:GLU:OE1	2:O:117:ARG:NH1	2.45	0.50
2:M:482:ARG:HG2	2:M:486:LYS:NZ	2.27	0.50
2:M:505:SER:HB3	2:M:551:ILE:HD11	1.94	0.50
1:B:377:ASN:H	1:B:377:ASN:HD22	1.58	0.49
1:C:487:GLU:HB2	8:C:907:HOH:O	2.11	0.49
2:M:707:THR:OG1	2:M:710:GLU:HG3	2.12	0.49
1:B:150:VAL:HG13	1:B:184:THR:HG21	1.93	0.49
2:N:372:ASP:OD1	2:N:373:ILE:N	2.41	0.49
1:C:278:PHE:HB3	1:C:312:LEU:HD23	1.94	0.49
2:N:342:MET:HG3	2:N:384:LEU:CD2	2.40	0.49
1:A:587:LYS:HE3	7:A:800:XCC:S4	2.52	0.49
1:B:351:VAL:HG21	1:B:356:ILE:HG12	1.93	0.49
1:C:415:ASN:HD22	1:C:415:ASN:C	2.15	0.49
2:M:622:THR:HB	2:M:623:PRO:HD2	1.95	0.49
1:B:601:PRO:HD3	1:B:652:ARG:CZ	2.42	0.49
1:A:31:PRO:HB2	1:A:423:ILE:HD13	1.93	0.49
1:C:510:LEU:O	1:C:543:PRO:HD2	2.13	0.49
1:A:150:VAL:HG13	1:A:184:THR:HG21	1.93	0.49
2:O:602:MET:HE2	2:O:647:ILE:HG21	1.94	0.49
2:O:445:GLY:O	2:O:449:VAL:HG23	2.12	0.49
2:M:568:ASN:OD1	2:M:581:GLN:HG3	2.12	0.49
2:O:700:ALA:CB	2:O:704:ILE:HD11	2.43	0.49
2:M:393:ARG:HG3	2:M:393:ARG:HH11	1.78	0.49
2:N:613:ILE:O	2:N:671:PRO:HD3	2.12	0.49
1:C:525:LYS:O	1:C:529:LYS:HG2	2.13	0.49
1:D:105:MET:HE1	1:D:609:PRO:HD2	1.95	0.49
1:C:176:ARG:O	1:C:207:GLY:HA3	2.13	0.49
2:P:473:LYS:HA	2:P:476:GLU:HB3	1.94	0.49
1:A:655:LYS:HG3	2:M:191:GLU:HG2	1.94	0.49
1:D:118:ASN:HD22	1:D:118:ASN:C	2.16	0.49
1:A:656:LEU:O	1:A:660:LYS:HG3	2.13	0.49
2:P:602:MET:HE2	2:P:647:ILE:HG21	1.93	0.49
1:D:313:VAL:CB	1:D:331:VAL:HG22	2.38	0.49
1:C:313:VAL:CB	1:C:331:VAL:HG22	2.38	0.49
1:B:559:LEU:HG	1:B:563:MET:HE3	1.95	0.49
1:B:653:THR:CG2	8:B:907:HOH:O	2.61	0.49
1:B:278:PHE:HB3	1:B:312:LEU:HD23	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:VAL:O	1:B:150:VAL:CG1	2.61	0.49
2:P:707:THR:OG1	2:P:710:GLU:HG3	2.12	0.49
2:M:424:ASN:N	2:M:424:ASN:HD22	2.05	0.48
1:B:68:CYS:HB2	1:B:97:ILE:HG23	1.96	0.48
1:D:24:ASN:O	1:D:27:ARG:HG2	2.13	0.48
2:O:602:MET:CE	2:O:647:ILE:HG21	2.43	0.48
2:P:210:GLY:HA3	2:P:214:GLN:HE21	1.78	0.48
2:N:626:MET:HB3	2:N:630:THR:HB	1.95	0.48
1:B:125:VAL:O	1:B:129:GLU:HG3	2.13	0.48
1:A:105:MET:CE	1:A:609:PRO:HD2	2.43	0.48
2:P:505:SER:HB3	2:P:551:ILE:HD11	1.95	0.48
2:O:707:THR:OG1	2:O:710:GLU:HG3	2.13	0.48
2:O:712:LEU:N	2:O:713:PRO:HD2	2.29	0.48
2:P:13:PRO:HB2	2:P:16:LYS:HG3	1.94	0.48
2:P:66:ARG:O	2:P:70:GLY:HA2	2.14	0.48
1:D:409:LYS:O	1:D:413:GLU:HG2	2.14	0.48
1:D:530:ARG:NH1	1:D:530:ARG:HB2	2.29	0.48
1:A:68:CYS:HB2	1:A:97:ILE:HG23	1.96	0.48
2:P:704:ILE:HD13	2:P:714:TYR:CG	2.49	0.48
1:D:480:SER:HB2	1:D:582:GLU:HG3	1.94	0.48
1:B:24:ASN:O	1:B:27:ARG:HG2	2.14	0.48
1:A:577:VAL:HG21	1:A:645:ILE:CG2	2.41	0.48
2:N:424:ASN:N	2:N:424:ASN:HD22	2.05	0.48
2:M:339:TYR:CG	2:M:435:VAL:HG21	2.49	0.48
1:C:217:ASN:ND2	1:D:112:ALA:HA	2.29	0.48
2:O:19:VAL:HG23	2:O:20:ALA:N	2.28	0.48
2:N:568:ASN:OD1	2:N:581:GLN:HG3	2.14	0.48
1:D:150:VAL:HG13	1:D:184:THR:HG21	1.96	0.48
2:N:61:TYR:O	2:N:63:PRO:HD3	2.14	0.48
2:N:587:LEU:CD2	2:N:588:MET:HE1	2.43	0.48
2:M:377:PRO:HG2	2:M:380:SER:CB	2.40	0.48
1:C:377:ASN:N	1:C:377:ASN:HD22	2.05	0.48
2:P:602:MET:CE	2:P:647:ILE:HG21	2.43	0.48
1:B:577:VAL:HG21	1:B:645:ILE:CG2	2.40	0.48
1:C:150:VAL:HG13	1:C:184:THR:HG21	1.96	0.48
1:B:559:LEU:HG	1:B:563:MET:HE2	1.94	0.48
1:C:559:LEU:HG	1:C:563:MET:HE2	1.96	0.48
1:A:335:ALA:HB2	1:A:471:ASN:HB3	1.96	0.48
1:B:335:ALA:HB2	1:B:471:ASN:HB3	1.96	0.48
2:N:266:ALA:HB1	2:N:276:VAL:HG21	1.96	0.48
1:A:351:VAL:HG21	1:A:356:ILE:HG12	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LYS:HA	1:A:416:ARG:HD3	1.96	0.48
2:N:479:GLU:HA	2:N:482:ARG:HG3	1.96	0.48
2:O:604:ILE:HD13	2:O:606:PRO:HD3	1.96	0.48
2:M:712:LEU:N	2:M:713:PRO:HD2	2.28	0.48
2:O:622:THR:HB	2:O:623:PRO:HD2	1.96	0.48
1:D:351:VAL:HG22	1:D:356:ILE:CD1	2.44	0.48
1:B:318:THR:HG21	8:B:855:HOH:O	2.14	0.47
1:B:615:LEU:CD2	2:N:27:HIS:HB3	2.44	0.47
1:D:460:GLU:OE1	1:D:530:ARG:NH2	2.47	0.47
1:D:525:LYS:O	1:D:529:LYS:HG2	2.14	0.47
2:P:604:ILE:HD13	2:P:606:PRO:HD3	1.96	0.47
2:N:406:ARG:HB3	2:N:406:ARG:HH11	1.78	0.47
1:A:601:PRO:HD3	1:A:652:ARG:CZ	2.45	0.47
1:A:176:ARG:O	1:A:207:GLY:HA3	2.13	0.47
2:N:19:VAL:HG22	8:N:1251:HOH:O	2.14	0.47
2:O:496:THR:O	2:O:500:VAL:HG12	2.15	0.47
2:O:568:ASN:OD1	2:O:581:GLN:HG3	2.14	0.47
2:P:712:LEU:N	2:P:713:PRO:HD2	2.28	0.47
2:O:350:PHE:HB3	2:O:478:MET:CE	2.44	0.47
2:M:468:PHE:CD2	2:M:473:LYS:HG3	2.50	0.47
1:A:525:LYS:O	1:A:529:LYS:HG2	2.15	0.47
2:O:410:PHE:CZ	2:O:455:GLU:HG3	2.50	0.47
1:C:581:PRO:O	1:C:605:GLY:HA3	2.14	0.47
2:N:564:TRP:CZ3	2:N:584:LEU:HD12	2.48	0.47
1:C:656:LEU:O	1:C:660:LYS:HG3	2.14	0.47
2:P:186:CYS:O	2:P:187:ASP:HB2	2.15	0.47
1:C:61:ILE:HD13	1:C:77:ARG:HE	1.78	0.47
2:O:371:PRO:HD2	2:O:469:THR:O	2.14	0.47
2:O:665:ALA:O	2:O:722:ALA:HB2	2.14	0.47
2:N:186:CYS:O	2:N:187:ASP:HB2	2.15	0.47
1:D:3:ARG:NH2	1:D:625:SER:CB	2.75	0.47
2:N:342:MET:SD	2:N:342:MET:N	2.88	0.47
2:P:496:THR:N	2:P:499:THR:HG1	2.13	0.47
1:D:154:VAL:HG13	1:D:162:LEU:HD11	1.97	0.47
2:M:597:CYS:HB3	5:M:950:ACT:O	2.14	0.47
1:B:615:LEU:HD23	2:N:27:HIS:CB	2.44	0.47
1:A:510:LEU:O	1:A:543:PRO:HD2	2.15	0.47
1:C:105:MET:CE	1:C:609:PRO:HD2	2.45	0.47
1:B:150:VAL:CG1	1:B:169:LYS:HG2	2.40	0.47
2:M:626:MET:HB3	2:M:630:THR:HB	1.97	0.47
2:P:564:TRP:CZ3	2:P:584:LEU:HD12	2.50	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:LYS:HG3	2:N:191:GLU:HG2	1.96	0.47
2:P:445:GLY:O	2:P:449:VAL:HG23	2.14	0.47
2:O:505:SER:HB3	2:O:551:ILE:HD11	1.95	0.47
1:A:318:THR:O	1:A:322:VAL:HG22	2.15	0.47
2:N:393:ARG:HG3	2:N:393:ARG:HH11	1.80	0.47
1:C:394:ILE:HG23	1:C:395:GLU:N	2.30	0.47
2:P:138:ASP:N	2:P:139:PRO:CD	2.77	0.47
1:B:460:GLU:CD	1:B:530:ARG:HH22	2.18	0.47
1:C:486:LYS:HE2	1:C:519:TYR:CE2	2.50	0.47
2:P:393:ARG:HG3	2:P:393:ARG:HH11	1.78	0.47
2:N:712:LEU:N	2:N:713:PRO:HD2	2.30	0.47
1:B:443:GLN:HB2	1:B:451:VAL:HG21	1.96	0.47
1:C:577:VAL:HG21	1:C:645:ILE:CG2	2.43	0.47
1:B:190:ILE:HG13	1:B:195:LYS:HG3	1.97	0.47
1:D:190:ILE:HG13	1:D:195:LYS:HG3	1.97	0.47
2:N:354:ARG:NH2	2:N:480:VAL:HG11	2.27	0.47
1:B:307:ALA:HB2	1:B:408:PHE:CE2	2.49	0.47
1:B:587:LYS:HE3	7:B:800:XCC:S4	2.55	0.47
1:D:176:ARG:O	1:D:207:GLY:HA3	2.15	0.47
1:A:443:GLN:HB2	1:A:451:VAL:HG21	1.96	0.46
2:O:356:VAL:CG2	2:O:361:ILE:HB	2.45	0.46
2:P:622:THR:HB	2:P:623:PRO:HD2	1.96	0.46
1:A:615:LEU:CD2	2:M:27:HIS:HB3	2.46	0.46
2:P:470:ASP:O	2:P:474:VAL:HG23	2.16	0.46
2:M:507:VAL:HB	2:M:510:GLN:HG3	1.97	0.46
1:D:601:PRO:HD3	1:D:652:ARG:CZ	2.45	0.46
1:B:412:LYS:NZ	1:B:416:ARG:CZ	2.79	0.46
2:P:372:ASP:OD1	2:P:373:ILE:N	2.43	0.46
1:C:377:ASN:HB2	1:D:218:GLN:HG3	1.97	0.46
2:M:372:ASP:OD1	2:M:373:ILE:N	2.41	0.46
1:D:469:GLY:O	7:D:800:XCC:S1	2.73	0.46
2:N:138:ASP:N	2:N:139:PRO:CD	2.79	0.46
1:C:480:SER:HB2	1:C:582:GLU:HG3	1.96	0.46
2:M:354:ARG:HD2	2:M:389:ASP:OD2	2.14	0.46
2:P:114:GLU:OE1	2:P:117:ARG:NH1	2.48	0.46
2:M:352:LEU:HD22	2:M:481:ALA:HB2	1.98	0.46
1:A:486:LYS:HE2	1:A:519:TYR:CE2	2.50	0.46
2:O:424:ASN:N	2:O:424:ASN:HD22	2.06	0.46
2:N:586:THR:HG22	2:N:587:LEU:N	2.30	0.46
2:P:419:HIS:HB2	2:P:428:LEU:HD13	1.97	0.46
2:P:365:LYS:HE2	2:P:367:GLU:OE2	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:371:PRO:HD2	2:O:469:THR:OG1	2.16	0.46
2:P:568:ASN:OD1	2:P:581:GLN:HG3	2.16	0.46
2:O:138:ASP:N	2:O:139:PRO:CD	2.77	0.46
2:P:410:PHE:CZ	2:P:455:GLU:HG3	2.50	0.46
2:O:247:ARG:HB3	2:O:512:PHE:CE2	2.51	0.46
1:A:480:SER:HB2	1:A:582:GLU:HG3	1.97	0.46
2:O:367:GLU:HG3	2:O:466:THR:HG23	1.97	0.46
1:C:615:LEU:HD22	2:O:260:MET:SD	2.55	0.46
1:C:190:ILE:HG13	1:C:195:LYS:HG3	1.97	0.46
2:M:365:LYS:HE2	2:M:367:GLU:OE2	2.15	0.46
1:B:61:ILE:HD13	1:B:77:ARG:HE	1.81	0.46
2:M:406:ARG:HH11	2:M:406:ARG:HB3	1.79	0.46
2:M:445:GLY:O	2:M:449:VAL:HG23	2.15	0.46
2:O:318:LEU:HD12	2:O:318:LEU:O	2.16	0.46
2:O:66:ARG:O	2:O:70:GLY:HA2	2.15	0.46
2:O:419:HIS:HB2	2:O:428:LEU:HD13	1.98	0.46
1:A:585:SER:OG	7:A:800:XCC:S4	2.65	0.46
1:D:656:LEU:O	1:D:660:LYS:HG3	2.16	0.46
2:M:66:ARG:O	2:M:70:GLY:HA2	2.15	0.46
1:B:411:ARG:CG	1:B:416:ARG:HD2	2.46	0.46
2:O:210:GLY:HA3	2:O:214:GLN:HE21	1.81	0.46
2:M:586:THR:HG22	2:M:587:LEU:N	2.31	0.46
2:O:586:THR:HG22	2:O:587:LEU:N	2.31	0.46
2:M:356:VAL:CG2	2:M:361:ILE:HB	2.45	0.46
1:B:149:ARG:NH2	1:B:250:ASP:OD2	2.41	0.46
2:M:439:PHE:CE1	2:M:443:ASN:HB2	2.51	0.46
1:A:415:ASN:O	1:A:417:PRO:CD	2.64	0.46
1:D:105:MET:CE	1:D:609:PRO:HD2	2.46	0.46
2:P:247:ARG:HB3	2:P:512:PHE:CE2	2.51	0.46
2:O:497:ASP:HA	2:O:500:VAL:CG1	2.43	0.45
2:O:381:LYS:O	2:O:382:LEU:HB2	2.16	0.45
2:P:482:ARG:HG2	2:P:486:LYS:HZ1	1.81	0.45
1:C:78:ILE:HD11	1:C:97:ILE:HD12	1.98	0.45
1:C:601:PRO:HD3	1:C:652:ARG:CZ	2.46	0.45
2:P:609:ASN:OD1	2:P:728:ILE:HG22	2.16	0.45
2:O:680:ASP:O	2:O:684:ARG:HG3	2.16	0.45
2:N:622:THR:HB	2:N:623:PRO:HD2	1.98	0.45
2:M:124:ASP:OD1	2:M:125:GLU:HG3	2.16	0.45
1:B:581:PRO:O	1:B:605:GLY:HA3	2.16	0.45
1:D:662:VAL:HG21	2:P:194:LEU:HD13	1.97	0.45
1:D:150:VAL:O	1:D:150:VAL:CG1	2.64	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:372:ASP:OD1	2:O:373:ILE:N	2.42	0.45
2:N:66:ARG:HD3	8:N:1160:HOH:O	2.16	0.45
2:P:680:ASP:O	2:P:684:ARG:HG3	2.16	0.45
1:B:525:LYS:O	1:B:529:LYS:HG2	2.16	0.45
1:C:149:ARG:NH2	1:C:250:ASP:OD2	2.45	0.45
2:N:350:PHE:CD1	2:N:350:PHE:C	2.90	0.45
1:B:105:MET:CE	1:B:609:PRO:HD2	2.46	0.45
1:C:105:MET:HE1	1:C:609:PRO:HD2	1.97	0.45
1:C:569:VAL:HB	1:C:573:LYS:HD3	1.97	0.45
1:B:415:ASN:O	1:B:417:PRO:CD	2.63	0.45
2:P:496:THR:O	2:P:500:VAL:N	2.49	0.45
1:A:615:LEU:HD23	2:M:27:HIS:CB	2.47	0.45
2:O:564:TRP:HZ3	2:O:584:LEU:HD12	1.81	0.45
2:M:726:ASP:HB2	2:M:727:PRO:HD2	1.97	0.45
2:M:199:LYS:HE2	2:M:199:LYS:CA	2.47	0.45
1:A:571:THR:OG1	1:A:572:PRO:HD3	2.16	0.45
2:O:376:ILE:HD12	2:O:376:ILE:O	2.17	0.45
2:O:475:LYS:HA	2:O:478:MET:CB	2.44	0.45
2:P:339:TYR:CG	2:P:435:VAL:HG21	2.52	0.45
1:A:468:CYS:HB2	8:A:803:HOH:O	2.16	0.45
2:P:356:VAL:CG2	2:P:361:ILE:HB	2.45	0.45
2:N:356:VAL:CG2	2:N:361:ILE:HB	2.46	0.45
2:M:564:TRP:CZ3	2:M:584:LEU:HD12	2.52	0.45
1:A:313:VAL:CB	1:A:331:VAL:HG22	2.37	0.45
2:M:419:HIS:HB2	2:M:428:LEU:HD13	1.98	0.45
1:D:150:VAL:CG1	1:D:169:LYS:HE2	2.46	0.45
1:D:3:ARG:O	2:P:162:ARG:NH1	2.49	0.45
2:P:473:LYS:HG2	2:P:476:GLU:OE2	2.17	0.45
2:M:367:GLU:HG3	2:M:466:THR:HG23	1.97	0.45
2:M:151:TRP:CE3	2:M:249:ARG:NH1	2.84	0.45
1:C:153:GLU:O	1:C:157:LYS:HD2	2.17	0.45
1:B:480:SER:HB2	1:B:582:GLU:HG3	1.99	0.45
2:P:376:ILE:HD12	2:P:376:ILE:O	2.16	0.45
1:B:273:PRO:HB2	1:B:416:ARG:HH21	1.82	0.45
2:N:586:THR:HG23	2:N:661:ASP:OD1	2.17	0.45
1:D:125:VAL:O	1:D:129:GLU:HG3	2.16	0.45
2:N:381:LYS:O	2:N:382:LEU:HB2	2.17	0.45
2:P:586:THR:HG22	2:P:587:LEU:N	2.32	0.45
2:M:439:PHE:C	2:M:440:ARG:HD2	2.37	0.45
1:C:466:LEU:HD22	1:C:595:TRP:CZ2	2.51	0.45
1:D:581:PRO:O	1:D:605:GLY:HA3	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:410:PHE:CZ	2:M:455:GLU:HG3	2.52	0.45
1:D:412:LYS:HD3	1:D:416:ARG:CD	2.47	0.45
1:B:607:MET:HE2	1:B:608:PRO:HD2	1.99	0.45
1:C:125:VAL:O	1:C:129:GLU:HG3	2.16	0.45
1:B:510:LEU:O	1:B:543:PRO:HD2	2.17	0.45
1:A:581:PRO:O	1:A:605:GLY:HA3	2.17	0.45
1:A:150:VAL:O	1:A:150:VAL:CG1	2.65	0.45
1:D:411:ARG:O	1:D:416:ARG:HB3	2.17	0.45
1:C:318:THR:O	1:C:322:VAL:HG22	2.17	0.45
2:O:365:LYS:HE2	2:O:367:GLU:OE2	2.16	0.45
1:C:559:LEU:HG	1:C:563:MET:HE3	1.98	0.45
1:A:235:ILE:HG23	1:A:597:SER:OG	2.17	0.45
1:B:569:VAL:HB	1:B:573:LYS:HD3	1.99	0.45
1:B:3:ARG:NH1	1:B:625:SER:HB3	2.31	0.44
1:A:3:ARG:HG2	1:A:3:ARG:NH1	2.32	0.44
1:B:486:LYS:HE2	1:B:519:TYR:CE2	2.52	0.44
1:C:150:VAL:CG1	1:C:150:VAL:O	2.65	0.44
2:N:382:LEU:HD12	2:N:383:PRO:HD2	1.99	0.44
1:D:235:ILE:HG23	1:D:597:SER:OG	2.17	0.44
1:A:394:ILE:HG23	1:A:395:GLU:N	2.33	0.44
2:O:3:ASP:O	2:O:6:LYS:HG2	2.17	0.44
2:N:210:GLY:HA3	2:N:214:GLN:HE21	1.81	0.44
2:O:424:ASN:HB2	2:O:478:MET:HE1	1.98	0.44
1:A:150:VAL:CG1	1:A:169:LYS:HG2	2.41	0.44
1:D:3:ARG:HH22	1:D:625:SER:HB2	1.78	0.44
1:C:439:LEU:CD1	1:C:537:ILE:HD13	2.47	0.44
2:N:410:PHE:CZ	2:N:455:GLU:HG3	2.52	0.44
2:O:348:PRO:HB3	2:O:475:LYS:HZ1	1.81	0.44
1:A:658:VAL:O	1:A:662:VAL:HG23	2.18	0.44
2:N:505:SER:HB3	2:N:551:ILE:HD11	2.00	0.44
2:N:456:PHE:HA	2:N:542:ILE:HD13	1.99	0.44
2:N:114:GLU:OE1	2:N:117:ARG:NH1	2.50	0.44
2:M:114:GLU:OE1	2:M:117:ARG:NH1	2.51	0.44
1:D:486:LYS:HE2	1:D:519:TYR:CE2	2.53	0.44
2:O:439:PHE:C	2:O:440:ARG:HD2	2.37	0.44
2:N:439:PHE:C	2:N:440:ARG:HD2	2.38	0.44
1:D:607:MET:HE2	1:D:608:PRO:HD2	1.96	0.44
1:A:415:ASN:HD22	1:A:415:ASN:C	2.19	0.44
2:N:66:ARG:O	2:N:70:GLY:HA2	2.17	0.44
1:A:125:VAL:O	1:A:129:GLU:HG3	2.18	0.44
2:M:224:ARG:O	2:M:228:MET:HG3	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:138:ASP:N	2:M:139:PRO:CD	2.79	0.44
2:M:604:ILE:HD13	2:M:606:PRO:HD3	2.00	0.44
1:A:283:HIS:CD2	1:A:317:CYS:HB2	2.52	0.44
1:D:150:VAL:CG1	1:D:169:LYS:HG2	2.42	0.44
1:B:282:GLY:C	1:B:318:THR:HG23	2.38	0.44
1:D:318:THR:O	1:D:322:VAL:HG22	2.17	0.44
2:P:363:ASP:OD1	2:P:462:ARG:HA	2.18	0.44
1:D:559:LEU:HG	1:D:563:MET:HE3	1.96	0.44
1:A:559:LEU:HG	1:A:563:MET:HE3	1.99	0.44
2:O:666:ARG:CZ	2:O:728:ILE:HB	2.48	0.44
1:B:466:LEU:HD22	1:B:595:TRP:CZ2	2.53	0.44
1:C:384:TYR:CE2	2:P:88:ALA:HB2	2.53	0.44
2:P:354:ARG:HD2	2:P:389:ASP:OD2	2.18	0.44
2:P:199:LYS:CA	2:P:199:LYS:HE2	2.47	0.44
2:M:587:LEU:CG	2:M:588:MET:HE1	2.48	0.44
2:O:393:ARG:HH11	2:O:393:ARG:HG3	1.82	0.44
1:A:652:ARG:O	1:A:656:LEU:HB2	2.18	0.44
2:M:553:LYS:HZ3	2:M:553:LYS:HB3	1.83	0.44
1:A:370:ARG:HG2	1:A:370:ARG:HH11	1.82	0.44
2:O:342:MET:SD	2:O:342:MET:N	2.91	0.44
1:C:150:VAL:CG1	1:C:169:LYS:HE2	2.47	0.44
1:A:411:ARG:CG	1:A:416:ARG:HD2	2.47	0.44
2:P:199:LYS:HE2	2:P:199:LYS:N	2.33	0.44
1:A:483:THR:HG23	1:A:639:GLN:HE21	1.82	0.44
2:O:14:GLU:OE1	2:O:15:GLY:N	2.50	0.44
1:C:186:LEU:CD2	1:C:205:PRO:HD2	2.48	0.44
2:O:382:LEU:HD12	2:O:383:PRO:HD2	1.99	0.44
2:P:352:LEU:HD22	2:P:481:ALA:CB	2.47	0.44
1:D:238:ALA:O	1:D:241:ASP:HB3	2.18	0.44
2:P:350:PHE:CD1	2:P:350:PHE:C	2.90	0.44
2:M:210:GLY:HA3	2:M:214:GLN:HE21	1.82	0.44
1:B:150:VAL:CG1	1:B:169:LYS:HE2	2.48	0.44
2:M:2:THR:HB	2:M:238:GLU:OE1	2.18	0.44
1:B:656:LEU:O	1:B:660:LYS:HG3	2.16	0.44
2:N:224:ARG:O	2:N:228:MET:HG3	2.16	0.44
1:C:52:PHE:CZ	1:C:474:LYS:HA	2.52	0.44
2:P:339:TYR:CD1	2:P:378:GLU:HG3	2.53	0.43
1:A:61:ILE:HD13	1:A:77:ARG:HE	1.82	0.43
1:B:3:ARG:HD3	1:B:4:PHE:CE1	2.54	0.43
1:B:273:PRO:HB2	1:B:416:ARG:NH2	2.33	0.43
2:M:381:LYS:O	2:M:382:LEU:HB2	2.17	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:VAL:HG21	1:C:356:ILE:HG12	1.99	0.43
2:O:568:ASN:CG	2:O:581:GLN:HG3	2.38	0.43
2:O:410:PHE:CE1	2:O:455:GLU:HG3	2.53	0.43
2:P:382:LEU:HD12	2:P:383:PRO:HD2	2.00	0.43
2:N:497:ASP:H	2:N:523:GLU:CD	2.18	0.43
2:O:314:THR:O	2:O:315:LYS:C	2.56	0.43
1:B:394:ILE:HG23	1:B:395:GLU:N	2.34	0.43
1:C:159:VAL:HG23	1:C:160:LEU:N	2.33	0.43
1:D:510:LEU:O	1:D:543:PRO:HD2	2.18	0.43
2:N:199:LYS:HE2	2:N:199:LYS:CA	2.48	0.43
1:B:313:VAL:CB	1:B:331:VAL:HG22	2.38	0.43
2:N:365:LYS:HE2	2:N:367:GLU:OE2	2.18	0.43
2:P:439:PHE:C	2:P:440:ARG:HD2	2.38	0.43
2:M:315:LYS:O	2:M:317:LYS:N	2.50	0.43
1:C:218:GLN:HG3	1:D:377:ASN:HB2	1.99	0.43
1:B:410:GLU:HA	1:B:413:GLU:HG2	2.00	0.43
1:A:223:MET:SD	1:B:353:VAL:HB	2.59	0.43
1:A:280:LEU:HD13	1:A:288:SER:HB2	1.99	0.43
2:N:124:ASP:OD1	2:N:125:GLU:HG3	2.18	0.43
2:M:71:GLU:CD	2:M:71:GLU:H	2.22	0.43
1:C:150:VAL:CG1	1:C:169:LYS:HG2	2.43	0.43
2:M:151:TRP:CE2	2:M:249:ARG:NH1	2.87	0.43
1:A:377:ASN:N	1:A:377:ASN:HD22	2.14	0.43
2:P:376:ILE:HD12	2:P:376:ILE:C	2.38	0.43
1:C:384:TYR:HE2	2:P:88:ALA:CB	2.31	0.43
2:P:399:PHE:O	2:P:403:LEU:HD13	2.19	0.43
1:D:466:LEU:HD22	1:D:595:TRP:CZ2	2.53	0.43
1:D:577:VAL:HG21	1:D:645:ILE:CG2	2.45	0.43
2:N:439:PHE:CE1	2:N:443:ASN:HB2	2.54	0.43
2:O:482:ARG:HG3	2:O:486:LYS:NZ	2.33	0.43
2:N:571:LEU:HD21	2:N:579:LEU:HD12	1.99	0.43
2:P:666:ARG:NH1	2:P:728:ILE:HB	2.34	0.43
2:N:419:HIS:HB2	2:N:428:LEU:HD13	2.01	0.43
1:A:158:SER:OG	1:A:161:GLU:HG3	2.18	0.43
1:A:305:ALA:CB	1:A:409:LYS:HE3	2.49	0.43
2:O:553:LYS:HZ3	2:O:553:LYS:HB3	1.83	0.43
1:D:280:LEU:HD13	1:D:288:SER:HB2	2.00	0.43
2:M:587:LEU:CD2	2:M:588:MET:HE1	2.49	0.43
1:A:317:CYS:O	1:A:321:GLU:HG2	2.19	0.43
1:A:150:VAL:CG1	1:A:169:LYS:HE2	2.48	0.43
2:N:666:ARG:HD3	2:N:725:MET:CE	2.48	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:199:LYS:HE2	2:M:199:LYS:N	2.34	0.43
1:A:299:GLU:O	1:A:303:LYS:HG3	2.19	0.43
2:M:316:ILE:O	2:M:316:ILE:HG22	2.19	0.43
2:O:604:ILE:CD1	2:O:606:PRO:HD3	2.48	0.43
2:P:342:MET:SD	2:P:342:MET:N	2.92	0.43
1:D:569:VAL:HB	1:D:573:LYS:HD3	2.01	0.43
2:P:595:CYS:HB2	5:P:950:ACT:H1	1.99	0.43
2:M:350:PHE:CD1	2:M:350:PHE:C	2.92	0.43
2:N:339:TYR:CD1	2:N:378:GLU:HG3	2.54	0.43
2:O:571:LEU:HD21	2:O:579:LEU:HD12	2.01	0.43
1:D:307:ALA:HB2	1:D:408:PHE:CE2	2.53	0.43
2:O:376:ILE:C	2:O:376:ILE:HD12	2.40	0.43
2:N:238:GLU:HG2	8:N:1293:HOH:O	2.19	0.43
1:C:223:MET:SD	1:D:353:VAL:HB	2.59	0.43
1:B:267:ASN:O	1:B:270:VAL:HG22	2.19	0.43
2:M:657:PHE:O	2:M:658:ILE:C	2.57	0.43
1:B:647:ASP:HB3	8:B:862:HOH:O	2.19	0.43
1:C:443:GLN:HB2	1:C:451:VAL:HG21	2.01	0.43
2:N:680:ASP:O	2:N:684:ARG:HG3	2.18	0.43
1:A:282:GLY:C	1:A:318:THR:HG23	2.38	0.42
2:P:367:GLU:HG3	2:P:466:THR:HG23	2.00	0.42
2:O:406:ARG:CB	2:O:406:ARG:HH11	2.32	0.42
1:C:466:LEU:HD22	1:C:595:TRP:HZ2	1.84	0.42
1:B:98:VAL:HG13	1:B:610:VAL:HA	2.01	0.42
1:C:352:ASP:OD1	1:C:353:VAL:N	2.43	0.42
2:P:587:LEU:CD2	2:P:588:MET:HE1	2.49	0.42
2:O:587:LEU:CD2	2:O:588:MET:HE1	2.49	0.42
1:A:377:ASN:N	1:A:377:ASN:ND2	2.64	0.42
1:A:411:ARG:HG2	1:A:416:ARG:HD2	2.01	0.42
2:P:657:PHE:O	2:P:658:ILE:C	2.57	0.42
1:B:351:VAL:CG2	1:B:356:ILE:CD1	2.98	0.42
1:D:78:ILE:HD11	1:D:97:ILE:HD12	2.02	0.42
1:C:652:ARG:O	1:C:656:LEU:HB2	2.19	0.42
1:B:238:ALA:O	1:B:241:ASP:HB3	2.19	0.42
1:B:241:ASP:OD2	1:B:245:GLU:OE2	2.37	0.42
1:C:326:GLN:HB2	1:C:328:ILE:HG12	2.00	0.42
2:O:657:PHE:O	2:O:658:ILE:C	2.56	0.42
2:O:199:LYS:CA	2:O:199:LYS:HE2	2.49	0.42
2:M:723:LEU:N	2:M:723:LEU:HD12	2.34	0.42
2:P:704:ILE:HD13	2:P:714:TYR:CD2	2.54	0.42
1:C:411:ARG:HH11	1:C:416:ARG:HD2	1.83	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:381:LYS:O	2:P:382:LEU:HB2	2.19	0.42
2:O:439:PHE:CE1	2:O:443:ASN:HB2	2.53	0.42
1:A:190:ILE:HG13	1:A:195:LYS:HG3	2.00	0.42
1:A:377:ASN:HB2	1:B:218:GLN:HG3	2.01	0.42
1:D:52:PHE:CZ	1:D:474:LYS:HA	2.54	0.42
1:D:326:GLN:HB2	1:D:328:ILE:HG12	2.02	0.42
2:O:86:LYS:HD3	2:O:86:LYS:HA	1.86	0.42
1:D:416:ARG:O	1:D:418:VAL:N	2.51	0.42
1:C:317:CYS:O	1:C:321:GLU:HG2	2.19	0.42
2:O:339:TYR:CD1	2:O:378:GLU:HG3	2.55	0.42
2:P:497:ASP:CA	2:P:500:VAL:HG12	2.46	0.42
1:B:377:ASN:N	1:B:377:ASN:ND2	2.66	0.42
2:M:199:LYS:HA	2:M:199:LYS:HE2	2.00	0.42
2:O:199:LYS:N	2:O:199:LYS:HE2	2.35	0.42
2:O:363:ASP:OD1	2:O:462:ARG:HA	2.19	0.42
2:N:564:TRP:HZ3	2:N:584:LEU:HD12	1.83	0.42
1:B:636:MET:N	1:B:636:MET:SD	2.93	0.42
1:C:3:ARG:NH1	1:C:625:SER:OG	2.50	0.42
2:O:350:PHE:CD1	2:O:350:PHE:C	2.92	0.42
2:O:587:LEU:CG	2:O:588:MET:HE1	2.50	0.42
2:M:339:TYR:CD1	2:M:378:GLU:HG3	2.55	0.42
1:A:158:SER:HG	1:A:161:GLU:HG3	1.85	0.42
1:C:235:ILE:HG23	1:C:597:SER:OG	2.19	0.42
2:N:376:ILE:HD12	2:N:376:ILE:O	2.19	0.42
1:A:241:ASP:OD2	1:A:245:GLU:OE2	2.37	0.42
1:B:280:LEU:HD13	1:B:288:SER:HB2	2.02	0.42
1:D:313:VAL:HB	1:D:331:VAL:CG2	2.41	0.42
2:P:410:PHE:CE1	2:P:455:GLU:HG3	2.55	0.42
1:D:394:ILE:HG23	1:D:395:GLU:N	2.34	0.42
2:O:720:HIS:HA	2:O:721:PRO:HD3	1.90	0.42
1:D:370:ARG:HH11	1:D:370:ARG:HG2	1.84	0.42
1:C:308:LYS:HD2	1:C:308:LYS:N	2.35	0.42
2:M:382:LEU:HD12	2:M:383:PRO:HD2	2.01	0.42
2:O:586:THR:HG22	2:O:588:MET:N	2.33	0.42
2:P:564:TRP:HZ3	2:P:584:LEU:HD12	1.85	0.42
1:D:652:ARG:O	1:D:656:LEU:HB2	2.19	0.42
2:O:280:GLN:HA	2:O:281:PRO:HD3	1.94	0.42
2:O:282:LEU:HA	2:O:283:PRO:HD3	1.96	0.42
2:M:376:ILE:O	2:M:376:ILE:HD12	2.19	0.42
1:B:445:ALA:HB3	1:C:38:VAL:HG13	2.01	0.41
2:P:604:ILE:CD1	2:P:606:PRO:HD3	2.50	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:496:THR:HB	2:N:523:GLU:OE2	2.20	0.41
2:N:314:THR:O	2:N:315:LYS:C	2.58	0.41
2:P:572:TYR:HA	2:P:579:LEU:O	2.20	0.41
2:N:199:LYS:N	2:N:199:LYS:HE2	2.35	0.41
1:C:409:LYS:O	1:C:413:GLU:HG2	2.20	0.41
1:D:439:LEU:CD1	1:D:537:ILE:HD13	2.49	0.41
1:C:370:ARG:HH11	1:C:370:ARG:HG2	1.85	0.41
1:C:412:LYS:HD3	1:C:416:ARG:HE	1.85	0.41
2:P:162:ARG:HB2	2:P:188:GLU:HB2	2.02	0.41
1:A:469:GLY:O	1:A:500:CYS:HB2	2.20	0.41
2:O:346:ARG:HG3	2:O:346:ARG:NH1	2.36	0.41
2:N:376:ILE:HD12	2:N:376:ILE:C	2.41	0.41
1:A:238:ALA:O	1:A:241:ASP:HB3	2.20	0.41
2:N:399:PHE:O	2:N:403:LEU:HD13	2.19	0.41
2:M:556:GLU:OE2	2:M:559:PRO:HB3	2.20	0.41
2:O:424:ASN:ND2	2:O:424:ASN:H	2.16	0.41
1:C:615:LEU:HD13	1:C:615:LEU:C	2.40	0.41
2:N:597:CYS:HB3	5:N:950:ACT:O	2.20	0.41
2:O:725:MET:HG2	2:O:726:ASP:OD1	2.20	0.41
1:D:443:GLN:HB2	1:D:451:VAL:HG21	2.02	0.41
1:A:52:PHE:CZ	1:A:474:LYS:HA	2.55	0.41
1:D:483:THR:HB	1:D:638:PRO:HB2	2.02	0.41
1:B:52:PHE:CZ	1:B:474:LYS:HA	2.55	0.41
2:O:471:GLU:O	2:O:475:LYS:CG	2.68	0.41
1:B:652:ARG:O	1:B:656:LEU:HB2	2.20	0.41
2:P:568:ASN:CG	2:P:581:GLN:HG3	2.41	0.41
1:B:12:ARG:HB3	1:B:13:PRO:HD2	2.02	0.41
2:M:405:ARG:CZ	8:M:1049:HOH:O	2.67	0.41
2:O:716:GLU:HG2	2:O:723:LEU:HD21	2.02	0.41
2:O:399:PHE:O	2:O:403:LEU:HD13	2.19	0.41
2:O:572:TYR:HA	2:O:579:LEU:O	2.19	0.41
2:P:510:GLN:HA	2:P:513:ALA:O	2.20	0.41
2:P:199:LYS:HE2	2:P:199:LYS:HA	2.02	0.41
2:O:560:ILE:O	2:O:660:ALA:HB2	2.20	0.41
1:C:483:THR:HG23	1:C:639:GLN:HE21	1.85	0.41
2:M:61:TYR:O	2:M:63:PRO:HD3	2.21	0.41
2:M:571:LEU:HD21	2:M:579:LEU:HD12	2.01	0.41
2:O:247:ARG:NH2	2:O:514:PRO:HG3	2.36	0.41
2:N:402:VAL:HG13	2:N:535:ASP:OD1	2.20	0.41
1:C:303:LYS:HA	1:C:307:ALA:O	2.21	0.41
1:B:398:LYS:O	1:B:402:ARG:HG3	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:419:HIS:ND1	2:M:419:HIS:C	2.74	0.41
2:M:315:LYS:HD2	8:M:1027:HOH:O	2.21	0.41
2:O:510:GLN:HA	2:O:513:ALA:O	2.20	0.41
2:M:376:ILE:HD12	2:M:376:ILE:C	2.41	0.41
1:D:483:THR:HG23	1:D:639:GLN:HE21	1.85	0.41
2:P:560:ILE:O	2:P:660:ALA:HB2	2.20	0.41
1:B:535:ALA:O	1:B:536:ASN:HB2	2.21	0.41
1:C:283:HIS:CD2	1:C:317:CYS:HB2	2.56	0.41
2:N:700:ALA:CB	2:N:704:ILE:HD11	2.51	0.41
1:C:439:LEU:HD12	1:C:537:ILE:HD13	2.03	0.41
1:D:352:ASP:OD1	1:D:353:VAL:N	2.42	0.41
1:D:317:CYS:O	1:D:321:GLU:HG2	2.21	0.41
2:N:445:GLY:O	2:N:449:VAL:HG23	2.20	0.41
2:M:86:LYS:HA	2:M:86:LYS:HD3	1.86	0.41
1:C:574:VAL:HA	1:C:575:PRO:HD3	1.91	0.41
2:M:342:MET:N	2:M:342:MET:SD	2.94	0.41
2:P:586:THR:HG23	2:P:661:ASP:OD1	2.21	0.41
2:O:704:ILE:HD13	2:O:714:TYR:CD2	2.55	0.41
1:A:182:GLU:HB3	1:A:204:VAL:HG11	2.02	0.41
2:P:579:LEU:HD21	2:P:640:GLN:HG3	2.03	0.41
2:M:568:ASN:CG	2:M:581:GLN:HG3	2.41	0.41
2:M:564:TRP:HZ3	2:M:584:LEU:HD12	1.86	0.41
2:M:282:LEU:HA	2:M:283:PRO:HD3	1.96	0.41
2:N:156:GLU:HG3	2:N:182:MET:HB3	2.03	0.41
1:B:370:ARG:HH11	1:B:370:ARG:HG2	1.86	0.41
2:O:605:LEU:HD11	2:O:612:MET:HB3	2.03	0.41
2:N:655:LYS:HE2	8:N:1272:HOH:O	2.20	0.41
2:O:496:THR:O	2:O:500:VAL:HB	2.21	0.41
2:M:588:MET:CE	2:M:604:ILE:HG21	2.51	0.41
1:A:469:GLY:O	7:A:800:XCC:S1	2.79	0.41
2:N:572:TYR:HA	2:N:579:LEU:O	2.21	0.41
2:O:156:GLU:HB2	2:O:250:ALA:HB2	2.03	0.41
2:O:354:ARG:HD2	2:O:389:ASP:OD2	2.21	0.41
1:D:152:ILE:HD12	1:D:166:VAL:CG1	2.51	0.40
2:O:289:PRO:O	2:O:290:ASP:HB2	2.21	0.40
2:P:289:PRO:O	2:P:290:ASP:HB2	2.20	0.40
2:O:419:HIS:ND1	2:O:419:HIS:C	2.75	0.40
2:P:419:HIS:ND1	2:P:419:HIS:C	2.74	0.40
2:O:373:ILE:HD11	2:O:435:VAL:CG2	2.50	0.40
2:N:363:ASP:OD1	2:N:462:ARG:HA	2.22	0.40
1:A:218:GLN:HG3	1:B:377:ASN:HB2	2.03	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:600:VAL:HG12	1:D:601:PRO:O	2.21	0.40
1:C:483:THR:HB	1:C:638:PRO:HB2	2.02	0.40
2:P:423:ARG:HB3	2:P:485:TYR:CE1	2.56	0.40
1:D:35:GLU:OE1	1:D:419:TYR:OH	2.30	0.40
2:O:496:THR:H	2:O:499:THR:HB	1.85	0.40
2:M:586:THR:HG23	2:M:661:ASP:OD1	2.21	0.40
2:N:384:LEU:HD11	2:N:467:ILE:HG23	2.04	0.40
2:M:424:ASN:H	2:M:424:ASN:ND2	2.15	0.40
1:C:33:VAL:HG12	1:C:37:LEU:CD2	2.51	0.40
2:M:723:LEU:H	2:M:723:LEU:CD1	2.35	0.40
1:A:326:GLN:HB2	1:A:328:ILE:HG12	2.03	0.40
2:P:124:ASP:OD1	2:P:125:GLU:HG3	2.21	0.40
1:A:267:ASN:O	1:A:270:VAL:HG22	2.21	0.40
2:N:657:PHE:O	2:N:658:ILE:C	2.59	0.40
2:N:71:GLU:CD	2:N:71:GLU:H	2.25	0.40
1:A:607:MET:HE2	1:A:610:VAL:HG22	2.02	0.40
2:N:579:LEU:HD11	2:N:593:THR:HG21	2.02	0.40
2:N:9:GLU:HA	2:N:9:GLU:OE1	2.22	0.40
1:D:305:ALA:CB	1:D:409:LYS:HE3	2.52	0.40
2:M:197:ASN:O	2:M:199:LYS:HE3	2.22	0.40
1:B:305:ALA:CB	1:B:409:LYS:HE3	2.52	0.40
1:A:637:ASP:HA	1:A:638:PRO:HD2	1.95	0.40
2:P:86:LYS:HD3	2:P:86:LYS:HA	1.83	0.40
2:P:424:ASN:ND2	2:P:424:ASN:H	2.16	0.40
1:C:157:LYS:NZ	8:C:870:HOH:O	2.54	0.40
2:N:199:LYS:HA	2:N:199:LYS:HE2	2.03	0.40
1:D:186:LEU:CD2	1:D:205:PRO:HD2	2.52	0.40
1:A:186:LEU:CD2	1:A:205:PRO:HD2	2.52	0.40
1:C:16:ALA:HB2	8:C:908:HOH:O	2.21	0.40
2:O:556:GLU:OE2	2:O:559:PRO:HB3	2.21	0.40
2:M:323:ASN:HD22	2:M:323:ASN:HA	1.74	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	670/674 (99%)	646 (96%)	21 (3%)	3 (0%)	39	42
1	B	670/674 (99%)	644 (96%)	22 (3%)	4 (1%)	30	29
1	C	670/674 (99%)	647 (97%)	21 (3%)	2 (0%)	46	50
1	D	670/674 (99%)	646 (96%)	22 (3%)	2 (0%)	46	50
2	M	726/729 (100%)	696 (96%)	26 (4%)	4 (1%)	30	29
2	N	726/729 (100%)	696 (96%)	26 (4%)	4 (1%)	30	29
2	O	726/729 (100%)	682 (94%)	34 (5%)	10 (1%)	14	10
2	P	726/729 (100%)	691 (95%)	29 (4%)	6 (1%)	24	22
All	All	5584/5612 (100%)	5348 (96%)	201 (4%)	35 (1%)	30	29

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	316	ILE
2	O	315	LYS
1	B	415	ASN
1	A	267	ASN
1	B	267	ASN
2	M	187	ASP
2	M	679	HIS
2	N	187	ASP
2	N	679	HIS
2	O	187	ASP
2	O	317	LYS
2	O	319	ASP
2	O	470	ASP
2	O	679	HIS
2	P	187	ASP
2	P	319	ASP
2	P	679	HIS
1	A	354	GLN
1	B	354	GLN
1	B	413	GLU
1	C	267	ASN
1	C	354	GLN
1	D	267	ASN
1	D	354	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	M	596	GLY
2	N	596	GLY
2	O	596	GLY
2	P	596	GLY
2	P	727	PRO
1	A	416	ARG
2	O	726	ASP
2	P	295	VAL
2	O	295	VAL
2	O	721	PRO
2	N	295	VAL

### 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	541/543 (100%)	528 (98%)	13 (2%)	57	69
1	B	541/543 (100%)	528 (98%)	13 (2%)	57	69
1	C	541/543 (100%)	526 (97%)	15 (3%)	51	63
1	D	541/543 (100%)	528 (98%)	13 (2%)	57	69
2	M	610/611 (100%)	593 (97%)	17 (3%)	51	63
2	N	610/611 (100%)	593 (97%)	17 (3%)	51	63
2	O	610/611 (100%)	593 (97%)	17 (3%)	51	63
2	P	610/611 (100%)	597 (98%)	13 (2%)	61	74
All	All	4604/4616 (100%)	4486 (97%)	118 (3%)	54	66

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	37	LEU
1	A	42	ASP
1	A	118	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	148	ARG
1	A	166	VAL
1	A	206	PHE
1	A	331	VAL
1	A	377	ASN
1	A	415	ASN
1	A	518	THR
1	A	653	THR
1	A	656	LEU
1	B	3	ARG
1	B	37	LEU
1	B	42	ASP
1	B	118	ASN
1	B	148	ARG
1	B	166	VAL
1	B	206	PHE
1	B	331	VAL
1	B	377	ASN
1	B	416	ARG
1	B	518	THR
1	B	653	THR
1	B	656	LEU
1	C	3	ARG
1	C	37	LEU
1	C	42	ASP
1	C	71	CYS
1	C	118	ASN
1	C	148	ARG
1	C	166	VAL
1	C	206	PHE
1	C	308	LYS
1	C	331	VAL
1	C	377	ASN
1	C	415	ASN
1	C	518	THR
1	C	653	THR
1	C	656	LEU
1	D	3	ARG
1	D	37	LEU
1	D	42	ASP
1	D	118	ASN
1	D	148	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	166	VAL
1	D	206	PHE
1	D	331	VAL
1	D	377	ASN
1	D	518	THR
1	D	539	ILE
1	D	653	THR
1	D	656	LEU
2	M	17	GLU
2	M	21	LEU
2	M	66	ARG
2	M	96	PHE
2	M	199	LYS
2	M	209	LEU
2	M	214	GLN
2	M	238	GLU
2	M	254	TYR
2	M	317	LYS
2	M	318	LEU
2	M	342	MET
2	M	424	ASN
2	M	428	LEU
2	M	571	LEU
2	M	702	GLU
2	M	704	ILE
2	N	9	GLU
2	N	21	LEU
2	N	66	ARG
2	N	71	GLU
2	N	96	PHE
2	N	199	LYS
2	N	209	LEU
2	N	214	GLN
2	N	238	GLU
2	N	315	LYS
2	N	342	MET
2	N	424	ASN
2	N	428	LEU
2	N	571	LEU
2	N	604	ILE
2	N	702	GLU
2	N	704	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	O	14	GLU
2	O	21	LEU
2	O	66	ARG
2	O	96	PHE
2	O	199	LYS
2	O	209	LEU
2	O	214	GLN
2	O	238	GLU
2	O	254	TYR
2	O	318	LEU
2	O	342	MET
2	O	424	ASN
2	O	428	LEU
2	O	482	ARG
2	O	571	LEU
2	O	702	GLU
2	O	704	ILE
2	P	21	LEU
2	P	66	ARG
2	P	96	PHE
2	P	199	LYS
2	P	209	LEU
2	P	214	GLN
2	P	238	GLU
2	P	318	LEU
2	P	342	MET
2	P	424	ASN
2	P	428	LEU
2	P	571	LEU
2	P	702	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	56	GLN
1	A	58	GLN
1	A	164	GLN
1	A	217	ASN
1	A	225	ASN
1	A	377	ASN
1	A	415	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	471	ASN
1	A	622	GLN
1	A	639	GLN
1	B	9	HIS
1	B	56	GLN
1	B	58	GLN
1	B	164	GLN
1	B	217	ASN
1	B	225	ASN
1	B	377	ASN
1	B	446	GLN
1	B	471	ASN
1	B	622	GLN
1	B	639	GLN
1	C	9	HIS
1	C	56	GLN
1	C	58	GLN
1	C	164	GLN
1	C	217	ASN
1	C	225	ASN
1	C	377	ASN
1	C	415	ASN
1	C	471	ASN
1	C	622	GLN
1	C	639	GLN
1	D	9	HIS
1	D	56	GLN
1	D	58	GLN
1	D	164	GLN
1	D	217	ASN
1	D	225	ASN
1	D	377	ASN
1	D	471	ASN
1	D	622	GLN
1	D	639	GLN
2	M	211	ASN
2	M	214	GLN
2	M	240	GLN
2	M	323	ASN
2	M	375	GLN
2	M	422	GLN
2	M	424	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	M	426	ASN
2	M	516	HIS
2	M	581	GLN
2	M	590	ASN
2	N	211	ASN
2	N	214	GLN
2	N	240	GLN
2	N	323	ASN
2	N	375	GLN
2	N	422	GLN
2	N	424	ASN
2	N	426	ASN
2	N	516	HIS
2	N	581	GLN
2	N	590	ASN
2	O	211	ASN
2	O	214	GLN
2	O	240	GLN
2	O	323	ASN
2	O	375	GLN
2	O	422	GLN
2	O	424	ASN
2	O	426	ASN
2	O	516	HIS
2	P	211	ASN
2	P	214	GLN
2	P	240	GLN
2	P	323	ASN
2	P	375	GLN
2	P	422	GLN
2	P	424	ASN
2	P	426	ASN
2	P	516	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 8 are monoatomic - leaving 18 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	$\# Z  > 2$
6	SF4	A	700	1	0,12,12	0.00	-	0,24,24	0.00	-
6	SF4	A	750	1	0,12,12	0.00	-	0,24,24	0.00	-
7	XCC	A	800	1	0,11,11	0.00	-	0,19,19	0.00	-
6	SF4	B	750	1	0,12,12	0.00	-	0,24,24	0.00	-
7	XCC	B	800	1	0,11,11	0.00	-	0,19,19	0.00	-
6	SF4	C	700	1	0,12,12	0.00	-	0,24,24	0.00	-
6	SF4	C	750	1	0,12,12	0.00	-	0,24,24	0.00	-
7	XCC	C	800	1	0,11,11	0.00	-	0,19,19	0.00	-
6	SF4	D	750	1	0,12,12	0.00	-	0,24,24	0.00	-
7	XCC	D	800	1	0,11,11	0.00	-	0,19,19	0.00	-
6	SF4	M	900	2	0,12,12	0.00	-	0,24,24	0.00	-
5	ACT	M	950	3	2,2,3	1.18	0	0,1,3	0.00	-
6	SF4	N	900	2	0,12,12	0.00	-	0,24,24	0.00	-
5	ACT	N	950	3	2,2,3	1.42	0	0,1,3	0.00	-
6	SF4	O	900	2	0,12,12	0.00	-	0,24,24	0.00	-
5	ACT	O	950	3	2,2,3	1.15	0	0,1,3	0.00	-
6	SF4	P	900	2	0,12,12	0.00	-	0,24,24	0.00	-
5	ACT	P	950	3	2,2,3	1.24	0	0,1,3	0.00	-

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
6	SF4	A	700	1	-	0/0/48/48	0/6/5/5
6	SF4	A	750	1	-	0/0/48/48	0/6/5/5

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	XCC	A	800	1	-	0/0/32/32	0/0/3/3
6	SF4	B	750	1	-	0/0/48/48	0/6/5/5
7	XCC	B	800	1	-	0/0/32/32	0/0/3/3
6	SF4	C	700	1	-	0/0/48/48	0/6/5/5
6	SF4	C	750	1	-	0/0/48/48	0/6/5/5
7	XCC	C	800	1	-	0/0/32/32	0/0/3/3
6	SF4	D	750	1	-	0/0/48/48	0/6/5/5
7	XCC	D	800	1	-	0/0/32/32	0/0/3/3
6	SF4	M	900	2	-	0/0/48/48	0/6/5/5
5	ACT	M	950	3	-	0/0/0/0	0/0/0/0
6	SF4	N	900	2	-	0/0/48/48	0/6/5/5
5	ACT	N	950	3	-	0/0/0/0	0/0/0/0
6	SF4	O	900	2	-	0/0/48/48	0/6/5/5
5	ACT	O	950	3	-	0/0/0/0	0/0/0/0
6	SF4	P	900	2	-	0/0/48/48	0/6/5/5
5	ACT	P	950	3	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	800	XCC	3	0
7	B	800	XCC	1	0
7	C	800	XCC	2	0
7	D	800	XCC	2	0
5	M	950	ACT	2	0
5	N	950	ACT	2	0
5	O	950	ACT	1	0
5	P	950	ACT	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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